Computational Fluid Dynamics (CFD) based spatial mapping of indoor air quality and thermal comfort in the indoor environment

Tripti Singh Rajput¹, Albert Thomas, Ph.D.¹
¹Department of Civil Engineering, Indian Institute of Technology Bombay, Mumbai, India

Abstract
Indoor environmental quality (IEQ) comprising indoor air quality (IAQ) and thermal comfort substantially impacts the health, well-being, and productivity of building occupants. However, no conclusive research is available to comprehend the spatial variation of the two crucial IEQ metrics, IAQ and thermal comfort, coupled, in a naturally ventilated building space. Previous studies have used Carbon Dioxide (CO₂) concentration as a stand-alone indicator to evaluate IAQ and PMV (predicted mean vote) measures for thermal comfort. Therefore, the proposed study aims at analysing the spatial variation of CO₂ concentration and indoor thermal comfort for a naturally ventilated (NV) classroom using a computational fluid dynamics (CFD) approach. The simulation results are validated with in-situ measurements of CO₂ concentration for the classroom, and they are found to be reasonably consistent. The results of the study show the importance of passive design solutions, such as the Opening-to-Wall Ratio (OWR), in reducing CO₂ exhaled in a breathing zone and improving indoor thermal comfort. Near windows and above the heads of seated occupants, CO₂ build-up is more noticeable in parametric models. The results indicate that with effective ventilation strategies and adequate air circulation in NV building spaces, IEQ can be improved.

Highlights
• Spatial variation of CO₂ concentration and indoor thermal comfort is assessed in the study.
• The implication of sustainable solutions to improve IAQ and thermal comfort is emphasized for naturally ventilated classroom set-ups.
• A full breathing cycle is modelled for each seated occupant to analyse the spatial variations of IEQ metrics.

Introduction
Humans spend 80% to 90% of their time inside buildings, and hence the buildings need to provide a healthy and comfortable indoor built environment (Al horr et al., 2016). However, factors including rapid urbanisation, rising vehicular traffic, and infrastructure development are contributing to extremely poor outdoor air quality. In urban regions with high levels of pollution, outdoor pollutants can enter indoor spaces through doors, windows, and ventilation systems. This causes indoor pollution levels to be high, which has a direct impact on building occupants’ productivity, well-being, and health. In addition to this, specifically in developing countries, the use of coal, wood, and other solid fuels for cooking, is also impacting the indoor environmental quality (IEQ), which includes thermal, acoustic, visual, and indoor air quality (IAQ) (Al horr et al., 2016; Tsantaki et al., 2020). In tropical nations, such as India, the IAQ in 76% of Indian buildings is believed to be subpar, which is 20 times above the World Health Organization (WHO) standard (Kumar et al., 2023). Many health conditions, such as respiratory disorders, allergies, cardiovascular problems, cancer, and asthma are brought on by poor IAQ.

To mitigate some of these effects, the Government of India (GOI) has implemented several programmes, including the IGBC Healthcare Rating System, the National Clean Air Programme, the National Program for Improved Cookstoves (NPIC), and the India Cooling Action Plan (ICAP) (Bhattacharya, 2020; Ganguly et al., 2020; Wei et al., 2015). Despite numerous such schemes and policies, the IEQ continues to decline due to expanding urbanisation, population growth, technological and financial constraints, and a lack of comprehension among stakeholders.

According to ASHRAE recommendations, the building design elements or passive design strategies are also related to acceptable IAQ (Falih, 2019). Therefore, there has been an upsurge in academic and professional interest in evaluating IAQ in relation to passive design features. One such effort was to identify the passive design parameters of rural kitchens in India using field survey data that enable improvement in IAQ without the inclusion of any external driver such as upgraded cookstoves or chimneys (Debnath et al., 2016). Passive design solutions include important considerations for the building’s exposure to convective airwaves and natural light. Nonetheless, a change in pressure between the inlet and outlet apertures (windows and doors) serves as a gauge of convective air movement in building spaces. Therefore, the opening-to-wall ratio (OWR) is among the significant passive design strategies that need to be considered while analysing IAQ in buildings.

