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Spiciness

by Trevor J. McDougall^{1,2} and Oliver A. Krzysik¹

ABSTRACT

We define and present algorithms for spiciness, which is an oceanographic variable whose isopycnal variations reflect isopycnal water-mass contrasts in density units. Discussion of spiciness in the oceanographic literature has often concentrated on its supposed orthogonality to isopycnals on the salinity-temperature diagram and how this orthogonal nature means that spiciness is a “passive” thermodynamic variable. Here we show that this “orthogonal” property is devoid of physical meaning. Moreover, it is emphasized that the notion of “orthogonality” on the salinity-temperature diagram does not give rise to a passive thermodynamic variable. Rather, the passive nature of variations of any thermodynamic variable is gained by evaluating those variations along isopycnals so that, for example, the isopycnal variations of both Absolute Salinity and Conservative Temperature are passive. The advantage of using isopycnal variations of our definition of spiciness is that this measures the passive spatial variations of water-mass properties in density units. The spiciness variables presented here have been derived using the equation of state from the *International Thermodynamic Equation of Seawater – 2010*.

Keywords: Ocean mixing, diapycnal mixing, spiciness

1. Introduction

The concept of a thermodynamic variable that is in some sense “orthogonal” to density on the salinity-temperature diagram has a long history, starting with Stommel (1962), Mamayev (1962), Veronis (1972), and Munk (1981). Mamayev (1962) and Veronis (1972) constructed their variable so that the isolines were orthogonal to contours of potential density on the salinity–potential temperature diagram; however, as pointed out by Veronis (1972), this definition of “orthogonal” is not unique because it depends on the relative scales chosen for the axes of the practical salinity–potential temperature (S_p, θ) diagram.

Jackett and McDougall (1985) avoided this dependence on the scaling of the (S_p, θ) axes, and they adopted a different definition of “orthogonality” for constructing their spiciness variable. They aimed to have the isolines of potential density and spiciness orthogonal to each other if the relative scales of the stretched (S_p, θ) diagram were chosen so that the isopycnals subtended an angle of 45° with the horizontal axis. In other words, their aim was

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to have the slopes of the isolines of potential density and spiciness on the (S_p, θ) diagram to be approximately the same magnitude but have opposite signs to each other.

Jackett and McDougall (1985) required that their spiciness variable obey another constraint—namely, that the variations of spiciness along isopycnals be proportional to the isopycnal integral of the saline contraction coefficient with respect to salinity, this being the strength of isopycnal water-mass contrasts (in density units) that is able to drive double-diffusive interleaving. The nonlinearity of the equation of state of seawater ensures that these two aims set out by Jackett and McDougall (1985) cannot both be obeyed. They opted to exactly satisfy the second criterion so that their spiciness variable did not exactly obey their adopted definition of orthogonality. Jackett and McDougall (1985) pointed out that no such definition of orthogonality ensures that a spiciness variable is dynamically passive as some have hoped, and because of this lack of an underpinning theoretical justification for any such orthogonality concept, Jackett and McDougall (1985) chose to relax this constraint in favor of exactly achieving the second desirable property of having the isopycnal variations of spiciness be water-mass contrasts, expressed in density units. Flament (2002) presented a very similar spiciness variable to that of Jackett and McDougall (1985) except that he chose to exactly enforce the Jackett and McDougall definition of orthogonality at the expense of sacrificing the accuracy of the isopycnal variations of spiciness so that his isopycnal variation of spiciness does not accurately represent the isopycnal contrast in water masses in density units.

Recently, Huang (2011) has defined a new version of “spicity,” but it has two fundamental drawbacks. First, this variable was constructed with the original definition of orthogonality, which is devoid of physical meaning. The second drawback of Huang’s (2011) spicity is the linear interpolation between several different polynomial expressions based on the pressure of one’s sample. In this way, the spicity that one finds is not a water-mass property but depends on the pressure of the parcel so that the spicity changes even for an adiabatic vertical motion in the ocean. Because potential density is a “potential” property that is independent of adiabatic heaving motion, it is desirable that spiciness also possess this potential property and be independent of adiabatic and isohaline changes in pressure.

There is a persistent belief in the oceanographic community that spiciness is (or should be) a dynamically passive variable. However, as pointed out by Jackett and McDougall (1985), there is no definition of orthogonality that yields a variable that is dynamically passive. Being “passive” is not a property of a thermodynamic variable, but rather, it is the construction of anomalies along isopycnals that yields variables that are dynamically passive.

