Determination of Potential Temperature and Density for Deep Fresh Waters*

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Abstract: As a rule, the hydrodynamic modeling of processes in fresh waters is performed with the use of potential temperature θ and potential density ρ^* . However, the formulae of potential temperature for natural waters given by Phillips (1977), Gill (1982) and others take into account only adiabatic correction. They do not consider such important characteristics of natural waters as temperature of maximal density T_{md} (S,P) remoting of real temperatures T(S,P) in situ from T_{md} ($T = T - T_{md}$), changes of Tmd with decreasing of pressure P (depth Z), and the equation of water state. $T_{md} = T_{md}(P)$ is the property of molecular structures of water (Horne, 1969). It is determined by the equation of water state: for example, for lacustrine waters in the form of Chen, Millero, (1986) $\rho = \rho(S,T,P)$, where ρ , S are density and salinity natural water. There is given and discussed a new formula for the calculation of potential temperature. It is established that potential densities calculated according to the new formula suggested by us show the entire thermodynamic similarity of characteristics within T in situ. It is not observed while using the old formulae.

Keywords: potential temperature, density, deep fresh waters, Lake Baikal

1. Introduction

The potential temperature $\theta(S, P)$ and potential density $\rho^*(S, P)$ are the most important oceanological and limnological characteristics for natural waters. There may occur greater difficulty and mistakes if the water temperature T is close to the temperature of maximum density T_{md} especially in deep water. We have come to the conclusion that the formulae for the calculation of the potential temperature θ (Phillips, 1977; Gill, 1982) is not complete. Therefore, it gives incorrect results. In fact, the calculation of potential temperature $\theta(S,P)$ takes into account only adiabatic correction $\Delta T_{ad}(T,S,P)$ to temperature T(S,P) measured in situ:

$$\theta(T,S,P) = T(S,P_a) = T(S,P) + \Delta T_{ad}(T,S,P), \tag{1}$$

where P_a is the atmospheric pressure.

Let us prove that it is insufficiently for the reasonable determination $\theta(T,S,P)$.

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2. Materials and Methods

We make use of the experimentally-theoretical approach.

3. Results

3.1 Theory

In order to elucidate that phenomenon, let's consider T as a function of $T_{md}(S,P)$. At normal atmospheric pressure Pa it is about 4°C, and decreases with the increase of pressure P (or Z). This peculiarity is due to the molecular structures of the water (Horne, 1969). This function may be expressed as follows:

$$T(S,P) = T_{md}(S,P) + T(T,S,P), \tag{2a}$$

or

$$T'(T,S,P)=T(S,P)-\operatorname{Tmd}(S,P). \tag{2b}$$

The absolute value of T(T,S,P) increases when T(S,P) becomes increasingly distant from $T_{md}(S,P)$ while water density $\rho(T,S,P)$ or $\rho^*(S,P)$ decreases.

Let us consider three main characteristics of the equation (2b):

- 1) Mathematically it involves any changes of $T_{md}(S,P)$ with pressure P (the depth Z);
- 2) Its physical sense it allows one to take into account the water molecular structures of water determined by any particular equation of the water state (e.g., in the Chen-Millero (1986) form), as $T_{md}(S,P)$ is determined only by the properties of molecular structures of water (Horne, 1969);
- 3) It is easy to obtain the potential temperature θ and θ for any pressure P (or Z) using the equation (1), (2a) or (2b) (Kamenkovich, 1973; Gill, 1982). It is necessary to perform an adiabatic transition to the surface, to the atmospheric pressure P_a (Z=0), i.e., the adiabatic correction $\Delta T_{ad}(T,S,P)$ should be taken into account:

$$\theta(T,S,P) = \theta_{md}(S,P_a) + \theta(T,S,P) \tag{3a}$$

or

$$\theta(T,S,P) = \theta(T,S,P) - \theta_{md}(S,Pa), \tag{3b}$$

where $\theta(T,S,P)=T(T,S,P)+\Delta T_{ad}(T,S,P)$; $\theta(T,S,P)$ - potential temperature for any T, S and P; $\theta_{md}(S,Pa)$ -potential temperature of maximal density for the atmospheric pressure P_a (Z=0) circa 4°C. Let us find the potential density $\rho^*(T,S,P)$ as (Kamenkovich, 1973; Gill, 1982)

$$\rho^*(T,S,P) = \rho (\theta,S,Pa). \tag{4}$$

Thus we deduce the main formulae for the potential temperature $\theta(T,S,P)$ in form 3a and 3b and the potential density $\rho^*(T,S,P)$ and let us compare them with formulae different authors.

