

MODELING CO₂ SPREAD IN INDOOR ENVIRONMENTS

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ABSTRACT

We introduce a hybrid modeling approach for simulating carbon dioxide (CO₂) dispersion in indoor environments by integrating Cellular Automata (CA), Discrete Event System Specification (DEVS), and agent-based modeling. The proposed framework enhances traditional models by incorporating dynamic CO₂ generators, random-walk algorithms, and CO₂ sinks. We show how the method can be used to examine the effects that room layouts, occupant movement, ventilation settings, and CO₂ sinks and sources placement have on indoor concentration patterns. The approach presented here enables the exploration of various configuration parameters and provides a flexible and scalable tool for understanding CO₂ diffusion.

1 INTRODUCTION

Recently, maintaining healthy indoor environments while ensuring energy efficiency has become a central concern. Carbon dioxide (CO₂) concentration is widely recognized as a key indicator of indoor air quality, with significant implications for occupant comfort, cognitive performance, and the implementation of demand-driven ventilation and occupancy detection systems (Mendell et al. 2024). Elevated CO₂ levels have been associated with reduced academic performance, productivity, respiratory health issues (Sadrizadeh et al. 2022; Deng et al. 2024). However, conducting physical experiments to assess CO₂ dispersion across diverse indoor scenarios is often impractical due to cost, time, and logistical constraints.

To address these challenges, Modeling and Simulation (M&S) techniques have emerged as powerful alternatives, enabling researchers to evaluate air quality under controlled virtual conditions. Existing approaches include statistical-based for occupancy estimation, as well as physics-based methods such as Computational Fluid Dynamics (CFD) for simulating airflow and CO₂ distribution. While effective, these techniques are often limited by high computational complexity or detailed input data and calibration (Labeodan et al. 2015; Mou et al. 2022). Other methods, in particular, the hybrid combination of Cellular Automata (CA) and Discrete Event System Specification (DEVS), known as Cell-DEVS formalism, has been successfully applied to incorporate spatial and temporal dynamics, including room geometry, HVAC systems, window and door locations, and occupant presence (Khalil et al. 2020; Khalil and Wainer 2024). These models are valuable for applications such as sensor placement optimization, air quality monitoring, and infection risk assessment. Despite their versatility, most current models are limited to two-dimensional representations, restricting their applicability in scenarios where the three-dimensional airflow interactions are significant.

To overcome these limitations, this study proposes a hybrid agent-based modeling approach that combines CA and DEVS to simulate CO₂ dispersion in three-dimensional indoor environments. The goal of this work is to enhance spatial realism and better capture the dynamic behaviors of both occupants and airflow patterns. Our approach incorporates dynamic CO₂ generators, random-walk algorithms for dispersion modeling, and the inclusion of CO₂ sinks to assess their impact on CO₂ reduction. The main contributions of this work are: i) the development of a 3D model to simulate CO₂ spread under dynamic occupancy behavior; ii) the evaluation of different CO₂ sinks to assess their impact on air quality; and iii) a set of simulation experiments that validate the proposed approach and highlight its practical implications for building design and environmental control strategies.

2 RELATED WORK

Modeling CO₂ dispersion in enclosed spaces is critical for addressing global warming, enhancing indoor air quality, optimizing sensor placement, and reducing energy use. Various computational methods have emerged, such as Labeodan et al. (2015), who noted challenges in obtaining reliable data for occupancy detection due to environmental variability and human behavior. Calì et al. (2015) developed an algorithm based on CO₂ levels to estimate occupancy in various settings, although it depends on knowledge of ventilation and outdoor CO₂. Ryu and Moon (2016) leveraged a statistical decision tree and Hidden Markov Model, finding that CO₂ measurements, particularly the indoor-to-outdoor concentration ratio, are key indicators of occupancy. Batog and Badura (2013) created a simplified bedroom model, focusing on key surfaces like the bed and wardrobe, and simulated CO₂ from a sleeping occupant over eight hours in two scenarios: one without fresh air inlets and another with airflow gaps. Their findings highlight the significance of proper CO₂ sensor placement for accurate readings. Similarly, Pantazaras et al. (2016) developed a method for predictive modeling of CO₂ levels in specific indoor spaces by integrating room characteristics, ventilation rates, and occupancy patterns, emphasizing the need for careful sensor placement to enhance model accuracy.

Recent studies have investigated Computational Fluid Dynamics (CFD) modeling for indoor environments. For instance, Mou et al. (2022) used CFD to simulate airflow and CO₂ distribution in a seminar room to optimize sensor placement, revealing that airflow patterns and occupant-generated CO₂ significantly affect concentration distributions. They stressed the importance of considering room layout, ventilation design, and occupant activity in simulations. However, while CFD offers high accuracy, it can be computationally demanding for large or complex environments and requires detailed boundary conditions and expert calibration (Zhang et al. 2024). Consequently, researchers are seeking alternative modeling techniques that provide a better balance of accuracy, efficiency, and scalability.

