CFD Investigation of Volatile Organic Compound (VOC) Emission from Building Material

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ABSTRACT

Volatile Organic Compounds or better known as VOCs are chemical emission from variety of sources such as paint, building materials, furnishes and adhesives. This paper focus more on the emission of VOC from wall paint with the aim of finding out the particle concentration and the effect of force ventilation to the particle concentration over time while also finding the effect of the layer thickness of paint to the concentration. Particle concentration of VOC is obtained as CFD simulation by using ANSYS software with a K-Ɛ turbulence model as the visual of velocity streamline and contour can be seen. The geometry of this simulation is a standard room where window and ceiling fan is present as outlet and inlet respectively. The results show that natural ventilation will decrease the VOCs emission over time but will take usually more than 8 hours to decrease to acceptable level. Forced ventilation was shorten the time period for VOCs emission to decrease to acceptable level. It has been found that paint layer thickness also affects the amount of VOCs emission concentration as thicker paint layer emits more VOCs than thin layer. A newly painted wall should be expose to a forced ventilation to decrease the VOCs concentration at shorter period of time so that it will not affects the building occupants.

Keywords: *CFD; VOCs; Ventilation; Paint*

Introduction

Volatile Organic Compound or better known as VOC emission is a type of emission that emit from variety of sources that exist in a closed space such as furniture, building materials, coating materials and varnishes [1][2][3]. It has become a major concern as people spend most of their time inside a building

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and this emission can cause adverse effects to health and wellbeing of building occupants [4][5]. A thorough study has been conducted in the past albeit mostly were set in cooler climate countries rather than countries in the equatorial climate [6] and the ventilation rate is much lower in cooler countries. Home is where people would want to be comfortable and spend most of their time but the presence of VOC that affects the wellbeing of tenants would prevent them for being comfortable. Such signs cause by the presence of VOC includes headache, irritating mucous membrane and overall drop of indoor air quality[7]. This paper is focusing on the emission of VOC from paint as it is always present in every house as people would use it to decorate their wall. The aim is to determine the VOC concentration in a forced ventilation room under four different cases and the concentration level at breathing height and bed height inside the indoor environment. Table 1 below would take a closer look at previous studies regarding VOC emission.

Most studies about measuring VOC emission that had been conducted in the past few years [13] comes from variety of sources and the sources are usually cramped in together in a closed indoor space. Some countries such as USA, Germany and Japan among others even set up guidelines and promoting programs to help people to reduce VOCs exposure in their indoor environments [14]. Further understanding of the behaviour of such emission are needed in order to really limiting the concentration and adverse health effects that would come together from the VOC. This study was run using CFD simulation on ANSYS FLUENT 2021 R1 where toluene is selected as the main emission from painted wall with the existence of forced ventilation in a standard bedroom.

Table 1: Recent research studies of VOC emission based on simulation and experiment

VOC	System Parameters	System Performance	Remarks	Reference
Toluene	Mass flowrate = 0.002525kg/s Temperature = 298 K Inlet velocity = 1 m/s	Concentration ranging from 30 – 70 kg/m^3 depending on cases and velocity condition Time = 3600 s	CFD simulation using Ansys Fluent	[8]
Toluene, Chlorobenzene, Ethylbenzene,	Coating thickness ranging from 5.2, 69.9 and 107.3 µm.	Emission rate for toluene ranging from 39.9, 66.7 and 156.1 mg/m^2/h	Experimental procedure	[9]

	Temperature = 25 °C Air Velocity = 10.0 ± 5.0 cms^{-1}	for 5.2, 69.9 and 107.3 μm respectively. Elapsed time = 100 min		
Decane	(Small-scale chamber case) Max Velocity = 0.15m/s Air exchange rate = 1 ACH Full-scale chamber case air exchange rate = 5 and 9 ACH Temperature = 23.5 ± 0.5 °C Inlet sizes are 0.00875 m, 0.015 m, 0.025 m for ACH = 1, 5, 9 respectively.	1. Emission characteristics from wet coating material may be affected by local airflow. 2. VOC emission dominated by evaporation at the start and internal diffusion afterward.	Chamber test experiment	[10]
Propane, Carbon Dioxide	(CFD) Kinematic diffusivities for Propane and Carbon Dioxide are 0.000012 m^2/s and 0.000016 m^2/s respectively Density: Propane = 1.8316 kg/m^3 CO_2 = 1.8080 kg/m^3 Air = 1.1800 kg/m^3 Timesteps = 1s (Experiment) Volume flow rate = 270-280 L/s Time = 60 min	CFD time period = 3200 s Concentration of VOC peak at 200 s, stabilize at 1800 s and start declining from 2000 s onwards. Average percentage difference between CFD and experiment for Propane is less than 10% while for CO_2 is between 10% to 20%	CFD simulation from Ansys CFX and experimental procedure	[11]

