

PAPER 103 – MODELLING OF VOCs EMISSION AND TRANSPORT IN INDOOR ENVIRONMENT USING FINITE ELEMENT ANALYSIS

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ABSTRACT

The concentration of Volatile Organic Compounds (VOCs) in an indoor environment like beauty depends on its emission rate and transportation. Consequently, a better understanding of the dynamic behaviour of this pollutant in the indoor environment improves estimates of human exposure to indoor air pollutants. This study systematically evaluated the influence of four computational parameters on pollutant dispersion in a beauty shop. The computation parameters include turbulence models, grid resolution, and discretization of time step size and length of the sampling period. For concentration simulations, the Large Eddy Simulation (LES) and Detached Eddy Simulation (DES) models did not give any result because it had limitations in areas near the source, whereas the realizable k- ϵ turbulence model did give a desirable result. An increase in the emission rate did not change the general dispersion characteristics, but it still affected the concentration distribution in the areas near the source and resulted in a larger polluted area. The findings of this study are intended to give a better understanding of the dynamic behaviour of VOCs in a beauty shop using CFD simulations, which will help develop a suitable control strategy.

KEYWORDS: Volatile Organic Compounds, indoor, beauty shop, ANSYS FLUENT, CFD, Modelling

12. INTRODUCTION

The quality of air in indoor environment is very important to work performance, productivity and the health of building users (Titiana, Andy, Marc, and Bluysen, 2019). Although Indoor Air Quality (IAQ) is not usually monitored, it must be perceived as a relevant issue to follow up for the inhabitants' well-being and comfort for enhanced living environments and occupational health (Vilčeková *et al.*, 017). The time spent in various types of indoor spaces depends on different social and environmental factors such as age, geographical latitude, occupation, lifestyle and quality of life (Śmiełowska, Marć, and Zabiegaj, 2017). Common air pollutants in indoors are particulate matter, photochemical oxidants (including ozone), carbon monoxide, sulfur oxides, nitrogen oxides, VOCs and lead. A lot of research has shown that commonly used materials such as wood products, floor coverings, wall coverings, household spray products emits a variety of VOCs which reduces the quality of the indoor air (Hussain *et al.*, 2015).

Volatile organic compounds (VOCs) are reactive organic compounds that are emitted into the atmosphere due to their high volatility at atmospheric conditions (Attia *et al.*, 2019; Guerra *et al.*, 2017; Tsai, 2016). They also have different types of reactive functional groups such as amines, amides, alcohols, carboxylic acids, aldehydes, and aromatic compounds (Attia *et al.*, 2019). VOCs are considered to be important air pollutants because of their persistence in the atmosphere (Kumar *et al.*, 2014) as well as their negative effects on respiratory and reproductive systems even at low levels of concentration (Tsai, Lu, Chung, and Chiang, 2020). The concentration of VOCs in the indoor environment depends on the pollutant emission sources, rate of removal, the air exchange rate with the outdoor air, and the outdoor VOCs concentrations (Guieysson *et al.*, 2008). VOCs can be classified into several groups based on their properties. Based on the boiling point, the VOCs can be divided into Very Volatile Organic Compounds (VVOCs), VOCs, Semi Volatile Organic Compounds (SVOCs) and Particulate Organic Matters (POMs) by WHO. Based on molecular structure, it is classified as alkanes, alkenes, aromatic hydrocarbons, alcohols, aldehydes, ketones etc, and based on molecular polarity they can be the polar and nonpolar VOCs in indoor environments. A better understanding of the dynamic behavior through Computational Fluid Dynamics will help in designing suitable control strategies.

CFD simulation programs are a powerful tool for estimating the airflow patterns and thermal environment of various heating, ventilation, and air conditioning systems in a very detailed way. They have been used for the estimation and control of the indoor environment and space ventilation when using different ventilation systems (Szczechpanik-Scislo and Lukasz Scislo, 2021). CFD divides a space into extremely fine grid cells, which can be used to predict the precise spatial distribution of target chemicals from spray products. Jung, Kim, Seol, Lee, and Kwon (2021) simulated inhalation exposure for an eight compartments room to an ethanol trigger and a propellant product. The well-mixed model overemphasized short-term exposure, particularly under the trigger spray scenario. The CFD based permeation model includes sorption/desorption, using a linear isotherm at inner and

outer surfaces and a blended wall function to account for the effects of near-wall turbulence. The model was used to show how vapor concentrations around a cardboard box containing a SVOC vary when some of the key input parameters are changed (Foat *et al.*, 2021). Indoor environment like beauty shops where numerous essential oil and scented products are used depends on their emission rate, decay and transportation. Consequently, a better understanding of the dynamic behaviour of this pollutant in the indoor environment improves estimates of human exposure to indoor air pollutants.