Cellular Automata (CA) models offer another promising approach by discretizing space into a grid of cells, where global system behavior emerges from simple local interactions and transition rules (Khalil and Wainer 2024). CA-based methods provide advantages in terms of computational efficiency, scalability, and the ability to model spatially heterogeneous environments, making them highly suitable for indoor CO₂ spread simulation. In this research we aim to model the spread of CO₂ using a hybrid approach that combines Discrete-Event models specified using the DEVS formalism (Zeigler et al. 2000) and CA (Wolfram 1984; Wolfram 1983). We propose an agent-based modeling framework in a spatial environment, incorporating a stochastic algorithm to simulate the dispersion of CO₂ particles as well as random walk.

CA is a method for modeling cell spaces using a regular n-dimensional grid, where each cell holds one of a finite set of possible states. The system evolves in *discrete time* steps, with all cells updating their states simultaneously according to a local transition rule. This rule determines the next state of a cell based on its current value and the values of its neighboring cells (the neighborhood). Figure 1(a) shows a two-dimensional CA, where each cell either contains a value or is empty, and its next state is computed based on its current state and those of the adjacent cells (shaded area).

CA allows for detailed mathematical analysis and can effectively model complex systems through simple computations in individual cells. While CA typically uses discrete-time updates suitable for asynchronous applications like pedestrian flow and traffic, it often employs synchronous rules, complicating the representation of time-triggered activities (Wang et al. 2023; Deng et al. 2022). Recently, combining CA with other modeling techniques for simulating CO₂ dispersion has gained interest. For example, Sonnenschein et al. (2025) proposed a hybrid model integrating Land Use Regression (LUR) for baseline CO₂ concentrations with CA to assess urban traffic-related CO₂ pollution by incorporating meteorological and morphological factors. However, research applying CA for indoor CO₂ dynamics remains limited. Integrating CA with DEVS formalism and other paradigms could provide a more flexible approach for simulating CO₂ spread, enhancing temporal precision, modularity, and asynchronous modeling capabilities. Cell-DEVS is a hybrid combination of both DEVS and CA.

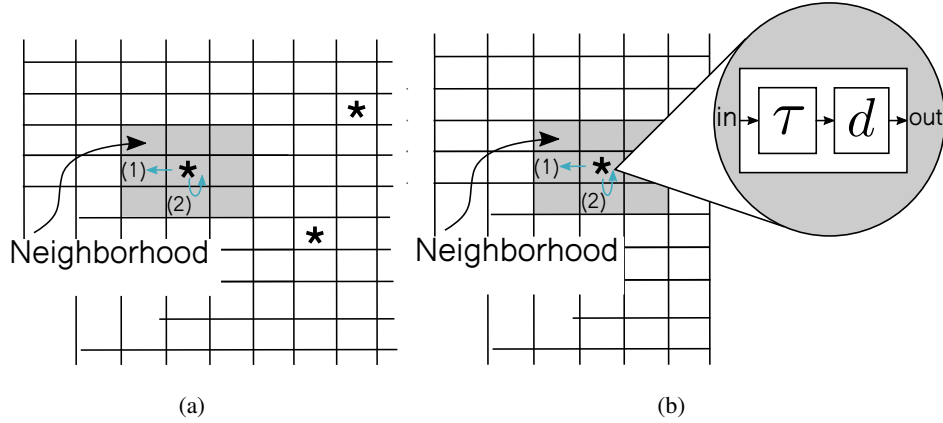


Figure 1: Two-dimensional cellular automaton with its neighborhood.

In Cell-DEVS, each agent in a cell is modeled using a hybrid combination of execution rules defined later as a DEVS atomic model. A structure coupling mechanism is used to interconnect the cells. Indeed, a Cell-DEVS model is an n -dimensional lattice where each cell is an atomic model, and the whole-cell space is a coupled DEVS model (Wainer 2009). These cells communicate with each other through input and output ports, allowing them to exchange information not only with neighboring cells but also with other models defined in different formalisms defined outside the defined cell space. Figure 1(b) provides an illustrative representation that highlights how Cell-DEVS integrates principles from both DEVS and CA.

To define a Cell-DEVS model, the first step is to define the atomic behavior of each cell a :

$$TDC = \langle X, Y, S, N, type, d, \delta_{int}, \delta_{ext}, \tau, \lambda, D \rangle,$$

where X and Y are the sets of external input and output events, respectively, S is the set of possible states, N is the set of input values, $type$ specifies the type of delay (transport, inertial, or other), and d denotes the delay duration. The local computing function τ determines the cell's future state, while the output function λ generates the corresponding output. Finally, D defines how long the state is held before a transition occurs. When using a transport delay, the output is sent after the delay time d has passed. In contrast, an inertial delay is used as a preemptive mechanism; it prevents any scheduled change from taking place upon receiving an external event from a neighbor cell before the scheduled time. Once the atomic behavior of each cell is specified, the next step is to define the complete cell space.

