# Prediction of Indoor Air Pollutant Concentrations Using Nazaroff-Cass Model

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## Abstract:

The mathematical modeling of the indoor air pollutants is an issue which draws interest today and also is promoted to work on. The objective of this study is to predict the indoor air pollutants' (such as CO, $SO_2$, $O_3$) concentration rates as a function of temperature, humidity, pressure and certain objects (odor sources) in a classroom using Nazaroff and Cass model. The effects of direct emission, filtration and ventilation are explained and the changes in the concentration of the pollutants in indoor air are determined by the modeling. In the study, specific software is also developed via MATLAB programming language to produce numerical values of the interested gas amount. The graphical output of this software shows emitted gas amount with respect to time.

**Key words:** Air quality, concentration, indoor air, mathematical model, pollutant

## Özet:

İç ortam hava kirleticilerinin matematiksel modellenmesi günümüzde ilgi çeken ve üzerinde çalışmak için de teşvik edilen bir konudur. Bu çalışmanın amacı, Nazaroff ve Cass modeli kullanarak bir sınıftaki iç ortam hava kirleticilerinin (CO, $SO_2$, $O_3$ gibi) sıcaklık, nem, basınç ve belli başlı nesnelerin (koku kaynakları) bir fonksiyonu olarak derişim oranlarını tahmin etmektir. Modelleme yardımıyla direkt yayım, filtreleme ve havalandırma etkileri açıklanmış ve iç ortamdaki kirleticilerin konsantrasyonlarındaki değişmeler ifade edilmiştir. Çalışmada, ilgili gaz miktarının sayısal değerlerini üretmek için MATLAB programlama dili kullanarak özel bir yazılım da geliştirilmiştir. Bu yazılımın grafiksel çıktısı, zamana bağlı yayılmış gaz miktarını göstermektedir.

**Anahtar kelimeler:** Hava kalitesi, derişim, iç ortam havası, matematiksel model, kirletici

## 1. Introduction

Air is vital for human life; people can tolerate hunger and thirst for a while but only survive for a few minutes without air. Breathing air is so important; hence it must be clean. The existence of harmful gases, biological agents or particulate matters in high enough concentrations can affect the air quality also human health.

In the developed world, people spend most of their time indoors so indoor air quality (IAQ) may cause adverse effects upon human health and productivity. Indoor levels of pollutants within a building depend on the physical and chemical properties of the pollutants, environmental

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parameters (temperature, pressure, relative humidity, concentrations of other indoor pollutants etc.), dispersion processes around the building, the ventilation of the building [1].

IAQ models are used to describe the dispersion of air pollutants in an indoor environment, to predict the indoor air pollutant concentration as a function of air exchange rates, sources, removal mechanism and other parameters, and to understand how the factors that affect IAQ [2]. The IAQ models can be generally classified into two main classes as macroscopic models and microscopic models. Macroscopic models are based on the mass balance equation and assume the well mixed air. Microscopic models are based on Navier-Stokes equations including the spatial and time dependency of all indoor variables. A sophisticated macroscopic model used in this study has been developed by Nazaroff and Cass [3].

Following this introduction section, the rest of the paper is organized as follows: the next section focuses on modeling methodology. In the third section, an overview of an application of a Nazaroff-Cass model is presented. The model is presented by Nazaroff and Cass [4] for estimating the concentrations of indoor pollutants. The fourth section provides information on the software. The final section summarizes and concludes the results.

## 2. Mathematical Formulation

Nazaroff-Cass model (1986) accounts for the effects of filtration, ventilation, direct emission and deposition on indoor surfaces (ceiling, floor, walls, and any items within the room). In this model, a building is considered as a group of interconnected compartments with the air exchange rate and each compartment is represented as a room or a set of rooms. The air within the building is assumed to be instantaneously well mixed. In this study, the predictions of the indoor air pollutant concentrations have been made using this model based on a mass balance approach.

A schematic diagram of the approach is presented in Fig. 1. In the model, air may enter from outdoors to the compartment (infiltration), leave from the compartment to the outdoors (exfiltration) and be recirculated through a filter. The ventilation system contributes to the removal of particles.

The mass balance equation (1) which is given the rate of change of the concentration of pollutant is the first-order differential-equation as

$$dC_{ijk}/dt = S_{ijk} - L_{ijk}C_{ijk} \tag{1}$$

where $C_{ijk}$ is the rate of change of the concentration of pollutant $k$ in room $j$ for compartment $i$, $S_{ijk}$ is the sum of all sources: direct emission inside the compartment, advective transport from other compartments, outside and ventilation system, $L_{ijk}$ is the sum of all sinks: removal by filtration and ventilation, loss to surfaces and a larger size by coagulation. The source and sink parameters vary with time.

