Accurate and Computationally Efficient Algorithms for Potential Temperature and Density of Seawater

TREVOR J. MCDougall and DAVID R. JACKETT
CSIRO Marine Research, Hobart, Tasmania, Australia

DANIEL G. WRIGHT
Department of Fisheries and Oceans, Bedford Institute of Oceanography, Dartmouth, Nova Scotia, Canada

RAINER FEISTEL
Institut für Ostseeforschung, Warnemünde, Germany

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ABSTRACT
An equation of state for seawater is presented that contains 25 terms and is an excellent fit to the Feistel and Hagen equation of state. It is written in terms of potential temperature (rather than in situ temperature), as required for efficient ocean model integrations. The maximum density error of the fit is $3 \times 10^{-3}$ kg m$^{-3}$ in the oceanographic ranges of temperature, salinity, and pressure. The corresponding maximum error in the thermal expansion coefficient is $4 \times 10^{-3}$ C$^{-1}$, which is a factor of 12 less than the corresponding maximum difference between the Feistel and Hagen equation of state and the widely used but less accurate international equation of state.

A method is presented to convert between potential temperature and in situ temperature using specific entropy based on the Gibbs function of Feistel and Hagen. The resulting values of potential temperature are substantially more accurate than those based on the lapse rate derived from the international equation of state.

1. Introduction
Ocean models carry conservation equations for salinity $S$ and for potential temperature $\theta$, and so the equation of state that is used by ocean models is a function of salinity, potential temperature and pressure, that is, $\rho = \rho(S, \theta, p)$. This is in contrast to the form of the international equation of state of seawater (Fofonoff and Millard 1983), which is written in terms of in situ temperature, that is, as $\rho = \rho(S, T, p)$. Two equations of state of the former kind are in common usage, namely, those of Jackett and McDougall (1995) and Wright (1997). The Jackett and McDougall (1995) equation has exactly the same terms as the international equation of state (but with different coefficients) and so it has a total of 41 coefficients. Wright’s (1997) equation of state is a rational polynomial function with just 15 coefficients that was designed to consume less computer time. It is computationally efficient, but the deviations from the international equation of state are larger than those obtained with the Jackett and McDougall (1995) formulation. The implications of this reduced accuracy for ocean models is not well documented, but it has been deemed to be sufficiently risky that most modeling groups have adopted the Jackett and McDougall (1995) formula, even though the extra computer time is bestowed upon the equation of state very grudgingly (Griffies et al. 2000).

While the international equation of state has served the community well for many years, it is no longer the most accurate choice. Feistel (1993) has advocated the procedure of using various measured thermodynamic quantities to determine the Gibbs thermodynamic potential (or specific free enthalpy) from which can be derived the internal energy, enthalpy, specific heat, entropy, specific volume, chemical potential, potential temperature, sound speed, and other quantities. This approach has the important advantage that all these derived quantities are then totally self-consistent. Feistel and Hagen (1995, henceforth referred to as FH95) have used this approach to derive a Gibbs function that combines among other things, the latest available data on the temperature of maximum density (TMD) from Caldwell (1978) and the sound speed data of Del Grosso (1974).
It is primarily the incorporation of these two types of observed data that has allowed the FH95 equation of state to be more accurate than the international equation of state.

A disadvantage of the FH95 equation of state is that it is substantially more computationally demanding than even the full international equation of state. For ocean modeling studies the computational requirements are compounded by the fact that the density obtained from FH95 is not easily expressed as a function of \( S, \theta, \) and \( p \). The present work was primarily motivated by the desire to obtain a computationally efficient equation of state that takes advantage of the improved accuracy of the FH95 Gibbs function. We decided to use the rational function approach of Wright (1997) with more terms included in order to improve the accuracy: our final choice being a rational function that has just 25 terms. This is more computationally efficient than the Jackett and McDougall (1995) formula, and the errors (relative to the improved FH95 formula) are about 15 and 20 times less than those in the Wright (1997) formula.

We emphasize that the equation of state that we present in this paper has not been fitted to the original laboratory data for density, sound speed, temperature of maximum density, etc. Rather, we have fitted to the equation of state of FH95. We have included sufficient terms in our equation of state so that the error in our fit is approximately the uncertainty in the original laboratory data to which FH95 fitted their Gibbs function.

As first pointed out by Brewer and Bradshaw (1975), the salinity and density of seawater cannot be accurately determined on the basis of conductivity measurements alone because of regional differences in alkalinity, total carbon dioxide, and silica content. Recent measurements reported in Millero (2000) have found the maximum density difference from this effect to be about 0.020 kg m\(^{-3}\) in the open ocean. However, the differences due to these variations in the composition of sea salt are thought to vary rather smoothly in space as they reflect differences between the forcing functions in different ocean basins. Also, there is some hope that at some stage in the future a correction function could be devised to account for a significant fraction of this effect. Hence, it seems worthwhile to derive a formula analogous to that of Wright (1997) that is as accurate as possible for standard seawater. The 25-term formula derived here achieves this goal. The issue of accounting for variations in sea salt composition needs to be addressed before further improvements will be warranted.

