

Article

Proposal for a Simplified Method to Calculate the Concentration of CO₂ in a Classroom Using CFD Simulation and Its Experimental Validation

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Abstract

The present study addresses the problems of predicting the distribution of CO₂ in a classroom where limited ventilation may compromise air quality. Through Computational Fluid Dynamics (CFD), a detailed analysis of airflow, temperature, and CO₂ dispersion was carried out; however, due to its high computational cost, real-time applications are limited. Therefore, this work proposes a simplified CFD approach to model human breathing based on a constant airflow velocity and an average CO₂ concentration, preserving mass balance while reducing computational demand. Three mathematical breathing models (constant, complete, and sinusoidal) were formulated and compared through CFD simulation with the classroom model. Subsequently, a CO₂ detection module based on SCD40 sensors was developed for the experimental validation of the simplified model, recreating the simulation conditions in a real environment. The results show strong agreement between the simplified model and the complex models, as well as with experimental measurements, with relative errors between 0.05% and 10% at different monitoring points. The proposed model reduced calculation time by more than 98% compared to the sinusoidal model, without compromising accuracy. These results show that the simplified model is an efficient alternative for predicting CO₂ concentration, allowing its integration into real-time control systems.

Keywords: CFD simulation; breathing models; experimental validation; CO₂; air quality



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1. Introduction

A fundamental factor in human health is indoor air quality, especially in enclosed spaces with little or no ventilation, which leads to the accumulation of pollutants. This is particularly true for pollutants naturally produced by the human body and exhaled through respiration, as they not only affect the body's ability to breathe but also contribute to the overall health of the environment. We release not only CO₂ but also other gases and respiratory aerosols that can carry pathogens [1]. Therefore, indoor spaces with high occupancy, such as school classrooms, represent a significant risk of exposure to contaminants and disease transmission, making it relevant to conduct studies on efficient and effective ventilation of these spaces.

Determining the quality of indoor air depends on several factors; however, CO₂ is an excellent parameter for measuring these levels: Ref. [2] demonstrated the correlation be-

tween CO₂ and the concentration of exhaled particles, while [3,4] argue for the appropriate use of CO₂ as an indicator of ventilation rate and, therefore, existing health risks. Therefore, knowing CO₂ concentration levels is essential for evaluating, designing, and optimizing ventilation strategies for indoor spaces.

CO₂ levels are measured by monitoring the gas with sensors placed at various points within the area of interest. However, these sensors only provide information about their specific location, without offering additional data to determine the spatial distribution of CO₂. Obtaining the complete spatial distribution and dynamics of CO₂ throughout the entire volume of an enclosed space would require filling the space with an excessively dense network of sensors, which is impractical. This is where computational fluid dynamics (CFD) becomes relevant, serving as a powerful tool to overcome this limitation. CFD allows for the virtual modeling of airflow, transport, and CO₂ concentration at each point in space by numerically solving fundamental fluid dynamics equations (Navier–Stokes, conservation of mass, energy, and species) without resorting to solutions that are too trivial in reality.

Despite this advantage, among many others, CFD simulations have a limitation when used in real-time control systems, primarily the high demand for computational resources, such as memory and processing time, which increases with the number of physical parameters considered. This complicates their implementation in closed-loop control systems, where they could aid in evaluating internal ventilation and activating certain actuators to maintain safe CO₂ levels.

Regarding CO₂ levels, international organizations have established recommended values to ensure air quality in indoor spaces. Some, such as ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers), do not establish a mandatory limit but consider concentrations around 700 ppm adequate for comfort and odor control, and concentrations above 1000 ppm indicate a deficiency in ventilation, causing an accumulation of pollutants and even drowsiness and fatigue [5,6]. Others, such as the U.S. Occupational Safety and Health Administration (OSHA), establish a permissible exposure limit of 5000 ppm during an eight-hour workday in relation to the workplace [7]. On the other hand, NIOSH (National Institute for Occupational Safety and Health) supports the above and adds that levels above 10,000 ppm are a short-term health risk, potentially causing symptoms such as headaches, dizziness, and difficulty concentrating [8]. Other research, such as studies conducted by the Harvard T.H. Chan School of Public Health, indicates that even moderately high concentrations of around 2500 ppm have health repercussions, negatively impacting cognitive performance, even without obvious physical symptoms [9]. At the other end of the spectrum, concentrations exceeding 40,000 ppm are potentially dangerous and lethal with prolonged exposure due to oxygen displacement and the gas's toxic effects. The data presented serve as valid reference values for evaluating indoor air quality and ventilation in CFD simulations [10], and in real-world applications for CO₂ level control, they would serve as a reference for triggering actuators that help maintain CO₂ concentrations below 1000 ppm [11,12].

Predicting the spatial distribution of CO₂ in classrooms is a topic frequently addressed in research, as high CO₂ levels negatively impact students' academic performance and health. For example, studies such as [11,13–15] demonstrate that increasing ventilation rates by improving air circulation effectively reduces CO₂ concentrations and other pollutants. Other studies maintain that factors such as wind direction, occupant density, heat sources, and building orientation also influence indoor air quality [16]. Analyzing all these factors using CFD has allowed for the optimization of space design, improving ventilation and air quality [12,17,18]. Even during the COVID-19 pandemic, CFD enabled the analysis of virus exposure in classrooms [19–21].

The main advantage of using CFD simulation is the ability to perform detailed analyses of airflow patterns and other fluids without the need for tedious experimental measurements. However, the reliability of these simulations must be rigorously validated against experimental data. Studies such as [11] show that CFD can simulate thermofluidic phenomena with an accuracy greater than 98% compared to experimental data. Other studies, such as [22–24], indicate that for CO₂ analysis, deviations can range from 4–5.2%, and up to 30% when heat transfer is considered. Furthermore, effectively validating a model requires an accurate characterization of the environment and its conditions, as well as multiple measurements and their statistical analysis for deviations [25,26].

As previously mentioned, one of the most relevant applications of CFD simulations is their integration into closed-loop control systems, enabling better temperature and airflow management within a system. Some studies focused on this type of application include [27], which used a combined response surface model (RSM) and CFD to optimize thermal distribution in servers and data center infrastructure. Similarly, ref. [28] used CFD to design a novel heat sink with adaptable fins to improve the thermal management of microchips. These systems demonstrate how CFD helps achieve better results in real-time systems, highlighting the importance of developing simplified CFD models to represent complex processes such as human respiration and CO₂ for integration into control systems.

