

Performance Evaluation of 3D Equipment Model for Laboratory Fume Hoods

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Abstract

Chemical exposure is a significant concern in occupational health, especially for personnel working in chemical laboratories. Laboratory workers have potential exposures to numerous hazardous substances, which can threaten their health. The effects of chemical exposure can vary based on variables such as the type of chemical, its concentration, the duration and frequency of exposure, and the susceptibility of the individual. Current laboratory fume hoods encounter significant challenges due to their heavy reliance on outdated methods, such as simplified models and empirical data, to predict performance. This reliance results in substantial drawbacks that compromise the effectiveness and efficiency of these crucial safety devices and to propose and validate numerical simulation which can predict flow of fume hoods 3D ventilation equipment model and mesh using ANSYS 2023 R1. 3D model and mesh being setup and validation of data using tracer gas test, flow visualization and face velocity measured. For flow visualization, the constricted opening directs the airflow directly onto the front source, potentially increasing its capture efficiency compared to a completely open sash. The fume hood is deemed to be functioning satisfactorily if the detected concentration of the tracer gas outside the hood is lower than the permissible threshold which is below 0.2 mg/m³. Also, Operating the system at half opening increases the air velocity, which improves the likelihood of meeting the required face velocity. Finally, The models confirmed the results obtained from tracer gas and smoke tests and enabled detailed examination of complex airflow dynamics that are difficult to observe physically.

1. Introduction

Chemical exposure is a significant concern in occupational health, especially for personnel working in chemical laboratories. Laboratory workers have potential exposures to numerous hazardous substances, which can threaten their health. The effects of chemical exposure can vary based on variables such as the type of chemical, its concentration, the duration and frequency of exposure, and the susceptibility of the individual [1]. Current laboratory fume hoods encounter significant challenges due to their heavy reliance on outdated methods, such as simplified models and empirical data, to predict performance. This reliance results in substantial drawbacks that compromise the effectiveness and efficiency of these crucial safety devices.

Creating a three-dimensional model of ventilation equipment specifically designed for laboratory fume hoods. This entails developing a comprehensive and precise virtual representation of the ventilation apparatus,

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considering parameters such as measurements, airflow dynamics, and component configuration. In addition, the comparison of numerical simulations with experimental data or established benchmarks is conducted to verify the accuracy and dependability of the simulation model. Finally, evaluating the effectiveness of the laboratory fume hoods using verified numerical simulations

The ASHRAE 110-2016 method is the prevailing industry standard in the United States for measuring the airflow of fume hoods, this procedure involves positioning a mannequin equipped with particle detectors near a fume hood. Subsequently, a sulphur hexafluoride tracer gas is introduced into the environment using a gas ejector located 6 inches away from the front of the hood. ASHRAE specifies that the height at which the breathing zone test should be conducted is 22 inches, which corresponds to the typical height of fume hood operators in the USA. During the test, particle concentrations are monitored digitally using a mannequin. This standard provides a set of instructions to guarantee that an unoccupied fume hood is functioning correctly and not causing air to flow into the area where people are inhaling [2].

It can be concluded that varying sash position which is half sash and full opening sash will affect the face velocity as well the airflow and that the insights gained from this work will help researchers improve their laboratory air quality simply by controlling the reaction placement within the volume of a fume hood. As evidenced in computational fluid dynamics (CFD) calculations and demonstrated using artificial smoke, it is apparent that the airflow is greatly affected by the sash. The position is determined not only by the height of the reaction.

2. Materials and Methods

There are more details and explanations about how the simulation will be run from the start of the study to the end, when the results will be gathered. Ansys Fluent, which is CFD software, is used for the main modelling. In this study, The Realizable $k-\epsilon$ model and boundary conditions will be studied to predict the data from CFD simulation result. Generally, a fume hoods geometry will be generated by any geometry software such as SolidWorks. As the model is ready, it can be transported to Ansys software for CFD analysis.

2.1 Flowchart

Flowcharts provide a visual representation of a process or system, as shown in Fig. 1 *Flowchart of this study* from the idea generation to conclusion of this study.

