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Multiple cell ventilation model with time-dependent emission sources

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ABSTRACT

A numerical model has been developed which predicts the concentration of contaminants in a multi-cell enclosure. This model calculates the transient concentration in each cell based upon the ventilation present in each cell and the emission rate. The numerical model incorporates emission sources that vary with time. Thus, the model may calculate accurate time-weighted-averages (TWA) and accurate maximum concentration levels in each cell. This allows designers of ventilation systems to perform proper engineering design for both commercial and industrial facilities.

INTRODUCTION

Air quality may be defined as the nature of air that affects an individuals health and well-being. Air quality is also an indication of how well the indoor air satisfies the three requirements for human occupancy: 1) Thermal acceptability; 2) Normal concentration of oxygen and carbon dioxide; 3) Control of the contaminants below their acceptable limits. The development and the application of validated mathematical and physical models provide the means to relate the design of the physical system to the expected exposure of the occupant, the related dose, and the resultant human response. A brief literature review of the available numerical models are presented in the following section.

LITERATURE REVIEW

The problem of predicting the effectiveness of ventilation systems is difficult due to the complex interaction of the system components within the ventilated space. There have been numerous numerical models developed which have varying degrees of sophistication, applicability and accuracy.

Horstman [1] developed a numerical model that predicts the velocity distribution, airflow circulation pattern, and airborne contamination distribution within an air exhaust passenger cabin. The model utilizes the finite difference approximations of the two-dimensional, time-varying Navier-Stokes equations. However, it is difficult to apply the model to other ventilated volumes, such as multi-cell volumes.

Meckler and Janssen [2] developed a model to calculate the amount of outdoor air required, concentration of filtered contaminants or the recirculation needed to meet an acceptable indoor air quality. This model is a one-cell, steady state model which includes recirculation of the indoor air through filters.

Sparks et al. [3] developed a multi-compartment model based on a well-mixed mixing model. The model estimates the effects of forced ventilation (HVAC), air cleaning, room-to-room air movement, and natural ventilation on pollutant concentrations.

Crommelin and Buringh [4] developed a multiple cell model to calculate temperatures and concentrations of indoor air pollution. Crommelin and Buringh concluded that a mathematical model which calculates the air flows in an enclosure requires the numerical solution of the Navier-Stokes equations with a large number of grid points. This requires a large computational effort. They decided to simplify the model by dividing the enclosure into cells and estimating the air flow between cells from measurements taken in the enclosure.

Awbi [5] developed a numerical model, called ROOMVENT, which solves two and three-dimensional ventilation problems. The model solves, in finite difference form, the steady-state conservation equations of mass, momentum and energy.

Siurna and Bragg [6] modelled room air diffusion based on a two cell geometry which enables room air concentrations to be described stochastically. Through stochastic analysis of the ventilation system, the model provides quantitative statistical conclusions concerning the ventilation performance.

Fletcher and Johnson [7] studied the build-up in concentration of a heavier than air gas emitted at various concentrations and positions within a room for different ventilation patterns.

Skäret [8] developed a ventilation model which is described in terms of the ventilation efficiency and quantified by means of a two-zone (compartment) flow and difference model.

Dellagi et al. [9] developed a three-dimensional, time-varying ventilation model. This model calculates only the velocity profiles. This model could be adapted so that concentration profiles could be calculated as well.

The model developed by Goodfellow Consultants (GCI) is a multi-cell, time-dependent model similar to the models of Crommelin and Buringh [4] and Sparks et al. [8]. Our model has been expanded to including multiple time-varying emission rates of the contaminants in question.

THEORY

Fundamental Model

The simple, one-compartment model, as shown in Figure 1, demonstrates the various factors that affect indoor exposure: indoor and outdoor sources, removal and dilution control. This model identifies the three most common methods of control: source control, removal control, and dilution control. In this model, source control, N, may be represented by isolation, product substitution or local exhaust. Removal control, E, may be represented by passive mechanisms such as settling or sorption, and active mechanism such as fan filter modules, clean benches, or central forced air systems with recirculated air. Dilution control, V_o, may be represented by infiltration, natural ventilation, or mechanical ventilation.

A mass balance of this uniformly mixed space in steady state may be expressed by:

$$C = C_i - C_o = \frac{N-E}{V_o}$$

This model indicates that the indoor air concentration of a contaminant, C_i, will exceed the outdoor concentration, C_o, unless the removal rate exceeds the net generation rate. This control method is commonly used for applications such as clean-rooms. This relationship also identifies the desired control strategy to achieve an acceptable C: 1) Reduce the net operation rate; (2) Apply techniques that will increase removal rate; (3) Increase the dilution rate.

