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Effect of dissolved air on the density of water at different temperatures and pressures

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According to the law of partial pressure, first discovered by John Dalton (1766-1844), “the total pressure, p_t , exerted by a mixture of gases is the sum of the partial pressures of component gases, p_g .” Considering the effect of the saturation pressure of water, $p_{s,f}$, on the total pressure, p_g is defined as:

$$p_g = \chi_g (p_t - p_{s,f}), \quad (1)$$

where χ_g is the molar fraction of the gas component in the gaseous mixture:

$$\chi_g = \frac{v_g}{v_{g,t}} = \frac{n_g}{n_{g,t}}. \quad (2)$$

For the gaseous mixture, the total pressure is $p_t = \sum_{i=1}^{N_{g,t}} p_i$, total volume is $v_{g,t} = \sum_{i=1}^{N_{g,t}} v_i$ and total number of molecules is $n_{g,t} = \sum_{i=1}^{N_{g,t}} n_i$, where $N_{g,t}$ is the number of gas species in the gas mixture. Air mainly consists of nitrogen (N_2), oxygen (O_2), Argon (Ar) and carbon dioxide (CO_2). The standard molar fractions of these gas species in atmospheric air are given in table 1. The saturation pressure of water is a function of temperature, i.e., $p_{s,f}(T)$. The effect of pressure on $p_{s,w}(T)$ was ignored here. The MATLAB code, XSteam, developed by [Holmgren \(2024\)](#), is capable of accurately calculating the steam and water properties for a wide range of pressures and temperatures based on the IF-97 standard of the International Association for the properties of water and steam (IAPWS). Xsteam was used here to calculate the water properties.

Henry's law states that “the amount of gas dissolved in an aqueous solution is proportional to the partial pressure of the gas component in the system, p_g ”. Henry's law is only valid for $p_g \leq 1$ atm and dilute solutions and is defined as ([Sander, 2015](#)):

$$x_g = \frac{p_g}{H_v^{px}}, \quad (3)$$

where x_g is the molar fraction of the gas component in the aqueous solution and H_v^{px} is Henry's law volatility constant. The SI unit of H_v^{px} is (Pa) and it varies with

temperature as (Harvey *et al.*, 2005):

$$H_v^{px} = e^{a_0 + a_1/T + a_2/T^2 + a_3/T^3}, \quad (4)$$

where T is the absolute temperature of the gas component in Kelvins (K). The constants a_0 to a_3 are listed in table 1 different gas species. These coefficients are presented by Harvey *et al.* (2005) as a collection of those available from reliable literature. Equation 4 properly approximates the H_s^{cp} values for $T_0 < T < T_1$, which are also listed in table 1. The molar fraction x_g is defined as:

$$x_g = \frac{n_g}{n_{s,t}}, \quad (5)$$

where $n_g = m_g/M_g$ and $n_{s,t} = \sum_{i=1}^{N_{s,t}} n_i$ are the number of gas molecules and total molecules in the solution. Here, $N_{s,t}$ is the number of the components in the solution, and m_g is the mass and M_g is the molar mass of the solute. Here, M_g has a unit of (gr mol⁻¹).

Table 1: The coefficients of H_v^{px} correlation, given in equation 4 for different gas species.

Gas species	a_0	$a_1 \times 10^{-3}$	$a_2 \times 10^{-6}$	$a_3 \times 10^{-8}$	$T_0(^{\circ}\text{C})$	$T_2(^{\circ}\text{C})$
N ₂	14.277	6.387	-1.140	0	0	50
O ₂	14.990	5.743	-1.071	0	0	55
Ar	15.350	5.470	-1.030	0	0	40
CO ₂	6.981	12.817	-3.767	2.997	0	160

Henry's laws can also be defined based on the molarity \mathcal{M}_g of the solute and Henry's law solubility constant, H_s^{cp} as:

$$\mathcal{M}_g = p_g H_s^{cp}. \quad (6)$$

The SI unit of the constant H_s^{cp} is (mol m⁻³ Pa⁻¹). Molarity \mathcal{M}_g is defined as the number of moles of solute present in a unit volume of the solution, typically one litre, i.e.,

$$\mathcal{M}_g = \frac{n_g}{v_{s,t}}, \quad (7)$$

where $v_{s,t}$ is the volume of the solution. The SI unit of molarity is (mol m⁻³). Assuming that (1) moles of solute are negligible compared to the moles of the solvent,