Xylene, 1,4-dimethylbenzene, 1,2-dimethylbenzene, 1,3-dimethylbenzene	Temperature = 20 °C Relative humidity = 44% Air flow rate = 0.7 m^3/h	CFD total timeflow = 6990 s Total xylene concentration dissipated at 4530 s but still remained at 6990 s Airflow in the workshop influence xylene diffusion	CFD simulation	[12]

Methodology

The CFD simulation was run using Ansys Fluent 2021 R1 software where the geometry was set up in the DesignModeler of the software. The geometry is a standard bedroom with dimension of 4.5 m length x 3.6 m width x 3.2 m height. Shown in Fig. 1 is the isometric view of the geometry and the inlet (1) and outlet position (2) of Case 1. The length and height of the outlet window is 1.6 m and 1 m respectively.

The surrounding wall is set as the mass-flow-inlet where it acts as the painted wall where Toluene will be emits to the indoor surrounding. The Toluene will start to emit from the start of the calculation and time will be taken to view when the emission start to stabilize. The stabilize value is viewed as the maximum value the emission can reach under the condition of forced ventilation inside the room. One consideration was made when deciding on the factors that could affect the simulation such as substrate considered to be impermeable to VOC from the paint as this could troublesome the simulation. The consideration was applied to simplifying the whole simulation based on the view of J. Xiong et al. [15]. Furthermore, this paper would not depend on the diffusion coefficient of VOC concentration as it will provide major difficulties to the simulation. Chang et al. [16] considered the diffusion as constant and the assumption was accepted by some researchers.

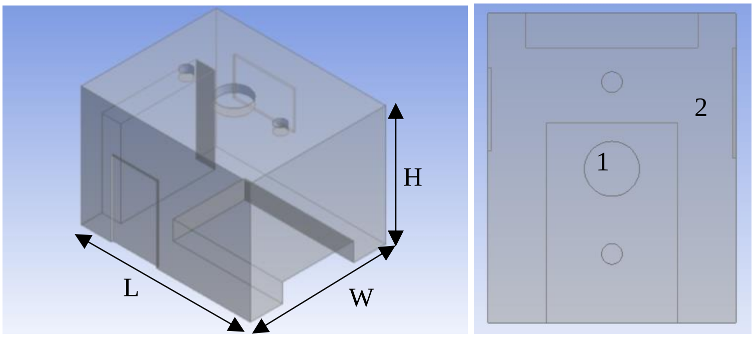

Figure 1: The schematic diagram of the geometry along with the position of (1) velocity inlet and (2) pressure outlet (Case 1)

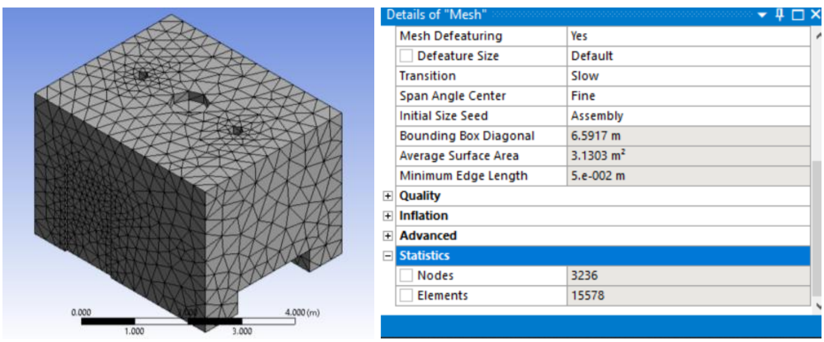

Figure 2: Mesh geometry details

The mesh of the geometry is done directly under the mesh setup of fluent. The transition and span angle center is set as slow and fine respectively. One main different between this paper and past research is that the mesh from previous studies was set in fluent meshing where detailed and much more refine mesh can be made. This mesh have 3236 nodes and 15578 elements. Detailed mesh would provide much more accurate result but would take longer time to simulate thus the limitation of time was also considered in taking the decision of making the current mesh.

