A mathematical modelling of the intensity of contaminants (CO_2) on occupancy level of a space in continuous use

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Abstract: This study investigates the Indoor Air Quality (IAQ) of a room apartment and focused on the number of occupants that a space or an apartment can accommodate as a result of increase in the concentration level of the CO_2 contaminant present within the space. The law of mass action was applied to generate a relation between the concentration of CO_2 produced and the concentration of the reactants (i.e., O_2 and CO). A decay equation was also used to relate the variation in the number of occupants with the level of the concentration of CO_2 within the space only at steady state conditions.

Keywords: contaminants; air quality; indoor; room ventilation; CO_2; concentration level.

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1 Introduction

From various research findings, it seems that a great number of people are exposed to an indoor air environment longer than they are to an outdoor environment (ASHRAE, 1996, 1989; Carpenter, 1996; Emmerich and Persily, 1997; Levine et al., 1994; Vaculik and Plett, 1993). The obvious reason is that many people spend most of their time for daily activities indoors. Apart from outright display and sales of goods in the open air, even marketing activities that are field-focused involve moving from one office to another or from one household to another. Thus, many activities such as manufacturing and maintenance operations, which are factory-based, are indoor activities. People engaged in indoor activities seem to be in the majority since the outdoor air environment may be uncomfortable to the delicate body of human being (Leephakpreeda et al., 2001). Although CO_2 is not the only indoor air pollutant, the focus of this paper seems to be on CO_2 since it can be used as an index of Indoor Air Quality (IAQ). As Leephakpreeda et al. (2001) noted, this may be because CO_2 is a human-waste fluid and if CO_2 concentration is controlled at the desired level, then other pollutants will be controlled at acceptably low levels as well.

Previous studies on modelling of the intensity of contaminants have been conducted on a worldwide scale in Mexico (Cynthia et al., 2008) and the UK (Kolokotroni and Katsoulas, 2002), among other locations, while no documentation seems to exist for the Nigerian case. Cynthia et al. (2008) evaluated the impact of an improved wood burning stove (Patsari) in reducing personal exposures and indoor concentrations of particulate matter ($PM_{2.5}$) and carbon monoxide (CO) in 60 homes in a rural community in Mexico. Kolkotroni et al. (2002) investigated the performance of thermal passive ventilation stacks in the classrooms of a school in the UK during the summer. Measurements of air temperature, carbon dioxide (CO_2) and air velocity were carried out, from which ventilation rates in the classrooms and stacks were calculated. Other studies relevant to the current work are as follows. Leephakpreeda et al. (2001) reported on the theoretical and experimental studies of occupancy-based control of the ventilation to demonstrate the practical usefulness of the occupancy-based scheme for real time air ventilation control and energy saving. In Carpenter (1996), it was reported that CO_2-based Demand Control Ventilation (DCV) was applicable and it saved energy when compared with constant ventilation. Ke and Mumma (1997) determined the changeable occupancy for the ventilation control based on the CO_2 concentration in the outdoor air and the return air.

Vaculik and Plett (1993) investigated the control strategies of the CO_2-based DCV by simulations for a typical occupancy profile during a working day. Kagi et al. (2007) noted that there are various emission sources of chemical contaminants. These emissions cause air pollution. Air pollution occurs as a result of the combustion of fossil fuels (i.e., petroleum, gasoline and natural gas) and the discharge of gaseous chemicals from industry and transport into the surrounding atmosphere.

Kagi et al. (2007) reported that in heavily industrialised areas, there is a high incidence of lung cancer and chronic bronchitis due to the inhaling of dust and smoke particles. In coal-mining areas, 'black lung' is a common occurrence in miners due to the inhalation of coal dust. In the plastic industry, asbestos dust, a carcinogen, causes pulmonary cancer. Various hydrocarbons that are released into the atmosphere from car exhausts include carbon monoxide. Carbon monoxide, a poisonous gas produced because of incomplete combustion, combines with haemoglobin in red blood corpuscles to form carboxyhaemoglobin. This substance impedes the transport of oxygen in the blood. Carbon dioxide (CO_2) is another contaminant present in the ambient air at a level of 0.03% and is generated by the respiration of human beings and animals. An individual is able to generate 4.72×10^{-3} litres per second of CO_2 during respiration. The effects of carbon dioxide contamination by volume (or concentration) become severe as the concentration increases. 1–2% CO_2 continuous exposure leads to headaches and dysproea, 3% CO_2 can lead to severe headaches, 5% CO_2 exposure can lead to mental depression, 6% CO_2 exposure can lead to visual impairment and a 10% concentration of CO_2 with respect to air volume can lead to unconsciousness.