The removal rate of particulate and gaseous contaminants may be considered to be comprised of two components: passive removal mechanisms and active removal mechanisms. During passive removal the concentrations of particulate and gaseous contaminants may be reduced by settling, condensation or sorption. Reactive gases, such as ozone, sulphur dioxide and nitrogen dioxide may be adsorbed or react with building surfaces. However, procedures to calculate passive removal rates of gases and vapour are
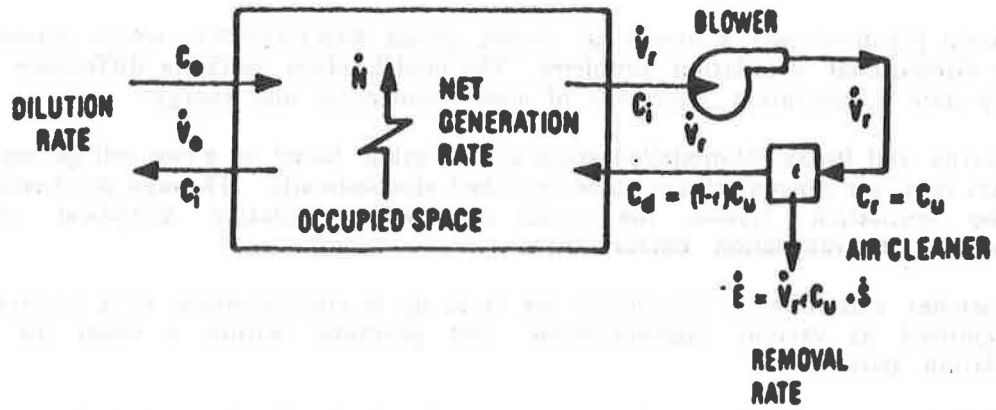
Figure 1. One-compartment, uniformly-mixed, steady-state model for indoor air quality control.
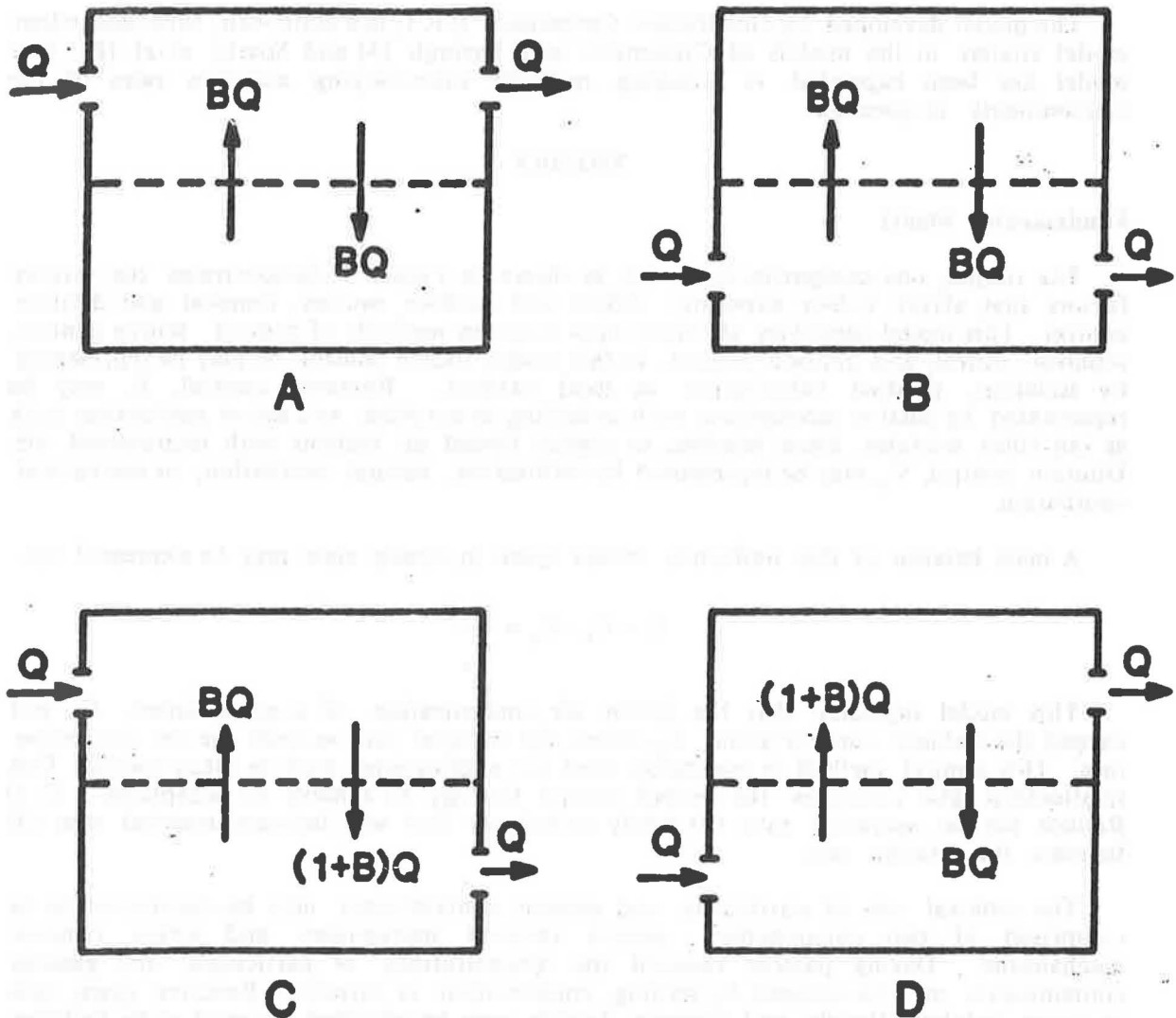

Figure 2 Flow Diagrams Of Two-Zone Models

not well developed at this time. In many circumstances, the recycled air is cleaned and then returned to the building to save on energy costs. The active removal rate of contaminant from the recycled air may be expressed as: $E = V_r \epsilon C_u$

where: ϵ = air cleaner efficiency
V_r = volumetric air flow through air cleaner
C_u = concentration of contaminant upstream of air cleaner.

Dilution control is the most commonly used method of air quality control in the introduction of outdoor air for dilution of the indoor air concentrations. Dilution control may be the most energy intensive and costly of the control methods available today. There are two different types of dilution control: 1) Infiltration and natural ventilation; and 2) Mechanical ventilation.

Infiltration is usually considered to be unwanted air leakage through cracks, joints and connections in the building, whereas natural ventilation is usually considered to be desired air exchange through intentional openings in the building such as doors and windows. Because of the large number of variables associated with infiltration ad natural ventilation, it is difficult to accurately estimate these variables. However, there are simple models to estimate both infiltration and natural ventilation rates.

For the case of no recirculated air within the occupied space (i.e. 100% outdoor air) and no removal central, the indoor concentration various inversely with the dilution rate, V_o. This relationship is the basis for the prescriptive ventilation rates commonly specified in ventilation codes and standards. However, the assumption of uniform mixing with the occupied space may lead to significant error in correctly estimating the amount of dilution air required to a given location within the occupied space.

The simple model, as discussed in Figure 1, assumes that the air within the occupied space is uniformly mixed. However, thermal and contaminant stratification can occur within the occupied space, resulting in occupant exposures much higher than predicted by models that assure uniform mixing. The effectiveness of the ventilation system for air quality control is dependent upon two system characteristics: the room air exchange rate, and the air flow patterns within the room.

