Modeling Carbon Dioxide Dispersion Indoors

A Cell-DEVS Experiment

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Abstract. Carbon dioxide concentration in closed spaces is an indication of air quality and a means of measuring the number of occupants for controlling energy consumption. However, the dispersion of the gas and the accuracy of the concentration measurements as logged by carbon dioxide sensors are highly sensitive to the configuration of the closed space. Conducting case by case studies for each closed space is neither practical nor cost-effective. We hereby propose a formal model using cellular discrete-event system specifications for studying carbon dioxide dispersion indoors and for analyzing the effect of different configurations on the sensors measurements of the concentration. We present a case study of the model and compare the simulation results to ground truth data collected from two physical systems of two computer laboratories. The results demonstrate that the proposed model can be used to study carbon dioxide dispersion and the change of sensors' readings in closed spaces based on the configurations of the space.

Keywords: Modeling, Simulation, Cell-DEVS, Sustainability.

1 Introduction

One reason for the substantial research effort in measuring CO_2 levels indoors is to maintain an acceptable level of air quality which in turn impacts the wellbeing of the space occupants [1]. Another reason is detecting the number of occupants to automatically control the environment (e.g. adjust heating and air conditioning) and consequently reduce energy consumption without compromising the occupants' comfort [2]. Although CO_2 sensors have advantages over many other kinds of ambient sensors (e.g. they are affordable and nonintrusive), CO_2 sensors are overly sensitive to configuration. The accuracy of CO_2 sensors differs case by case depending on several factors such as heating, ventilation, and air conditioning (HVAC) settings. Although researchers have conducted experiments on CO_2 sensors' accuracy for indoor occupants' detection [3], more research is required to measure the effect of the different configurations of closed spaces on the measurements recorded by CO_2 sensors. Observing the effects of such parameters on the indoor CO_2 level and the readings of CO_2 sensors is the motivation for this research. Real-life experiments for measuring the effect of room configuration are impractical, time-consuming, and sometimes impossible. This motivates us to use modeling and simulation (M&S) to perform the required experiments for the objective of developing a robust general model that can be adapted to any closed space. This model can be reused, while adjusting the different required parameters (e.g. dimensions and windows locations), to measure their effect on the logged CO_2 concentration.

We use cellular discrete-event system specifications (Cell-DEVS) to model CO_2 behavior in closed spaces. Cell-DEVS is a "modification" of cellular automata (CA) modeling that has several advantages over other modeling techniques (section 2.2). This makes it suitable for modeling complex systems. In previous work [4], we presented a simple 2-D toy model to demo the effect of placing the sensor in two different positions on the recorded CO_2 concentration. In this paper, we develop an advanced 3-D model with possible variable parameters (e.g. windows, furniture layout, and different arrival and departure times of occupants) and multiple occupants. We implement a case study model of a computer laboratory that physically exists at Carleton University and we use it to calibrate the model. We base the calibration on the ground truth data collected from the physical laboratory. Then, we validate the model by comparing the simulation results to a set of ground truth data collected from the sensors installed in another laboratory on a different floor in the same building.

We first explain essential background information to position the presented work (section 2) and present examples from the literature of modeling CO_2 behavior indoors (section 3). Then, we introduce the experimental setup. Previously, we used the CD++ simulator, while in this work we use an improved simulator (Cadmium) (section 4). Then we present two versions of the model that are replicas of real-life laboratories: one for calibration and the other for validation (section 5). We compare the simulation results to the ground truth data and discuss them (section 6). Finally, we present the conclusion and propose future possible improvements (section 7).

2 Background

In this section, we provide background information that is necessary for understanding the research problem and the experimentation process. In section 2.1, we explore sensor-based occupant detection, while in section 2.2 we offer basic information about the M&S methodology we use, and we emphasize its advantages.

