CHEMICAL ENGINEERING TRANSACTIONS
VOL. 106, 2023

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Jeng Shiun Lim, Nor Alafiza Yunus, Peck Loo Kiew, Hon Huin Chin

ISBN 979-12-81206-05-2; **ISSN** 2283-9216
DOI: 10.3303/CET23106085

Simulation of Benzene Leakage and Dispersion in the Laboratory via Computational Fluid Dynamics

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This study investigates the internal conditions of laboratory and effectiveness of ventilation system with evaporation of benzene from a hypothetical accident by using a computational fluid dynamic program. There are five inlets which moist air enter and exits through four vent hoods connecting with the exhaust fan was placed on the ceiling. The species model and the realizable k-ε turbulence model with standard wall function are used to investigate the effects of turbulence. The benzene leakage source in laboratory was modelled as vapour phase with natural evaporation rate and the ventilation system was set up with different modes such as 1,000 m^3/h, 2,000 m^3/h, 3,000 m^3/h, and 4,000 m^3/h. The objective of this research is to investigate chemical leakage and dispersion in indoor environments and consider the performance of ventilation system of different exhaust fan modes and various layout designs (single-inlet or multi-inlets). Based on the analysis of air flow patterns and the distribution of pollutant concentrations, the performance of the ventilation system is evaluated and appropriate solutions are proposed to manage the problem. The results show that in both cases of opening all doors and opening only doors, the ventilation rate of 3,000 m^3/h is considered to be the most effective in terms of pollutant removal because the benzene concentration meets the safety standard (< 10 ppm), namely 4.6 ppm in the multi-inlets and 2.8 ppm in the single-inlet.

1. Introduction

Chemical exposure remains a significant concern for laboratory personnel, especially those who work directly with chemicals (Ustolin et al., 2021). Both direct and indirect exposure have a high likelihood of leading to serious diseases, including cancer, leukemia, and brain tumors (Liu et al., 2017). In order to ensure safety in the laboratory, ventilation and laboratory layout not only play an important role in creating a healthy working environment, but also ensure the safety and health of workers.In order to advance research in process safety, experimental and quantitative studies are essential for understanding the underlying mechanisms. Conducting experimental research can be resource-intensive due to the large number of tests required for evaluation, especially when it comes to conducting dangerous leakage tests. To overcome this barrier, many studies have focused on the evaluation of ventilation systems and the diffusion of toxic organic solvents by simulation to assess the overall safety of the process (Jin et al., 2012). Numerous studies have focused on ventilation and employed simulations to assess ventilation performance, particularly investigating the impact of air changes per hour (ACH). Jin et al. (2012) examined the relationship between ACH and laboratory air quality, demonstrating that ACH values ranging from 8 to 12 effectively controlled the release of organic solvents. Jiao et al. (2019) evaluated the efficiency of air supply equipment and exhaust systems to determine their overall effectiveness. Dong et al. (2017) indicated that various factors, such as ventilation efficiency, ventilation equipment, and the arrangement of open or closed exhaust fans, influence the diffusion of solvents in the air. During the COVID-19 pandemic, a number of simulation studies to improve indoor air quality were also performed similarly, predicting and evaluating the dispersion direction, concentration of chemical vapour or the direction of diffusion of chemicals. Liquid droplets containing the covid-19 virus are extensively studied (Tran et al., 2023).

Paper Received: 14 June 2023; Revised: 11 August 2023; Accepted: 28 August 2023
Please cite this article as: Duong Y.H., Dang N.T., Le T.M., Le D.T., Le K.N., Nguyen D.K., Tran V.T., 2023, Simulation of Benzene Leakage and Dispersion in the Laboratory via Computational Fluid Dynamics, Chemical Engineering Transactions, 106, 505-510 DOI:10.3303/CET23106085

This not only shows the concern about air quality in living, studying and working environment but also raising safety standards, towards sustainable socio-economic development.
Computational Fluid Dynamics (CFD) software is a commonly used method for simulating and evaluating indoor environments, as demonstrated in numerous studies (Wang et al., 2020). In this study, CFD was used to analyse the efficiency of ventilation systems in a laboratory environment assuming the presence of the harmful organic solvent benzene. According to Threshold limit values (TLVs) standards, benzene concentrations below 10 ppm are safe standards. The objective of the study is to evaluate the ventilation efficiency of different design layouts to investigate benzene concentrations at exhaust fan ventilation levels. Two separate ventilation profiles with different ventilation rates were proposed for evaluation.

