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Calculating density of water in geochemical lake stratification models

Bertram Boehrer[1], Peter Herzsprung[1], Martin Schultze[1], and Frank. J. Millero[2]*
[1]Helmholtz-Centre for Environmental Research - UFZ, Brueckstrasse 3a, 39114 Magdeburg, Germany
[2]Rosenstiel School of Marine and Atmospheric Science, Miami, FL 33149, USA

Abstract

To model chemically stratified lakes numerically, chemical transformations must be reflected in the density function. In this contribution, partial molal volumes are used to calculate density from the chemical composition of lake water. Such values have been evaluated for cations and anions separately, to facilitate an easy implementation into geochemical stratification models for lakes. Coefficients for temperature dependence and variation for higher ionic strengths were evaluated from previously published data. An algorithm RHOMV to calculate density with a second order approximation for temperature dependence and ionic strength dependence is proposed. The accuracy is tested for seawater composition. We conclude that this approach delivers a representation of density based on the actual chemical composition of the lake water, which is accurate enough for most limnological purposes. The implementation of RHOMV into geochemical stratification models facilitates the numerical tackling of pressing questions, such as meromixis or double diffusive features or altered circulation patterns of lakes due to changing climate or change of use.

Density is one of the crucial physical quantities that control currents and flows, such as the vertical circulation of lakes and the propagation of internal waves (e.g., Turner 1973). The stability of density stratification is quantified by the gradient of potential density, in oceanography usually called simply "density." Whether a lake will experience a full overturn during winter or will be perennially stratified depends on the density difference, which remains in the deep waters during times of deep circulation (e.g., Hutchinson 1957).

Lakes show gradients of dissolved substances. In some cases, vertical gradients are formed, which can withstand the deep circulation in winter (Findenegg 1935; Campbell and Torgersen 1980). Iron accumulation in deep water (Kjensmo 1967) combined with carbon dioxide production (Hongve 2002) as well as calcite production (Rodrigo et al. 2001) have been documented to turn lakes meromictic. In the iron meromictic Waldsee in Lusatia (Germany), it was shown that chemical reactions can even drive double diffusive convection (Boehrer et al. 2009a). Dietz et al. (pers. comm.) quantified the contribution of the relevant solutes for the density gradient in the iron meromictic Waldsee.

Whereas stratification models have recently been developed to simulate geochemical evolution in many water bodies on Earth by incorporating geochemical models (New Zealand: Castendyk and Webster-Brown 2007a, 2007b; Germany: Müller et al. 2008; Australia: Salmon et al. 2008; Spain: Samper et al. 2008), a feedback of the geochemical model to the stratification of the lake was not included. However, geochemical transformations can be decisive for the circulation of a lake (e.g., meromixis). As a consequence, a most recent simulation tried to attempt this challenge with promising results (Moreira et al. 2009). The stratification of Waldsee was modeled with DYRESM for a period of 6 months: first using the conductivity-based standard salinity for density and second calculating density from molal volumes and concentrations of dissolved substances as delivered by the geochemical model. Only the second approach reproduced the stable stratification over the entire period.

Besides chemical gradients in the vertical, also temporal evolution of the lake chemistry requires density functions, which adjust implicitly to changing conditions, i.e., (1) if remediation strategies are implemented, which change the chemical characteristics of a lake fundamentally (e.g., Boehrer et al. 2003; Fisher and Lawrence 2006; Stottmeister et al. 2010), (2) if climate change or (3) change of lake use impact

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*Corresponding author: E-mail: Bertram.Boehrer@ufz.de,
phone + 49 391 810 9441, fax + 49 391 810 9150

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its circulation pattern, (4) if temperature boundary conditions change (Hirae et al. 1987; Danis et al. 2004; Boehrer et al. 2009b), or (5) indirectly if there are changes in the regional hydrology (Jellison et al. 1998).