With regard to the above, recent studies have demonstrated strong agreement between CFD simulations and experimental data in modeling human respiration, particularly in research on nasal cavities, airways, and tracheae [29–31], with relative deviations of approximately 10% [32]. Ref. [33] highlights a critical point: static airway models can vary by up to 237% compared to dynamic simulations, underscoring the importance of incorporating physiological motion into CFD analysis. Other studies specifically evaluate the prediction of inhaled CO₂ concentration and gas exchange efficiency [34,35].

Considering all the variables involved in human respiration in classroom simulations (exact anatomical geometry, flow variables such as velocity, pressure, density, viscosity, relative humidity, temperature, rhythmic movement of the rib cage and diaphragm, metabolism, respiratory diseases, among others) requires considerable computational effort. Therefore, researchers resort to simplified models that describe the process using three main approaches: the constant model, the full-breath model (square curve), and the sinusoidal model [34,36–39]. The accuracy of these models depends on more general parameters such as mass flow rate, exhaled air velocity, body and exhaled air temperature, and simplified nasal geometry.

The literature reports various parameters for modeling human respiration in CFD simulations, focusing on boundary conditions and the geometric representation of the real world.

In general, there are primarily four boundary conditions in this type of simulation. The first is the concentration of exhaled CO₂, with reported values ranging from 36,000 ppm [36] to 52,778 ppm [40], although some authors express it as a percentage: 4.0% [16], 5% [18], or as a volumetric flow rate of 0.31 L/min [19]. Ref. [39] used a sinusoidal function for respiratory flow and a concentration of 40,000 ppm in their study with realistic human models. The second is the exhaled airflow, for which [36] reports that a sleeping person has an average flow rate of 6 L/min, a value also used by [40] for nasal breathing.

In [16], they define a mass flow rate of 0.000164 kg/s. The third parameter is the temperature of the exhaled air, with reported values ranging from 34.0 °C [16] to 37 °C [18]. The fourth is the exhalation velocity, which [18] reports as 0.37 m/s, while [40] manually calculated 0.8 m/s for a mouth area of 1.3 cm².

Regarding geometric representation, ref. [41] compared the use of mannequins with simplified “human-box” models, obtaining similar results and concluding that the latter yielded reliable results. Works such as [36] used a simplified human-box geometry, simulating three breathing models (constant, full, and sinusoidal), and subsequently validated them experimentally by measuring CO₂ levels for three hours with four sensors, concluding that the three models produced results close to the measurements.

The cited studies show that CFD models typically define exhalation using an airflow (in terms of mass or volume), which can vary over time or remain constant depending on the respiratory model used, and that the CO₂ concentration is usually set as a constant number or as a percentage in the exhaled air. This traditional approach can be computationally expensive.

Therefore, the main objective of this work is to propose a simplified CFD model of human respiration using an alternative approach based solely on airflow velocity and a constant CO₂ concentration, while maintaining a correct mass balance of CO₂ supplied during exhalation. This aims to minimize the computational resources and simulation time required for calculations, making the model more suitable for implementation in a real-time closed-loop control system. Finally, the resulting model will be validated through experimental measurements.

2. Materials and Methods

This work consists of the following stages: (1) Differences between the proposed method and traditional methods; (2) Mathematical modeling of respiratory patterns; (3) Development of equations by the model; (4) CFD Model and Boundary Conditions; (5) CFD Simulation and Validation of the Proposed Breathing Model; (6) Development of the detection module; and (7) Experimental validation of the proposed breathing model. Each of these stages is described in detail below.

2.1. Differences Between the Proposed Method and Traditional Methods

Table 1 presents an ordered comparison of the method proposed in this work with traditional CFD models used for CO₂ concentration studies. The main differences lie in how exhaled air and CO₂ concentration are modeled.

Table 1. Differences between models.

Exhaled Air	Proposed Method (Constant Breathing)	Methods Reported in the Literature
CO ₂ flow	Constant air velocity in m/s based on mouth geometry.	Variable air flow in kg/s or L/min, value defined according to the breathing models (constant, square, sinusoidal).
CO ₂ concentration	Average value in ppm according to the respiration models (constant, square, sinusoidal).	Given in ppm or as a constant percentage.

As shown in Table 1, the proposed method simplifies the representation of human respiration by using constant values for both exhaled air velocity and CO₂ concentration, whereas traditional methods employ variable flows and constant or percentage concentration. This simplification aims to reduce computational load without compromising result accuracy. The most commonly used respiration models are described below.

2.2. Mathematical Modeling of Breathing Models

Human respiration, like many physiological processes, can be mathematically modeled. Because it is a periodic process, it is common to analyze a complete cycle to obtain an

equation that describes its general behavior. Refs. [36–38] report three ways of representing breathing. Each will be described below. The complete breathing model (Figure 1, red line) considers the average of a complete respiratory cycle for a resting adult, with a respiratory rate of 10 min^{-1} , so a respiratory cycle has a period of approximately 6 s. This model states that inhalation and exhalation have approximately equal durations of 2.5 s, with a 0.5 s pause before the start of the next cycle.

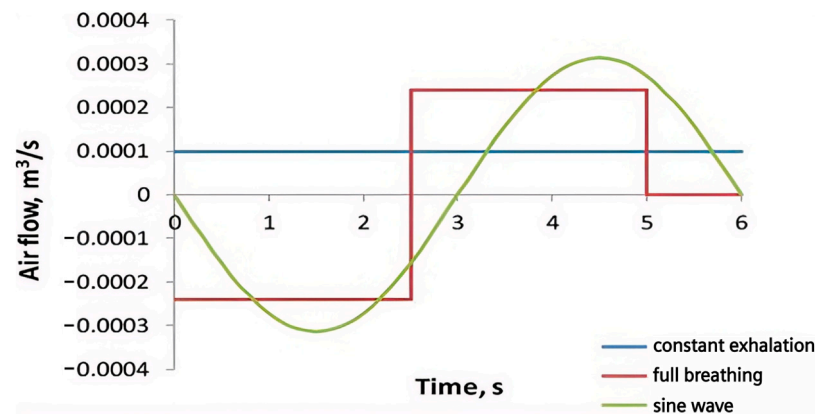


Figure 1. Models of breathing [36].