The structure of the paper is as follows: introduction, methodology, case study, discussion and conclusion. The introduction provides the motivation for the study and a justification for the choice of topic. In Section 2, methodology discuses the approach utilised to solve the problem. Section 3 is a case description of practical instances that verify the workability of the model. Section 4 presents a discussion of important points. Section 5 presents the concluding remarks.

2 Mathematical modelling

2.1 Definition of terms

y: The concentration of carbon (IV) oxide produced; it is represented by percentage of air volume in that environment

f: The velocity constant, which is similar to the frequency of the chemical reaction, the unit is cycles/sec

A_a: The initial concentration of oxygen in the air; it is also represented by percentage of air volume

B_b: The initial concentration of carbon (II) oxide, it is expressed as percentage of air volume

a and b: Combining moles of oxygen and carbon (II) oxide, respectively

y_c: Complementary function

y_p: Particular solution

ψ: Constant

C: Increase in contamination concentration
Q: Volumetric flow per second per person of the incoming air into the space
Q_c: Volume of pollutant (Carbon (IV) oxide) produced per person within the space
C_i: Initial concentration of contaminant in the space at time zero
C_o: Concentration of the contaminant in the incoming air to the space
V: Volume of the space ≠ IV per person
n: Number of air changes per hour for the whole space
v_n: Volume at the instant of n.

2.2 *Problem analysis*

The concentration of carbon (IV) oxide produced by the chemical reaction between carbon (II) oxide and oxygen can be determined by using the Law of Mass Action, which states that under constant temperature, the velocity of a chemical reaction is proportional to the product of the concentrations of the reacting substances.

Considering the chemical reaction: $2CO_{(g)} + O_{2(g)} \longrightarrow 2CO_{2(g)}$

The combining ratio of CO to O_2 is 2 : 1. Mathematically, the Law of Mass Action is:

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f\left(A_o - \frac{ay}{a+b}\right)\left(B_b - \frac{by}{a+b}\right). \tag{1}$$

As carbon (II) oxide is released to the atmosphere, it reacts almost immediately with the oxygen in the air, depending on the temperature of the air, to yield carbon (IV) oxide. This paper assumes that the concentration of CO_2 produced as a result of this reaction is the same of the volume of CO produced was stored and made to accumulate for the same period of time it took to release the CO to the atmosphere, and the gas reacted with oxygen. Then, the gas was released, with an initial percentage by volume of air, B_b and consequently reacted with oxygen, having an initial percentage by volume of air, A. By solving the ordinary differential equation in equation (1), we have:

$$\frac{\mathrm{d}y}{\mathrm{d}t} + f\left(\frac{Ab+aB}{a+b}\right)y = \left(\frac{fab}{(a+b)^2}\right)y^2 + fAB. \tag{2}$$

The solution to the equation above can be classified into complementary and particular equations, i.e., $y = y_c + y_p$.

Now, solving for the particular function:

$$\frac{\mathrm{d}y}{\mathrm{d}t} + f\left(\frac{Ab+aB}{a+b}\right)y = f\left(\frac{ab}{(a+b)^2}\right)y^2. \tag{3}$$

Let $R = \left(\frac{Ab+aB}{a+b}\right)f$ and $P = f\left(\frac{ab}{(a+b)^2}\right)$.