The CFD is set as a transient simulation with gravitational acceleration acting in the opposite Y direction. The models for this simulation use energy equation, standard k-Ɛ model with standard wall function and species transport with Toluene-air chosen as the mixture material

Boundary Condition, model parameters and other settings

The boundary conditions are important setup to make sure the CFD simulation running smoothly. Velocity inlet, mass flow inlet and pressure outlet are set as the fan_inlet, painted_wall and window_outlet respectively. The mass flow rate of air is 0.002525 kg/s [8] in which Toluene mass fractions is describe with value of 1 while the velocity is valued at 1 m/s based on the same reference article. The recommended inlet turbulence is set as default on Ansys Fluent at “Medium (Intensity = 5%)” and the viscosity ratio is 10. The temperature for both inlets is 24.85 °C [8] while the pressure outlet is default at 30 °C.

The CFD simulations were performed with target for residual set at 10^{-4} with time step size began at low value of 0.0015 to stabilize the calculation before increasing after every 1000 time steps to reach the targeted time of 600 s.This paper conducted the CFD simulation through 4 different cases where some parameters were change to get the desired result. The different cases are explain in the Table 2 below.

Table 2: Simulation Cases

Cases	Velocity (m/s)	Outlet
1	1	Window
2	0.25	Window
3	1	Door
4	1	Window & Door

The aim is to see the different VOC concentration level for each cases with regards to normal tenant behaviour in the indoor environment. This also would help in the decision making of tenant regarding on whether just by opening the window would be enough to decrease the concentration level or should the door be open to achieve optimum level of concentration.

Mathematical Modelling

The governing equation use in the ANSYS FLUENT software are summarized in the Table 3 below:

Table 3: Governing equations use in ANSYS FLUENT software

Equation Name	Mathematical Equation
Continuity Equation	$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$ (1) $u_i = \bar{u}_i + u'_i$ (2) Where $\bar{u}_i$ and u'_i are the instantaneous fluctuate of velocity components
Momentum Equation	$\frac{\partial p}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_l}{\partial x_l}\right)\right] + \frac{\partial}{\partial x_j}(-\rho \overline{u'_i \bar{u}_j})$ (3) where μ is the dynamic viscosity of air
Turbulent kinetic energy and dissipation equations	$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right] + G_k - \rho\varepsilon$ (4) $\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial \varepsilon}{\partial x_i}\right] + G_{1_\varepsilon}\frac{\varepsilon}{k}G_k - C_{2_\varepsilon}\rho\frac{\varepsilon^2}{k}$ (5) where $\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$ (6) $G_k = -\rho\overline{u'_i u'_j}\frac{\partial u_j}{\partial x_i}$ (7) The values of model constant $C_{1_\varepsilon}, C_{2_\varepsilon}, C_\mu$ is as follows [16] $C_{1_\varepsilon} = 1.44, C_{2_\varepsilon} = 1.92, C_\mu = 0.09$
Mass Conservation Equation	$\frac{\partial}{\partial t}(\rho m) + \frac{\partial}{\partial x_i}(\rho u_i m) = -\frac{\partial}{\partial x_i}J_i$ (8) m = local mass fraction J_i = diffusion flux of toluene in air $J_i = -\left(\rho D_m + \frac{\mu_t}{S_{c_t}}\right)\frac{\partial m}{\partial x_i}$ (9) S_{c_t} = Turbulent Schmidt Number

Result and Discussion

Figure 3 illustrates the CFD simulation results of four mentioned cases inside the forced ventilated indoor environment. The blue, yellow, orange and grey line represents case 1, 2, 3 and 4 respectively. As mention before, the main case which is Case 1 where the velocity is set at 1m/s with pressure outlet set at the window. From the graph, the pattern for each cases are consistent where the emission rises up to around 50 s to 70 s mark before it starts to consistently emits until 600 s mark. This is because the simulation does not consider the dry effect acting onto the paint where the emission off-gassing rate will eventually decrease and disappear after a very long time [15][16][17] since the time taken to run the CFD simulation up to 700 s is two days. The emission started at 1.145596 kg/m^3 since the paint is already on the wall and no painting process took place like usually found in past researches. These results were obtained by setting up point of interest in the centre of the room on FLUENT thus explain as to why Case 1 where velocity is 1 m/s has a little higher amount of concentration compared to Case 2 where the velocity is 0.25 m/s. The emission is carried over by the air velocity thus the amount of concentration directly below the air velocity of Case 1 is higher than Case 2 albeit by not too much. This shows that low value of velocity can not carry out most of the emission from the wall. For Case 3 and 4, the outlet position is change to door and window plus door respectively. The difference in concentration between setting the window as outlet and door as the outlet is quite big. This is due to the door having higher area compared to the window. Case 4 having the lowest amount of concentration is expected due to having two outlets compare to other three cases. The curve trend is validated with other study as it follows the same pattern which is a sharp increase during early emission before it became constant emission after certain time [8].