In the constant-breathing model (blue line), typically half of the volumetric contribution of a complete cycle is considered. The sinusoidal breathing model (green curve), on the other hand, is represented by equation $\dot{Q}_b = a \sin \beta t$ [36–38], where $\dot{Q}_b$ is the instantaneous volumetric flow rate of exhaled CO_2 , t is time, a is the maximum concentration of exhaled CO_2 , and β is the exhalation frequency. Unlike previous work that models volumetric flow, this study addresses respiration from the perspective of CO_2 concentration. This methodological difference requires adapting the characteristic equations of each model, as explained later.

2.3. Development of Equations by Model

In Figure 2, the area under the curve represents the cumulative exposure to exhaled CO_2 in each respiratory cycle; therefore, for each model, this area is equivalent to the integral with respect to time t . Let be T the period and C_0 the CO_2 concentration for the constant-breathing model (blue). Then, the equations describing each model are obtained as follows:

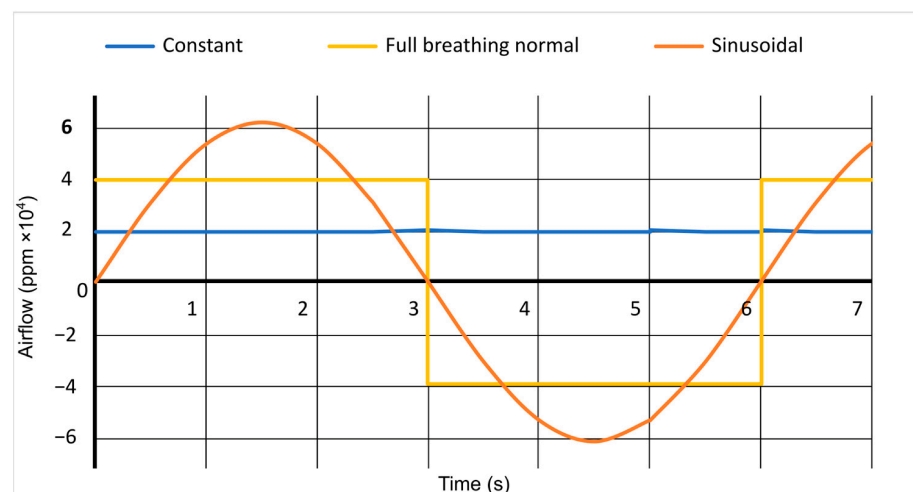


Figure 2. Breathing model curves.

Constant Model: The concentration $C(t) = C_0$ remains constant over time. The area under the curve during the period T for constant concentration is:

$$A_{cte} = \int_0^T C_0 dt = C_0 T \quad (1)$$

Full (square) breathing model: Complete breathing has two variations. One considers the pause a person makes between breathing cycle, and the second variation is a simplification of the first (yellow), in which the square cycle has a maximum C_s and a $-C_s$ minimum value. When exhaling, the curve is positive only for a fraction d_s of the period (50% of the complete cycle in this case). Therefore, the positive portion will last $d_s \times T$ for half the period, and its maximum value is the missing value C_s . Mathematically, this can be written as:

$$A_{cda} = \int_0^{d_s T} C_s dt = C_s d_s T \quad (2)$$

Since the full-breath model must exhale the same amount as the constant model, equating Equations (1) and (2) gives the following equation:

$$C_s d_s T = C_0 T C_s = \frac{C_0}{d_s}, \quad (3)$$

Sinusoidal Model: The sinusoidal model has the following form

$$C(t) = A \times (\sin \omega t) \quad (4)$$

where A is the amplitude of the function, in this case the maximum concentration of exhaled CO_2 , and $\omega = \frac{2\pi}{T}$ is the frequency of the given function in terms of the period. Analyzing the positive part of the curve from $t = 0$ to $t = \frac{\pi}{\omega} = \frac{T}{2}$, then the integral of the positive area per cycle is:

$$A_{\sin} = \int_0^{\frac{\pi}{\omega}} A(\sin \omega t) dt = -A \left[\frac{\cos \omega t}{\omega} \right]_0^{\frac{\pi}{\omega}} = -A \left(\frac{\cos \pi - \cos 0}{\omega} \right) = A \left(\frac{2}{\omega} \right), \quad (5)$$

$$\text{As } \omega = \frac{2\pi}{T}$$

$$A_{\sin} = A \left(\frac{2}{\omega} \right) = \frac{2A}{\frac{2\pi}{T}} = \frac{AT}{\pi}, \quad (6)$$

Equating the area of the sinusoidal function with that of the constant function (Equations (1) and (6)).

$$\frac{AT}{\pi} = C_0 T, \quad (7)$$

Therefore, the amplitude of the sinusoidal function will be

$$A = \pi C_0, \quad (8)$$

In the studies cited above, the CO_2 concentration during inhalation and exhalation is approximately 40,000 ppm. That is, for a complete breath $C_s = 40,000$ ppm. Therefore, for constant breathing, the CO_2 intake will be

$$C_0 = C_s d_s = 40,000 \times 0.5 = 20,000 \text{ ppm} \quad (9)$$

This approach allows for the representation of a sustained average CO₂ concentration over time, eliminating the need to define parameters such as mass flow rate and time-dependent functions. This significantly reduces the computational load when modeling respiration, limiting it to just two variables: the velocity of exhaled air and the CO₂ concentration.

To verify this claim, three independent CFD simulations were performed—one for each breathing model—with the aim of comparing their results and evaluating the accuracy of the proposed method.

2.4. CFD Model and Boundary Conditions

The space selected for the CFD study was classroom A009 in building A on the TECNAM Veracruz campus. The classroom has the following dimensions and characteristics: 6 m wide, 8 m long, 2.5 m high, and a total volume of 120 m³. Figure 3 shows the interior of the classroom, which has the following characteristics: an air conditioning system (air supply), two windows, one measuring 1.7×1.7 m and the other 3×1 m (considered closed during the study), twenty-eight student chairs, a teacher's desk, and a closed door. A total of 28 students were included in the model, matching the actual class size that will subsequently be employed during the experimental phase. Likewise, it was assumed that the occupants exhibited behavior consistent with light speaking activity (not just nasal), resulting in a greater contribution of CO₂.



Figure 3. Selected classroom.