2. Materials and methods

2.1 Experimental setup

The laboratory used in this study is based on organic chemistry laboratory 403 in B2 building at Ho Chi Minh City University of Technology. The dimensions of the room are as follows: a height of 3.05 m, a length of 9.6 m, and a width of 8 m, resulting in a floor area of 76.8 m^2. There are 5 inlets which moist air enters and exits through 4 vent hoods connecting with the exhaust fan was placed on the ceiling.

2.2 Modelling and analysis

2.2.1 Geometry model and meshing

Figure 1 illustrates the geometric model and grid domain of the laboratory. The meshing was performed independently, using three different mesh quality levels: coarse, medium and fine. Poly-hexcore meshing method is used, which showed a reduction in the number of cells and bringing a faster overall solution time. The coarse mesh consisted of 303,311 nodes, the medium mesh contained 600,991 nodes, and the fine mesh comprised 1,190,903 nodes.

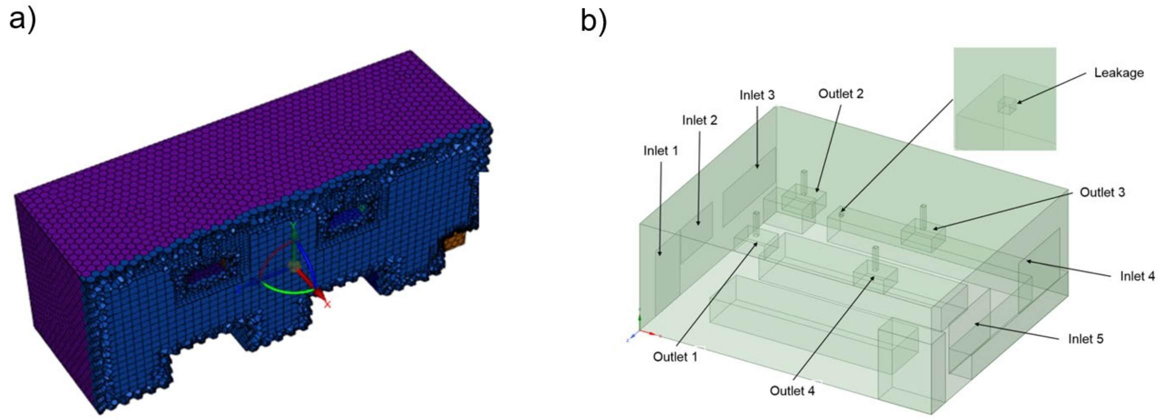

Figure 1: (a) Mesh model and (b) Geometric domain of the laboratory

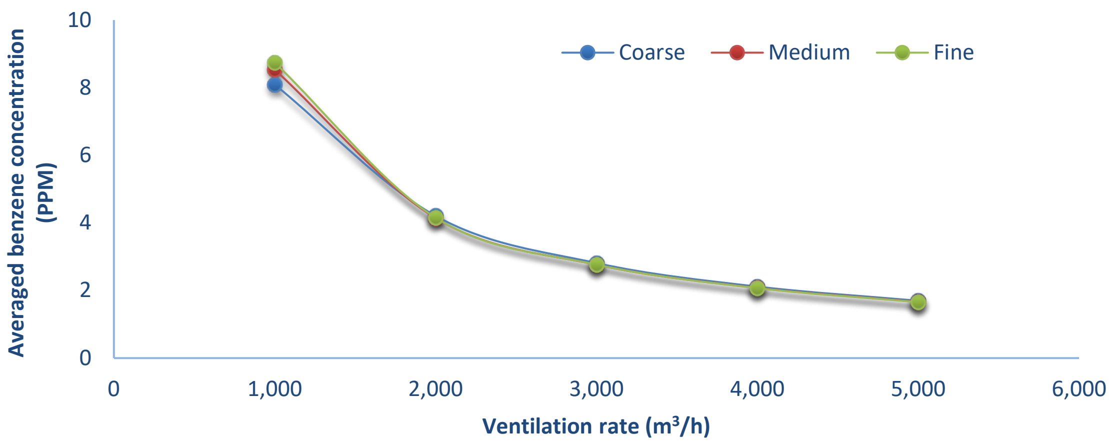

Figure 2: The average benzene concentration in three quality of mesh levels

To ensure the reliability and accuracy of the simulation results, the grid independence is assessed by solving the average benzene concentration in the laboratory as shown in Figure 2. Considering the computational accuracy and cost, the medium grid is selected as the most appropriate.

