Simulation approach of chamber purging experiment by nitrogen gas

R Marjunus

University of Lampung, Jl. Prof. Dr. Soemantri Brodjonegoro No.1, Bandar Lampung 35145, Indonesia
roniyus.1977@fmipa.unila.ac.id

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. An experiment shows 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% O$_2$ and 80% of N$_2$). It was also obtained the same condition when N$_2$ gas was used instead of synthetic air. In order to understand this experiment’s results, a simulation has been done. The simulation approach using a 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 the chamber purging experiment instead of pure diffusion or pure convection. For the future step, it is needed further investigation (experiment and simulation) in order to reach 0% RH.

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 purging experiments that were planned to reach expected R.H. i.e., 0% and 50% at room temperature (30°C) using flow variations. According to figure 1, if it was used 100 sccm (standard cubic centimeter) air, the chamber would only achieve 32.2% after 30 minutes. It would be 4% RH for 300 sccm air. The first 30 minutes was aimed for temperature stabilization in the chamber. Then, there were no significantly different results between 100 sccm and 300 sccm for expected R.H= 50%, and it was obtained 47% after it was waited for 10 minutes.

![Figure 1](image1.png)

**Figure 1**. Purging experiments in a gas sensor experiment [1]

![Figure 2](image2.png)

**Figure 2.** Reproducibility of purging experiments [1]
If it used nitrogen ($N_2$), the results are as given in figure 2 [1]. $N_2$ was used because synthetic air is more expensive than $N_2$. Based on figure 2.(a) and (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 makes the dehumidification faster but the humidification slower.

**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 [2,3,4,5,6,7,8]. 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) [9],

$$\frac{dC}{dt} = D \nabla^2 C$$  \hspace{1cm} (1)

where $C$ is the water vapor concentration, $D$ is water vapor diffusion constant in $N_2$ for temperature $T$ (in K) and at pressure $p$ (in atm). $D$ in Equation (1) can be calculated as presented in Equation (2) [9],

$$D = D_0 \frac{p_0}{p} \left(\frac{T}{T_0}\right)^\alpha$$  \hspace{1cm} (2)

where $D_0$ is diffusion constant of water vapor in $N_2$ (i.e. 0.2178 cm$^2$/s) at $T_0 = 273.15$ K and $p_0 = 1$ atm; and $\alpha$ is a constant (1.81) in Massman’s Equation [9]. Afterward, specific humidity will also be used in this simulation as reveals in Equation (3) [10]

$$\omega = \frac{m_w}{m_a}$$  \hspace{1cm} (3)
where \( m_w \) and \( m_a \) are the water vapor mass (kg), which is in the \( N_2 \) and the \( N_2 \)-mass, 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 mass balance equation for \( N_2 \) as given in Equation (4) [10],

\[
\frac{dm_{a \text{ in}}}{dt} = \frac{dm_{a \text{ out}}}{dt}
\]

where \( m_{a \text{ in}} \) is \( N_2 \)-mass (kg), which goes in and \( m_{a \text{ out}} \) which is out from the system. It also employs the mass balance equation for the water vapor as presented in Equation (5) [10],

\[
\frac{dm_{w \text{ in}}}{dt} = \frac{dm_{w \text{ out}}}{dt}
\]

where \( m_{w \text{ chamber}} \), \( m_{w \text{ in}} \) and \( m_{w \text{ out}} \) are the water vapor mass (in kg) which is in, goes into and flows out from the system, respectively. 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)

\[
\frac{d\omega}{dt} = D \nabla^2 \omega
\]