In Cell-DEVS, this space is modeled as a coupled DEVS model, formally represented as follows:

$$GCC = \langle X_{list}, Y_{list}, I, X, Y, \eta, \{t_1, \dots, t_n\}, N, C, B, Z \rangle,$$

where X_{list} and Y_{list} denote the list of external input and output couplings, respectively; I is the set of states, X and Y are the sets of external input and output events, respectively; $\eta \in N$ defines the neighborhood size; and $\{t_1, \dots, t_n\}$ is the number of cells in each dimension of the lattice. The cell space itself is denoted by C , with N being the neighboring cells. B represents the set of border cells, which can have different behavior than the interior cells or can be configured with wrap-around boundaries. The function Z is the translation function that maps the output port of a cell to the input port of another cell.

Random walk algorithms have shown to be useful to include stochastic behavior in the movement of particles within indoor environments. These algorithms simulate the trajectories of individual particles based on probabilistic rules, effectively capturing the effects of turbulent diffusion and airflow variability (Wang and Mu 2011; Marashian et al. 2023). In this context, a hybrid model integrating random walk algorithms with agents defined using CA and DEVS modeling and simulation could offer a more comprehensive and flexible modeling framework for simulating CO₂ dynamics in realistic indoor scenarios.

3 MODELING THE SPREAD OF CO₂ PARTICLES

In this section we present various CO₂ spread models that combine a cellular model with a discrete-event specification. Khalil et al. (2020) introduced such hybrid models to study CO₂ dispersion in a room and to identify the optimal placement and detection latency of CO₂ sensors, a complex problem in building design. A closed space was modeled as a set of neighboring cells representing the 2D layout of a room. The formal specification of the two-dimensional Cell-DEVS CO₂ model presented in (Khalil et al. 2020) is:

$$CO_2 = \langle X_{list}, Y_{list}, S, X, Y, \eta, N, \{t1, t2\}, C, B, Z \rangle,$$

where $X_{list} = Y_{list} = \{\emptyset\}$; $S = \text{type} : \{0, 1, 2, 3, 4, 5\}$ and $\text{conc} : \{\text{double}\}$; $X = Y = \emptyset$; $\eta = 5$; $N = \{(0, 0), (-1, 0), (0, -1), (0, 1), (1, 0)\}$; $t1 = 14$; $t2 = 20$; $C = \{C_{ij} | i \in [0, 14] \wedge j \in [0, 23]\}$; and $B = \{\emptyset\}$ (unwrapped cell space); Z is the translation function that defines the internal and external function. The local computing function τ of the atomic model of each cell and the duration function D are shown in Table 1 and Table 2, respectively. The neighborhood is a Von Neumann and only the North (N), East

Table 1: Values of $\tau(N)$.

$\tau(N)$	N
conc = average of neighbors	type = 0
conc = neighbors average + 12.16 ppm	type = 1
conc = - 10 ppm	type = 2
conc = 500 ppm	type = 3
conc = 400 ppm	type = 4
conc = 300 ppm	type = 5

Table 2: Values of $D(s)$.

$D(S)$	S
R0 += 1,000	type = 0
R0 += 5,000	type = 1
R0 += 1,000	type = 2
R0 += 1,000	type = 3
R0 += 1,000	type = 4
R0 += 1,000	type = 5

(E), West (W), and South (S) neighbors are considered. This model was implemented using the CD++ tool. Each area could use one of six model types, representing CO₂ levels in particles per million (ppm), based on gas diffusion rules: open-air space (constant 500 ppm); CO₂ sources (fixed emissions); walls (no diffusion); open doors, windows, and vents (diffusers with baseline CO₂ concentrations of 500, 400, and <300 ppm, respectively). Each cell in the cell space was defined by its model type. Diffuser cells were unaffected by surrounding CO₂ levels. CO₂ sources were modeled as an occupant at rest, with an average breathing interval that emitted CO₂ every 5 seconds and a diffusion interval set at 1.

We validated this model with real-world data and showed that the model effectively represented CO₂ diffusion, dissipation and latency. Based on these results, we modified the static generator (a DEVS model that represented a stationary occupant) as well as CO₂ behavior after the generator left the room. We modeled scheduled emissions and effects of movement (such as a person walking) on CO₂ distribution.