Density differences within one lake are small. In general, density varies by only a few parts per thousand in a lake. Only in exceptionally highly stratified lakes, higher gradients are encountered (e.g., Boehrer and Schultze 2008; Böhrer et al. 1998). As a consequence, highly accurate numerical approaches are required to reflect the small differences that control vertical circulation and wave propagation.

Hence, in most applications, density is calculated as a function of temperature and a term reflecting the contribution of dissolved substances (Fofonoff and Millard 1983; Chen and Millero 1986). All dissolved substances are comprised in one single quantity (electrical conductivity or salinity), even if lake specific density curves are developed (Jellison et al. 1999; Millero 2000, Karakas et al. 2003; Boehrer et al. 2009a). Also numerical stratification models for lakes use this type of density functions (Imberger and Patterson 1981; Cole and Buchak 1995; Jöhnk 2001). Wüest et al. (1996) used partial molal volumes and specific electrical conductances of a small number of salts to correlate measured conductivity to density under chemical conditions as given in deep waters of Lake Malawi. Local variability of chemical composition and temporal evolution cannot be reflected with such approaches. As a consequence, separate terms were dedicated to the inclusion of CO_2 and CH_4 in the density function for Lake Kivu/East Africa and Lake Nyos/Cameroun by Schmid et al. (2003, 2004) to account for the variable concentrations as a consequence of submersed sources and artificial degassing.

In this publication, we show how density of lake water can be based on the composition of the solutes. On purpose, we avoid using quantities like electrical conductivity or salinity for the derivation of density (for a recent detailed study, see Pawlowicz 2008). Concentrations of dissolved substances—as delivered by geochemical water quality models—are directly converted into density contributions by using partial molal volumes for separate chemical species. As far as documented in the scientific literature of physical chemistry, the required coefficients are included in this paper. Beyond this, some coefficients had to be evaluated from published empirical data on other physical quantities. A numerical approach is proposed that uses molal volumes of the solutes and can easily be handled by contemporary computer hardware and software. We provide an algorithm RHOMV (from ρ_{mv} see below) for practical and simple implementation in numerical, geochemical lake stratification models. This approach allows the calculation of density in each node at any time step directly from the actual chemical composition.

Numerical models using this density approach can attempt an entirely new category of challenges in limnological science, such as the geochemistry in mixolimnion and monimolimnion of meromictic lakes, the stratification of acidic lakes during remediation, or the formation of meromixis, e.g., by changing climate conditions.

Numerical approach

Density of water is calculated by dividing the mass m [kg] by its volume V [L]

$$\rho = m/V \tag{1}$$

We use an index W, when we deal with pure water: $\rho_W = m_W/V_W$. If a lake model uses molal units for concentrations, both volume and mass can be calculated implementing coefficients evaluated below. For concentrations in other units, a conversion may be required, especially for salt lakes (*see* Web appendix).

Lake water represents an aqueous solution of a number of substances. We consider a solution of b_i [kg mol^{-1}] moles of several substances (indexed i) of molar mass M_i [kg mol^{-1}] per water volume of mass m_w [kg] (i.e., molal units). The mass of the solution is simply the sum of the contributions:

$$m = m_W + m_W \cdot \sum b_i M_i \tag{2}$$

Molar masses of common solutes in lake waters are listed in Table 1.

However, substances dissolving in water also change its volume. For many substances, the volume increases, but in a few cases, the volume is reduced. In total, the volume of this solution is given by the volume of the water, and the specific contributions of the substances, called partial molal volumes V_i [L mol^{-1}]:

$$V = V_W + m_W \sum b_i V_i \tag{3}$$

Under atmospheric pressure, the specific volume V_W/m_W of water lies slightly above 1 L kg^{-1} (see also Fig. 1). Both V_W and V_i are functions of temperature and pressure. In addition, the coefficients V_i may also depend on the concentrations of dissolved substances.

