# Mathematical Modeling for Carbon Dioxide Level Within Confined Spaces

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Federal regulations require refuge alternatives (RAs) in underground coal mines to provide a life-sustaining environment for miners trapped underground when escape is impossible. A breathable air supply is among those requirements. For built-in-place (BIP) RAs, a borehole air supply (BAS) is commonly used to supply fresh air from the surface. Federal regulations require that such a BAS must supply fresh air at 12.5 cfm or more per person to maintain the oxygen concentration between 18.5% and 23% and carbon dioxide level below the 1% limit specified. However, it is unclear whether 12.5 cfm is indeed needed to maintain this carbon dioxide level. The minimal fresh air flow (FAF) rate needed to maintain the 1% CO2 level will depend on multiple factors, including the number of people and the volume of the BIP RA. In the past, to predict the interior CO<sub>2</sub> concentration in an occupied RA, 96-h tests were performed using a physical human breathing simulator. However, given the infinite possibility of the combinations (number of people, size of the BIP RA), it would be impractical to fully investigate the range of parameters that can affect the CO<sub>2</sub> concentration using physical tests. In this paper, researchers at the National Institute for Occupational Safety and Health (NIOSH) developed a model that can predict how the %CO2 in an occupied confined space changes with time given the number of occupants and the FAF rate. The model was then compared to and validated with test data. The benchmarked model can be used to predict the %CO2 for any number of people and FAF rate without conducting a 96-h test. The methodology used in this model can also be used to estimate other gas levels within a confined space. [DOI: 10.1115/1.4055389]

Keywords: confined space, gas concentration, breathing air, mathematical model

#### 1 Introduction

Human breathing generates a significant amount of carbon dioxide. High levels of carbon dioxide can be extremely hazardous [1–3]. Carbon dioxide mitigation methods, such as soda lime carbon dioxide scrubber curtains, and purging with high volume air flows, can prevent carbon dioxide levels from reaching

dangerous levels. This is especially critical for confined spaces, such as refuge chambers—also known as refuge alternatives (RAs)—that federal regulation require in underground coal mines to provide miners with a life-sustaining environment in case of an inescapable mine disaster [4–6]. According to federal regulations, the average carbon dioxide concentration in the occupied structure shall not exceed 1.0%, and excursions shall not exceed 2.5% while maintaining the oxygen concentration between 18.5% and 23% [2,5,6]. A 1.0% carbon dioxide (CO<sub>2</sub>) atmosphere is the threshold of a serious health risk. The 15-min short-term exposure limit for carbon dioxide set by the National Institute for Occupational Safety and Health (NIOSH) and the American Conference of Governmental Industrial Hygienists (ACGIH, Cincinnati, OH) is 3% [2]. Therefore, excursions to 2.5% carbon dioxide must be mitigated quickly.

While occupied and without a breathable air supply, the RA interior oxygen level will decrease, and the carbon dioxide level will increase quickly due to breathing [4]. For built-in-place (BIP) RAs, one mitigation strategy is to implement a borehole air supply (BAS) to supply fresh air from the surface. Federal regulations require the supply of fresh air of 12.5 cfm or more per person to maintain the oxygen and carbon dioxide levels within the safety range specified in the RA regulations [5,6]. While the oxygen level is mainly determined by the fresh air flow rate, the CO<sub>2</sub> concentration within the RA will depend on multiple factors including the number of occupants, the volume of the BIP, and the fresh air flow (FAF) rate. The CO<sub>2</sub> concentration can exceed the 1% limit even when the oxygen level is within the 18.5%–23% range. It is crucial to estimate or predict the CO<sub>2</sub> concentration for RA or other occupied confined space.

Recently, research has been conducted to examine the gas level within confined spaces based on either experiment or modeling [7–10]. In this paper, researchers at NIOSH developed a model that can predict the  $\%\text{CO}_2$  within an occupied confined space. The model was then validated with test data. The benchmarked model was used to predict the  $\%\text{CO}_2$  given the number of people and FAF rate without conducting a physical test. The methodology used in this model can also be used to estimate other types of gas levels within a confined space.

## 2 Mathematic Modeling

As illustrated in Fig. 1, a confined space has an inward fresh air flow. The confined space is also equipped with a pressure relief valve which allows air to release to outside of the space when the internal pressure reaches the set point of the relief valve. Two models were developed to represent the change in  $\%\text{CO}_2$  over time. The simplified model relies on a number of assumptions to provide an approximation of the  $\%\text{CO}_2$  level. The differential model uses differential equations to more accurately represent the change in  $\%\text{CO}_2$  over time. In Secs. 2.1 and 2.2, these two models are described.