For assessing IAQ, carbon dioxide (CO₂) concentration is used as a standalone indicator by several studies (Szcurek et al., 2015; Persily, 2022). The ambient air contains carbon dioxide, with a normal concentration being, and productivity of building occupants. However, factors including rapid urbanisation, urban re...
CO₂ content, rendering them the primary sources of CO₂ in buildings (Persily & Polidoro, 2022). The volume of the air that enters the building space and the strength of the sources, therefore, together contribute to the CO₂ concentration in naturally ventilated (NV) buildings.

Furthermore, elevated CO₂ levels are a sign of the non-existence of fresh air, which has an immediate effect on the health and thermal comfort of building occupants. The two important IEQ metrics, IAQ indicated by CO₂ concentration and thermal comfort integrated into a single study, are not, however, the subject of any decisive research. Few researchers, though, have examined CO₂ concentration and thermal comfort using field surveys and in-situ measurements. One such study investigated the indoor comfort levels in a classroom environment in a school (Heracleous & Michael, 2019a). The authors used a field survey to obtain data, and correlation findings show that incorporating natural ventilation strategies at each break time had a positive effect on the reduction of CO₂ concentration without jeopardizing indoor thermal comfort. Similarly, using year-long field surveys that included simultaneous indoor thermal conditions monitoring and surveys of students’ subjective responses, Wang et al. (2021) explored seasonal changes in the thermal environment and comfort in classrooms in the cold region of China. Likewise, using in-situ measurements of IAQ indicators and the use of statistical models, Sahu et al. (2020) investigated the spatial and seasonal variations of CO₂ in various microenvironments of an Indian technical institution.

As a consequence, in situ, measurements are primarily used to assist investigations of the distribution of CO₂ within building spaces. Due to the restricted number of CO₂ sensors available and the limited number of locations where measurements can be collected in space, it is extremely difficult to analyse the spatial distribution of exhaled CO₂ in building space caused by improper mixing. A numerical simulation, on the other hand, can deliver CO₂ concentration at every point in the computational domain, which is one of the aims of this study. Similarly, because of the imperfect air mixing, indoor thermal comfort will also vary from point to point, making it insufficient to utilise a single value or its ranges for the entire indoor space. Although numerical simulation is a cutting-edge concept for analysing the complexity of the building space and capturing the momentum effect of airflow in the imperfect mixing of air, it is rarely used to simultaneously evaluate IAQ and indoor thermal comfort in a digital simulation environment. Therefore, it will be beneficial in this domain to study the spatial variation of CO₂ concentration and thermal comfort indices with passive design components, particularly for a configuration where occupants are indeed distributed all through the building spaces, such as in classrooms in academic buildings.

Based on the aforementioned limitations, the following are the study’s primary goals:

1. To assess CO₂ distribution and indoor thermal comfort in academic buildings using a spatial mapping technique in a simulation environment.
2. To incentivize the use of sustainable and cost-effective building solutions by highlighting passive design strategies, in particular, opening characteristics such as OWR to concurrently enhance IEQ comprised of IAQ and thermal comfort in the indoor built environment.

**Methodology**

The proposed methodology employed in this research is outlined in Figure 1 below and can be split down into five key steps. The first phase involves gathering the data from the building’s test case study room that would be needed for modelling the building space. In the second phase, the reference test case study room is modelled and simulated using the commercial Computational Fluid Dynamics (CFD) code (Fluent) of the variant ANSYS Fluent 2020 R2 (Matssson, 2022), and the details of the simulation environment will be further explained in the next section. The simulated outcomes are then retrieved for the variables, including temperature, CO₂ concentration, and thermal comfort index.

![Figure 1: Flowchart of the proposed methodology](https://doi.org/10.26868/25222708.2023.1306)

The field data from the test case study room is used to validate the CO₂ concentration. The same test case study room is the basis for the parametric simulations of passive design strategies that are run in the next step. The dataset is eventually put together in the final stage, as depicted in Figure 1, to understand the relationships between IAQ and thermal comfort with regard to the passive design elements for buildings.
Airflow and species dispersion analysis in CFD

The conservation of mass, momentum, and energy equations are used to solve the 3D indoor airflow problem. The equations are given as follows which are adapted from Ashgriz & Mostaghimi (2002):

**Continuity equation:**

\[
\frac{\partial \rho}{\partial t} + \nabla . (\rho \vec{v}) = 0 \quad (1)
\]

where \(\rho\) [kg/m\(^3\)] represents air density, and \(v\) (m/s) is the velocity.