We conclude that there is no compelling fundamental physical meaning to the concept of orthogonality on the salinity-temperature diagram, which leads us to adopt the approach of Jackett and McDougall (1985) and choose not to strictly enforce our particular choice of the meaning of orthogonal. Rather, we strictly enforce that the variation of spiciness along isopycnals be proportional to the water-mass contrast along isopycnals, expressed in density units. Jackett and McDougall (1985) showed (in their Fig. 6) that their spiciness

variable achieved this “water-mass” property along isopycnals by a factor of three better than Veronis’s (1972) variable, which was based on the ordinary geometric meaning of orthogonality. It should be noted that near the temperature of maximum density the variations of our spiciness variable along isopycnals tends to zero (as it should, along with the isopycnal water-mass contrast and the isopycnal Absolute Salinity contrast), but that there remains a substantial nonzero dynamically passive isopycnal variation of Conservative Temperature (Stipa 2002).

In this article, we develop a spiciness variable along the lines of Jackett and McDougall (1985), but for the *International Thermodynamic Equation of Seawater – 2010* (TEOS-10; see IOC et al. 2010), the new international definition of the thermophysical properties of seawater, ice, and humid air. The expression for density that we use is the function $\text{gsw_rho}(S_A, CT, p)$ of the Gibbs Seawater (GSW) Oceanographic Toolbox of TEOS-10 (McDougall and Barker 2011). This function calculates the in situ density (or the potential density) of seawater as a function of Absolute Salinity (S_A), Conservative Temperature (Θ), and pressure (p ; or reference pressure [p_r]). This expression for density is the 75-term polynomial of Roquet et al. (2015), which is a computationally efficient expression for density in terms of the basic thermodynamic variables of TEOS-10—namely, (S_A , Θ , p). Note that Absolute Salinity (S_A) is defined on the TEOS-10 Reference-Composition Salinity Scale of Millero et al. (2008) using the McDougall et al. (2012) algorithm for Absolute Salinity in terms of practical salinity, whereas Conservative Temperature is a temperature-like variable that more accurately (by two orders of magnitude) encapsulates the “heat content per unit mass of seawater” than does potential temperature (McDougall 2003; Graham and McDougall 2013). Absolute Salinity can be calculated from practical salinity using an approach based on a lookup table of Absolute Salinity anomaly ratios or by using measurements of the nutrient and carbon chemistry variables of a seawater sample. The estimation of Absolute Salinity in the ocean is an aspect of TEOS-10 that is expected to improve over time as more measurements become available.

2. Construction of the spiciness variables

We have constructed three different spiciness variables, one appropriate for use with shallow data, constructed using potential density referenced to $p_r = 0$ dbar; a second for $p_r = 1,000$ dbar; and a third for $p_r = 2,000$ dbar. These reference pressures have been selected because they correspond to commonly used potential density surfaces. In this section, we describe how, for each of these three cases, we first construct a fine mesh of spiciness values on the (S_A , Θ) diagram, and then we fit a polynomial in S_A and Θ to this data.

Noting that the differential of potential density with reference pressure (p_r) can be written as

$$d\rho^\Theta = b(S_A, \Theta, p_r) dS_A - a(S_A, \Theta, p_r) d\Theta, \quad (1)$$

where $b(S_A, \Theta, p_r)$ and $-a(S_A, \Theta, p_r)$ are the partial derivatives of potential density given by

$$b(S_A, \Theta, p_r) = \left. \frac{\partial \rho^\Theta}{\partial S_A} \right|_{\Theta, p_r} \quad \text{and} \quad a(S_A, \Theta, p_r) = - \left. \frac{\partial \rho^\Theta}{\partial \Theta} \right|_{S_A, p_r}, \quad (2)$$

the original aim of Stommel (1962), Munk (1981), and Jackett and McDougall (1985) was to construct a spiciness variable, τ , whose differential approximately obeyed

$$d\tau \approx b(S_A, \Theta, p_r) dS_A + a(S_A, \Theta, p_r) d\Theta. \quad (3)$$

Equation (3) cannot be exactly satisfied by τ because the partial derivative of $b(S_A, \Theta, p_r)$ with respect to Θ is not equal to the partial derivative of $a(S_A, \Theta, p_r)$ with respect to S_A , and so the right-hand side of equation (3) is not a total derivative. In fact, we know that instead of having b_Θ equal to a_{S_A} , rather, $b_\Theta = -a_{S_A}$. For differences along a potential density surface, we know that $b(S_A, \Theta, p_r) \delta S_A = a(S_A, \Theta, p_r) \delta \Theta$, and we choose to enforce equation (3) only in this direction. That is, we insist that the integral of spiciness along each and every isoline of potential density satisfies

$$\int_{\rho^\Theta} d\tau = 2 \int_{\rho^\Theta} b(S_A, \Theta, p_r) dS_A. \quad (4)$$