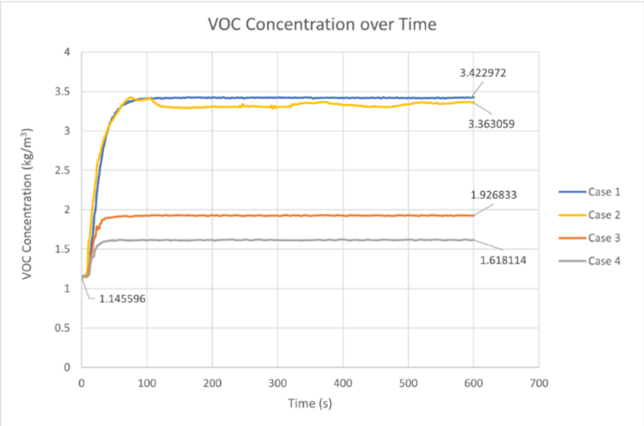

Figure 3: Result of VOC Concentration over Time

Below is the density volume rendering of the bedroom. It can be seen that the least amount of VOC concentration are situated in the centre of the room and at the top near the velocity inlet. This shows that the VOC emission is being carried away by air velocity coming from the inlet. One worthy note is that the value of 1 m/s is not strong enough to really carry away all the emission as 2/3 of the room volume has high amount of VOC concentration with the maximum value of 3.422972 kg/m^3 coming near the bottom of the room. The airflow velocity is important in the resulting concentration as concentration should have decrease due to effect of airflow over time [11] and because of the high concentration of VOC near the bottom of the room, airflow from inlet might have not reach to the bottom thus fail to decrease the concentration. Local recirculation and existence of stagnant air could also cause the high concentration at the bottom of the bedroom thus highlighting the importance of inlet air location [18]. Since there is no obstacle preventing the direct airflow from the inlet then velocity value, local recirculation and stagnant air could be some of the reasons for the high concentration.

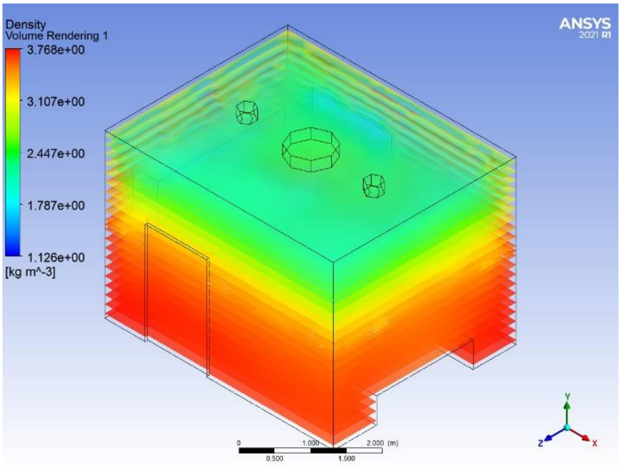

Figure 4: Density Volume Rendering of Geometry

Figure 5 is showing results for VOC concentration across the room at breathing line level of 1.6 m considering the standard of most Malaysian's height. Top left is the result for Case 1, top right is Case 2, bottom left is Case 3 and bottom right is for Case 4. The centre of the room was set at 0 or the origin of axis meaning the the value 2.5 m moves to the right of the room where the bed is located while -2 m moves to the left of the room where it ended on the surface of the cupboard. The fan inlet location is located in between -1 m to 0 m thus showing why on all the four charts that the concentration has the same decrease pattern at around the fan inlet location. Case 4 showing an increase of concentration around the fan inlet location albeit still lesser than most cases. This is because only Case 4 that is using both window and door as outlets thus the airflow from inlet and air turbulence would be different than most cases thus showing generally low VOC concentration on breathing line. Airflow direction and turbulence also shows why Case 1 and 2 have the same pattern throughout the room as the only changes made is on the velocity value while Case 3 and 4 have quite the same pattern due to outlet parameter changes. Case 3 and 4 shows a massive drop in concentration early in the chart are due to the location of door outlet near the left side of the room as both cases has door which is bigger in area compare to window as the outlet.

