# From $H_2O_2$ volume strength to mass fraction and *vice versa*

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Last updated: May 3, 2022

## Summary

Volume strength has been used in past publications to express the concentration of water/hydrogen peroxide ($H_2O/H_2O_2$) systems. This concentration quantity, like mass fraction, is dimensionless. Whereas the latter is a physical quantity based on the mass of the two system components, solvent strength was defined via chemical transformation considering the theoretical decomposition of $H_2O_2$ to oxygen gas, $O_2(g)$. Herein, formulas establishing the conversion between volume strength and mass fraction are given. Calculated data for various concentrations of $H_2O/H_2O_2$ compositions are provided.

**Keywords.** Hydrogen peroxide, aqueous solution, volume strength, mass fraction, percentage of weight, density data, liberated oxygen.

## 1 Introduction

**Volume strength**, also termed **volume percent** and **volume concentration**, is an outdated concentration concept referring to the volume of oxygen gas liberated from a unit volume of a $H_2O/H_2O_2$ mixture [1, 2]. Solvent strength actually is a practical definition concerning handling and safety of $H_2O/H_2O_2$ mixtures with respect to the theoretical maximum of possible oxygen gas evolution. Since physicochemical data in the older literature is sometimes given by using solvent strength as the quantity for concentration, conversion to mass fraction or other common measures of concentration (see Appendix 1) is needed when incorporating such resources into the comparison and discussion of concentration-based data of $H_2O/H_2O_2$ solutions or mixtures. Herein, I derive the formula that relates volume strength to $H_2O_2$ mass fraction, $w_2$, by including empirical equations to calculate the density of $H_2O/H_2O_2$ mixtures as a function of composition and temperature.

## 2 Definition of volume strength of water/hydrogen peroxide mixtures

In the following, the volume strength definition as provided by Reichert and Hull is applied [1]. These authors use the term "volume concentration"and write that this "commonly used term" is defined "as the number of cubic centimeters of oxygen gas, measured at 0 °C and 760 mm pressure, liberated from 1 cc. of the solution (measured at 20 °C) when the peroxide is completely decomposed." Based on this definition, volume strength is the ratio of the volume of deliberated oxygen gas over the "original" volume of a $H_2O/H_2O_2$ mixture:

$$R_{\mathrm{sv}}^{T} = \frac{V_{\mathrm{O}_2}}{V_{1,2}} \tag{1}$$

$R_{\mathrm{sv}}^{T}$ is the solvent strength based on a unit volume of the mixture, $V_{1,2}$, at temperature $T$. $V_{\mathrm{O}_2}$ is the volume of deliberated oxygen gas at 0 °C and 760 mm pressure. In the definition cited by Reichert and Hull, $T$ equals 20 °C; but the use of other reference temperatures is possible.

Within this document, the indices 1 and 2 denote the components $H_2O$ and $H_2O_2$, respectively. The subscript "$1, 2$" refers to the mixed system.

## 3 Relation between $R_{\mathrm{sv}^T}$ and $w_2$

The density of the $H_2O/H_2O_2$ mixture, $d_{1,2}$, at 20 °C has to be known to calculate $R_{\mathrm{sv}^T}$ for a given value of $w_t = m_2/(m_1 + m_2)$ or *vice versa*. We calculate the mass of the mixture:

$$m_{1,2} = m_1 + m_2 = d_{1,2} \cdot V_{1,2} \tag{2}$$

The mass of $H_2O_2$ in the mixture is

$$m_2 = m_{1,2} \cdot w_2 = d_{1,2} \cdot V_{1,2} \cdot w_2 \tag{3}$$

The corresponding amount of moles is

$$n_2 = \frac{m_2}{M_2} = \frac{d_{1,2} \cdot V_{1,2} \cdot w_2}{M_2} \tag{4}$$

With the decomposition reaction

$$2\mathrm{H_2O_2(l)} \rightarrow 2\mathrm{H_2O(l)} + \mathrm{O_2(g)} \tag{5}$$

we find the number of moles of oxygen gas after complete liberation:

$$n_{\mathrm{O_2}} = \frac{n_2}{2} = \frac{d_{1,2} \cdot V_{1,2} \cdot w_2}{2 \cdot M_2} \tag{6}$$

