How to calculate the density of aqueous solutions of chemical substances for given temperature and concentration values

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Apply DENS1

DENS1, an Axeleratio Chemistry Online Calculator (ACOC), is available to calculate the density of aqueous solutions of chemical substances as a function of temperature and solute concentration. This online calculator implements an equation published in 1988 by Novotný and Söhnel. DENS1 is accessible via a web browser: its design is based on HTML, CSS and JavaScript, while the required arrays with substance-specific data were exported from a table in Axeleratio's PostgreSQL database into JavaScript-conform arrays using a Python script. This document is available at
www.axeleratio.com/calc/solution_density/doc/dens1.pdf.

Keywords. Solution chemistry, binary aqueous solutions, empirical equation, online calculator, estimator, JavaScript.

1 Open Access

The calculator is available at
www.axeleratio.com/calc/solution_density/form/dens1.htm.
Testing of DENS1 under Windows 10 with Firefox Quantum Version 64.0

(64-bit) and Google Chrome Version 71 (64-bit) showed that the calculator functions as intended. Any feedback is welcome. Axeleratio accepts no liability for the data obtained with DENS1, or for the consequences of any actions taken on the basis of the results and information provided by DENS1.

2 Application

DENS1 allows aqueous-solution density calculations for a large number of substances over a wide range of temperature and concentration values. Most of the substances are inorganic acids and salts consisting of a metal ion and an inorganic-acid anion. A few salts contain an organic-acid anion such as formate (Form), acetate (Ac), oxalate (Ox) or tartrate (Tart). Densities of solutions of these substances within the given temperature and concentration ranges are often required in physical chemistry studies, chemical engineering and hydrometallurgy. Estimation methods for liquid viscosities and other important properties of aqueous solutions frequently ask for densities under variable conditions. Also, DENS1 allows the conversion of a solution concentration for a selected substance at a given temperature from molarity to molality [1].

3 Implemented

Based on the definition of the apparent molar volume of a solute in a binary solution and a relation by Masson [2], Söhnel, Novotný and Šolc derived the following relation that describes the concentration-temperature dependence of binary aqueous solutions [3, 4]:

$$\rho_{\mathrm{sln}} = \rho_{\mathrm{w}} + Ac + Bct + Cct^2 + Dc^{3/2} + Ec^{3/2}t + Fc^{3/2}t^2 \qquad (1)$$

The coefficients A to F are available for 167 substances in Table I in [3]. The density of water, ρ_w, is:

$$\rho_{\mathrm{w}} = 999.65 + 2.0438 \cdot 10^{-1}t - 6.174 \cdot 10^{-2}t^{3/2} \qquad (2)$$

These equations are used by DENS1 to calculate solution densities as a function of $t/^{\circ}\mathrm{C}$ and $c/(\mathrm{mol} \cdot \mathrm{L}^{-1})$.

4 Input

First, a substance needs to be selected. The drop-down selection box of DENS1 lists substance notations in alphabetical order. The notations are