Though pressure effects on the "in-situ density" are important in the deeper layers of most freshwater lakes, they do not contribute to the stability of the stratification. Consequently, the density under atmospheric pressure is used as a reference: the so-called "potential density," or as common in oceanography simply "density." This article is an approach to potential density. Temperatures also refer to "potential temperature" throughout this paper. The rare case where the potential density concept fails (thermobaric stratification, e.g., Boehrer et al. 2008) is not covered by this approach. However three points need further consideration: first the effect of temperature on specific volume of water, second the effect of temperature on molal volumes, and third the effect of ionic strength on molal volumes.

Temperature effect on specific volume of water—A very accurate regression for the density of water was published by Kell

Table 1. Coefficients for calculating conventional partial molal volumes (see text) under different conditions (from Tables A1 and A2 in Web Appendix A except for Lide 2008*, Enns et al 1965†, Tiepel and Gubbins 1972‡, Duedall et al. 1976§, and Lo Surdo and Millero 1980‖) used in Eq. 10. More substances in Table A3.

Substance	Charge	Molar mass*	Coefficient at 25°C and *I* = 0	Coefficient for ionic strength	Coefficient for ionic strength	Temperature coefficient	Temperature coefficient
Symbol	Z_i	M_i	$\overline{\Phi_i}$	$\overline{A_i}$	$\overline{B_i}$	$\overline{C_i}$	$\overline{D_i}$
	—	g/mol	mL/mol	mL kg$^{1/2}$/mol$^{3/2}$	mL · kg/mol^2	mL/(mol · K)	mL/(mol · K^2)
H^+	1	1.008	0	0	0	0	0
Na^+	1	22.990	–1.2410	0.351	0.401	0.0700	–0.0008000
K^+	1	39.098	8.996	0.379	0.394	0.0521	–0.0007429
NH_4^+	1	18.039	17.961	0.257	0.160	0.0391	0.0010571
Mg^{2+}	2	24.305	–21.186	0.235	0.720	0.0065	–0.0016143
Ca^{2+}	2	40.078	–17.850	0.691	0.497	0.0430	–0.0012476
Mn^{2+}	2	54.938	–17.6‖				
Fe^{2+}	2	55.845	–26.1				
Al^{3+}	3	26.982	–41.5				
Fe^{3+}	3	55.845	–33.5				
F^-	–1	18.998	–1.130	1.488	0.160	0.0241	–0.0020619
Cl^-	–1	35.453	17.854	1.460	–0.307	0.0262	–0.0012714
OH^-	–1	17.007	–4.005	1.697	0.583	0.0558	–0.0035286
NO_3^-	–1	62.004	29.046	2.235	–0.693	0.0896	–0.0019857
HCO_3^-	–1	61.016	24.359	3.311	–0.516	0.0726	–0.0022476
CO_3^{2-}	–2	60.008	–3.713	7.008	–1.185	0.0967	–0.0040667
SO_4^{2-}	–2	96.062	14.041	6.048	–0.715	0.0935	–0.0038143
$Si(OH)_4$	0	96.114	(~61.5)§				
O_2	0	31.998	31†	(~0)	(~0)		
N_2	0	28.014	33.3†				
CO_2	0	44.009	34.8†	(~0)	(~0)		
CH_4	0	16.043	37.4‡				

Values in this table are given in the usual units as they appear in the literature for easier reading and better comparison with the scientific literature. For the use in equations, they need to be multiplied by the unity factor 1000 g/kg or 1000 mL/L, respectively, so that units cancel each other properly.