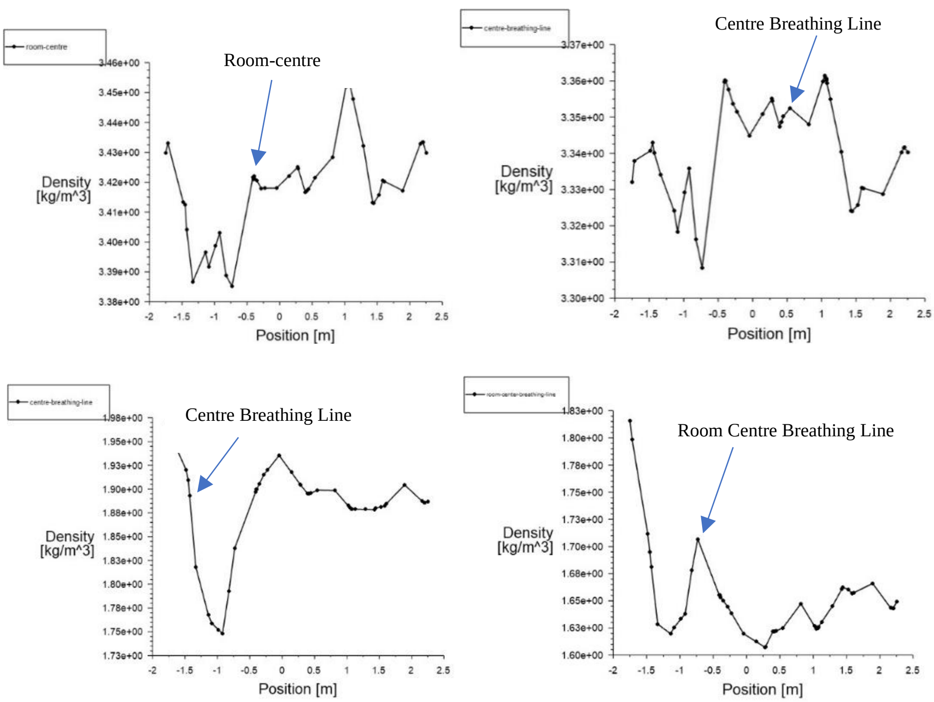

Figure 5: Breathing Line Concentration of Case 1 (Top Left), Case 2 (Top Right), Case 3 (Bottom Left) and Case 4 (Bottom Right)

Below is the illustration of VOC concentration across the bed length and height. This position is taken into account to find out what is the concentration of the VOC when tenant would lied down onto the bed. With the positioning of the chart and cases the same as Figure 5, it can be seen that Case 1 and 2 has the same concentration pattern across the bed while Case 3 and 4 illustrate a sharp rise in concentration between position 1m to 2m but still generally lesser than result shown for Case 1 and 2. This shows that the surface area of outlet plays important role in determining the concentration emission across the room in general. The result pattern also shows that as the location moves further away from the fan inlet, the VOC concentration will start to increase as it moves closer to the source which is the painted wall. As mentioned for Figure 4, near the bottom of the bedroom is where recirculation and stagnant air exist thus explain why the concentration level is higher compare to breathing line level. The bed level also moves further away from the fan inlet in y-direction.