Finally, we note that the in situ and potential temperatures are also most accurately related through the Gibbs function approach of FH95. This relation is useful in general and is required in order to determine the density as a function of \( S, \theta, \) and \( p \). A procedure for accurately converting between \( T \) and \( \theta \) is described in the next section.

2. The evaluation of potential temperature

When the pressure of a fluid parcel with salinity \( S \) and in situ temperature \( T \) is changed from \( p \) to a reference pressure \( p_r \), without exchange of heat or salt, the in situ temperature changes and the new in situ temperature is called the potential temperature of the fluid parcel \( \theta \) referenced to \( p_r \). The process of changing the pressure of a fluid parcel in an isohaline and adiabatic manner does not cause any change in either the potential temperature or the specific entropy of the fluid parcel.

The specific entropy \( \sigma \) (henceforth simply called entropy, with the “per unit mass” concept implied) is derived from the Gibbs function \( G \) by differentiating it with respect to temperature, \( \sigma(S, T, p) = -G_T(S, T, p) \). To find the potential temperature referenced to pressure \( p_r \), of the seawater parcel \((S, T, p)\), we need to solve

\[
\sigma(S, \theta, p_r) = \sigma(S, T, p),
\]

for \( \theta \), and the remainder of this section describes how this is done.

We begin with a very simple approximate functional form for \( \theta \) as a function of \( S, T, (p + p_r) \), and \((p - p_r)\) (see appendix A). This gives the zeroth estimate of potential temperature, namely, \( \theta_0 \). A Newton–Raphson technique is then used to accurately determine the potential temperature using the derivative of entropy with respect to temperature. This derivative is found by twice differentiating the Gibbs function and is closely related to the specific heat at constant pressure \( C_p \) since (from FH95)

\[
\sigma_T(S, T, p) = -G_{TT}(S, T, p) = C_p(S, T, p)/(273.15 + T),
\]

where in situ temperature \( T \) is measured in degrees Celsius on the ITS-90 temperature scale.

An improved estimate of potential temperature is found from the following approximate solution to (1):

\[
\theta_i = \theta_0 - \frac{[\sigma(S, \theta_0, p_r) - \sigma(S, T, p)]}{(13.9 \text{ J kg}^{-1} \text{ K}^{-2})},
\]

which involves two evaluations of entropy, and uses 13.9 J kg\(^{-1}\) K\(^{-2}\) as a first-guess (constant) estimate of \( \sigma_T \). Using a million random points drawn from the \((S-T-p)\) cube (0 psu, 40 psu) \(\times(-3^\circ\text{C}, 40^\circ\text{C})\) \(\times(0 \text{ db}, 10^4 \text{ db})\), and with potential temperature referenced to another \(10^6\) random pressures also in the range \(0 \text{ db}, 10^4 \text{ db}\), the rms and maximum errors of the intermediate estimate \( \theta_i \) are 0.001°C and 0.015°C, respectively. While these errors are about a factor of about 10 less than those of \( \theta_0 \), they are still too large for oceanographic use. Note that while salinity is a dimensionless quantity, we use the common terminology of 35 psu (standing for practical salinity units) to describe a salinity of 0.035 because it tells the reader exactly how the salinity has been calculated [viz., from measurements of conductivity, see Fofonoff (1985)].
Further savings in computer time have been obtained by using the relation of salinity (including a term in the logarithm of salinity). This eliminates the need to evaluate two lots of six coefficients, then

\[ u_5 = u_2 + [\sigma(S, \theta_0, p_r) - \sigma(S, T, p)] / \sigma_r(S, [\theta_0 + \theta_1] / 2, p_r). \]  

(4)

This procedure could be iterated further, but as we will show, (4) is sufficiently accurate for all foreseeable purposes.

Note that since both \( \alpha(S, \theta_0, p_r) \) and \( \alpha(S, T, p) \) in (3) are evaluated at the same salinity, the terms in the polynomial for entropy that are functions of salinity alone need not be evaluated since they cancel in (3) and (4). This eliminates the need to evaluate two lots of six terms (including a term in the logarithm of salinity). Further savings in computer time have been obtained by grouping terms in \( \alpha(S, \theta_0, p_r) \) and \( \alpha(S, T, p) \) in terms of their powers of salinity and using Horner’s rule to reduce a few multiplications in the code.

FH95 discuss a very similar Newton–Raphson procedure to that described above but actually recommend using a different approach for evaluating potential temperature. They present a polynomial for enthalpy as a function of salinity, entropy, and pressure, namely, \( h(S, \alpha, p) \), and suggest potential temperature be determined using their equation (7.1), namely, \( 273.15 + \theta = h_\alpha(S, \alpha, p_r) \), a thermodynamic identity. This method requires first the evaluation of entropy, \( \alpha(S, T, p) \), which involves 64 coefficients, then \( h_\alpha \), involving 129 coefficients for a general reference pressure but only 28 coefficients if \( p_r = 0 \). In comparison, our technique requires one evaluation of \( \alpha_r \) (involving 43 coefficients for a general reference pressure) and two evaluations of entropy (64 coefficients each, but note that we save about 20 multiplications by recognizing that the salinities are the same). When the reference pressure is set to zero (i.e., for potential temperature referenced to the sea surface), there are only 18 and 12 coefficients, respectively, involved in evaluating \( \alpha \) and \( \alpha_r \). The computational requirements of the two methods are thus about the same. However, our method can be evaluated to any required precision by controlling the number of loops through the Newton–Raphson technique. In contrast, the method based on \( h(S, \alpha, p) \) has limited accuracy with errors of about \( 2 \times 10^{-4} \) °C being common near the freezing line (see Fig. 7.2 of FH95).