To address these limitations, we introduced a dynamic CO₂ generator to the original Cell-DEVS model. Each cell contained the concentration, type, a counter, and a direction. The rules for this model are defined as follows:

```
% rules for CO2 generator
rule : {counter += 1;} 1000 {if cell type 1 AND counter != 2 OR 5}
rule : {type = 0; add 12.16ppm of CO2; counter += 1;} 1000 {if cell type 1 AND counter = 2}
rule : {add 12.16ppm of CO2; counter = 0;} 1000 {if cell type 1 AND counter = 5}

% rules when open cells are affected by CO2 neighbors
rule: {type = CO2; counter = neighbors counter; direction = randInt(100) or neighbor
      direction; (depends if scheduled or random movement)} 1000 {if cell type 0 AND
      neighbors(counter = 2 AND type = 1 AND direction is correct)} (4 rules)

% set of rules if type 0 for CO2 dissipation
rule: {calculate average concentration of all surrounding cells} 1000 {if cell type
```

```

open air}

% set of rules for the remaining cases
rule: {maintain preset CO2 concentration;} 1000 {if cell of other types}

rule: {counter += 1;} 1000 {any type} % default rule

```

These rules included logic to prevent generator from passing through walls, regulate CO₂ emission timing, handle transitions between cell types, and model diffusion in open-air spaces.

We tested the dynamic CO₂ generator with two types of scenarios: i) randomly, to model organic movement and distribution, and ii) a scheduled path representing a person arriving and visiting specific rooms in sequence. The environment represents a bachelor apartment layout with a door and vents in the kitchen and bathroom. To simulate active breathing, CO₂ emissions were increased every 3 seconds. The left panel in Figure 2 shows CO₂ concentration, while the right panel shows the generator's position. We can see the results from the random scenario starting at the entrance (green door). The generator remains



Figure 2: Random CO₂ generation. Start at the entrance at 0 (left), 5 (middle), and 10 (right) minutes.

near its starting point, saturating that area with CO₂ leaving other regions mostly unaffected (similar to the static scenario) as we used a uniform distribution for movement direction, which resulted in a tendency for circular paths. Next, we run a scheduled scenario representing a person entering at home, leaving the door open, staying around 1 minute and 30 seconds in the living room, 2 minutes in the kitchen, and finishing in the bathroom. Figure 3 illustrates CO₂ distribution over the course of this planned movement. As expected,

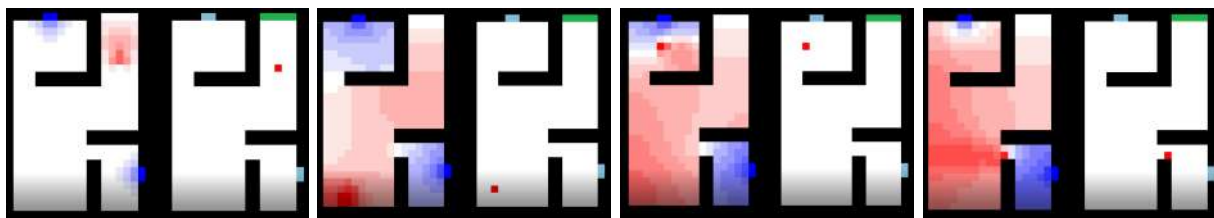


Figure 3: Scheduled CO₂ generation for times 0, 1.45, 3.45, and 4 minutes (left to right).

CO₂ spread across the apartment. Notably, a significant concentration remained in the entrance hallway, even with the door open. This highlights both the rapid spread of CO₂ and its slow dissipation, even in well-ventilated conditions.

3.1 Effect of Plants and CO₂ Sinks on Indoor CO₂ Levels

The model above was further extended to investigate CO₂ level variations in a closed indoor environment, where moving occupants act as CO₂ sources. We evaluate the effectiveness of adding plants and CO₂ sinks placed in various positions throughout the room. Each cell now considers the `type` and `concentration` of CO₂. Walls are modeled as impermeable structures that block CO₂ diffusion and maintain constant

values (barrier). Doors are initialized with a typical indoor baseline CO₂ level (500 ppm), while windows maintain lower concentration to simulate the influence of outdoor air. Ventilation cells actively reduce CO₂ concentration to simulate mechanical air extraction. Workstations behave as passive air cells, averaging the CO₂ levels of their non-wall neighbors. Simulations were carried out using the Cell-DEVS formalism and Cadmium tool.