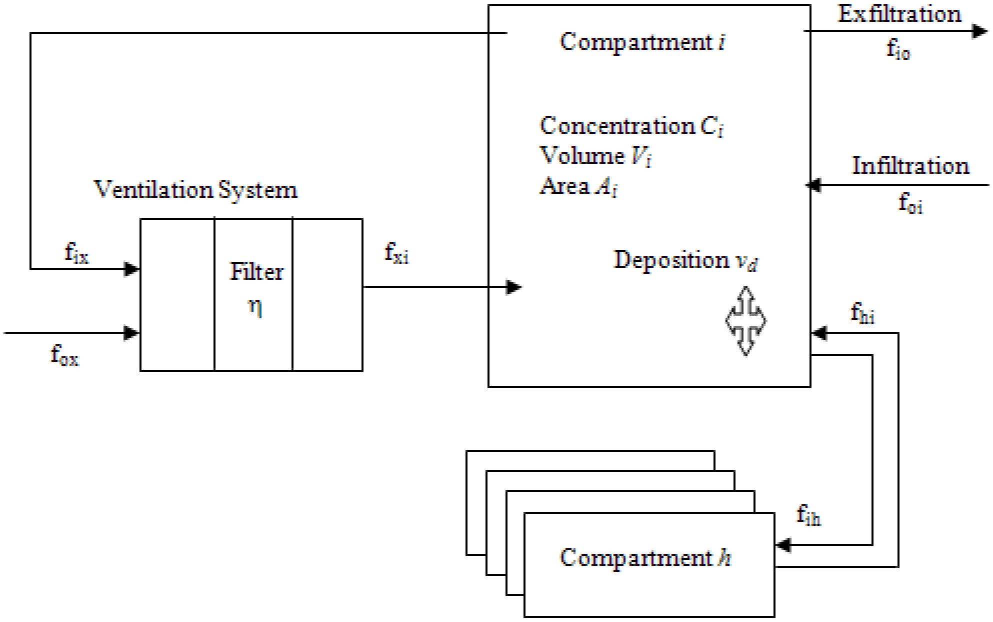

**Figure 1.** Schematic representation of multi-compartment IAQ model [3, 4]

The filtration efficiency may be determined by the user for each pollutant. In mathematical terms, the effects of the ventilation and filtration systems may be described by (2) and (3) equations

$$dC_{ijk}/dt = \sum_{h=0}^{n}\left[(f_{hi}C_{hjk} - f_{ih}C_{ijk})/V_i\right] + \left[(f_{xi}C_{xjk} - f_{ix}C_{ijk})/V_i\right] - (\eta_{iij}f_{ii}C_{ijk})/V_i \quad (2)$$

$$C_{xjk} = \sum_{h=0}^{n}(1 - \eta_{hxj})f_{hx}C_{hjk}/\sum_{h=0}^{n} f_{hx} \quad (3)$$

where $\eta_{ihj}$ is the efficiency of removal in size room $j$ by the filter located in the air stream connecting chamber $i$ to compartment $h$, $V_i$ is the volume of compartment $i$, $f_{ih}$ is the volume flow rate to compartment $h$ from compartment $i$. Subscript $x$ denotes the mechanical ventilation system and 0 outdoor air [5].

The infiltration rate $f_{i0}$ can be calculated by Eq. (4) for the specific period the end of time interval $t_e$ to the beginning of time interval $t_0$.

$$f_{i0} = \ln(C_i/C_0)/\Delta t\,,\ \Delta t = t_e - t_0 \quad (4)$$

where $\Delta t$ is the end of time interval minus the beginning of time interval, $C_i$ is the pollutant concentration at time $t_e$ and $C_0$ is the initial indoor concentration of the pollutant at time $t_0$ ($t_0 = 0$) in compartment $i$ [6].

When the source and sink parameters in Eq. (1) are time-dependent, an analytical solution is obtained as [3]

$$C_{ijk} = C_0 e^{-L_{ijk}t} + \int_0^t e^{-L_{ijk}t} S_{ijk} dt \tag{5}$$

Deposition is a secondary important loss mechanism in determining indoor particle concentrations. The particle deposition rate $\lambda_d$ onto surfaces that is characterized by its deposition velocity $v_d$ can be calculated by Eq. (6) or Eq. (7).

$$\lambda_d = \Delta t^{-1} ln(C_0/C_i) - f_{i0} \tag{6}$$

$$\lambda_d = v_d A_d / V \tag{7}$$

where $A_s$ is the indoor surface area of contact for deposition, V is the volume of the building [6]. $v_d$ can be theoretically defined as the particle deposition flux divided by the undistributed particle concentration [3].

