CFD analysis on the effect of temperature on gas distribution in indoor environment

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Abstract. There are times when people are required to spend time indoors, especially due to unhealthy outdoor air quality as well during a pandemic when lockdowns are imposed. However, spending time indoors can also at times be dangerous due to the release of harmful gasses if left unchecked. This has very much to do with many parameters, among which is the indoor environment and its ventilation. The latter is affected by the way gases distribute inside the building. It is influenced by many factors such as temperature, wind, air circulation, and also ventilation system itself. The knowledge on how the gases spread in different conditions within the indoor environment can be utilized in many applications such as improving the smoke detector safety system and identifying as well as predicting the potential risks. This paper presents the investigation of the effect of different temperatures on gas distribution in an indoor environment. A three-dimensional simulation was performed of different temperature gas released in a closed room that has different ambient temperatures. The effect of temperature on the gas dispersion was observed. The results revealed that there is a significant effect of temperature on the way gas spread in the indoor environment support by the theoretical knowledge on the relationship between temperature and gas in the gas law.

1. Introduction

The occurrence of a major accident involving hazardous substances or chemicals comes from industrial sites, office buildings, and the farming industries [1] attracted the interest of researchers around the world to study the behaviour of those hazardous substances. Many researchers have done remarkable jobs via theoretical, experimental, and numerical approaches [2]. Those accidents such as harmful gases leakage may happen due to the hazardous chemical substances poor handling system. In detail, it can cause death or serious injuries if suitable safety measures are not taken, among which an appropriate room with ventilation, alarms, gas detectors, and other necessary equipment for keeping cylinders or tanks

The accident involving hazardous substances not only happened in the outdoor environment but also happened in an indoor environment. It is important to make sure the indoor air quality is always good quality since people's health could be affected due to the contaminated air. Moreover, it is found that humans spend 80% to 90% of their daily life indoor compared to the outdoor environment [3]. There are three types of airborne contaminants which are biological contaminants, particular contaminants,
and gaseous contaminants. The gaseous contaminant is known as the smallest type and is commonly found in the airborne in real indoor environments [2].

The gas contaminants move freely in our indoor space and people may not realize their presence. A certain number of hazardous gaseous also known to be odourless and colourless which can be a silent killer to a human being. Their molecules have fast thermal motion speed in a random direction and several researchers mentioned that the movement of their molecules is governed by the convection and diffusion law [2]. However, there is also a certain researcher in the mobile robot olfaction field that mentioned that gas molecules are significantly governed by the airflow while diffusion of the gas molecule into the air is generally an extremely slow process [4], [5]. It is important to know the behaviour of contaminated gas dispersion in the indoor environment for future risk assessment [6]. In addition, the dispersion of gas contaminants in the indoor environment may also be affected by several environmental factors such as wind, convection, temperature, humidity, and pressure [7].

In a structured indoor environment, there are typically different enclosed spaces and each of the spaces may have a different environmental condition. For example, there may be rooms with an air-conditioning system while the others may have windows or a ventilation system. This condition causes the temperature reading at different indoor spaces could be different. The heat can come from many sources such as windows, machines, electronic devices, ceilings, and also the human body. These sources of heat can directly increase the temperature inside the indoor space. If the same type of harmful gas is released inside two different rooms with different temperatures at the same time, the dispersion of both harmful gas molecules will be different from each other. This is because Charles’ Law shown that there is a relationship between the volume of gas with the temperature [8]. Different temperatures will result in a different effect on gas molecule dispersion.

The most critical step in indoor risk assessment is to model the dispersion of hazardous gas. It may impact negatively on both human and financial resources if the model design is inadequate and also lead to the wrong estimation of concentration prediction. With increasing computing power and widespread availability of commercial and open-source codes, CFD techniques have been used to predict the airflows and chemical plumes in indoor environments for search algorithm development and testing [9]. This study focuses on the analysis of the various temperature effect on the gas dispersion inside the indoor environment through Computational fluid dynamic (CFD). These studies will help to ensure consistency in the gas plume propagation and fluid fields at different test runs. It also provides useful information for safety precautions when dealing with harmful substances.

2. Experimental setup
In CFD, the fundamental equations describing the conservation of mass, momentum, and energy balance are solved numerically for a given flow domain, initial, and boundary conditions. The flow of a Newtonian fluid is governed by the continuity and the momentum conservation equations for total energy flow, described by equation (1) and equation (2) respectively;

Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0$$  \hspace{1cm} (1)

Momentum balance:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \frac{\partial u_k}{\partial x_k} \right] + \rho g_i$$  \hspace{1cm} (2)