13. THEORETICAL ANALYSIS

CFD solves Reynolds-Averaged Navier–Stokes Equations for turbulent buoyant flow, heat and mass transfer established based on conservation equations of mass, momentum, energy, turbulent kinetic energy equation, turbulent energy dissipation equation, and contaminants (Davardsoot and Kahfooroushan, 2018; Panagopoulos, Karayannis, Kassomenos, and Aravossis, 2021).

For the mass conservation as shown in Equation 1

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad 1$$

Equation 2 represents momentum conservation

$$\frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left\{ (\mu + \mu_t) \left(\frac{\partial v_i}{\partial x_i} \right) \right\} + \rho g_i \beta (T - T_m) \quad 2$$

Turbulent kinetic Energy can be estimated with Equation 3

$$\frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_j} \left\{ (\mu + \frac{\mu_t}{\sigma_k}) \left(\frac{\partial k}{\partial x_i} \right) \right\} + G_k + G_b - \rho \varepsilon \quad 3$$

Equation 4 represents turbulent kinetic energy dissipation equation

$$\frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_j} \left\{ (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \left(\frac{\partial \varepsilon}{\partial x_i} \right) \right\} + \frac{C_{1\varepsilon} \varepsilon}{k} (G_k + C_{3\varepsilon}) G_b - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \quad 4$$

Energy conservation equation as indicated in Equation 5

$$\frac{\partial}{\partial x_i}(\rho u_i T) = \frac{\partial}{\partial x_j} \left\{ (\frac{\mu}{Pr} + \frac{\mu_t}{Pr_t}) \left(\frac{\partial T}{\partial x_i} \right) \right\} + S_T \quad 5$$

Contaminants conservation equations are indicated by Equation 6 -9;

$$\frac{\partial}{\partial x_i}(\rho u_i C) = \frac{\partial}{\partial x_j} \left\{ (\frac{\mu}{\sigma} + \frac{\mu_t}{\sigma_T}) \left(\frac{\partial C}{\partial x_i} \right) \right\} + S_c \quad 6$$

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad 7$$

$$G_k = \mu_t \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_j}{\partial x_i} \quad 8$$

$$G_b = -g_i \left(\frac{\mu_t}{\rho \sigma_h} \right) \frac{\partial u_j}{\partial x_i} \quad 9$$

$$C_{1\varepsilon} = 1.44 \quad C_{2\varepsilon} = 1.92 \quad C_{3\varepsilon} = 0.09$$

$$\sigma_k = 1.0 \quad \sigma_\varepsilon = 1.0$$

Where ρ is the fluid density, u_i is the flow velocity vector field in x_i direction, P is the pressure, k is the turbulent kinetic energy, μ_t is the turbulent viscosity, μ molecular viscosity, g is acceleration due to gravity, C , $C_{1\varepsilon}$, $C_{2\varepsilon}$ and $C_{3\varepsilon}$ are coefficient in approximated turbulent transport equations, σ_h molecular prandtl number, σ_t is effective turbulent prandtl number, ε rate of dissipation of turbulence energy, T is the temperature, T_m is the reference temperature, G_k is the kinetic energy produced by buoyancy, C is molar concentration of the VOC.

14. METHODOLOGY

The transportation of VOCs in beauty shops was simulated using ANSYS Fluent (2016) which is an application-based software that helps in physical modelling. There are five major steps involve in the numerical simulation with ANSYS Fluent which describes flow of air pollutant include

- (i) Geometry is set up according to the dimensions of the indoor space.
- (ii) Setting up material properties and boundary conditions or a turbulent forced-convection problem, material properties considered/chosen were equivalent to n-butane (n-butane), which is selected from the gas list present in software.
- (iii) Boundary condition for concentration change was considered zero at zeroth time, and change in the concentration with respect to time has been determined by mass flow equation through software.
- (iv) Calculating a solution using the pressure-based solver wherein mass and energy balance equations are used.
- (v) Examining the flow fields using ANSYS Fluent.

