# A numerical method to determine the steady state distribution of passive contaminant in generic ventilation systems

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## ARTICLE INFO

## ABSTRACT

Ventilation system with air recirculation is designed to conserve energy, yet at the same time may result in transporting hazardous substance among different rooms in the same building, which is a concern in indoor air quality control. There is a lack of effective methods to predict indoor contaminant distribution primarily because of uncertainty of the contaminant concentration in supply air which in turn due to the mixing ratio of fresh and recirculation air. In this paper, a versatile numerical method to determine the pollutant distribution of ventilation system with recirculation at steady state is proposed based on typical ventilation systems with accessibility of supply air (ASA) and accessibility of contaminant source (ACS). The relationship is established between contaminant concentrations of supply air and return air in a ventilated room or zone. The concentrations of supply air and contaminant distribution in each room can be determined using such parameters as ASA and ACS. The proposed method is validated by both experimental data and numerical simulation result. The computing speed of the proposed method is compared with the iteration method. The comparisons between the proposed method and the lumped parameter model are also conducted. The advantages of the proposed method in terms of accuracy, speed and versatility make it advantageous to be applied in air quality control of complex ventilation systems with recirculation.

## 1. Introduction

People spend most of their life time, 87% in U.S. as an example indoors and 7% in various types of vehicles [1]. By that measure indoor air quality is a critical element affecting human health and wellbeing [2]. Buildings are especially vulnerable to hazardous substances such as chemical and biological agents, which can severely contaminate the indoor environment once they are released in the building naturally or deliberately [3]. Some extreme cases such as the anthrax attacks (2001), the Severe Acute Respiratory Syndrome (SARS, 2003) and H1N1 Type A influenza (2009) pandemic serve as reminder how important to protect people in buildings by preventing contaminants spreading or re-entrainment.

One of the causes of poor air quality in buildings is their central air handling systems, which act as a carrier and distributor of the hazardous substances [3]. Once a contaminant is released in one room, it may re-enter the recirculation air and transport to other rooms, causing the entire building contaminated. Methods to predict contaminant distributions in multi-zone buildings are in great need for the evaluation of exposure levels and the appropriateness of counter measures for different rooms.

Contaminant distribution in different kinds of ventilation modes has been widely studied [4–8], including experimental investigation and using numerical technique [9–11]. The past studies were focused on single room/zone, where the boundary conditions for contaminant concentration are defined. However, in a multi-zone building where room air handling systems are inter-connected, or a building with several air handling units (AHUs), air is provided to individual rooms with a recirculation loop. In this case, the contaminant in one room or AHU will affect other rooms or AHUs, making the concentration of each supply air uncertain, causing numerical methods to fail to calculate the contaminant distribution.

In order to determine the contaminant distribution in building ventilation systems with recirculation, lumped parameter model is usually used, where full mixing is assumed in individual rooms [12–14]. However, the contaminant distribution is non-uniform, especially for displacement and personalized ventilation [4,5,11]. In this case, the contaminant concentration in exhaust air is not

## Nomenclature

$A_{C,k}^n$　steady state accessibility of contaminant source to the $k$th outlet of the $m$th GAHU in room $n$

$A_{C,p}^n$　steady state accessibility of contaminant source to arbitrary point $p$ in room $n$

$A_{C,p}^n(\tau)$　accessibility of contaminant source to arbitrary point $p$ in room $n$ within time period $\tau$

$A_{Ci,p}(\tau)$　accessibility of the $i$th source to point $p$ within time period $\tau$

$A_{DF,k}^n$　steady state accessibility of direct fresh air to the $k$th outlet of the $m$th GAHU in room $n$

$A_{DF,p}^n$　steady state accessibility of direct fresh air to point $p$ in room $n$

$A_{Sm,k}^n$　steady state accessibility of the $m$th GAHU to the $k$th outlet of the $m$th GAHU in room $n$