$n_{s,t} \approx n_f$, and (2) the solution occupies almost all of the system volume, $v_{s,t} \approx v_f$, and combining equation 3 to 7, H_s^{cp} can be defined as a function of H_v^{px} as:

$$H_s^{cp} = \frac{\rho_f}{M_f} \frac{1}{H_v^{px}}. \quad (8)$$

The mass concentration of a gas component in an aqueous solution, c_g , is defined as:

$$c_g = \frac{m_g}{m_{s,t}}, \quad (9)$$

where $m_{s,t} = \sum_{i=1}^{N_{s,t}} m_i$ is the total mass of the solution. The unit of c_g is ($\text{kg}_g \text{ kg}_s^{-1}$) or conveniently ($\text{g}_g \text{ kg}_s^{-1}$). Assuming that (1) the mass of the solute is negligible compared to the solvent, i.e., $m_{s,t} \approx m_f$, and (2) moles of solute are negligible compared to the moles of the solvent, $n_{s,t} \approx n_f$, c_g can be formulated as a function of x_g as:

$$c_g \approx x_g \frac{M_g}{M_f}. \quad (10)$$

Table 2 lists the main molar and fractional properties of dissolved air gas components at $T = 25^\circ\text{C}$ and $p_t = 101.325 \text{ kPa}$. The mass fraction of the dissolved air under these ambient conditions is 22.64 (mg kg^{-1}).

Table 1 lists the H_v^{px} values of the common gas species found in air (Sander, 2023) for a range of temperatures and pressures. Figure 0.1 illustrates the variation of isobaric c_g profiles with temperature. For a constant temperature, the amount of dissolved air increases as the total pressure of the solution increases. Under constant pressure, increasing the solution's temperature reduces the amount of dissolved air in the water.

Table 2: Properties of the main dissolved air components at $T = 25^\circ\text{C}$ and $p_t = 101.325 \text{ kPa}$. Under these conditions, $p_{s,f} = 3.17 \text{ kPa}$ and $\rho_f = 997.05 \text{ kg m}^{-3}$ (Holmgren, 2024).

Gas name	N_2	O_2	Ar	CO_2
$M_g(\text{gr mol})$	28.01	32	39.95	44.01
χ_g	0.781	0.2094	0.0092	0.0004
$p_g(\text{kPa})$	76.66	20.55	0.90	0.039
$x_g \times 10^6$	8.91	4.67	0.23	0.24
\mathcal{M}_g	0.493	0.258	0.012	0.013
$H_v^{px}(\text{MPa})$	8 605	4 404	4 003	162
$H_s^{cp}(\text{mol m}^{-3} \text{ Pa}^{-1})$	6.432	12.567	13.828	341.704
$c_g(\text{mg kg}^{-1})$	13.852	8.290	0.499	0.592

Table 3: Concentration of air in water at different temperatures and total pressures. The water properties are obtained using XSteam ([Holmgren, 2024](#)).

$T(^{\circ}\text{C}) / p_t(\text{kPa})$	101.325	250	400	550	700	850	1000
0	38.8	96.09	153.88	211.68	269.47	327.26	385.06
5	34.06	84.48	135.35	186.22	237.08	287.95	338.82
10	30.29	75.27	120.66	166.04	211.43	256.81	302.2
15	27.23	67.87	108.87	149.88	190.88	231.88	272.88
20	24.73	61.86	99.33	136.8	174.27	211.74	249.21
25	22.64	56.93	91.53	126.13	160.73	195.33	229.93
30	20.88	52.85	85.1	117.36	149.62	181.87	214.13
35	19.35	49.42	79.76	110.1	140.44	170.77	201.11
40	18.01	46.52	75.29	104.05	132.81	161.58	190.34
45	16.8	44.03	71.51	98.98	126.45	153.93	181.4
50	15.67	41.86	68.28	94.7	121.12	147.54	173.96