With equation (4) defining the variation of τ along isopycnals, all that remains is to specify the value of τ at some point along each isopycnal, and we have chosen to do this in the following two-step procedure. First, we chose the horizontal line $\Theta = 20^\circ\text{C}$ on the (S_A, Θ) diagram, and we applied the ‘‘orthogonal’’ property of equation (3) only along this line so that along $\Theta = 20^\circ\text{C}$ we specify $d\tau$ by

$$d\tau|_{\Theta=20^\circ\text{C}} = b(S_A, \Theta, p_r) dS_A = d\rho^\Theta|_{\Theta=20^\circ\text{C}}. \quad (5)$$

That is, along the line $\Theta = 20^\circ\text{C}$ the changes of spiciness are set to be exactly equal to changes in potential density referenced to p_r . We temporarily assigned a specific value to $\tau(S_A = 0 \text{ g kg}^{-1}, \Theta = 20^\circ\text{C})$ so that spiciness is defined by equation (5) for all values of Absolute Salinity at $\Theta = 20^\circ\text{C}$. A grid of points was then established over the (S_A, Θ) plane at given fixed intervals of Conservative Temperature and potential density. The GSW function `gsw_SA_from_rho` (obtained from <http://www.TEOS-10.org>) was then used to find the Absolute Salinity of these points. The integral given by the right-hand side of equation (4) was performed along each isopycnal from $\Theta = 20^\circ\text{C}$, integrating first to warmer temperatures and then to cooler temperatures from $\Theta = 20^\circ\text{C}$.

This procedure labeled much of the (S_A, Θ) plane with values of spiciness, but there was a region of warm fresh seawater that was not reached by this integration procedure. Specifically, this unlabeled ‘‘minority region’’ on the (S_A, Θ) plane is warmer than $\Theta = 20^\circ\text{C}$ and has potential density less than $\rho^\Theta = \rho(S_A = 0 \text{ g kg}^{-1}, \Theta = 20^\circ\text{C}, p_r)$. We labeled

this minority region by first fitting an eighth-order polynomial in Absolute Salinity to the spiciness data at $\Theta = 45^\circ\text{C}$ that were already labeled (and therefore whose potential density exceeded $\rho^\ominus = \rho[S_A = 0 \text{ g kg}^{-1}, \Theta = 20^\circ\text{C}, p_r]$). This provided values of spiciness at low salinities at $\Theta = 45^\circ\text{C}$, and the integral on the right-hand side of equation (4) was performed to label the minority region with values of spiciness.

The spiciness data over the full (S_A, Θ) plane up to $S_A = 42 \text{ g kg}^{-1}$, to $\Theta = 45^\circ\text{C}$, and down to 2°C below the freezing temperature were fitted with a 49-term polynomial as described in the Appendix. The final step in this fitting procedure was to add a constant value to the fit to ensure that $\tau(S_A = 35.16504 \text{ g kg}^{-1}, \Theta = 0^\circ\text{C})$ was zero. This value of Absolute Salinity corresponds to a practical salinity of 35 on the Reference-Composition Salinity Scale of TEOS-10 (as defined by Millero et al. 2008) for seawater of standard composition. The root-mean-square error in these polynomial fits to the underlying labeled spiciness data over the full (S_A, Θ) plane is no larger than $6 \times 10^{-6} \text{ kg m}^{-3}$ (or 0.15 ppm) in each case.

We performed the previously described procedure for three values of the reference pressure: $p_r = 0 \text{ dbar}$, $p_r = 1,000 \text{ dbar}$, and $p_r = 2,000 \text{ dbar}$. Note that each of the three polynomial definitions of spiciness is forced to be zero at $S_A = 35.16504 \text{ g kg}^{-1}$, $\Theta = 0^\circ\text{C}$.

The contours of the resulting three polynomials for spiciness are shown in Figure 1. In each panel are also plotted contours of the potential density referenced to that pressure, minus $1,000 \text{ kg m}^{-3}$. The dashed lines in the panels of Figure 1 are the freezing lines at the respective pressures.

