Preface

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The International Conference on Theoretical and Applied Physics (The ICTAP 2019) is a conference organized by Physical Society of Indonesia (PSI), University of Lampung (Dept. of Physics, Dept. of Physics Education, and Dept. of Geophysics Engineering); Dept. of Physics Education - Raden Intan State Islamic University of Lampung; Dept. of Physics - Technology Institut of Sumatera; Dept. of Physics Education- Univ. of Muhammadiyah Metro; Research Unit for Mineral Technology Lampung- Indonesian Institute of Sciences; Research & Standardization Industry Lampung, and Physics Teacher Forum of Bandar Lampung. It is an annual conference of the Society and moves from one major city to another, started seven years back in Bandung (Capital city of West Java Province), then consecutively moved to Palangkaraya (Capital city of Central Kalimantan Province, 2012), Malang (East Java, 2013), Denpasar (Capital city of Bali Province, 2014), Kendari (Capital city of South-East Sulawesi Province, 2015), Makasar (Capital city of South Sulawesi Province, 2016). Yogyakarta (Capital city of Special Region of Yogyakarta Province, 2017), and Medan (Capital city of South Sumatera Province, 2018).

The ICTAP 2019 was held in Bandar Lampung, Lampung, on 26th-28th September 2019, with the main theme "Physics and Smart Society." It was aimed for promoting, developing, and disseminating interdisciplinary research from many different fields of physics. Researchers from universities, institutes, and related industries, working on various fields of physics were invited to participate to present papers or just as a participant.

We would like to acknowledge all of those who have supported ICTAP 2019. Each individual and institutional help were very important for the success of this conference. Especially we would like to thank the organizing committee for their valuable advices in the organization and helpful peer review of the papers.

We hope that ICTAP 2019 will be a forum for excellent discussions that will put forward new ideas and promote collaborative researches. We are sure that the proceedings will serve as an important research source of references and the knowledge, which will lead to not only scientific and engineering progress but also other new products and processes.

Dr. rer. nat. Roniyus Marjunus

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Bandung, 25 Januari 2019
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Prof. Dr.-Ing Mitra Djamal

Simulation approach of chamber purging experiment by nitrogen gas

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. 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

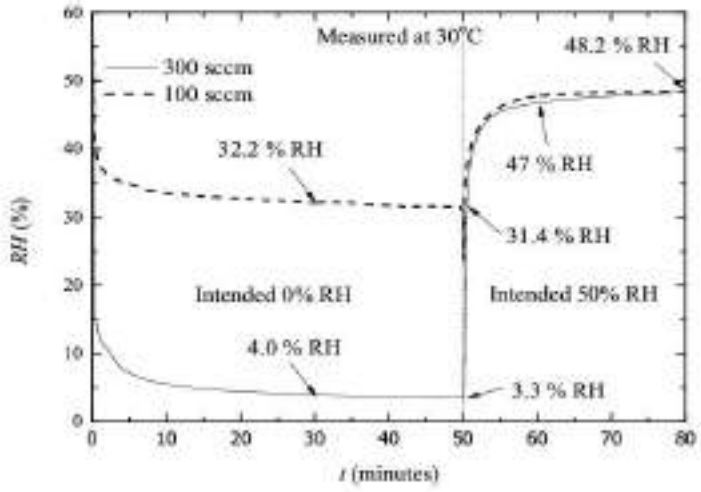
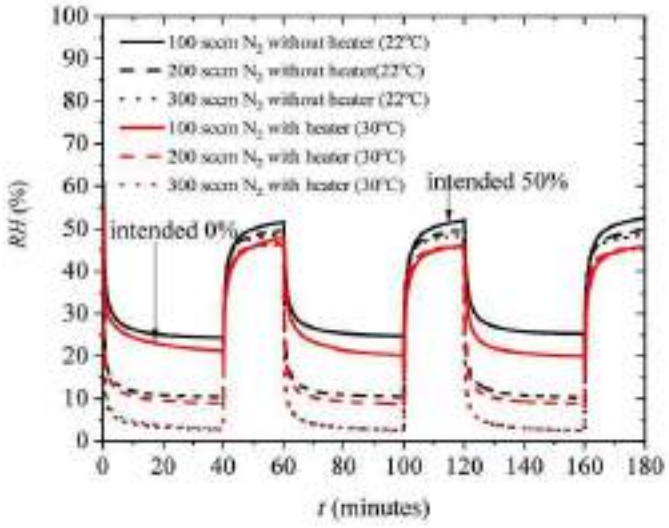
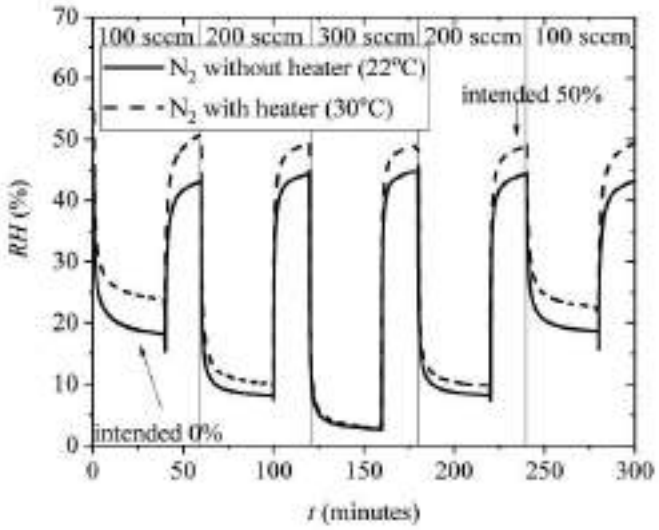