Table 1 compares the accuracy and computational efficiency of the three different potential temperature algorithms: the Fofonoff and Millard (1983) algorithm, which uses one Runge–Kutta integration of their lapse rate, the technique recommended by FH95, and Eq. (4) above. One million random points were generated in the \((S–T–p)\) cube (0 psu, 40 psu) × (−3°C, 40°C) × (0 db, 104 db), and potential temperature was referenced to another one million random pressures also in the range (0 db, 104 db). The data points were restricted to be above the freezing temperature when the fluid parcels were brought adiabatically to a pressure of 500 db. The standard against which we compare the three algorithms is the result obtained after four iterations of the Newton–Raphson algorithm described above, although in practice, the algorithm converged to machine precision after two iterations. This method is believed to give the most accurate estimate of potential temperature currently available since (1) is satisfied to machine precision. All computations in this paper have been performed in double precision.

Table 1 shows that the new routine to estimate potential temperature requires roughly between 2 and 3 times the CPU time used by the Fofonoff and Millard (1983) algorithm. This increased computational cost provides a substantial increase in accuracy. The method based on \( h(S, \alpha, p) \) as suggested by FH95 is slightly more expensive than the method developed here, but is not quite as accurate. The last column shows the improvements in execution speed when the reference pressure \( p_r = 0 \).

Table 1 should not be interpreted as implying that our algorithm has an absolute accuracy of \( 3.4 \times 10^{-4} \) °C but rather that it approximates the best available expression for specific entropy (viz, FH95) to this level of accuracy. Using the maximum uncertainty in the thermal expansion coefficient that can be derived from FH95 of \( 6 \times 10^{-7} \) °C⁻¹ (this estimate of uncertainty is discussed by FH95 and is reviewed at the end of our section 3) in Eq. (A2) and then substituting this error in the lapse rate into (A1) gives a maximum uncertainty in \( \theta - T \) of \( 4 \times 10^{-3} \) °C for a pressure difference of 10 000 db. That is, the maximum uncertainty in the FH95 Gibbs function translates into a maximum uncertainty of \( 4 \times 10^{-3} \) °C in \( \theta - T \). Because the maximum error in Table 1 for our method, at \( 3.4 \times 10^{-6} \) °C, is much less than \( 4 \times 10^{-3} \) °C we conclude that our method for evaluating potential temperature is essentially as accurate as entropy derived from the FH95 Gibbs function and is more accurate than the Fofonoff and Millard (1983) algorithm. The \( h(S, \alpha, p) \) method of FH95 does not conform
to the FH95 Gibbs function as precisely as our algorithm, but for practical purposes it could be used with no significant loss of accuracy.

Another test, which is also a test of the internal consistency of each of the algorithms, is the degree to which the function obtained by interchanging the two pressure arguments in the call to potential temperature gives the “physical inverse” to potential temperature. Since the movements from one pressure to the other are done without exchanges of heat or salt, the movement from one pressure to another and then back to the original pressure should have no net effect. Table 2 shows the accuracy achieved by comparing the in situ temperatures corresponding to $10^4$ randomly generated points in the $(S-T-p)$ cube described above, with the temperatures obtained by moving these parcels from their in situ pressures to another $10^4$ randomly generated pressures in the range (0 db, 10$^4$ db), and then back again to the original pressures. The table shows the rms and maximum absolute errors for the same three algorithms as in Table 1 above. For this test the Fofonoff and Millard (1983) algorithm outperforms the $h(S, \sigma, p)$ of FH95 by almost two orders of magnitude, but the algorithm developed here is substantially more precise than the Fofonoff and Millard (1983) algorithm. 

Feistel (1993) compares his potential temperature algorithm with that of Fofonoff and Millard (1983) and notes that “maximum differences of 0.04°C appear at $S = 25$ and high pressures mainly as a result of the better consistency of the Gibbs function with sound speed data.” This refers to the high-pressure part of the international equation of state, which is not fully consistent with the Chen–Millero sound speed data from which it was derived. The Gibbs function of FH95, on which our potential temperature algorithm is based, makes use of more reliable sound speed data than that of Feistel (1993) and earlier work. It is thus of interest to examine the differences between our algorithm and that of Fofonoff and Millard (1983). In Fig. 1 we plot this difference on the $S-T$ plane at $p = 5000$ db using a reference pressure of $p_s = 0$ db. Although maximum differences of only 0.02°C are seen along the $S = 25$ psu line (and similarly for deeper pressures), maximum differences of 0.04°C are still evident in the full $S-T$ plane. On the other hand, for realistic ocean data such as given by the Levitus (1982) ocean atlas at 5000 db, the maximum difference between the potential temperatures obtained with the two different approaches is only 0.0025°C, more than an order of magnitude less than the maximum difference over the full $S-T$ range shown in Fig. 1.