2.1 Sensor-Based Occupants Detection

Automatically sensing occupants and adjusting the building systems based on the number of occupants have become paramount for saving energy. The use of sensors to detect occupants in closed spaces has been addressed in many theoretical and experimental work. Researchers have proposed ways of detecting the presence of occupants including cameras, computer applications, and sensor fusion. They have used different kinds of sensors for occupancy detection such as passive infrared (PIR) sensors, electromagnetic sensors (EM), image sensors, and CO_2 sensors. Each type of sensor has its advantages and disadvantages. We focus on CO_2 sensors for their proven advantages and since there is potential for improving their performance [3-5]. CO_2 sensors are sensitive to factors such as the level of HVAC, dimensions (width, length, and height), locations of the ventilation port, the presence of open windows and doors, and the location where the sensor is installed. Testing each physical closed room to know how its configuration parameters affect the readings of an installed sensor is an impractical time-consuming approach. Hence, we propose M&S as a solution.

2.2 Methodology

With M&S, we can achieve the goal of understanding the dynamics of CO_2 dispersion less expensively and more practically. We model CO_2 dispersion using Cell-DEVS which solves some of the shortcomings of CA by combining it with discrete-event system specifications (DEVS) [6]. Cell-DEVS defines a grid of cells where each cell is specified as a DEVS model. The next state of each cell is defined based on the current state of that cell and the states of the neighboring cells. Cell-DEVS has been used extensively to model social and environmental complex systems [7-9]. One advantage of Cell-DEVS, and its supporting tools, is the improved execution time. This is attributed to the fact that Cell-DEVS provides asynchronous execution to model the asynchronous nature of complex systems [6]. Also, Cell-DEVS formalism offers ways to define complex timing conditions. Besides, there is an extensive set of tools available for translating the formalism into an executable model. This facilitates validating the conceptual model against the physical system and allows for verifying the simulation.

A Cell-DEVS model can be formalized as follows: GCC = (X_{list}, Y_{list}, I, X, Y, η, N, $\{t_1, . . . , t_n\}$, C, B, Z), where X_{list} is the list of external input couplings (i.e. input values to the cell that couples it with its defined neighbors), Y_{list} is the list of external output couplings, I is the set of states, X is the external input events set, Y is the external output events set, η is the neighborhood size, N is the neighborhood set, $\{t_1, . . . , t_n\}$ is the number of cells in each dimension, C is the cell space, B defines the border cells, and Z is a translation function that defines internal and external coupling.

3 Literature Review

In this section, we review some research efforts for modeling CO_2 dispersion in closed spaces while considering occupants. In their work, researchers have raised the issue of the importance of considering the location of CO_2 sensors and other configuration parameters in the modeled space, but no clear solution has been provided. Instead, a case by case solution for modeling is suggested.

Batog and Badura [10] present a model of a bedroom that contains big solid surfaces (e.g. bed and wardrobe) and one occupant. The authors perform two simulations: one with the possibility of CO_2 escaping through gaps around the windows and doors, and the other without such gaps. The occupant is assumed to spend eight hours sleeping in the room. The result of the simulations proves that the strategic placement of CO_2 sensors is important for accurate measurement. In particular, the authors do not recommend placing CO_2 sensors in corners nor near windows or doors. They also recommend that the height at which the sensor is installed should be above the level of the bed for the specific environment they model [10].

Pantazaras et al. [11] propose a method for tailoring models for specific spaces. The model takes into consideration the CO_2 concentration, ventilation, and multiple occupants. This is used to predict CO_2 concentration levels in the room. The model is only effective for short term predictions of CO_2 concentration levels [11].

A study that is not focused on CO_2 modeling but rather on the dispersion of hazardous gasses in closed spaces is presented by Makmul [12]. The study uses CA to model the influence of the spread of gas on the behavior of pedestrians. Makmul's objective is to aid designers in building safe public spaces that are practical during evacuations. The authors offer an experiment on a specific model of a closed space with two exits. The used model is a 2-D model that does not consider indoor space height [12].