If the room air distribution is not sufficient to dilute or remove contaminants from the location of most likely exposure, the effectiveness of the system will be impaired as excessive air exchange rates will probably be used as compensation, with the expected results of increased energy consumption and non-uniform mixing. These air distribution patterns within the room may be as important to the effectiveness of the ventilation system as the room air exchange rate.

Two Zone Models

In general, flow patterns in a room are quite complicated due to: 1) warm and cold surfaces; 2) unevenly distributed heat sources; 3) supply diffuser design; 4) air supply and exhaust locations; 5) infiltration and exfiltration; 6) unevenly distributed pollutants with regard to; and 7) thermal stratification.

This situation is modelled in practice using a two-zone model with reasonable results (Rodahl, 1987, Jansenn et al., [11], Skåret [8, 12], Woods, [13], Persily, [13]). This type of model has been used extensively by scientists in Scandinavia for designing displacement ventilation systems (Skåret [8]). Simplified models have been used for cases where there is no infiltration, exfiltration or recirculation to calculate ventilation effectiveness for various supply and exhaust configurations (Figure 2).

In these diagrams, Q is the airflow into and out of the total space volume, and BQ is the flow between the zones where B is a fraction which ranges from zero to infinity which corresponds to complete mixing between the zones. Within each zone, the air is assumed to be perfectly mixed. Case A in Figure 2 is typical of most office designs with the supply

and exhaust located at ceiling level. It is suggested that this may lead to a situation in which a significant portion of the supply air short-circuits the occupied zone. This model has been used extensively by Sandberg [15], Skäret [8,12] and others.

For an actual installation, mechanical ventilation systems almost always employ recirculation of exhaust air as an energy saving measure (Persily, [14]). A two-zone approach has been developed which includes recirculation and is based on the schematic of office ventilation shown in Figure 3 by Meckler and Janssen [2].

To ensure acceptable air quality, care must be taken in the location of the supply and exhaust devices. For example, the common procedure of locating both supply and exhaust devices in the ceiling has been shown to result in a ventilation efficiency of less than 50 per cent.

Central, forced air systems may be constant air volume (CAV) or variable air volume (VAV) systems. The basic difference is that the CAV system provides the same amount of air flow into an occupied space, independently of thermal load, whereas the VAV system reduces the air flow rate into the occupied space as a function of thermal load. The VAV system is inherently more energy efficient for applications where variable thermal loads exist, as the reduction for power can be significant. Conversely, VAV systems may at time operate at less than required ventilation capacities because these systems reduce their air flow rates to occupied spaces in response to thermal loads.

Meckler and Janssen [2] proposed the use of air cleaners to reduce outdoor air requirements. The objective of air cleaners is to increase the fraction of return air and thus reducing the energy required to condition the ventilating air. They found that there are a number of design considerations which affect the performance of air-cleaning systems. The type of air cleaner used, the location in the system, and the amount of air passed through the air cleaner all affect the amount of reduction in contaminants. The air cleaner can be placed in one of two different locations: recirculated stream, identified as A in Figure 3 or the mixed stream identified as B in Figure 3.

The volumetric flow through the air cleaner and its effectiveness determines the amount of material that can be removed. When the volumetric flow is reduced in a variable air volume (VAV) system, the contaminant removal capacity is reduced. This effect is incorporated in the flow reduction factor, F_r. The filter effectiveness is given by E_f. In general, the effectiveness increases as velocity through the air cleaner is reduced.

The recirculation flow factor, R, is the fraction of the return air that is recirculated. As the ventilation requirements increase, the amount of outdoor air needed to dilute the occupied space increases. This causes the recirculation factor to decrease.

Multi-Compartment Models

Sparks et al. [3] developed a multi-compartment model based on a well-mixed mixing model. They noted that air movement in a building consists of: 1) Natural air movement between rooms; 2) Air movement driven by a forced air system (HVAC); 3) Air movement between the building and the outside.