**2.1 Simplified Model.** At the point when the test starts, t = 0,  $x = x_0$ , and the total  $CO_2$  mass within the confined space is  $mx_0$ . As shown in Fig. 1, there are two sources that bring  $CO_2$  into the confined space: fresh air flow and breathing. There is one outward flow that allows  $CO_2$  to exit the confined space through the exhaust pipe. It is reasonable to assume that the amount of air exiting the space equals the amount of air entering the space, i.e., the outward air flow rate and inward air flow rate both have a value of f. At time t, the total  $CO_2$  mass, mx, within the confined space is given by

$$mx = mx_0 + x_0 f t + G t - \mu x f t$$
 (1)

where  $\mu$  is a coefficient to average the %CO<sub>2</sub> (by mass) value from time t=0 to time t,  $0 < \mu < 1$ . Consider  $x_0 \to 0$ , (1) can be rewritten as

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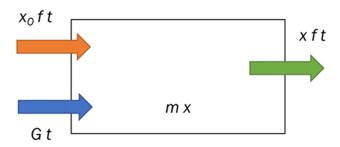


Fig. 1 The gas  $(CO_2)$  movement into and out of a confined space (dimension of  $a \times b \times c$ ) with fresh air flow. The  $CO_2$  gas moving into the confined space includes breathing (blue) and fresh air flow (orange). The  $CO_2$  gas moves out of the confined space through the exhaust pipe (green).

$$x \approx \frac{Gt}{m + \mu ft} \tag{2}$$

**2.2 Differential Model.** Define  $x_{\rm ini}$  as the initial %CO<sub>2</sub> by mass in the confined space. At the point when the test starts, t=0 and  $x=x_{\rm ini}$  (refer to Fig. 1). For a small time interval,  $\Delta t = t_2 - t_1$ , the CO<sub>2</sub> mass change within the confined space from  $t_1$  to  $t_2$  is given by

$$\Delta(mx) = \Delta(Gt + x_0ft - xft) \tag{3}$$

Equation (3) can be rewritten as

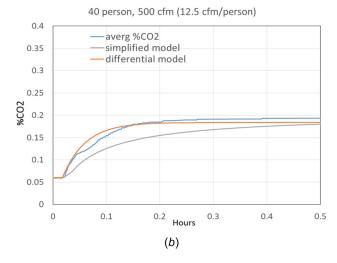


Fig. 2 The %CO<sub>2</sub> (by volume) based on test data and model prediction for 40 people and 100 cfm (a) or 500 cfm (b) FAF rate

$$m\Delta x = G\Delta t + x_0 f \Delta t - x f \Delta t \tag{4}$$

Let  $\Delta t = dt \rightarrow 0$ , then  $\Delta x = dx \rightarrow 0$ . Equation (4) can be rewritten as

$$mdx = Gdt + x_0 f dt - x f dt ag{5}$$

$$m\frac{dx}{dt} = G + x_0 f - xf \tag{6}$$

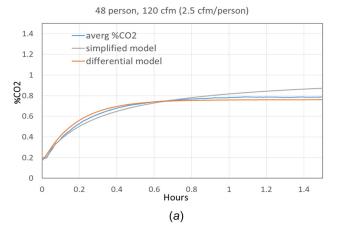
$$mx'(t) + fx(t) = G + x_0 f$$
 (7)

Equation (7) is the boundary value problem with the boundary condition:  $x(t=0)=x_{\rm ini}$ . Equation (7) is the mathematical and accurate description of the event. Solving the boundary value problem above will give the analytical solution of x as a function of t.

### 3 Test Setup

In order to conduct testing to examine the  $CO_2$  levels inside an occupied confined space, a test lab was created using a 20-ft-long by 8-ft-wide by 8-ft-high shipping container, and a human breathing simulator was created to consume oxygen and generate  $CO_2$  to represent human breathing. For the human breathing simulator, the concept was to burn propane at the rate necessary to match the rate of human oxygen consumption.

Multiple gas monitors were used to measure the  $\%CO_2$  and  $\%O_2$  inside the test lab. For each test, all flow rates were set based on an assumed number of occupants. The propane flow rate was set based on the rate needed to consume the oxygen of the assumed number of occupants.



