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MATHEMATICAL MODELING FOR CARBON DIOXIDE LEVEL WITHIN CONFINED SPACES

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ABSTRACT

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. It is assumed that the fresh air has an oxygen concentration of 20.9%. 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% to 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 CO₂ concentration in an occupied RA, 96-hour 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 CO₂ 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 fresh air flow (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-hour test. The methodology used in this model can also be used to estimate other gas levels within a confined space.

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

NOMENCLATURE

t	time after test starts
x	%CO ₂ (by mass) at time t within the confined space
x_0	%CO ₂ (by mass) in the atmosphere
ρ	air density within the confined space
m	total air mass within the confined space
G	CO ₂ generation rate due to breathing
f	fresh air flow rate
P	air pressure in the confined space
R	universal gas constant
T	air temperature in the confined space
CO ₂	carbon dioxide
%CO ₂ _v	CO ₂ gas concentration by volume
%CO ₂ _m	CO ₂ gas concentration by mass
%O ₂ _m	O ₂ gas concentration by mass
%N ₂ _m	N ₂ gas concentration by mass
M_{CO_2} :	the molar mass for CO ₂ gas
M_{O_2} :	the molar mass for O ₂ gas
M_{N_2} :	the molar mass for N ₂ gas
MSHA	Mine Safety and Health Administration
NIOSH	the National Institute for Occupational Safety and Health
BIP	built-in-place
RA	refuge alternative
BAS	borehole air supply
FAF	fresh air flow

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1. INTRODUCTION

Human breathing generates a significant amount of carbon dioxide. High levels of carbon dioxide can be extremely hazardous [1]. 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 regulations require in underground coal mines to provide miners with a life-sustaining environment in case of an inescapable mine disaster [2] [3]. 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%. A 1.0% carbon dioxide (CO₂) atmosphere is the threshold of a serious health risk [2] [3]. The 15-minute short-term exposure limit (STEL) for carbon dioxide set by the National Institute for Occupational Safety and Health (NIOSH) and the American Conference of Governmental Industrial Hygienists (ACGIH) is 3% [4]. 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 [5]. 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 as specified in the RA regulations [2] [3]. While the oxygen level is mainly determined by the fresh air flow rate, the CO₂ 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 CO₂ concentration can exceed the 1% limit even the oxygen level is within the 18.5% - 23% range. It is crucial to estimate or predict the CO₂ concentration before the RA or other confined being occupied.

In this paper, researchers at NIOSH developed a model that can predict the %CO₂ within an occupied confined space. The model was then compared and validated with test data. The benchmarked model was used to predict the %CO₂ given the number of people and FAF rate without conducting 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 Figure 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. The variables involved in determining the carbon dioxide concentration are defined as in the Nomenclature section. Two models were developed to represent the change in %CO₂ over time. The simplified model relies on a number of assumptions to provide an approximation of the %CO₂ level. The differential

model uses differential equations to more accurately represent the change in %CO₂ over time. In the following sections, these two models are described.

2.1 Simplified model

At the point when the test starts, $t=0$, $x=x_0$, and the total CO₂ mass within the confined space is mx_0 . As shown in Figure 1, there are two sources that bring CO₂ into the confined space: the fresh air flow and the breathing. There is one outward flow that allows CO₂ to exit the confined space through the exhaust pipe. It is reasonable to assume that the amount of the 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 CO₂ mass, mx , within the confined space is given by

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

Where μ is a coefficient to average the %CO₂ (by mass) value from time $t=0$ to time t , $0 < \mu < 1$. Consider $x_0 \rightarrow 0$, (1) can be rewritten as:

$$x \approx \frac{Gt}{m + \mu ft} \quad (2)$$

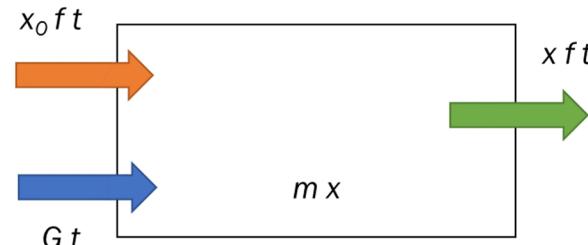


Figure 1. The gas (CO₂) movement into and out of a confined space (dimension of $a \times b \times c$) with fresh air flow. The CO₂ gas moving into the confined space includes breathing (blue) and fresh air flow (orange). The CO₂ gas moves out of the confined space through the exhaust pipe (green).

2.2 Differential model

Define x_{ini} as the initial %CO₂ by mass in the confined space. At the point when the test starts, $t=0$ and $x=x_{ini}$ (refer to Figure 1). For a small time interval, $\Delta t = t_2 - t_1$, the CO₂ mass change within the confined space from t_1 to t_2 is given by:

$$\Delta(mx) = \Delta(Gt + x_0 ft - x ft) \quad (3)$$

Equation (3) can be rewritten as:

$$m\Delta x = G\Delta t + x_0 f \Delta t - x f \Delta t \quad (4)$$

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

$$mdx = Gdt + x_0fdt - xfdt \quad (5)$$

$$m \frac{dx}{dt} = G + x_0f - xf \quad (6)$$

$$m x'(t) + f x(t) = G + x_0f \quad (7)$$

Equation (7) is the boundary value problem with the boundary condition: $x(t = 0) = x_{ini}$. 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 (HBS) was created to consume oxygen and generate CO_2 to represent human breathing. For the HBS, the concept was to burn propane at the rate necessary to match the rate of human oxygen consumption. Because burning propane generates less CO_2 than human breathing for a set oxygen consumption rate, supplemental CO_2 would have to be added to match both oxygen consumption and CO_2 generation.

