An Approximate Equation of State for Numerical Models of Ocean Circulation

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The Knudsen formula (Fofonoff, 1962) is the standard method for computing the density of sea water from the temperature, salinity and pressure. However, the Knudsen formula is designed to fit experimental data over a wide range of temperatures and salinities, a much wider range, in fact, than is ordinarily encountered in the ocean. In a numerical model of ocean circulation, it is usually necessary to calculate the density only at a discrete set of levels which are determined in advance. In that case, it is possible to calculate the density from simple polynomial formulas if the constant coefficients in these formulas are a function of pressure and are determined in such a way as to give a good fit to the classical Knudsen formula for a realistic range of temperatures and salinities in the World Ocean.

In many previous studies of ocean circulation the mathematical models do not include temperature and salinity explicitly. The models in these studies only predict the density field and heating, while the effects of evaporation and precipitation only enter through the specification of boundary conditions on density.

Such models are quite adequate for studying many aspects of the dynamics of the ocean circulation. In the case of large-scale, ocean-atmosphere interaction, however, we are interested in the transfer of heat and salinity in the ocean *per se*. For such studies the model must include predictive equations for temperature and salinity and an equation of state is required as an additional diagnostic relation.

An extensive body of hydrographic data is available on magnetic tape files at the National Oceanographic Data Center in Washington, D. C. In Table 1, the ranges which include 98% of the volume of the World Ocean are shown for temperature and salinity at different depths. The ranges are rounded off to the nearest 1C in temperature and 0.1‰ in salinity. It can be seen that near the surface, the range of temperature is nearly 30C, but decreases to only a few degrees at great depths. In the same way, the greatest range of salinities is found at the surface and decreases to only 1‰ at greater depths.

Let ρ_{0k}, T_{0k} and S_{0k} be the density, temperature and salinity corresponding to the mid-point of the ranges shown in Table 1 for any given level Z_k. Let δT, $\delta S \equiv (T-T_{0k})$, $(S-S_{0k})$ represent the departures of temperature from the mid-point values. We can express the density as

$$x_{1k}\delta T+x_{2k}\delta S+x_{3k}(\delta T)^2+x_{4k}(\delta S)^2+x_{5k}\delta T\delta S+x_{6k}(\delta T)^3 +x_{7k}(\delta S)^2\delta T+x_{8k}(\delta T)^2\delta S+x_{9k}(\delta S)^3+\cdots =[\rho(T,S,Z_k)-\rho_{0k}]\times 10^3. \quad (1)$$

To find the set of coefficients, $x_{1k}, x_{2k}, x_{3k}\cdots x_{mk}$, which provides the best fit to the Knudsen formula, we first compute the density from the Knudsen formula for m evenly spaced points in the T-S range shown in Table 1. It is then possible to write a series of m linear equation of the form of (1):

$$\begin{bmatrix} \delta T_1 & \delta S_1 & \delta T_1^2 & \cdots \\ \delta T_2 & \delta S_2 & \delta S_1^2 & \cdots \\ \vdots & \vdots & & \\ \vdots & \vdots & & \\ \delta T_m & \delta S_m & \cdots & \cdots \end{bmatrix} \begin{bmatrix} x_{1k} \\ x_{2k} \\ \vdots \\ x_{nk} \end{bmatrix} = \begin{bmatrix} \rho_1-\rho_{0k} \\ \rho_2-\rho_{0k} \\ \vdots \\ \rho_m-\rho_{0k} \end{bmatrix}. \quad (2)$$

TABLE 1. 98% range of temperatures and salinities given by the NODC data for the World Ocean rounded off to 1C and 0.1‰ of salinity.

