

Simulation Approach of Chamber Purging Experiment by Nitrogen Gas

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Abstract. Chamber purging is usually required in a gas sensing research, in order to make a perfect dry air condition (Relative Humidity/ $RH = 0\%$) in the chamber. Experimentally, it was found that RH of the cylindrical chamber (volume = 7.5 cm^3) never touch 0% (only 32% and 4%) although it was purged by 100 and 300 sccm of synthetic air (consists of $20\% \text{ O}_2$ and 80% of N_2). It was also obtained the same condition when N_2 gas was used instead of synthetic air. Simulation approach using box-form chamber (volume = 9.6 cm^3) shows that the combination of the diffusion-convection process of N_2 gas is responsible for the results of chamber purging experiment instead of pure diffusion or pure convection.

1. Introduction

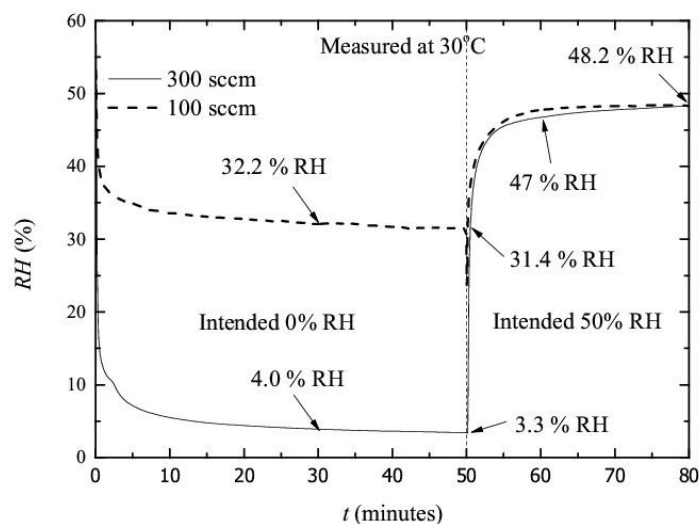
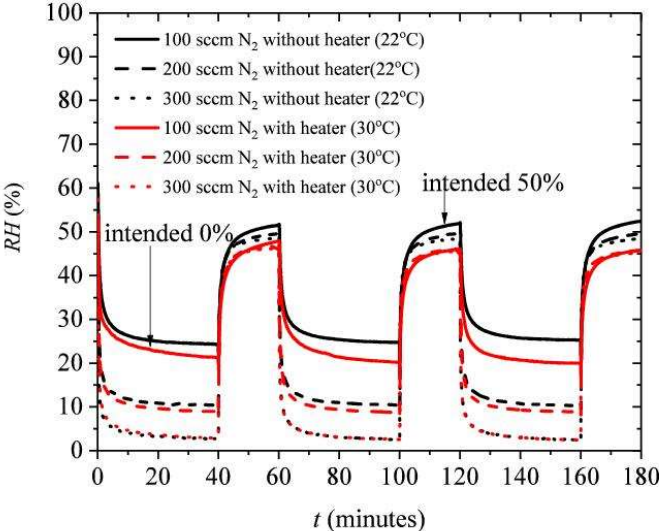
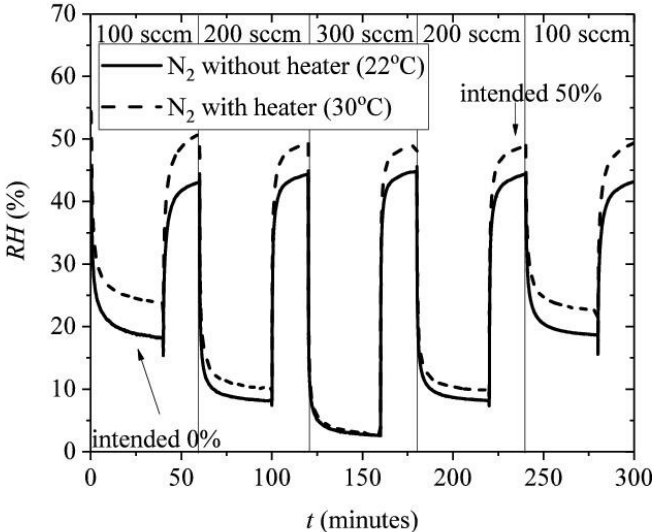


Figure 1. Humidity achievement with flow variations [1]

