

Short Note

Adapting molar data (without density) for molal models[☆]

Giles M. Marion^{*}

Desert Research Institute, 2215 Raggio Parkway, Reno, NV 89512, USA

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Abstract

Theoretical geochemical models for electrolyte solutions based on classical thermodynamic principles rely largely upon molal concentrations as input because molality (wt/wt) is independent of temperature and pressure. On the other hand, there are countless studies in the literature where concentrations are expressed as molarity (wt/vol) because these units are more easily measured. To convert from molarity to molality requires an estimate of solution density. Unfortunately, in many, if not most, cases where molarity is the concentration of choice, solution densities are not measured. For concentrated brines such as seawater or even more dense brines, the difference between molarity and molality is significant. Without knowledge of density, these brinish, molar-based studies are closed to theoretical electrolyte solution models. The objective of this paper is to present an algorithm that can accurately calculate the density of molar-based solutions, and, as a consequence, molality.

The algorithm consist of molar inputs into a molal-based model that can calculate density (FREZCHEM). The algorithm uses an iterative process for calculating absolute salinity (S_A), density (ρ), and the conversion factor (CF) for molarity to molality. Three cases were examined ranging in density from 1.023 to 1.203 kg(soln.)/l. In all three cases, the S_A , ρ , and CF values converged to within 1ppm by nine iterations. In all three cases, the calculated densities agreed with experimental measurements to within $\pm 0.1\%$. This algorithm opens a large literature based on molar concentrations to exploration with theoretical models based on molal concentrations and classical thermodynamic principles.

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1. Introduction

Theoretical geochemical models for electrolyte solutions based on classical thermodynamic principles rely largely upon molal concentrations as input because molality (wt/wt) is independent of temperature and pressure, which greatly facilitates model

development (e.g., Marion et al., 2005; Millero, 2001; Nordstrom and Munoz, 1994, Pitzer, 1991, 1995). These theoretical models can further our understanding of natural processes by exploring facets such as degree of mineral saturation and evolution of solutions with changing temperature, pressure, and gas concentrations. On the other hand, there are countless studies in the literature where concentrations are expressed as molarity (wt/vol) because these units are more easily measured (e.g., Bockheim, 1997; Kohut and Dudas, 1994; Lyons et al., 2005; Ouellet et al., 1989; Skarie

[☆]Code available from server at <http://www.iamg.org/CGEditor/index.htm>.

^{*}Tel.: +1 775 673 7349; fax: +1 775 673 7485.

E-mail address: giles.marion@dri.edu.

et al., 1987). To convert from molarity to molality requires an estimate of density (ρ). Unfortunately, in many, if not most, cases where molarity is the concentration of choice, aqueous solution densities are not measured. In dilute aqueous solutions [ionic strength (I) ≤ 0.1 m], molarity and molality are nearly equivalent [$\rho \approx 1.00$ kg(soln.)/l], and lack of density is a nonsignificant issue. However, for concentrated brines such as seawater or even more dense brines, the difference between molarity and molality is significant. Without knowledge of density, these brinish, molar-based studies are closed to theoretical aqueous solution models. For example, in Lyons et al. (2005), molal data from nonsaline Lakes Fryxell and Hoare (Antarctica) were used with the FREZCHEM model to explore saline Lake Bonney processes rather than Lake Bonney data because only molar data were available

for Lake Bonney (see Table 1 in Lyons et al., 2005). The objective of this paper is to open these closed cases to theoretical models by demonstrating how density can be estimated based on molar inputs used in conjunction with a theoretical molal model that can estimate density.

2. Theory

The conversion of molarity (M_j) to molality (m_j) of the j th species is given by

$$M_j \left(\frac{1}{\rho} \right) \left(\frac{\text{kg(soln.)}}{\text{kg(water)}} \right) = m_j, \quad (1)$$

where

$$\frac{\text{kg(soln.)}}{\text{kg(water)}} = \left(\frac{1.00}{1.00 - S_A/1000} \right) \quad (2)$$

and S_A is absolute salinity [g salt/kg(soln.)]. In what follows, the expression

$$CF = \left(\frac{1}{\rho} \right) \left(\frac{\text{kg(soln.)}}{\text{kg(water)}} \right) \quad (3)$$

will be referred to as the conversion factor (see Eq. (1)).

The approach to estimate the density of aqueous molar solutions requires a geochemical model that can estimate solution density based on molal concentrations. The model that will be used in this study is called FREZCHEM and is based on the Pitzer approach (Pitzer, 1991, 1995) for estimating activity coefficients, the activity of water, density, and solubility products as functions of temperature

Table 1

A FORTRAN code for calculating density and molal concentrations from molar data (see text for definition of terms)

Table 2

A comparison of model inputs (molar concentrations and S_L) and resulting model outputs (S_A , ρ , and conversion factors)

	Lake Bonney, West Lobe ^a	Lake Bonney, East Lobe ^a	Seawater ^b
Na (mol/l)	1.734	3.2844	0.47995
K (mol/l)	0.041	0.071	0.01045
Mg (mol/l)	0.378	1.074	0.05406
Ca (mol/l)	0.041	0.037	0.01060
Cl (mol/l)	2.433	5.499	0.55955
SO ₄ (mol/l)	0.051	0.037	0.02890
Alkalinity (equil./l)	0.078	0.0044	0.00237
S_L (g salt/l)	148.47	305.45	35.99
S_A [g salt/kg(soln.)]	134.84	253.99	35.17
$\rho_{calc.}$ [kg(soln.)/l]	1.1011	1.2026	1.023302
$\rho_{expt.}$ [kg(soln.)/l]	1.102	1.203	1.023344
Conversion factor [l/kg(H ₂ O)]	1.04972	1.11465	1.01285
Convergence (± 1 ppm) iterations	6	9	5

^aData from Torii and Yamagata (1981) and Lyons et al. (2005).

^bData from Feistel (2003).

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