Finally, a comment on the significance of the additional computational overhead involved in obtaining a very accurate determination of $\theta$ is warranted. For most purposes the additional CPU time is not of great concern, but it would obviously be a concern if this conversion had to be made at every grid cell for every time step in a numerical integration. This conversion is required in order to determine density as a function of $S$, $\theta$, and $p$ from the FH95 equation of state. However, once a formula is determined that gives density directly in terms of these quantities without intermediate reference to the in situ temperature, the conversion will not be required as part of ocean model integrations and hence the extra computational load will be of little consequence. The derivation of an appropriate expression for $\rho(S, \theta, p)$ is discussed in the next section.

### 3. The 25-term equation of state

We are now in a position to determine a formula for $\rho$ as a function of $S$, $\theta$, and $p$ that is consistent with the FH95 equation of state. We fit the equation of state over the pressure range from 0 to 8000 db (0 to 80 Mpa), but noting that the deep ocean contains neither freshwater nor warm water, we have concentrated the fit on water of environmental relevance. The salinity range used in the fit is 0–40 psu at the surface, but the range is reduced to 30–40 psu at pressures below 5500 db. The minimum salinity used in the fit varies linearly with pressure from 0 to 30 psu between 0 and 5500 db. Similarly, the maximum potential temperature used in the calculation of the fit is $33^\circ$C at 0 db, varying linearly with pressure thereafter down to $12^\circ$C at 5500 db. The minimum potential temperature of data that is included

<table>
<thead>
<tr>
<th>Potential temperature algorithm</th>
<th>Rms error</th>
<th>Max absolute error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fofonoff and Millard (1983)</td>
<td>$4.9 \times 10^{-4}$</td>
<td>$1.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>Using $h(S, \sigma, p)$ of FH95</td>
<td>$2.3 \times 10^{-4}$</td>
<td>$8.6 \times 10^{-4}$</td>
</tr>
<tr>
<td>This paper</td>
<td>$1.2 \times 10^{-2}$</td>
<td>$3.7 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

**Table 2. Accuracy (in °C) of the inverse property of the potential temperature algorithms.**
in the evaluation of the fit corresponds to the freezing temperature at a pressure of 500 db. That is, for a given salinity, the minimum potential temperature (with a reference pressure of 0 db) was chosen so that if the fluid parcel was moved to a pressure of 500 db, its in situ temperature was the freezing temperature at that salinity and pressure. The rationale for this choice is that icebergs and ice shelves are rarely if ever deeper than 500 db and there are no sources of cooling away from the sea surface (there are only sources of heat, viz. geothermal heating and the dissipation of mechanical energy). This procedure thus defines the coolest potential temperature that can be found anywhere in unfrozen water. In practice we calculated the freezing point of seawater at 500 db from the polynomial appearing in Fofonoff and Millard (1983), the corresponding potential temperatures (with a reference pressure of 0 db) ranging from \(-0.36^\circ\text{C}\) at 0 psu to \(-2.6^\circ\text{C}\) at 40 psu.

The above paragraph describes a “funnel” over which we evaluated our fit to the equation of state, and this funnel is shown in Fig. 2. In order to better control the errors in density and particularly the errors in the thermal expansion coefficient, we included a larger range of potential temperature in the fitting procedure but did not include this larger range in the evaluation of the errors of the fitted equation of state. The minimum potential temperature used in the fit was actually \(2^\circ\text{C}\) less than the freezing line described above. These potential temperatures would correspond to frozen water at a pressure of approximately 3000 db, which is clearly unphysical since, for example, there is no water of in situ temperature of \(-4^\circ\text{C}\) observed at this pressure. The maximum potential temperatures that are included in the fit range up to \(40^\circ\text{C}\) at 0 db and up to \(15^\circ\text{C}\) at 5500 db (and below), varying linearly with pressure between these two pressure limits. We include the extra temperature data in the fit so as to control the well-known problems that can occur when extrapolating polynomials beyond their range of validity, particularly when the equation of state is differentiated with respect to potential temperature to obtain the thermal expansion coefficient.

The functional form used to approximate the FH95 equation of state is based on the rational function approach of Wright (1997) and is of the form (see appendix B for the coefficients of the two polynomials and check values)

\[
\rho(S, \theta, p) = \frac{P_1(S, \theta, p)}{P_2(S, \theta, p)}. \tag{5}
\]

Note that potential density referenced to a variety of reference pressures such as 2000 db and 4000 db can be evaluated from our equation of state as \(\rho(S, \theta, 2000)\) and \(\rho(S, \theta, 4000)\) without having to evaluate potential temperature with reference to 2000 and 4000 db. This amounts to a substantial reduction in computer time when evaluating these potential densities.