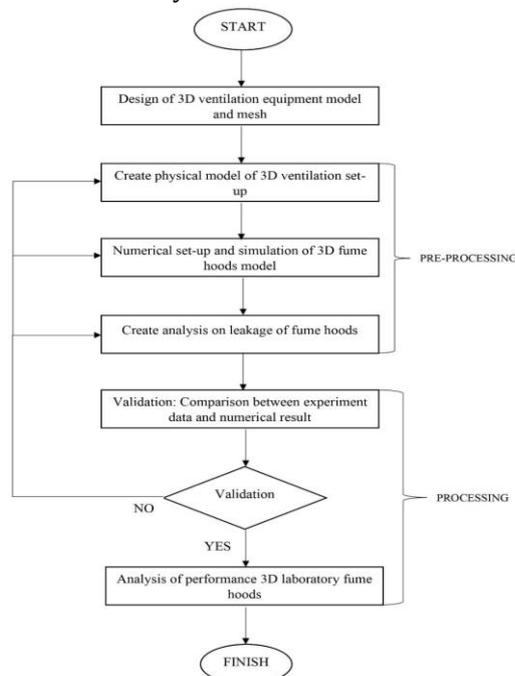


Fig. 1 Flowchart of this study

2.2 Simulation Setup

This simulation begins with a few steps which are geometry construction, meshing, setup, solution, and post result.

2.2.1 Geometry

Geometry is the first step in CFD simulation. In this project, the fume hoods model is drawn by using SolidWorks software. Based on the original parameter of fume hood labs in Nanosurf Laboratory FKMP, geometry is taken to construct the 3D model using SolidWorks software. The drawing file is saved as Parasolid Files (*.x_t, *.x_b). After finishing meshing the surface, the boundary condition must be identified before running the simulation.

2.2.2 Meshing

From this section, by dividing the solid geometry and the boundary condition into several elements of order called mesh. The process of obtaining an appropriate mesh or grid is termed meshed generation or grid generation. The good meshing construction will give a better solution and fast converging result for the simulation. The consideration of geometry also takes part in the meshing process.

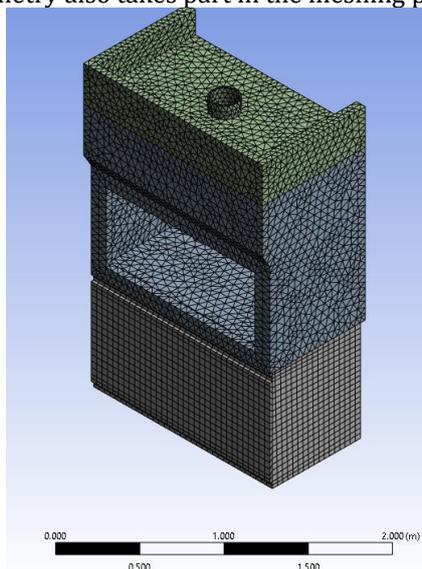


Fig. 2 Meshing of the Design

2.2.3 Numerical Model

The CFD method is employed by using a commercial CFD program, ANSYS Fluent 16.2, which solves the governing equations through a finite-volume procedure. The Realizable $k-\epsilon$ model provides the best performance of all the $k-\epsilon$ model versions for several validations of separated flows and flows with complex secondary flow features and the use of the model is recommended relative to other variants of the $k-\epsilon$ family.

Therefore, the Realizable $k-\epsilon$ model with the standard wall function is used to simulate the turbulent effect. The discretization scheme used for all variables except the pressure is second order up-wind to ensure the computational accuracy and the pressure is discretized by a staggered scheme named PRESTO [3]. Radiant heat transfer between different surfaces is calculated using the Discrete Ordinates model.

2.2.4 Boundary conditions

Returns have a pressure-outlet boundary condition, but the exhaust has inlet boundary condition with a negative number. This is done to make sure that the same amount of air is exhausted through the fume hood. The constant heat flow boundary condition is put on the surfaces of heat sources. The adiabatic boundary condition is put on the other surfaces.

2.3 Experimental Setup

The purpose of the fume hood smoke plume experiments was to generate easily distinguishable and information-rich data. This data would be used to study the evolution of smoke plumes in laboratory environments, considering that the mesh sizes used in computational fluid dynamics models are not sensitive enough to capture fine-grained changes. White smoke is useful for quickly and visually observing how effluent plumes change over time and space. It may also be used to verify the accuracy of CFD simulations.