Here, \(\rho\) is the density, \(u_i\) is the velocity component in the \(i\)th direction, \(p\) is the pressure, \(\mu\) is the viscosity of the medium, \(\lambda\) is the second coefficient viscosity (the term involving this variable is assumed to be negligible) and \(g_i\) is the component of gravitational acceleration in the \(i\)th direction.
A consistent environment with controlled variables (i.e., pressure, temperature, wind,) is essential for developing experiments related to gas distribution in an indoor environment. Therefore, ANSYS application was used in this experiment as a platform to perform the simulation of gas distribution at different ambient temperatures and different gas temperatures itself. This is because many variables that can affect gas distribution in real-environment can be controlled easily. Figure 1(a) shows a model of a closed empty room that will be utilized to perform the simulation. This simulation model is similar to the standard office room which has the dimension of \( L_x = 6 \, \text{m}, \, L_y = 6 \, \text{m}, \, \text{and} \, L_z = 3 \, \text{m} \) in the x, y, and z directions, respectively. It consists of four non-slip walls, a ceiling, and a flat floor. There was an access door with a dimension of width (1.2m) x height (2.4m) which are normally closed. There was no presence of obstacles inside the room which was different from the experiment done by the researcher in [2]. It is to prevent the obstacles to influence the dispersion of the gas inside the room. There is no air inlet to prevent airflow caused by the ventilation system inside the room. Hence, there was no air entering the room and no air going out which is also known as an airtight room [7]. A petri dish with 0.09m diameter was placed at the center of the room to simulate the release point of the harmful gas. Ethanol vapor was used in this research to simulate the gas release since it is widely used in mobile robot olfaction experiments to simulate gas leaks [10]–[12]. The gas is also not harmful to humans and therefore could be suitable for validation purposes in real experiments. Any gas with a density greater than that of the ambient air through which it is dispersed is referred to as a dense gas [13]. Therefore, ethanol is a type of dense gas because it has a density greater than ambient air density.

![Figure 1. (a) 3-dimensional closed empty room simulation model. (b) Mesh grid for room model.](image)

The Computational Fluid Dynamic (CFD) simulation was run using the commercial CFX program in ANSYS/DESIGNMODELER 14.0 for transient mode under different ambient temperatures inside the room. The simulations of the gas spread were performed on an Intel® i5 Core computer with a typical time step size of 1 second. Initial spreading calculations with a time step of 0.1 second were performed and the comparison showed that a step size of 1 second would be adequate. The total simulation time is 60 seconds. Typically, each simulation took about an hour to perform the computation. For transient simulation, assuming that there is no airflow movement inside the room at the beginning of the simulation. Since the velocities in the present study are fairly low and no heat transfer is considered, it is expected that no special, wall-induced effect will be adequate. In terms of boundary conditions, all the components in the design except the gas inlet were treated to be used wall function. Two experiments have been conducted. The first experiment was to observe the effect of different ambient temperatures
on gas dispersion. While the second experiment was done to observe the effect of gas temperature itself toward gas dispersion.

For the first experiment, the temperature of ethanol vapor and air humidity was maintained at the reading of 25 °C and 50% respectively. The manipulation variable in this experiment was the room ambient temperature setting (i.e., -3 °C, 25 °C, and 40 °C). It is to make sure that all the changes in the dispersion of the gas are only caused by the variability in ambient temperature.

For the second experiment, the room ambient temperature and air humidity were maintained at a reading of 25 °C and 50% respectively. The manipulation variable in this experiment was the temperature of ethanol vapor release inside the room which was set to 40 °C, 100 °C, 200 °C, and 300 °C. It is to make sure all the changes in the dispersion of the gas are only caused by the variability of release gas temperature itself.

The ethanol vapor was released at the rate of 0.0010 kg/s with low turbulence intensity (1%) for both experiments. As mentioned before, the total time of the simulation is 60 seconds while the ethanol vapor is released in the early of 5 seconds only. The remaining time left is used to allow the ethanol vapor to reach its equilibrium condition. Then, the k-epsilon model (k-ε) was utilized as the turbulence model for this simulation. It is able to provide reasonable results in many cases[9]. The turbulent viscosity \( \mu_t \) was calculated by the k-ε turbulence closure model defined as follows:

\[
\mu_t = C_\mu \frac{k^2}{\varepsilon}
\] (3)

\[
\frac{\partial \rho k}{\partial t} + \nabla \cdot (\rho u_j k) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_t} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \frac{\partial}{\partial x_j} \left[ \frac{\partial}{\partial x_j} \right] (c_{1k} \varepsilon G_k - c_{2k} \varepsilon^2) - \rho \varepsilon
\] (4)

\[
\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho u_j \varepsilon) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_t} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + c_{1}\varepsilon G_k - c_{2}\varepsilon^2 \frac{\varepsilon^2}{k}
\] (5)

In equation (3) – (5), the constants are: \( C_\mu = 0.09, c_{1\varepsilon} = 1.44, c_{2\varepsilon} = 1.92, \sigma_t = 1.3, \sigma_k = 1.0 \). The k-ε turbulence model was chosen because of its relative simplicity and it was used by previous author[14].

The unstructured mesh grid applied in this study has the average size of 0.2m² and produced about 116,058 computational cells as shown in figure 1(b). Previous researchers [2] mentioned that the calculation result of the simulation does not depend on the mesh size of the model. Therefore, the number of cells produces is enough for this simulation and will save computer calculation running time. For this reason, this study will not perform the experiment on different mesh numbers for the number of mesh validation.