There are 12 terms in the polynomial \(P_1(S, \theta, p)\) in the numerator and 13 terms in the polynomial \(P_2(S, \theta, p)\) in the denominator of (5). The highest power of pressure in the numerator in (5) is quadratic and this facilitates the evaluation of the pressure integral of specific volume (see appendix C). The constant term in the denominator was set to unity, thus making the problem well posed [see (7) below]. The latter being calculated from simple finite differences of in situ density. The reason for including errors in the thermal expansion coefficient in the penalty function is discussed below. The relative weighting between density and the thermal expansion coefficient was chosen so that the errors in density and in the thermal expansion coefficient contributed about equally to the penalty function. Introducing this relative weighting on the thermal expansion coefficient had the effect of re-

![Fig. 2. The “funnel” over which the error in the fit of our 25-term equation was calculated.](image-url)
dicing its maximum error by 40%. At the same time the maximum error in density decreased by about 10% (although the rms density error increased by 20%). We also up-weighted (in a spatially smooth fashion) several regions at the extremities of the funnel in order to reduce the maximum errors of the fit.

The difference between our 25-term equation of state and the FH95 “truth” is illustrated in Fig. 3. Both the root-mean-square (rms) and the maximum absolute errors are shown as a function of pressure for data in the (S–θ–p) funnel shown in Fig. 2. Figure 3a shows that the maximum error in density is always less than 0.003 kg m⁻³ while the rms error is closer to 0.001 kg m⁻³. The other panels of Fig. 3 show the errors in the thermal expansion coefficient α, the haline contraction coefficient β, and the sound speed c, that result from the errors in our 25-term equation of state, compared with the corresponding coefficients obtained from the full Gibbs function of FH95. These coefficients are defined in the “adiabatic” sense (rather than in the isothermal sense since temperature in these derivatives is taken to be potential temperature rather than in situ temperature) by

\[
\alpha = -\frac{1}{\rho} \frac{\partial \rho}{\partial \theta} \bigg|_{S,p},
\]

\[
\beta = \frac{1}{\rho} \frac{\partial \rho}{\partial S} \bigg|_{S,p},
\]

\[
(c^b)^{-2} = \frac{\partial \rho}{\partial S} \bigg|_{S,\theta}.
\]

Figure 3b shows that the maximum error in the thermal expansion coefficient is less than \(4 \times 10^{-7} \, {^\circ}C^{-1}\) while the rms value is generally about \(1.2 \times 10^{-7} \, {^\circ}C^{-1}\). The haline contraction coefficient shows a different error pattern (as a function of pressure), having its largest deviations at the extremes of the pressure range. The maximum error in β, at almost \(8 \times 10^{-7} \, \text{psu}^{-1}\), amounts to a relative error of about one-quarter that found for the thermal expansion coefficient. This occurs at very low salinities (near 0 psu) and very high temperatures. We have not paid much attention to the error in sound speed, but we note that the errors in our Fig. 3d are significantly less than the difference between Feistel and Hagen’s (1995) sound speed and those derived from the international equation of state (see Fig. 3.3c of FH95).

Maps of the error in the 25-term fit show that the maximum errors tend to occur on the boundaries of our funnel, as is illustrated in Fig. 4. We suggest that the errors at large potential temperature are less important than those near the freezing line, since it is at low temperatures that deep waters are formed and subsequently spread throughout the world ocean basins. Because of this fact and because the largest errors often occur near the freezing line, a useful measure of error at a given pressure is the typical error at cold temperatures on the S–θ plane of the funnel. This error measure is more stringent and more relevant than the rms error over all the data on the S–θ plane at this pressure. Because of the greater concern with the accuracy at low potential temperatures than at high potential temperatures, we have excluded the warmest few degrees Celsius of the larger funnel when calculating both the maximum and the rms error measures, so forming the smaller funnel of Fig. 2 for this purpose. (If we do include potential temperatures up to 40°C in the error evaluation, the relative error in the maximum thermal expansion coefficient doubles.)

The significance of a certain error in the evaluation of density is not immediately obvious. This is primarily because an offset in density that is a function of pressure alone, \(\delta \rho(p)\), affects the evaluation of sound speed, but has no dynamical consequences for the ocean circulation since the isobaric (quasi-horizontal) density gradients that drive the thermal wind are unaffected. Also, such an error does not affect the calculation of the buoyancy frequency N. For this reason we advocate that the error in the thermal expansion coefficient (and saline contraction coefficient) be used as the most relevant measure of the error in an equation of state for dynamical oceanography.

The key accuracy measure would then seem to be the maximum error in the thermal expansion coefficient, namely, \(4 \times 10^{-7} \, {^\circ}C^{-1}\), as described above in relation to Fig. 3b. Over much of the S–θ plane the thermal expansion coefficient is greater than \(1 \times 10^{-4} \, {^\circ}C^{-1}\) so our maximum error corresponds to a relative error in the thermal expansion coefficient of less than 0.4%. The maximum error in the saline contraction coefficient of \(8 \times 10^{-7} \, \text{psu}^{-1}\) corresponds to 0.1% of the mean value of the saline contraction coefficient, and so is less important than the error in the thermal expansion coefficient. Because there is often some cancellation between the effects of salinity and potential temperature on both the horizontal density gradient and the relevant pressure-corrected vertical density gradient (where the buoyancy frequency N is given by \(g^{-1} N^2 = \alpha \theta - \beta S\), with \(\alpha \theta\) and \(\beta S\), often having the same sign), we may expect that the maximum errors in the thermal expansion coefficient will result in maximum relative errors in the dynamically important density gradients of about 1%. It was the desire to have a maximum error in \(\nabla \rho\) and in \(N^2\) of no more than 1% that drove us to include as many as 25 terms in our fit to the FH95 equation of state.