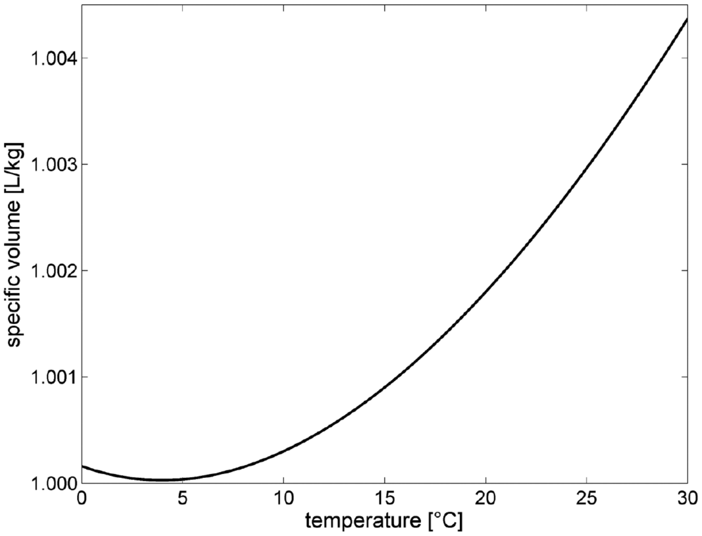

Fig. 1. Specific volume of water against temperature (after Kell 1975) under normal pressure conditions.

(1975), claiming a relative accuracy of 10^{-7}. Since then, a new international definition has shifted temperature readings slightly. Hence more recent publications (Spieweck and Bettin 1992) indicate that deviations from the real value are close to 10^{-6} for the interval between 0 and 30°C, which is fully sufficient for our approach:

$$\rho_W(T) = \frac{\sum_{i=0}^{5} a_i T^i}{1+aT} \cdot \rho_{\max} \tag{4}$$

In units [g/L] with coefficients a_i = [0.9998676; 17.801161·10^{-3}; -7.942501·10^{-6}; -52.56328·10^{-9}; 137.6891·10^{-12}; 364.4647·10^{-15}] and a = 17.735441·10^{-3}. The coefficients are valid for temperatures in °C. The maximum density of degassed Standard Ocean Water (SMOW) is $\rho_{\max}$ = 999.975 gL^{-1}, while for isotopically different lake water, this value can be slightly different (for details see Tanaka et al. 2001).

The volume of pure water then can be calculated as:

$$V_W(T) = m_W / \rho_W(T) \tag{5}$$

Temperature effect on molal volumes—Salts dissociate in the water. Cations and anions can be involved in chemical reactions separately. As a consequence, geochemical models most practically and most realistically treat each ion as separate substance. For a most accurate and most practical density calculation molal volumes V_i of each ion are desirable. However, these values are supplied for salts, i.e., combinations of cations and anions (e.g., Millero 2001; Table 3.19). A division cannot be done purely empirically.

The common approach nowadays is defining "conventional" partial molal volume of any ion of charge Z_i (dimensionless number of charges; $Z_i < 0$ for anions), where the partial molal volume of the H^+ ion is used as a reference (Millero 2001; see also appendix A.1).

$$\overline{V_i} = V_i - Z_i V_{H+} \tag{6}$$

Any other ion than H^+ could have served for the same purpose (e.g., Moreira et al. 2009). Here we follow the established convention. Values and coefficients are marked with a bar in this paper. The sum of all conventional molal volumes (*see* Eq. 3) amounts to

$$\sum b_i \overline{V_i} = \sum b_i (V_i - Z_i V_{H+}) = \sum b_i V_i - V_{H+} \sum b_i Z_i \tag{7}$$

In a geochemical model, any water parcel conserves its electrical charge at zero: $\sum b_i Z_i = 0$. Hence the last term of Eq. 7 vanishes. Thus for a water volume of total electrical charge of zero, the procedure using conventional molal volumes does not involve any inaccuracy.

For the most common ions, conventional partial molal volumes are listed in the book by Millero (2001; Table 5.27). For limnological purposes, the values between 0°C and 30°C are the most relevant. Hence we used this range for a second order regression against temperature under dilute conditions:

$$\overline{V_i}\,(T, dilute) = \overline{\Phi_i} + \overline{C_i}(T - 25°C) + \overline{D_i}(T - 25°C)^2 \tag{8}$$

where $\overline{V_i}(25°C, dilute) = \overline{\Phi_i}$ is the conventional partial molal volume at 25°C and dilute conditions. Respective coefficients were evaluated in Web Appendix A2 and results were listed in Table 1. Conventional molal volumes were calculated following Eq. 8 (see Fig. 2). To exemplify the temperature dependence, we also displayed the results with the constant term $\overline{\Phi_i}$ removed from Eq. 8 (Fig. 3). Hence all lines intersect 0 at 25°C. Obviously, the conventional values of partial molal volumes show a different behavior for cations and anions.

