Solution to gas weighing challenge

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This Analytical Challenge sets out to develop an equation to obtain mass of gases added to cylinders while accounting for buoyancy corrections [1]. The gas containers have tare masses, e.g., m_s , encasing the inner volume V_{gas} . This volume contains an amount of gas, e.g., m_A . The total mass of the container and the gas m_{s+A} is:

$$m_{s+A} = m_s + m_A = K_{s+A} \times m'_{s+A} = \frac{1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}}}{\rho_{s+A}} \times m'_{s+A} \quad (1)$$

where K_{s+A} is the buoyancy correction factor, m'_{s+A} is the balance reading, $\rho_{\text{air},1}$ is the density of air at the time t_1 when the mass is recorded, ρ_{cal} is the density of the calibration mass, and ρ_{s+A} is the density of the container filled with gas. The latter can be expressed as follows:

$$\rho_{s+A} = \frac{m_s + m_A}{V_s + V_{\text{gas}}} \quad (2)$$

The numerator is the sum of the mass of the container m_s and the mass of the contained gas m_A . This is divided by the sum of the inner volume, V_{gas} , which is the volume occupied by the gas, and the outer volume, V_s , which is the volume occupied by the container walls (and valves). If m_A becomes zero (the container is evacuated), Eq. 2 can be rewritten to yield the density ρ_s of the empty container

$$\rho_s = \frac{m_s}{V_s + V_{\text{gas}}} \quad (3)$$

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The inverse of ρ_s can be written as:

$$\frac{1}{\rho_s} = \frac{V_s + V_{\text{gas}}}{m_s} = \frac{1}{\rho_m} + \frac{V_{\text{gas}}}{m_s} \quad (4)$$

Here, ρ_m is the combined density of all metallic parts the container is made from (the walls, the valve etc.). Equation 4 and Equation 1 can be used to find the mass of the evacuated container at time t_0 ($m_A = 0$):

$$m_s = \frac{1 - \frac{\rho_{\text{air},0}}{\rho_{\text{cal}}}}{1 - \rho_{\text{air},0} \times \left(\frac{1}{\rho_m} + \frac{V_{\text{gas}}}{m_s} \right)} \times m'_{s,0} \quad (5)$$

where $m'_{s,0}$ is the balance reading of the empty container “s.” We assume that the densities of the two evacuated containers are the same within the limits of their uncertainties. We also assume that the ambient conditions (air temperature, humidity, and pressure) do not change significantly during weighing the two containers (for a better understanding of the applied weighing procedure, please see the figure 1 in the challenge [1]). At the time t_0 (before container “s” is filled with gas), both containers “s” and “r” are evacuated and weighed which provide the following equations:

$$m_s = K_{s,0} \times m'_{s,0} \quad (6)$$

$$m_r = K_{r,0} \times m'_{r,0} \quad (7)$$

The masses m_s and m_r are the (tare) masses of the to-be filled container “s” and the empty reference container “r,” respectively, whereas $m'_{r,0}$ and $m'_{s,0}$ are the balance readings.

After filling the container “s” with gas A and weighing it (at the time t_1), the total mass of the container “s” is the sum of m_s and m_A :

$$m_{s+A} = m_s + m_A \quad (8)$$

The tare mass m_s at time point t_1 is

$$m_s = K_{s,1} \times m'_{s,1} \quad (9)$$

Also, container “r” is weighed at time point t_1 and its tare mass is

$$m_r = K_{r,1} \times m'_{r,1} \quad (10)$$

From Eqs. 6 and 9, we can obtain the following:

$$m'_{s,1} = \frac{m_s}{K_{s,1}} = \frac{K_{s,0}}{K_{s,1}} \times m'_{s,0} \quad (11)$$

Since the densities of the two containers are nearly identical, the following relations are valid.

$$K_{s,0} \approx K_{r,0} \text{ and } K_{s,1} \approx K_{r,1} \quad (12)$$

From Eqs. 11 and 12, it follows that

$$\frac{K_{s,0}}{K_{s,1}} \approx \frac{K_{r,0}}{K_{r,1}} = \frac{m'_{r,1}}{m'_{r,0}} \quad (13)$$

Now, Eq. 13 is introduced in Eq. 11 and one obtains

$$m'_{s,1} = \frac{m_s}{K_{s,1}} = \frac{m'_{r,1}}{m'_{r,0}} \times m'_{s,0} \quad (14)$$

Together, Eqs. 14 and 9 give m_s (following along the lines of Eq. 5):

$$m_s = \frac{1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}}}{1 - \rho_{\text{air},1} \times \left(\frac{1}{\rho_m} + \frac{V_{\text{gas}}}{m_s} \right)} \times \frac{m'_{r,1}}{m'_{r,0}} \times m'_{s,0} \quad (15)$$

Rearranging Eq. 15 leads to

$$m_s - \rho_{\text{air},1} \times \left(\frac{m_s}{\rho_m} + V_{\text{gas}} \right) = \left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right) \times \frac{m'_{r,1}}{m'_{r,0}} \times m'_{s,0} \quad (16)$$

The next step is to derive an expression for m_{s+A} by combining Eqs. 1 and 2:

$$m_{s+A} = \frac{\left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right)}{1 - \rho_{\text{air},1} \times \left(\frac{\rho_m}{m_s + m_A} \right)} \times m'_{s+A} \quad (17)$$