Level (m)	T_{Min}	T_{Max}	S_{Min}	S_{Max}
0	−2.000	29.000	28.500	36.700
250	−2.000	19.000	33.700	36.600
500	−2.000	14.000	34.000	35.800
750	−2.000	11.000	34.100	35.700
1000	−1.000	9.000	34.200	35.300
1250	−1.000	7.000	34.400	35.100
1500	−1.000	5.000	34.500	35.100
1750	−1.000	4.000	34.500	35.000
2000	−1.000	4.000	34.600	35.000
2250	−1.000	4.000	34.600	35.000
2500	−1.000	3.000	34.600	35.000
2750	−1.000	3.000	34.600	35.000
3000	−1.000	3.000	34.600	35.000
3250	−1.000	3.000	34.600	35.000
3500	−1.000	3.000	34.600	34.900
3750	−1.000	2.000	34.600	34.900
4000	−1.000	2.000	34.600	34.900
4250	−1.000	2.000	34.600	34.900
4500	−1.000	2.000	34.600	34.900
4750	0.000	2.000	34.600	34.900
5000	0.000	2.000	34.600	34.900
5250	0.000	2.000	34.600	34.900
5500	0.000	2.000	34.600	34.900
5750	0.000	2.000	34.700	34.800
6000	0.000	2.000	34.700	34.800

TABLE 2. The constants in the polynomial formula (1), retaining only the first three terms on the left. $m=50$.

Z	$(\rho_0-1)10^{-3}$	T_0	S_0	$X1$	$X2$	$X3$
0	24.458	13.50	32.600	−0.19494−00	0.77475−00	−0.49038−02
250	28.475	8.50	35.150	−0.15781−00	0.78318−00	−0.52669−02
500	29.797	6.00	34.900	−0.13728−00	0.78650−00	−0.55278−02
750	31.144	4.50	34.900	−0.12720−00	0.78807−00	−0.56610−02
1000	32.236	4.00	34.750	−0.12795−00	0.78710−00	−0.56274−02
1250	33.505	3.00	34.750	−0.12312+00	0.78763−00	−0.56972−02
1500	34.808	2.00	34.800	−0.11837+00	0.78822−00	−0.57761−02
1750	35.969	1.50	34.750	−0.11896+00	0.78751−00	−0.57631−02
2000	37.143	1.50	34.800	−0.12543−00	0.78560−00	−0.56422−02
2250	38.272	1.50	34.800	−0.13168−00	0.78368−00	−0.55239−02
2500	39.462	1.00	34.800	−0.13250−00	0.78300−00	−0.55116−02
2750	40.582	1.00	34.800	−0.13871−00	0.78109−00	−0.53946−02
3000	41.695	1.00	34.800	−0.14483−00	0.77920−00	−0.52793−02
3250	42.801	1.00	34.800	−0.15088−00	0.77733−00	−0.51654−02
3500	43.863	1.00	34.750	−0.15673−00	0.77544−00	−0.50557−02
3750	45.038	0.50	34.750	−0.15771−00	0.77475−00	−0.50466−02
4000	46.130	0.50	34.750	−0.16363−00	0.77292−00	−0.49360−02
4250	47.216	0.50	34.750	−0.16948−00	0.77110−00	−0.48268−02
4500	48.296	0.50	34.750	−0.17524−00	0.76930−00	−0.47193−02
4750	49.278	1.00	34.750	−0.18556−00	0.76641−00	−0.45102−02
5000	50.344	1.00	34.750	−0.19107−00	0.76467−00	−0.44074−02
5250	51.404	1.00	34.750	−0.19650−00	0.76295−00	−0.43061−02
5500	52.459	1.00	34.750	−0.20186−00	0.76126−00	−0.42068−02
5750	53.508	1.00	34.750	−0.20715−00	0.75958−00	−0.41138−02
6000	54.552	1.00	34.750	−0.21237−00	0.75792−00	−0.40172−02

TABLE 3. The constants in the polynomial formula (1), retaining the first nine terms on the left. $m=50$.