Though the partial molal volumes are known for 25°C, temperature dependences are not listed for all common ions, which are stratification relevant in lakes (e.g., Fe^{2+} for iron meromixis). Hence we calculated the average coefficients for cations ($\overline{C_C}$ = 0.0498 mL mol^{-1} K^{-1} and $\overline{D_C}$ = –0.000561 mL

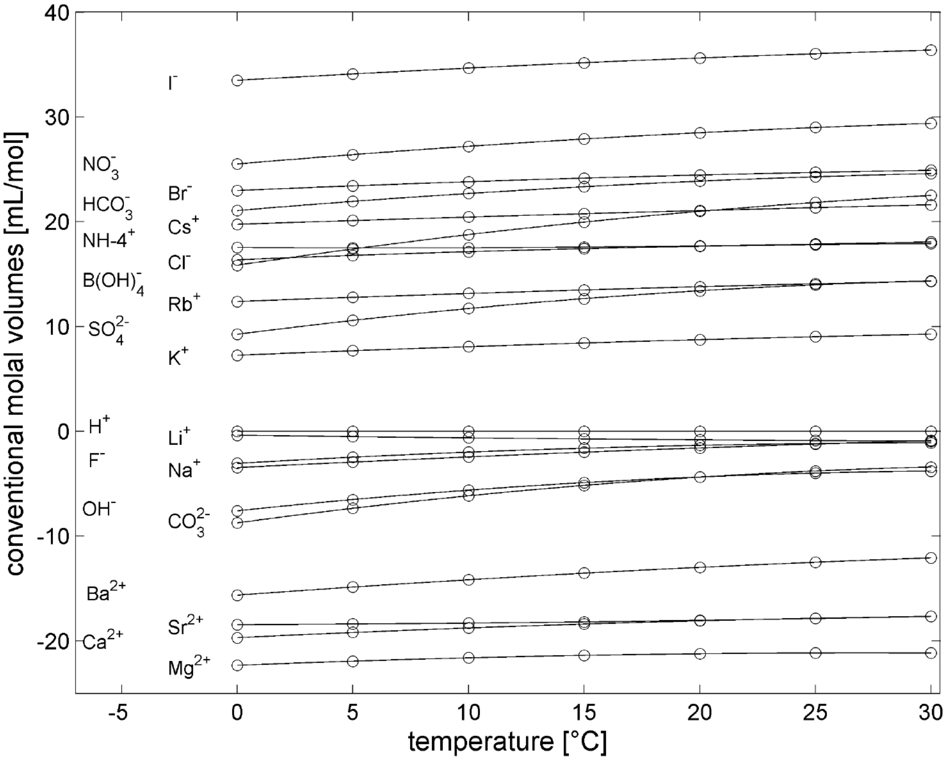

Fig. 2. Conventional molal volumes of several ions in freshwater against temperature. Open circles: data from Millero 2001, Table 5.27, lines: regressions according to Eq. 8.