3.2 Result of field observation

It is very convenient to check our conclusions on Lake Baikal with its deepwater zone where the temperature is close to the temperature of maximum density, $T_{md}(S,P)$ (Vereshagin, 1927; Weiss *et al.*, 1991; Peeters *et al.*, 1996). Let us take field observations with data of $\theta(T,S,P)$ and $\rho^*(T,S,P)$ and take only extreme points for deepwater zone by way of example of 300 and 1 600 m (Fig.1.).

We see that for deep water zone all θ (*T,S,P*) from data Weiss *et al.* (1991) and Peeters *et al.* (1996) are less than 4 °C but our similar data are more than 4 °C.

4. Discussion

According to a more complete identification of potential temperature $\theta(T,S,P)$ (Kamenkovich, 1973), "it is the temperature the system will get at equilibrium adiabatic transition from pressure P to atmospheric pressure P_a ".

The analysis shows that the equation (1) for the calculation of potential temperature $\theta(T,S,P)$ does not take into account the following characteristics: equilibrium transition; maximal density temperature T_{md} for natural waters; changes of T_{md} with pressure P (depth Z), i.e. $T_{md} = T_{md}(S,P)$; remote of real temperature T from T_{md} or $T(S,P)=T(S,P)-T_{md}(S,P)$; water state equation (Weiss et al., 1991; Sherstyankin, Kuimova, 1995; Peeters et al., 1996). The formula reveals only the features of the surface waters. The temperature of maximal density of the water Tmd(S,Pa) and its dependence on P are the properties of molecular structures of the water (Horne, 1969). It is calculated according to the equation of water state, e.g. for fresh waters (Chen, Millero, 1986), and it is not reduced to adiabatic corrections. The formal use of (1) results in incorrect determination of $\theta(T,S,P)$.

To eliminate the deficiency mentioned above, it is necessary to transform (1) according into (2a). Then the equilibrium transition from pressure P to P_a is performed (it is shown with an arrow $P \rightarrow P_a$). $T_{md}(S,P \rightarrow P_a)$ will be transformed into $T_{md}(S,P_a)=\theta_{md}(S,P_a)$; $\Delta T_{ad}(T,S,P \rightarrow P_a)$ will act only on T(S,P) as the adiabatic correction (lapse) to $T_{md}(S,P)$ at any P equals $\theta(T,S,P)$ identically (the coefficient of thermic extension $\alpha(T,S,P)$ at $T=T_{md}$ which is included in $\Delta T_{ad}(T,S,P)$ as a cofactor equals 0). The equilibrium transition will be observed if the transition is carried out along the T_{md} line or will be equidistant from the density constancy, $\alpha(T,S,P)$ and other thermodynamic properties of water are preserved (Fig.1).

The analysis of (2a) shows: any points on the line $T_{md}(S,P)$ are transformed only into a single point $\theta_{md}(S, P_a)$ with $\Delta T_{ad}(T_{md}, S, P) \equiv 0$. The points lying in situ to the right (to the left) of the $T_{md}(S,P)$ curve after the transformation into potential temperature $\theta(T,S,P)$ are situated to the right (to the left) of $\theta_{md}(S,P_a)$. As a result, the transformation of (2a) has thermodynamic properties from the T vicinity in situ to the θ vicinity taking into account density features of corresponding water densities $\rho(T,S,P)$ and potential densities $\rho^*(T,S,P) = \rho(\theta,S,P_a)$. It testifies the equilibrium of the transition $P \rightarrow P_a$ performed (Fig.). At $P = P_a$ the equation (2) is transformed into (3) where $\theta(T,S,P) = \theta_{md}(S,P_a) + \theta'(T,S,P)$. It again emphasizes that (1) is applicable only for surface waters, i.e. for $P = P_a$. While using (1) for P = 180 bars, the error in the calculation of $\Delta T_{ad}(T,S,180)$ at $T < 4^{\circ}C$ may be 0.04 °C (for $T > 4^{\circ}C$ and to 30 °C - 0.4 °C). The error for $\theta(T,S,180)$ calculation reaches 4°C. It is evidently clear that maximal errors of qualitative and quantitative character in θ calculation and ρ^* are within the range of $T(P) < 4^{\circ}C$; e.g., for deep zone of Lake Baikal (Weiss et al., 1991; Sherstyankin, Kuimova, 1995; Peeters et.al., 1996) which is given in (Sherstyankin, Kuimova, Potemkin, 1996). We are going to show only one example from Weiss et al. (1991): T(P = 160)