To enhance comprehension of a typical synthesis setup, it was crucial to ascertain the influence of components on airflow patterns. The airflow was visualized and documented under various fume hood settings using a smoke generator machine. In this study, two conditions are being focused on which are sash opening and position of obstruction.

2.3.1 Sash Opening Variation

An essential aspect of assuring the proper containment of hazardous vapors and the protection of laboratory personnel is the study of airflow patterns in fume hoods, considering various sash openings and source positions. Employing a smoke generating apparatus can offer a tangible depiction of air movement, facilitating the evaluation of the effectiveness of a hood. As shown in Table , experimental variable for sash openings including type of opening, dimensions and face area.

Table 1 *Experimental Variable of Sash Openings*

Type Of Opening	Dimensions (Height x Length)	Face Area
Full	25-inch x 49 inch	8.51 sqft
Half	12.5-inch x 49 inch	4.25 sqft

2.3.2 Source Position Variation

Smoke was released in each of two positions from a smoke generator as shown in Figure below. The location of the contamination source within the fume hood can affect the hood's capacity to catch and confine the emitted compounds. An analysis of several source positions aids in assessing the efficacy of the fume hood in capturing and confining pollutants.

2.3.3 Local Visualization

To obtain an accurate test result, it is crucial to remove the smoke efficiently and smoothly, preventing it from getting stuck in the swirling motion at the top of the hood. Produce a steady stream of smoke from the small smoke emitter, directing it along the walls and work surface of the hood. The smoke should form a line that is parallel to the front of the hood and positioned 150 mm behind the front edge of the hood, at the top of the opening. Conduct a comprehensive analysis of the activity taking on in the corners.

To visualize how smoke flows in hoods, imaginary grid is with length of 30.5 cm and width of 63.5 cm is being done. When it is required, be mindful of the influence of air entering the hood via the gap between the sash and the header panel. Imaginary grids need to be done to easily visualize airflow patterns.

2.3.4 Tracer Gas Test

The detector needs to be triggered and allowed enough time to achieve equilibrium. Before, during, and after the testing period, ensure the operation of the detector by subjecting it to periodic exposure of a tiny quantity of tracer gas. The hood test should only be performed if the detector is functioning properly unless the problem has been resolved. The detector must be continually turned on.

Place the sash at the specified position. Place the smoke source and detector at a specified position for the purpose of conducting tests. The probe will be positioned near the breathing area, precisely at 75 mm from the plane of the sash. The detector probe must be firmly placed, with its midpoint positioned 560 mm above the work surface and 75 mm in front of the sash. Begin recording after a 20-second pause, and continue for 20 minutes, making sure to take a reading at least every 4 minutes. The positioning control level is established by computing the average of the tracer gas concentrations measured during the 20-minute test.

3. Results and Discussion

This chapter will cover the step-by-step process for utilizing ANSYS fluent to stimulate the fume hood capture rate. The fundamental analysis of a fume hood as well as the examination of air flow characteristics and concentration profiles will also be covered in this chapter. Prior to initiating the simulation, the 3D model of the fume hoods laboratory needs to be prepared.

3.1 Face Velocity Measured

Face velocity is a key indicator of how effectively the hood is capturing and containing these substances. Insufficient face velocity can lead to the escape of hazardous materials into the laboratory, posing serious health and safety risks.

3.1.1 Full Opening Fume Hood

Average face velocity is being measured by adding them up and dividing them by total number of points. The average face velocity for Table 2, calculated is 0.458 m/s. Check the average face velocity against the recommended standards for your specific type of fume hood and the materials for certain experiments. Common standards range from 0.3 m/s (60 fpm) to 0.5 m/s (100 fpm).

Table 2 Face Velocity for Full Opening

P1	0.4925	P2	0.508	P3	0.503	P4	0.493
P5	0.2615	P6	0.4903	P7	0.4295	P8	0.409
P9	0.4748	P10	0.531	P11	0.475	P12	0.4295

3.1.2 Half Opening Fume Hood

Average face velocity measured by adding them up and dividing it by total number of points which is 4 points as shown in Table 3. The average face velocity calculated is 0.767 m/s.