As discussed in Section 1, it is not possible to achieve both our water-mass requirement (equation 4) regarding the variation of spiciness along isopycnals and a definition of orthogonality such as in our equation (3), and we have chosen to impose the water-mass variation constraint and to sacrifice any attempt to enforce orthogonality over the (S_A, Θ) plane; we have only imposed this orthogonality constraint along the line $\Theta = 20^\circ\text{C}$. In Figure 2, it is clear that along the line $\Theta = 20^\circ\text{C}$ the spiciness isolines almost exactly obey our orthogonal property in that if the relative axes of the (S_A, Θ) diagram are stretched so that the isopycnals subtend an angle of 45° with the Absolute Salinity axis, then the isolines of τ are rotated 90° with respect to the isopycnals. This is the meaning of the horizontal contours labeled 90° in the three panels of Figure 2. At warmer temperatures, the angle between the τ contours and the isopycnals becomes as much as 96° (when the isopycnals are arranged to be at 45° to the horizontal), whereas at cooler temperatures this included angle is less than 82° . Again, we emphasize that because there is no physical argument that can justify any particular meaning of the concept of orthogonality, the fact that this included angle is not a constant is of no consequence.

3. Discussion

We have provided three different expressions for spiciness, using reference pressures of $p_r = 0 \text{ dbar}$, $p_r = 1,000 \text{ dbar}$, and $p_r = 2,000 \text{ dbar}$, for the TEOS-10

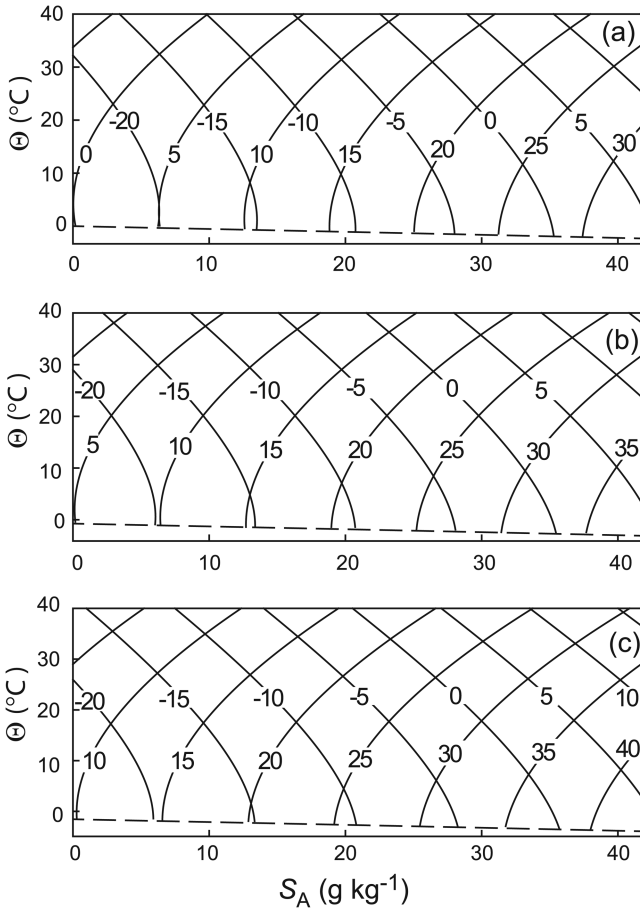


Figure 1. Contours of potential density and spiciness for reference pressures of (a) 0 dbar, (b) 1,000 dbar, and (c) 2,000 dbar. The dashed line in each panel is where seawater freezes at the pressure appropriate to each panel.

thermodynamic description of seawater (IOC et al. 2010). Unlike Huang (2011), we strongly recommend against linearly interpolating between these three spiciness variables using the pressure of an observation. Although these three spiciness variables coincide at $S_A = 35.16504 \text{ g kg}^{-1}$, $\Theta = 0^\circ\text{C}$, they differ over the (S_A, Θ) plane, as illustrated in Figure 3. A linearly pressure-interpolated spiciness variable would mean that a purely adiabatic and isohaline heaving motion of a seawater parcel would result in a change in the interpolated spiciness variable. That is, such an interpolated spiciness variable would not possess the potential property, and because potential density possesses this potential property, so should spiciness.