Then equation (3) becomes:

$$\frac{dy}{dt} + Ry = Py^2. \tag{4}$$

Equation (4) is a first order linear and non-homogeneous differential equation. Hence, using Bernoulli's equation to solve it,

$$y^{-2}\frac{dy}{dt} + Ry^{-1} = P. \tag{5}$$

Let

$$Z = y^{-1}. \tag{6}$$

Therefore

$$\frac{dz}{dt} = -y^{-2}\frac{dy}{dt}. \tag{7}$$

Multiply through equation (5) by –1:

$$-y^{-2}\frac{dy}{dt} - Ry^{-1} = -P. \tag{8}$$

Substituting equations (6) and (7) into (8) yields:

$$\frac{dz}{dt} - Rz = -P. \tag{9}$$

Solving equation (9) by the use of Integrating Factor (IF),

$$\mathrm{IF} = \exp\int -R\,dt = e^{-Rt} \tag{10}$$

$$Z\,.\,\mathrm{IF} = \int -P\,.\,\mathrm{IF}\,dt \tag{11}$$

$$Ze^{-Rt} = \int -Pe^{-Rt}dt = \frac{P}{R}e^{-Rt} + \psi. \tag{12}$$

But

$$Z = \frac{P}{R} + \psi e^{-Rt} = \frac{P + \psi Re^{Rt}}{R}. \tag{13}$$

Also, $Z = 1/y$ for equation (6), which implies that $y = 1/z$.

Therefore,

$$y_p = \frac{R}{P + \psi\, Re^{Rt}}. \tag{14}$$

This is the particular solution.

Now, solving for the complementary function,

$$y_c = \text{constant} = \phi \tag{15}$$

$$\frac{\mathrm{d}y_c}{\mathrm{d}t} = 0. \tag{16}$$

Putting equations (15) and (16) into the differential equation:

$$\phi R = fAB \tag{17}$$

$$\phi = \frac{fAB}{R}. \tag{18}$$

Hence,

$$y_c = \frac{fAB}{R}. \tag{19}$$

Thus,

$$y = \frac{R}{P + \psi Re^{Rt}} + \frac{fAB}{R}. \tag{20}$$

Equation (20) gives the value of the concentration of carbon (IV) oxide produced due to the chemical reaction between carbon (II) oxide and oxygen. Carbon (IV) oxide can be regarded as a pollutant for man but an important gas for the photosynthesis in plants. This paper focuses on its effect on man; hence, we can conclude against this background that it is a contaminant. In a time increment dt, the contamination in a space increases due to the influx of the contaminated outside air into the space and that generated by the occupants.

Therefore,

$$C^{i} = \left(\frac{QC_o}{10000} + Q_c\right)\mathrm{d}t \text{ per person in the space.} \tag{21}$$

Contamination levels are usually referred to as parts per 10,000. Now, let us assume that there is no build up of pressure in the space and that natural ventilation occurs, so that no air storage term exists in the continuity of air flow equation. Contamination leaves with the effluent air. The concentration that leaves = C^{o}. For natural ventilation, the extract air flow is equal to the inflow air rate; only, the level of contamination carried by this flow differs.

$$C^{o} = \left(\frac{QC}{10000}\right)\mathrm{d}t \text{ per person in the space.} \tag{22}$$

The net change in the contamination level in the space over the time increment dt is $C^{i} - C^{o}$,

$$\mathrm{d}c = \left(\left(\frac{QC_o}{10000} + Q_c\right) - \left(\frac{Q_c}{10000}\right)\right)\mathrm{d}t \text{ per person in the space.} \tag{23}$$

Expressing dc as a concentration in parts per 10,000 of air/volume of room space, we have:

$$\frac{\mathrm{d}c}{10000} = \frac{1}{v}\left(\left(\frac{QC_o}{10000} + Q_c\right) - \left(\frac{Q_c}{10000}\right)\right)\mathrm{d}t. \tag{24}$$

Re-arranging

$$\frac{\mathrm{d}c}{\mathrm{d}t} + \frac{QC}{v} = \frac{QC_o + 10000\,Q_c}{v}. \tag{25}$$

Equation (25) can be solved by the use of an IF

$$\mathrm{IF} = \exp\int\frac{Q}{v}\mathrm{d}t = \mathrm{e}^{\frac{Qt}{v}}.$$

Therefore

$$C\,.\,\mathrm{IF}\int\frac{1}{v}(QC_o + 10000Q_c)\,.\,\mathrm{e}^{\frac{Qt}{v}}\,\mathrm{d}t \tag{26}$$

$$C\,\mathrm{e}^{\frac{Qt}{v}} = \left(\frac{v}{Q}\right).\frac{1}{v}(QC_o + 10000Q_c)\,\mathrm{e}^{\frac{Qt}{v}} + \beta \tag{27}$$

$$C\,\mathrm{e}^{\frac{Qt}{v}} = \frac{1}{Q}(QC_o + 10000Q_c)\,\mathrm{e}^{\frac{Qt}{v}} + \beta. \tag{28}$$