Figure 4 presents the geometric models used in the CFD simulation: (Figure 4a) shows the occupants (human-box model) and (Figure 4b) shows the study space. The virtual model of classroom A009 developed in the CFD simulator presents simplifications implemented to optimize computational consumption without compromising the accuracy of the results, which are:

- Removal of rounded edges and chamfers;
- Simplifying complex geometries in desks and chairs;
- Representation of occupants using human-box models [41].

The materials used in the CFD model are detailed in Table 2. The selection of these materials and their thermal properties are fundamental to correctly simulating heat transfer and fluid dynamics in the classroom.

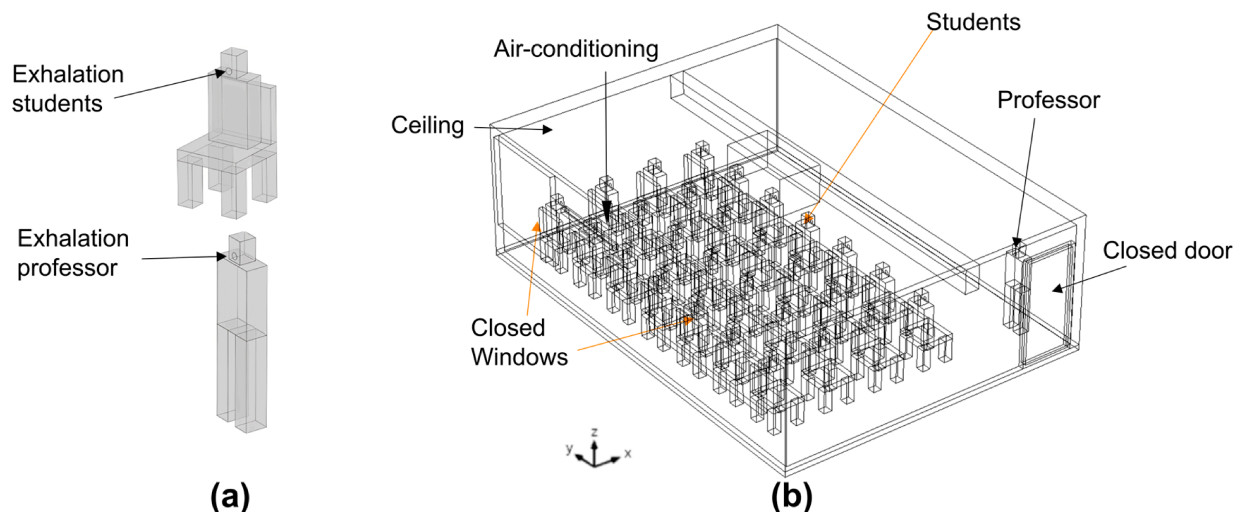


Figure 4. Geometric models for CFD simulation. (a) Human-box model; (b) study space.

Table 2. Materials and characteristics.

Material	Density (kg/m ³)	Cp (J/Kg × K)	Thermal Conductivity (W/m × K)
Air	1.29	1005.2	0.02
Concrete (Roof and walls)	2300	880	1.8
Human tissue (Human-box models)	1090	3421	0.49
PVC (Student Seats)	1200	1500	0.2
Glass (Doors and windows)	2203	703	1.38
Pino (Teacher's Desk)	560	1500	0.163

Boundary conditions are parameters defined in the CFD model, such as air velocity, temperature, and concentration. These values are presented in Tables 3–5, and their locations in the model are shown in Figure 4.

Table 3. Airflow parameters.

Element	Geometry Size	Boundary Condition	Value
Air conditioning supply	1.5 × 0.1 m	Speed	2.06 m/s
Exhalation students	Radius 0.03 m	Speed	0.1 m/s
Exhalation, professor	Radius 0.03 m	Speed	0.1 m/s

Table 4. Mass transport parameters.

Breathing Pattern	Parameter	Geometry	Boundary Condition	Value
Constant	Air conditioning supply	1.5 × 0.1 m	Concentration	430 ppm
	Exhalation students	Radius 0.03 m	Concentration	20,000 ppm
	Exhalation, professor	Radius 0.03 m	Concentration	20,000 ppm
Complete	Air conditioning supply	1.5 × 0.1 m	Concentration	430 ppm
	Exhalation students	Radius 0.03 m	Concentration	$C(t) = \begin{cases} 40,000, & \text{if } (t \bmod 6) < 3 \\ 0, & \text{if } (t \bmod 6) \geq 3 \end{cases} \text{ ppm}$
	Exhalation, professor	Radius 0.03 m	Concentration	
Sinusoidal	Air conditioning supply	1.5 × 0.1 m	Concentration	430 ppm
	Exhalation students	Radius 0.03 m	Concentration	$C(t) = 20,000\pi \sin \frac{2\pi t}{6} \text{ ppm}$
	Exhalation, professor	Radius 0.03 m	Concentration	

Table 5. Heat transfer parameters.

Element	Geometry	Boundary Condition	Value
Ceiling	6×8 m	Temperature	$30\text{ }^{\circ}\text{C}$
Windows	2.7×0.38 m	Temperature	$40\text{ }^{\circ}\text{C}$
People		Temperature	$37\text{ }^{\circ}\text{C}$
Walls	$6 \times 2.5; 8 \times 2.5$ m	Temperature	$40\text{ }^{\circ}\text{C}$
Air conditioning	1.5×0.1 m	Temperature	$25\text{ }^{\circ}\text{C}$

For the CFD simulation, a time of 2000 s was used, and it was assumed that the classroom occupants were at rest (seated) and participating in class (speaking moderately). Studies such as [42–44] indicate ranges of $10 \frac{\text{L}}{\text{min}}$ to $20 \frac{\text{L}}{\text{min}}$ for normal/moderate speech. Therefore, taking a flow rate $Q = 17 \frac{\text{L}}{\text{min}}$ and an exhalation radius of $r = 0.03$ m the exit velocity will be

$$v = Q/\pi r^2 \approx 0.1 \frac{\text{m}}{\text{s}} \quad (10)$$

The CFD simulations were performed using the same parameters, including the mesh and boundary conditions. The specifications of the numerical implementation of the CFD simulations are described in Appendix A.

3. Results

3.1. CFD Simulation to Compare the Proposed Model with Other Models

The purpose of this simulation is to compare the behavior of the 3 breathing models (constant, complete, and sinusoidal) under equal conditions to verify that their behavior is equivalent.