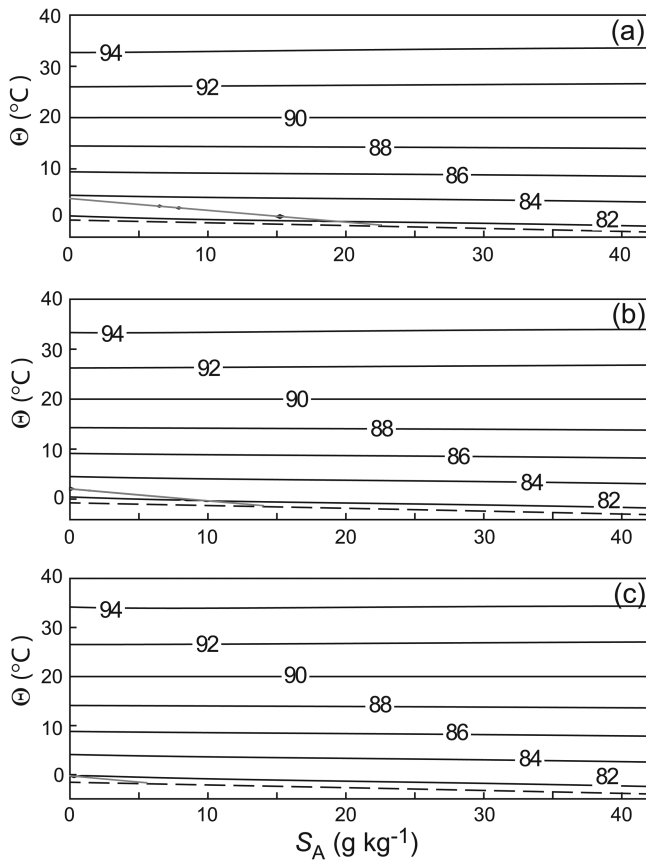


Figure 2. Contours of the angle between the isolines of potential density and spiciness once the (S_A, Θ) diagram has been stretched so that the isopycnals subtend an angle of 45° with the horizontal axis. The three panels are for (a) 0 dbar, (b) 1,000 dbar, and (c) 2,000 dbar. The dashed line in each panel is where seawater freezes at the pressure appropriate to each panel, and the gray line is the locus of locations where the thermal expansion coefficient is zero (i.e., the temperature of maximum density).

Like Jackett and McDougall (1985), we have opted to have the isopycnal variations of spiciness be proportional to the isopycnal water-mass variations, expressed in terms of density, as given by equation (4). Because of the nonlinear nature of the equation of state of seawater, this water-mass variation constraint cannot be simultaneously satisfied with any definition of orthogonality. We have argued that there is no theoretical justification for any meaning of orthogonality, and so we have allowed our spiciness variables to not be orthogonal to potential density isolines on the (S_A, Θ) plane, even in the sense of our equation (3), except along the line $\Theta = 20^\circ\text{C}$.

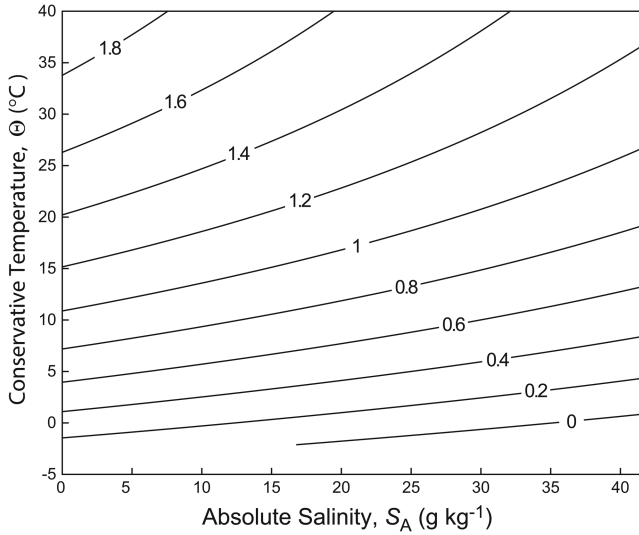


Figure 3. Contours of the difference between the spiciness variables defined for 2,000 dbar and 0 dbar—that is, contours of $\tau_2(S_A, \Theta) - \tau_0(S_A, \Theta)$.

In particular, we emphasize that the notion of orthogonality on the (S_A, Θ) diagram does not give rise to a passive thermodynamic variable. Rather, the passive nature of variations of a thermodynamic variable is gained by evaluating those variations along isopycnals (Montgomery 1938). For example, the isopycnal variations of Absolute Salinity are passive, as are the isopycnal variations of Conservative Temperature. The advantage with using the isopycnal variations of spiciness is that this provides the passive spatial variations of water-mass properties in density units.