To determine the value of the constant β, let us consider the boundary condition at time $t = 0$, $c = C_i$.

$$C_i = C_o + 10000\frac{Q_c}{Q} + \beta. \tag{29}$$

Therefore

$$\beta = C_i - \left(C_o + 10000\frac{Q_c}{Q}\right). \tag{30}$$

Hence, putting equation (30) into (28)

$$C\mathrm{e}^{\frac{Qt}{v}} = \left(C_o + \frac{10000Q_c}{Q}\right)\mathrm{e}^{\frac{Qt}{v}} + C_i - \left(C_o + 10000\frac{Q_c}{Q}\right). \tag{31}$$

Dividing through by $\mathrm{e}^{Qt/v}$, we have:

$$C = \left(C_o + \frac{10000Q_c}{Q}\right) + C_i\mathrm{e}^{-\frac{Qt}{v}}\left(C_o + 10000\frac{Q_c}{Q}\right)\mathrm{e}^{-\frac{Qt}{v}}. \tag{32}$$

Re-arranging and factorising, we have:

$$C = \left(C_o + \frac{10000Q_c}{Q}\right)\left(1 - e^{-\frac{Qt}{v}}\right) + C_i\mathrm{e}^{-\frac{Qt}{v}}. \tag{33}$$

Equation (33) is the general expression for the contamination within a space at any time t.

Consider the fact that,

$$Q = \frac{v_n}{3600} \tag{34}$$

where n is the number of air changes per hour for the whole space. Putting equation (34) into equation (33) yields:

$$C = \left(C_n + \frac{10000 Q_c}{\left({}^{v_n}\!/_{3600} \right)} \right) = (1 - e^{-nt}) + C_i e^{-nt}. \tag{35}$$

Note that n is different from v_n since n refers to number of air changes per hour for the whole space, while v_n is the volume at that instant. We further state that

$$\frac{C - C_i e^{-nt}}{(1 - e^{-nt})} - C_o = \frac{3.6 \times 10^7 \, Q_c}{nV} \tag{36}$$

$$\frac{C - C_i e^{-nt} - C_o (1 - e^{-nt})}{(1 - e^{-nt})} = \frac{3.6 \times 10^7 \, Q_c}{nV}. \tag{37}$$

By taking the inverse of both sides of equation (37), we have:

$$\frac{(1 - e^{-nt})}{\left(C - C_i e^{-nt} - C_o (1 - e^{-nt}) \right)} = \frac{nV}{3.6 \times 10^7 \, Q_c}. \tag{38}$$

From equation (38),

$$V = \frac{3.6 \times 10^7 \, Q_c (1 - e^{-nt})}{\left(C - C_i e^{-nt} - C_o (1 - e^{-nt}) \right)}. \tag{39}$$

Now, let the volume of the space be represented by V^s while the expected number of occupants be N. This implies that

$$N = \frac{V^s}{N}. \tag{40}$$

Therefore, putting equation (40) into (39) yields:

$$\frac{V^s}{N} = \frac{3.6 \times 10^7 \, Q_c (1 - e^{-nt})}{\left(C - C_i e^{-nt} - C_o (1 - e^{-nt}) \right)}. \tag{41}$$

From equation (41),

$$N = \frac{V^s \left\{ C - C_i e^{-nt} - C_o (1 - e^{-nt}) \right\}}{3.6 \times 10^7 \, Q_c (1 - e^{-nt})}. \tag{42}$$

Under normal atmospheric conditions, i.e., when there are no pollutants like carbon (II) oxide or carbon (IV) oxide released into the air by any human activity, the volume of carbon (IV) oxide is 0.03% air volume. This paper assumes that the concentration of these gases should be represented by their percentage composition of air volume.
It implies that:

$$C_o = 0.03 + y. \tag{43}$$

By putting equation (20) into (43) yields:

$$C_o = 0.03 + \frac{R}{P + \psi \mathrm{Re}^{Rt}} + \frac{fAB}{R}. \tag{44}$$

Recall that: $R = \left(\frac{Ab + aB}{a + b}\right) f$, and $P = f\left(\frac{ab}{(a+b)^2}\right)$.