In a gas sensor experiment, chamber purging is one of the important steps in order to get an adjusted humidity condition (dry or wet) in the chamber. Experimentally, it was found that to achieve a perfectly dry condition (0 % *R.H.*/Relative Humidity) was unreachable [1]. Figure 1 shows humidity experiments which had been done to know the humidity condition, which can be achieved in the measurement chamber based on flow variations. According to figure 1, if it was used 100 sccm (standard cubic centimeter) air and it was intended $RH = 0\%$ at room temperature (30°C), after 30 minutes chamber would only reach 32.2%. It would be 4% *RH* if it was used 300 sccm air. The waiting time 30 minutes was used because this waiting time which was needed to stabilize the temperature in the chamber at room temperature in the gas sensing measurement. On the other hand, there was no significant difference between using 100 sccm or 300 sccm if it was intended $RH = 50\%$, it would be obtained 47% after 10 minutes.



(a)



(b)

Figure 2. Reproducibility of purging experiments [1]

Other experiments using nitrogen (N_2) instead of the synthetic air also have been done as revealed in figure 2 [1]. N_2 was used because synthetic air is more expensive than N_2 . Based on figure 2.a and 2.b, it proves that measurements of the purging experiments which have been done are reproducible. If a heater was used in the chamber (figure 3), it shows that the heater accelerates the dehumidification but slows the humidification.

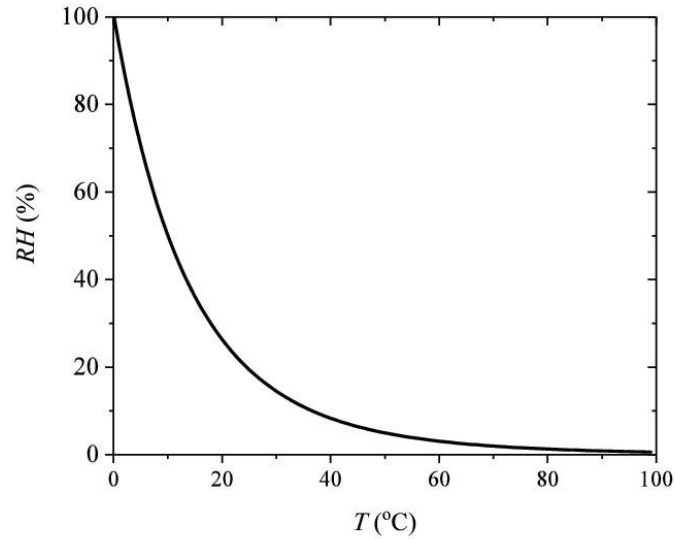


Figure 3. RH and chamber temperature [1]

According to those explanations, it should be an explanation for these phenomena. Literature searching concludes that there is no report yet, which is similar to this case. Some researches regarding the simulation approach of the humidification and dehumidification process have been conducted, but their cases are actually not the same as this report [2], [3], [4], [5], [6]. This article will investigate the explained phenomena based on diffusion and convection concept.

2. Data/Materials and Methods

As explained before, this investigation based on the diffusion process which uses the Diffusion Equation as given by Equation 1 [7],

$$\frac{dc}{dt} = D\nabla^2 C, \quad (1)$$

where C is the concentration of water vapor, D is diffusion constant of water vapor in N_2 at temperature T (in K) and pressure p (in atm). D in Equation (1) can be calculated as presented in Equation (2) [7],

$$D = D_0 \frac{p_0}{p} \left(\frac{T}{T_0}\right)^\alpha, \quad (2)$$

where D_0 is diffusion constant of water vapor in N_2 (i.e. $0.2178 \text{ cm}^2/\text{s}$) at temperature $T_0 = 273.15 \text{ K}$ and pressure $p_0 = 1 \text{ atm}$; and α is a constraint (1.81) in Massman's Equation [4]. Afterward, specific humidity will also be used in this simulation as reveals in Equation (3) [8]

$$\omega = \frac{m_w}{m_a}, \quad (3)$$

where m_w and m_a are the mass (kg) of water vapor which is in the N_2 and mass of the N_2 , respectively. By combining Equation (1) – (3), it will be obtained a new form of Equation (1) which will be used in this simulation for the diffusion process.

This simulation will also compare the diffusion and the convection process, which employs the equation of mass balance for N_2 as given in Equation (4) [8],

$$\frac{dm_{a \text{ in}}}{dt} = \frac{dm_{a \text{ out}}}{dt}, \quad (4)$$

where $m_{a \text{ in}}$ and $m_{a \text{ out}}$ are mass (kg) of N_2 which flows into and out from the chamber respectively. It also uses equation of mass balance for the water vapor as presented in Equation (5) [8],

$$\frac{dm_{w \text{ chamber}}}{dt} = \frac{dm_{w \text{ in}}}{dt} - \frac{dm_{w \text{ out}}}{dt}, \quad (5)$$

where $m_{w \text{ chamber}}$, $m_{w \text{ in}}$ and $m_{w \text{ out}}$ are the mass (in kg) of water vapor which is in, flows into and flows out from the chamber. Then, by combining Equation (3) – (5), it will be produced a new form of Equation (5) will be the basic equation in this simulation for the convection process.