A code snippet used to compute concentration values for plants, CO₂ sinks, and sources is shown below:

```

switch(state.current_state.type) {
  case PLANT: { ...
    if(neighbors.type != IMPERMEABLE) {
      concentration +=
        neighbors.concentration;
      num_neighbors++; }
    new_state.concentration =
      concentration / num_neighbors -
      (plant_decrease / 480); break; }
  case SCRUBBER: { ...
    if(neighbors.type != IMPERMEABLE) {
      concentration +=
        neighbors.concentration;
      num_neighbors++; }
    new_state.concentration =
      concentration / num_neighbors - 10;
  }
  case CO2_SOURCE: { ...
    if(neighbors.type != IMPERMEABLE) {
      concentration +=
        neighbors.concentration;
      num_neighbors++; }
    new_state.concentration =
      (concentration / num_neighbors) +
      concentration_increase;
    ...
  }
}

```

CO₂ sources simulate human breathing by adding a fixed amount of CO₂ to their cell every ten minutes. Plants absorb a small portion of CO₂, decreasing the local concentration slightly, whereas CO₂ sinks remove a larger amount, simulating active filtration mechanisms.

Figure 4 illustrates the results for a scenario in this model. The simulation, run for 1440 minutes, examines how CO₂ levels are affected by occupants, plants, and sinks in a closed space. The initial condition, shown in Figure 4(a), features all occupants outside the room and active ventilation. Under these conditions, CO₂ remains below 500 ppm (blue cells), aided by sinks and plants absorbing CO₂. Figure 4(b)

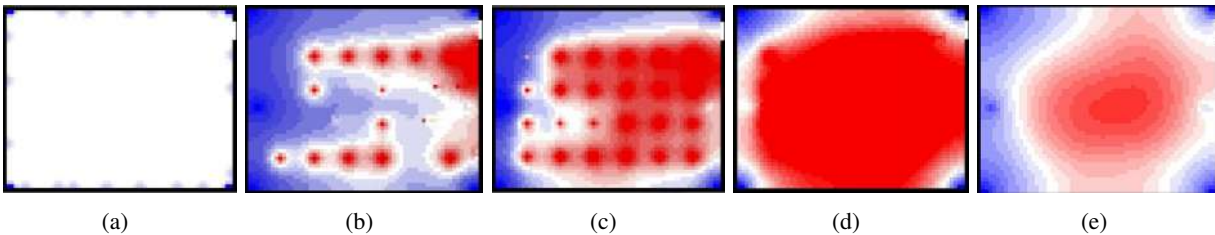


Figure 4: Indoor CO₂ concentration with moving occupants, plants and CO₂ sinks.

depicts thirteen occupants entering the room, shown as red cells moving toward assigned workstations (gray cells). As they move, expanding red zones in the left panel indicate rising CO₂ levels, with the size of these zones varying to reflect individual breathing rates, which were randomly assigned. Over time, CO₂ concentration steadily increases due to ongoing respiration. Figure 4(c) shows all occupants at their workstations. The red regions have expanded compared to (b), indicating increased CO₂ levels, especially from occupants with higher breathing rates. As more people enter, overall CO₂ rises, but ventilation units and sinks (blue cells) help circulate air and reduce CO₂, especially near the edges where devices are present. The central area has higher CO₂ due to lack of vents, while plants along the walls have minimal impact.

Figure 4(d) shows ten occupants leaving, causing red CO₂ zones to shrink as vents, sinks, and plants absorb CO₂. The central area remains more concentrated with CO₂ than the edges, where changes are minimal, indicating that the plants had little impact on overall CO₂ levels. Figure 4(e) depicts the final scene with all occupants gone; fresh air (blue) expanded, and CO₂ (red) decreased as ventilation and sinks

removed residual CO₂. Plants, specifically Prayer plants, had minimal impact, absorbing about 215 ppm over 1440 minutes, compared to 18,158 ppm produced by a single person in the same period, showing their limited role in reducing CO₂ levels.

3.2 Effect of Distance between CO₂ Sources

This example investigates how varying the distance between CO₂ sources influences the overall indoor CO₂ concentration. Simulations were carried out using the Cell-DEVS formalism and CD++ tool. Different distances between CO₂ sources were tested to analyze how their separation affects diffusion patterns and concentration levels over time.

Each cell in the model represent an agent characterized by `type`, `counter`, and `concentration`. As before, the behavior of the model is defined by the τ function. The rules to generate cells simulating occupants are as follows:

```
{...}
% Moving person
rule : { ~c := $conc; ~ty := $type; } { $conc := ((121.6*2) + (((-1,0)~c + (0,-1)~c
+ (0,0)~c + (0,1)~c + (1,0)~c)/5)); $counter:= $counter + 1; } 5000
{ $type = -900 AND $counter < 125 }

rule : { ~c := $conc; ~ty := $type; } { $conc := (((-1,0)~c + (0,-1)~c + (0,0)~c
+ (0,1)~c + (1,0)~c)/5); $counter:= $counter + 1; $type:=-100; } 5000
{ $type = -900 AND $counter = 125 }
{...}
```

These dynamic source cells emit CO₂ for 125 update cycles to simulate active breathing, and then revert to standard air cells, simulating the departure of human activity.