The model of Sparks et al. [3] consists of pollutant mass balance on each room. The amount of air entering a room from all sources (HVAC, outdoors, other rooms) must equal the amount of air leaving the room. They also assumed a well mixed model. Each differential equation represents a mass balance for each room. The resulting differential equations can be solved using standard numerical techniques, resulting in concentration profiles, with respect to time, for each room.
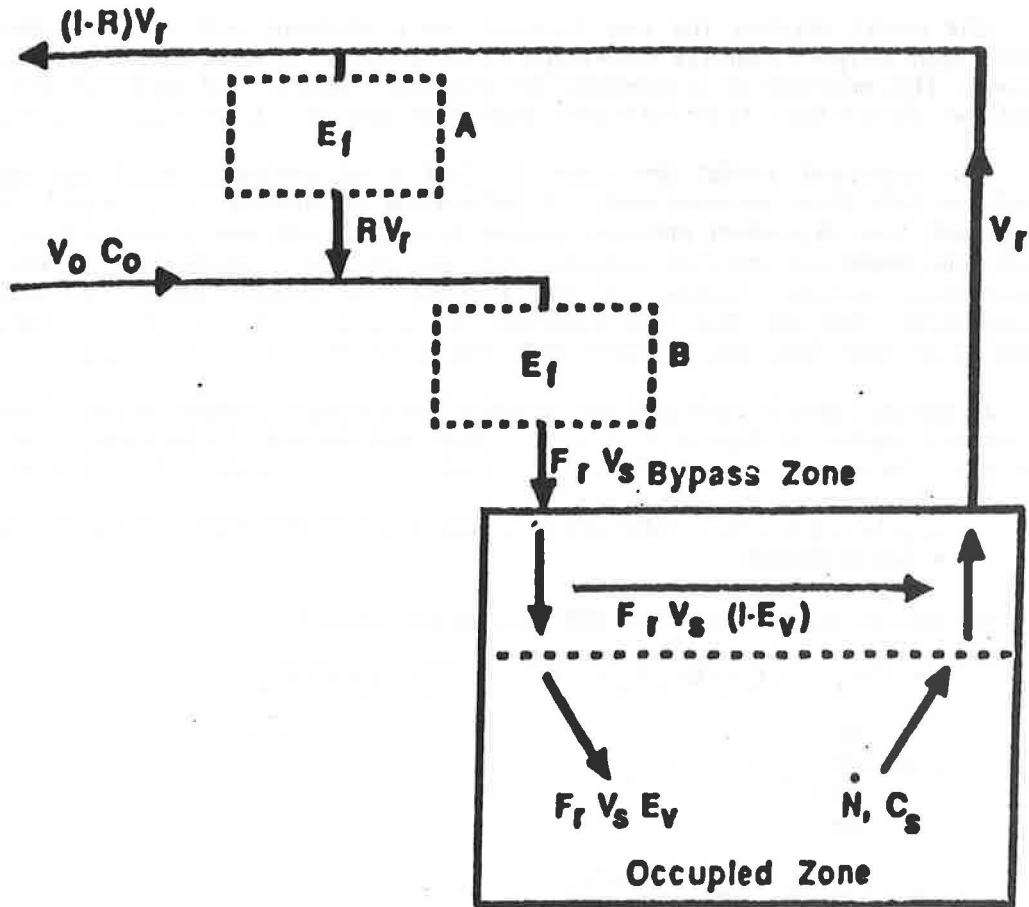
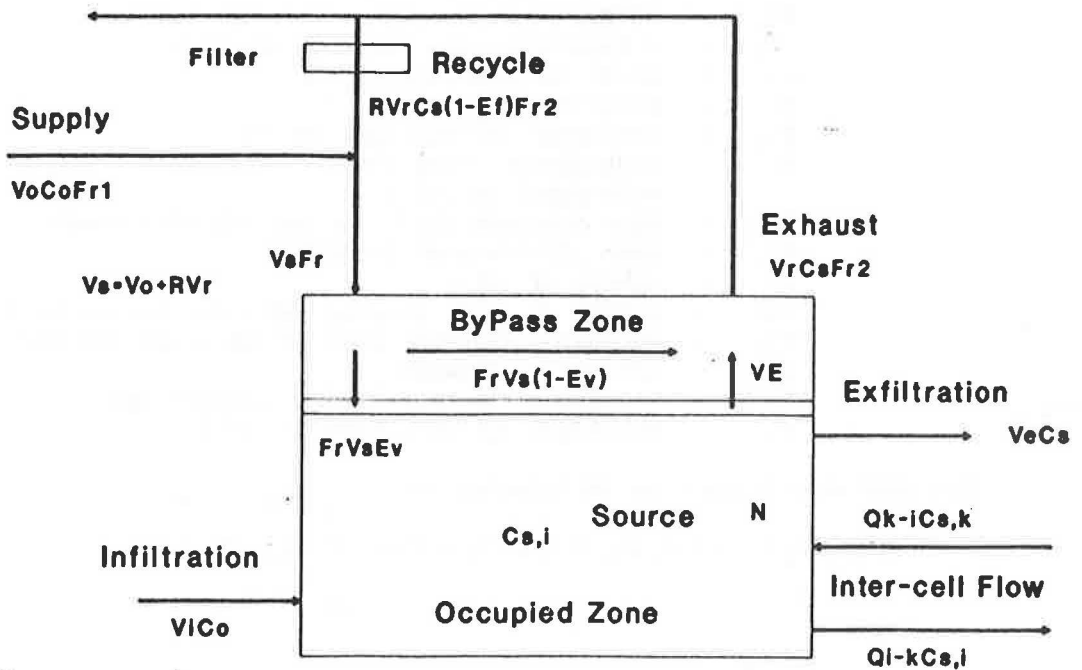**Figure 3. ASHRAE Two-Zone Model with Recirculation**

Figure 4   TYPICAL CELL

The model requires the user to enter the inter-room airflows. Calculation of the inter-room airflows requires knowledge of the temperature and pressure gradients between rooms. This information is generally not available. Sparks et al. [3] found that inter-room airflows do not have to be estimated with high precision to produce good model results.

The numerical model developed by GCI is an unsteady, multi-cell model which includes bulk flows between each cell, infiltration/exfiltration to each cell, recycle air to each cell, time-dependent emission sources from each cell, and mixing efficiency of each cell. The model can calculate concentration profiles for a maximum of 15 cells. The input parameters include: number of cells (rooms), cell volume, initial cell concentration, infiltration flowrate and concentration, exfiltration flowrate, HVAC flowrates and interconnecting flowrates between cells and emission rate for each cell.

In the GCI model, each cell was modelled in a similar manner to the ASHRAE model discussed earlier in Figure 3. The air filter was assumed to be located in the recycle stream. The species mass balance on occupied zone, as shown in Figure 4, is:

Supply + Recycle + Infiltration + Source + Intercell Flow - Exhaust - Exfiltration = Accumulation

The species mass balance for cell i (occupied zone) is:

$$Ev_i \ Vo_{i,i} \ Fr1_i \ Co_i + Ev_i \ R_i \ Vr_i \ Fr2_i \ (1-Ef_i) \ Cs_i + Vi_i \ Co_i$$

$$+ \ N_i + \sum_{\substack{k=1 \\ k=i}}^{N} (Q_{k-i} \ Cs_k - Q_{i-k} \ Cs_i)$$

$$- VE_i \ Cs_i - Ve_i \ Cs_i = Vi \ \frac{dCs_i}{dt}$$

where

N	-	number of cells
Q_{k-i}	-	volumetric flowrate from cell k to cell i
Q_{i-k}	-	volumetric flowrate from cell i to cell k
Cs_i	-	concentration in cell i
Vi_i	-	infiltration/exfiltration flowrate to cell i
Co_i	-	concentration of outside air to cell i
Ci_i	-	initial concentration in cell i
N_i	-	emission rate in cell i
Ev_i	-	ventilation effectiveness in cell i
R_i	-	recirculation flow factor - fraction of return air that is recirculated to cell i
$Fr1_i$	-	flow reduction factor for cell i (VAV system)
Ef_i	-	filter effectiveness for cell i
V_i	-	volume of cell i
Vo_i	-	outdoor flowrate entering cell i through HVAC system
Vr_i	-	volumetric flowrate from HVAC system for cell
Ve_i	-	exfiltration flowrate
VE,i	-	volumetric flowrate leaving occupied zone
V_i	-	volumetric flowrate entering cell i