Figure 5 shows the results obtained, illustrating the CO₂ concentration distribution for each respiration model: constant (Figure 5a), complete (Figure 5b), and sinusoidal (Figure 5c). The cross-section is located 1.2 m above ground level. Visually, it can be inferred that the CO₂ concentration results for the three respiration models are similar, particularly in areas with high concentrations.

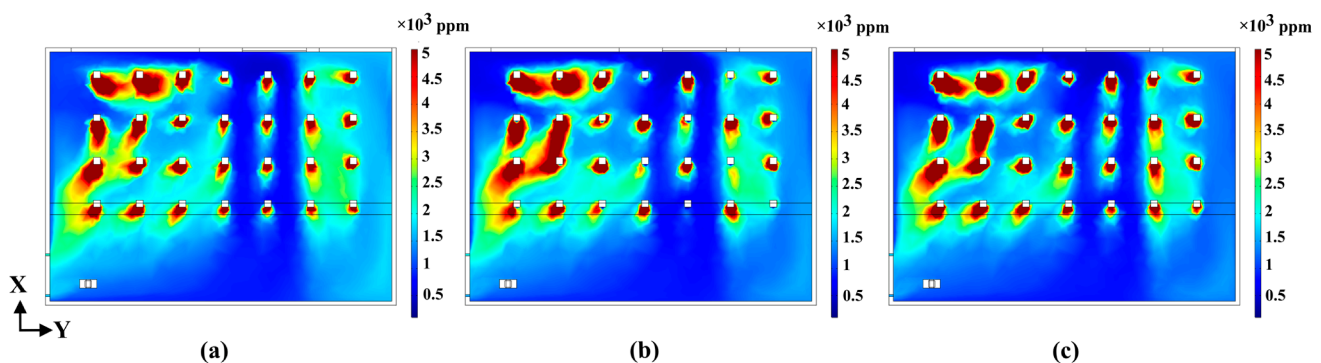


Figure 5. CO₂ concentration in the x-y plane. (a) Constant breathing; (b) Complete breathing; (c) Sinusoidal breathing.

To quantitatively assess the similarity among the three breathing models, nine strategic points were selected and distributed throughout the classroom (Figure 6). These points are located at strategic locations near areas of interest: the student area, the teacher area, and the area near the door.

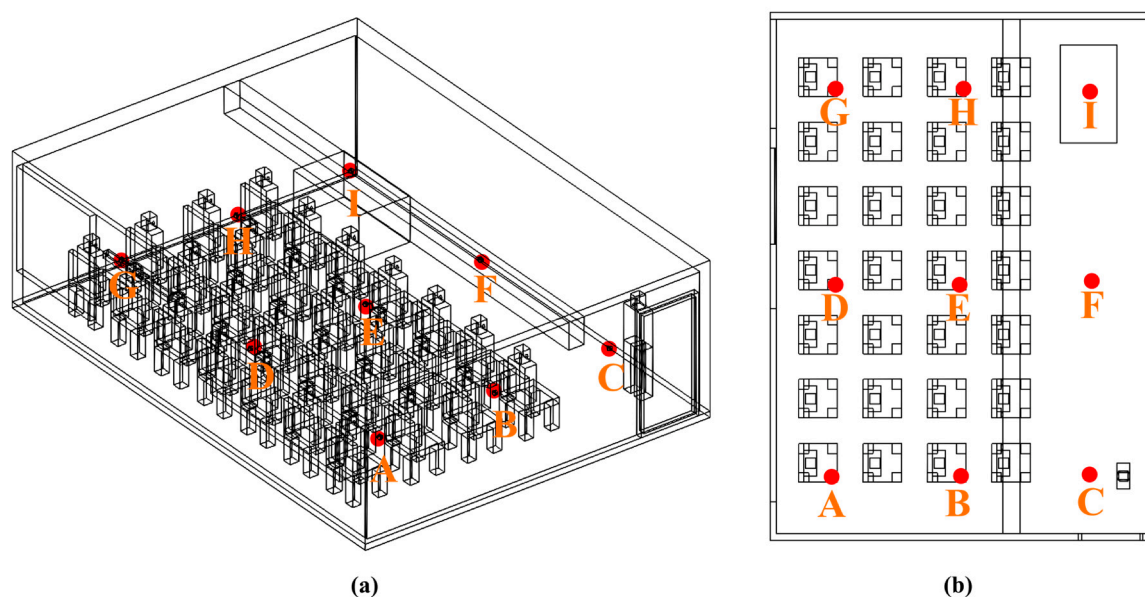


Figure 6. Simulation points for the three models. (a) Isometric view; (b) x-y plane.

In Figure 7, we can observe the results obtained for a simulation time of 2000 s for each breathing model, showing at a glance that there is a strong relationship between the three, such that:

1. The constant breathing model (blue line) shows smoother, more predictable behavior, with minimal variation over time.
2. The full and sinusoidal breathing models (yellow and red lines) exhibit more unpredictable behavior, with more pronounced variations due to the periodic nature of their associated functions.

The results show that the three models follow a similar trend, suggesting that, for practical air quality monitoring applications, the simplified Constant breathing model yields results comparable to those of the complex models. One result that is highly relevant when comparing the three models and deciding which is most feasible to implement in a real-time control system is the computation time. Table 6 presents the computation time for the three simulations.

Table 6. Resources demanded by simulations.

CFD Breathing Model	Calculation Time
Constant	242 s
Complete	6360 s
Sinusoidal	13,080 s

As shown, the constant-breathing model has a considerably shorter simulation time than the other two, reducing it by 98% compared to the sinusoidal-breathing model. However, this did not compromise the accuracy of the results. Figure 8a shows (red lines) the air streamlines within the classroom, obtained from the CFD model, illustrating how the supplied air moves from one end of the room to the other. Some of this cool airflow recirculates at the back of the room, while the rest is distributed toward the front, reaching the areas near the door and the desk. Figure 8b shows the simulated temperature distribution on the classroom surfaces (ceiling and walls) using previously measured temperature conditions.