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

\[
\frac{d\omega_{a \text{ chamber}}}{dt} = \frac{d\omega_{a \text{ in}}}{dt} = \frac{d\omega_{a \text{ out}}}{dt}
\]

where \( \omega_{a \text{ in}} \), \( \omega_{a \text{ out}} \), \( m_{a \text{ chamber}} \), \( m_{a \text{ in}} \) and \( m_{a \text{ out}} \) are water vapor specific humidity which goes into and out from the system, \( N_2 \)-mass which is in, goes into and out from the system, respectively. Afterward, it is assumed

\[
\frac{dm_{a \text{ in}}}{dt} = \frac{dm_{a \text{ out}}}{dt} = \frac{dm_{a}}{dt}
\]

Equation (8) causes Equation (7) can be represented as written in Equation (9)
\[ m_{\text{a chamber}} \frac{d\omega_{\text{chamber}}}{dt} = \frac{d}{dt} \left( \omega_{\text{in}} - \omega_{\text{out}} \right) - m_{\text{a}} \frac{d\omega_{\text{out}}}{dt} \]  

(9)

Afterward, it is already understood that [1]

\[ \omega_{\text{out}} = \omega_{\text{chamber}} \]

(10)

\[ \omega_{\text{in}} = \text{constant}, \]

(11)

\[ m_{\text{a chamber}} = \rho_{\text{N}_2} V_{\text{chamber}}, \]

(12)

\[ m_{\text{a}} = \rho_{\text{N}_2} V, \]

(13)

where \( \rho_{\text{N}_2} \), \( m_{\text{a}} \), \( V_{\text{chamber}} \), and \( V \) are the \( \text{N}_2 \)-density (in kg/m\(^3\)), the \( \text{N}_2 \)-mass which flows (in kg), the chamber volume (in m\(^3\)), and the atmosphere volume which flows (in m\(^3\)), respectively. Because of these equations/Equation (10) – (13), Equation (9) can be redisplayed as given in Equation (14)

\[ \frac{d\omega}{dt} = \dot{V} \frac{(\omega_{\text{in}} - \omega)}{(V_{\text{chamber}} + V_{\text{a}})} \]  

(14)

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

\[ \frac{d\omega}{dt} = D \nabla^2 \omega + \frac{(\omega_{\text{in}} - \omega)}{(V_{\text{chamber}} + V_{\text{a}})} \]  

(15)

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

\[
\begin{align*}
\omega_{i,j,k+1} &= \omega_{i,j,k} \\
&+ D \Delta t \left( \frac{\omega_{i+1,j,k+1} - 2\omega_{i,j,k+1} + \omega_{i-1,j,k+1}}{\Delta x^2} \right) \\
&+ \frac{\omega_{i,j+1,k+1} - 2\omega_{i,j,k+1} + \omega_{i,j-1,k+1}}{\Delta y^2} \right) + \Delta t \dot{V} \frac{(\omega_{\text{in}} - \omega_{i,j,k})}{(V_{\text{chamber}} + \Delta t \dot{V})}
\end{align*}
\]  

(16)

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

\[ \frac{d\omega}{dx} = \frac{d\omega}{dy} = \frac{d\omega}{dz} = 0. \]

(17)

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

\[ \omega_{i,j,k+1} = \omega_{i,j,k-1}. \]

(18)

Afterward, based on \( \omega \)-form solution, it be formed the \( RH \)-form as the followed procedure. Based on the Ideal Gas Equation, the gas mass \((m)\) can be computed as exhibited in Equation (19)

\[ m = \frac{pVM}{RT}, \]

(19)

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

\[ \omega = \frac{M_{\text{a}}P_{\text{a}}}{m_{\text{a}}P_{\text{a}}}, \]

(20)
where $p_w$ is the water vapor pressure (Pa), $p_a$ is the $N_2$-pressure in Pa, $M_w$ is the water vapor molecular mass (18 kg/mol), and $M_a$ is the $N_2$-molecular mass (28 kg/mol). Then, because of

$$p_a = p - p_w,$$

(21)

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

$$\omega = 0.629 \frac{p_w}{p - p_a}.$$  

(22)

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

$$RH = \frac{p_w}{p_{sat}},$$

(23)