Table 3 Face Velocity for Half Opening

	P1	P2	P3	P4
V	0.7654	0.7773	0.7663	0.745

From this study, it can be concluded that when the sash is only slightly open, there is less cross-sectional area for air to enter than when it is fully open. This creates a bottleneck in the airflow, resulting in increased air velocity to maintain a constant volumetric flow rate (the total amount of air passing through the hood per unit time).

3.2 Validation of Result

By using function calculator in Post Fluid simulation, the simulation itself will help in calculating value such as flow rate, velocity, and area. To validate the experimental value with simulation, the outlet boundary condition being set up as 211.53 kg/s.

The data shows that the velocity of inlet almost proximity from experimental data calculated which is 0.46m/s. Velocity measurements at inlet for half opening sash position is 0.767 m/s. By comparing both results, it shows that the design simulated is closely proximate to real dimensions of fume hoods.

3.3 Impact of Source Position

While still efficient, placing the source at the front while full opening of sash may lead to the release of smoke before it is completely contained, especially if the source generates a strong upward plume that can be expelled by the surrounding air. Positioning the source at the front enhances the effective dissipation of heat from the sash opening, hence minimizing the risk of thermal stress on the hood and the potential emission of hot exhaust. Placing the source exactly in the middle can disrupt the natural, continuous movement of air, causing swirling currents and temporary pockets where smoke or odours may gather before being removed. Positioning the source at the centre maximizes the efficiency of capturing by utilizing the converging airflow patterns from all directions, effectively directing the pollutants into the exhaust system.

Smoke Pattern at Centre during Half Opening Sash, the airflow velocity increases because of the reduced cross-sectional area, which has the potential to enhance capture, even in the presence of a central source. When a sash is partially open, it creates more turbulence along the edge that is exposed, resulting in the production of extra eddies. This could impact the uniformity of air capture throughout the hood. **Error! Reference source not found.**, it can be concluded that the constricted opening directs the airflow directly onto the front source, potentially increasing its capture efficiency compared to a completely open sash.

3.4 Tracer Gas Test

The tracer gas test is a crucial technique for ensuring the safety of laboratory staff by thoroughly evaluating the effectiveness of fume hoods containing hazardous compounds. By regularly conducting tracer gas testing, laboratories may verify that their fume hoods are operating at optimal efficiency, so successfully protecting people from potential harmful exposures. As shown in Figure 3, the concentration of the experiment for 20 minutes.

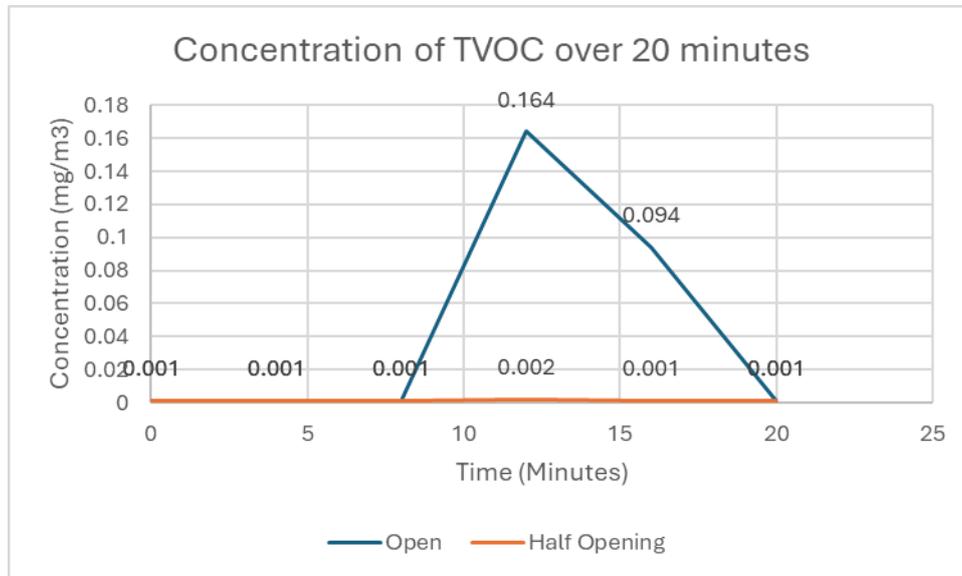


Fig. 3 Concentration in mg/m³ over 20 minutes.