Z (m)	$(\rho_0-1)10^{-3}$	T_0	S_0	$X1$	$X2$	$X3$	$X4$	$X5$	$X6$	$X7$	$X8$	$X9$
0	24.458	13.50	32.600	−0.20134−00	0.77096−00	−0.49261−02	0.46092−03	−0.20105−02	0.36597−04	0.47371−05	0.37735−04	0.65493−05
250	28.475	8.50	35.150	−0.16175−00	0.78144−00	−0.52769−02	0.75722−03	−0.23216−02	0.49230−04	0.51236−05	0.38366−04	0.65903−05
500	29.797	6.00	34.900	−0.13993−00	0.78549−00	−0.55345−02	0.75780−03	−0.24758−02	0.57307−04	0.60986−05	0.38758−04	0.66124−05
750	31.144	4.50	34.900	−0.12911−00	0.78740−00	−0.56670−02	0.56653−03	−0.25505−02	0.62594−04	0.68808−05	0.38692−04	0.66235−05
1000	32.236	4.00	34.750	−0.12910−00	0.78671−00	−0.56315−02	0.49614−03	−0.25491−02	0.63658−04	0.70626−05	0.38377−04	0.64420−05
1250	33.505	3.00	34.750	−0.12391+00	0.78738−00	−0.57000−02	0.51205−03	−0.25839−02	0.67480−04	0.77630−05	0.38187−04	0.72748−05
1500	34.808	2.00	34.800	−0.11884+00	0.78808−00	−0.57787−02	0.37875−03	−0.26168−02	0.71687−04	0.84025−05	0.37987−04	0.45243−05
1750	35.969	1.50	34.750	−0.11930+00	0.78742−00	−0.57655−02	0.34884−03	−0.26132−02	0.73473−04	0.85132−05	0.37725−04	0.60659−05
2000	37.143	1.50	34.800	−0.12575−00	0.78551−00	−0.56439−02	0.39420−03	−0.25705−02	0.72506−04	0.89350−05	0.37149−04	0.44399−05
2250	38.272	1.50	34.800	−0.13200−00	0.78359−00	−0.55256−02	0.39655−03	−0.25290−02	0.71549−04	0.85260−05	0.36616−04	0.12463−04
2500	39.462	1.00	34.800	−0.13271−00	0.78294−00	−0.55138−02	0.32413−03	−0.25239−02	0.73429−04	0.10282−04	0.36109−04	0.16525−04
2750	40.582	1.00	34.800	−0.13892−00	0.78103−00	−0.53969−02	0.33409−03	−0.24835−02	0.72448−04	0.99097−05	0.35560−04	0.12621−04
3000	41.695	1.00	34.800	−0.14504−00	0.77914−00	−0.52816−02	0.33539−03	−0.24432−02	0.71438−04	0.91199−05	0.35204−04	0.87250−05
3250	42.801	1.00	34.800	−0.15109−00	0.77727−00	−0.51678−02	0.33845−03	−0.24036−02	0.70442−04	0.93518−05	0.34838−04	0.12774−04
3500	43.863	1.00	34.750	−0.15693−00	0.77539−00	−0.50572−02	0.38111−03	−0.23652−02	0.69451−04	0.74599−05	0.34235−04	0.39869−04
3750	45.038	0.50	34.750	−0.15783−00	0.77472−00	−0.50488−02	0.32700−03	−0.23606−02	0.71438−04	0.71846−05	0.34354−04	0.21159−04
4000	46.130	0.50	34.750	−0.16375−00	0.77289−00	−0.49382−02	0.32053−03	−0.23220−02	0.70448−04	0.13349−04	0.33704−04	0.11926−04
4250	47.216	0.50	34.750	−0.16959−00	0.77107−00	−0.48290−02	0.32045−03	−0.22846−02	0.69403−04	0.63029−05	0.33422−04	−0.16154−04
4500	48.296	0.50	34.750	−0.17536−00	0.76927−00	−0.47215−02	0.32345−03	−0.22472−02	0.68376−04	0.10706−04	0.33227−04	−0.34828−04
4750	49.278	1.00	34.750	−0.18561−00	0.76640−00	−0.45150−02	0.30913−03	−0.21784−02	0.64295−04	0.63017−05	0.32674−04	0.31481−05
5000	50.344	1.00	34.750	−0.19111−00	0.76466−00	−0.44123−02	0.31778−03	−0.21430−02	0.63184−04	0.96040−05	0.32820−04	0.22144−04
5250	51.404	1.00	34.750	−0.19655−00	0.76294−00	−0.43111−02	0.32116−03	−0.21081−02	0.62171−04	0.13567−04	0.32430−04	−0.34214−04
5500	52.459	1.00	34.750	−0.20191−00	0.76124−00	−0.42118−02	0.32078−03	−0.20739−02	0.61268−04	0.14557−04	0.30528−04	−0.43468−04
5750	53.508	1.00	34.750	−0.20720−00	0.75957−00	−0.41144−02	0.30341−03	−0.20398−02	0.60008−04	−0.48824−04	0.32333−04	−0.10261−03
6000	54.552	1.00	34.750	−0.21242−00	0.75791−00	−0.40180−02	0.45242−03	−0.20072−02	0.58999−04	0.26971−04	0.30869−04	−0.36297−03