Simulation results are shown in Figure 5, where magenta cells indicate the position of occupants actively emitting CO₂, red cells represent fixed CO₂ sources, white cells correspond to impermeable walls that block CO₂ diffusion, blue cells denote ventilation units maintaining ambient CO₂ levels at 300 ppm, and yellow cells depict the room's air duct system. At the beginning of the simulation, two individuals are placed

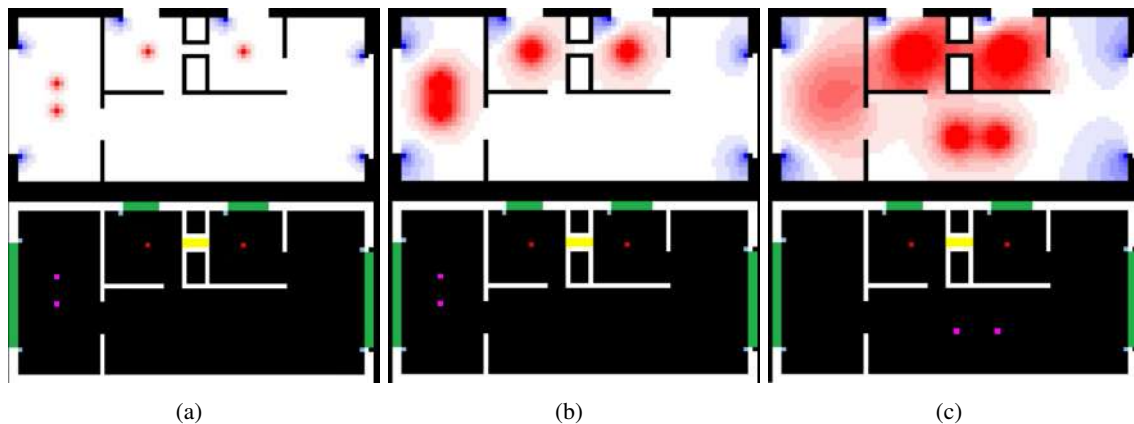


Figure 5: Effect of Distance on CO₂ sources.

1.25 meters apart (Figure 5(a)), and CO₂ concentration begins to rise around them (Figure 5(b)). After 125 breathing cycles, they move to the bottom room and are positioned 3.25 meters apart (Figure 5(c)). As a result, CO₂ concentration in the left room decreases due the absence of a source, while it begins to rise in the bottom room with the arrival of the new sources. The duct system enables CO₂ spread between the two upper rooms. CO₂ diffuses in all directions from the emitting cells, and the concentration

gradually increases over time. The simulation results indicate that when sources are close together, CO₂ levels rise more quickly. In contrast, when the distance between sources increases, the concentration builds up more slowly. These findings suggest that the distance between individuals influences how quickly CO₂ accumulates in indoor environments.

3.3 CO₂ Cell-DEVS Model with Random Walk Algorithm

In this section, we show how to combine cellular modeling, discrete-event simulation and random walk algorithms (in 2D and 3D environments). The idea is to model the indoor spread of CO₂ particles in a 3D environment. The cell space is used to build an agent based model in which each cell contains the behavior of the particles in a room, discretizing a continuous space using a rectangular grid. Each of the cells are updated using a continuous-time specification. In addition, a random walk algorithm is used to represent the movement of the CO₂ particles in a more realistic fashion using a stochastic model, because the randomness of the movements, makes the random walk algorithm a good approach to model the spread of air particles in 2D and 3D space. The three methods are combined and simulated for different indoor scenarios using the Cadmium tool.

To define the behavior of the agents on each cell, which is then reproduced in all the cells in the cell space, first we need to define a local transition function. This should take into consideration the random walk algorithm, where each object can move freely in all directions based on a stochastic rule. In Figure 6,

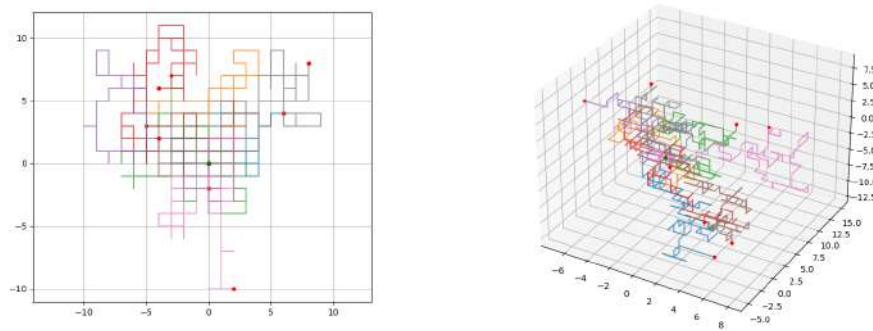


Figure 6: 2D and 3D Random Walk Models.

we show a 2D (left) and 3D (right) example of how the random walk works. In the former, the objects move up, down, left, and right at random; while in the latter the object can also move upward and downward. The probability of choosing the direction is varied and can be changed in each calculation, which is activated using a discrete-event simulation algorithm based on the DEVS formalism.