Typically, the results of a tracer gas test can be classified into three distinct categories which is fail, pass and inconclusive. As shown by data calculated it can be considered pass. The fume hood is deemed to be functioning satisfactorily if the detected concentration of the tracer gas outside the hood is lower than the permissible threshold which is below 0.2 mg/m³.

Tracer gas tests, which are used to evaluate the effectiveness of fume hoods, may sometimes result in unwanted little leaks, such as when the fume hood is completely open and the air velocity surpasses the required capture velocity to effectively contain all contaminants, including the tracer gas. If the pressure in the laboratory is not high enough compared to the pressure in the hood, it can cause air to flow inward instead of outward, leading to the release of tracer gas.

3.5 Flow Visualization

Flow visualization challenges pertain to the execution of tests aimed at assessing the airflow patterns within a fume hood. By employing flow visualization challenges, researchers can validate that the airflow under the hood is functioning properly and effectively containing these dangerous substances. As shown in Figure 4, it shows the flow visualization for full opening fume hoods.

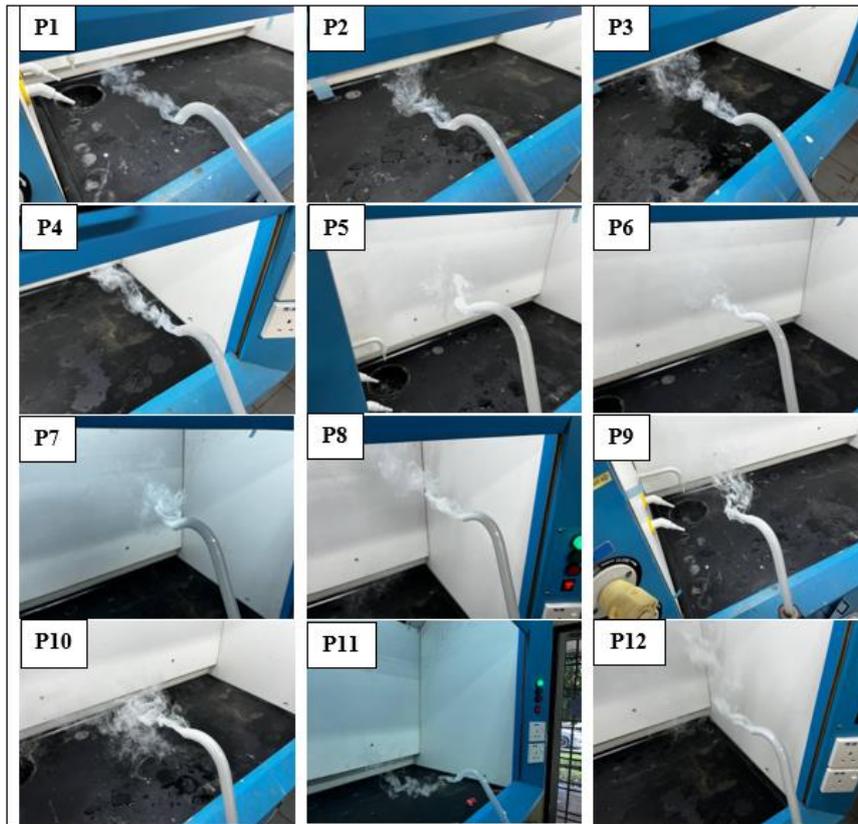


Fig. 4 Flow Visualization for Full Opening Fume Hoods

When confronted with partially ajar sashes as shown in Figure 5, the rate at which air is pulled into the opening may diminish towards the lower half. The airflow pattern becomes more complex when the sash is partially open. Air normally enters the hood through the lower section and follows a curved path upwards towards the opening. This leads to the creation of turbulent zones and stagnant regions, particularly at the corners and near the lower part of the sash.