3. Experimental Result
This section discusses the observation gained from both experiments performed in Section 2. Noted that all the results afterward displayed the dispersion of ethanol vapor at the time step of 60 seconds. The blue color indicates the isosurface of ethanol vapor dispersion inside the room.

3.1. Ambient indoor temperature variation
This subsection will present the result of the first experiment as mention earlier. All the results in this subsection will be related to the variation of ambient temperature while the ethanol gas temperature is fixed at room temperature. All the results can be seen in figure 2.
Figure 2. (a) Horizontal view of ethanol dispersion when temperature of ethanol vapor is 25°C and ambient room temperature is -3°C. (b) Top view of ethanol dispersion when temperature of ethanol vapor is 25°C and ambient room temperature is -3°C. (c) Horizontal view of ethanol dispersion when temperature of ethanol vapor is 25°C and ambient room temperature is 25 °C. (d) Top view of ethanol dispersion when temperature of ethanol vapor is 25°C and ambient room temperature is 25°C. (e) Horizontal view of ethanol dispersion when temperature of ethanol vapor is 25°C and ambient room temperature is 40°C. (f) Top view of ethanol dispersion when temperature of ethanol vapor is 25°C and ambient room temperature is 40 °C

Figure 2 displays the side view of the simulation result isosurface of ethanol vapor that was released inside a closed room which does not present any airflow and also has different ambient temperatures (i.e., -3 °C, 25 °C, and 40 °C respectively). From the observation, the heat from the surrounding air does not cause the ethanol vapor to rise upward. This is because the density of the surrounding air decreases as its temperature increases. Even though ethanol vapor was heated up by the surrounding air and had
its density decreased, the density of ethanol vapor was still higher compared to surrounding air density. This is the reason why the ethanol vapor cloud did not elevate toward the ceiling of the room and stayed on the ground level. However, it can be seen that the ethanol vapor spread horizontally further as the room ambient temperature was increased.

From the top view of the simulation result, it can be observed that the ethanol dispersion radius varies by ambient temperature. At -3 °C ambient temperature, the ethanol vapor disperses and covered a small area even it has been released at a similar time and flow rate. As the ambient temperature increase, the area of ethanol vapor dispersion also increased. This phenomenon can be explained by the increase in the average kinetic energy of ethanol vapor molecules. The average kinetic energy molecules of ethanol vapor at -3 °C are lower compared to its average kinetic energy molecule at 40 °C. This result is supported by Max-Boltzman distribution on gas law [15]. It shows that the relationship between the velocity distribution of the gas and temperature. The average kinetic energy of gas molecules is directly proportional to absolute temperature. In terms of diffusion, when the average kinetic energy is increasing the diffusion rate of ethanol vapor also will be increased.

3.2. Temperature variation of gas in an indoor environment

This simulation was performed to observe the effect of the different temperature levels of the gas itself toward its dispersion in an indoor environment. The ethanol vapor with different temperatures (i.e., 50°C, 100°C, 150°C, and 200°C respectively) was released into the indoor environment that maintained within room ambient temperature (i.e., 25°C). Figure 3 below shows the simulation result.

![Figure 3](image_url)

**Figure 3.** (a) Ethanol distribution when the temperature of ethanol vapor is 50°C while the ambient temperature is 25°C. (b) Ethanol distribution when the temperature of ethanol vapor is 100°C while the ambient temperature is 25°C. (c) Ethanol distribution when the temperature of ethanol vapor is 150°C while the ambient temperature is 25°C. (d) Ethanol distribution when the temperature of ethanol vapor is 200°C while the ambient temperature is 25°C.
When the ethanol vapor was released at a temperature of 50 °C it tends to spread on the ground level. This is caused by the density of ethanol vapor at 50 °C is heavier compared to the density of surrounding air inside the room. However, when the temperature of released ethanol vapor was increased up to 100 °C, the ethanol vapor starts to float upwards due to the ethanol vapor density start to decrease compared to the density of surrounding air. As the vapor temperature raised beyond 150 °C, the gas accumulates nearby the ceiling. At this level of temperature, the density of ethanol vapor has become lighter than the density of surrounding air. This phenomenon explained why victims who trap in a fire building or house should be crawling to save their lives because the hot smoke will spread at ceiling level. The hot smoke spreads in the upper space of the building when it has a high temperature because it has a lower density compared to the surrounding air inside the building.

4. Conclusion
This paper presented the effect of temperature on the behavior of gas distribution in an indoor environment. For workplace health and safety, gas emissions from early-stage fires, poisonous gas discharge, and explosives in an indoor environment are major important. The study of the gas behavior spreading in the indoor environment can be utilized to identify potential risks of harmful gas and for future risk assessment. The usage of such a computational model would provide useful information for the ventilation system's safe design and exploration of evacuation/mitigation measures. The results of the simulation show that there is an effect of temperature on gas distribution in an indoor environment. The temperature affects the vertical and horizontal dispersion of the gas release in an indoor environment. If there is harmful gas release inside a closed building, it will spread wider when the ambient temperature is high. The simulation also shows that if the harmful gases release at a high degree of temperature they will tend to elevate towards the ceiling level. This is because when the temperature of the released gas is higher the density of the gas will become lower compared to the density of surrounding air.

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