Afterward, these two equations (diffusion and convection) will be applied for the experiment chamber, which is replaced by the chamber model as presented in figure 4. Finally, it will be shown, which one is the best approach to explain these phenomena: is it diffusion, convection or combination of diffusion and convection?

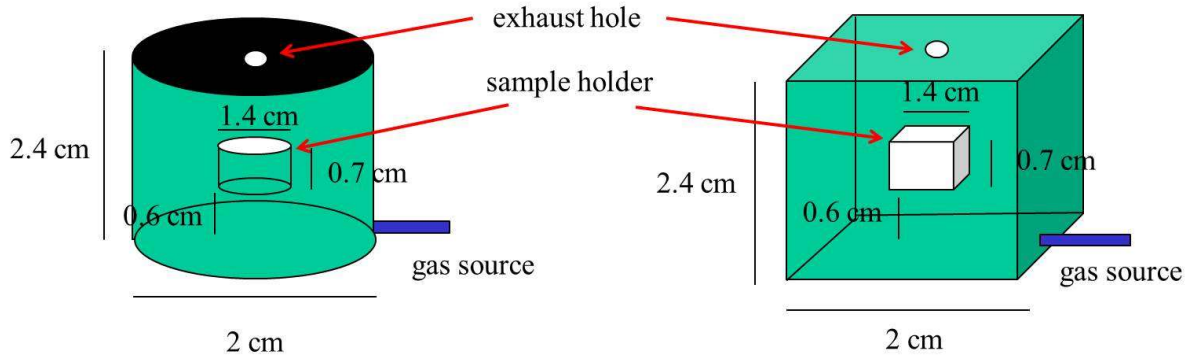


Figure 4. Experiment Chamber (left) and its model (right) [1]

3. Results and discussion.

As mentioned before, this simulation starts with the diffusion process. By substituting Equation (3) to Equation (1), it is obtained a new form of Equation (1) as exhibited in Equation (6)

$$\frac{d\omega}{dt} = D\nabla^2\omega. \quad (6)$$

Then, for the convection process, by using Equation (3), Equation (5) can be reformed as presented in Equation (7)

$$\frac{d\omega m_{a \text{ chamber}}}{dt} = \frac{d\omega_{in} m_{a \text{ in}}}{dt} - \frac{d\omega_{out} m_{a \text{ out}}}{dt}, \quad (7)$$

where ω_{in} , ω_{out} , $m_{a \text{ chamber}}$, $m_{a \text{ in}}$ and $m_{a \text{ out}}$ are specific humidity of water vapor which flows into and out from the chamber, mass of N_2 which is in, flows into and out from the chamber, respectively.

Afterward, it is assumed

$$\frac{dm_{a \text{ in}}}{dt} = \frac{dm_{a \text{ out}}}{dt} = \frac{dm_a}{dt}. \quad (8)$$

Equation (8) causes Equation (7) can be represented as written in Equation (9)

$$m_{a \text{ chamber}} \frac{d\omega_{\text{chamber}}}{dt} = \frac{dm_a}{dt} (\omega_{in} - \omega_{out}) - m_a \frac{d\omega_{out}}{dt}. \quad (9)$$

Afterward, it is already understood that [1]

$$\omega_{out} = \omega_{\text{chamber}} = \omega, \quad (10)$$

$$\omega_{in} = \text{constant}, \quad (11)$$

$$m_{a \text{ chamber}} = \rho_{N_2} V_{\text{chamber}}, \quad (12)$$

$$m_a = \rho_{N_2} V, \quad (13)$$

where ρ_{N_2} , m_a , V_{chamber} , and V are the density of N_2 (in kg/m^3), mass of N_2 which flows (in kg), volume of the chamber (in m^3), and volume of atmosphere which flows (in m^3), respectively. Because of these equations/Equation (10) – (13), Equation (9) can be redisplayed as given in Equation (14)

$$\frac{d\omega}{dt} = \dot{V} \frac{(\omega_{\text{in}} - \omega)}{(V_{\text{chamber}} + V_a)}. \quad (14)$$