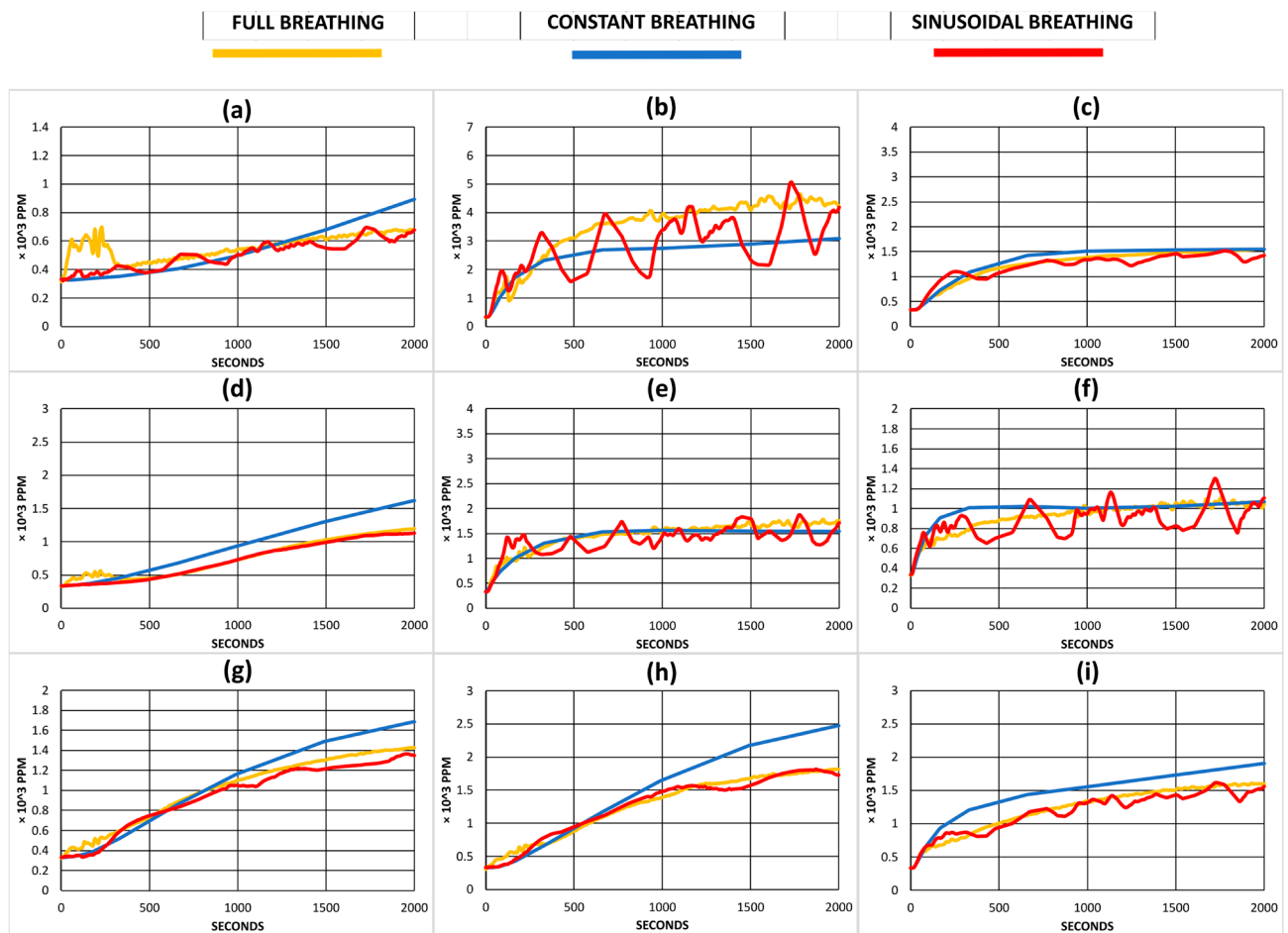


Figure 7. CO₂ concentration as a function of time for the three breathing models.

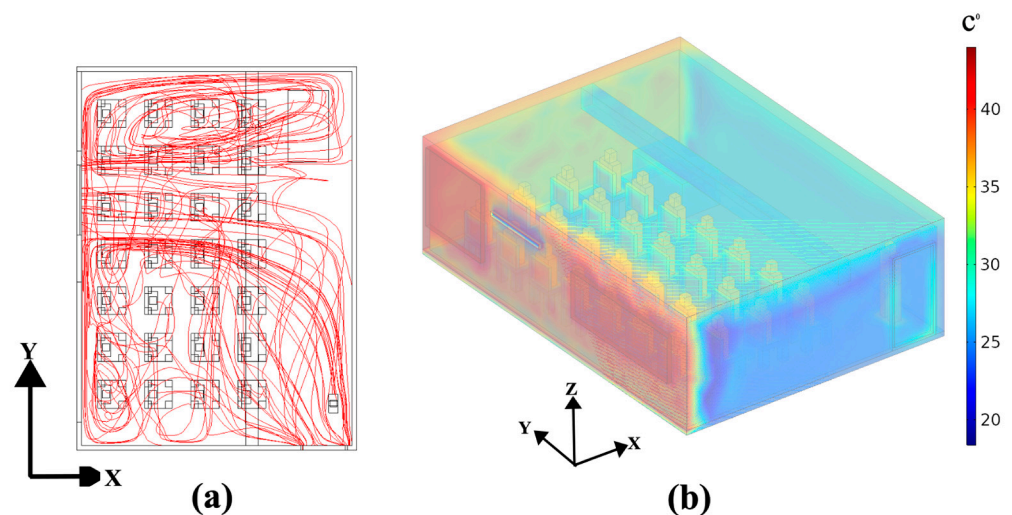


Figure 8. Results obtained using CFD. (a) Air streamlines; (b) Temperature field.

3.2. Development of the Sensing Module

The sensor module consists of two main components that work together to measure and transmit data on air quality:

1. ESP32 Microcontroller: Manufactured by Espressif Systems (Shanghai, China), it serves as the processing and communication unit of the module.

- Low power consumption system (SoC—System on Chip);
- Tensilica Xtensa LX6 Processor (dual core or single core);

- Clock frequency: up to 240 MHz;
- Connectivity: Dual mode Wi-Fi and Bluetooth;
- Capacity for local processing and remote transmission of data is required [45].