The behavior of the model is defined in τ function, which is used to define the behavior of the agent on each cell. In this case, the cells defined as sources increase the concentration of CO₂, while cells defined as vents, doors, and windows decrease it. The implementation of this behavior is as follows:

```

switch(state.current_state.type) {
  case IMPERMEABLE:
    new_state.concentration = 0; break; // Neighbor on right
  case DOOR:
    new_state.concentration = base; break; else if((neighbors.first[0] - 1) ==
  case WINDOW:
    new_state.concentration =          std::get<0>(currentLocation) &&
    window_conc; break;                neighbors.first[1] ==
    std::get<1>(currentLocation)){
  case VENTILATION:
    ...                                concentration +=
    std::get<1>(currentLocation) +
  case AIR:
    ...                                neighbors.concentration +
    floor(neighbors.concentration*
  case WORKSTATION:
    ...                                distneg(rng)/500 );
    num_neighbors++;
  case CO2_SOURCE:{ ...                }
  if(neighbors.type != IMPERMEABLE){ // Similar for Neighbor on bottom, left,
  // Neighbor on top                    // itself and above
  if (neighbors.first[0] ==            else if((neighbors.first[2] - 1) ==
  std::get<0>(currentLocation) &&      std::get<2>(currentLocation)){
  (neighbors.first[1] - 1) ==          concentration +=
  std::get<1>(currentLocation) ){      neighbors.concentration +
  concentration +=                    floor(neighbors.concentration*
  neighbors.concentration +            distneg(rng)/500 );
  floor(neighbors.concentration*      num_neighbors++;
  distneg(rng)/500 );                }
  num_neighbors++;                    // behind
  }                                    {...}
}
}

```

In this code, the τ function first checks the type of each cell. Cells classified as walls (IMPERMEABLE) are assigned a concentration of zero, while doors, windows, and ventilation cells are updated with predefined concentration values that represent air exchange characteristics. For CO₂ source cells, the concentration is increased by considering the contribution of neighboring cells. The CO₂ concentration of cells classified as air and workstation is updated in a similar way. To simulate the variability introduced by the random walk algorithm, a random number generator based on the Mersenne Twister algorithm was initialized using a non-deterministic seed to ensure variability across runs. A uniform integer distribution in the range [-70, 70] was used to produce evenly distributed random values within this interval.

In existing CO₂ models, particles move to the neighbor cells using a uniform method for spreading, as shown in Figure 7. The dark brown cell in the middle of the first image represents a CO₂ source that increase the concentration of the cell. In the following iterations, the CO₂ particles move to the neighbor cells and increase their CO₂ concentration.

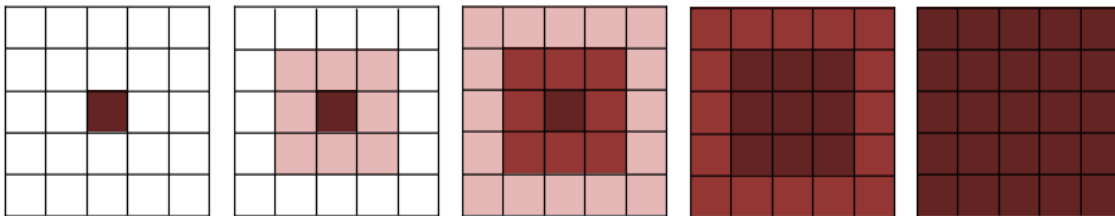


Figure 7: Deterministic spreading of CO₂ particles - Iterations #1(left) to #5 (right).

As we can see in Figure 8, when we combine the model with a random walk method, the use of a more realistic spread of CO₂ particles add randomness to the increase of CO₂ in the neighboring cells as it is done in a random way.

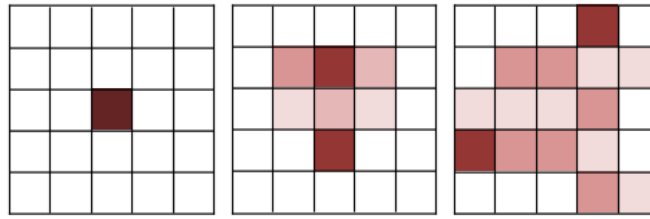


Figure 8: Random Walk spreading of CO₂ particles - Iterations #1(left) to #3 (right).