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APPENDIX

The three spiciness variables, τ_0 , τ_1 , and τ_2 , referenced to 0 dbar, 1,000 dbar, and 2,000 dbar, respectively, are given by the following three polynomial expressions:

$$\tau_0(S_A, \Theta) = \tau_u \sum_{j=0}^6 \sum_{k=0}^6 A_{jk} S^j y^k, \tag{A1}$$

$$\tau_1(S_A, \Theta) = \tau_u \sum_{j=0}^6 \sum_{k=0}^6 B_{jk} S^j y^k, \quad \text{and} \tag{A2}$$

Table A1. The coefficients of the polynomials for spiciness: A_{jk} .

j	k	A_{jk}	j	k	A_{jk}
0	0	$-9.229\ 828\ 983\ 716\ 78 \times 10^1$	3	4	$6.696\ 265\ 651\ 695\ 29 \times 10^1$
0	1	$-1.357\ 278\ 736\ 288\ 66 \times 10^1$	3	5	$3.028\ 512\ 350\ 507\ 66 \times 10^2$
0	2	$1.873\ 536\ 509\ 940\ 10 \times 10^1$	3	6	$-1.963\ 452\ 856\ 046\ 21 \times 10^2$
0	3	$-1.613\ 600\ 473\ 734\ 55 \times 10^1$	4	0	$-5.740\ 408\ 067\ 135\ 26 \times 10^2$
0	4	$3.761\ 127\ 622\ 864\ 25 \times 10^1$	4	1	$7.032\ 859\ 054\ 783\ 33 \times 10^1$
0	5	$-4.270\ 866\ 714\ 612\ 57 \times 10^1$	4	2	$-2.978\ 702\ 988\ 797\ 16 \times 10^2$
0	6	$2.008\ 201\ 110\ 415\ 94 \times 10^1$	4	3	$3.883\ 403\ 737\ 351\ 18 \times 10^2$
1	0	$2.879\ 697\ 175\ 840\ 45 \times 10^2$	4	4	$-8.291\ 889\ 360\ 891\ 22 \times 10^1$
1	1	$1.137\ 471\ 119\ 596\ 74 \times 10^1$	4	5	$-1.876\ 021\ 371\ 953\ 54 \times 10^2$
1	2	$6.073\ 771\ 929\ 906\ 80 \times 10^1$	4	6	$1.270\ 969\ 444\ 257\ 93 \times 10^2$
1	3	$-7.375\ 140\ 335\ 701\ 87 \times 10^1$	5	0	$2.116\ 711\ 678\ 921\ 47 \times 10^2$
1	4	$-7.511\ 718\ 789\ 535\ 74 \times 10^1$	5	1	$-3.151\ 409\ 198\ 762\ 85 \times 10^1$
1	5	$1.633\ 109\ 897\ 215\ 04 \times 10^2$	5	2	$1.164\ 588\ 649\ 536\ 02 \times 10^2$
1	6	$-8.832\ 227\ 516\ 380\ 95 \times 10^1$	5	3	$-1.500\ 297\ 308\ 023\ 44 \times 10^2$
2	0	$-6.417\ 253\ 0223\ 70\ 48 \times 10^2$	5	4	$3.762\ 938\ 486\ 605\ 89 \times 10^1$
2	1	$2.797\ 325\ 307\ 892\ 61 \times 10^1$	5	5	$6.472\ 474\ 243\ 732\ 00 \times 10^1$
2	2	$-2.494\ 669\ 019\ 937\ 28 \times 10^2$	5	6	$-4.471\ 599\ 944\ 088\ 67 \times 10^1$
2	3	$3.266\ 912\ 950\ 354\ 16 \times 10^2$	6	0	$-3.235\ 333\ 394\ 490\ 55 \times 10^1$
2	4	$2.663\ 892\ 437\ 081\ 81 \times 10^1$	6	1	$5.306\ 485\ 620\ 976\ 67 \times 10^0$
2	5	$-2.931\ 709\ 057\ 575\ 79 \times 10^2$	6	2	$-1.820\ 512\ 491\ 779\ 48 \times 10^1$
2	6	$1.760\ 539\ 071\ 445\ 24 \times 10^2$	6	3	$2.331\ 843\ 510\ 904\ 95 \times 10^1$
3	0	$8.276\ 343\ 181\ 202\ 24 \times 10^2$	6	4	$-6.229\ 099\ 034\ 603\ 68 \times 10^0$
3	1	$-7.021\ 562\ 201\ 269\ 26 \times 10^1$	6	5	$-9.559\ 754\ 643\ 014\ 46 \times 10^0$
3	2	$3.829\ 733\ 365\ 908\ 03 \times 10^2$	6	6	$6.618\ 770\ 739\ 601\ 13 \times 10^0$
3	3	$-5.062\ 068\ 280\ 839\ 59 \times 10^2$			