2. SCD40 Sensor: The SCD40 sensor of Sensirion AG (Stäfa, Switzerland) specializes in indoor carbon dioxide monitoring using photoacoustic sensing technology. Its operating principle is based on:

- Detection of CO₂ concentration through photoacoustic non-dispersive infrared (NDIR) measurement.
- Emission and absorption of infrared light are proportional to the concentration of carbon dioxide present in the air.
- Generation of calibrated digital measurements of CO₂, temperature, and relative humidity through an internal signal processing system.
- It is compatible with Arduino and ESP32 microcontrollers through I²C communication and specialized libraries provided by Sensirion [46].

The functionality of the module (see Figure 9) consists of executing an algorithm for CO₂ detection that includes the following phases:

- Data Acquisition: The ESP32 acquires, via I²C and the specialized Sensirion library for the SCD4x series, information on CO₂ concentration, temperature, and relative humidity. Furthermore, this sensor does not require prior calibration since it incorporates an automatic self-calibration system.
- Storage and transmission: Locally stores processed data while transmitting it via Wi-Fi to a .csv file in the cloud, enabling real-time viewing of the data.

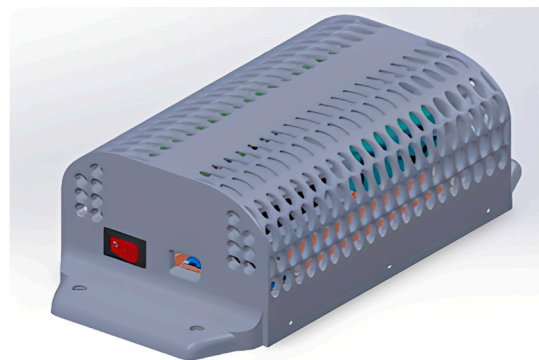


Figure 9. Detection module.

3.3. Experimental Validation of the Proposed Breathing Model

The validation of the proposed breathing model was carried out through in situ experimental measurements in classroom A009. Five sensing modules were used, built according to the methodology described in Section 3.2. To experimentally validate the proposed breathing model, a second CFD simulation was carried out, reproducing in the simulator the classroom conditions as closely to reality as possible. For this, the following was considered:

- Total time of the experiment: The experimental measurements were conducted on Wednesday, 29 April 2026, from 10:40 a.m. to 12:00 p.m. (± 3 min), which corresponds to an approximate time of 5000 s.
- Initial Conditions from classroom: The classroom had remained empty since the previous day, which allowed the CO₂ levels to stabilize around 500 ppm. The air conditioning had been turned on before the start of the measurements, maintaining the internal temperature at 22.7 °C, and the initial relative humidity was 37.24%.

- Occupant breathing: Although students remained seated during the class, the group activity resembled loud speaking rather than moderate speaking. Consequently, a higher airflow rate of approximately 34 L/min was selected, corresponding to an air velocity of about 0.2 m/s, as defined in Equation (10). This and the two previous points are summarized in Table 7.
- Occupancy of the classroom during the experiment: The students entered the classroom in a staggered manner during the experimental period. Table 8 presents the number of students in the classroom and their arrival times.

Table 7. Experimental conditions from the classroom.

Conditions Considered for the CFD Simulation	
Initial CO ₂ concentration (ppm)	500
Initial classroom temperature with the air conditioner turned on (°C)	22.7
Initial relative humidity (%)	37.24
Total time of the experiment (seconds)	5000
Exhalation velocity of the occupants (m/s)	0.2

Table 8. Temporal Occupancy Distribution.

Temporal Occupancy Distribution			
	Time (s)	New students	Cumulative total
Arrival interval	0–1000	7	7
	1000–2000	7	14
	2000–3000	7	21
	3000–5000	7	28

For the experimental measurements, strategically distributed points were used to observe CO₂ concentration in different areas of the classroom. These measurement points are shown in Figure 10, and their spatial coordinates (x, y, z) are as follows: M1 (5.8, 6.8, 0.9); M2 (4.6, 0.2, 0.75); M3 (3, 4.2, 1); M4 (0.4, 0.2, 0.75); and M5 (1.2, 7.9, 0.9).

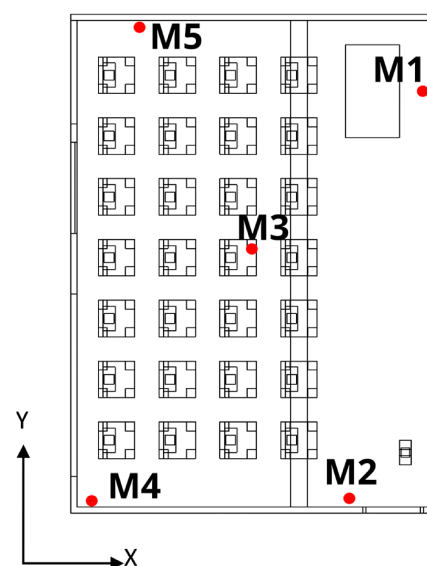


Figure 10. Sensing points in the classroom.

Figure 11 shows the values recorded by the five sensors (blue lines) and their respective values in the CFD simulation (gray lines). Visually, they exhibit similar behavior; however, a quantitative analysis can be performed using the recorded data.



Figure 11. SCD40 data vs. CFD simulation.

Table 9 presents two statistical indicators which validate the predictive capacity of the proposed constant-respiration CFD model. The first is the relative error, which measures the discrepancy between the simulated data and the actual data at each of the five positions considered. The second is Pearson's correlation coefficient, which describes the relationship between the two variables for each position. Based on these values, the average of the Pearson's correlation coefficients for the five positions is also calculated.

Table 9. Relative error and Pearson correlation coefficient between real and simulated values.

	M1	M2	M3	M4	M5	Units
Simulated average concentration:	1507.99	1676.24	1342.66	1014.23	1443.54	ppm
Average measured concentration	1.48420	1.67599	1.27670	1.11754	1.54508	ppm
Relative error	1.60%	0.02%	5.17%	9.24%	6.57%	
Pearson coefficient	0.99	0.97	0.85	0.93	0.98	
Average Pearson coefficients	0.94					

4. Discussion

According to the results shown in Table 9, the CO₂ levels recorded by the sensing modules at the five points show a high degree of agreement with the values obtained in the

CFD simulation. The results can be analyzed as follows. According to the relative error, they are classified into two groups: the first, the best-performing modules M1, M2, and M3, with relative errors below 6%; and the second group, with acceptable performance, consisting of modules M4 and M5, with relative errors below 10%. On the other hand, the average Pearson coefficient (0.94) shows a strong positive correlation between the real and sensed data. This results in favorable approximations for the proposed model, which experimentally validates the constant respiration model well, although the accuracy is slightly reduced due to the simplification of the model. The parameters used in the CFD (constant air velocity and CO₂ concentration = 20,000 ppm) are suitable for representing real-world conditions; furthermore, the geometric simplifications (human box and simplified geometries) are appropriate for reducing computational costs in this type of application.