To create the HBS, a commercially available propane smoker was modified, and additional test equipment were used to create a well-controlled combustion device. A sealed combustion chamber was created by sealing the bottom of the propane smoker to the floor of the shipping container. Propane was delivered to the sealed combustion chamber from tanks stored outside the shipping container via a gas line that passed through a pressure regulator and a propane mass flow controller. An air pump was used to deliver air from inside the shipping container to the sealed combustion chamber via an airline that was connected to an air mass flow controller. The mass flow rate of propane was determined based on the desired number of people to represent. The air mass flow rate was set 20% higher than the rate needed to provide enough oxygen to support complete propane combustion. To match the CO_2 generation, supplemental CO_2 was provided from a cylinder outside the test lab. A CO_2 mass flow controller was used to provide the additional CO_2 needed to match the CO_2 generated by people.

A previously developed pressure relief valve test stand (PRVTS) was used as the source of fresh air. The PRVTS uses a centrifugal fan connected to a variable frequency drive (VFD) to allow for adjustment of the fresh air provided to the test lab. The PRVTS uses a VELTRON airflow measurement station to measure the provided volume flow of air corrected based on standard atmospheric conditions. The VFD keypad was used to set the FAF to the desired value for a given test.

Multiple gas monitors were used to measure the $\% \text{CO}_2$ and $\% \text{O}_2$ inside the test lab. To measure the $\% \text{CO}_2$, two CTI GG- CO_2

carbon dioxide sensors were positioned within the shipping container. The two sensors were located approximately 6 inches and 3 inches from the floor and positioned around 6.5 feet and 13 feet from the end-wall of the laboratory, respectively. To measure the $\% \text{O}_2$, two Macurco OX-6 oxygen sensors were positioned approximately 6 inches and 3 inches from the floor and positioned around 6.5 feet and 13 feet from the end-wall of the laboratory, respectively. One additional O_2 monitor was positioned near the air pump to document the $\% \text{O}_2$ in the combustion air.

To record the FAF rate, the CO_2 concentrations, and the oxygen concentrations, a Data Translation DT-9874 data acquisition system was used. All data were recorded at a sample rate of 2 samples per second with 24-bit resolution.

Multiple steps were taken to ensure research safety during the tests. The propane delivery line and the interior of the HBS were checked with a gas leak detector before lighting the propane burner. A Beacon 800 gas monitoring system with multiple CO_2 sensors, an O_2 sensor, a carbon monoxide sensor, and $\% \text{ lower explosive limit}$ sensor was used to ensure all gases within the test lab were at safe levels. If the gas levels exceeded predetermined levels, the Beacon 800 would activate an audible alarm to alert researchers. The presence of a flame in the HBS was monitored using a flame detector and a video camera. If the flame went out, the flame detector would activate an audible alarm and automatically turn off the propane flow via a solenoid valve. Gas monitors at the data acquisition table were used to ensure the O_2 , CO_2 , CO , and propane levels were at safe levels.

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. The combustion air flow rate was set at 1.2 times the air flow rate needed to provide sufficient oxygen to achieve complete combustion. The supplemental CO_2 flow rate was set based on the total CO_2 generation of the assumed number of occupants less the CO_2 generated due to burning propane. The FAF provided by the PRVTS was varied to examine the resulting CO_2 concentration for FAF rates based on dividing the RA regulation requirement of 12.5 cfm per person by integer values from 2 through 7. For each FAF rate, individual tests were conducted until the $\% \text{CO}_2$ inside the test lab stabilized.

The CO_2 concentration was measured using two carbon dioxide sensors located within the shipping container. The average $\% \text{CO}_2$ was calculated from the readings of the two sensors. All the gas concentrations in Section 3 and Section 4 were either measured or calculated by volume. However, the gas concentration in this section was denoted by mass. For CO_2 , the volume concentration relates to the mass concentration through

$$\% \text{CO}_{2v} = \frac{\% \text{CO}_{2m} / M_{\text{CO}_2}}{\frac{\% \text{O}_{2m} + \% \text{N}_{2m} + \% \text{CO}_{2m}}{M_{\text{O}_2} + M_{\text{N}_2} + M_{\text{CO}_2}}} \quad (8)$$

where

$\% \text{CO}_{2v}$: the CO_2 gas concentration by volume

$\% \text{CO}_{2m}$: the CO_2 gas concentration by mass

$\% \text{O}_{2m}$: the O_2 gas concentration by mass

$\%N_{2m}$:	the N_2 gas concentration by mass
M_{CO_2} :	the molar mass for CO_2 gas
M_{O_2} :	the molar mass for O_2 gas
M_{N_2} :	the molar mass for N_2 gas.

4. RESULTS

A series of tests was 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). Since the air flow meter did not have the capacity of measuring flow rate below 100 cfm, a large number of people (in our case, a higher propane burning rate to simulate more human breathing) was selected in order to bring down the FAF rate/person.

The first test was to look at the $\%CO_2$ level at various FAF rates for 40 people. The $\%CO_2$ test data was plotted in Figure 2 for FAF rates of 100 cfm (Figure 2a) and 500 cfm (Figure 2b). For 40 people and 100 cfm, the FAF rate is 2.5 cfm/person. For 40 people and 500 cfm, the FAF rate is 12.5 cfm/person. The model prediction of $\%CO_2$ value was also plotted and compared with test data in Figure 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 $\%CO_2$ reaches a steady level in about one hour. For the high FAF rate (500 cfm), the test data and the differential model show the $\%CO_2$ reaches a steady level within 15 minutes.