The temperature-of-maximum-density data of Caldwell (1978) have been incorporated into FH95 into their Gibbs function and this data, together with the more modern sound speed measurements, are credited with most of the improvements in the FH95 equation of state compared with the international equation of state. As previously discussed by FH95 [see the paragraph following their Eq. (3.4)], information from the vicinity of the TMD can be used to provide an estimate of the uncertainty in the thermal expansion coefficient. Right
Fig. 3. (a) The rms and the maximum absolute errors in density as a function of pressure for data in the $(S-\theta-p)$ funnel of Fig. 2. (b), (c), and (d) Error measures for the thermal expansion coefficient, the haline contraction coefficient, and the sound speed, respectively. These figures are for the differences between our 25-term equation of state and the full FH95 form of the equation of state [our Eq. (6)].
at the TMD, \( \alpha \) is exactly zero by definition. Also, the second derivative of density with respect to temperature near the TMD is about \(-1.5 \times 10^{-2} \text{ kg m}^{-3} (\text{C})^{-2}\), which implies that \( \frac{\partial \rho}{\partial \theta} \) \( |_{S,p} \) is about \( 1.5 \times 10^{-3} \text{ C}^{-2}\). Thus, an error \( \Delta(TMD) \) in the estimate of the TMD, implies a corresponding error in the thermal expansion coefficient \( \Delta \alpha \sim 1.5 \times 10^{-5} \Delta(TMD) \). This immediately provides an estimate of the absolute magnitude of the error in the thermal expansion coefficient in just the region of parameter space of most concern to oceanographers, namely, the cool parts of the world ocean. As discussed by FH95, the Caldwell (1978) TMD data are thought to be known to 0.04°C and this error estimate translates into an error in the thermal expansion coefficient at the TMD of \( 6 \times 10^{-7} \text{ C}^{-1}\). Since our 25-term fit has achieved a maximum error in the thermal expansion coefficient in our reduced funnel of \( 4 \times 10^{-7} \text{ C}^{-1}\), we believe that our equation is about as accurate as the data used by FH95 to obtain their Gibbs function.

4. Comparisons with the international and Wright equations of state

Figure 5 shows the differences between the standard UNESCO form of the international equation of state (Fofonoff and Millard 1983), the Wright (1997) equation of state and the FH95 equation of state. We mainly compare the former two equations with the latter “truth.” The data here are taken over the same nonfrozen funnel of Fig. 2 so that the results are directly comparable with those of Fig. 3. The solid lines depict the errors for the UNESCO equation while the dashed lines are the errors for the Wright (1997) equation.

The solid lines in Fig. 5a are consistent with the density differences plotted in Feistel and Hagen’s (1995) Fig. 3a, which shows differences between their equation of state and that of Fofonoff and Millard (1983). Comparing Figs. 3a and 5a shows that the maximum error in the fit to density of our 25-term equation is a factor of 4 less than the maximum error of the UNESCO equation and 15 times smaller than the maximum error of the Wright (1997) fit.

In terms of the thermal expansion coefficient, Fig. 5b indicates that the Wright (1997) and UNESCO equations are of about the same accuracy, both being about an order of magnitude less accurate than our 25-term equation. (The bold line with dots in Fig. 5b is a repeat of the maximum curve of Fig. 3b, emphasizing the improved accuracy of our new 25-term formula.) This implies that whereas our 25-term equation of state has a maximum error that can cause a 1% error in typical values of the dynamically important quantities \( \nabla_h \rho \) and in \( N^2 \), use of the Wright (1997) and UNESCO equations of state will lead to maximum errors in \( \nabla_h \rho \) and in \( N^2 \) that are up to 10% of their typical values.

Based on the comparison in Fig. 5b and our argument that the errors in the thermal expansion coefficient are the best indication of dynamically significant errors, it appears that the use of the more accurate FH95 equation of state is required to significantly improve on Wright’s (1997) simple formula. The dashed-dotted line in Fig. 5b depicts the maximum absolute errors between the UNESCO and Wright (1997) equations of state. Clearly the discrepancies between UNESCO and Wright (1997) are of the same order as the errors in each of these formulas, which was the desired goal for Wright’s (1997) formulation. This result is somewhat surprising since the density errors permitted by Wright are about 4 times larger than Fig. 5a suggests are actually present in the UNESCO formula.