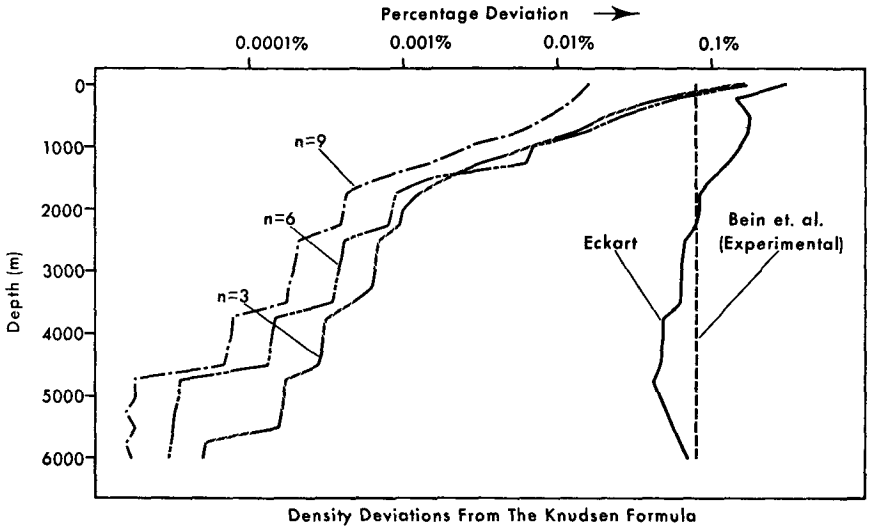

FIG. 1. The average percentage error in $(\rho-1)\times10^{-3}$ over the ranges given in Table 1, where the Knudsen formula is taken as a standard.

If $m=n$, the vector **x** can be determined by directly solving (2). However, the case of interest is for $m>n$. In that case, we have an overdetermined system and an iterative procedure must be used to find the best least-squares fit. The algorithm used in the present study is outlined by Hanson and Lawson (1969). The actual calculation is carried out with a Jet Propulsion Laboratory Fortran subroutine designated LSQL2.

A set of coefficients computed by this procedure is shown in Tables 2 and 3. In Table 2, n is set equal to 3, while in Table 3 n is set to 9. In Fig. 1 the average absolute error over the ranges of Table 1 is plotted in terms of percent of sigma-t units. The average is calculated from 2400 equally spaced points. The error is compared to the difference between the Eckart (1958) formula and the Knudsen formula, as well as the average difference found by Bein *et al.* (1935) between laboratory measurements and Knudsen's formula. Note that the polynomials give a much better fit to the Knudsen formula than Eckart's formula, and also that the fit of the polynomials is particularly accurate at greater depths where the range is small. The steps in the curves are due to the fact that round-off has not allowed the ranges to vary continuously with respect to depth.

To present a more complete picture of the relative difference between the present polynomials, and the Eckart and Knudsen formulas, we refer to Figs. 2a and 2b. These figures show lines of constant density plotted on a conventional T-S diagram. Fig. 2a compares the density corresponding to surface pressure calculated from the Eckart and Knudsen formulas. Note that the Eckart formula gives consistently higher values of density at lower temperatures. On the other hand, the third-order polynomial curves based on the

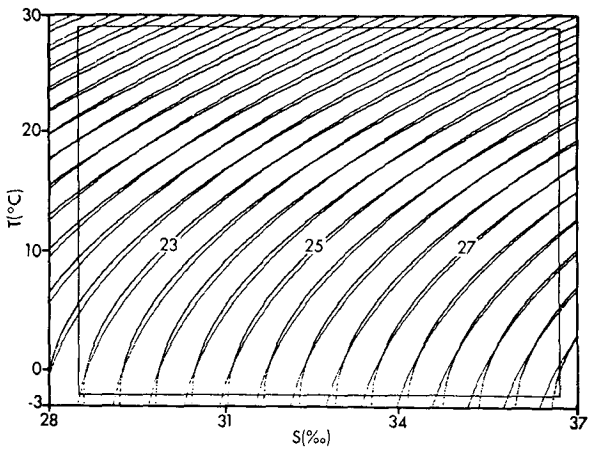

FIG. 2a. Lines of constant density based on the Knudsen and Eckart formulas. The Eckart curves are shifted slightly to the left at low temperatures.