Figure 1. Humidity achievement with flow variations [1]

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 *RH*= 50%, and it was obtained 47% after it was waited for 10 minutes.



(a)



(b)

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.

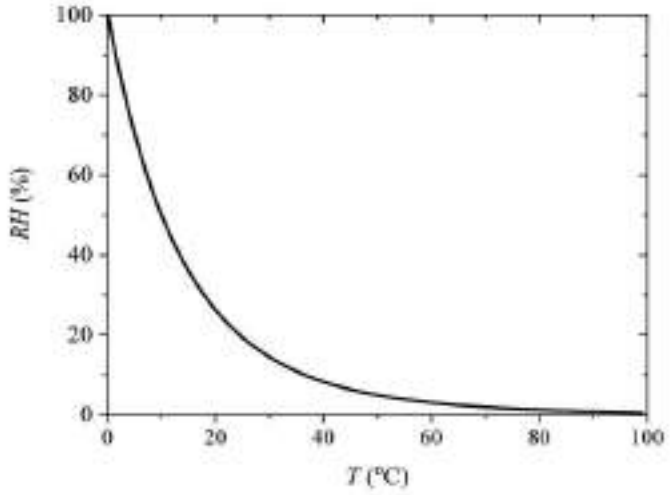


Figure 3. *RH* and chamber temperature [1]

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],

$$\frac{dC}{dt} = D\nabla^2 C \tag{1}$$

where C is the water vaporconcentration, 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],

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

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]

$$\omega = \frac{m_{\mathrm{w}}}{m_{\mathrm{a}}} \tag{3}$$

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 usedin 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],

$$\frac{dm_{\mathrm{a\ in}}}{dt} = \frac{dm_{\mathrm{a\ out}}}{dt} \tag{4}$$

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

$$\frac{dm_{\mathrm{w\ chamber}}}{dt} = \frac{dm_{\mathrm{w\ in}}}{dt} - \frac{dm_{\mathrm{w\ out}}}{dt} \tag{5}$$

where $m_{\mathrm{w\ chamber}}$, $m_{\mathrm{w\ in}}$ and $m_{\mathrm{w\ out}}$ 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?

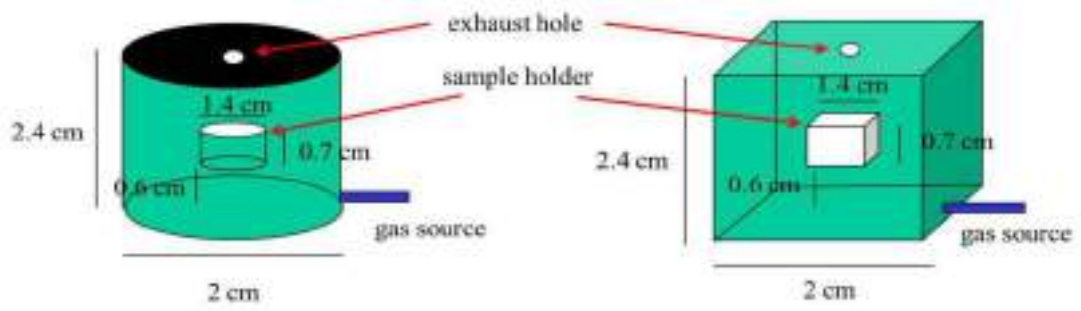


Figure 4. Experiment Chamber (left) and its model (right) [1]