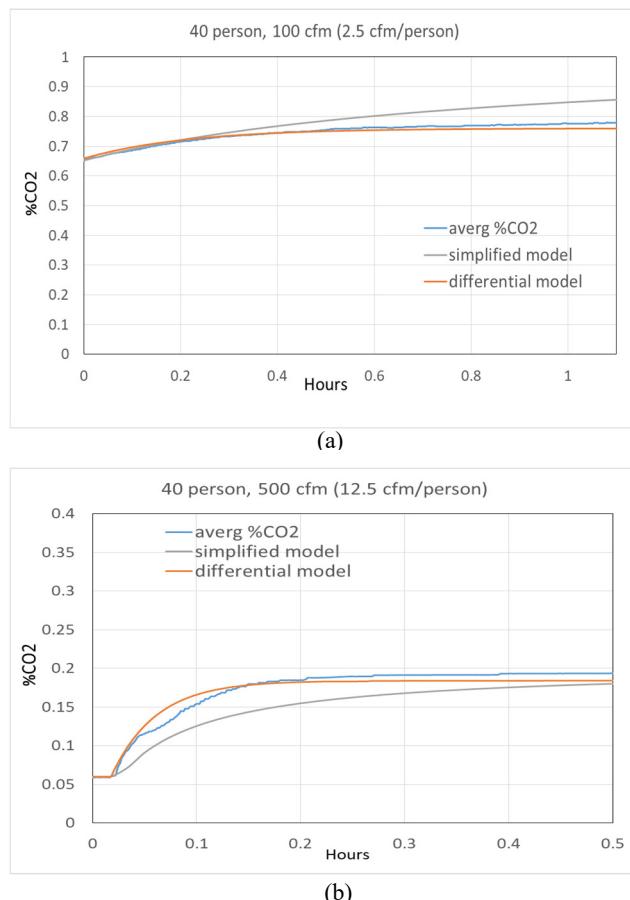


Figure 2. The $\%CO_2$ (by volume) based on test data and model prediction for 40 people and 100 cfm (a) or 500 cfm (b) FAF rate.

Another test was conducted for 48 people, with FAF rates of 120 cfm and 600 cfm. The $\%CO_2$ test data was plotted in Figure 3 for FAF rates of 120 cfm (Figure 3a) and 600 cfm (Figure 3b). For 48 people and 120 cfm, the FAF rate is 2.5 cfm/person. For 48 people and 600 cfm, the FAF rate is 12.5 cfm/person. The predicted $\%CO_2$ values based on the simplified model and the differential model were also plotted and compared with test data in Figure 3. Again, the figure shows that the differential model predicts the $\%CO_2$ value better than the simplified model. For 120 cfm (Figure 3a), both the test data and the differential model show that the $\%CO_2$ would reach a steady level within one hour. For 600 cfm (Figure 3b), both the test data, the simplified model, and the differential model show that the $\%CO_2$ would reach a steady level within 0.5 hour.

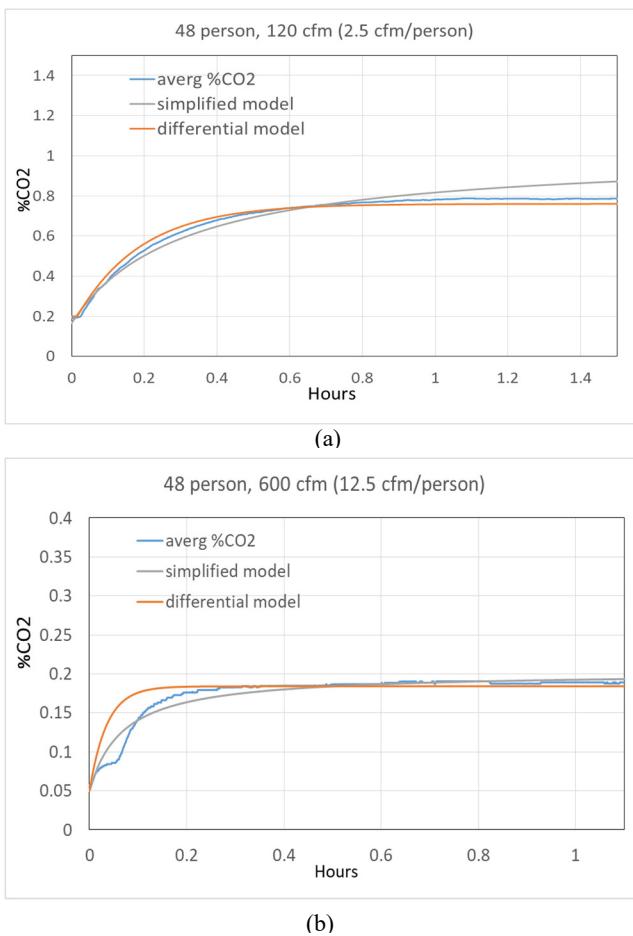


Figure 3. The %CO₂ (by volume) based on test data and model prediction for 48 people and 120 cfm (a) or 600 cfm (b) FAF rate.

The test data and the differential model show that for FAF rates higher than 2.5 cfm/person, the %CO₂ level within the shipping container will stabilize below 1% (Figure 2 and Figure 3).

An additional test was conducted with 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 (Figure 4a) and 725 cfm (Figure 4b) FAF rate. For 58 people, the FAF rate is 1.81 cfm/person for 105 cfm and 12.5 cfm/person for 725 cfm.