3.1 Geometry and Mesh generation

A 7.725 m × 6.000 m × 1.989 m (L × H × W) numerical model of the 3-D room as shown in Figure 1 was designed with SOLIDWORKS software and then saved in IGS format that is acceptable in ANSYS Fluent. The SOLID WORK modelled room has no furniture and occupants. The empty room as shown in Figure 1a was modeled to study indoor environmental conditions. An empty room consists of the glazed glass window, adiabatically insulated walls, and a source of aerosol placed on the table.

Meshing was carried with a high smoothing, slow transition and fine relevance center as shown in Figure 1b. The realizable k-ε turbulence model with standard wall functions in Fluent was used to model the effects of turbulence on airflow and aerosols transport.

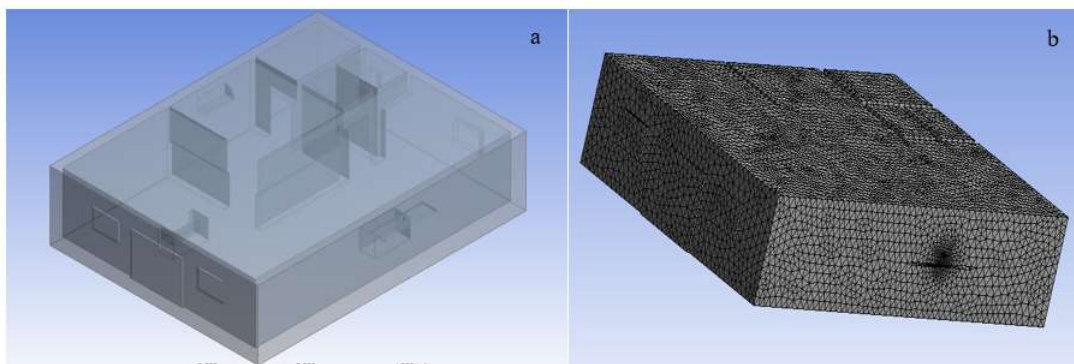


Figure 1: (a) geometry of modelled room (b) mesh generated

3.2 Setup and solution

The realizable k-ε turbulence model with standard wall functions in Fluent was used to model the effects of turbulence on airflow and aerosols transport (Adeniran *et al.*, 2021). The solver was set to be pressure based with two Eulerian phases with implicit body force. The VOCs was represented by n-butane which was chosen from the fluent data base. The VOCs inlet (Hair spray Bottle), wind inlet and outlet was specified to be velocity inlet and pressure outlet respectively in the software. The wind velocity was varied from 2 to 6 m/s. The solution of the model was initialized using the hybrid initialization

15. RESULTS AND DISCUSSION

Air flow velocity is an important parameter to be considered when studying airflow in an indoor environment wind velocity was varied from 2 to 6 m/s the result obtained for 2, 4, 6 m/s are presented in Fig. 2, 3 and 4 (Scenerio A, Scenerio B and Scenerio C) respectively.

Scenerio A

About one thousand (1000) iteration was carried out the volume fraction of VOCs emitted reduced swiftly with time and slightly reduced for some time until steady state was reached at about 800 iteration. The spread of the pollutant was not much this could be attributed to the wind velocity, which did not make the VOCs to spread to other part of the beauty shop. This can result excessive chemical exposure conditions in beauty shops that can lead include irritation to eyes and nose, headache, dizziness, drowsiness, *etc.* Therefore, the appearance of a mixture of compounds in high concentrations can cause similar symptoms to both employees and customers (Tsigonia, Lagoudi, Chandrinou, Linos, Evlogias, and Alexopoulos, 2010). For Scenerio B presented in Figure 3a and b there was a sharp decrease the volume fraction of the VOCs until uniform concentration is attained with the part of the room. A uniform spread was attained at a shorter time span around 700 iteration. When the wind velocity was increased to about 6 m/s the spread was very fast and steady state was attained at about 600 iteration. These findings predicts the highest concentration near the source of the pollutant concentration gradually decreases and then transported towards the direction of the wind this result corresponds to the findings of Mohammadi and Calautit (2021). Environmental conditions such as meteorology, temperature difference across the building, indoor activity, furnishings, *etc.*, alter the rate of air exchange and consequent pollution transmission. For the model considered in this study it was observed that there was negligible spread of the VOCs to other compartment separated by walls.