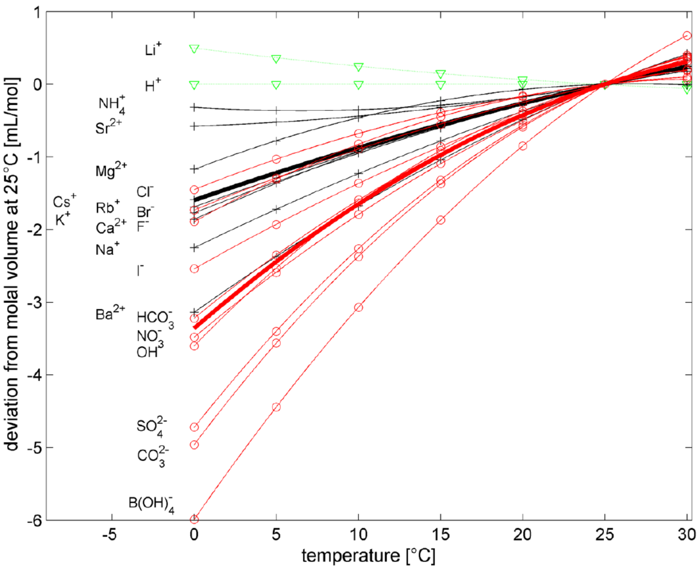

Fig. 3. Temperature dependence of partial molal volumes for the most common ions (same data as Fig. 2). Open circles: data calculated based on Millero 2001, Table 5.27, lines: regressions based on Eq. 8 (red: anions; black: cations except H^+ and Li^+; green: H^+ and Li^+). Thick lines without symbols show the average temperature dependence of anions (red) or cations (black, except for H^+ and Li^+).

mol^{-1} K^{-2}) and for anions ($\overline{C_A}$ = 0.0731 mL mol^{-1} K^{-1} and $\overline{D_A}$ = –0.00245 mL mol^{-1} K^{-2}) included in the figure, where we excluded the very light cations H^+ and Li^+ because of their different temperature behavior.

Also gases dissolve in water. In particular, CO_2 can show high concentrations in deep waters. Like CO_2, other important gases in limnic waters have been included in Table 1. Partial molal volumes were taken from Millero's work (2001; Table 5.3). We used the first number in the list citing earlier publications (Enns et al. 1965; Tiepel and Gubbins 1972; Duedall et al. 1976). No information was available on the temperature dependence of the molal volumes of gases.

Effect of ionic strength on molal volumes—Partial molal volumes depend weakly on the presence of other solutes. For freshwater lakes, this probably plays a subordinate role, but for any salt lake, this dependence must be considered. This effect has been characterized by determining the dependence of coefficients versus ionic strength:

$$I = \frac{1}{2}\sum_i b_i Z_i^2 \qquad (9)$$

units [mol kg^{-1}]. The dependence on ionic strength is given as a second order regression for $\sqrt{I}$ with terms

$$\overline{V_i}\,(25°C, I) = \overline{\Phi_i} + \overline{A_i}\sqrt{I} + \overline{B_i}I \qquad (10)$$

For cases, where we were missing coefficients for the dependence on ionic strength in the literature, we derived the conventional partial molal volumes of cations and anions from given data in Millero's work (Millero et al. 1977; Millero 2001 Tab. 3.19) as shown in Web Appendix A.2. Conventional partial molal volumes can only be used when the electrical charge of a water parcel is 0 (*see* Web Appendix A.2). For calculating the density contribution of a single ion, the values presented by Millero (1969) are the better approach. For two gases (O_2 and CO_2), molal volumes for freshwater and seawater were given. As the difference was not significant, 0 was included for coefficients $\overline{A_i}$ and $\overline{B_i}$ in Table 1.

Calculating the volume of lake water—Finally, to comprise the specific contribution of one particular ion in the solution, the coefficients $\overline{A_i}$, $\overline{B_i}$, $\overline{C_i}$ and $\overline{D_i}$ must be known besides temperature T and ionic strength I of the solution. Using the set of coefficients from Table 1, and inserting temperature and ionic strength,

$$\overline{V_i}\,(T, I) = \overline{\Phi_i} + \overline{A_i}\sqrt{I} + \overline{B_i}I + \overline{C_i}(T - 25°\mathrm{C}) + \overline{D_i}(T - 25°\mathrm{C})^2 \qquad (11)$$

can be calculated for each solute i. Using Eq. 3, density can be calculated by using molal volumes:

$$\rho_{mv} = \frac{m}{V} = \frac{m_W + m_W\sum b_i M_i}{m_W/\rho_W + m_W\sum b_i \overline{V_i}} = \frac{1 + \sum b_i M_i}{1/\rho_W + \sum b_i \overline{V_i}} \qquad (12)$$

Assessment

For a crucial test of the approach, we needed a reference water, of which the composition and density were known at a high accuracy. Ocean water is suited for this approach: the required density correlation (UNESCO) is applicable from salinities on the Practical Salinity Scale (PSS-1978) from 2 to 42 and is valid for more than the required temperature interval. In addition, the reference is well known and truly independent from our calculation. On purpose, we had not included very detailed information on ocean salts and interaction known between the dominant ions in the ocean. We approached all dissolved substances with the same second order fit against temperature and ionic strength.