2.2.2 Turbulent model

In this case, the flow was characterized as unstable and turbulent, primarily caused by the significantly high flow rates in the field. To address this turbulence, the realizable turbulence model k-ε was employed, which is built upon the transport equations for turbulent kinetic energy (k) and its dissipation rate (ε). The Boussinesq model had been applied to treat density as a constant value in all equation.

2.2.3 Species transport

This model represents air as a mixture of dry air, water vapour and benzene vapour. Benzene release from beaker was considered as vapour phase. When choosing to preserve the equation for chemical components, the software will predict the local mass fraction of each substance (Yi) by solving the convective diffusion equation for the i^{th} substance in the mixture.

2.2.4 Boundary conditions

In this study, the laboratory was assumed in the absence of people, set up at natural ventilation conditions with the exhaust fan. Benzene was set up at vapour phase at initial and natural evaporation in steady state. In this study, thermal transfer is not considered. All details are indicated in Table 1.

Table 1: Boundary conditions

Boundary conditions	Type	Value
Chemical leakage	Mass flow rate	0.025 [g/s]
Inlet 1	Pressure	1 [atm]
Inlet 2	Pressure	1 [atm]
Inlet 3	Pressure	1 [atm]
Inlet 4	Pressure	1 [atm]
Inlet 5	Pressure	1 [atm]
Case 1: Outlet 1, 2, 3, 4	Velocity	1,000 [m^3/h]
Case 2: Outlet 1, 2, 3, 4	Velocity	2,000 [m^3/h]
Case 3: Outlet 1, 2, 3, 4	Velocity	3,000 [m^3/h]
Case 4: Outlet 1, 2, 3, 4	Velocity	4,000 [m^3/h]

3. Result analysis and discussion

3.1 Air velocity in single – inlet and multi – inlet cases

Figure 3 shows the results of the intensity of air velocity in the laboratory in two cases with only one door open (single-inlet) and all door and windows open (multi-inlets). The results are taken at the XZ plane, with the corresponding different heights of 0.2 m, 0.4 m, 1.47 m and 2.29 m, respectively. The results indicate that the velocity near the inlet and outlet areas is higher than elsewhere, with the highest velocity observed at the exhaust surface, where it matches the ventilation rate (0.35 m/s at case 1,000 m^3/h). Notably, the velocity magnitude varies significantly based on local positions. Some areas exhibit high velocity levels, while other areas far from the exhaust duct have very low values (ranging from 0 m/s to 0.1 m/s at case 1,000 m^3/h). It appears that the ventilation rate has a considerable impact on the velocity magnitude in windless laboratory environments.

When all the windows are closed, the velocity of the airflow originates primarily from the entrance door and maintains a relatively constant magnitude, typically ranging from 0.2 m/s to 0.35 m/s (in the case of a ventilation rate of 1,000 m^3/h). This velocity is significantly higher compared to the scenario where all windows are open. The horizontal section velocity contour at a height of 1.47 m indicates that the inflow velocity is better developed in comparison to the case with open windows (as depicted by the orange region). At higher positions, such as 2.29 m, the airflow entering the room continues to circulate within the range of 0.1 m/s to 0.2 m/s (represented by a combination of light green and light blue colours).