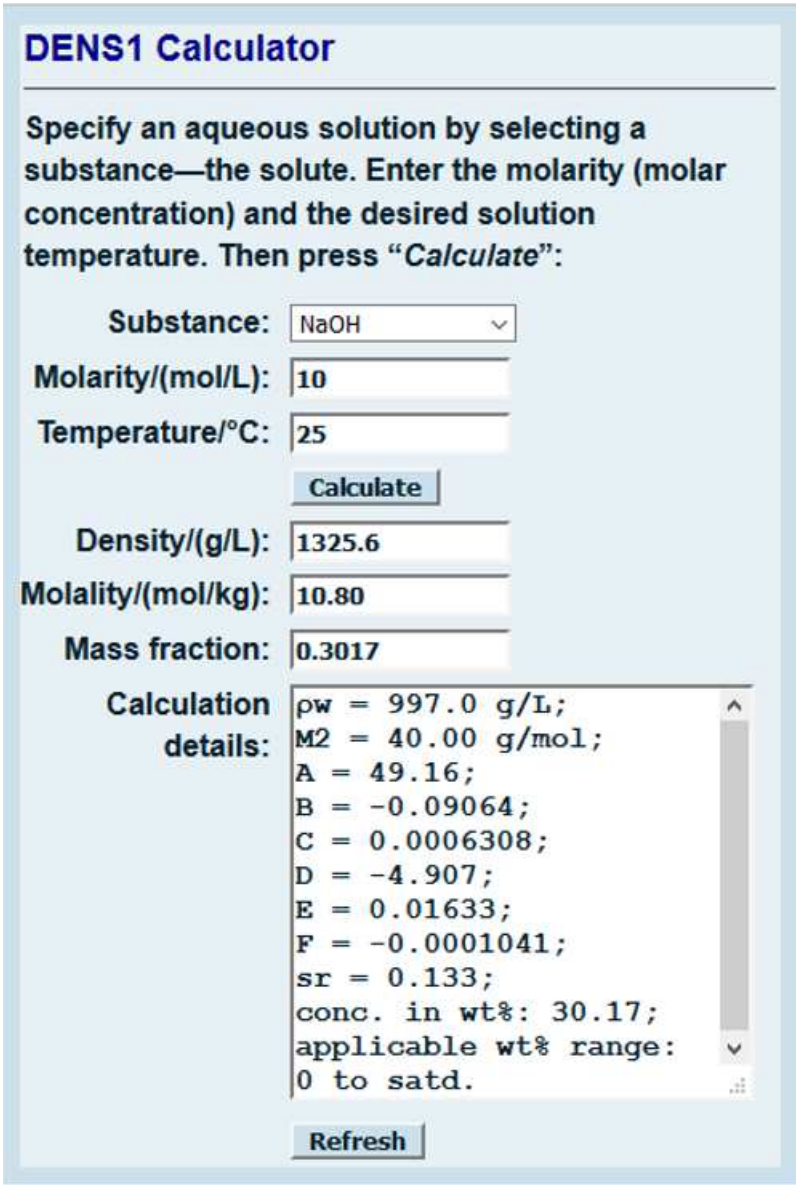

Figure 1: DENS1 calculation of the density of an aqueous NaOH solution (10 molar) at 25.0 °C

the same as in Table I in [3], using the typical salt notation, in which the cation symbol (metal symbol or "H" or "UO2" or "NH4") is followed by the anion notation. We have not changed the originally given salt notations KTart, NH4Ox, NaOx and NaTart, although they are assumed to stand for dipotassium tartrate, diammonium tartrate, disodium oxalate and disodium tartrate with corresponding notations K2Tart, (NH4)2Ox, Na2Ox and Na2Tart. For example, in the referenced paper [4], providing density data for NH4Ox (!), the stoichiometrically expected notation (NH4)2C2O4 was used (C2O4 = Ox). The concentration of the substance in the solution, for which the density is going to be calculated, is required as molar concentration (molarity) in $\mathrm{mol \cdot L^{-1}}$. The solution temperature needs to be entered in °C. The applicable temperature range is (0 to 100) °C for most substances, but is smaller for some.

5 Output

The calculated solution density is represented in $\mathrm{g \cdot L^{-1}}$. This density is applied to calculate the molality of the solution in $\mathrm{mol \cdot kg^{-1}}$, using equation (5) in [1]. Figure 1 shows the output for a 10 molar sodium hydroxide (NaOH) solution at 25°C. The density calculated for this solution is 1325.6 $\mathrm{g \cdot L^{-1}}$. The derived concentration values are: 10.8 $\mathrm{mol \cdot L^{-1}}$ for molality and 0.3017 for mass fraction. The "Calculation details" field gives the following data:

- ρw: density of pure water
- M2: molar mass of solute
- A-F: substance-specific coefficients of equation 1
- sr: goodness of fit for substance-specific instance of equation 1
- conc. in wt%: 100 · mass fraction
- applicable wt% range: for comparison, wt% range as given in [3] (satd = saturated solution)

It is left to the user to verify if, based on the derived wt%, the calculation was done within an acceptable concentration range.