The maximum error in the saline contraction coefficient from our 25-term equation is a factor of 2.5 less than the maximum error of the UNESCO equation, as seen in Figs. 3c and 5c. The corresponding estimate from the Wright (1997) equation is more than 5 times less accurate than the UNESCO equation. In spite of this reduced accuracy, it should be noted that the relative errors in \( \alpha \) and \( \beta \) are similar in the Wright (1997) formula so that relative errors in the dynamically important density variations should not be significantly increased by the reduced accuracy of the haline contraction coefficient. Comparison of Figs. 3d and 5d shows that our 25-term equation and the UNESCO equation give sound speed estimates of similar accuracy (except at the surface where the UNESCO equation is remarkably accurate), while the Wright (1997) equation is 3.5 times less accurate.

The differences between the international and Wright (1997) equations of state and the full FH95 equation of state as shown in Fig. 5 are consistent with the improvement in FH95 in the shallowest 4000 db being due to the incorporation of the more accurate data on the...
Fig. 5. Error measures of the differences between the international equation of state (solid line) and Wright’s (1997) equation of state (dashed line) when compared with the full FH95 form of the equation of state. (a) The rms and the maximum absolute errors in density as a function of pressure. (b), (c), and (d) Error measures for the thermal expansion coefficient, the haline contraction coefficient, and the sound speed, respectively. Also shown in (b) is a repeat of the maximum curve of Fig. 3b (bold line with dots) as well as the magnitude of the maximum errors between the UNESCO and Wright (1997) equations of state (the dotted–dashed line).
temperature of maximum density. This was a known weakness of the UNESCO formula, especially at medium salinities. At larger pressures, the more accurate sound speed data is probably the dominant cause of the differences.

5. Summary

We have utilized the most accurate thermodynamic knowledge of seawater to derive more accurate algorithms for potential temperature and for density. The equation for density has been written in terms of potential temperature referenced to the sea surface, rather than in terms of in situ temperature, as this is the form that is required by prognostic ocean models. In addition, we have provided an accurate and computationally efficient algorithm for potential temperature, and also sketched (in appendix C) how enthalpy in the form \( h(S, \theta, p) \) can be regarded as a thermodynamic potential in place of the Gibbs function.

Fofonoff (1985) states that the standard deviation between the international equation of state of seawater and the measurements that were used to define it is 0.009 kg m\(^{-3}\). This rms error has been interpreted as the rms error of the international equation of state, but it now appears that the international equation of state is substantially more accurate than this, and that the above error estimate reflects the accuracy of the individual laboratory and other measurements that were used. We regard the FH95 equation of state as substantially more accurate than the international equation of state and Fig. 5a shows that the rms difference between these two equations of state is only about 0.003 kg m\(^{-3}\) when measured over our funnel that includes all environmentally relevant fluid. This supports the view that for standard seawater, the international equation of state has an rms error of no more than 0.003 kg m\(^{-3}\), and (again from Fig. 5a) a maximum error of about 0.012 kg m\(^{-3}\). Our 25-term equation of state fits the full FH95 equation of state with a maximum error of no more than 0.003 kg m\(^{-3}\), which is probably close to the absolute accuracy of the FH95 expression.

We have argued that the more relevant measure of accuracy for dynamical oceanography is the error in the thermal expansion coefficient, (7), and that the maximum error is more relevant than the rms error because the maximum error tends to occur at very cold temperatures where it is most critical to have accuracy in the equation of state. At the temperature of maximum density we are confident that we have a good measure of the accuracy of the thermal expansion coefficient derived from Feistel and Hagen’s (1995) Gibbs function, namely, a maximum error in the thermal expansion coefficient of no more than 6 \( \times \) 10\(^{-7}\) °C\(^{-1}\). Our 25-term equation of state achieves a fit to Feistel and Hagen’s (1995) thermal expansion coefficient with a maximum error of 4 \( \times \) 10\(^{-7}\) °C\(^{-1}\) and so we believe that our equation of state is as accurate as is warranted by present knowledge of the Gibbs function of standard seawater. Figure 5b is perhaps the key figure of this paper and it shows that the maximum error in the thermal expansion coefficient of the international equation of state is an order of magnitude larger than the corresponding maximum error in our 25-term equation of state.

It should be noted that all the results in this paper apply to so-called standard seawater and there remains the issue of determining the true salinity of seawater (since the use of only conductivity, temperature, and pressure limits the accuracy of salinity determination) and the extent to which the different composition of sea salt affects density.

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APPENDIX A

The Approximate Polynomial for Potential Temperature

The potential temperature \( \theta \) with respect to the reference pressure \( p_r \) of a fluid parcel \((S, T, p)\) is defined in terms of the adiabatic lapse rate by the integral (Fofonoff 1977, 1985)

\[
\theta(S, T, p, p_r) = T + \int_{p_r}^{p} \Gamma(S, \theta(S, T, p, p'), p') \, dp'. \tag{A1}
\]

