An Equation of State for Numerical Models of Oceans and Estuaries

GEORGE L. MELLOR

Atmospheric and Oceanics Sciences Program, Princeton University, Princeton, New Jersey

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1. Introduction

Numerical models of oceans or estuaries require an equation of state in order to relate density, salinity, temperature, and pressure. The needs are for an equation that is reasonably efficient numerically and has a wide range of application. In addition, since numerical models solve for potential temperature, one would like an equation of state in the form

$$\rho = \rho(S, \Theta, p) \tag{1}$$

where ρ is density, S is salinity, Θ is potential temperature, and p is pressure.

In the following we will denote property functions as in Eq. (1) where, for example, $\partial\rho/\partial S$ denotes the partial derivative of density with respect to S holding θ and p constant. We denote spatial functions with a superposed tilde so that, for example, $\partial\tilde{\rho}/\partial x$ denotes the partial derivative of density with respect to x holding y and z constant.

Models require horizontal density gradients, $(\partial\tilde{\rho}/\partial x, \partial\tilde{\rho}/\partial y)$, which are readily obtained from Eq. (1) and known spatial fields of $\tilde{T}$, $\tilde{S}$, and $\tilde{p}$. They also require the vertical static stability obtained either from

$$\frac{N^2}{g} = -\frac{1}{\rho}\left[\frac{\partial\rho}{\partial S}\frac{\partial\tilde{S}}{\partial z} + \frac{\partial\rho}{\partial\theta}\frac{\partial\tilde{\theta}}{\partial z}\right] \tag{2a}$$

or from

$$\frac{N^2}{g} = -\frac{1}{\rho}\left[\frac{\partial\tilde{\rho}}{\partial z} - \frac{1}{c_s^2}\frac{\partial\tilde{p}}{\partial z}\right] \tag{2b}$$

where $c_s^2 \equiv [(\partial\rho/\partial p)_{s,\theta}]^{-1}$ is the speed of sound squared. The term N^2 governs vertical mixing either through a Richardson number formulation (e.g., Munk and Anderson 1948) or by a turbulence closure scheme (e.g., Mellor and Yamada 1982). Equations (2a) and (2b) are equivalent since $\partial\tilde{\rho}/\partial z - (\partial\rho/\partial S)(\partial\tilde{S}/\partial z) + (\partial\rho/\partial\theta)(\partial\tilde{\theta}/\partial z) + (\partial\rho/\partial p)(\partial\tilde{p}/\partial z)$. However, numerical calculations using (2a) or (2b) may differ as discussed below.

Bryan and Cox (1972) use a three-dimensional model whose vertical coordinate corresponds to constant depth levels. To obtain density they preprocess a table of coefficients for each depth. On the other hand, we have a three-dimensional, primitive-equation ocean model that uses a sigma coordinate system in the vertical (Oey et al. 1986a,b; Blumberg and Mellor 1987). It has been applied to coastal oceans and estuaries but, increasingly, is also applied to deep water ocean domains. Other sigma coordinate models have appeared and are still appearing in the literature. For sigma coordinate models, the Bryan–Cox scheme is inappropriate.

2. Analysis

The now standard, UNESCO (United Nations Educational, Scientific, and Cultural Organization) equation of state is fairly expensive computationally and is overly precise relative to the capability of numerical models to produce comparable precision. Furthermore, it is an equation of the form, $\rho = \rho(S, T, p)$; i.e., in situ temperature is an independent variable rather than potential temperature.

A less precise but substantially simpler formula of the desired form is

$$\rho(S, \Theta, p) = \rho(S, \Theta, 0) + \frac{p}{c^2}\left(1 - C\frac{p}{c^2}\right) \tag{3}$$

where $\rho(S, \Theta, 0)$ can be taken from the UNESCO formula [the complete formula, $\rho(S, T, p)$, increases the computational time by about a factor of 3] since $\Theta = T$ for $p = 0$. The second term in Eq. (3), the pressure dependent part, contains $c = c(S, \Theta, p)$ and a constant C. It should be noted that c is not exactly the speed of sound. Thus, from Eq. (3)

$$c_s^2 = \frac{1}{(\partial\rho/\partial p)_{s,\theta}} = c^2\left[\left(1 - \frac{2p}{c}\frac{\partial c}{\partial p}\right)\left(1 - 2C\frac{p}{c^2}\right)\right]^{-1}. \tag{4}$$

To approximate the complete UNESCO function, we have determined that

$$\rho(S, \Theta, p) = \rho(S, \Theta, 0) + 10^4\frac{p}{c^2}\left(1 - 0.20\frac{p}{c^2}\right) \tag{5a}$$

Corresponding author address: Dr. George L. Mellor, Program in Atmospheric and Oceanic Sciences, P.O. Box CN710, Sayre Hall, Princeton University, Princeton, NJ 08544-6571.