$A_{Sk,p}(\tau)$　accessibility of supply air from the $k$th inlet to point $p$ within time period $\tau$

$A_{Sm,p}^n$　steady state accessibility of supply air from the $m$th GAHU to point $p$ in room $n$

$A_{Sm,p}^n(\tau)$　accessibility of supply air from the $m$th GAHU to point $p$ in room $n$ within time period $\tau$

$C_0$　initial contaminant concentration in ventilated space at moment $t=0$ [kg/m$^3$]

$C_{e,i}$　average exhausted contaminant concentration under steady-state conditions only when the $i$th source exists [kg/m$^3$]

$C_e^n$　average exhausted contaminant concentration in room $n$ under steady-state conditions when contaminant source exists [kg/m$^3$]

$C_{od}$　contaminant concentration of outdoor air [kg/m$^3$]

$C_p(t)$　contaminant concentration of point $p$ at moment $t$ [kg/m$^3$]

$C_p^n$　contaminant concentration of point $p$ in room $n$ at steady state [kg/m$^3$]

$C_p^n(t)$　contaminant concentration of point $p$ in room $n$ at moment $t$ [kg/m$^3$]

$\overline{C_p}(\tau)$　average concentration at point $p$ within time period $\tau$ [kg/m$^3$]

$C_{Rm}^T$　total return air concentration of the $m$th GAHU [kg/m$^3$]

$C_{RM}^n$　contaminant concentration at steady state in room $n$ [kg/m$^3$]

$C_{S0}$　contaminant concentration of all direct fresh air inlets [kg/m$^3$]

$C_{S,k}$　contaminant concentration of supply air of the $k$th inlet [kg/m$^3$]

$C_{S,m}$　contaminant concentration of supply air of the $m$th GAHU [kg/m$^3$]

$f_m$　fresh air ratio of the $m$th GAHU

$I$　number of contaminant sources in ventilated space

$K$　number of inlets in ventilated space

$K_m^n$　number of exhaust outlets for the $m$th GAHU in room $n$

$M$　number of GAHUs

$N$　number of independent rooms

$Q$　total air flow rate for the ventilated space [m$^3$/s]

$Q_{Fm}$　fresh air flow rate of the $m$th GAHU [m$^3$/s]

$Q^n$　total air flow rate in room $n$ [m$^3$/s]

$Q_{Rm}^n$　return air flow rate of the $m$th GAHU from room $n$ [m$^3$/s]

$Q_{Rm}$　total return air flow rate of the $m$th GAHU [m$^3$/s]

$Q_{Sm}$　supply air flow rate of the $m$th GAHU [m$^3$/s]

$r_{mk}^n$　ratio of the $k$th outlet air flow rate to $Q_{Rm}^n$

$R_{Rm}^n$　ratio of return air flow rate from room $n$ of the $m$th GAHU to the total return air flow rate of the $m$th GAHU

$S_i$　emission rate of the $i$th contaminant source [kg/s]

$S^n$　total emission rate of contaminant source in room $n$ [kg/s]

$t$　time [s]

*Greek symbols*

$\alpha_m$　coefficients determined by the flow characteristic of the $m$th GAHU

$\beta_m$　coefficients determined by the flow characteristic and contaminant source of the $m$th GAHU

$\delta_m$　coefficient determined by the flow characteristic, contaminant source and cleaning performance of the $m$th GAHU

$\eta_{DF}^n$　cleaning efficiency of contaminant for direct fresh air supply in room $n$

$\eta_m$　cleaning efficiency of the $m$th GAHU to contaminant

$\tau$　time elapsed since moment $t=0$ [s]

equal to average concentration in the room, which may result in substantial discrepancy or even misleading information about the contaminant distribution.