If the Diffusion Process/Equation (6) is combined with the Convection Process/Equation(14), then it is obtained

$$\frac{d\omega}{dt} = D\dot{V}^2\omega + \frac{(\omega_{\text{in}} - \omega)}{(V_{\text{chamber}} + V_a)}. \quad (15)$$

Equation (15) can only be solved numerically as given in Equation (16),

$$\omega_{i,j,k,l+1} = \omega_{i,j,k,l} + D\Delta t \left(\left(\frac{\omega_{i+1,j,k,l} - 2\omega_{i,j,k,l} + \omega_{i-1,j,k,l}}{\Delta x^2} \right) + \left(\frac{\omega_{i,j+1,k,l} - 2\omega_{i,j,k,l} + \omega_{i,j-1,k,l}}{\Delta y^2} \right) + \left(\frac{\omega_{i,j,k,l+1} - 2\omega_{i,j,k,l} + \omega_{i,j,k,l-1}}{\Delta z^2} \right) \right) + \Delta t \dot{V} \frac{(\omega_{\text{in}} - \omega_{i,j,k,l})}{(V_{\text{chamber}} + \Delta t \dot{V})}. \quad (16)$$

Then, according to figure 4, the sample holder is as a barrier which causes the followed condition at the boundary of the sample holder

$$\frac{d\omega}{dx} = \frac{d\omega}{dy} = \frac{d\omega}{dz} = 0. \quad (17)$$

Numerically, the meaning of Equation (17) is as given by Equation (18)

$$\omega_{i,j,k,l+1} = \omega_{i,j,k,l}. \quad (18)$$

Afterward, because the solution is still in ω -form, the RH can be formed as the followed procedure. Based on the Ideal Gas Equation, the mass of the gas (m) can be computed as exhibited in Equation (19)

$$m = \frac{pVM}{RT}, \quad (19)$$

where p is the pressure of the gas (Pa), V is the volume of the gas (m^3), M is the molecular mass of the gas (kg/mol), and T is the temperature of the gas (K). According to Equation (19), Equation (3) can be redisplayed as presented in Equation (20)

$$\omega = \frac{M_w p_w}{M_a p_a}, \quad (20)$$

where p_w is the pressure of the water vapor (Pa), p_a is the pressure of N_2 in Pa, M_w is the molecular mass of the water vapor (18 kg/mol) and M_a is the molecular mass of N_2 (28 kg/mol). Then, because of

$$p_a = p - p_w, \quad (21)$$

where p is total pressure of water vapor and N_2 (in Pa), then Equation (20) can be reformed as exhibited in Equation (22)

$$\omega = 0.629 \frac{p_w}{p - p_w}. \quad (22)$$

Since, RH is as given in Equation (23) [8]

$$RH = \frac{p_w}{p_{\text{sat}}}, \quad (23)$$

where p_{sat} is saturated water vapor pressure of N_2 (in Pa) as presented in Equation (24)

$$p_{\text{sat}} = \frac{(1.0007 + 3.46 \times 10^{-6} \times 1013.250) \times 6.1121 \exp\left(\frac{17502T}{240.97 + T}\right) \times 1.01 \times 10^5}{1013.250} \quad (24)$$

where T is temperature (in $^{\circ}\text{C}$). Afterward, if Equation (22) is substituted to (23), it changes the form of Equation (23) as presented in Equation (25)

$$RH = \frac{\omega p}{(0.6429 + \omega)p_{\text{sat}}}. \quad (25)$$

Then, substitution Equation (16) to (25) produces the RH as function of time. If it is only diffusion, then Equation (16) is simplified as presented in Equation (26)

$$\omega_{i,j,k,l+1} = \omega_{i,j,k,l} + D\Delta t \left(\left(\frac{\omega_{i+1,j,k,l} - 2\omega_{i,j,k,l} + \omega_{i-1,j,k,l}}{\Delta x^2} \right) + \left(\frac{\omega_{i,j+1,k,l} - 2\omega_{i,j,k,l} + \omega_{i,j-1,k,l}}{\Delta y^2} \right) + \left(\frac{\omega_{i,j,k,l+1} - 2\omega_{i,j,k,l} + \omega_{i,j,k-1,l}}{\Delta z^2} \right) \right). \quad (26)$$

If simulation results of pure diffusion case/Equation (26) is compared to the experiment results, it is as presented in figure 5. It can be seen that there is no change of RH when wet/dry N_2 is applied. Simulated- RH is always at the same value, i.e. 60%. It happens because the process of this approach is very slow.