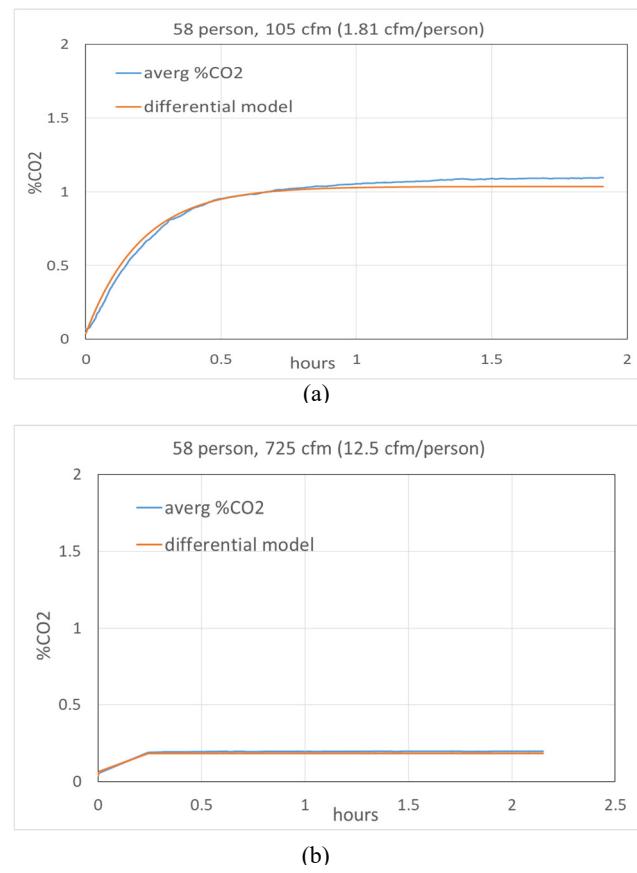


Figure 4. The %CO₂ (by volume) based on test data and model prediction for 58 people and 105 cfm (a) or 725 cfm (b) FAF rate.

5. DISCUSSION

While fresh air was delivered to the shipping container, the interior pressure would increase until the exhaust valve opened to release the air out. When stabilized, the differential pressure gauge read about 0.3–0.5 inch-of-water (74.7–124.4 Pa) of the interior air pressure. The interior air temperature also increased due to propane burning. It could reach to ~85°F (302.6°K) from ambient temperature (~75°F or 297°K) when the test started. For ideal gas (air),

$$P = \rho RT = \frac{m}{abc} RT \quad (9)$$

where P is the air pressure, R is the universal gas constant, T is the air temperature, and ρ is the air density.

Equation (9) can be rewritten as:

$$m = \frac{Pabc}{RT} \quad (10)$$

The pressure fluctuation has a range of 0.074% – 0.123%. The temperature fluctuated at about 1.89% [(302.6°K–297°K)/297°K]. So, the total air mass m should have a fluctuation less than 1.89% due to interior air pressure and temperature

increasing. It is reasonable to assume the total air mass remained the same during the test and the pressure/temperature fluctuation can be ignored.

Another observation based on Figure 2–Figure 4 is that the steady state %CO₂ 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 %CO₂ level stabilized at ~0.8% for 2.5 cfm/person as shown in Figure 2a and Figure 3a, regardless of the number of people and the total FAF rate.

Figure 5 shows the %CO₂ predicted by the differential model for various number of people and total FAF rate. The model predicted that the %CO₂ level will approach to 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 %CO₂ < 1% are listed in Table 1. The model predicts the minimal FAF rate to maintain 1% CO₂ to be ~1.87 cfm/person, regardless of the number of people and the total FAF rate.

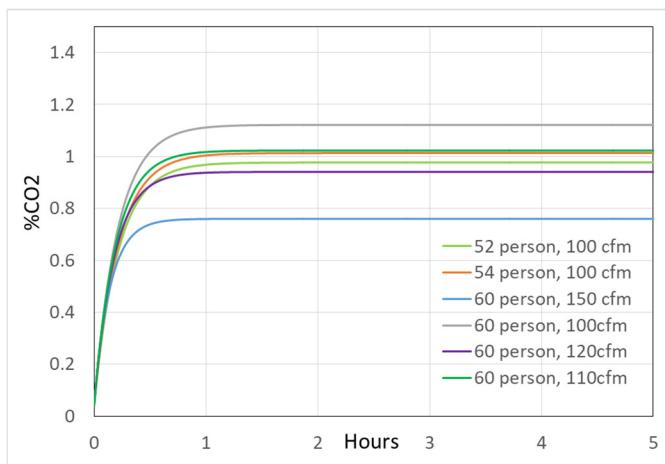


Figure 5. The %CO₂ by volume predicted by the differential model for various numbers of people and FAF rates.

Table 1. The simulation results for the minimum FAF rate for different numbers of people to maintain %CO₂ < 1%.

N	Federal regulation of CFR FAF at 12.5 cfm/person (cfm)	Model Min FAF for CO ₂ < 1% (cfm)	
		Model Min FAF for CO ₂ < 1% (cfm)	Model Min FAF for CO ₂ < 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

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 %CO₂ to stabilize below 1%. However, safety factors must be taken into consideration when implementing regulations [3]. Because of that, the minimal FAF of 12.5 cfm specified in federal regulations is indeed needed to maintain this carbon dioxide and other gases level within the safe range for 96 hours. The model also predicts the %CO₂ level will reach to steady state within 1 hour or less. Another observation is that the %CO₂ level depends on the cfm/person value rather than the number of people or the total FAF rate. Additionally, the %CO₂ 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 %CO₂ for various numbers of occupants, size of the confined space, and FAF rate without conducting a 96-hour test for every scenario. The model and testing confirm 12.5 cfm of supplied air will sustain miners for 96 hours and comply with the federal regulations. The model may also be useful to help manufacturers and mines to make decisions on RA design and implementation to comply with federal regulations.

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The findings and conclusions in this paper are those of the authors and do not necessarily represent the official position of the National Institute for Occupational Safety and Health, Centers for Disease Control and Prevention. Mention of any company or product does not constitute endorsement by NIOSH.

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6. CONCLUSION

The mathematical models presented in this study agree with test data well. They can be used to predict the %CO₂ level based

**Proceedings of
ASME 2021 International Mechanical
Engineering Congress and Exposition
(IMECE2021)**

Volume 13

**November 1-5, 2021
Virtual, Online**

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ISBN: 978-0-7918-8569-7

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- Dr. Shery Welsh, Director of AFOSR with \$500M in Basic Research (Aerospace Track Plenary)
- Dr. Nancy Sottos, Member of the NAE (Materials Track Plenary)
- Dr. Mehrdad Zangeneh, Founding Director of Advanced Design Technology, Ltd (Fluids Track Plenary)
- Dr. Yi Cui, one of the world's most cited scientists (Materials Track Plenary)

And these are just a few of the amazing speakers that will be available to you! Go to (<https://event.asme.org/IMECE/Keynote-Speakers>) and (<https://event.asme.org/IMECE/Program/Track-Plenary>) for the full list.