To the contrary to previous research that deals with the problem in a case by case manner and considers a small subset of the configuration parameters, we offer a generic model of CO_2 dispersion using well-established formalism that is supported by tools. It is worth noting that the objective of this research is not to estimate the number of occupants in the room based on CO_2 levels, but rather to provide a mechanism for studying the effect of the space settings on the measurement and the dispersion behavior of CO_2. The presented solution reaches this objective while considering different configurations in the space where the CO_2 sensor is to be installed; a problem that was raised by researchers in the field of occupants' detection [3, 5, 11].

4 Experimental Setup

In previous work [8], we used CD++ (a toolkit that implements DEVS and Cell-DEVS theoretical concepts) to implement and simulate the model [13]. For the model presented in this paper, we use a newer Cell-DEVS simulator. Cell-DEVS Cadmium is a cross-platform header-only C++ library that can be used to implement and simulate Cell-DEVS models. A model simulated using Cadmium is defined in a header (.hpp) file and coded in C++. The simulator allows defining a general category of models using the programming language (C++) while reading specific configuration details for each model from a JavaScript Object Notation (JSON) file that is parsed by the simulator. On the one hand, we have implemented one general model in C++ for CO_2 dispersion and the breathing of occupants. On the other hand, the JSON file describes different initial configurations per cell. Each cell represents a specific segment of the physical space. The JSON file also specifies the dimensions of the room, the shape of the cells' neighborhood, and other configuration parameters. For visualizing the simulation results, we use Advanced Real-time Simulation Laboratory (ARSLab) DEVSWeb Viewer [14].

The general model we are presenting considers the dimensions of the closed space, ambient CO_2 concentration, size and location of CO_2 sinks (i.e. windows, doors, and ventilation ports), possible locations where occupants may exist, the breathing rate of occupants based on their activity level, concentration increase due to breathing occupants, and dimensions of the room. The model assumes ambient outdoor CO_2

concentration of 400 particles per minute (ppm) based on the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) standards [15]. However, this value can be adjusted as a parameter specified for each JSON scenario. Human breathing is calculated based on the fact that humans breathe every five seconds, and the produced CO_2 in every breath (exhaling and inhaling) is a parameter that depends on the activity level [16]. The general model has seven types of cells: (1) walls and obstacles that do not allow CO_2 diffusion, (2) air cells whose CO_2 concentration is dependent on the concentration values in their neighborhoods, (3) CO_2 sources with a periodic increase in the CO_2 level added at an interval to mimic breathing in addition to the CO_2 diffused from the neighborhood, (4) open doors that diffuse CO_2 to the rest of the building with a fixed indoor background CO_2 level, (5) open windows that are also CO_2 sinks with a fixed outdoor background CO_2, (6) vents that diffuse gas through HVAC system with a reduced constant CO_2 level, and (7) workstation cells that act as normal air cells when not occupied and as CO_2 sources when occupied. The CO_2 diffusion is calculated by averaging the concentration level in the Moore neighborhood of each cell. This means that to get the concentration of each cell, the concentrations in either 27 or 9 cells are averaged in the cases of 3-D and 2-D models, respectively.

5 Case Study

In this section, we present a case study for two computer laboratories at Carleton University. We use the first physical system to calibrate the parameters of the model and the second to validate the calibrated model.

5.1 Calibration Model

The general model has flexible parameters, some of which are not available in the set of ground truth data that we have. For example, although the exact number of attendees in the lab is available, the arrival time of each person at the computer workstation they have used is not available. Also, the exact CO_2 concentration in the vents is not available. Thus, we had the space to change this data to calibrate the model to get simulation results that are as close as possible to the ground truth data. The parameters that we adjusted are the arrival and departure times of the occupants, the workstations that the occupants chose to use, ambient CO_2 concentration, and CO_2 concentration in the air pumped to the room through the ventilation ports. The exact steps to run the model, the code, and the parameter settings are available through the ARSLab repository [17].