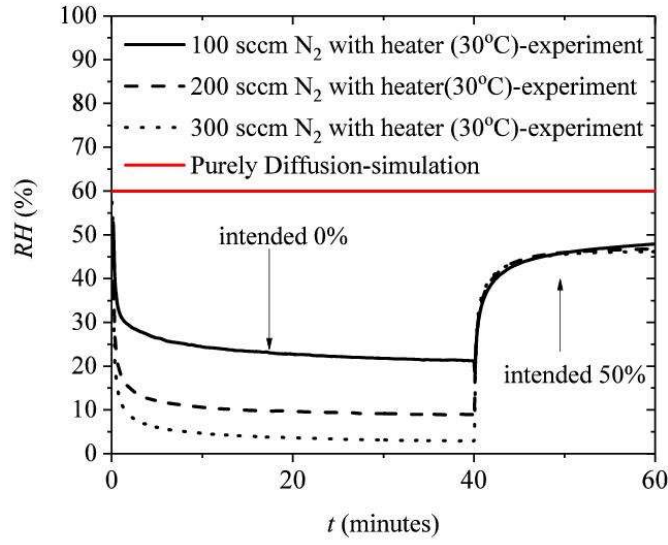


Figure 4. Simulation results of pure diffusion versus experiment results [1]

If it is only convection, then Equation (16) is reformed as given in Equation (27) and shown in figure 5.

$$\omega_{i,j,k,l+1} = \Delta t \dot{V} \frac{(\omega_{in} - \omega_{i,j,k,l})}{(V_{chamber} + \Delta t \dot{V})}. \quad (27)$$

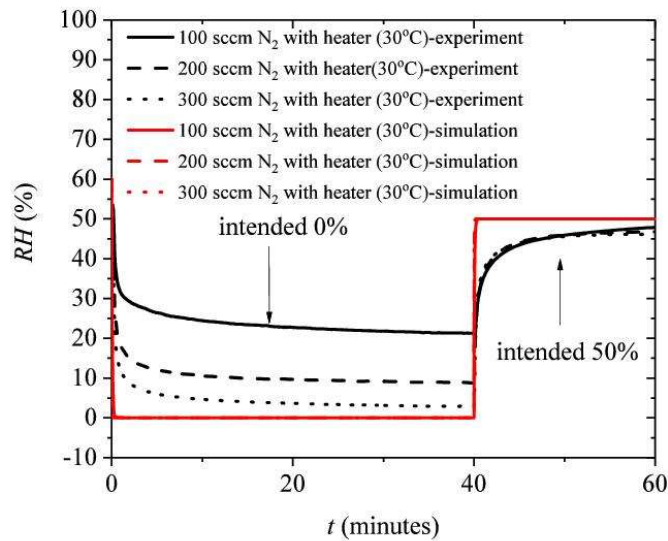


Figure 5. Simulation results of pure convection versus experiment results [1]

According to figure 5, if it is pure convection, then simulated-*RH* is always at the same value, although the flow rate of N_2 is variated. It is obtained because the process is very fast.

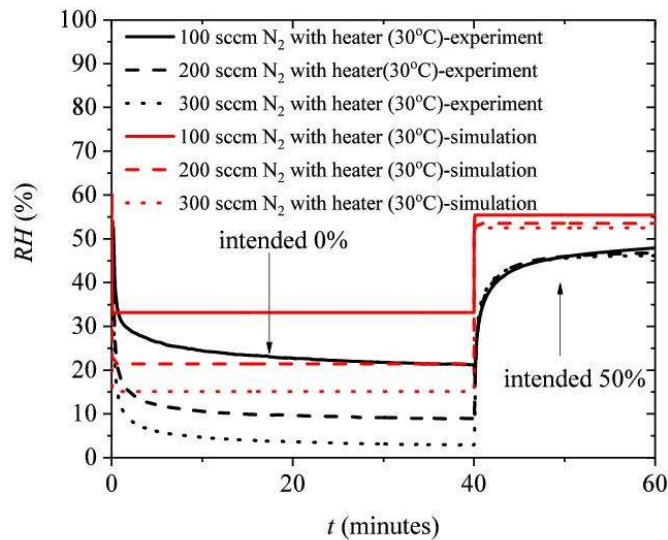


Figure 6. Simulation results of diffusion-convection versus experiment results [1]

The last result is a combination of diffusion and convection process (Equation (16)) as presented in figure 6. Based on figure 6, the combination of diffusion and convection is the best approach because the simulation results have a tendency to the experiment results.

4. Conclusion

The simulations which have been done proving that combination of diffusion and convection is the best approach because it can close experiment results instead of using only diffusion or convection approach.

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