$$\tau_2(S_A, \Theta) = \tau_u \sum_{j=0}^6 \sum_{k=0}^6 C_{jk} s^j y^k, \quad (\text{A3})$$

where the unit-related scaling constants are

$$\tau_u \equiv 1 \text{ kg m}^{-3}, S_{A_u} \equiv (40 \times 35.16504 \text{ g kg}^{-1})/35 \quad \text{and} \quad \Theta_u = 40^\circ\text{C}, \quad (\text{A4})$$

the nondimensional (root) salinity (s) and temperature (y) variables are

$$s \equiv \sqrt{\frac{S_A + 24 \text{ gkg}^{-1}}{S_{A_u}}} \quad \text{and} \quad y \equiv \frac{\Theta}{\Theta_u}, \quad (\text{A5})$$

and the coefficients A_{jk} , B_{jk} , and C_{jk} are given in Tables A1–A3, respectively. Computer code to evaluate τ_0 , τ_1 , and τ_2 is available online (<http://www.TEOS-10.org>) as the functions `gsw_spiciness0`, `gsw_spiciness1`, and `gsw_spiciness2`, respectively, in the Gibbs Seawater Oceanographic Toolbox.

Table A2. The coefficients of the polynomials for spiciness: B_{jk} .

j	k	B_{jk}	j	k	B_{jk}
0	0	$-9.198\,745\,848\,689\,12 \times 10^1$	3	4	$6.483\,071\,899\,194\,33 \times 10^1$
0	1	$-1.335\,172\,685\,294\,08 \times 10^1$	3	5	$2.164\,333\,347\,015\,78 \times 10^2$
0	2	$2.183\,522\,116\,481\,07 \times 10^1$	3	6	$-1.482\,730\,327\,743\,05 \times 10^2$
0	3	$-2.014\,917\,441\,141\,73 \times 10^1$	4	0	$-5.745\,456\,487\,997\,54 \times 10^2$
0	4	$3.700\,042\,043\,551\,32 \times 10^1$	4	1	$4.504\,464\,311\,274\,21 \times 10^1$
0	5	$-3.788\,315\,432\,262\,61 \times 10^1$	4	2	$-2.307\,149\,813\,437\,72 \times 10^2$
0	6	$1.763\,378\,342\,945\,54 \times 10^1$	4	3	$3.159\,583\,892\,530\,65 \times 10^2$
1	0	$2.878\,388\,427\,733\,96 \times 10^2$	4	4	$-8.606\,353\,139\,301\,06 \times 10^1$
1	1	$2.145\,314\,205\,545\,22 \times 10^1$	4	5	$-1.229\,784\,550\,690\,97 \times 10^2$
1	2	$3.146\,797\,051\,987\,96 \times 10^1$	4	6	$9.182\,872\,826\,262\,61 \times 10^1$
1	3	$-4.043\,988\,647\,506\,92 \times 10^1$	5	0	$2.121\,204\,730\,622\,03 \times 10^2$
1	4	$-7.707\,964\,289\,504\,87 \times 10^1$	5	1	$-2.215\,282\,169\,738\,20 \times 10^1$
1	5	$1.367\,838\,338\,209\,55 \times 10^2$	5	2	$9.190\,134\,179\,232\,70 \times 10^1$
1	6	$-7.368\,343\,170\,448\,50 \times 10^1$	5	3	$-1.244\,007\,760\,260\,14 \times 10^2$
2	0	$-6.417\,534\,151\,807\,01 \times 10^2$	5	4	$4.085\,128\,711\,638\,39 \times 10^1$
2	1	$1.337\,019\,816\,855\,90 \times 10^0$	5	5	$3.911\,273\,522\,135\,16 \times 10^1$
2	2	$-1.752\,893\,279\,484\,12 \times 10^2$	5	6	$-3.105\,080\,218\,530\,93 \times 10^1$
2	3	$2.426\,661\,606\,575\,36 \times 10^2$	6	0	$-3.247\,900\,358\,991\,52 \times 10^1$
2	4	$3.170\,624\,007\,991\,14 \times 10^1$	6	1	$3.910\,290\,165\,567\,86 \times 10^0$
2	5	$-2.281\,314\,904\,408\,65 \times 10^2$	6	2	$-1.453\,627\,193\,854\,12 \times 10^1$
2	6	$1.395\,642\,450\,684\,68 \times 10^2$	6	3	$1.961\,361\,942\,463\,55 \times 10^1$
3	0	$8.277\,479\,345\,064\,35 \times 10^2$	6	4	$-7.060\,354\,746\,890\,88 \times 10^0$
3	1	$-3.509\,015\,906\,947\,75 \times 10^1$	6	5	$-5.368\,846\,886\,140\,09 \times 10^0$
3	2	$2.874\,739\,072\,620\,29 \times 10^2$	6	6	$4.432\,473\,030\,924\,48 \times 10^0$
3	3	$-4.002\,273\,411\,449\,28 \times 10^2$			