Waters and Simon [15] proposed a method to take the influence of recirculation on contaminant distribution in simple ventilated space into account. Contaminant distributions in typical buildings, such as the building with fan-coil units, fresh air system and recirculation air were investigated by Li et al. [16] and Yang et al. [17]. There is a lack of a versatile method to determine the contaminant distribution in generic buildings with recirculation air. Hiyama et al. [18] proposed an algorithm to calculate the transient contaminant transport using a concentration response factor method. This method can be used to obtain the concentration for some interested locations but the spatial and temporal computation is intensive, making it difficult to be used in real-case evaluation and implementation.

Li et al. [19] has constructed a generic ventilation system which covers many typical existing ventilation systems such as all-air system with air recirculation, fan coil unit (FCU), room air conditioner (RAC) and air cleaner system. In this paper a versatile method to determine the contaminant distribution at steady state is proposed based on the generic ventilation system. In addition, the accuracy and computing speed of the proposed method and the versatility of the lumped parameter model are further discussed.

## 2. Algorithm of contaminant distribution in generic ventilation system

In order to calculate the contaminant distribution in a ventilation system with recirculation, the following assumptions are made to simplify the problem:

(1) The air flow and contaminant are at steady state and the density of air is constant.
(2) The contaminant is passive gas, which has no effect on the flow field.
(3) There is no air leakage in ductwork and the airflow in ductwork is completely mixed.
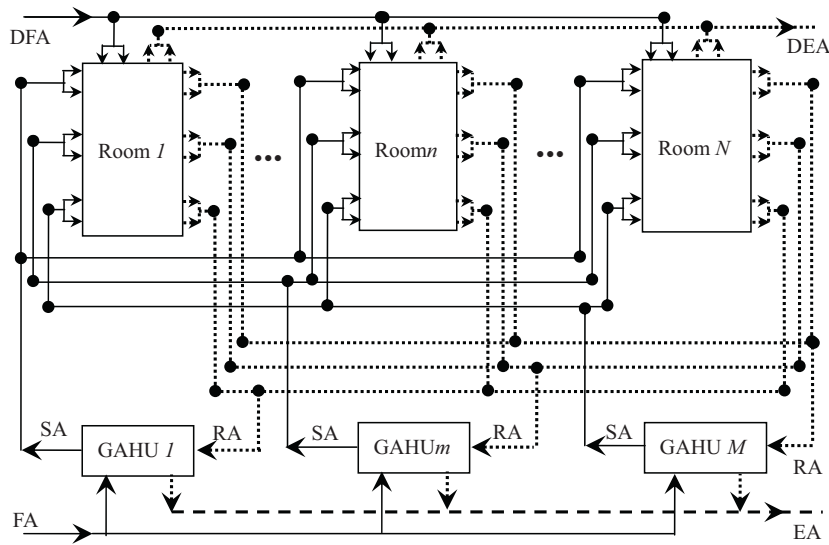
DEA: Direct exhaust air; DFA: Direct fresh air supply; EA: Exhaust air of GAHUs; FA: Fresh air for GAHUs; SA: Supply air of GAHUs; RA: Return air of GAHUs.

**Fig. 1.** Schematic representation of generic ventilation system (by Li et al. [19]).

## 2.1. Description of generic ventilation system

The generic ventilation system constructed by Li et al. [19] consists of three parts, i.e. ventilated rooms, generalized air handling units (GAHUs) and air openings and ductwork connecting rooms with GAHUs (Fig. 1). GAHU is an air handling unit in which return air is handled with or without fresh air mixing. Openings between adjacent spaces such as doors and windows exist in actual buildings to allow the air from one airspace to another. The interacting air flow inevitably transports the contaminant from one airspace to the adjacent airspace. In this case, the interacting air flow between airspaces can be treated as a virtual AHU, as shown in Fig. 2. In this virtual AHU, the interacting air is treated as 'return air' for one airspace and the same air is treated as 'supply air' for the adjacent airspace. No fresh air exists in the virtual AHU. Essentially, the interacting air flow has the same feature as the ventilation system with air recirculation, so it can also be included into the generic ventilation system.