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Finally, on behalf of the IMECE Congress Steering Committee, I express my sincere thanks to and recognition of the hundreds of volunteers and the ASME staff that have dedicated time and effort to strengthening the fields of Mechanical Engineering R&D through organizing and leading sessions, topics, and tracks at this year's IMECE. It is never convenient to serve, and we have all continued to face frustrations of schedule, deadlines, conference websites, and more. Thank

you for your service. Your efforts have resulted in a strong congress that will continue to drive research forward both now and in the next generation. Thank you.

Sincerely,

Marriner H. Merrill, PhD
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Guangchao Song
Li Song
Zhengyi Song
Xiaolei Song
Hoanan Song
Yooseob Song
Mehmet Sozen
McKay Sperry
Vinod Srinivasan
Rajeshwar Sripada
Ankit Srivastava
Terrin Stachiw
John Steimke
Vesselin Stoilov
Gabriel Streitmatter
Samuel Subia
Harish Subramanyan
Prathik Jain Sudhir
Taylor Suess
C. Steve Suh
Yunyun Sun
Lei Sun
Haining Sun
Wangping Sun
Shung-hsing Sung
Vyshak Sureshkumar
Ehsan Taati
Alireza Tabarraei
Alex Tacescu
Luca Tagliafico
Hossein Taheri
Abdul Raouf Tajik
Siddharth Talapatra
Lorenzo Talluri
Ilie Talpasanu
Atsutaka Tamura
Kwek-Tze Tan
Hua Tan
X. Gary Tan

Martin Tanaka	Ankit Verma	Zhijun Wu
Hui Tang	Riccardo Vescovini	Chenglin Wu
Jinsong Tang	Carlos Ramón Vidal Tovar	Mingtao Wu
Yash Tank	Jose L. Viesca	C.T. Wu
Khalid Tantawi	Umberto Villa	Wenxuan Xia
Buddi Tanya	Vimal Viswanathan	Yingxiang Xia
Akin Tatoglu	Andrea Vitali	Xiao Xiangyu
Dorothy Taylor	Diego Vittorini	Xinyi Xiao
Mehran Tehrani	Kelen Cristiane Teixeira	Angran Xiao
Khashayar Teimoori	Vivaldini	Gongnan Xie
Ayse Tekes	Gabriele Volpato	Zhuowen Xie
Halil Tekinalp	Tung Vuong	Siyuan Xing
John Tencer	Anand Vyas	Ruitong Xiong
Zhiqiang Teng	Adam Wachtor	Luoyu Xu
Alp Tezbasharan	Ian Walker	Jun Xu
Mishal Thapa	Graham Walker	Yongfeng Xu
Scott Thompson	D.K. Walters	Yeyin Xu
Zhenhua Tian	Xingyu Wang	Minghan Xu
Ang Tian	Michael Cai Wang	Tongge Xu
Saeed Tiari	Xinwei Wang	Baoxing Xu
Juan Tibaquira	Yeqing Wang	Wei Xue
Ankit Tiwari	Qiming Wang	Reza Yaghmaie
Beth Todd	Jingyu Wang	Sami
Ravi Pratap Singh Tomar	Wei Wang	Yamanidouzisorkhabi
Mukul Tomar	Junzhen Wang	Karen Chang Yan
Robert Tomko	Curtis Wang	Ling Yan
Casey Troxler	Zhenyu Wang	Lincan Yan
Eleonora Tubaldi	Yan Wang	Chen Yan
Göker Türkakar	Peng Wang	Zhuo Yang
Pawan Tyagi	Jianhua Wang	Chun-Lin Yang
James V. Cox	Wenxi Wang	Yichao Yang
Luca Valdarno	Shiyan Wang	Mengqiao Yang
R. Michael Van Auken	Xueju (Sophie) Wang	Bingen (Ben) Yang
Kenneth Van Treuren	Kristina Warmefjord	Haoqing Yang
K. Philip Varghese	Ronald Warzoha	Song Yang
Thomas Vasko	Dane Wedgeworth	Shujie Yang
Kostiantyn Vasylevskyi	Justin Weinmeister	Xiaolong Yang
Andrea Vecchi	Miri Weiss Cohen	Weizhu Yang
Arun Veeramany	Yi Wen	Zhonghua Yang
Ruben Venegas	John Wiechel	Yifei Yao
Holalu Venkatdas	Enakshi Wikramanayake	Wei Yao
Ravindra	Sara Wilson	Timothy Yap
Chadalavada	Stephanie Wimmer	Taiho Yeom
Venkateswara Babu	Keo-Yuan Wu	Ravinder Yerram

Sumith Yesudasan Daisy	Wei Zhang	Qinqiang Zhang
Steven Yip Fun Yeung	Lin Zhang	Haipeng Zhang
Ho Yeung	Kaihao Zhang	Dianyun Zhang
Guilian Yi	Yanmei Zhang	Yating Zhang
Salih Yildiz	Wen Zhang	Xian Zhang
Sha Yin	Zhou Zhang	Man Zhao
Akio Yonezu	Zilong Zhang	Huijuan Zhao
William Young	Jianan Zhang	Shijia Zhao
Kianoosh Yousefi	Xiaoliang Zhang	Kai Zhao
Cunjiang Yu	Jing Zhang	Changlong Zheng
Kai Yu	Chao Zhang	Cao Zhi
Hong Yu	Zhifeng Zhang	Allan Zhong
Zexing Yu	Xiaoyu Zhang	Hong Zhou
Pengyu Yuan	Liang Zhang	Yanguang Zhou
Chunhao Yuan	Chen Zhang	Min Zhou
Sichen Yuan	Yue Zhang	Zenghao Zhu
Zhangxian Yuan	Jian Zhang	Linda Zhu
Andrei Zagrai	Nathan Zhang	Linqi Zhuang
Md. Zahid Hasan	He Zhang	Wei Zhuang
Guiyan Zang	Min Zhang	Metodi Zlatinov
Jian Zeng	Yongqing Zhang	Hamidreza Zobeiri
Chi Zhan	Mingshao Zhang	An Zou
Lufan Zhang	Peiran Zhang	Ahmad Zueter
Ning Zhang	Peter Zhang	