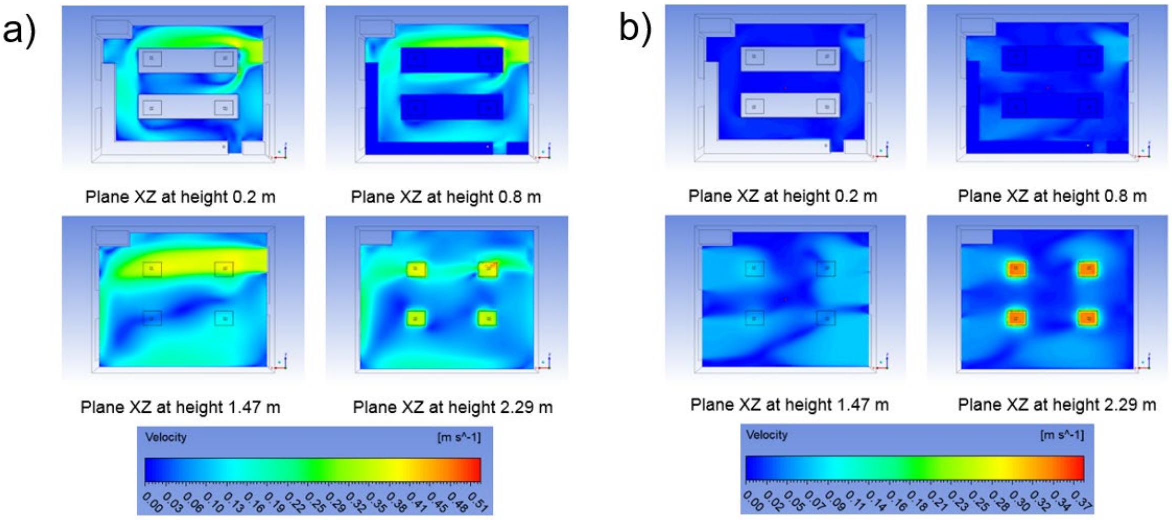

Figure 3: (a) The air velocity distribution at single – inlet and (b) The air velocity distribution at multi – inlets of the laboratory at XZ plane

3.2 Concentration distribution of benzene in single – inlet and multi – inlet cases

According to Figure 4, the presence of a blue region near the inlets indicates the influx of fresh air from the outside, which fills the room and displaces the indoor air. Despite the fact that the average concentration of benzene in cases where the airflow rates were set at 2,000 m^3/h, 3,000 m^3/h, and 4,000 m^3/h remained below 10 parts per million (ppm), certain locations still exceeded this threshold. For instance, in case 4, the average benzene concentration was approximately 2.8 ppm, but the areas near the source release and outlet 2 were depicted in red (indicating concentrations over 10 ppm), surpassing the safety threshold.

It shows that the amount of benzene is widely and strongly dispersed, leading to the benzene content being widely distributed, reducing the concentration in different areas. The concentration of benzene exists below the threshold 10 ppm completely in case 4,000 m^3/h.

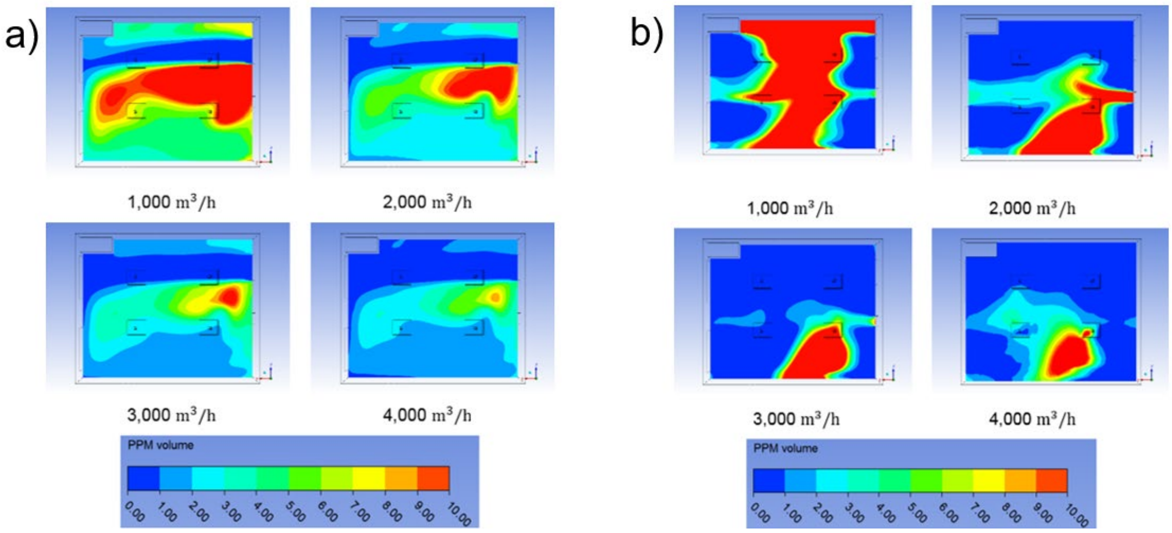

Figure 4: (a) The benzene concentration distribution at single – inlet and (b) The benzene concentration distribution at multi – inlets of the laboratory at XZ plane