The adiabatic lapse rate \( \Gamma \) is the change in in situ temperature per unit change in pressure under adiabatic and isohaline conditions. This is related to the Gibbs function, \( G(S, T, p) \), by (see FH95)

\[
\Gamma = -G_{T_p}/G_{TT} = -\sigma_{T_T} \sigma_p = (273.15 + T) V_p / C_p
\]

\[
= (273.15 + T) \alpha \rho C_p, \tag{A2}
\]

where \( T \) is in degrees Celsius on the ITS-90 temperature scale (Preston-Thomas 1990). Here \( V \) is the specific volume, \( \rho \) is the in situ density, and \( \alpha \) is the thermal expansion coefficient (defined with respect to changes of in situ rather than of potential temperature). Since the thermal expansion coefficient is a strong function of pressure, we sought an approximation to the integral in (A1) of the form \( (p_p - p_r) \Gamma(S, T, [p + p_p]/2) \) leading to the following approximate expression for potential temperature

\[
\theta_0(S, T, p, p_r) = T + (p - p_r) P(S, T, \{p + p_p\}), \tag{A3}
\]

where the polynomial, \( P(S, T, \{p + p_p\}) \), is given by

\[
P(S, T, \{p + p_p\}) = a_1 + a_2 S + a_3 \{p + p_p\} + a_4 T
\]

\[
+ a_5 S T + a_6 T^2 + a_7 [p + p_p], \tag{A4}
\]

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salinity $S$ being in psu, temperature $T$ in degrees C, and pressure $p$ in db. The best-fit coefficients for this polynomial are given in Table A1. A check value for the polynomial is $\theta_0 = 19.621$ 967°C corresponding to $S = 35$ psu, $T = 20^\circ$C, $p = 2000$ db, and $p_r = 0$ db. The rms and maximum absolute errors of $\theta_0$ are 0.016°C and 0.123°C over the range of data for which it is defined, namely, the $(S-\theta-p-p_r)$ hypercube ($0$ psu, 40 psu) $\times$ $(-3^\circ$C, 40°C) $\times$ (0 db, 10 000 db) $\times$ (0 db, 10 000 db).

APPENDIX B

The Rational Function Equation of State

The 25-term equation of state is of the form

$$\rho(S, \theta, p) = P_1(S, \theta, p)/P_2(S, \theta, p)$$ (B1)

where the polynomials $P_1(S, \theta, p)$ and $P_2(S, \theta, p)$ are defined as in Table B1. Note that $p$ in (B1) is in decibars and $\theta$ is potential temperature referenced to the sea surface where $p_r = 0$. A check value for this equation is $\rho(35, 25, 2000) = 1031.654$ 229 kg m$^{-3}$, corresponding to $S = 35$ psu, $\theta = 25^\circ$C, and $p = 2000$ db. Other check values are $\rho(20, 20, 1000) = 1017.726$ 743 kg m$^{-3}$, and $\rho(40, 12, 8000) = 1062.928$ 258 kg m$^{-3}$. Over the very large $(S-\theta-p)$ cube ($0$ psu, 50 psu) $\times$ $(-10^\circ$C, 50°C) $\times$ (0 db, 10$^4$ db), $P_1$ and $P_2$ are very well behaved: $P_1$ varies from just less than 1000 kg m$^{-3}$ to about 1500 kg m$^{-3}$ while $P_2$ varies from 1.0 to about 1.5.

APPENDIX C

Enthalpy, $h(S, \theta, p)$, as Thermodynamic Potential

From the definition of entropy $\sigma$ and the fact that entropy can be regarded as a function of salinity and potential temperature alone [i.e., $\sigma = \sigma(S, \theta)$], it follows from the total differential $dh$ of $h(S, \sigma, p)$ that

$$(273.15 + T)\sigma_r d\theta + [\mu + (273.15 + T)\sigma_r]dS$$

$$= dh - (1/p)dp,$$ (C1)

where $\mu$ is the chemical potential and subscripts denote partial differentiation. Hence for adiabatic and isohaline excursions in pressure, the dependence of enthalpy on pressure is simply given by the pressure integral of specific volume, namely,

$$h(S, \theta, p) = h(S, \theta, 0) + \int_0^p 1/\rho(S, \theta, p') dp'.$$ (C2)

We have specifically chosen the form of our rational function, (5), so that the integral in (C2) may be easily formed analytically. The numerator in (5), $P_1(S, \theta, p)$, which becomes the denominator in the integrand in (C2), is a quadratic in pressure whose discriminant is positive definite for all conceivable values of the arguments, giving two real roots for the quadratic. The integral can then be written down in terms of natural logarithms (see, e.g., Gradshteyn and Ryzhik 1980). This integral is augmented by the expression for enthalpy at zero pressure from FH95, $h(S, \theta, 0) = h(S, T, 0)$, so giving the full expression, (C2), for enthalpy in terms of potential temperature.

When combined with the expression for entropy as a function of $S$ and $\theta$ from FH95 $[\sigma(S, \theta) = \sigma(S, T, 0)]$ the above expression for $h(S, \theta, p)$ can be regarded as a complete thermodynamic potential from which all thermodynamic quantities can be derived. For example, the relationship between in situ and potential temperature can be found from (C1) to be

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\[ h_s \big|_{s_p} = (273.15 + T)\sigma_p, \quad (C3) \]

and the Gibbs function is
\[ G = h - \sigma h_p/\sigma_p, \quad (C4) \]

REFERENCES