CONTENTS

Proceedings of ASME 2021 International Mechanical Engineering Congress and Exposition Volume 13

Safety Engineering, Risk, and Reliability Analysis

Congress-Wide Symposium on Prognostic and Health Management: NDE and Prognostics of Structures and Systems

IMECE2021-69162	V013T14A001
Probabilistic Optimization Approach for Damage Identification Using Frequency Response <i>Hussain Altammar, Sudhir Kaul, and Anoop Dhingra</i>	
IMECE2021-71878	V013T14A002
Applications of High-Dimensional Data Analytics in Structural Health Monitoring and Non-Destructive Evaluation: Thermal Videos Processing Using Tensor-Based Analysis <i>Hamed Momeni and Arvin Ebrahimkhanlou</i>	
IMECE2021-73153	V013T14A003
A Review of SQL vs NoSQL Database for Nuclear Reactor Digital Twin Applications: With Example MongoDB Based NoSQL Database for Digital Twin Model of a Pressurized-Water- Reactor Steam-Generator <i>Subhasish Mohanty, Thomas W. Elmer, Sasan Bakhtiari, and Richard B. Vilim</i>	
IMECE2021-73194	V013T14A004
Spindle Bearings Fault Diagnosis Technique Based on Integration of Zero Resonator Frequency Filter and Discrete Wavelet Packet Transform <i>Avitus Titus Mwelinde, Hongyu Jin, Jamal Banzi, Hongya Fu, and Zhenyu Han</i>	
IMECE2021-73504	V013T14A005
Fatigue Crack Growth Prognosis With the Particle Filter and On-Line Guided Wave Structural Monitoring Data <i>Jian Chen, Shenfang Yuan, Lei Qiu, and Yuanqiang Ren</i>	
Crashworthiness, Occupant Protection, and Biomechanics	
IMECE2021-66627	V013T14A006
Reinforced Concrete Barrier Modeling In-Series Impacts in LS-DYNA <i>Roshan Sharma, Chiara Silvestri Dobrovolny, Stefan Hurlebaus, and Maysam Kiani</i>	
IMECE2021-69776	V013T14A007
Damage Assessment Method of Battery Pack of Electric Vehicle in Undercarriage Collision <i>Powen Chen, Yong Xia, Qing Zhou, Yunlong Qu, and Xinqi Wei</i>	
IMECE2021-70137	V013T14A008
Equivalent Energy Absorption (EEA) - A Methodology for Improved Automotive Crash & Safety Design <i>Peddi Sai Rama Narayana, Raghu V. Prakash, Srinivas Gunti, and Kanugula Raghu</i>	
General Topics on Risk, Safety, and Reliability	
IMECE2021-66623	V013T14A009
Improving Overall Equipment Effectiveness by Enabling Autonomous Maintenance Pillar for Integrated Work Systems <i>Aneesh A. Chand, Kushal A. Prasad, Krishneel R. Sharma, Sumesh Narayan, Kabir A. Mamun, F. R. Islam, Nallapaneni Manoj Kumar, and Shauhrat S. Chopra</i>	

IMECE2021-67665	V013T14A010
Implementation of Reliability Design Theory on a Thin-Wall Vessel Structure	
<i>Xiaobin Le</i>	
IMECE2021-68096	V013T14A011
Compression Analysis Tests for Prototypes Made of Different Polymers	
<i>Taher Deemyad, Vincent Akula, and Anish Sebastian</i>	
IMECE2021-68452	V013T14A012
Mathematical Modeling for Carbon Dioxide Level Within Confined Spaces	
<i>Lincan Yan, Dave S. Yantek, Cory R. DeGennaro, and Rohan D. Fernando</i>	
IMECE2021-68680	V013T14A013
Fresh Air Flow Required to Maintain Safe Carbon Dioxide Levels and Provide a Breathable Air Environment in a Refuge Alternative	
<i>Cory DeGennaro, Lincan Yan, and David Yantek</i>	
IMECE2021-69709	V013T14A014
Improving Real-Time Methane Monitoring in Longwall Coal Mines Through System Response Characterization of a Multi-Nodal Methane Detection Network	
<i>Brian Cappellini, Derek Johnson, Nigel Clark, and Amber Barr</i>	
IMECE2021-70198	V013T14A015
Establishment of the Off-Center Embedded Crack Stress Intensity Factor Database for Probabilistic Risk Assessment Based on Universal Weight Function	
<i>Tongge Xu, Shuiting Ding, and Guo Li</i>	
IMECE2021-71001	V013T14A016
Multiobjective Reliability-Based Design of an Aircraft Wing Using a Fuzzy-Based Metaheuristic	
<i>Suwin Slesongsom, Saksan Winyangkul, and Sujin Bureerat</i>	
IMECE2021-71215	V013T14A017
A Systematic Study of Pedestrian Contrast and Detection From Vehicle Headlights	
<i>Fawzi P. Bayan, Thomas A. Timbario, Jonathan D. Nelson, Stuart Sheldon, II, Ronny E. Wahba, and Brandon Keys</i>	
IMECE2021-71294	V013T14A018
Increased Vehicle Intrusion as a Result of Vehicle Weight	
<i>Lauren Eichaker, Cameron Trebeck, Michael Arnett, H. Fred Chen, John Wiechel, and Dennis Guenther</i>	
IMECE2021-71359	V013T14A019
Verification Study of the Nuclear PRA for the Mars 2020 Mission Following Accidental Orbital Re-Entry	
<i>Arjun Earthperson and Mihai A. Diaconeasa</i>	
IMECE2021-71836	V013T14A020
Attempting To Establish Design Margins for Glassy Polymers In Critical Structural Service	
<i>Bart Kemper and Kaylie Kling Williams</i>	
IMECE2021-72943	V013T14A021
A Multi-Attribute Knowledge Criticality Framework for Ranking Major Maintenance Activities: A Case Study of Cement Raw Mill Plant	
<i>Lilian O. Iheukwumere-Esotu and Akilu Yunusa-Kaltungo</i>	
IMECE2021-73021	V013T14A022
A Framework for Integrating Reliability, Robustness, Resilience, and Vulnerability to Assess System Adaptivity	
<i>Milad Rostami and Scott Bucking</i>	
IMECE2021-73696	V013T14A023
A Quantitative Approach to Assess the Likelihood of Supply Chain Shortages	
<i>Priyanka Pandit, Arjun Earthperson, Alp Tezbasar, and Mihai A. Diaconeasa</i>	
IMECE2021-73770	V013T14A024
Effect of Weather on the Performance of Autonomous Vehicle LiDAR Sensors	
<i>Jamil Abdo, Spencer Hamblin, and Genshe Chen</i>	