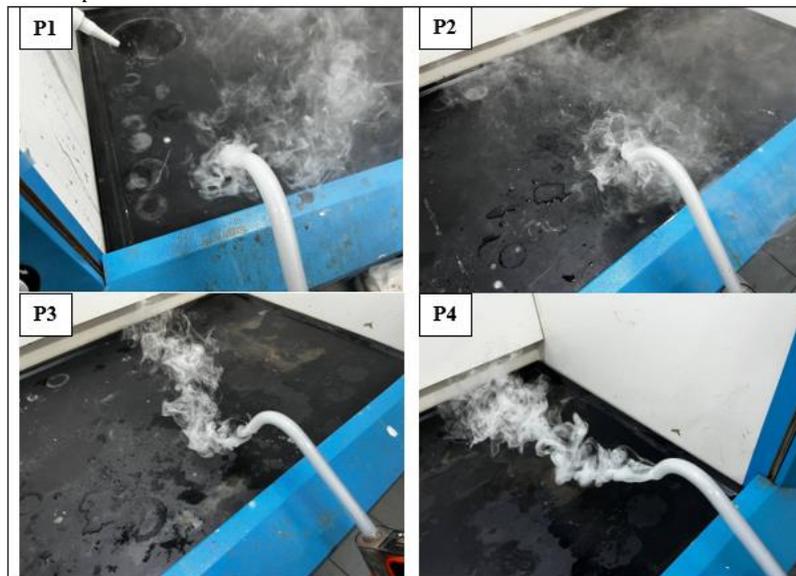


Fig. 5 Flow Visualization of Half Opening Fume Hoods

3.6 Ansys Fluent Setups

A few configurations need to be set up before running the simulation. The model that will be used to stimulate fume hood is $k-\omega$ epsilon SST and the energy settings need to activate to have input for both inlet and outlet of geometry. For the materials, air will be selected as this study is to predict airflow patterns of fume hoods. Also, we need to set up the volume fractions of the model so that simulation will run smoothly.

3.6.1 Airflow Patterns

A type of simulation has been done in this project which is to study air flow in fume hoods. Airflow patterns analysis to predict how air moves from inlet to outlet. The huge cross-sectional area causes the air velocity at the sash opening to be comparatively low. The airflow is accelerated as it passes through the exhaust duct, a phenomenon caused by the venturi effect. The maximum velocity is measured at proximity to the exhaust exit.

Although the complete opening of the sash makes it easier to reach the workplace as shown in Figure 6, it can reduce the effectiveness of capturing contaminants because of the decreased air speed at the sash and the possibility of contaminants escaping from the margin.

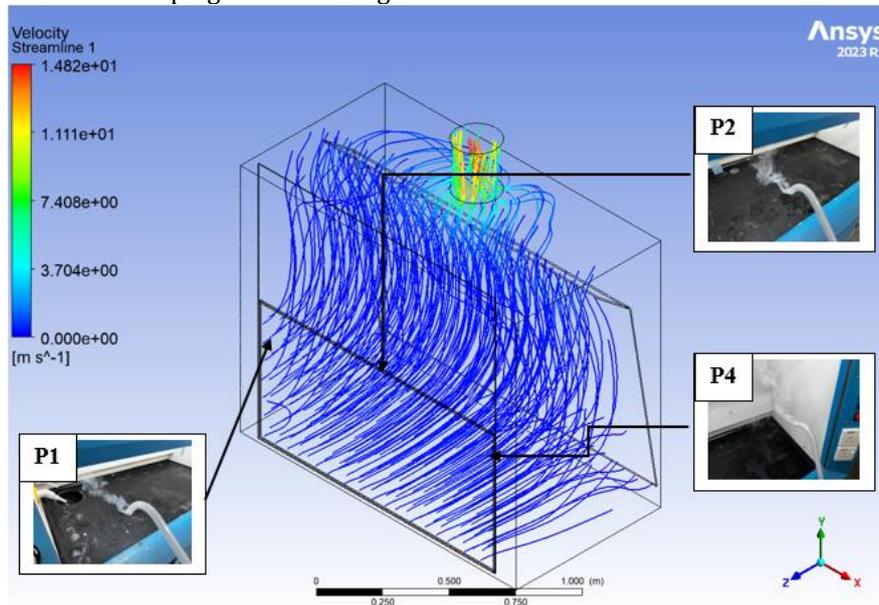


Fig. 6 Velocity Distribution of Airflow in Full Opening

The air velocity is greater at the sash opening than at full aperture because of the reduced cross-sectional area. The airflow experiences a substantial increase in velocity as it passes through the exhaust duct, owing to the venturi effect. The maximum velocity is measured at proximity to the exhaust exit. Streamlines exhibit a greater concentration of airflow directed towards the exhaust duct in comparison to when it is fully open as shown in Figure 7.