3.3 Benzene concentration compared between two cases

The notable difference of benzene concentration between 2 cases is illustrated in Figure 5. Mostly, case open only door achieve better efficiency in terms of ventilation. In the 1,000 m^3/h and 2,000 m^3/h modes, the mean

benzene concentrations accounted for 26 ppm and 10 ppm in the all-open case, while in the other modes it is 8.5 ppm and 4.1 ppm. As the ventilation rate increases, the difference in benzene concentration between both cases becomes less pronounced. In the case of 3,000 m^3/h, when a higher ventilation rate is used, the average benzene concentration fell below the hazardous threshold, recording values of 4.6 ppm and 2.8 ppm. Based on these results, it was found that the safety threshold for benzene concentration was met in both the 2,000 m^3/h and 3,000 m^3/h regimens, with the 3,000 m^3/h mode showing better safety outcomes. Increasing the ventilation flow resulted in lower benzene concentrations, and beyond the 4,000 m^3/h and 5,000 m^3/h thresholds, the benzene concentration in these two levels of ventilation does not differ significantly.
The permissible threshold for benzene concentration, as per TLV-TWA standards (<10 ppm), is utilized as the safety criterion. The laboratory actual volume is measured at 268.8 m^3. At 2,000 m^3/h, the ACH value is 7, which remains within the safe threshold. The CFD simulations demonstrate that both the 2,000 m^3/h and 3,000 m^3/h scenarios maintain benzene concentrations below the permissible limit. At the higher flow rate of 3,000 m^3/h, the concentration threshold exhibits a more substantial decrease in both cases. The attained ACH at 3,000 m^3/h is 11, which falls within the recommended range of 8-12 for effective organic solvent removal while optimizing operational costs (Jin et al., 2012). Based on these results, the selection of the 3,000 m^3/h flow rate appropriates for the intended application.

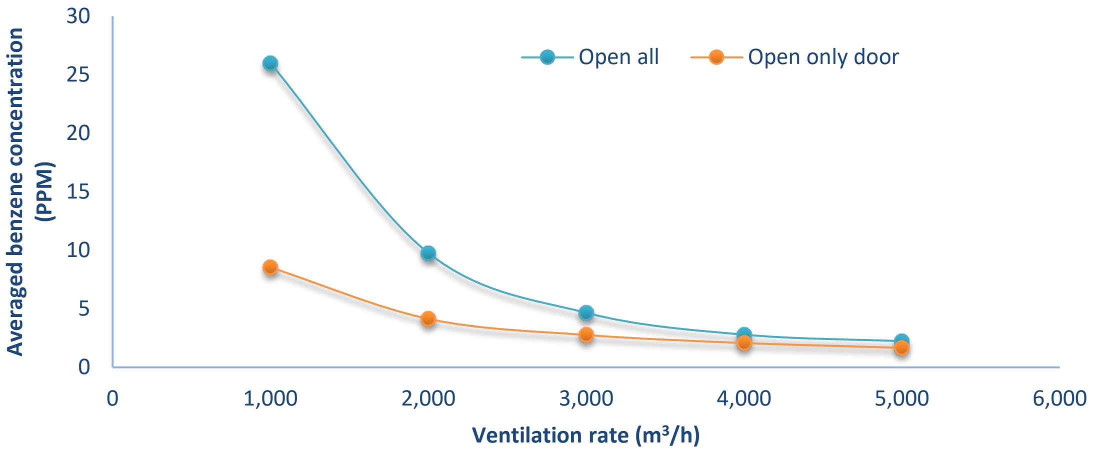

Figure 5: The comparison of the averaged benzene concentration in two cases open all and open only door

The results of benzene distribution in the laboratory environment are presented in Figure 6, at the cross-sectional position Y = 0.2 m from the floor. The results indicate that at a ventilation rate of 1,000 m^3/h, there is a significant amount of red area, indicating high levels of benzene concentration (>10 ppm).