**Momentum equation:**

\[
\frac{\partial (\rho \vec{v})}{\partial t} + \nabla . (\rho \vec{v} \vec{v}) = -\nabla P + \nabla \cdot \tau + \rho \vec{g} \quad (2)
\]

where \(\vec{\tau}\) denotes stress tensor, \(P\) is the static pressure, and \(\rho \vec{g}\) stands for gravitational body force.

**Energy equation:**

\[
\frac{\partial (\rho E)}{\partial t} + \nabla . (\rho \vec{v} E) = \nabla \cdot (\rho k \nabla T - h \cdot \nabla T) \quad (3)
\]

where \(k\) represents effective conductivity, \(E\) is the specific internal energy, \(h\) is sensible enthalpy and \(T\) is the fluid temperature.

Moreover, the set of governing equations is closed using the standard \(k-\varepsilon\) model. The \(k-\varepsilon\) model simulates turbulence by solving transport equations to determine the values of turbulent kinetic energy \(k\) and its dissipation rate \(\varepsilon\).

\[
\mu_t = c_p \rho \frac{k}{\varepsilon} \quad (4)
\]

where \(\mu_t\) is turbulent viscosity.

The species transport equations are solved to simulate the \(CO_2\) concentrations in the proposed methodology:

\[
\nabla (\rho \vec{u} Y_i) - \nabla \cdot \vec{J}_i = S_i \quad (5)
\]

\[
\vec{J}_i = -\rho D_{i,m} \nabla Y_i - D_{i,t} \frac{\nabla T}{T} \quad (6)
\]

where \(S_i\) represents source term, \(Y_i\) is the mass fraction of \(CO_2\), and \(D_i\) is the diffusion coefficient.

The aforementioned airflow modelling and species transport equations are solved in ANSYS Fluent 2020 R2 in the study. Moreover, the study uses the domain-decoupling approach (Kurabuchi et al., 2009) to analyse wind-driven natural ventilation strategy considering the above equations, which are under-explored in earlier studies.

**Formulation of the base test study room**

To present the applicability of the proposed methodology in a tropical climatic region such as India, the study takes a test study classroom from an academic building into account. The reference building is situated in Mumbai, Maharashtra, India. Figure 2 below shows the reference building’s location on Google 3D map. It is approximately 19.07°N latitude and 72.87°E longitude. Mumbai’s climate is described as warm and humid, with an annual mean temperature of 27.2 °C and 242.2 cm of precipitation on average. In Mumbai, February and March serve as the transition months between winter and summer. These months are typically warm and humid. The investigation is carried out in mid-March, when the average temperature ranges from 23°C to 34°C, the relative humidity ranges from 60% to 90%, and the mean wind speed is predicted to be 1–1.5 m/s (ISHRAE data Mumbai). As it reduces the possibility of temperature-related fluctuations in IAQ measurements, the moderate temperature range of this month is appropriate for analysing IAQ and the microclimatic conditions in the built environment.

The second floor of the two-story academic building comprises the test study classroom. The classroom's 40 benches occupy a total of 76.2 m\(^2\) in space. The test study classroom has an aspect ratio of 1:0.75 and its longer axis is aligned east-west. The estimated floor-to-floor height is 3.5 metres, while the external walls' standard thickness is 0.23 metres. Two entrances are positioned in the south and two windows are facing north as shown in Figure 3 below. The study uses sitting mannequins that are 1.22 metres height and have shoulders that are 0.4 metres wide to represent the pupils in the classroom. The area for the mouth opening of the mannequin is kept equal to 1.3 cm\(^2\) for the breathing process consistent with the past literature for the numerical analysis (Katramiz et al., 2022). This is equivalent to 1.3 cm\(^2\) x 1.0 cm in size.