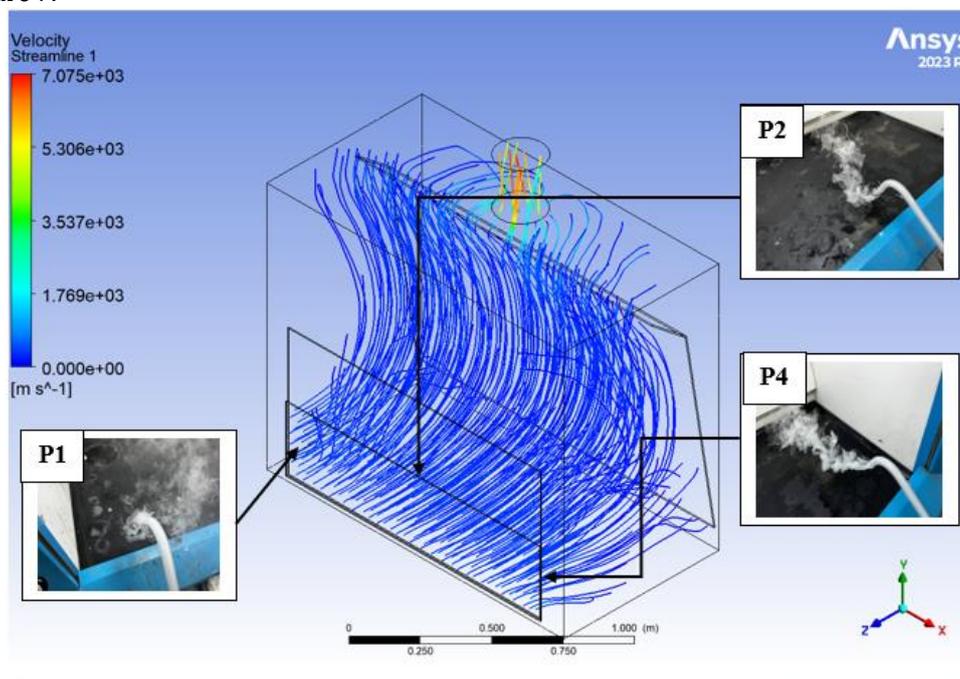


Fig. 7 Velocity Streamline of Half Opening

When comparing a fully opened sash to a half-open sash, the latter generally has better capture efficiency because of the increased air velocity at the sash and the directed airflow towards the exhaust. Operating the system at half opening increases the air velocity, which improves the likelihood of meeting the required face velocity standards for hazardous materials. This, in turn, enhances the safety of the operation.

4. Conclusions

The aim of this study was to comprehensively evaluate the efficiency of fume hoods by employing tracer gas tests, flow visualization, changes in sash position, and computational fluid dynamics (CFD) simulations for both fully open and partially open setups. The integrated methodology produced substantial results on the airflow patterns, capture efficiency, and the impact of operating factors on the performance of the fume hood. The tracer gas tests validated that the capture efficiency reached its maximum level when the sash was completely opened, as expected. However, there were slight reductions observed when the areas were partially open, highlighting the importance of adjusting ventilation settings or maintaining full opening whenever possible. Flow visualization approaches, such as the utilization of smoke generators, effectively revealed stationary regions and areas of turbulence within the hood, particularly when the sashes were only partially ajar. This information is crucial for optimizing the design and functioning of hoods to minimize the buildup of contaminants and mitigate the risks of exposure. CFD models provided accurate numerical data on the flow patterns and velocities of air, augmenting the qualitative information obtained via flow visualization. The models confirmed the results obtained from tracer gas and smoke tests and enabled detailed examination of complex airflow dynamics that are difficult to observe physically.

It is recommended to always utilise fume hoods with the sash fully open whenever feasible. This ensures optimal efficiency in capturing vapours and minimises the risks of exposure. To address the reduction in capture efficiency and mitigate any areas of stagnant air or turbulence, adjust the ventilation settings when operating in a partially open position. Utilise computational fluid dynamics (CFD) simulations as a crucial tool for improving the design of hoods, ventilation settings, and operational operations, resulting in increased safety and performance of fume hoods.

Acknowledgement

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