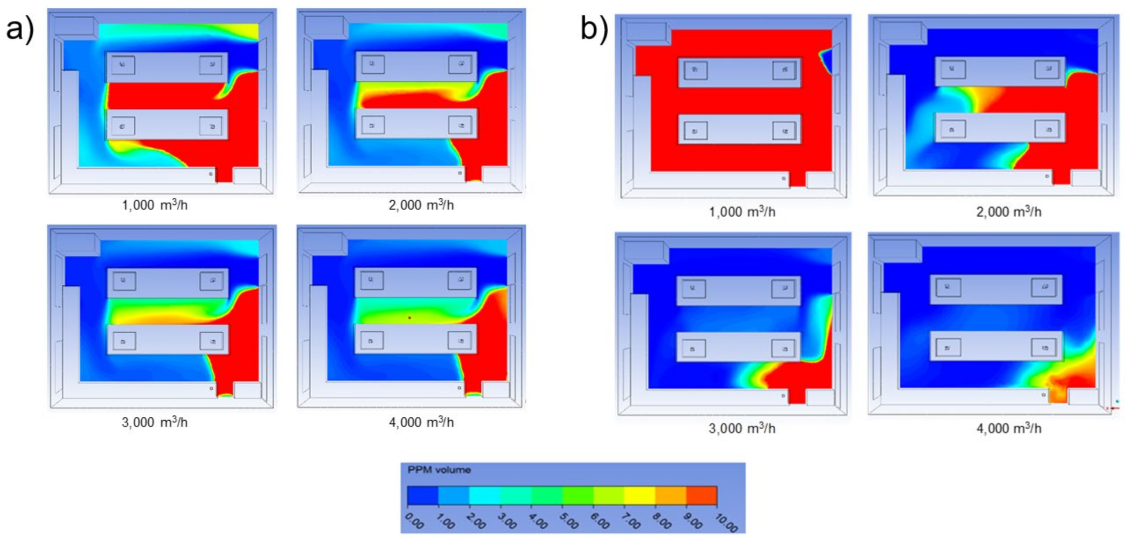

Figure 6: The comparison of the benzene distribution in two cases (a) single - inlet and (b) multi - inlets at the plane Y = 0.2 m

At a ventilation rate of 2,000 m^3/h, with both cases open all and open only door, the red area is significantly reduced but still occupies half of the room area from the emission source to the inlet. When the ventilation rate is further increased to 3,000 m^3/h and 4,000 m^3/h, the red zone persists but appears in a smaller area near the lower right corner compared to the previous cases. At 4,000 m^3/h, the red colour transitions to orange and light green, indicating lower contaminant concentrations. Comparing the cases, the distribution of benzene is better in open all at the modes 2,000 m^3/h, 3,000 m^3/h, and 4,000 m^3/h. The dispersion of benzene vapour is compacted at a corner, rather than spreading evenly as observed in the case of opening only door.
Overall, these findings suggest that increasing ventilation rates can significantly reduce the amount of benzene present in a laboratory setting. However, even at high ventilation rates, there may still be areas where benzene concentrations remain elevated. This highlights the importance of properly arranging ventilation and carefully considering the layout of the laboratory ventilation system.

4. Conclusions

Overall, the CFD simulation results indicate that both the multiple-inlets (open all) and single-inlet (open only door) cases achieve a safe standard concentration at steady-state conditions in the 3,000 m^3/h and 4,000 m^3/h modes. Concerning the distribution of benzene inside the laboratory, the results favour the multi-inlets case, which gives better results. Based on CFD simulation results, ventilation rates of 3,000 m^3/h and 4,000 m^3/h are the most effective for pollutant removal. The increasing the ventilation rate will increase operating costs, so corresponding to ACH in the range of 8-12, the mode of 3,000 m^3/h is appropriate. These findings suggest that although increasing ventilation rates could reduce benzene concentrations, there are limitations to its effectiveness. The average pollutant concentration could be reduced by increasing the ventilation rate, but the relationship between ventilation rate and pollutant reduction is not linear.
In general, optimizing ventilation arrangements and considering specific laboratory layouts are significant for contaminant removal. This CFD simulation study contributes to the importance of balancing energy consumption and pollution reduction, as a premise for further studies. The study contributes to an overview before the actual future ventilation system layout is developed, contributing a friendly working environment, minimizing costs incurred and towards sustainable development.

Acknowledgments

We acknowledge Ho Chi Minh City University of Technology (HCMUT), VNU-HCM for supporting this study.

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