The corresponding volume is:

$$V_{\mathrm{O_2}} = n_{\mathrm{O_2}} \cdot V_{\mathrm{m}} \tag{7}$$

where $V_{\mathrm{m}}$ is the molar volume of an ideal gas. According to the definition of volume strength, the value for $V_{\mathrm{m}}$ has be for $O_2$ at 0 °C and 1 atmosphere. Combining equations 1, 4, 6, and 7 we obtain for the formula to convert from mass ratio to volume strength:

$$R_{\mathrm{sv}}^{T} = \frac{V_m \cdot d_{1,2}}{2 \cdot M_2} \cdot w_2 \tag{8}$$

The formula to convert from volume strength to mass ratio is

$$w_2 = \frac{2 \cdot M_2}{V_m \cdot d_{1,2}} \cdot R_{\mathrm{sv}}^{T} \tag{9}$$

The molar mass of $H_2O_2$ is $M_2 = 34.016\mathrm{g} \cdot \mathrm{mol}^{-1}$. Further, we know that $V_{\mathrm{m}} = 22.414\mathrm{L} \cdot \mathrm{mol}^{-1}$ for $O_2$ at 0 °C and 1 atmosphere (equal to 760 mm Hg or 101.325 Pa).

## 4 Volume strength depending on reference temperature

By definition, solvent strength depends on the reference temperature, which is the temperature of the solution or mixture making up the unit volume.

Let's think of taking a unit volume of a $H_2O/H_2O_2$ mixture at 0 °C with a given mass fraction and warming it up: the mass fraction will not change while the volume increases and the density decreases. According to equation 8, $R_{\text{sv}}^{T}$ decreases directly with decreasing $d_{1,2}$. Note that $T = \text{const}$, since the temperature of the reference state stays by definition the same irrespective of the actual mixture temperature.

However, if we consider two mixtures that have the same unit volume and equal mass fraction values at the reference state, but at different reference temperatures, then the mixture with the higher reference temperature has a lower density, resulting in different volume strengths. We have

$$R_{\text{sv}}^{T_1} > R_{\text{sv}}^{T_2}, \text{for } T_1 < T_2 \tag{10}$$

because the density is increasing with decreasing temperature. In Table 1 solvent strength values within the molar fraction range from 0.05 to 0.90 based on two reference temperatures, $T = 20°\text{C}$ and $T = 0°\text{C}$, are compared for the different refence temperatures. Calculations were made by using equation 8. The densities were derived by using equation 16 in Appendix 2. The right-most column of Table 1 lists values given on the USP technologies$^{\text{TM}}$ webpage with $H_2O_2$ equivalent values of concentration for different wt% values [2]. The USP values differ slightly from those calculated herein, which is not surprising, assuming that slightly different density values may have been used. We also don't know $T$ for the USP values. But the USP values come very close to the $R_{\text{SV}}^{0}$ values, suggesting that they are based on $T = 0$. Where no USP solvent strength is available, this is indicated by nvg (for "no value given").

## Literature and Web Pages Cited

[1] Reichert, J.S., Hull, H. G. "Control of pH in Peroxide Solutions," *Ind. Eng. Chem. Anal. Ed.* 1939, 11 (6), 311-314. DOI: 10.1021/ac50134a005.

[2] "H2O2 Equivalent Values of Concentration," *USP Technologies*$^{\text{TM}}$, 2022. URL: USP Technologies (accessed: 4/30/2022).

[3] Lide, D. R. (Editor-in-Chief). "Handbook of Chemistry and Physics," *CRC Press* Boca Raton, FL, 88th Edition, 2007-2008.

[4] Easton, M.F., Mitchell, A.G., Wynne-Jones, W.F.K. "The behaviour of mixtures of hydrogen peroxide and water. Part 1.—Determination of the densities of mixtures of hydrogen peroxide and water," *Trans. Faraday Soc.* 1952, 48, 796-801. DOI: 10.1039/TF9524800796.