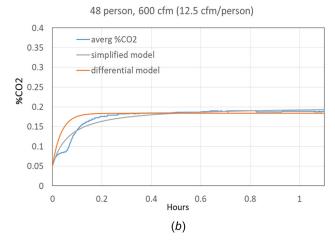


Fig. 3 The %CO<sub>2</sub> (by volume) based on test data and model prediction for 48 people and 120 cfm (a) or 600 cfm (b) FAF rate

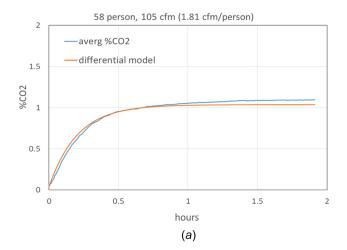
#### 4 Results

A series of tests were conducted for various numbers of people and FAF rates to observe the  $CO_2$  concentration within the confined space (the shipping container). The first run of the test was to look at the  $\%CO_2$  by volume with 40 people and various FAF rates. Two FAF rates were chosen, one low rate (100 cfm) and one high rate (500 cfm).

The first test was to look at the %CO<sub>2</sub> level at various FAF rates for 40 people. The %CO<sub>2</sub> test data was plotted in Fig. 2 for FAF rates of 100 cfm (Fig. 2(a)) and 500 cfm (Fig. 2(b)). The model prediction of %CO<sub>2</sub> value was also plotted and compared with test data in Fig. 2. The figure clearly shows that for both the low FAF rate and high FAF rate, the differential model agrees with test data better than the simplified model. Both the test data and the differential model prediction show that the %CO<sub>2</sub> reaches a steady level in about 1 h. For the high FAF rate (500 cfm), the test data and the differential model show the %CO<sub>2</sub> reaches a steady level within 15 min.

Another test was conducted for 48 people, with FAF rates of 120 cfm and 600 cfm. The  $\%\text{CO}_2$  test data was plotted in Fig. 3 for FAF rates of 120 cfm (Fig. 3(a)) and 600 cfm (Fig. 3(b)). Again, the figure shows that the differential model predicts the  $\%\text{CO}_2$  value better than the simplified model. For 120 cfm (Fig. 3(a)), both the test data and the differential model show that the  $\%\text{CO}_2$  would reach a steady level within 1 h. For 600 cfm (Fig. 3(b)), the data and the models show that the  $\%\text{CO}_2$  would reach a steady level within 0.5 h.

The test data and the differential model show that for FAF rates higher than 2.5 cfm/person, the %CO<sub>2</sub> level within the shipping container will stabilize below 1% (Figs. 2 and 3).



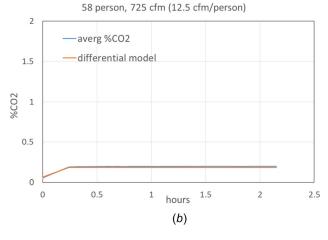


Fig. 4 The %CO<sub>2</sub> (by volume) based on test data and model prediction for 58 people and 105 cfm (a) or 725 cfm (b) FAF rate

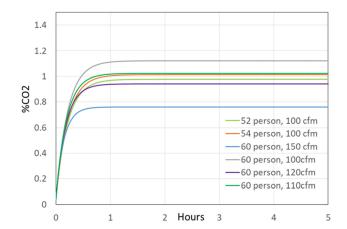


Fig. 5 The %CO<sub>2</sub> by volume predicted by the differential model for various numbers of people and FAF rates

Table 1 The simulation results for the minimum FAF rate for different numbers of people to maintain %CO<sub>2</sub><1%

N	Federal regulation of CFR FAF at 12.5 cfm/person (cfm)	Model minimum FAF for CO <sub>2</sub> < 1% (cfm)	Model minimum FAF for CO <sub>2</sub> < 1% (cfm/person)
1	12.5	NA	NA
54	675	101	1.87
55	687.5	103	1.87
56	700	105	1.88
57	712.5	107	1.88
58	725	108	1.86
59	737.5	110	1.86
60	750	112	1.87

An additional test was conducted with a smaller cfm/person value (less than 2.5 cfm/person) by increasing the number of people. Figure 4 shows the differential model validated by test data for 58 people with 105 cfm (Fig. 4(*a*)) and 725 cfm (Fig. 4(*b*)) FAF rate.

# 5 Discussion

An observation based on Figs. 2–4 is that the steady-state  $\%\text{CO}_2$  level depended on the cfm/person value rather than the number of people or the total FAF rate, given other parameters are unchanged. For example, the  $\%\text{CO}_2$  level stabilized at  $\sim$ 0.8% for 2.5 cfm/person as shown in Figs. 2(a) and 3(a), regardless of the number of people and the total FAF rate.

Figure 5 shows the  $\%\text{CO}_2$  predicted by the differential model for a various number of people and total FAF rate. The model predicted that the  $\%\text{CO}_2$  level will approach 1% for 60 people and 110 cfm or 54 people and 100 cfm. The simulation results for the minimum FAF rate for different numbers of people to maintain  $\%\text{CO}_2 < 1\%$  are listed in Table 1. The model predicts the minimal FAF rate to maintain 1% CO<sub>2</sub> to be  $\sim 1.87$  cfm/person, regardless of the number of people and the total FAF rate.