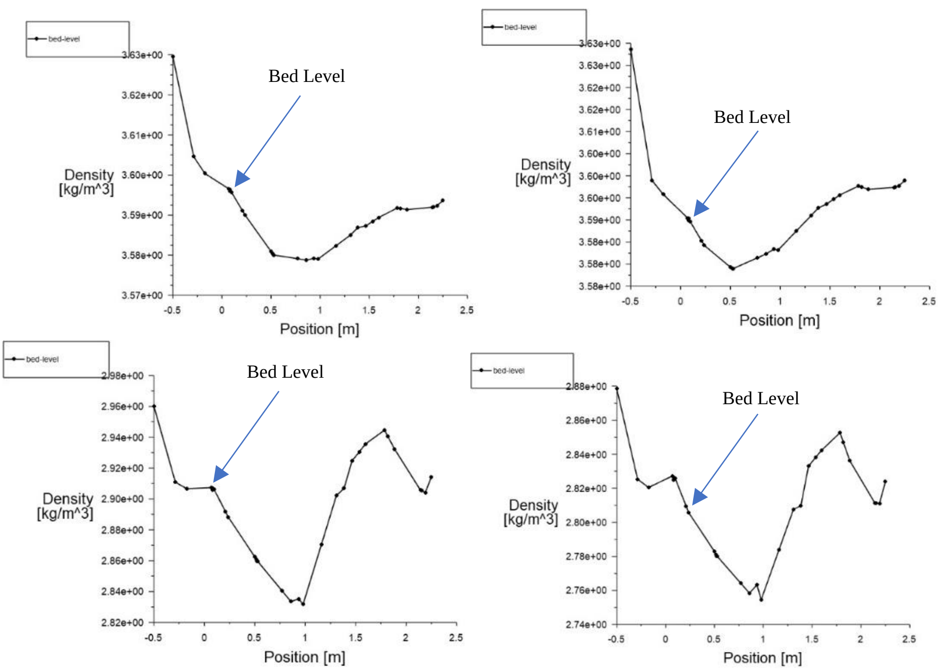

Figure 6: Bed Level of VOC Concentration of Case 1 (Top Left), Case 2 (Top Right), Case 3 (Bottom Left) and Case 4 (Bottom Right)

Figure 7 shows the concentration contour at bed level (top) and breathing line level of 1.6 m (bottom) for the main case which is Case 1 where it can be seen that for the bed level, the concentration level drop down from position -0.5 m based on the chart to position 1 m before rising slightly as the position moves near to the painted wall. The concentration at level breathing line is lesser than bed level due to being close to the fan inlet in term of y-direction thus the airflow velocity could reach and carry away the concentration bringing it down as a result. The figure below is graphic explanations of the concentration behaviour illustrates on the line chart from figure 6.

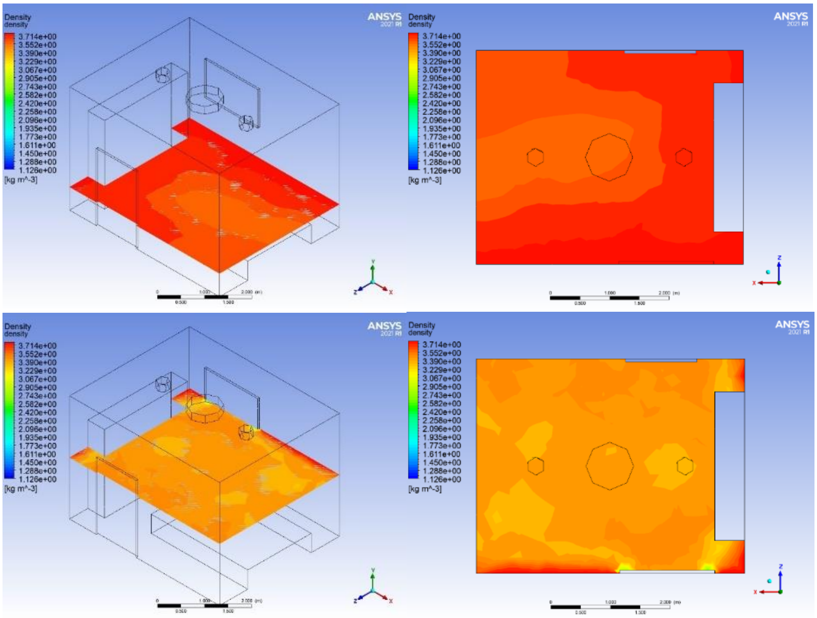

Figure 7: Concentration Contour of Case 1 at Bed Level (top) and Breathing Line Level (bottom)

Conclusion

Overall, the objectives for this paper which are to find the concentration of VOC in forced ventilation room under four different cases and the VOC concentration at breathing height and bed height has been achieved and discussed. The simulation is run through ANSYS FLUENT 2021 R1 and result is compared with past researches. The pattern of the result follows exactly as previous research in terms of concentration emission and concentration position. The CFD simulation validated the obtained result as past researches show that most emission would rise in the first hours of the experiment and would take longer time to finally decrease, something that is limited as personal computer capacity is insufficient to run complex setting of the simulation.

Recommendation

For future recommendation, some of the ways to improve result accuracy can be made by using different approach such as below:

- Make a geometry with no obstructions inside the indoor environment to obtain result throughout the geometry.
- Use high performance laptop/computer to run the calculation so that bigger time step size can be use to get faster result of time more than 1 hour and to prevent crash during calculation.
- Types of VOC to be compare with toluene behaviour.
- Different inlet location to get better VOC positioning chart.

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