**Computational domain**

In Ansys 2020 R2 package, the AutoCAD model was imported into SpaceClaim. The geometry of the model was cleaned up in SpaceClaim to be processed further. The geometry’s interferences were also removed for refinement. The computational domain’s dimensions were chosen to be sufficiently large to prevent an interruption of the air movement in the test study room’s inlet path for modelling it in an NV set-up, in line with the recommended practices suggested by Franke (2004) and Ghadiri et al. (2013). The classroom has the following dimensions: 10.08 m (L) x 7.56 m (W) x 2.5 m (H), and
the computational domain that was included in the study was 5L x 5W x 3H. The wind logarithmic profile was factored in parallel to the inlet boundary. In addition, the blockage ratio was kept below 3% for the study.

**Grid generation**

The next step is grid generation, which is comprised of breaking up the geometry's entire volume into discrete, distinguishable volumes allowing for the truncation error in numerical simulation to be ignored. In the study, grid generation was carried out using an unstructured mesh using tetrahedral elements, as shown in Figure 4.

![Image](https://example.com/image1.png)

**Figure 3:** (a) Front view of the test study classroom in an AutoCAD model (b) Top view of the test study classroom in an AutoCAD model with a seated mannequin used in CFD simulations

The mesh sensitivity analysis/grid independence test was carried out using two distinct grid sizes of fine and coarse in order to ascertain whether the simulation findings are independent of the grid size and will not vary either by grid density.

**Boundary conditions**

The buoyancy impact is ignored in this analysis as the wind-driven flow supersedes it (Sheikhshahrokhdehkordi et al., 2020; Goudarzi et al., 2021). This assumption is supported by the fact that convective flow, which in this instance is brought on by wind, is the primary mechanism of heat transfer. The walls and ground of the test study room model were referred to as "Walls" and "Ground," respectively. The top and sides of the computational domain were described as "Symmetry". The inlet was a mass flow inlet, and the outlet was kept as a pressure outflow. The walls, ceiling, and floor, temperatures were set to be between 26.5-28°C. A no-slip boundary requirement was set for the walls. Concrete was considered to be the material for walls.

![Image](https://example.com/image2.png)

**Figure 4:** (a) Grid generated for test study classroom model without computational domain (b) Mannequin’s grid generation

The air was modelled as an incompressible fluid made up of four species: oxygen (O₂), carbon dioxide (CO₂), water steam (H₂O), and nitrogen (N₂). Inflow air was considered with a 400ppm volume fraction of CO₂. The species transport equation was solved in the Fluent package to analyse the spatial distribution of CO₂, and the Reynolds Average Navier Strokes Equation (RANS) and standard k-ε were used to simulate turbulence of the airflow. 5% turbulence intensity was considered in simulations. The semi-implicit technique for the pressure-linked equations (SIMPLE) algorithm was used to accomplish the pressure-velocity coupling, and all residuals were set to 10⁻⁵ as the convergence threshold. The air temperature and wind speed for Mumbai are derived from hourly-based ISHRAE data for March. The constant heat flux on the seated mannequin was maintained at 70 W/mannequin.

**Results and discussion**

**Grid independence test**

In the study, the relationship between CO₂ concentration, air velocity, and temperature for two monitoring locations with different occupancies was analysed and can be depicted in Figure 5 below. The study made use of a portable air quality sensor called Huma-i (HI-150), which can measure CO₂ content, air temperature, and air velocity with an accuracy of 5.0% + 50 characters. The sensor's data logging frequency was every 5 minutes. Figure 5 (a) shows the outcome for a sensor with a 17-person occupancy positioned in the middle of the bench (X = 5<m> metres from the back, Z = 1.1 metres from the floor, and Y = 3.3 metres from the outlet). Similarly, Figure 5 (b) displays the findings for the sensor placed at the first-row last bench (X = 0.32 m from the rear side; Z = 1.1 m of floor height; and Y = 3.78 m from the outlet of the test study classroom) with 33 students seated there. Figure 5 reveals that while increased air velocity can reduce CO₂ in the test study classroom, higher temperatures have been
reported for increasing the metabolic CO$_2$ concentration. Next, in the study, two different grid sizes were tested for grid independence analysis. Elements in the coarse grid of the test study room model had a size of around 0.1 metres. Elements on the fine grid were about 0.05 m in size. The comparison of measured CO$_2$ data from the two monitoring sites stated above to the CO$_2$ concentration determined by the CFD using both grids is shown in Figure 6 below. Results from two different grid sizes were found to differ by no more than 85 ppm.