After defining the cell's behavior, we define specific parameters and a configuration of the cell space as well as of each cell. An extract of a JSON configuration file, where we can include different objects like doors, walls, windows, vent, and CO₂ sources, together with their specific parameters is shown below:

```

"scenario": {
  "shape": [ 43, 40, 8],
  "wrapped": false,
  "default_delay": "transport",
  "default_cell_type": "CO2_cell",
  "default_state": {
    "counter": -1,
    "concentration": 500,
    "type": -100
  },
  "default_config": {
    "CO2_cell": {
      "conc_increase": 143.2,
      "base": 500,
      "resp_time": 1,
      "window_conc": 400,
      "vent_conc": 300
    },
    "neighborhood": [
      {"type": "von_neumann",
       "range": 1}]
  },
  "cells": [{}]}

```

Figures 9 and 10 present simulation results comparing CO₂ dispersion patterns using a deterministic method (left) versus the proposed random walk approach (right), for both 2D and 3D building layouts. In both scenarios, the introduction of the random walk algorithm significantly alters the CO₂ dispersion dynamics. In Figure 9, the 2D simulations highlight how the deterministic method results in smoother and

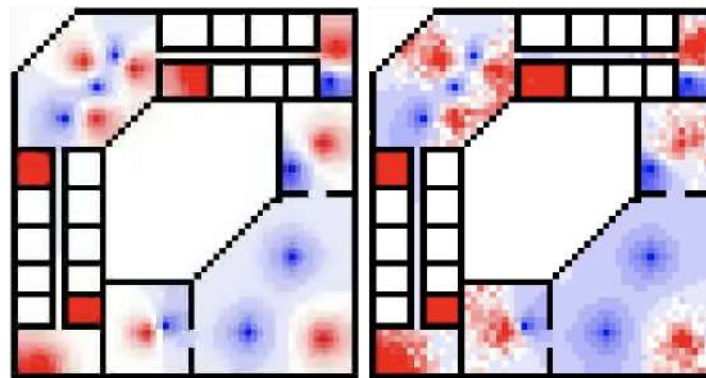
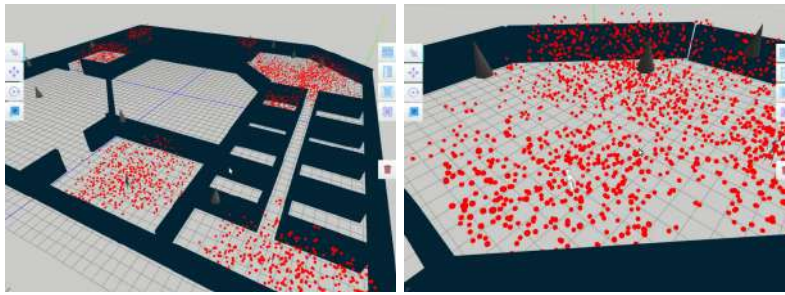


Figure 9: 2D CO₂ spread. Deterministic (left) and with Random Walk (right).

more uniform diffusion patterns centered around the CO₂ sources. In contrast, the random walk approach introduces localized variations and asymmetries, reflecting the stochastic nature of particle movement. Indeed, some regions near sources exhibit lower concentrations than surrounding cells, emphasizing the irregular dispersion introduced by random motion. Figure 10 shows similar behavior in a 3D environment. The deterministic simulation again yields a more structured and symmetric distribution, while the random

Figure 10: 3D CO₂ spread.

walk approach introduces more irregular and diffuse spread of CO₂ particles. This results in faster propagation and more realistic dispersion.

From a methodological perspective, the deterministic CO₂ model, computes the concentration of each cell as the average of the neighboring cells' concentrations, resulting in a smooth but uniform spread. Using random walk, the concentration update in each cell reflects a randomized fraction of the neighboring cells' CO₂ concentration. This modification includes local fluctuations without imposing a significant computational burden, as it avoids the need to track individual particles explicitly. In this context, the random walk approach provides a way to approximate the natural stochastic behavior of gas diffusion.

4 CONCLUSION

We presented a hybrid modeling approach for simulating CO₂ dispersion in indoor environments by integrating CA, DEVS, random walk algorithms and 2D and 3D modeling techniques. We addressed the limitations of traditional models by incorporating dynamic CO₂ generators, random-walk dispersion algorithms, and CO₂ sinks to capture more realistic indoor air behavior. Through a series of simulation experiments, we demonstrated how room layout, occupant movement, and source placement significantly influence CO₂ distribution patterns.

The proposed models are well-suited for studying CO₂ spread in enclosed spaces. They provide a flexible framework for evaluating the impact of various design and operational parameters, including sensor placement, ventilation strategies, occupancy levels, and furniture arrangements. This approach can support more informed decisions in the design and management of healthy and energy-efficient indoor environments.

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