If the entered temperature is not within the applicable temperature range, this temperature range will be displayed in the "Calculation details" field

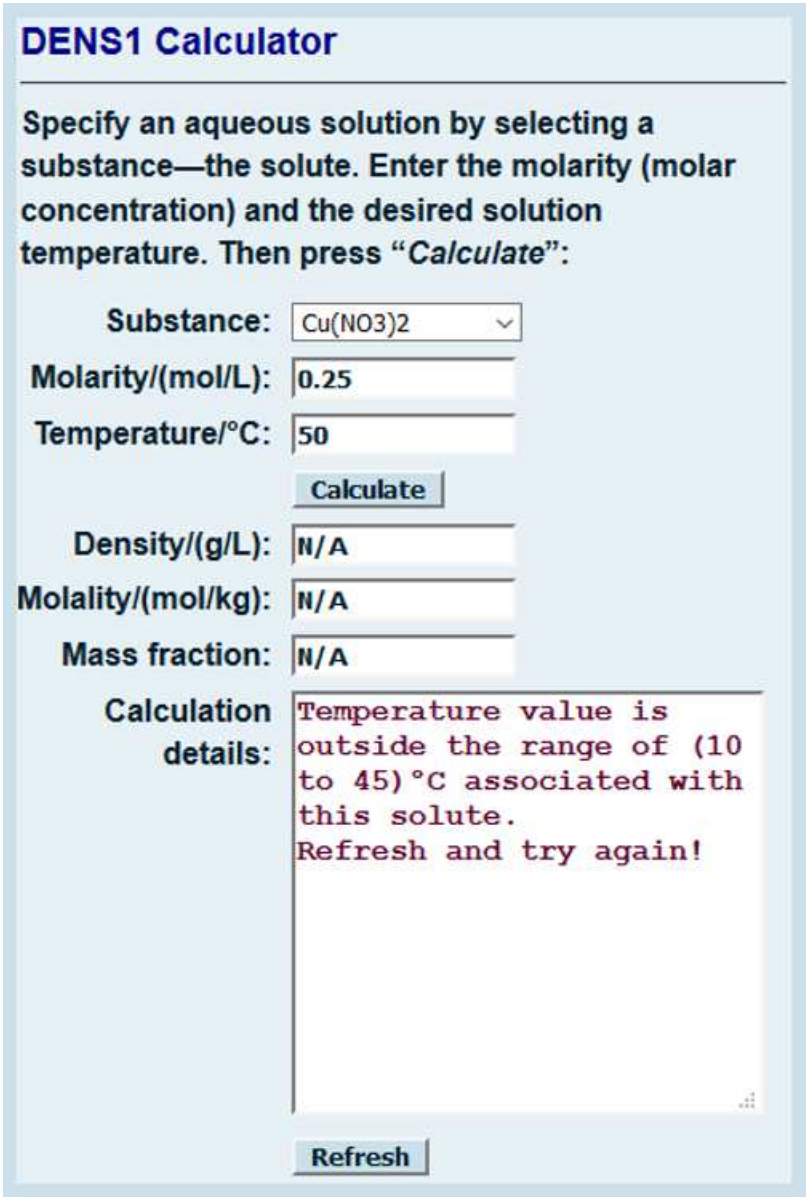

Figure 2: Example of DENS1 performance when the entered temperature value is outside the applicable range

and the user then is asked to refresh and start again with a temperature value in that range. Figure 2 illustrates such as a case for copper nitrate, for which a temperature value between 10 and 45 °C is expected.

6 Also good to know

Novotný and Söhnel further derived equations for 139 substances expressing aqueous-solution densities as a function of concentration at a constant temperature. Density calculation using those equations can be done with calculator DENS2, which is described in a document available at www.axeleratio.com/calc/solution_density/doc/dens2.pdf.

Literature

[1] Drefahl, A. "From molarity to molality and *vice versa*." www.axeleratio.com/chem/conc/molarity_molality_conversion.pdf.

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[3] Novotný, P. and Söhnel, O. "Densities of Binary Aqueous Solutions of 306 Inorganic Substances." *J. Chem. Eng. Data* 1988, *33*, 49-55. DOI: 10.1021/je00051a018.

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