The CO$_2$ concentrations resulting from CFD were found to be lower than the measured levels as shown in Figure 6. The range of uncertainty of the CO$_2$ sensor accounts for the discrepancy between the measured and estimated CO$_2$ readings. Since the percentage error of the CO$_2$ concentration between the measured and fine grids is in the range of 5-10% whereas it is between 8-15% for the coarse grid at different time intervals, it is concluded that the fine grid is more appropriate. Finally, with 6.3 million grid cells contained, the simulation results produced with the fine grid were used for all subsequent simulations.

Figure 5 (a) and (b): Measured CO$_2$ concentration, air velocity, and temperature

Breathing model results

The spatial distribution of the CO$_2$ concentration within the room is considerably impacted by the breathing process modelling of the occupants in the building space. The study models a full breathing cycle using User defined function (UDF) in C programming language for transient simulation runs in CFD.

Figure 6 (a) and (b): Comparison of measured and simulated CO$_2$ concentration for coarse and fine grid elements

The model’s implementation of a full breathing cycle included an inhaling period lasting 2.5 seconds, an exhalation period lasting 2.5 seconds, and a 1-second pause. Figure 7 displays the distribution of CO$_2$ concentrations near the mouth during the subsequent period of the full breathing cycle of the seated mannequin. A model with a full breathing cycle imparts an exhalation velocity of 1.58 m/s and a maximum CO$_2$ concentration of 1000 ppm. The air being breathed by the person is approximately 34 °C in temperature and 95% relative humidity (Hyldgård, 1994).

CO$_2$ spatial distribution and thermal comfort assessment

The study analysed the spatial distribution of IEQ parameters, namely CO$_2$ concentration and thermal comfort, for the end of the class period in an NV classroom environment when doors and windows are left fully open to external conditions (cross-ventilated strategy) while considering the full breathing cycle of occupants in the test study classroom. The height of 1.5 m above the floor, or the heads of seated occupants, is used to analyse CO$_2$ concentrations. It is immensely significant because it provides a more accurate representation of the air quality they are breathing in. Since CO$_2$ tends to build up close to the ceiling, measuring at this level can provide a more precise picture of the air quality in the student’s breathing zones. In compliance with ASHRAE code
regulation for NV buildings, thermal comfort is measured using the corrective predicted mean vote (PMV), which takes 0.5 as an adaptive factor into consideration (Fanger, 1986).

During the simulation run, a UDF file is compiled using the PMV equation from the ASHRAE code (ASHRAE, 2009). To perform the simulations, the constant values of relative humidity (72%), clothing insulation (0.55), radiant temperature (air temperature), and metabolic rate (1.2) are assumed.

The study considered the scenarios, which are given in Figure 8 for performing the parametric simulations of OWR. For warm and humid areas, OWR should not be lower than 5%. Moreover, apertures for adjacent classrooms are not allowed on the walls of academic buildings. As a result, the study considered three OWR cases: the base scenario, the minimum OWR advised, and the maximum OWR feasible in the indoor functional area. For these simulations, the standard dimensions of windows and doors are maintained. Further, the study uses the domain-decoupling approach to analyse wind-driven natural ventilation. By employing outdoor flow field simulations with airflow parameter data from the ISHRAE weather file, the modelling for the domain inside the models is developed using the boundary condition data acquired at the building surface. In the CFD environment, parametric simulations are solved using the same boundary conditions and solver parameters as that of the base test study classroom model.

### Table 1: Summary table of simulated outcomes

<table>
<thead>
<tr>
<th>OWR</th>
<th>Velocity (m/s)</th>
<th>Temp. (°C)</th>
<th>CO₂ con. (ppm)</th>
<th>PMV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model 1</td>
<td>0.19</td>
<td>27.3</td>
<td>1254</td>
<td>0.58</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.23</td>
<td>28.1</td>
<td>1623</td>
<td>0.61</td>
</tr>
<tr>
<td>Model 3</td>
<td>0.3</td>
<td>27.7</td>
<td>710</td>
<td>0.51</td>
</tr>
</tbody>
</table>

Figure 9 depicts the spatial variation of CO₂ concentration and PMV for parametric cases of OWR. Table 1 provides a summary table for each model and displays the area-averaged values for velocity, temperature, CO₂ concentration, and PMV that were determined in a simulated environment.