Machine Learning for Safety, Reliability, and Maintenance

IMECE2021-70258 V013T14A025

KrakenBox: Deep Learning-Based Error Detector for Industrial Cyber-Physical Systems

Sheng Ding, Andrey Morozov, Tagir Fabarisov, and Silvia Vock

IMECE2021-70387 V013T14A026

Deep Learning-Based Error Mitigation for Assistive Exoskeleton With Computational-Resource-Limited Platform and Edge Tensor Processing Unit

Tagir Fabarisov, Andrey Morozov, Ilshat Mamaev, and Klaus Janschek

IMECE2021-70759 V013T14A027

Dynamic Placement of Rapidly Deployable Mobile Sensor Robots Using Machine Learning and Expected Value of Information

Alice Agogino, Hae Young Jang, Vivek Rao, Ritik Batra, Felicity Liao, Rohan Sood, Irving Fang, R. Lily Hu, Emerson Shoichet-Bartus, and John Matranga

IMECE2021-70783 V013T14A028

Prognostic Health Monitoring Method for Thermal Fatigue Failure of Power Modules Based on Finite Element Method-Based Lagrangian Neural Networks

Akira Kano, Tomoko Monda, Tomoyuki Suzuki, Hideaki Uehara, Tomoya Fumikura, and Kenji Hirohata

IMECE2021-73702 V013T14A029

Fault Diagnosis With Deep Learning for Standard and Asymmetric Involute Spur Gears

Fatih Karpat, Ahmet Emir Dirik, Onur Can Kalay, Celalettin Yüce, Oğuz Doğan, and Burak Korcuklu

Models and Methods for Probabilistic Risk Analysis

IMECE2021-69998 V013T14A030

Demonstration of a Limited Scope Probabilistic Risk Assessment for Autonomous Warehouse Robots With OpenPRA

Philipp Grimmeisen, Artur Karimov, Mihai A. Diaconeasa, and Andrey Morozov

IMECE2021-72345 V013T14A031

Performance of Iterative Network Uncertainty Quantification for Multicomponent System Qualification

Edward Rojas and John Tencer

Probabilistic Risk Assessment of Protective Systems

IMECE2021-69562 V013T14A032

The Role of Protective System Reliability Analysis in the Study of System Safety

Martin Wortman, Ernie Kee, and Pranav Kannan

IMECE2021-70716 V013T14A033

Application of Bayesian Calibration to Improve Multiple Ballistic Impact Modeling

Gregory A. Langone, Brad G. Davis, and Nicholas A. Reisweber

IMECE2021-73035 V013T14A034

Nuclear Power: On PRA and Protective System Maintenance

Ernie Kee and Martin Wortman

Reliability and Risk in Energy Systems

IMECE2021-69881 V013T14A035

Effect of Particle Overlapping Impacts in Erosion Process

Xuerui Zang, Xuewen Cao, Zhenqiang Xie, Jun Zhang, and Yijie Li

IMECE2021-69942 V013T14A036

A Proposed Method for Online Condition Monitoring of Pneumatic Systems Under Different Operating Conditions and Parameters for Optimal Energy Consumption

Anil U. Peerapur, Mangesh N. Dhavalikar, Sunil V. Dingare, and Bhumeshwar K. Patle

IMECE2021-71460 V013T14A037
On the Modeling of Wildfires-Induced Release and Atmospheric Dispersion in Radioactively Contaminated Regions
Damla Polat and Mihai A. Diaconeasa

Reliability and Safety in Industrial Automation Systems

IMECE2021-69395 V013T14A038
Anomaly Detection for Cyber-Physical Systems Using Transformers
Yuliang Ma, Andrey Morozov, and Sheng Ding

IMECE2021-73087 V013T14A039
An Approach for Safeguarding Autonomous Mobile Robots Using Monitoring Tools
Manuel Müller, Natalie Schinzel, Nasser Jazdi, and Michael Weyrich

Reliability and Safety in Transportation Systems

IMECE2021-67732 V013T14A040
Development of Algorithms for Improving Fiber-Optical Rail Circuit on Railway Spans
Nikoloz Mgebrishvili, Maksim lavich, Tengiz Tabidze, and Amiran Nodia