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

$$p_{sat} = \left( \frac{1013.250}{1.0007 \times 6.1121 \times 10^{10} \times 1013.250} \right)^{\frac{17507}{240.57^2}} \times 1.01 \times 10^5,$$

(24)

where $T$ is the temperature (in °C). Afterward, if Equation (22) is substituted to (23), it changes the display of Equation (23) as presented in Equation (25)

$$RH = \frac{\omega p}{(0.629 + \frac{1}{p_{sat}})}.$$  

(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)

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

(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 $RH$ change when wet/dry $N_2$ is applied. Simulated-$RH$ is always at the same value, i.e. 60%. It happens because of very slow process in this approach.

![Figure 5. Simulation of pure diffusion versus experiment [1]](image-url)
If it is only convection, then Equation (16) can be reformed as given in Equation (27) and shown in figure 6.

\[ \omega_{i,j,k,l+1} = \Delta t \hat{V} \frac{(\omega_{in} - \omega_{i,j,k,l})}{(V_{chamber} + \Delta t \hat{V})} \]  

(27)

Figure 6. Simulation of pure convection versus experiment [1]

According to figure 6, if it is pure convection, then simulated-RH is always at the same value, although the flow rate of N\(_2\) is varied. It is obtained because the process is very fast.

Figure 7. Simulation of diffusion-convection versus experiment [1]

The last result is a diffusion-convection combination (Equation (16)) as given in figure 7. According to figure 7, 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 the combination of diffusion and convection is the best approach because it can close experiment results instead of using only diffusion or convection approach. For the future step, it is needed further investigation (experiment and simulation) in order to reach 0% RH.

5. References
[1] Roniyus M 2018 Development of Pt-based sensitive layer for carbon monoxide work function change based sensor in air at room temperature Ph D Thesis (München: Universität der Bundeswehr)
[2] Faissal A, Mohammed A, Mazherb A K and Abdulrahim A 2019 Simulation and optimization study of the humidification–dehumidification desalination process Desalination and Water Treatment 141 p 23-25
[3] Yang L, Xin H, Hao P, Xiang L and Shan D T 2018 Simulation and optimization of humidification-dehumidification evaporation system Energy 145 p 128-140
[4] He W F and Han D 2017 Performance simulation of an air-heated humidification dehumidification desalination system IOP Conference Series: Earth and Environmental Science 73 012004 p 1-6
[5] Chiranjeevi C and Srinivas T 2015 Experimental and simulation studies on two stage humidification–dehumidification desalination and cooling plant Desalination 376 p 9-16
[6] Yoshinori H, Hideo M and Fumio M 2008 Simulation of a dehumidification/humidification performance of a desiccant rotor using pore size controlled material regenerated by low grade thermal energy International Refrigeration and Air Conditioning Conference at Purdue (2008) p 1-8
[7] Haris P G, Rajendra S A and Rakesh K 2003 Experimental design and computer simulation of multi-effect humidification (MEH)-dehumidification solar distillation Desalination 153 p 81-86
[8] Naser K N, Mohammed M F, Abdul A O, Said M A H and Abdul R T A 1997 Simulation study to improve the performance of a solar humidification-dehumidification desalination unit constructed in Jordan Desalination 109 p 277-284
[9] William J M 1998 A review of the molecular diffusivities of H2O, CO2, CH4, CO, O3, SO2, NH3, N2O, NO, and NO2 in air, O2 and N2 near STP Atmospheric Environment 32 (6) p 1111–1127
[10] Yunus A Ç, John M C and Robert H T 2017 Fundamentals of thermal-fluid sciences (5th Edition. Mc Graw-Hill Education)

Acknowledgment
The author would like to thank Ministry of Research and Higher Education, Republic of Indonesia and also to Institut für Physik, Fakultät Elektrotechnik und Informationstechnik, Universität der Bundeswehr München, Germany, for supporting this research.