The first computer laboratory we are modeling in this paper represents a $(9.5\times14.24\times3.25)$ m^3 closed space, with 48 workstations where students can sit to work on their computer assignments. The floor plan of the laboratory and the furniture layout are shown in Fig 1. The ground truth data is based on the number of attendees for a 110-minute tutorial that has taken place in the Winter term of the year 2019. Thirty nine students have attended the tutorial in addition to the teaching assistant (TA) who has been present throughout the tutorial. Students arrive and leave at different times along the period of the lab tutorial. The logged data (Fig. 3) for this period is based on one

CO_2 sensor installed close to the door at 1.5 m height and logs the concentration level every 30 minutes. As the occupants arrive at the room, the readings of CO_2 concentration start to increase reaching the peak after the middle of the lab tutorial period when all students are present. The CO_2 starts to decrease again until all students leave the room (Fig. 3).

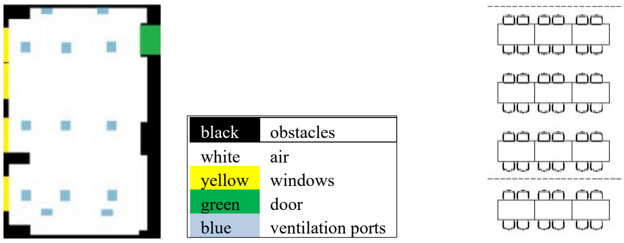


Fig. 1. Floor plan and furniture layout of the physical system of the calibration model

The physical 9.5×14.24×3.25 m^3 system is mapped to a 23×35×8 cell^3 model. Table 1 shows how the physical system maps to the 3D model. Each cross-section of the room of 40 cm height maps to a 23×35 cell grid.

Table 1. Mapping the physical system to the 3D model

cross-section (cm) (physical system)	0-40	40-80	80-120	120-160	120-200	200-240	240-280	280-320
grid number (model)	0	1	2	3	4	5	6	7
significance for simulation	floor	air	air	breathing	CO_2 sensors	air	air	ceiling-vents

The 3-D Cell-DEVS model is formally specified as follows: $CO_2 = < X_{list}, Y_{list}, Z_{list}, I, X, Y, Z, \eta, N, \{t_1, t_2, t_3\}, C, B, Z >$, where $X_{list} = Y_{list} = Z_{list} = \{Ø\}$; I = type: {0, 1, 2, 3, 4, 5, 6} and conc: {float}; $X = Y = Z = Ø$; $\eta = 27$; N = { (0,0,0), (-1,0,0), (1,0,0), (0,1,0), (0,-1,0), (-1,1,0), (1,1,0), (-1,-1,0), (1,-1,0), (0,0,1), (-1,0,1), (1,0,1), (0,1,1), (0,-1,1), (-1,1,1), (1,1,1), (-1,-1,1), (1,-1,1), (0,0,-1), (-1,0,-1), (1,0,-1), (0,1,-1), (0,-1,-1), (-1,1,-1), (1,1,-1), (-1,-1,-1), (1,-1,-1) }; $t_1 = 23$; $t_2 = 35$; $t_3 = 8$; $C = \{C_{ijk} \mid i \in [0, 23[\wedge j \in [0, 35[\wedge k \in [0, 8[\}$; and B = {Ø} (unwrapped cell space).

For this case study, we specify a 40×40×40 cm^3 cell size. Therefore, the physical system is translated to an approximated (23×35×8) cell model. To replicate the physical system, the CO_2 production for each occupant is calculated as follows based on two facts: (1) an average-sized person doing normal low-activity office work produces 0.31 liter/minute/person of CO_2 [11] and (2) breathing occurs every 5 seconds on average. Therefore, an average person produces 0.02583 liters of CO_2 per breath. Hence, every occupant breath increases the concentration of CO_2 in each occupied cell by:

$$\frac{0.02583}{cell\ volume} = \frac{0.02583 \times 1000}{40 \times 40 \times 40} \approx 0.000403 \tag{1}$$

It is worth noting that equation (1) gets calculated automatically based on the model parameters (i.e. cell volume and produced CO2 per breath specified in the input JSON settings file). We are including here how this calculation is done for the parameters we specify for the presented case study.