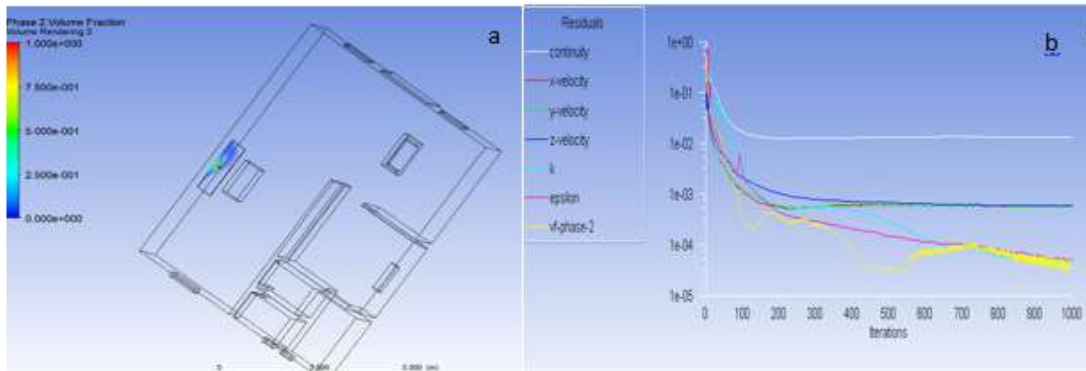


Figure 2:(a) Volume rendering of VOCs dispersion (b) decay of VOCs with time steps at wind velocity

Scenario B

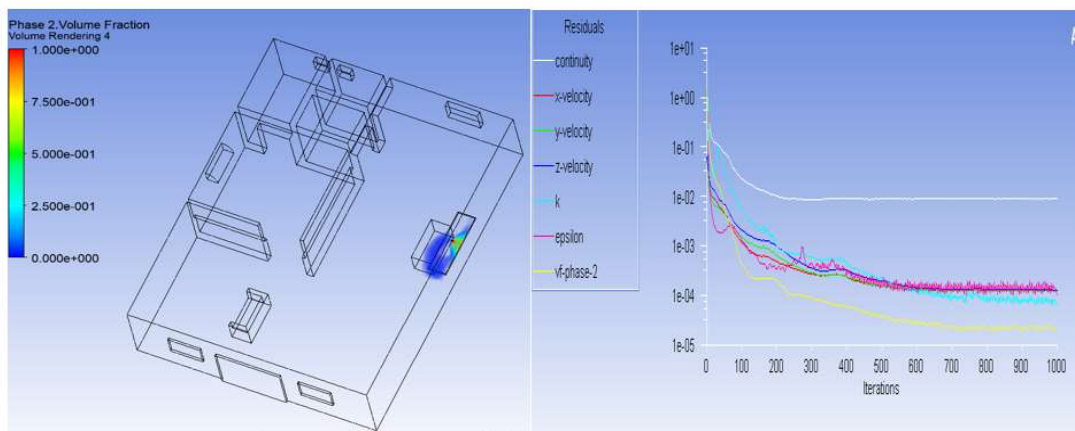


Figure 3:(a) Volume rendering of VOCs dispersion (b) decay of VOCs with time steps at wind velocity at 4 m/s