Putting the corresponding value of P and R into equation (44) yields:

$$C_o = 0.03 + \left(\frac{(Ab + aB)\, f}{(a+b)\, f\left(ab \big/ (a+b)^2 \right) + \psi \frac{(Ab + aB)}{a+b} e^{\left(\frac{Ab+aB}{a+b}\right)t}} \right) + \left(\frac{AB(a+b)}{(Ab + aB)} \right) \tag{45}$$

But $a = 1$, $b = 2$, and

$$C_o = 0.03 + \left(\frac{(2A + B)\, f}{\frac{2}{3} f + \psi (2A + B) e^{\left(\frac{2A+B}{3}\right)t}} \right) + \left(\frac{3AB}{2A + B} \right). \tag{46}$$

Therefore, putting equation (46) into (42), we have:

$$N = \frac{V' \left\{ C - C_i e^{-nt} - \left[0.03 + \left(\frac{(2A + B)\, f}{2/3\, f + \psi (2A + B) e^{\left(2A + B/3\right)t}} \right) + \left(\frac{3AB}{2A + B} \right) \right] (1 - e^{-nt}) \right\}}{\left\{ 3.6 \times 10^7\, Q_c (1 - e^{-nt}) \right\}}. \tag{47}$$

3 Case study

3.1 Case study I

A classroom having a volume of 283 m^3 undergoes 1–5 air changes per hour due to natural ventilation. The school is located in an industrial estate where the environment is seriously polluted by CO from the manufacturing companies within the estate. Now, assuming that the concentration of CO_2 a person can produce during respiration is 4.72×10^{-6} m^3/s. The critical value of the concentration of CO_2 under consideration here is 1%.

S/N	*A*%	*B*%	*C*%	*N*
1	21.00	0.020	0.030	242.0
2	20.90	0.030	0.045	238.0
3	20.70	0.050	0.075	213.0
4	20.30	0.080	0.120	220.0
5	20.10	0.085	0.127	218.0
6	19.90	0.087	0.130	217.0
7	19.80	0.088	0.132	217.0

Specimen calculation

For case I

Given that $A = 21\%$, $B = 0.02\%$ and $b = 2$, $a = 1$; $C_c = 1\%$ or 100 parts per 10,000

$$C_o = \frac{AB\,(a+b)}{Ab + aB} = \frac{21 \times 0.02 \times 3}{21 \times 2 + 0.02} = 0.03\% \text{ or 3 parts per 10,000.}$$

Therefore, $N = \dfrac{(C_c - C_o)\,nV}{3.6 \times w^7 \times Q_c} = \dfrac{(100-3) \times 1.5 \times 283}{3.6 \times w^7 \times 10^{-6}} = 242.$

3.2 *Case study II*

A media house planned on building a cinema hall that would operate for six hours a day with the use of mechanical ventilating equipment having air changes per hour value of four. The company has two pieces of land located at different places where patronage rates are almost the same. The environmental conditions of the two areas are as stated below:

	L	*V*
Relative humidity	50%	51%
Ambient temperature	20°C	21°C
Atmospheric pressure	1.013 bars	1.013 bars
Percentage of CO released by other companies	0.02%	0.08%
Percentage of O_2 available in air	21%	20%

The critical concentration of CO_2 is assumed to be 1%. The initial concentration of CO_2 present in the supposed hall is assumed to be equal to that of the ambient environment. The company needs advice on where to build the cinema hall for maximum profit. Assuming that $f = 1$ cycle per hour and $\psi = 1$.