TABLE 1. A comparison of ρ_1, the density obtained from the full UNESCO formula, and ρ_2, the density obtained from Eqs. (5a) and (5b). The units of ρ, c, S, Θ, and p are kilograms per cubic meter, meters per second, parts per thousand, degrees Celsius, and decibars, respectively. The quantity, 1000 kg m^{-3}, has been subtracted from the densities.

p	S	T	Θ	ρ_1	ρ_2	$\rho_2 - \rho_1$
0	35	0	0.00	28.106	28.106	0.000
0	35	4	4.00	27.786	27.786	0.000
0	35	8	8.00	27.274	27.274	0.000
0	35	12	12.00	26.590	26.590	0.000
0	35	16	16.00	25.748	25.748	0.000
0	35	20	20.00	24.763	24.763	0.000
0	35	24	24.00	23.643	23.643	0.000
0	35	28	28.00	22.397	22.397	0.000
1000	35	0	−0.05	32.818	32.818	−0.001
1000	35	4	3.92	32.393	32.393	0.000
1000	35	8	7.89	31.792	31.791	−0.001
1000	35	12	11.87	31.031	31.029	−0.002
2000	35	0	−0.11	37.429	37.427	−0.002
2000	35	4	3.83	36.903	36.903	−0.001
2000	35	8	7.78	36.216	36.215	−0.001
4000	35	0	−0.28	46.356	46.351	−0.005
4000	35	4	3.61	45.643	45.642	0.000
6000	35	0	−0.51	54.908	54.902	−0.005
6000	35	4	3.34	54.025	54.026	0.001
10 000	35	0	−1.10	70.958	70.965	0.007
10 000	35	4	2.68	69.792	69.790	−0.002
0	37	0	0.00	29.722	29.722	0.000
0	37	4	4.00	29.378	29.378	0.000
0	37	8	8.00	28.846	28.846	0.000
0	37	12	12.00	28.144	28.144	0.000
0	37	16	16.00	27.288	27.288	0.000
0	37	20	20.00	26.290	26.290	0.000
0	37	24	24.00	25.158	25.158	0.000
0	37	28	28.00	23.902	23.902	0.000
1000	37	0	−0.05	34.417	34.416	−0.001
1000	37	4	3.92	33.970	33.969	−0.001
1000	37	8	7.89	33.350	33.348	−0.002
1000	37	12	11.86	32.573	32.569	−0.004
2000	37	0	−0.11	39.012	39.010	−0.002
2000	37	4	3.83	38.465	38.464	−0.002
2000	37	8	7.77	37.760	37.757	−0.003
4000	37	0	−0.29	47.909	47.904	−0.004
4000	37	4	3.60	47.177	47.175	−0.002
6000	37	0	−0.52	56.432	56.430	−0.003
6000	37	4	3.32	55.534	55.533	0.000
10 000	37	0	−1.12	72.443	72.446	0.013
10 000	37	4	2.66	71.255	71.252	−0.003

where

$$c = 1449.2 + 1.34(S - 35) + 4.55\Theta - 0.045\Theta^2 + 0.00821p + 15.0 \times 10^{-9} p^2. \quad (5b)$$

In Eqs. (5a) and (5b) the constants have been specialized so that the units of ρ, c, S, Θ, and p are kilograms per cubic meter, meters per second, parts per thousand, degrees Celsius, and decibars, respectively. A comparison of ρ from Eqs. (5a) and (5b) with a result taken from the full UNESCO formulation is shown in Table 1. In the latter case, the relation between temperature and potential temperature, $\Theta = \Theta(S, T, p)$, is obtained from a formula by Bryden (1973).

We use the word "error" to denote the difference between the approximate formula and the full UNESCO formula. Thus, the error when $p = 0$ is identically zero for all values of S and Θ since the UNESCO formula is used for $\rho(S, \Theta, 0)$ in Eq. (5a); otherwise, the error is given in the last column of Table 1. The resulting error in calculating horizontal density gradients using Eqs. (5a) and (5b) are, in the deepest water, about 1%, and it decreases with decreasing depth; errors in geostrophic velocities, dependent on the vertical integral of the density gradients, are much less. Note that the maximum temperatures at each pressure in Table 1 are outside the climatological envelope of 98% of the World Ocean (Bryan and Cox 1972; see also Gill 1982).