IMECE2021-67822 V013T14A041
Study of Carbody Structure Design Under Different Standards
Jianran Wang, Xiaofang Liu, Haifeng Zhang, Qi Luo, Shihong Jiang, and Haifeng Hong

IMECE2021-69313 V013T14A042
A Hybrid Methodology for Risk Mitigation During Development of Safety-Critical Autonomy Features
Pez Zarifian, Divya Garikapati, Julia Pralle, Jennifer Dawson, Constantin Hubmann, Brielle Reiff, Raymond Tam, and Gopi Gaddamadugu

IMECE2021-70802 V013T14A043
Safety Technology Advancements for Autonomous Cars; Prospective of Manufacturing, Regulatory and Society
Mohammad Pourgol Mohamad and Amin Pourgol Mohamad

IMECE2021-72955 V013T14A044
An Imperfect Usage-Based Preventive Maintenance Planning Model for Railway Track Superstructures
Fateme Dinmohammadi, Mahmood Shafiee, and Enrico Zio

Reliability and Safety of Deep Learning-Based Components

IMECE2021-69390 V013T14A045
An Overview of the Research Landscape in the Field of Safe Machine Learning
Georg Siedel, Stefan Voß, and Silvia Vock

IMECE2021-72891 V013T14A046
Automated Hardening of Deep Neural Network Architectures
Michael Beyer, Christoph Schorn, Tagir Fabarisov, Andrey Morozov, and Klaus Janschek

Student Safety Innovation Challenge

IMECE2021-69308 V013T14A047
Design of an Efficient, Low-Cost, Stationary LiDAR System for Roadway Condition Monitoring
Jarod Bennett, Mather Saladin, Daniel Sizoo, Spencer Stewart, Graham Wood, Thomas DeAgostino, and Christopher Depcik

Users, Technology, and Human Reliability in Safety Engineering

IMECE2021-71261 **V013T14A048**
An Integrative and Transdisciplinary Approach for a Human-Centered Design of AI-Based Work Systems

Larissa Schlicht, Marlen Melzer, Ulrike Rösler, Stefan Voß, and Silvia Vock

IMECE2021-71504 **V013T14A049**
On the Use of Probabilistic Risk Assessment for the Protection of Small Modular Reactors Against Terrorist Attacks

Burak Polat and Mihai A. Diaconeasa

Research Posters

Acoustics, Vibration, and Phononics

IMECE2021-72041 **V013T15A001**
On the Vibration Transfer Characteristics From the Seat of the Vehicle to the Occupant
Ryoma Morisaki, Osamu Terashima, Fumiya Kinoshita, and Hideaki Touyama

IMECE2021-72083 **V013T15A002**
Acoustic Emission Detection and Signal Source Analysis of Boiler Water Wall Tube
Yilin Yuan, Gongtian Shen, Yongna Shen, Junjiao Zhang, Wenjun Zhang, and Qiang Wan

Advanced Materials: Design, Processing, Characterization, and Applications

IMECE2021-69648 **V013T15A003**
Mechanical Properties and Durometer Testing Relationship of Thermoplastic Polyurethane
Edwar Romero-Ramirez, Charisma Clarke, Sanna F. Siddiqui, and Gerardo Carbajal

Design, Systems, and Complexity

IMECE2021-69333 **V013T15A004**
Modular Printed Powered Air Purifying Respirator
J. Brown, M. Clifford, J. Magana, M. Salman, and D. Tran

IMECE2021-69459 **V013T15A005**
Terrestrial Mission Extender for Weather Balloon Radiosonde
Carrington Chun, Joseph McBride, Kaveh Torabzadeh, Andrew Smith, and Santana Roberts

IMECE2021-71881 **V013T15A006**
Mechanical Design and Development of a Suborbital Payload for Real-Time Data Acquisition and Structural Health Monitoring
Dillon Cvetic-Thomas, Amy Tattershall, Eli Jackson, Dane Robergs, Funmilola Nwokocha, and Andrei Zagrai

IMECE2021-72492 **V013T15A007**
Design, Modeling, and Fabrication of a Ventilator Prototype - A Successful Student Project Story
Haoyee Yeong, Francis Iloeje, Eli Kindomba, Sunday Folorunso, Yafeng Li, and Jing Zhang

Dynamics, Vibration, and Control

IMECE2021-69771 **V013T15A008**
A Time-Frequency Domain Adaptive Control Approach for Vibration of Active Magnetic Bearing System
Xuan Yao and Zhaobo Chen

IMECE2021-70469 **V013T15A009**
Active Vibration Control of Aerospace Structural Systems for Specified Damping
Sathya Hanagud

Heat Transfer and Thermal Engineering

IMECE2021-70833 **V013T15A010**

Senior Capstone Project: A Classroom Heat Exchanger Demonstration Kit

Matthew Quigley, Jason Klebba, Badih Jawad, and Liping Liu

Mechanics of Solids, Structures, and Fluids

IMECE2021-70925 **V013T15A011**

A Prediction Software to Evaluate Frisbee Movement

Haowen Yang

IMECE2021-71806 **V013T15A012**

Verification and Validation of a Small Wind Tunnel Data Acquisition System

Alex J. Doorn, Elena Hollingsworth, Riley Bishop, Wesley Fisher, Brian Mazzoni, and Chidurala Manohar

Safety Engineering, Risk, and Reliability Analysis

IMECE2021-66606 **V013T15A013**

Scaled Crash Testing Using Modeling, Similitude, and Experimentation

Richard Melnyk, Olivia Beattie, and Bogue Waller

IMECE2021-72082 **V013T15A014**

Robotic-Based Repair of Concrete Structures: A Surface Crack Filler Robot

Melinda Stevens, Samuel Arellano, Diego Rodriguez, James Wilson, Zady Gutierrez, Noah Trudell, Hamed Momeni, and Arvin Ebrahimkhanlou