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

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Apply DENS2

DENS2, an Axeleratio Chemistry Online Calculator (ACOC), is provided to calculate the density of aqueous solutions of chemical substances as a function of solute concentration at a constant temperature. This online calculator implements an equation published in 1988 by Novotný and Söhnel. DENS2 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. A Python script was written to exchange the required data. This document is available at
www.axeleratio.com/calc/solution_density/doc/dens2.pdf.

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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/dens2.htm.

Testing of DENS2 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 DENS2, or for the consequences of any actions taken on the basis of the results and information provided by DENS2.

2 Application

DENS2 allows aqueous-solution density calculations for a large number of substances over a wide range of concentration values at a constant temperature. 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), tartrate (Tart), citrate (Citr) or benzoate (Benz).
Densities of solutions of these substances 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. DENS2 also executes the conversion of a solution concentration for a selected substance from molarity to molality [1].

3 Implemented

Novotný and Söhnel derived the following relation that describes the concentration dependence of aqueous solutions at constant temperature [3]:

$$\rho_{\mathrm{sln}} = \rho_{\mathrm{w}} + Gc + Hc^{3/2} \tag{1}$$

The coefficients G to H are available for 131 substances, for some at more than one temperature, in Table II in [3]. The density of water, ρ_w, as a function of temperature, $t/^{\circ}\mathrm{C}$, is:

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

These equations are used by DENS2 to calculate solution densities as a function of $c/(\mathrm{mol} \cdot \mathrm{L}^{-1})$.

4 Input

First, a substance-temperature pair needs to be selected. The drop-down selection box of DENS2 lists substance notations (followed by the tempera-

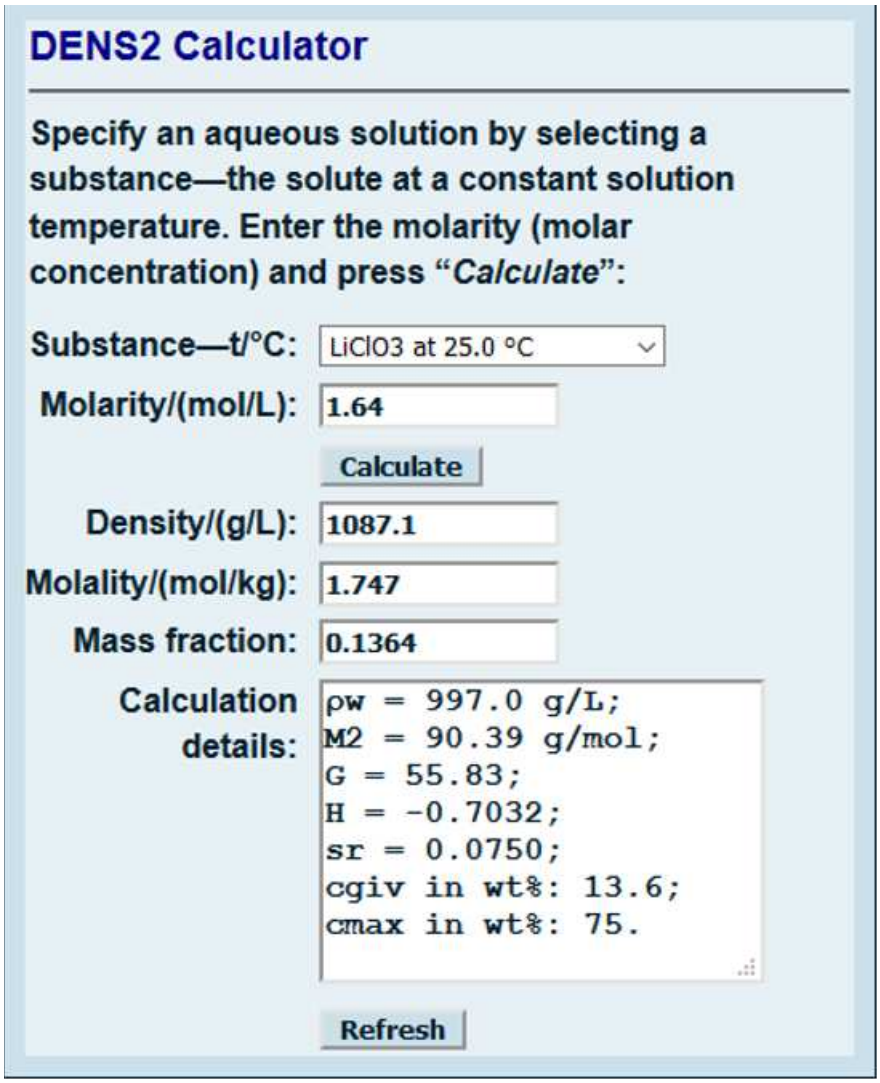

Figure 1: DENS2 calculation of the density of an aqueous $LiClO_3$ solution (1.64 molar) at 25.0 °C

ture constant) in alphabetical order. The notations are the same as in Table II 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 KOx and KCitr, although they are assumed to stand for dipotassium oxalate and tripotassium citrate with corresponding notations K2Ox and K3Citr.

The concentration of the substance in the solution, for which the density is going to be calculated, is required as molar concentration (molarity) in $\mathrm{mol} \cdot \mathrm{L}^{-1}$.

5 Output

The calculated solution density is represented in $\mathrm{g} \cdot \mathrm{L}^{-1}$. This density is applied to calculate the molality of the solution in $\mathrm{mol} \cdot \mathrm{kg}^{-1}$, 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 $\mathrm{g} \cdot \mathrm{L}^{-1}$. The derived concentration values are: 10.8 $\mathrm{mol} \cdot \mathrm{L}^{-1}$ 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
- G, H: substance-specific coefficients of equation 1
- sr: goodness of fit for substance-specific instance of equation 1
- cmfr in wt%: $100 \cdot$ mass fraction
- cmax in wt%: 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.

6 Also good to know

Novotný and Söhnel further derived equations for 167 substances expressing aqueous-solution densities as a function of both concentration and solution temperature. Density calculation using those equations can be done with calculator DENS1, which is described in a document available at www.axeleratio.com/calc/solution_density/doc/dens1.pdf.

Literature

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