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)

$$\frac{d\omega}{dt} = D\nabla^2\omega \tag{6}$$

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

$$\frac{d\omega m_{\mathrm{a\ chamber}}}{dt} = \frac{d\omega_{\mathrm{in}} m_{\mathrm{a\ in}}}{dt} - \frac{d\omega_{\mathrm{out}} m_{\mathrm{a\ out}}}{dt} \tag{7}$$

where ω_{in}, ω_{out}, $m_{\mathrm{a\ chamber}}$, $m_{\mathrm{a\ in}}$ and $m_{\mathrm{a\ out}}$ 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

$$\frac{dm_{\mathrm{a\ in}}}{dt} = \frac{dm_{\mathrm{a\ out}}}{dt} = \frac{dm_{\mathrm{a}}}{dt} \tag{8}$$

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

$$m_{\mathrm{a\ chamber}}\frac{d\omega_{\mathrm{chamber}}}{dt}=\frac{dm_{\mathrm{a}}}{dt}(\omega_{\mathrm{in}}-\omega_{\mathrm{out}})-m_{\mathrm{a}}\frac{d\omega_{\mathrm{out}}}{dt} \tag{9}$$

Afterward, it is already understood that [1]

$$\omega_{\mathrm{out}}=\omega_{\mathrm{chamber}}=\omega \tag{10}$$

$$\omega_{\mathrm{in}}=\mathrm{constant}, \tag{11}$$

$$m_{\mathrm{a\ chamber}}=\rho_{N_2}V_{\mathrm{chamber}}, \tag{12}$$

$$m_{\mathrm{a}}=\rho_{N_2}V, \tag{13}$$

where ρ_{N_2}, m_{a}, V_{chamber}, and V are the N_2-density (in kg/m^3),the 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)

$$\frac{d\omega}{dt}=\dot{V}\frac{(\omega_{\mathrm{in}}-\omega)}{(V_{\mathrm{chamber}}+V_{\mathrm{a}})}, \tag{14}$$

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

$$\frac{d\omega}{dt}=D\dot{\nabla}^2\omega+\frac{(\omega_{\mathrm{in}}-\omega)}{(V_{\mathrm{chamber}}+V_{\mathrm{a}})}. \tag{15}$$

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

$$\begin{aligned}\omega_{\mathrm{i,j,k,l+1}}=\omega_{\mathrm{i,j,k,l}}&\\+D\Delta t\Bigg(&\left(\frac{\omega_{\mathrm{i+1,j,k,l}}-2\omega_{\mathrm{i,j,k,l}}+\omega_{\mathrm{i-1,j,k,l}}}{\Delta x^2}\right)+\left(\frac{\omega_{\mathrm{i,j+1,k,l}}-2\omega_{\mathrm{i,j,k,l}}+\omega_{\mathrm{i,j-1,k,l}}}{\Delta y^2}\right)\\&+\left(\frac{\omega_{\mathrm{i,j,k,l+1}}-2\omega_{\mathrm{i,j,k,l}}+\omega_{\mathrm{i,j,k-1,l}}}{\Delta z^2}\right)\Bigg)+\Delta t\dot{V}\frac{\left(\omega_{\mathrm{in}}-\omega_{\mathrm{i,j,k,l}}\right)}{\left(V_{\mathrm{chamber}}+\Delta t\dot{V}\right)}\end{aligned} \tag{16}$$