## 2.2. Relation of contaminant distribution with inlet conditions and source in rooms

In developing the method, the geometry, positions and types of inlets and outlets for each GAHU, direct fresh air and exhaust air, and positions and emission rates of contaminant sources are defined. The air flow rates supplied and returned by GAHU, direct fresh air flow rates and direct exhaust air flow rates are also defined.
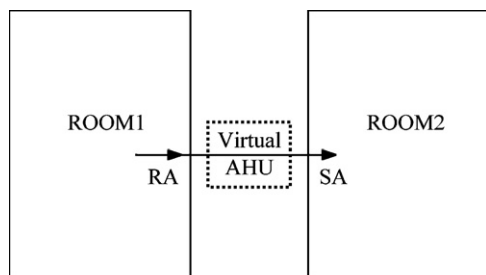


**Fig. 2.** Interacting air flow between rooms in a complex ventilation system.

The contaminant concentration is known for direct fresh air, but is unknown for supply air of GAHU because of utilization of return air. The contaminant concentrations of direct exhaust air and return air of GAHU are unknown because the contaminant distribution is non-uniform and cannot be obtained simply by mass balance. If the concentrations of supply air from GAHUs are known, the contaminant distribution in the room can be calculated using appropriate CFD tools. Yang et al. [20] proposed a formula to correlate contaminant distribution in ventilated rooms with supply air and contaminant sources, which is the basis of the proposed method in this paper.

### 2.2.1. Contaminant distribution in ventilated room with multiple inlets and sources

In order to quantify the effect of supply air and contaminant source on contaminant distribution, Li and Zhao [21] proposed the concept of accessibility of supply air (ASA) and accessibility of contaminant source (ACS). Yang et al. [20] defined the ASA to an arbitrary point $p$ from the $k$th inlet and ACS to an arbitrary point $p$ from the $i$th source as:

$$A_{Sk,p}(\tau) = \frac{\int_0^\tau C_p(t)\,dt}{C_{S,k} \cdot \tau} \tag{1}$$

where $C_{S,k}$ is the contaminant concentration of the $k$th inlet, $C_p(t)$ is the contaminant concentration of point $p$ at moment $t$ when the initial concentration is 0 and all the inlets concentrations are 0 except that the $k$th inlet is $C_{S,k}$.

$$A_{Ci,p}(\tau) = \frac{\int_0^\tau C_p(t)\,dt}{C_{e,i} \cdot \tau} \tag{2}$$

where $C_p(t)$ is the contaminant concentration of point $p$ at moment $t$ when the initial concentration is 0, all the inlets concentrations are 0 and only the $i$th contaminant source exists; $C_{e,i}$ is the average exhausted contaminant concentration under steady-state conditions only when the $i$th source exists:

$$C_{e,i} = \frac{S_i}{Q} \tag{3}$$

where $S_i$ is emission rate of the $i$th contaminant source; $Q$ is the air flow rate in ventilated space.

ASA quantifies how the air from a supply inlet is continuously delivered to an indoor location. It is a function of the flow characteristic regardless of contaminant type and source. ACS quantifies how the contaminant is continuously diffused into an indoor location. It is a function of both the flow characteristic and the source location regardless of emission rate and contaminant type. ASA and ACS can be calculated using CFD tools when the flow field and source position are available [20,21].

When the airflow is at steady state, the concentration of supply air and emission rate of contaminant source are constant and the contaminant can be treated as passive gas, the time weighted average (TWA) concentration at arbitrary indoor point $p$ can be expressed as [20]:

$$\overline{C_p}(\tau) = C_0 + \sum_{k=1}^{K}\{(C_{S,k} - C_0)A_{Sk,p}(\tau)\} + \sum_{i=1}^{I}\left\{\frac{S_i}{Q}A_{Ci,p}(\tau)\right\} \tag{4}$$