The total mass balance on the occupied zone is

$$Fr2_i \ Ev_i \ R_i \ Vr_i + Ev_i \ Vo_i \ Fr1_i + Vi_i = VE_i + \sum_{\substack{k=1 \\ k=i}}^{N} (Q_{i-k} - Q_{k-i})$$

The species mass balance was simplified by substituting VE_i into the expression.

$$Ev_i\, Fr1_i\, Vo_i\, (Co_i - Cs_i) + N_i - Ev_i\, Fr2_i\, R_i\, Vr_i\, Ef_i\, Cs_i$$

$$+ Vi_i\, (Co_i - Cs_i) + \sum_{\substack{k=1 \\ k=i}}^{N} Q_{k-i}\, (Cs_k - Cs_i) = V_i\, \frac{dCs_i}{dt}$$

The total mass balance on cell i is:

Supply + Recycle + Infiltration + Intercell = Exhaust + Exfiltration

$$Vo_i\, Fr1_i + R_i\, Vr_i + Vi_i + \sum_{\substack{k=1 \\ k=i}}^{N} (Q_{k-i} - Q_{-k}) - Vr_i\, Fr2_i - Ve_i = 0$$

The total mass balance must be satisfied to ensure correct results.

Both constant air volume (CAV) and variable air volume (VAV) systems have been incorporated into the model. In general, for a CAV system, the volumetric flowrate through the air cleaner is constant. Thus, $Fr1_i$ and $Fr2_i$ equal 1.0. When the volumetric flowrate is variable (VAV), $Fr1_i$ and $Fr2_i$ are not equal to 1.0. The flow reduction factor is equal to the ratio of the mean volumetric flowrate and the maximum volumetric flowrate through the air filter.

There are two flow reduction factors $Fr1_i$ and $Fr2_i$ for a VAV system. $Fr1_i$ is the flow reduction that applies to the make-up air and $Fr2_i$ applies to the exhaust recycle air.

There are a number of emission rates defined in the numerical model: 1) A constant source in the entire time interval; 2) A constant source for a set time interval; 3) An exponential decay from an initial value; 4) An exponential increase from an initial value; 5) An asymptotic increase to a final value; 6) A linear increase/decrease from an initial value; and 7) A combination of these types of emission rates. Schematics of the different emission rates, N, are presented in Figure 5.
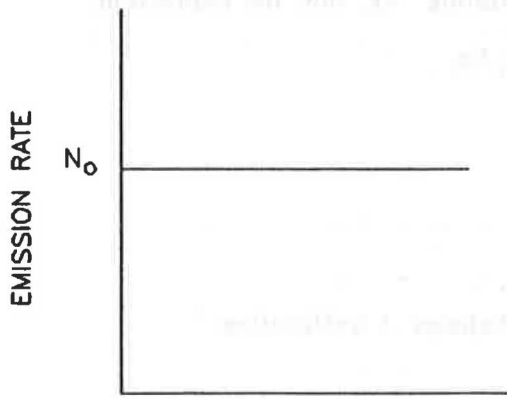
Emission Rates

The most significant factor to be quantified in air quality models is the generation rate of the contaminants. There are thousands of gases, vapours, particulates and radionuclides that are emitted from three primary sources: 1) Human occupants; 2) Materials and furnishings within the occupied space; 3) Processes conducted within the occupied space.
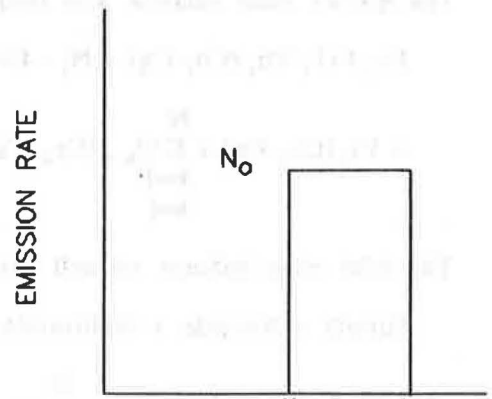
The emission sources vary from "single point" (e.g. occupants, tobacco smoking) to large "surface areas" (e.g. building material outgassing). Contaminant emissions may be independent of other indoor environmental conditions (e.g. tobacco smoking) or may be interactive with the environment (e.g. bacterial growth).

The simplest assumption for modelling emissions is that the rates are independent of other environmental factors. With this assumption, contaminant emission rates may be considered to be constant for specific time intervals which are dependent on the mobility of the source (e.g. human occupants) or by the frequency of the occurrence.
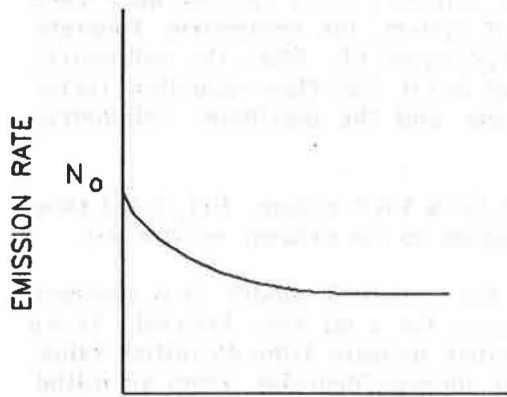
The assumption that emissions are independent of environmental factors simplifies calculations, but significant errors in predicting exposures can result. There are two types of interactions: 1) Interactions with thermal factors; 2) Interactions with other contaminants.
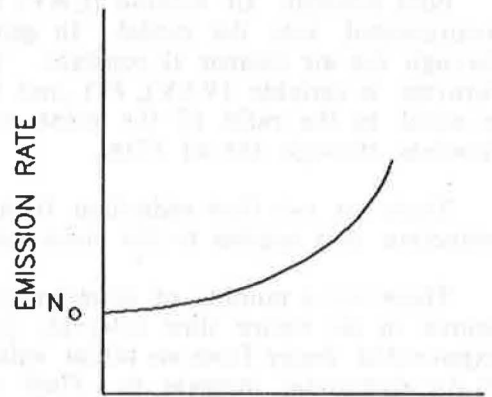
FIGURE 5 — Emission Rates