Scenario C

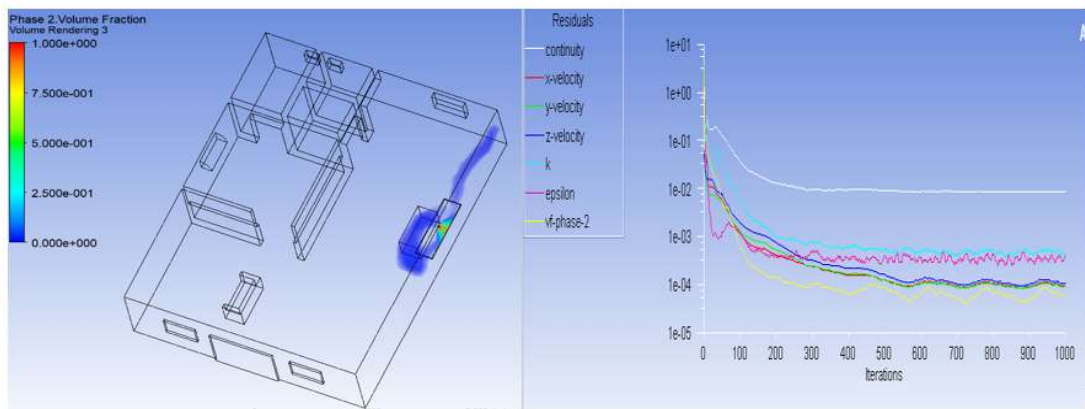


Figure 4: (a) Volume rendering of VOCs dispersion (b) decay of VOCs with time steps at wind velocity at 6 m/s

The emission rate of the pollutant was varied by increasing the emission rate thus altering the velocity of the VOCs inlet. It was found that an increase in emission rate did not affect the flow characteristics but increases the polluted area. The airflow velocity have impact on the transportation of the VOCs in the indoor environment.

16. CONCLUSIONS

This study concentrated on the transportation of VOCs in a beauty shop. The transportation pattern did not change an increase in emission rather there was a spread in the larger parts of the room. There was an increase in dispersion of the VOCs (n-butane) when the wind speed was increased from 2m/s to 6 m/s. Operation of saloons in confined places with poor ventilation leads to the emission of VOCs that might have pleasant smell in some cases but are actually deadly, poisonous, colourless, and odourless. Symptoms of poisoning are dull headache, blurred vision, shortness of breath, weakness, dizziness, and nausea or vomiting. Hence, this has adverse health effect on both the beauty shop operator and the customer. Measures must be taken in such indoor environment to reduce its impact on health and the environment. A great part of the effect of using spray products in beauty shop can be controlled by carrying out awareness campaigns, adopting air cleaning technology, introducing common house plants in work, proper engineering measures, and a well-designed awareness campaign. Where there is high usage of this hair product, which contains high concentration of VOCs, there should be a proper ventilation and vent can be installed around where these hair products are being used. However, a well-ventilated room with modern air purification systems should be used in most beauty shops

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APPENDICES

The outer dimension of the geometry used for Figure A1

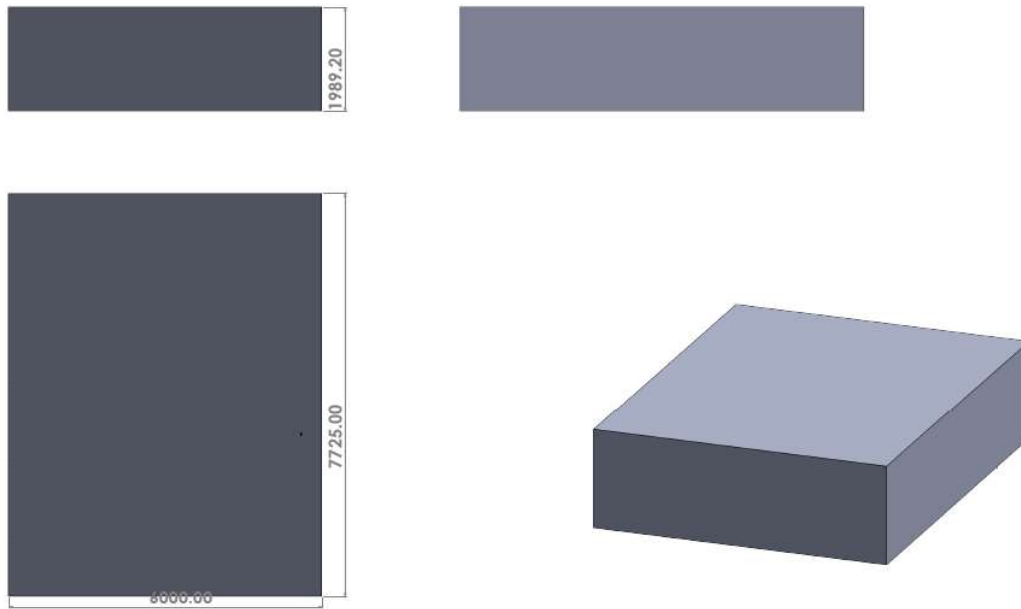


Figure A1: Dimension of the proposed geometry