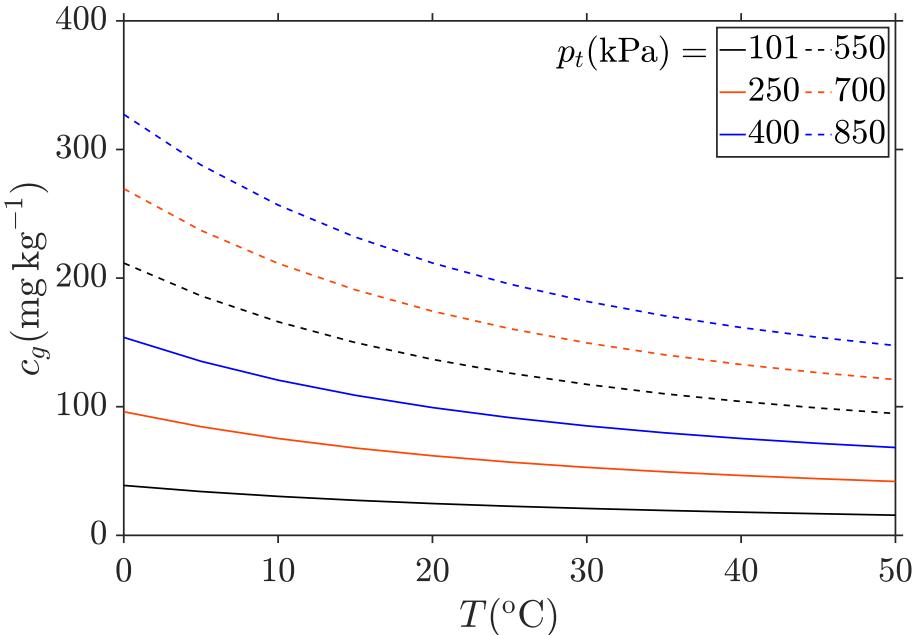


Figure 1: Variation of the mass concentration of air in water with absolute temperature and total pressure.

Variation of the density

The total molar volume of the air-water solution can be defined as ([Harvey *et al.*, 2005](#)):

$$\mathcal{V}_s = x_f \mathcal{V}_f + \sum_{i=1}^{N_g} x_{g,i} \mathcal{V}_{g,i} \quad (11)$$

where \mathcal{V} is the partial molar volume with a unit of ($\text{m}^3 \text{mol}^{-1}$). The subscripts 'f' and 'g' denote the solvent (water) and the solute (gas species of air), with $N_g = 4$ as the number of gas species in air. The molar fraction of water in the solution is $x_f = 1 - \sum_{i=1}^{N_g} x_{g,i}$. As discussed by [Harvey et al. \(2005\)](#), \mathcal{V}_f can be assumed to be the molar volume of water in pure state: $\mathcal{V}_f = M_f/\rho_f(p_t, T)$. Empirical correlations provided by [Harvey et al. \(2005\)](#) were utilised to estimate \mathcal{V}_g of each gas component, which has a form of:

$$\mathcal{V}_g = b_1 T + b_2. \quad (12)$$

The coefficients b_1 and b_2 are listed in table 3 for the main gas components of the dissolved air. The change in water density due to the dissolution of air is defined as ([Harvey et al., 2005](#)):

$$\Delta\rho = \frac{M_s}{\mathcal{V}_s} - \rho_f, \quad (13)$$

where $M_s = \sum_{i=1}^{N_g} x_{g,i}$ is the total molar-fraction weighted molar mass of the solution.

Table 4: Coefficients of the correlation to calculate the partial molar volume of gas species, given in equation 12.

Reference	Gas name	N_2	O_2	Ar	CO_2
(Harvey et al., 2005)	$b_1 \times 10^6$	34.5	31.7	32.7	34.2
	$b_2 \times 10^6$	-0.03	-0.04	-0.06	0.00
(Watanabe & Iizuka, 1985)	$b_1 \times 10^6$	35.359	31.265	30.092	33.520
	$b_2 \times 10^6$	0.0075	-0.0285	-0.0277	0.0071

[Watanabe & Iizuka \(1985\)](#) also provided values for b_1 and b_2 of equation 12, which are listed in table 4. Using their approach, the density changes in the water due to the dissolution of each gas component is defined as:

$$\Delta\rho_{g,i} = \frac{x_{g,i}}{\mathcal{V}_f} (M_{g,i} - \rho_f \mathcal{V}_{g,i}). \quad (14)$$

Here, $\Delta\rho = \sum_{i=1}^{N_g} \Delta\rho_{g,i}$. Table 5 lists the change of the water density due to dissolved air at different temperatures at $p_t = 101.325 \text{ kPa}$, calculated using equation 13 and 14.