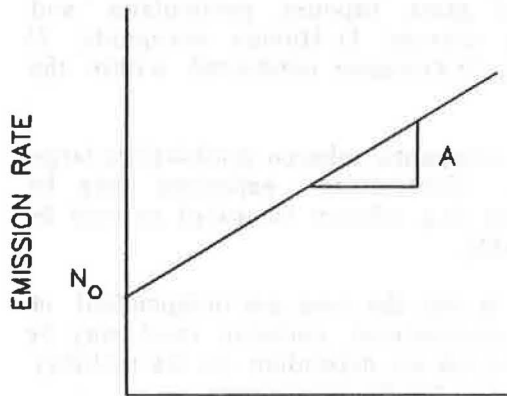GOODFELLOW CONSULTANTS INC.

SKETCH NO.

Formaldehyde is an example of a contaminant affected by thermal interactions. Net generation rates may double if the temperature increase 6 degrees Celsius. Radon is an example of a contaminant affected by interactions with other contaminants. When radon is in equilibrium with its progeny, the radiation dose may be 500 times that due to the radon itself.

The emission rate of a contaminant from a liquid surface can be calculated based on mass-transfer mechanisms. The emission rate is highly dependent of the air velocity over the liquid surface where the emission is occurring. If the air flow is zero, the emission rate is primarily through stagnant diffusion. Conversely, if the air flow is non-zero, the emission rate increases markedly.

Fick's law, for the case of diffusion through a stagnant film of thickness y_o [16], is:

$$n_A = \frac{D_{AB} \, A \, M_w \, P^{\cdot}_A \, x_A}{RT \, y_o}$$

where

n_A = emission rate, g/s
D_{AB} = diffusion coefficient, m^2/s
R = gas constant
T = temperature (K)
A = surface area (m^2)
M_w = molecular weight
x_A = liquid phase mole fraction.
$P^{\cdot}_A$ = vapour pressure of component A (Pa)
y_o = thickness of the stagnant film (m)

In this expression, the concentration in the free stream is equal to zero. In polymeric solutions, the liquid mole fraction is replaced by the volume fraction, v_A.

Incropera and Dewitt [17] developed methods to calculate the mass transfer rate of a contaminant (emission rate) to or from liquid surface for different flow geometries. They developed correlations which may be applied to problems of low-velocity, forced convection, with no phase change occurring within the fluid. Forced convection refers to situation in which the relative motion between the fluid and the surface is maintained by external means, such as a fan or a pump, and not by buoyancy forces due to temperature gradients in the fluid (natural convection).

The mass transfer rate may be calculated using the theoretical approach which involves solving the boundary layer equations for a particular geometry. Unfortunately, solving the boundary layer equations is often extremely difficult. Therefore an experimental approach is generally used to obtain the mass transfer correlations.

The mass transfer rate, for ideal solution, can be calculated from

$$n_A = \frac{h_m \, A \, Mw \, P^{\cdot\cdot}_A \, x_A}{RT}$$

where h_m = mass transer coefficient

The average mass transfer coefficient, h_m, can be calculated for laminar flow over a flat plate from:

$$Sh = \frac{h_m L}{D_{AB}} = 0.664 \, Re_L^{0.5} \, Sc^{0.33}$$

where   Sh   = Sherwood number
           L   = length (m)
           Re_L = Reynolds number
           Sc   = Schmidt number

The Reynolds number may be computed from

$$Re_L = \frac{u_\infty L}{\nu}$$

where u_∞ = free stream velocity (m/s)
           ν = kinematic viscosity (m²/s)

The Schmidt number may be computed from

$$Sc = \frac{\nu}{D_{AB}}$$

If the flow is turbulent, that is, if the Reynolds number, Re_L, is greater than 5×10^5, the mass transfer coefficient may be computed from

$$Sh = (0.037\ Re_L^{0.8} - 871)\ Sc^{0.33}$$

Incropera and DeWitt [17] outlined a mass transfer analogy, based on experiments results, of the external flow involving a circular cylinder in cross flow.

The analogy is based on the Sherwood number, Sh.

$$Sh = CRe_D^m\ Sc^n$$

where $Re_D = \frac{u_\infty D}{\nu}$

The constants C and m are listed below:

Table 1   Constants of equation for the circular cylinder in cross flow

Re_D	C	m
1-40	0.75	0.4
40-100	0.51	0.5
$1 \times 10^3 - 2 \times 10^5$	0.26	0.6
$2 \times 10^5 - 2 \times 10^6$	0.076	0.7

The value of n is determined from the value of the Schmidt number, Sc. If Sc < 10, n = 0.37; if Sc > 10, n = 0.36.

In this model, the density of component A in the free stream was assumed to be small and thus equal to zero. For polymeric solutions, the mole fraction is replaced by the volume fraction, as outlined by Flory [18].

In summary, the parameters required to calculate the emission rate are: surface area (A), length of surface (L), air velocity (u_∞), temperature (T), liquid mole fraction (x_A), vapour pressure, $P_A^\circ(T)$, and the physical properties: binary mass diffusion coefficient (D_{AB}), kinematic viscosity of air (ν) and the molecular weight of the chemical (M_w).

RESULTS

A two-cell model with recycled air in one of the cells was used as an example for the general GCI model. The input parameters are listed in Table 2.

The steady state solution is:

$$Cs_1 = 2.71 \text{ g/m}^3, \quad Cs_2 = 2.0 \text{ g/m}^3$$

The concentration profiles as a function of time for both cells are presented in Figure 7.