It is important to note that the objective was to adequately replicate the environmental conditions in the simulation, considering parameters such as the distribution and number of occupants, the dimensions of the classroom, the temperature of the walls and the environment, the air conditioning flow, and the behavior of the occupants during the class.

5. Conclusions

The constant breathing model developed in this work accurately approximates the CO₂ dispersion dynamics in an enclosed classroom. The results obtained in this work show that the constant model exhibits a high correlation with the following:

- Complex breathing patterns (complete and sinusoidal);
- Experimental in situ measurements.

This cross-validation, using both numerical and experimental data, supports the viability of the proposed method for indoor air quality monitoring applications. The results demonstrate a significant advantage of the constant-breathing model in terms of computational resources, particularly in simulation times, which were as follows:

- For the constant model, 242 s;
- For the full breathing model, 6360 s, which is approximately 26 times slower;
- For the sinusoidal model, 13,080 s, which is 54 times slower than the constant model.

Despite this drastic reduction in computation time, the convergence analysis across the three simulations shows that the simplified model exhibits good accuracy in predicting CO₂ concentration. The average values and trends of the three models converge to very similar results.

The development of this work opens the following lines of research for future work: extension to other spaces with characteristics different from those of the classroom studied, such as offices (workspaces), hospitals, gyms, and auditoriums; implementation in a closed-loop control system based on the proposed CFD model, considering existing HVAC systems, automatic activation of ventilation based on CO₂ predictions, and energy optimization through predictive control; and finally, extension of its application to other pollutants, to model the dispersion of respiratory aerosols, volatile organic compounds (VOCs), or particulate matter (PM_{2.5}, PM₁₀). In all cases, the low computational load characteristic of the proposed method will be maintained.

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Abbreviations

The following abbreviations are used in this manuscript:

CFD	Computational Fluid Dynamics
ASHRAE	American Society of Heating, Refrigerating, and Air-Conditioning Engineers
OSHA	Occupational Safety and Health Administration
NIOSH	National Institute for Occupational Safety and Health
HVAC	Heating, Ventilation, and Air Conditioning

Appendix A

In the present research, simulations of CO₂ concentration were conducted in a three-dimensional space representing a classroom. The study considered governing equations that describe the turbulent flow of an incompressible fluid.

$$\rho \frac{\partial u_i}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \rho \overline{u'_i u'_j} \right] + F_i \quad (\text{A1})$$

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (\text{A2})$$

$$\rho \frac{\partial T}{\partial t} + \frac{\partial(\rho u_j T)}{\partial x_j} = \frac{1}{C_p} \frac{\partial}{\partial x_j} \left[\lambda \frac{\partial T}{\partial x_j} - \rho C_p \overline{u'_j T'} \right] \quad (\text{A3})$$

$$\rho \frac{\partial C}{\partial t} + \frac{\partial(\rho u_j C)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\rho D \frac{\partial C}{\partial x_j} - \rho \overline{u'_j C'} \right] \quad (\text{A4})$$

In the above equations, ρ is the density, p is the pressure, μ is the dynamic viscosity, F_i is the i component for the external body force, T is the temperature, D is the diffusion coefficient, C is the concentration, λ is the thermal conductivity, and C_p is the specific heat. Furthermore, u_i and x_i are the i -component of velocity and spatial coordinate, respectively.

The Reynolds stress tensor, the turbulent heat flux, and the turbulent mass flux in Equations (A1)–(A4) are calculated as follows:

$$\overline{\rho u'_i u'_j} = -\mu_t \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] + \frac{2}{3} \rho K \delta_{ij} \quad (\text{A5})$$

$$\overline{\rho u'_j T'} = -\frac{\mu_t}{\sigma_t} \frac{\partial T}{\partial x_j} \quad (\text{A6})$$

$$\overline{\rho u'_j C'} = -\frac{\mu_t}{Sc_t} \frac{\partial C}{\partial x_j} \quad (\text{A7})$$

where Sc_t is the turbulent Schmidt number. Turbulent kinetic energy K and turbulent kinetic energy dissipation ε are calculated by:

$$\rho \frac{\partial K}{\partial t} + \frac{\partial(\rho u_i K)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_K} \right) \frac{\partial K}{\partial x_i} \right] + P_K + G_K - \rho \varepsilon \quad (A8)$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \frac{\partial(\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + C_{\varepsilon 1} \frac{\varepsilon}{K} (P_K + C_{\varepsilon 3} G_K) - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{K} \quad (A9)$$

In these equations, μ_t is the turbulent viscosity, G_K represents turbulence generation or destruction, and P_K is the kinetic energy production rate.

The governing Equations (A1)–(A9) describing the velocity and temperature of the air, as well as the concentration of CO₂ inside a classroom, were discretized by the finite volume method [47,48]. The general time-dependent convection-diffusion equation that enables the simulation of flow within a classroom is given by:

$$\frac{\partial(\rho \phi)}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i \phi) = \frac{\partial}{\partial x_i} \left(\Gamma_\phi \frac{\partial \phi}{\partial x_i} \right) + S_\phi \quad (A10)$$

Equation (A10) is integrated over a control volume V to obtain the following integral form:

$$\int_V \frac{\partial(\rho \phi)}{\partial t} dV + \int_A \rho \phi u_i n_i dA = \int_A \Gamma_\phi \frac{\partial \phi}{\partial x_i} n_i dA + \int_V S_\phi dV \quad (A11)$$

where S is the source term, Γ is the diffusion coefficient, ϕ is the variable to be discretized, n_i is the unit normal vector, and A is the area.

The numerical simulations were performed in a transient, turbulent regime using the finite-volume method; specifically OpenFOAM v2212 was used. The coupling between pressure and velocity over time was treated using the PIMPLE algorithm. Spatial discretization was performed considering a tetrahedral mesh. For the terms convective and divergence, second-order discretization schemes were employed to minimize numerical diffusion, while the temporal integration was performed with an implicit second-order scheme.

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