Table 1: Comparison of solvent strength for $H_2O/H_2O_2$ mixtures with increasing $H_2O_2$ content

| $w_2$ | $R_{\mathrm{SV}}^{20}$ | $R_{\mathrm{SV}}^{0}$ | $R_{\mathrm{SV}}(\mathrm{USP})$ |
|---|---|---|---|
| 0.05 | 16.73 | 16.80 | nvg |
| 0.10 | 34.07 | 34.27 | 34.03 |
| 0.15 | 52.02 | 52.40 | nvg |
| 0.20 | 70.61 | 71.22 | 71.21 |
| 0.25 | 89.86 | 90.74 | nvg |
| 0.30 | 109.80 | 110.97 | 110.96 |
| 0.35 | 130.44 | 131.94 | nvg |
| 0.40 | 151.82 | 153.66 | 153.68 |
| 0.45 | 173.96 | 176.16 | nvg |
| 0.50 | 196.90 | 199.46 | 199.49 |
| 0.55 | 220.65 | 223.60 | nvg |
| 0.60 | 245.26 | 248.61 | 248.66 |
| 0.65 | 270.75 | 274.53 | nvg |
| 0.70 | 297.16 | 301.39 | 301.46 |
| 0.75 | 324.53 | 329.23 | nvg |
| 0.80 | 352.89 | 358.10 | 358.17 |
| 0.85 | 382.29 | 388.05 | nvg |
| 0.90 | 412.76 | 419.12 | 419.16 |

# Appendix 1

**Common measures of concentration**.
The mass fraction of a $H_2O_2$ solution is defined as

$$w_2 = \frac{m_2}{m_1 + m_2} \tag{11}$$

and the percentage of $H_2O_2$ by weight is then given as

$$\mathrm{wt}\% = w_2 \cdot 100\% \tag{12}$$

Also frequently used are mole fraction, molarity and molality (see, for example, page 8-116 in [3]), for which the formulas are given below using our notation.
Mole fraction:

$$x_2 = \frac{w_2/M_2}{w_2/M_2 + (1 - w_2)M_1} \tag{13}$$

Molarity:

$$c_2 = \frac{1000 \cdot d_{1,2} \cdot w_2}{M_2} \tag{14}$$

Molality:

$$b_2 = \frac{1000 \cdot w_2}{M_2 \cdot (1 - w_2)} \tag{15}$$

# Appendix 2

**Density of $H_2O/H_2O_2$ mixtures as a function of temperature and composition**.
The densities at 0, 10, 25, 50 and 96 °C over a large range of compositions have have been determined by Easton, Mitchell and Wynne-Jones [4]. For each experimental temperature, they fitted the data by the method of least square to a cubic equation of the following form:

$$d_{12}/(\mathrm{g} \cdot \mathrm{mL}^{-1}) = A + Bw_2 + Cw_2^2 + Dw_2^3 \tag{16}$$

The coefficients are listed in Table 2. The coefficient for $T = 0$°C are used in calculating $R^0_{\mathrm{SV}}$. To calculate $R^{20}_{\mathrm{SV}}$, the densities at $T = 10$°C and $T = 25$°C were calculated and then densities at $T = 20$°C were derived by interpolation:

Table 2: Temperature-dependent coefficients of equation 16

| $T$/°C | $A$ | $B$ | $C$ | $D$ |
|---|---|---|---|---|
| 0 | 0.9998 | 0.39939 | 0.01758 | 0.05470 |
| 10 | 0.9997 | 0.36790 | 0.06208 | 0.02954 |
| 25 | 0.9970 | 0.34672 | 0.06995 | 0.02885 |
| 50 | 0.9880 | 0.31382 | 0.09402 | 0.01910 |
| 96 | 0.9612 | 0.27652 | 0.11956 | 0 |

$$d_{1,2}(20\,^\circ\mathrm{C}) = d_{1,2}(10\,^\circ\mathrm{C}) + 2/3(d_{1,2}(25\,^\circ\mathrm{C}) - d_{1,2}(10\,^\circ\mathrm{C}) \tag{17}$$

The calculated values are available in a OpenOffice Calc spreadsheet at:
http://www.axeleratio.com/chem/conc/H2O2_volume_strength.ods