If now we specialize Eq. (4) for the same units as above and use Eq. (5b) to obtain $\partial c/\partial p$, we obtain

TABLE 2. A comparison of c_{s1}, speed of sound obtained from the full UNESCO formula together with Bryden's potential temperature formula, and c_{s2}, the speed of sound from Eq. (6).

p	S	Θ	T	c_{s1}	c_{s2}	$c_{s2} - c_{s1}$
0	35	0	0.00	1449.2	1449.2	0.0
0	35	4	4.00	1466.6	1466.7	0.1
0	35	8	8.00	1482.5	1482.7	0.3
0	35	12	12.00	1496.8	1497.3	0.5
0	35	16	16.00	1509.8	1510.5	0.7
0	35	20	20.00	1521.5	1522.2	0.7
0	35	24	24.00	1532.0	1532.5	0.5
0	35	28	28.00	1541.4	1541.3	0.0
1000	35	0	0.05	1465.7	1465.9	0.2
1000	35	4	4.08	1483.3	1483.3	0.0
1000	35	8	8.11	1499.3	1499.4	0.1
1000	35	12	12.14	1513.8	1514.0	0.2
2000	35	0	0.11	1482.5	1482.7	0.2
2000	35	4	4.17	1500.3	1500.2	−0.1
2000	35	8	8.23	1516.3	1516.2	−0.1
4000	35	0	0.29	1517.2	1517.1	−0.2
4000	35	4	4.40	1534.9	1534.5	−0.4
6000	35	0	0.53	1553.1	1552.3	−0.8
6000	35	4	4.69	1570.3	1569.7	−0.6
10 000	35	0	1.16	1627.6	1625.3	−2.3
10 000	35	4	5.39	1643.0	1642.7	−0.3
0	37	0	0.00	1451.8	1451.9	0.1
0	37	4	4.00	1469.2	1469.4	0.2
0	37	8	8.00	1484.9	1485.4	0.5
0	37	12	12.00	1499.2	1500.0	0.8
0	37	16	16.00	1512.1	1513.2	1.1
0	37	20	20.00	1523.7	1524.9	1.1
0	37	24	24.00	1534.2	1535.2	1.0
0	37	28	28.00	1543.4	1544.0	0.6
1000	37	0	0.05	1468.4	1468.5	0.2
1000	37	4	4.08	1485.9	1486.0	0.1
1000	37	8	8.11	1501.8	1502.1	0.3
1000	37	12	12.14	1516.2	1516.7	0.5
2000	37	0	0.12	1485.3	1485.4	0.1
2000	37	4	4.18	1502.9	1502.9	0.0
2000	37	8	8.23	1518.8	1518.9	0.1
4000	37	0	0.30	1520.0	1519.7	−0.3
4000	37	4	4.41	1537.5	1537.2	−0.3
6000	37	0	0.55	1555.9	1554.9	−1.0
6000	37	4	4.70	1573.0	1572.4	−0.6
10 000	37	0	1.19	1630.3	1628.0	−2.3
10 000	37	4	5.42	1645.6	1645.3	−0.2

$$c_s = c\left[1 - \frac{2}{c}(0.00821p + 15.0 \times 10^{-9}p^2)\left(1 - 0.40\frac{p}{c^2}\right)\right]^{-1/2} \quad (6)$$

Table 2 is a comparison of Eq. (5b) and Eq. (6) with a more precise determination of c_s. The latter is obtained by numerical differentiation (in double precision) of ρ to obtain $(\partial\rho/\partial p)_{s,\theta}$ using the complete UNESCO formula, $\rho(S, T, p)$, after conversion to $\rho(S, \Theta, p)$, using Bryden's formula for $\Theta = \Theta(S, T, p)$; an iteration is required but convergence is fast. Thus, c_s, obtained from Eq. (5b) and Eq. (6), can be used to obtain the static stability in (2b).

The use of (2b) rather than (2a) to obtain N^2 may be preferred numerically if one had previously stored $\tilde{\rho}(x, y, z)$ in memory. However, this could involve some roundoff error (dependent on word length) or truncation error (dependent on grid resolution). For indefinitely small grid size and indefinitely large word length the difference is null. As a counter example, consider $\delta\tilde{S} - \delta\tilde{\theta} - 0$ and $\partial\tilde{p} - 1000$ db; here the roundoff error is negligible but the truncation error for this rather large increment in $\tilde{p}$ may not be. From (2a) we obtain $N^2 = 0$, the correct result, whereas, from (2b) and Tables 1 and 2 (using a midpoint value of c_s) we obtain $N^2 - O(10^{-7})\ \mathrm{s}^{-2}$. Typical oceanic values of N^2 are $O(10^{-4} - 10^{-3})\ \mathrm{s}^{-2}$.

Note that, in (2), the hydrostatic relation, $\partial p/\partial z = -\rho g$, can be used. If one approximates this relation such that ρ = constant = ρ_0, then it is necessary to use the same approximation to obtain p in (5a), (5b), and (6).

3. Summary

The equation of state according to Eqs. (5a) and (5b) is an equation for density whose independent variables are salinity, potential temperature, and pressure. It should cover the small range in pressure and the large range of Θ and S found in estuaries and other shallow waters, as well as the large pressure range and smaller range of Θ and S of the deeper ocean basins. The use of Eq. (2a) or the combination of Eq. (6) and Eq. (2b) enables one to obtain the static stability. All of these equations are relatively efficient computationally and suitable for numerical ocean models.

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