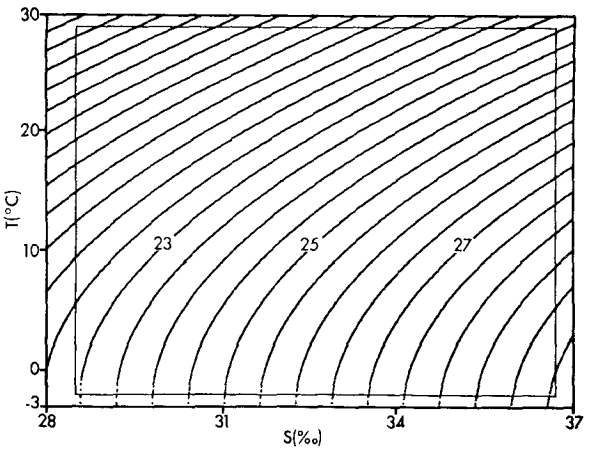

FIG. 2b. Nearly coincident lines of constant density based on the third-order polynomial formula (1) and the Knudsen formula.

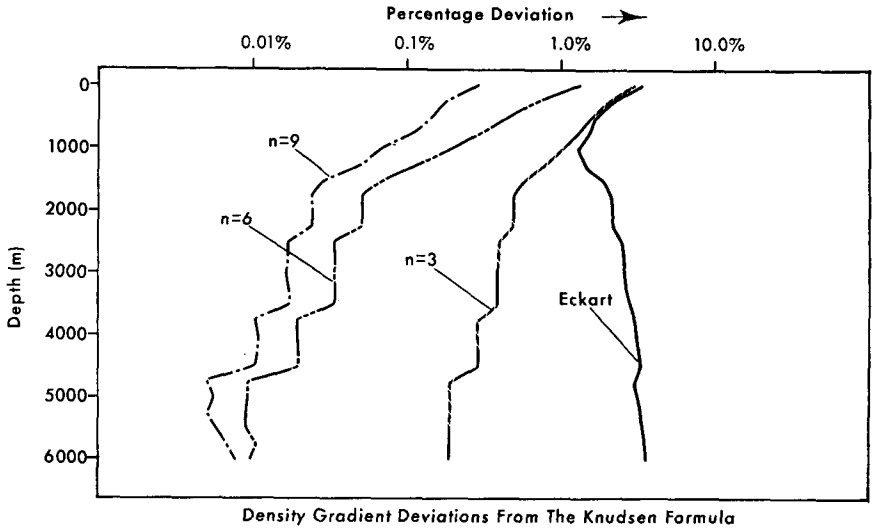

FIG. 3. The percentage error in gradients of density over the ranges given in Table 1.

coefficients given in Table 3 coincide so closely with the Knudsen formula that the resolution of the diagram does not allow us to discriminate between the two.

In dynamic calculations, horizontal gradients of density are more important than the density itself. In Fig. 3, the difference between the density gradients computed from the polynomials and the density gradients computed from the Knudsen formula are expressed as a percentage of the density gradient computed from the Knudsen formula. The gradients are computed over intervals of 0.05C and 0.05‰ of salinity. As in Fig. 1, the percentage deviation at each level is based on the average of 2400 evenly spaced points. Note that the results are similar to Fig. 1. The fit is superior to that of the Eckart formula and is much more accurate over the smaller ranges at great depths.

For special model studies it may be desirable to find polynomial formulas for different levels, and fitted to different ranges of temperature and salinity than those of Table 1. The authors would be happy to make their Fortran program available to their colleagues upon request.

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