### Discussion

According to Table 1 above, when the cross-ventilation technique is implemented in the test study classroom, the CO₂ concentration lowers while the OWR percentage increases and the PMV simultaneously rises. The PMV value between +0.5 to -0.5 and the CO₂ concentration range within 1000 ppm offer an acceptable level of indoor thermal comfort and IAQ, respectively (ASHRAE, 2009). Figure 9 shows that CO₂ build-up is evident in all models near windows and above the heads of seated occupants. In all three test study models, with windows acting as inlets and doors as outlets, the venturi effect can help enhance airflow within the classroom space. When the windows are opened, they provide a larger opening area than the doors, creating a higher air pressure outside the building. As a result, air flows from the windows towards the lower-pressure area inside the classroom models. However, Model 1 performs better than Model 2 overall, although it delivers less air volume into the classroom and has a lower proportion of OWR. In Model 1, the smaller inlet aperture results in an airflow path constriction that resembles a venturi tube. The air’s velocity increases as it flows through these narrow inlets, causing a pressure drop. The air is further prompted to move towards the doors, which serve as outlets, contributing to improved IAQ and thermal comfort performance. This draws attention to a key aspect of designing sustainable buildings, specifically the careful consideration of the relative positioning and dimensioning of opening apertures in cross-ventilation strategies. Moreover, Model 3 with the highest OWR percentage represents the best IAQ and thermal comfort performance, with an area-averaged CO₂ concentration of 710 ppm and PMV of 0.51, respectively, that fall within the acceptable range. The findings demonstrate that implementing the venturi effect and adequate ventilation strategy in NV building spaces can enhance both IAQ and thermal comfort. However, it is vital to note here that in some circumstances, the venturi effect might not be enough to deliver the optimum ventilation rates to dilute air contaminants and enhance air circulation within building spaces. Factors such as building orientation, outdoor air...
quality, and indoor air distribution systems should also be considered to achieve efficient airflow indoors.

Furthermore, the study's findings emphasise the need for passive design features and sustainable indoor built environments to be integrated when designing academic spaces. OWR is an essential design strategy that needs to be assessed for NV efficacy and IEQ factors, such as IAQ and thermal comfort. Additionally, the proposed methodology in the study enables decision-making regarding the layout of the space and passive design elements without having to be physically present in the built environment by allowing navigation through spaces and mapping locations that are identified with higher CO₂ concentration and discomfort.

Nonetheless, two key limitations of this study should be acknowledged. First, the constant heat flux emitted by the seated mannequin was the only heat source that was taken into consideration. There were no provisions made for additional heat sources, such as electronic equipment. Second, the study did not evaluate the occupant’s breathing rates in the classroom space directly. Instead, it made use of usual breathing rates from prior research. When interpreting the findings and implementing them in real-world scenarios, these limitations should be factored in.

Conclusion
The study examined the spatial distribution of critical IEQ metrics, including IAQ and thermal comfort, while incorporating the building envelope's opening characteristics, or OWR, in a CFD environment. In the working plane of 1.5 m from the floor height of the classroom model, the proposed framework exhibited its capability for predicting the spatial variation of CO₂ distribution and PMV to evaluate IAQ and thermal comfort, respectively. The results show that the accumulation of CO₂ concentration can be decreased by incorporating greater OWR percentages within building envelopes. Cross-ventilation techniques must, however, take into account the relative location and dimensioning of opening apertures. Near windows and above the heads of sitting occupants, CO₂ buildup is more noticeable in parametric classrooms. The results indicate that with effective ventilation strategies and adequate air circulation in NV building spaces, IAQ and thermal comfort can be improved.

Future studies should concentrate on developing IoT devices, sensors, and transducers that can precisely monitor and analyse CO₂ concentration and indoor thermal comfort at various points across an indoor environment for identifying the problem areas. As a result of combining these elements into the indoor environment design, would aid in determining the optimum passive design parameters for sustainable habitats.

References


---

**Figure 9:** Spatial variation of IEQ parameters, CO₂ concentration, and thermal comfort at 1.5 m floor height with the same occupancy for Models 1, 2, and 3 (top view). The dotted rectangle represents the area of seated mannequins.