bars)=3.08 °C. According to (1), θ =3.05 °C; the sign $\alpha(T,S,P)$ changes. According to (3), $\theta(T=3.08,P=160)=6.37$ °C retaining the character of thermodynamic features of surrounding point in situ and on the surface (It is conserving the sign α).

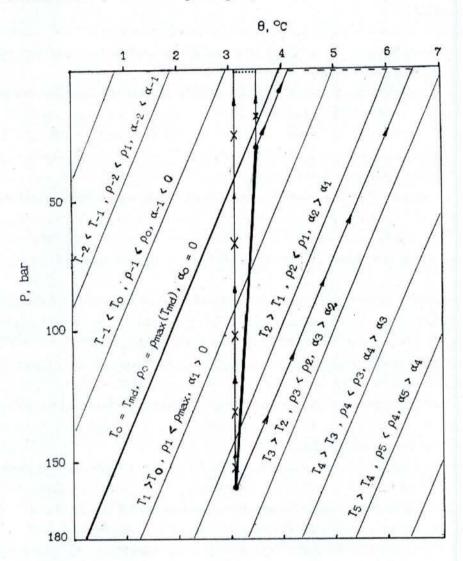


Fig. 1 The example of calculation of potential temperature θ for equilibrium correct transition from pressure P to P_a according to (2) (\rightarrow) and for non-equilibrium incorrect transition from pressure P to P_a according to (1) (\rightarrow x \rightarrow) for the equation of water state in the form (Chen, Millero, 1986). The adiabatic correction • Tad is less than the point size. The diapason of changes $\theta(T,S,P)$ for the formala (1) show by the dotted line, for the formala (3) show by the dashed line.

Let us calculate $\rho^*(T,S,P) = \rho$ (θ,S,P_a) according formulae (1) and (3) or $\sigma^*=(\rho^*-1)10^3$ and to receive at different S, Table 1.

It is seen in Table 1 that potential temperatures $\theta(T,S,P)$ and potential densities $\rho^*(T,S,P)$ between

the horizons 300 and 1600 m (30 and 160 bars) calculated using formules (1) and (3) change very strongly. The range of their changes for Baikal water (S=0.096 g·kg⁻¹) is 0.48 and 2.24 °C for θ or 5.2 10^{-6} and 44.8 10^{-6} g·cm⁻³ for potential density ρ *. It is quite clear the using of formule (1) misinterpret the character of θ and ρ * vertical distributions.

Table.1. $\rho^*(T,S,P) = \rho (\theta,S,P_a)$ according formulae (1) and (3) or $\sigma^*=(\rho^*-1)10^3$ at different S

P, bars	θ ,°C(of(1))	σ^* , g·mm ⁻³	S, g·kg-1	θ ,°C(of(3a))	σ*, g·mm ⁻³	S, g·kg-1
30	3.53^{x}	-0.0297	0.000	4.13 ^{xxx}	-0.0282	0.000
		0.0475	0.096		0.0488	0.096
		0.0508	0.100		0.0521	0.100
160	3.05^{xx}	-0.0351	0.000	6.37xxx	-0.0724	0.000
		0.0423	0.096		0.0040	0.096
		0.0455	0.100		0.0071	0.100

x-of Peeters et al. (1996), xx - of Weiss et al. (1991), xxx - our calculation

We see that at calculation according to formula (1) we receive more narrow-band potential temperature θ (less 1 °C) than at our calculations according to formula (3) (more 2 °C, Fig.1.) and respectively different potential density ρ^* (Table 1).

It is possible to obtain the correct conclusion for practical and theoretic problems with the use of potential densities $\rho^*(T,S,P)$ only according to (3) which takes into account not only adiabatic correction but also the equilibrium transition in accordance with the equation of water state, i.e. with regard to the properties of molecular structures of water.

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