The chemical composition of seawater was inferred from Millero's book (2001; Table 4.2). After a few numerical steps (Web Appendix A.4) molal concentrations could be attained for any desired salinity S. Hence density was evaluated from Eq. 12 and compared with density from the UNESCO formula at the same salinity. The results of both approaches have been included in Fig. 4. In general, densities calculated from molal volumes follow the empirical formulas well. For pure water, Kell's formula (1975) is also used in our approach. Hence there is no difference.

We chose the conventional delineation of fresh to salt water lakes, salt content of 3 g/kg (Williams 1994) as our first test case. $S = 3$ lay well inside the validity of the UNESCO equation ($2 < S < 42$). Density differences between UNESCO and our approach were smaller than 0.015 gL^{-1} for all temperatures, which meant a relative accuracy of $1.5 \cdot 10^{-5}$. At salinity $S = 3$, the salt contribution to density amounted to about 2.4 gL^{-1}. Hence the

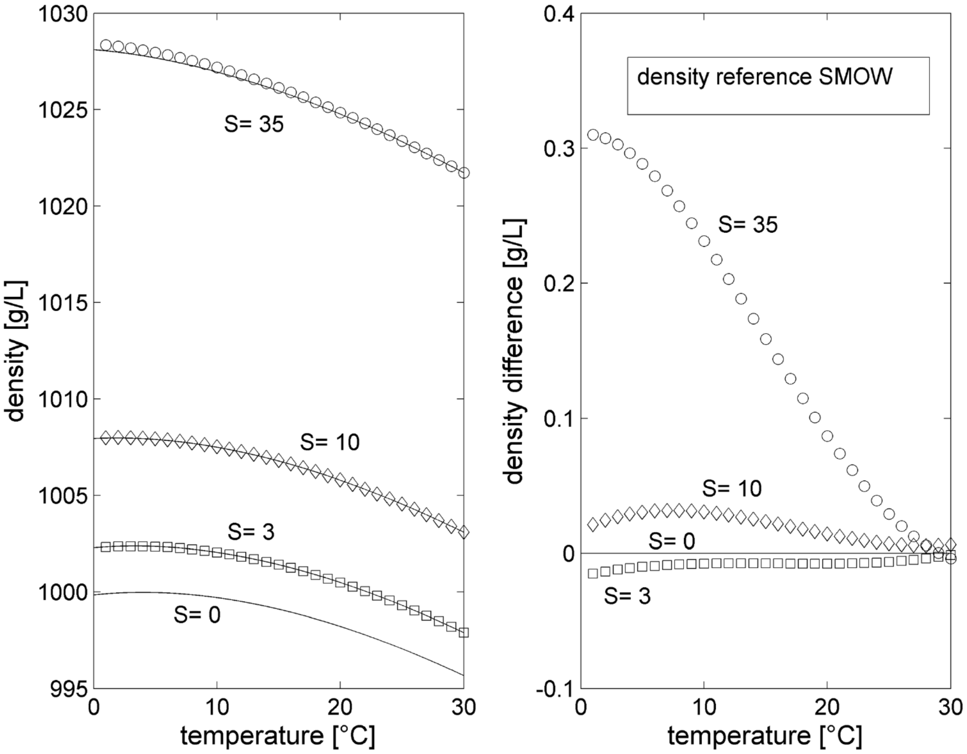

Fig. 4. Densities calculated for various salinities for water of ocean composition: Left panel: densities calculated after UNESCO (practical salinity: S = 3, 10, 35, solid lines) or Kell (1975) (S = 0, solid line). Symbols: densities ρ_{mv} from present approach using molal volumes. Right panel: differences between approaches.

salinity contribution was reflected within an accuracy in the order of 1%. As no special knowledge about sea salt was included, we would expect a similar accuracy for freshwater lakes of other salt compositions.