## 6 Conclusion

The mathematical models presented in this study agree with test data well. They can be used to predict the %CO<sub>2</sub> level based on the parameters of confined space such as the dimension of the confined space, the number of occupants, and the FAF rate. The differential model predicts that a FAF of about 1.87 cfm/person is needed for the %CO<sub>2</sub> to stabilize below 1%. However, safety factors must be taken into consideration when implementing regulations. Because of this, the minimal FAF of 12.5 cfm specified in federal regulations is indeed needed to maintain this carbon dioxide level and the level of other gases within the safe range for 96 h. The model also

predicts the  $\%CO_2$  level will reach a steady-state within 1 h or less. Another observation is that the  $\%CO_2$  level depends on the cfm/ person value rather than the number of people or the total FAF rate. Additionally, the  $\%CO_2$  level is more sensitive to the total FAF rate variation than to the number of people.

The benchmarked model can be used to predict the  $\%\text{CO}_2$  for various numbers of occupants, size of the confined space, and FAF rate without conducting a 96-h test for every scenario. The model and testing confirm 12.5 cfm of supplied air will sustain miners for 96 h and comply with federal regulations. The model may also be useful in helping manufacturers and mines to make decisions on RA design and implementation to comply with federal regulations.

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#### References

- [1] Harper, P., Wilday, J., and Bilio, M., 2011, "Assessment of the Major Hazard Potential of Carbon Dioxide (CO<sub>2</sub>)," Health and Safety Executive, pp. 1–28.
- [2] NIOSH, 2018, Occupational Exposure Limits, The National Institute for Occupational Safety and Health, Morgantown, WV, accessed Aug. 19, 2022, https://www.cdc.gov/niosh/topics/flavorings/limits.html

- [3] Permentier, K., Vercammen, S., Soetaert, S., and Schellemans, C., 2017, "Carbon Dioxide Poisoning: A Literature Review of an Often Forgotten Cause of Intoxication in the Emergency Department," Int. J. Emer. Med., 10(1), pp. 1–4.
- [4] Bauer, E. R., Matty, T. J., and Thimons, E. D., 2014, "Investigation of Purging and Airlock Contamination of Mobile Refuge Alternatives (Report of Investigatons 9694)," *Department of Health and Human Services, Centers for Disease Control and Prevention (CDC)*, National Institute for Occupational Safety and Health (NIOSH), Pittsburgh, PA.
- [5] MSHA, 2008, "Regulatory Economic Analysis for Refuge Alternatives for Underground Coal Mines," Mine Safety and Health Administration, U.S. Department of Labor, Office of Standards, Regulations, and Variances, Arlington, VA, accessed Sept. 7, 2022, https://arlweb.msha.gov/ REGS/rea/refuge-alternatives.pdf
- [6] MSHA, 2008, "30 CFR Parts 7 and 75; Refuge Alternatives for Underground Coal Mines; Final Rule," Mine Safety and Health Administration, U.S. Department of Labor, Office of Standards, Regulations, and Variances, Arlington, VA. https://www.federalregister.gov/documents/2008/12/31/E8-30669/refuge-alternativesfor-underground-coal-mines
- [7] He, B., Jiang, X., Yang, G., and Xu, J., 2017, "A Numerical Simulation Study on the Formation and Dispersion of Flammable Vapor Cloud in Underground Confined Space," Process Saf. Environ. Prot., 107, pp. 1–11.
- [8] Shi, G., He, Y., Zhang, Y., Yin, B., and Ali, F., 2019, "Detection and Determination of Harmful Gases in Confined Spaces for the Internet of Things Based on Cataluminescence Sensor," Sens. Actuators B Chem., 296, p. 126686.
- [9] Stefana, E., Marciano, F., Cocca, P., Rossi, D., and Tomasoni, G., 2021, "Oxygen Deficiency Hazard in Confined Spaces in the Steel Industry: Assessment Through Predictive Models," Int. J. Occup. Saf. Ergon., 27(4), pp. 990–1004.
- [10] Zhan, G., Bai, L., Wu, B., Cao, F., Duan, Y., Chang, F., Shang, D., Bai, Y., Li, Z., Zhang, X., and Zhang, S., 2021, "Dynamic Process Simulation and Optimization of CO<sub>2</sub> Removal From Confined Space With Pressure and Temperature Swing Adsorption," Chem. Eng. J., 416, p. 129104.