The simulation runs of 7,200 timesteps which is equivalent to two hours; each time step is one second. The session lasted for 110 minutes and we added five minutes before and after the session to get a better picture of the CO_2 level changes due to the arrival and departure of occupants. Fig. 2 (a) shows the simulation results at the beginning of the simulation where only one occupant is present (the TA), and during other timestamps as occupants start to arrive (Fig. 2 (b) and Fig. 2 (c)). CO_2 concentration is to the left of each figure (a, b, and c) and the occupants' locations are at the right. Occupants are represented as red squares and empty workstations are in grey. The two grids shown in the figure are layer 4 (left), which is the cross-section of the room representing the height at which the CO_2 sensor is installed (120-160 cm), and layer 3 (right) representing the height at which the seated occupants are breathing (80-120 cm). The legend below Fig. 2 maps the CO_2 concentration to the color used to visualize the simulation. Comparing the simulation results to the floor map of Fig. 1 shows how the area below the vents has less CO_2 concentration than other areas as the vents try to offset the CO_2 increase that occurs where the occupants are concentrated.

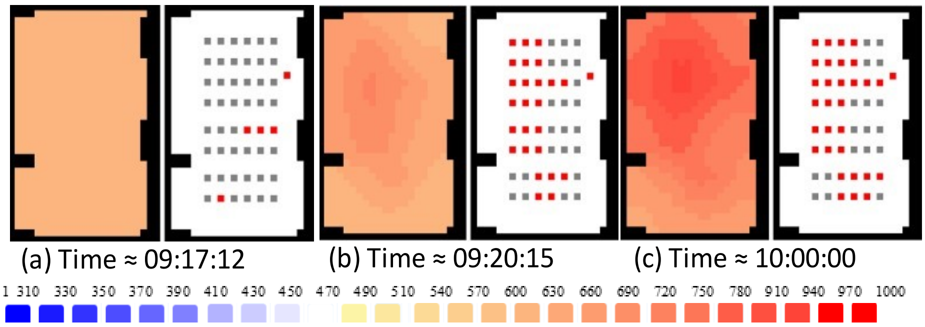


Fig. 2. Simulation results during different timestamps (hh:mm:ss)

Fig. 4 is a plot of the simulation results. The figure shows that the simulation results after calibrating the model are similar to the ground truth data (Fig. 3).

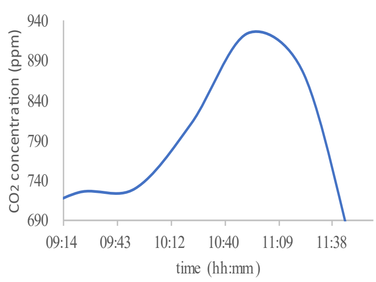


Fig. 3. Ground truth data plot

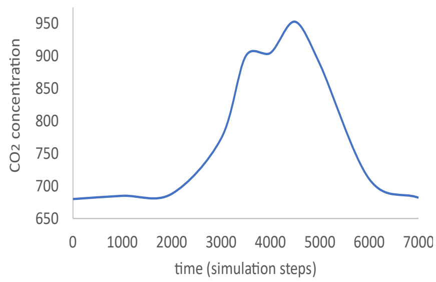
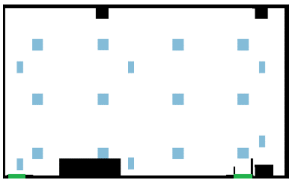


Fig. 4. Simulation results plot

Note that while the simulation results are logged every second, the ground truth data is logged every 15-30 minutes. This justifies a possible minor difference between the ground truth data and the simulation results. The plots of the simulation results are generated using Microsoft Excel© for ease of comparison. However, plots of the simulation results can be regenerated using the ARSLab charting tool [18].