## 3. Numerical Application

The classroom is shown in Fig. 2 is about 7 m in length, 3.5 m in width, 2.4 m in height. The classroom has been divided into 8 and the size of each room is 1.75 m × 1.75 m × 2.4 m. The total area and volume of the classroom which contains one window (height 2 m and width 1 m) and one door (height 2.1 m and width 1 m) is 95.3 $m^2$ and 58.8 $m^3$, respectively.

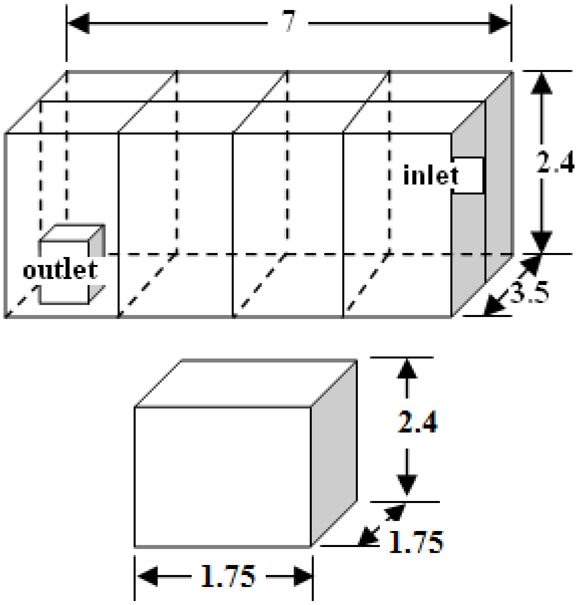

**Figure 2.** Schematic representation of the classroom

The classroom is represented as a single well-mixed compartment, so i = 1. The values of other variables in Eq. (1) are j = 1, 2, …, 8 and k = 1, 2, 3, 4. *k* refers to the pollutant sources. The pollutants are CO (carbon monoxide), $CO_2$ (carbon dioxide), $SO_2$ (sulfur dioxide) and $O_3$ (ozone). The pollutants have been generated by indoor sources and removed by natural and/or mechanical ventilation.

The indoor activity (such as smoking, walking, cleaning) and meteorological conditions that will affect air flow rates are constrained. It is assumed that the air flow rates and air filter efficiency are constant for the time of interest. The classroom is vacant during the study.

The indoor temperature should be between 22.5 $^{o}$C and 25.5 $^{o}$C and the relative humidity indoor shouldn't exceed 70% according to the United States Environmental Protection Agency (U.S. EPA) [7]. The standard values of the indoor air pollutants which have been used in this study are given in Table 1.

**Table 1.** The standard values of the pollutants by EPA [7]

| Pollutant | Molecular Weight (MW) | ppm | mg/m$^3$ |
|---|---|---|---|
| CO | 28.01 | 9 | 10.332 |
| $CO_2$ | 44.01 | 1000 | 1803.689 |
| $SO_2$ | 64.06 | 70 | 183.779 |
| $O_3$ | 48 | 0.05 | 0.098 |

The conversion Eq. (8) is used to convert from ppm to mg/m$^3$ under the standard conditions of 25$^{o}$ C and 1 atmosphere pressure. 24.4 is a conversion constant that represents molar volume [8].

$$C_{mg/m3} = MW \times C_{ppm}/24.4 \tag{8}$$

The deposition velocities for the gas pollutants have been determined according to literature values and are 0.036 cm/s for $SO_2$ and $O_3$, 0 cm/s for CO [9, 10] and 0.3 cm/s for $CO_2$ [11, 12].

The indoor concentrations of CO, $CO_2$, $SO_2$ and $O_3$ have been initialized at 10, 1500, 160, 0.09 mg/m$^3$, respectively. The outdoor concentrations of the pollutants are constant. The operating time of interest is 1 hour.

The time-dependent pollutant generation rate (source strength) can be calculated by Eq. (9)

$$G(t) = C_{avg}Q^2t/(Ve^{\frac{-QV}{t}} + Qt - V) \tag{9}$$

where Q is the volumetric air flow rate and $C_{avg}$ is the average of the pollutant concentrations for the time interval of interest [13].