At a salinity of S = 10, we found about double the deviation, while at ocean concentration S = 35, differences amounted to nearly 0.33 g L^{-1} at temperatures close to 0°C, while at temperatures around 25 to 30°C, the results agreed much better with UNESCO. Comparing the deviation at 25°C, the salinity contribution to density was reflected within 0.5% over the range of compared salinities. At S = 35 the temperature effect is overestimated by less than 5%, i.e., 0.32 gL^{-1} deviation (Fig. 4, right panel) divided by an effect of about 7 gL^{-1} over the temperature range 0 to 30°C (Fig.4, left panel).

Discussion

As the quantifications of temperature dependence and dependence on ionic strength were supplied by different sources, no mixed term between temperature and ionic strength, (i.e., a term of the form $\sim (T - 25°C) \cdot \sqrt{I}$) could be evaluated for equation 10. However, this information was not available in the scientific literature. Such a term would improve the accuracy of the approach for very high salinities and temperatures far away from 25°C. The evaluation of respective coefficients would require a separate research programme.

Conventional molal volumes are well suited for calculating density in geochemical models, as the electrical charge can be conserved. However, as they implicitly include the molal volume of the H^+ ion, their use for the evaluation of the density contribution of one single ion species is limited. Knowledge about the molal volume of H^+ is required. In his work, Millero (1969) tried to evaluate the molal volume of H^+ from a combination of theoretical and empirical arguments. Later Lo Surdo and Millero (1980) used a molal volume of $V_{H+} = -5.5$ mL mol^{-1} at 25°C and dilute conditions. The accuracy of this value cannot be quantified empirically. However, based on this approximation, the coefficient V_i for dilute conditions and 25°C can be calculated for an ion *i* of charge Z_i [dimensionless] by solving Eq. 6:

$$V_i = \overline{V}_i - Z_i \cdot 5.5 \text{ mL mol}^{-1} \qquad (13)$$

Whereas exact numbers for the molal volumes of single ion species seem desirable, the application more urgently requires the missing coefficients for temperature and ionic strengths of manganese, iron, and aluminium, as well as for silicate and the listed gases in Table 1. Finally, there are no published values for the density contribution of dissolved organic matter (DOC) at any accuracy.

Concluding comments and recommendations

Density calculation for lake water can be based on the composition of the dissolved substances. An easy-to-apply approach is presented in this article, consisting of five coefficients for each considered substance, for temperature variation and higher ionic strength. The approach is simple enough that it can be implemented in stratification models and calculated in each time step for each layer or node. The approach has been tested for seawater composition against the UNESCO equation. The accuracy was better than $1.5 \cdot 10^{-5}$ for freshwater. Only for higher salinities greater deviations must be anticipated: up to $3.3 \cdot 10^{-4}$at ocean concentration and low temperatures. Even at high salt concentrations as found in the ocean, the contributions of salts are reproduced within 1%, but the temperature effect on density was overestimated by less than 5%. The conclusions about the accuracy of the solute contribution to density are not affected by the choice of the pure water reference.

As a consequence, the presented approach can be used for freshwater lakes (S<3). In many applications, even the ionic strength terms may be neglected when salinity is low. On the contrary, salt lakes require the full set of coefficients. At S = 10, very accurate results can be anticipated from this model, while for salt concentrations higher than ocean conditions, density may be reflected less accurately, which can be of concern for some applications that require a particularly high accuracy. In these cases, a lake specific approach to density may be mandatory. Further improvements for high salt concentrations and inclusion of more organic substances, e.g., fulvic and humic acids, should be subject of further research. A web access to the numerical model RHOMV has been implemented on www.ufz.de/webax.

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