Figure 0.2(a)-(b) demonstrates the variation of the density change of water due to the dissolution of air at different temperatures and pressures. Equation 14 and 13 were used to generate the figures in (a) and (b). Under constant total pressure, an increase in the temperature reduces the amount of dissolved air in the water,

Table 5: Changes of the water density due to the dissolution of different gas species and air in total at different temperatures and $p_t = 101.325 \text{ kPa}$. The results from equation 13 and 14 are denoted by subscripts 'H' and 'W'. The $\Delta\rho$ values are in $(\text{kg m}^{-3}) \times 10^3$.

$T(^{\circ}\text{C})$	$\Delta\rho_{\text{N}_2}$	$\Delta\rho_{\text{O}_2}$	$\Delta\rho_{\text{Ar}}$	$\Delta\rho_{\text{CO}_2}$	$\Delta\rho_{\text{W}}$	$\Delta\rho_{\text{H}}$	$\left(\frac{\Delta\rho_{\text{W}}}{\rho_f}\right) \times 10^5$	$\left(\frac{\Delta\rho_{\text{H}}}{\rho_f}\right) \times 10^5$
0	-6.105	0.338	0.216	0.316	-5.235	-4.797	-0.524	-0.480
5	-5.411	0.351	0.192	0.263	-4.605	-4.052	-0.461	-0.405
10	-4.846	0.363	0.172	0.222	-4.089	-3.447	-0.409	-0.345
15	-4.381	0.375	0.156	0.188	-3.661	-2.949	-0.366	-0.295
20	-3.993	0.386	0.143	0.162	-3.301	-2.532	-0.331	-0.254
25	-3.664	0.397	0.132	0.140	-2.995	-2.179	-0.300	-0.219
30	-3.382	0.407	0.123	0.122	-2.73	-1.875	-0.274	-0.188
35	-3.134	0.416	0.115	0.107	-2.496	-1.609	-0.251	-0.162
40	-2.912	0.423	0.108	0.094	-2.287	-1.373	-0.230	-0.138
45	-2.709	0.429	0.102	0.083	-2.095	-1.162	-0.212	-0.117
50	-2.517	0.432	0.096	0.073	-1.916	-0.971	-0.194	-0.098

and as a result, the changes in the water density are less pronounced. At a constant temperature, water density decreases by increasing the pressure.

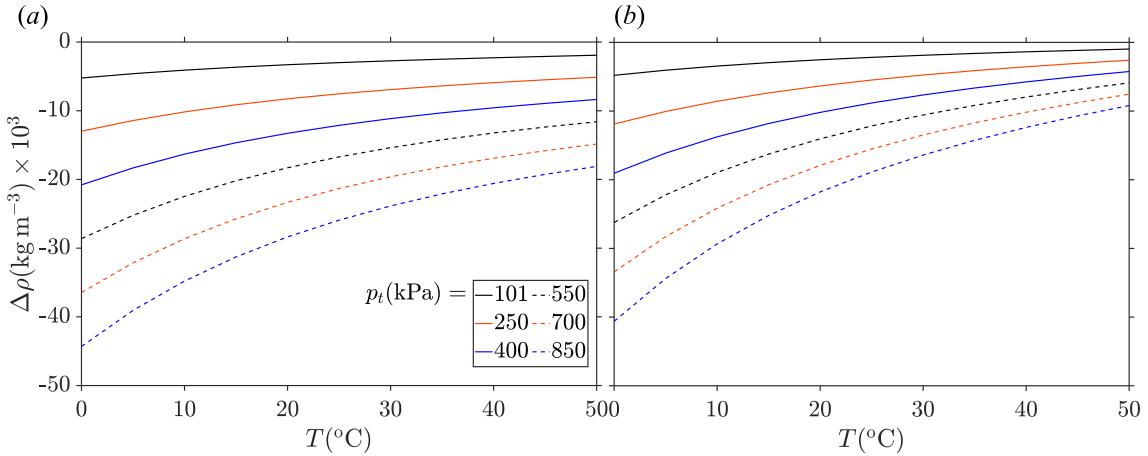


Figure 2: Changes of water density with temperature under different applied pressures, calculated using (a) Watanabe & Iizuka (1985) and (b) Harvey *et al.* (2005) approach.

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