Considering location L:

$$C = C_o + \left(\frac{10{,}000 Q_c N}{Q}\right)\left(1 - e^{\frac{Qt}{v}}\right) + c_i e^{-\frac{Qt}{v}}$$

but $C_o = y = \dfrac{R}{p + \psi R e^{Rt}} + \dfrac{fAB}{R}$ and $R = \dfrac{(Ab + aB)f}{a + b}$, $p = f\left(\dfrac{ab}{(a+b)^2}\right)$

$$R = \frac{21 \times 2 + 0.02}{3} = 14.0067, \text{ and } p = \frac{2}{3^2} = 0.222$$

$$C_o = \frac{14.0067}{0.222 + 14.0067e^{14.0067\times 6}} + \frac{21 \times 0.02}{14.0067} = \frac{14.0067}{4.411 \times 10^{37}} + 0.03 = 0.03\%$$

or 3 parts per 10,000

Now, determining the volume of persons per volume of room space.

$$100 = \left(3 + \frac{10000 \times 4.72 \times 10^{-6} \times N \times 3600}{V \times 4}\right)(1 - e^{-4t}) + 3e^{-4t}.$$

Since $t = 6$ hrs, $n = 4$,

$$100 = \left(3 + \frac{169.92\, N}{4\, V}\right)(1 - e^{-24}) + 3e^{-24}.$$

This is approximately equal to:

$$100 = 3 + \frac{169.92\, N}{4V}$$

$$\frac{97 \times 4}{169.92} = \frac{N}{V} = \text{ 2.283 persons per 1m}^3; \quad \frac{V}{N} = 0.438 \text{ m}^3 \text{ per person.}$$

3.3 Case study III

A lecture theatre has a volume of 1500 cm^3. The maximum level of carbon dioxide at the end of the maximum usable time of the theatre is 0.1%, assuming an initial concentration of 0.03%, equal to that in the outside air used for ventilation. Natural ventilation can provide 1.5 air changes per hour. If each occupant generates CO$_2$ at a rate of 5×10^{-6} m^3/s and the maximum number of occupants that can use the space for the maximum time is 113, we can determine the maximum allowable time as follows.

$$C = \left(C_o + \frac{10000 Q_c N}{Q}\right)\left(1 - e^{-\frac{Qt}{v}}\right) + \left(c_i e^{-\frac{Qt}{v}}\right)$$

$$10 = \left(3 + \frac{10000 \times 5 \times 10^{-6} \times 113 \times 3600}{1500 \times 1.5}\right)(1 - e^{-1.5t}) + 3e^{-1.5t}$$

$$\frac{2.04}{9.04} = e^{-1.5t}$$

$t = 1$ hr.

Considering location V:

$$C_n = \frac{R}{p + \psi R e^{Rt}} + \frac{fAB}{R}$$

$$R = \frac{20 \times 2 + 0.08}{3} = 13.36$$

$$P = \frac{2}{3^2} = 0.222$$

$$C_n = \frac{13.36}{0.222 + 13.36e^{13.36 \times 6}} + \frac{20 \times 0.08}{13.36} = 0.12\% \text{ or 12 parts per 10000.}$$

Now determining the space per person:

$$100 = 12 + \frac{169.92N}{4V}$$

$$\frac{N}{V} = \frac{88 \times 4}{169.92} = 2.07 \text{ persons per m}^3.$$

4 Discussion

The results obtained have been able to affirm the concept that the number of occupants that can conveniently stay in an apartment or space reduces as the concentration of the contaminant (especially CO_2) increases. Consequently, the percentage by volume of O_2 needed to respire comfortably drops. This has been verified by case study I. In case study II, the adverse effect, of the indiscriminate release of CO into the atmosphere, has been seen on profit maximisation. The increase in the amount of CO in location V reduced the number of persons per m^3 (volume). Consequently, for a specific hall volume, the number of people that can conveniently stay in the hall in V, will be lower than that in L, hence, the company will not make as much profit in V as in L. Therefore, it will be advisable, based on the foundation of convenience on the part of the viewers and profit on the part of the company, to build the cinema house in location L.

5 Conclusion

The decay equation introduced in this paper has been restricted to fully mixed contamination, and is also applicable so long as there is no change in the contamination generation rate during the time period covered by the integration. However, the expressions are general in that they may be applied sequentially to time periods having constant contamination generation rates or constant occupation levels. It may be applied in parallel to any number of non-reacting contaminants that may be present together within the space under study (Douglas). The paper has been able to validate the fact that the occupancy rate is adversely affected by the concentration (volume in air) of the contamination generated within the vicinity of the space utilised.

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