TABLE 2
Two-Cell Input Parameters (Figure 6)

Parameter	Cell 1	Cell 2
Ev_i	1.0	1.0
N_i	5 g/s	10 g/s
Vo_i	5 m^3/s	2 m^3/s
Vr_i	0.0	5 m^3/s
Vi_i	0.0	5 m^3/s
Ve_i	0.0	11 m^3/s
R_i	0.0	0.8
Ef_i	1.0	1.0
V_i	50.0 m^3	75.0 m^3
Ci_i	0.0	0.0
Co_i	2 g/m^3	1 g/m^3

$$Q_{1-2} = 7.0 \text{ m}^3/\text{s}$$
$$Q_{2-1} = 2.0 \text{ m}^3/\text{s}$$
$$Mw = 100 \text{ g/gmole}$$

The GCI model is able to calculate concentration profile for systems where the emission rate is a function of time. In Figure 8, the emission rate (g/s) varies considerable as a function of time. In the first 100 seconds, the emission rate is constant (5 g/s). Between 100 and 200 seconds, the emission rate increases linearly at a rate of 0.1 g/s^2. From 200 to 300 seconds, the emission rate decrease exponentially at a rate of exp(-0.01t) to 5.5 g/s. Between 300 and 350 seconds, the emission rate decreases linearly at a rate of 0.05 g/s^2. From 350 to 400 seconds, the emission rate is constant and equal to 8 g/s. After 400 seconds, the emission rate is 0. The input parameters are listed in Table 3. The resulting concentration profile is also plotted in Figure 8.

TABLE 3

Vo_1	0.5 m^3/s
Vr_1	0.5 m^3/s
Vi_1	0
Ve_1	0
Co_1	0
R_1	0
Ef	0
V_1	5.0 m^3
Frl	1.0
Fr2	1.0

For these parameters, there is a lag between the emission rate and the resulting concentration profile, as expected.
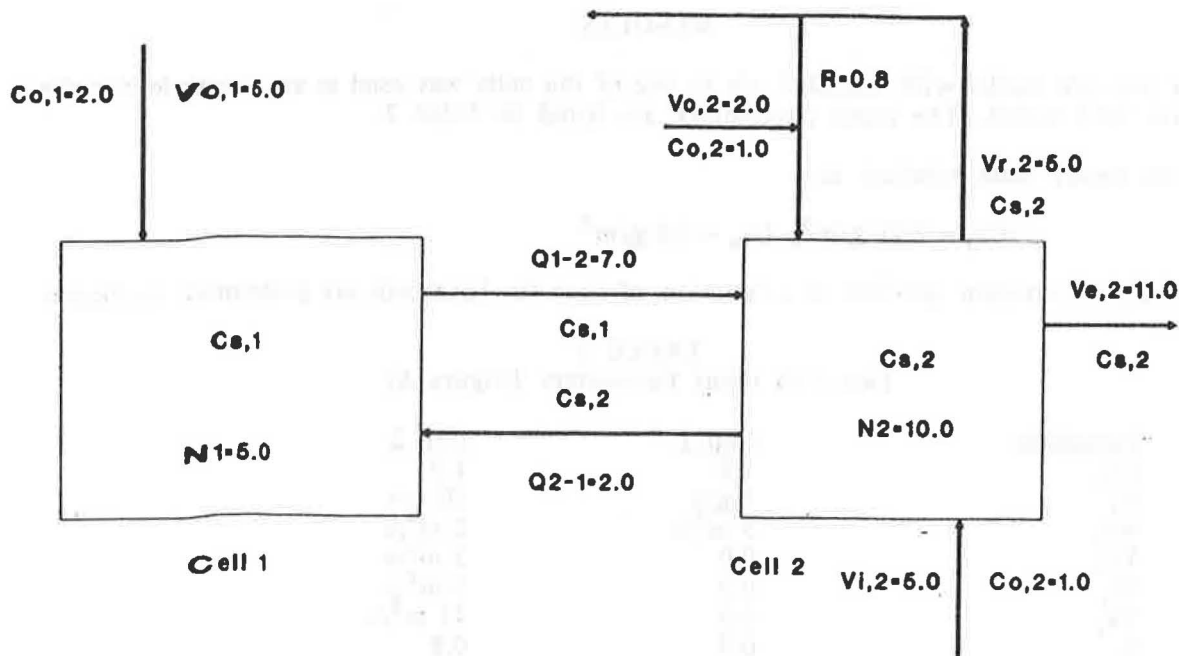
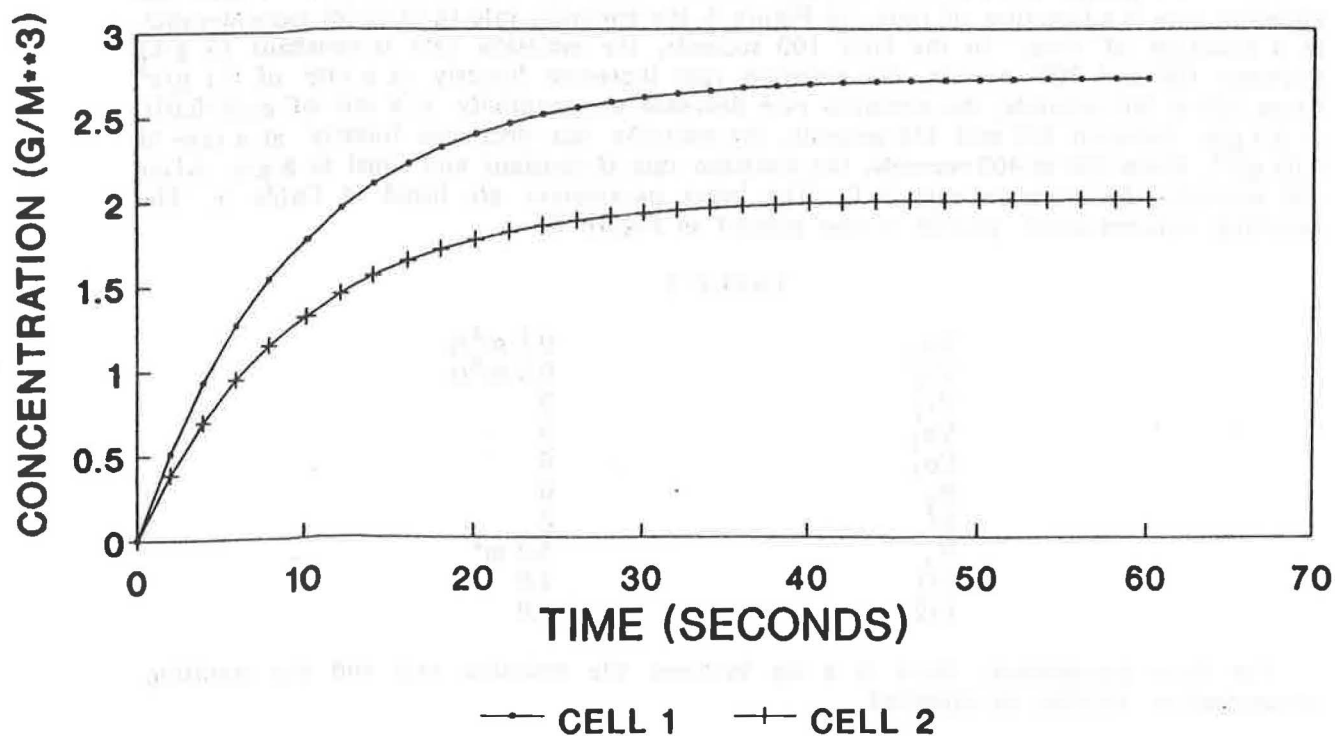FIGURE 6   Two-Cell Model with Recycle