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

$$\frac{d\omega}{dx}=\frac{d\omega}{dy}=\frac{d\omega}{dz}=0. \tag{17}$$

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

$$\omega_{\mathrm{i,j,k,l+1}}=\omega_{\mathrm{i,j,k,l}}. \tag{18}$$

Afterward, based on ω-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)

$$m=\frac{pVM}{RT}, \tag{19}$$

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)

$$\omega=\frac{M_{\mathrm{w}}p_{\mathrm{w}}}{M_{\mathrm{a}}p_{\mathrm{a}}}, \tag{20}$$

where p_w is the water vapor pressure (Pa), pa 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

$$p_a = p - p_w, \tag{21}$$

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)

$$\omega = 0.629 \frac{p_w}{p - p_w}. \tag{22}$$

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

$$RH = \frac{p_w}{p_{sat}}, \tag{23}$$

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

$$p_{sat} = \frac{\left(1.0007 \quad .46\times10^{-6}\times1013.250\right)\times6.1121\exp\left(\frac{17502T}{240.97+}\right)\times1.01\times10^{5}}{1013.250} \tag{24}$$

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

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

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)

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

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.

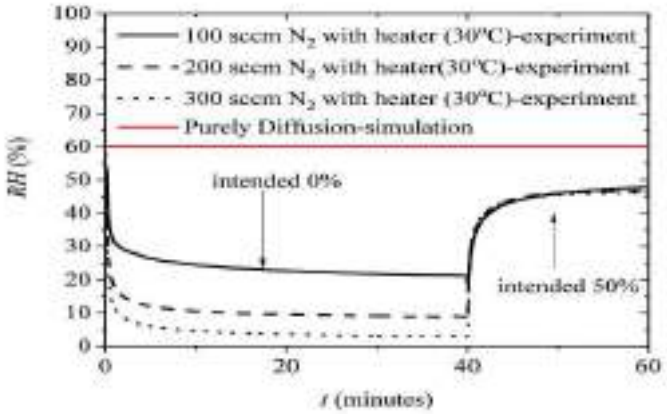


Figure 5. Simulation of pure diffusion versus experiment [1]

If it is only convection, then Equation (16) can be reformed as given in Equation (27) and shown in figure 6.

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

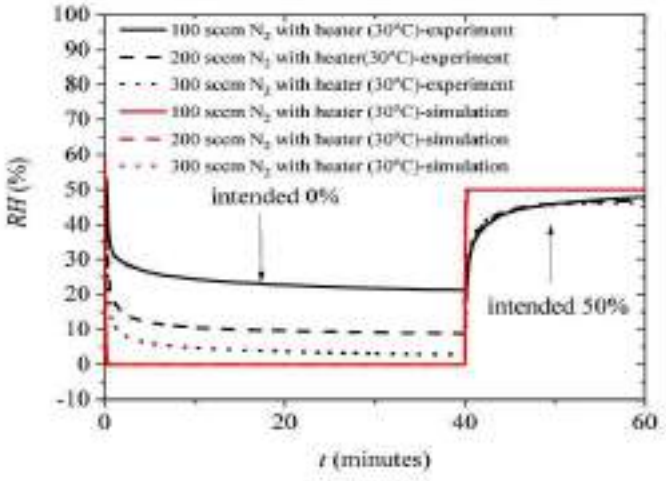


Figure 6. Simulation of pure convection versus experiment [1]

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 variated. It is obtained because the process is very fast.

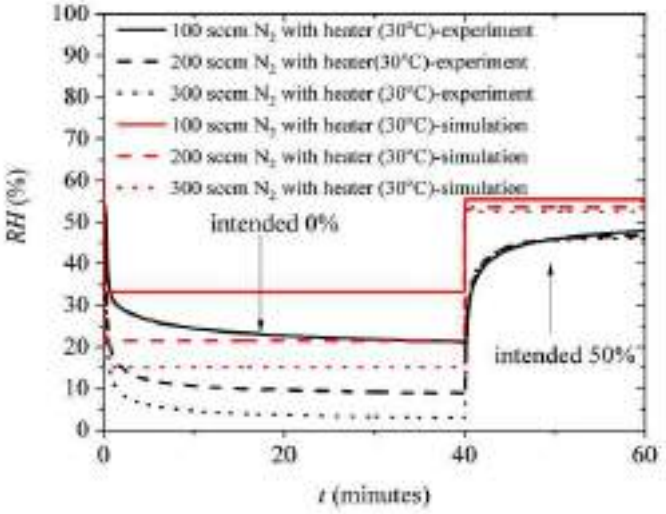


Figure 7. Simulation of diffusion-convection versus experiment [1]

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*.

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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.