## 4. Results and Discussion

Mechanical ventilation denotes to using fan systems to move air, and natural ventilation to opening windows and/or doors to increase the entry of outside air [14]. The models have been developed for a classroom with a Heating, Ventilating and Air Conditioning (HVAC) system and a classroom with natural ventilation. Both the generation rates of the pollutants have been changed dynamically and selected constant for each developed model.

When the generation rates are constant over the time interval, the pollutant concentrations in the classrooms have been calculated according to the methodology described by Nazaroff and Cass [4] and the indoor model predictions have been presented in Figure 3.

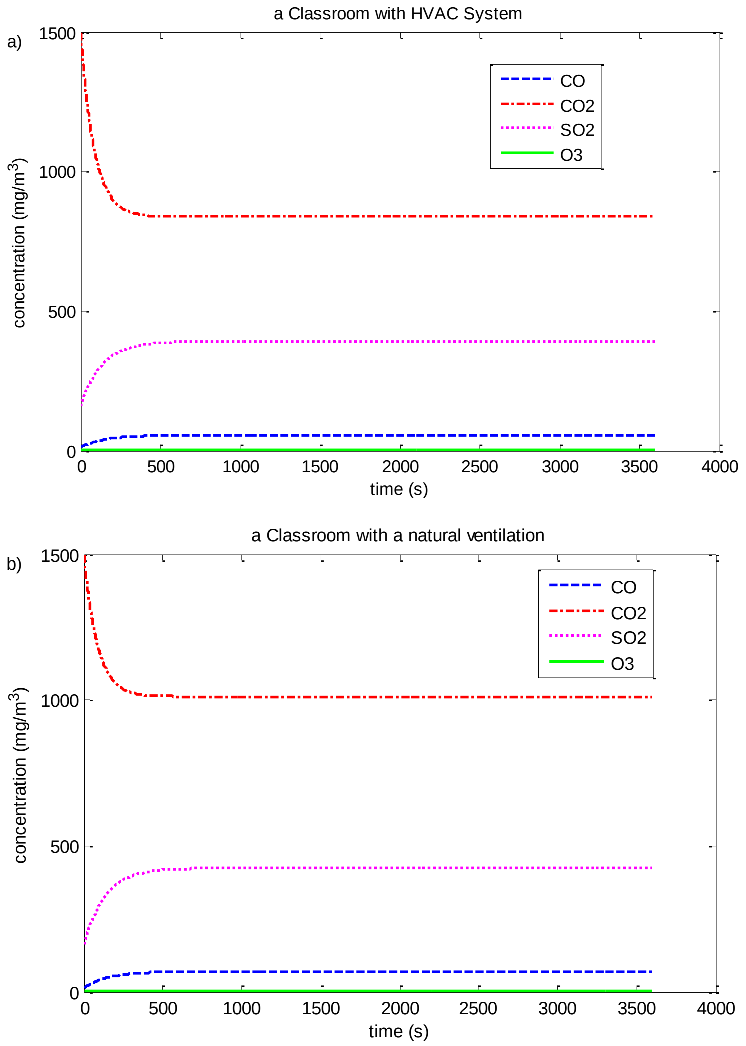

**Figure 3.** Indoor concentrations of the pollutants with constant generation rates within a classroom a) with a continually HVAC system b) ventilated naturally

As can be seen in Figure 3, $CO_2$ concentration have been decreased by more than, CO, $SO_2$ and $O_3$ concentrations have been increased less when the generation rates of the pollutant generation rates are kept in the operation times of the HVAC system.

The generation rates of the limited amount of the pollutant sources can be updated by Eq. (9). The pollutant concentrations in ventilated mechanically and naturally classrooms are calculated using by time-dependent generation rates and presented in Figure 4.