Table A3. The coefficients of the polynomials for spiciness: C_{jk} .

j	k	C_{jk}	j	k	C_{jk}
0	0	$-9.173\,273\,207\,322\,65 \times 10^1$	3	4	$5.144\,859\,945\,976\,35 \times 10^1$
0	1	$-1.312\,002\,351\,479\,12 \times 10^1$	3	5	$1.299\,757\,550\,626\,96 \times 10^2$
0	2	$2.495\,743\,457\,825\,03 \times 10^1$	3	6	$-9.365\,265\,883\,774\,56 \times 10^1$
0	3	$-2.416\,780\,752\,473\,98 \times 10^1$	4	0	$-5.749\,117\,289\,729\,48 \times 10^2$
0	4	$3.616\,546\,314\,020\,53 \times 10^1$	4	1	$1.911\,758\,518\,627\,72 \times 10^1$
0	5	$-3.225\,821\,646\,677\,10 \times 10^1$	4	2	$-1.593\,472\,319\,688\,41 \times 10^2$
0	6	$1.450\,926\,239\,825\,09 \times 10^1$	4	3	$2.338\,847\,257\,449\,38 \times 10^2$
1	0	$2.877\,766\,459\,831\,95 \times 10^2$	4	4	$-7.877\,440\,105\,461\,57 \times 10^1$
1	1	$3.139\,023\,076\,724\,47 \times 10^1$	4	5	$-6.047\,572\,354\,436\,85 \times 10^1$
1	2	$1.697\,774\,675\,344\,59 \times 10^0$	4	6	$5.278\,696\,955\,996\,57 \times 10^1$
1	3	$-5.696\,301\,157\,404\,38 \times 10^0$	5	0	$2.125\,177\,584\,788\,78 \times 10^2$

(Continued)

Table A3. (Continued)

j	k	C_{jk}	j	k	C_{jk}
1	4	$-7.975\ 863\ 590\ 179\ 87 \times 10^1$	5	1	$-1.243\ 517\ 947\ 405\ 28 \times 10^1$
1	5	$1.075\ 074\ 603\ 877\ 51 \times 10^2$	5	2	$6.539\ 043\ 089\ 374\ 90 \times 10^1$
1	6	$-5.582\ 344\ 049\ 647\ 87 \times 10^1$	5	3	$-9.448\ 040\ 807\ 637\ 88 \times 10^1$
2	0	$-6.417\ 080\ 687\ 665\ 57 \times 10^2$	5	4	$3.938\ 742\ 578\ 873\ 64 \times 10^1$
2	1	$-2.534\ 948\ 012\ 861\ 61 \times 10^1$	5	5	$1.494\ 254\ 488\ 889\ 96 \times 10^1$
2	2	$-9.867\ 554\ 373\ 853\ 64 \times 10^1$	5	6	$-1.623\ 507\ 216\ 563\ 67 \times 10^1$
2	3	$1.524\ 069\ 307\ 958\ 42 \times 10^2$	6	0	$-3.259\ 368\ 442\ 766\ 69 \times 10^1$
2	4	$4.238\ 882\ 582\ 641\ 05 \times 10^1$	6	1	$2.440\ 357\ 003\ 015\ 95 \times 10^0$
2	5	$-1.601\ 188\ 111\ 414\ 38 \times 10^2$	6	2	$-1.050\ 796\ 336\ 837\ 95 \times 10^1$
2	6	$9.674\ 978\ 980\ 539\ 89 \times 10^1$	6	3	$1.515\ 157\ 962\ 590\ 82 \times 10^1$
3	0	$8.276\ 743\ 554\ 786\ 37 \times 10^2$	6	4	$-7.066\ 098\ 864\ 606\ 83 \times 10^0$
3	1	$5.275\ 612\ 344\ 121\ 33 \times 10^{-1}$	6	5	$-1.480\ 433\ 370\ 529\ 68 \times 10^0$
3	2	$1.874\ 402\ 069\ 923\ 96 \times 10^2$	6	6	$2.100\ 666\ 539\ 785\ 15 \times 10^0$
3	3	$-2.832\ 953\ 923\ 451\ 71 \times 10^2$			

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