5.2 Validation Model

In this section, we validate the rules used in the presented CO_2 model, using another room in the same building but on a different floor and with a different configuration. This physical system used for validation is another laboratory setting during a different time of the day, with only eleven occupants, a larger space, and no windows. The dimensions of this room are $15.8 \times 9 \times 3.25$ m^3. Fig. 5 shows the floor plan of the room and the furniture layout. In the physical system, there is another lab session following this one and hence more students enter the room at the end of the laboratory, and we have tried to mimic this in the model. The CO_2 sensor is installed close to the door and logs the concentration level every 15 minutes. Fig. 6 is a chart of the ground truth data of the CO_2 concentration during the studied period.



black	obstacles
white	air
blue	ventilation ports
green	doors

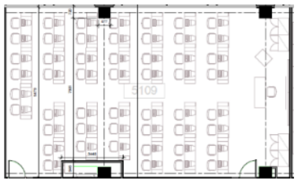


Fig. 5. Floor plan and furniture layout of the validation model

The formal model specification is the same as the one explained in section 5.1 except for the following: $t_1 = 23$; $t_2 = 40$; and $C = \{C_{ijk} \mid i \in [0, 23[\wedge j \in [0, 40[\wedge k \in [0, 8[\}$. We have used the same ambient CO_2 concentration and ventilation concentration that have resulted from calibrating the model. We have executed the model for a simulation period equivalent to 7200 seconds (two hours) and Fig. 7 shows data collected from the simulation results. Comparing that simulation results (Fig. 7) to the data logged by the real sensors in the physical system (Fig. 6) demonstrates the resemblance between the model's data and the system's data. Simulation videos of the validation model and the original CO_2 model are available online through the ARSLab YouTube channel [19].

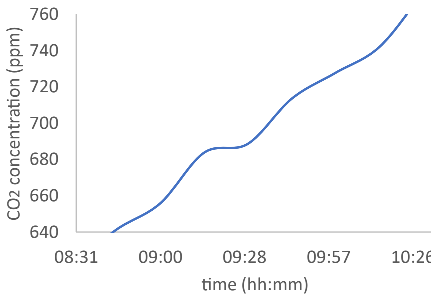


Fig. 6. Validation model ground truth data

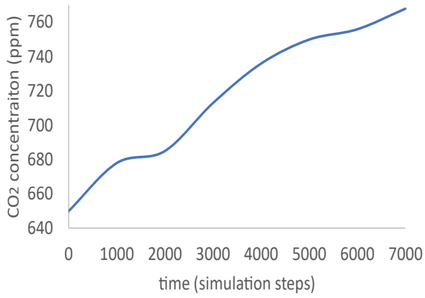


Fig. 7. Validation model simulation results

6 Discussion

The model proposed is evinced successful at replicating the physical indoor space. However, as in any other experimental study, there are some threats to validity that are worthy of discussion. A minor validity threat is the existence of some approximations when converting the physical system into a model. Nevertheless, this does not affect the usability of the model as the model user is aware of it and can handle the slight approximations if needed. A second validity threat is that the current model assumes that the air in the room is at a steady-state and the CO_2 is diffused evenly in all directions. This is not usually the case due to the different types of HVAC and occupants breathing in different directions. Incorporating airflow in the room is a future feature that we are planning to add to the model. However, the model at the current state has successfully mimicked the physical system.

7 Conclusion

Motivated by the need for studying the effects of room configuration on recorded CO_2 concentration and the way CO_2 diffuses in closed areas, we present a generic model for indoor CO_2 diffusion. We have developed a generic Cell-DEVS model that accepts different room configurations as input parameters. We have calibrated the model using the settings of a real physical system of a computer laboratory at Carleton University. Then, we validated the model using another closed space in the same building during a different time and with different configurations. The simulation results resemble the physical systems as presented by the plot of CO_2 concentration in both the simulation and the physical system. The results suggest that the model is suitable for studying the spread of CO_2 indoors. The model can help to study the effect of placing sensors in different locations, the effect of changing the ventilation, increasing the number of occupants, changing the furniture layout, and many other configuration parameters.

Future improvements to the model will target the flow field of the air in the room and conducting statistical analysis of the results of different case studies.

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