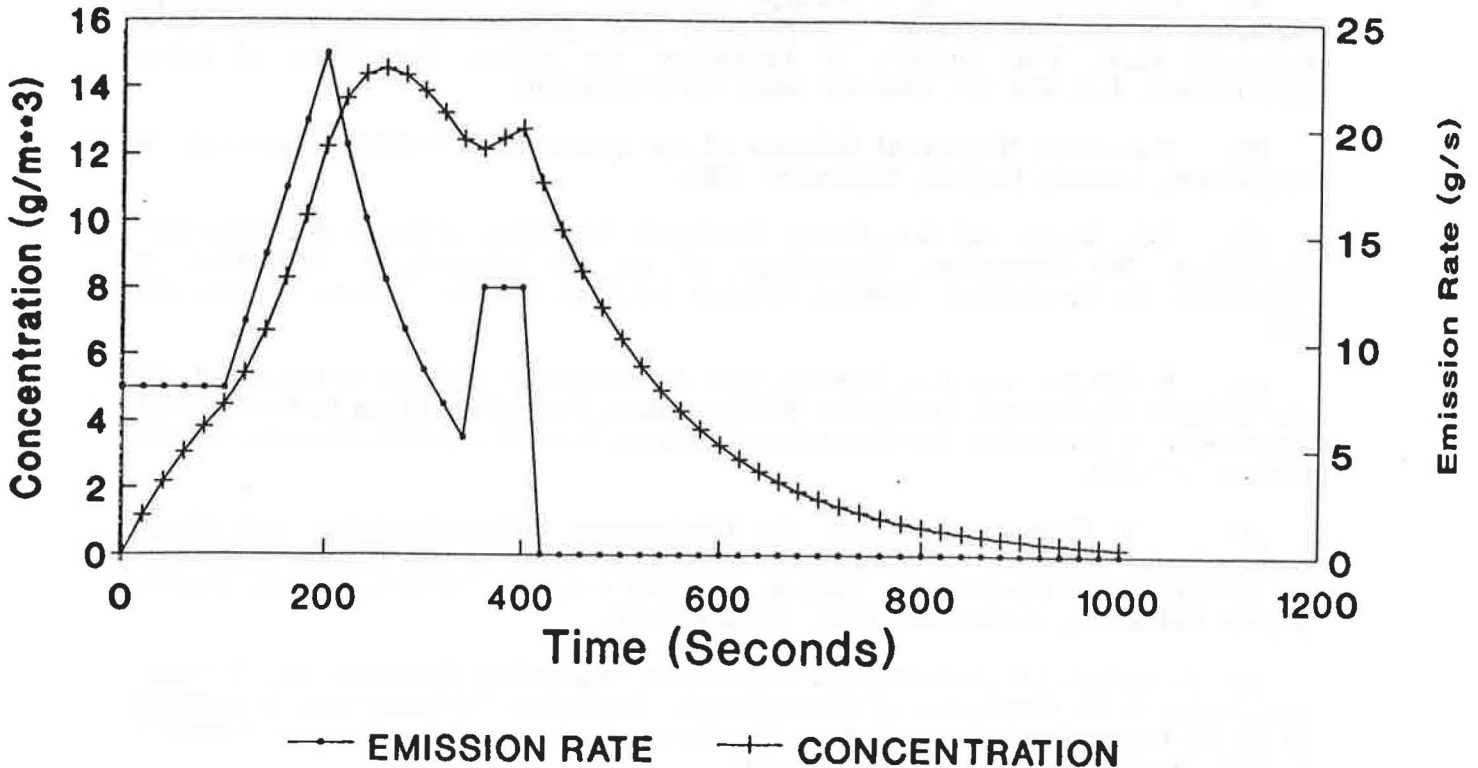FIGURE 7   Two-Cell Model with Recycle

Figure 8. Multiple Emission Rates

CONCLUSIONS

The numerical model developed by GCI, allows the user to calculate the concentration profile in each cell of a multi-cell complex as a function of time. Further, the model also calculates the emission rate of contaminants evaporating from a liquid surface. This type of emission rate is prevalent in many coating and process operations. As emission rates usually vary with time, the model can accommodate a time-variable emission rate. This allows the GCI model to accurately determine the maximum concentrations and the time-weighted average (TWA).

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