Now, it is important to remember that $m_s + m_A = m_{s+A}$ and thus Eq. 17 can be rearranged to

$$m_{s+A} - \rho_{\text{air},1} \times \left(\frac{m_s}{\rho_m} + V_{\text{gas}} \right) = \left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right) \times m'_{s+A} \quad (18)$$

To obtain m_A , we need to subtract Eq. 16 from Eq. 18:

$$m_{s+A} - m_s + \rho_{\text{air},1} \times \left(\frac{m_s}{\rho_m} + V_{\text{gas}} \right) - \rho_{\text{air},1} \times \left(\frac{m_s}{\rho_m} + V_{\text{gas}} \right) = \left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right) \times m'_{s+A} - \left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right) \times \frac{m'_{r,1}}{m'_{r,0}} \times m'_{s,0} \quad (19)$$

This equation can be further simplified which leads to

$$m_{s+A} - m_s = \left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right) \times \left(m'_{s+A} - \frac{m'_{r,1}}{m'_{r,0}} \times m'_{s,0} \right) \quad (20)$$

As $m_{s+A} = m_s + m_A$, Eq. 20 is the wanted solution for m_A :

$$m_A = \left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right) \times \left(m'_{s+A} - \frac{m'_{r,1}}{m'_{r,0}} \times m'_{s,0} \right) \quad (21)$$

If a second gas is added, its mass (m_B) can be calculated in a similar fashion. At first, an equation just like Eq. 18 must be

set up, describing the total mass of container “s” at the time t_2 . This equation would be

$$m_{s+A+B} - \rho_{\text{air},2} \times \left(\frac{m_s}{\rho_m} + V_{\text{gas}} \right) = 1 - \frac{\rho_{\text{air},2}}{\rho_{\text{cal}}} \times m'_{s+A+B} \quad (22)$$

where $\rho_{\text{air},2}$ is the density of air at the time t_2 , when container “s” (containing gases A and B) and container “r” are both weighed again (m_{s+A+B} is the total mass of container “s”). The second step is to set up an equation which describes the tare mass of container “s” at the time t_2 ; it can be derived like Eq. 18:

$$m_s - \rho_{\text{air},2} \times \left(\frac{m_s}{\rho_m} + V_{\text{gas}} \right) = \left(1 - \frac{\rho_{\text{air},2}}{\rho_{\text{cal}}} \right) \times \frac{m'_{r,2}}{m'_{r,0}} \times m'_{s,0} \quad (23)$$

Eq. 23 from Eq. 22, the net gas mass $m_{A+B} = m_A + m_B$ can be calculated:

Note that the density of air at t_2 is different from $\rho_{\text{air},1}$ and thus also the balance reading for container “r.” By subtracting

$$\begin{aligned} m_{s+A+B} - \rho_{\text{air},2} \times \left(\frac{m_s}{\rho_m} + V_{\text{gas}} \right) - m_s + \rho_{\text{air},2} \times \left(\frac{m_s}{\rho_m} + V_{\text{gas}} \right) &= \left(1 - \frac{\rho_{\text{air},2}}{\rho_{\text{cal}}} \right) \times m'_{s+A+B} - \left(1 - \frac{\rho_{\text{air},2}}{\rho_{\text{cal}}} \right) \times \frac{m'_{r,2}}{m'_{r,0}} \times m'_{s,0} = \\ m_{s+A+B} - m_s &= m_A + m_B = \left(1 - \frac{\rho_{\text{air},2}}{\rho_{\text{cal}}} \right) \times \left(m'_{s+A+B} - \frac{m'_{r,2}}{m'_{r,0}} \times m'_{s,0} \right) \end{aligned} \quad (24)$$

As Eq. 24 is the total mass of both gases, m_A must be subtracted to obtain m_B . This operation (subtracting Eq. 21

from Eq. 24) is summarized in Eq. 26 and the final result is shown in Eq. 26:

$$m_{s+A+B} - m_s - (m_{s+A} - m_s) = \left(1 - \frac{\rho_{\text{air},2}}{\rho_{\text{cal}}} \right) \times \left(m'_{s+A+B} - \frac{m'_{r,2}}{m'_{r,0}} \times m'_{s,0} \right) - \left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right) \times \left(m'_{s+A} - \frac{m'_{r,1}}{m'_{r,0}} \times m'_{s,0} \right) \quad (25)$$

$$m_B = \left(1 - \frac{\rho_{\text{air},2}}{\rho_{\text{cal}}} \right) \times \left(m'_{s+A+B} - \frac{m'_{r,2}}{m'_{r,0}} \times m'_{s,0} \right) - \left(1 - \frac{\rho_{\text{air},1}}{\rho_{\text{cal}}} \right) \times \left(m'_{s+A} - \frac{m'_{r,1}}{m'_{r,0}} \times m'_{s,0} \right) \quad (26)$$

Inserting the given quantities from the challenge [1] gives the following values:

$$m_A = 0.9672 \text{ g and } m_B = 1.0389 \text{ g} \quad (27)$$

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1. Flierl, L., Rienitz, O., Pramann, A. Gas weighing challenge. *Anal Bioanal Chem.* 2020;412:1–3. <https://doi.org/10.1007/s00216-019-02168-4>.

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