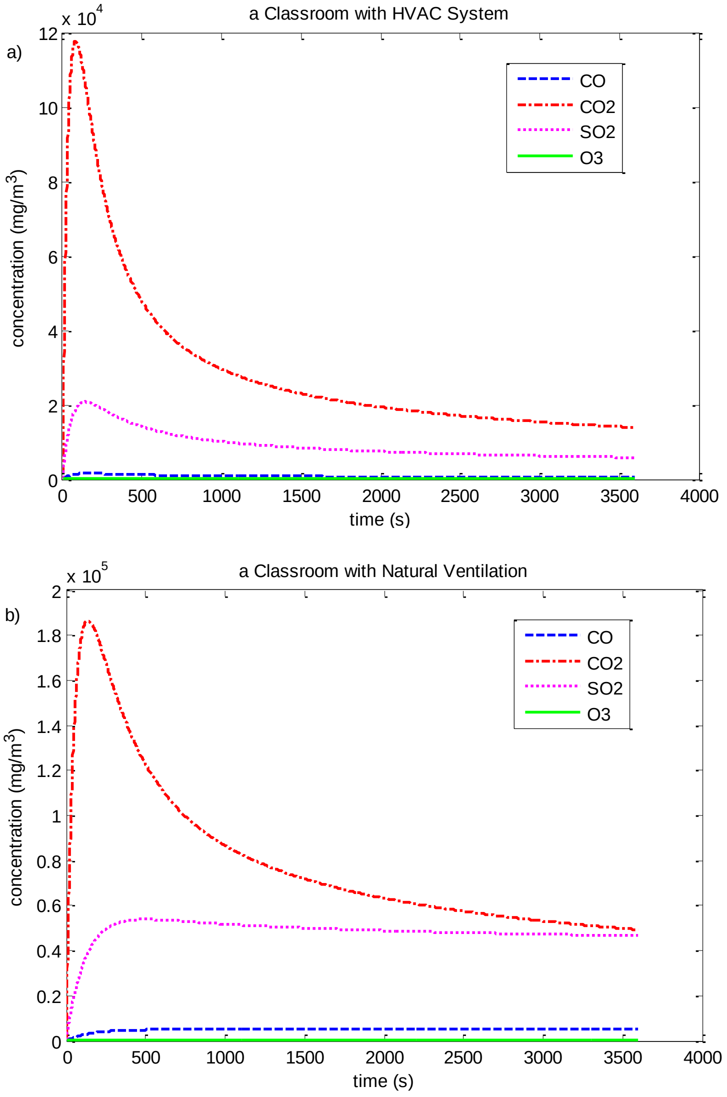

**Figure 4.** Indoor concentrations of the pollutants with time-dependent generation rates within a classroom a) with a continually HVAC system b) ventilated naturally

Figure 4 shows that when the generation rates of pollutants vary with time, the pollutant concentrations within the classroom with natural ventilation are higher. The concentrations have been increased with the release of pollutant sources and then decreased depending on the generation rates in indoor environment because the limited amount of the pollutant sources.

## 5. Conclusions

In this paper, the formulation of the Nazaroff-Cass model used for predicting pollutant concentrations in indoor air is described. The model provides to analyze airflows and the distributions of pollutant concentration so that IAQ problems and HVAC systems can be evaluated.

The concentrations of the pollutants with constant generation rates in the classrooms which are ventilated naturally and mechanically with an operated continuously HVAC system are examined and compared according to the changes in their generation rates. The effects on the indoor air pollutant concentrations in the changes of generation rates are investigated and interpreted.

## Nomenclature

| | |
|---|---|
| $A_d$ | indoor surface area, $m^2$ |
| $C_0$ | initial pollutant concentration, $mg/m^3$ |
| $C_{avg}$ | mean of the pollutant concentration for the time interval of interest, $mg/m^3$ |
| $C_i$ | pollutant concentration in compartment *i*, $mg/m^3$ |
| $C_{ppm}$ | concentration in ppm |
| $f_{0i}$ | the exfiltration rate, $s^{-1}$ |
| $f_{i0}$ | the infiltration rate, $s^{-1}$ |
| $f_{ih}$ | rate of air flow from compartment *i* compartment *h*, $s^{-1}$ |
| G | generation rate, mg/s |
| h | compartment number |
| i | compartment number |
| j | room number |
| k | pollutant number |
| L | sum of all sinks, $s^{-1}$ |
| MW | molecular weight |
| n | total number of compartments |
| ppm | parts per million |
| Q | air flow volume, $m^3/s$ |
| S | sum of all sources, $mg\ s^{-1}/m^3$ |
| t | time, s |
| $t_0$ | the beginning of time interval, s |
| $t_e$ | the end of time interval, s |
| x | mechanical ventilation system |
| V | volume of the classroom, $m^3$ |
| $V_i$ | volume of compartment *i*, $m^3$ |
| $v_d$ | deposition velocity, m/s |
| $\eta$ | filtration efficiency (dimensionless) |
| $\Delta t$ | time difference between the end and beginning of the time interval, s |
| $\lambda_d$ | particle deposition rate, $s^{-1}$ |

## Abbreviations

| | |
|---|---|
| HVAC | Heating, Ventilating and Air Conditioning |
| IAQ | Indoor Air Quality |
| U.S. EPA | United States Environmental Protection Agency |

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