### 2.2.2. Contaminant distribution in ventilated rooms with multiple GAHUs and sources

Since the supply air to each room may come from multiple GAHUs and each GAHU in a room may have more than one inlet, it will be complicated to define the accessibility with each inlet as what Yang et al. [20] did. Here we define the accessibility of each GAHU in each room based on Eq. (1):

$$A_{Sm,p}^n(\tau) = \frac{\int_0^{\tau} C_p(t)\,\mathrm{d}t}{C_{S,m}\cdot\tau} \tag{5}$$

where $C_{S,m}$ is the contaminant concentration of $m$th GAHU inlets, $C_p^n(t)$ is the contaminant concentration at moment $t$ when the initial concentration is 0, all the inlets concentrations are 0 except that the inlets of the $m$th GAHU supply contaminant with a concentration $C_{S,m}$ in room $n$. When it is at steady state, the accessibility of the $m$th GAHU to point $p$ in room $n$ becomes:

$$A_{Sm,p}^n = \frac{C_p^n}{C_{S,m}} \tag{6}$$

where $C_p^n$ is the contaminant concentration at steady state when all the inlets concentrations are 0 except that the inlets of $m$th GAHU supply contaminant with a concentration $C_{S,m}$ in room $n$. For all the direct fresh supply inlets, we define their accessibility as:

$$A_{DF,p}^n = \frac{C_p^n}{C_{S0}} \tag{7}$$

where $C_{S0}$ is the contaminant concentration of all direct fresh air inlets, $C_p^n$ is the contaminant concentration of point $p$ at steady state when all the inlets concentrations are 0 except that concentrations at all direct fresh air inlets are $C_{S0}$ in room $n$.

Since we do not investigate the relationship between different contaminant sources, here we take all the contaminant sources in one room as one source. Then the accessibility of the source to arbitrary point $p$ in room $n$ can be defined as:

$$A_{C,p}^n(\tau) = \frac{\int_0^{\tau} C_p^n(t)\,\mathrm{d}t}{C_e^n\cdot\tau} \tag{8}$$

where $C_p^n(t)$ is the contaminant concentration at moment $t$ when the initial concentration is 0, all the inlets concentrations are 0 and the contaminant source exists in room $n$. $C_e^n$ is the average exhausted contaminant concentration in room $n$ under steady-state conditions when the source exists in the room:

$$C_e^n = \frac{S^n}{Q^n} \tag{9}$$

where $S^n$ is the total emission rate of contaminant source in room $n$; $Q^n$ is the total air flow rate in room $n$. When it is at steady state, the accessibility of the source to point $p$ in room $n$ is:

$$A_{C,p}^n = \frac{C_p^n}{C_e^n} \tag{10}$$

where $C_p^n$ is the contaminant concentration at steady state when all the inlets concentrations are 0 and the contaminant source exists in room $n$.

The accessibility of the $m$th GAHU, direct fresh air and the accessibility of the source to arbitrary point $p$ at steady state in room $n$ can be calculated using CFD tools based on Eqs. (6), (7) and (10). The accessibility of the $m$th GAHU will be 0 if the $m$th GAHU does not supply air to room $n$, and the accessibility of the source will be 0 if there is no contaminant source in room $n$. Then the contaminant concentration at arbitrary point $p$ at steady state can be written as:

$$C_p^n = \sum_{m=1}^{M}(C_{S,m}A_{Sm,p}^n) + \frac{S^n}{Q^n}A_{C,p}^n + C_{od}(1 - \eta_{DF}^n)A_{DF,p}^n \tag{11}$$

where $C_p^n$ is the contaminant concentration of point $p$ in room $n$; $C_{S,m}$ is the contaminant concentration of the $m$th GAHU inlets in room $n$; $S^n$ is the total emission rate of contaminant source in room $n$; $Q^n$ is the total air flow rate in room $n$; $C_{od}$ is the contaminant concentration of outdoor air; and $\eta_{DF}^n$ is the cleaning efficiency of contaminant for direct fresh air supply in room $n$ ($0 \le \eta_{DF}^n < 1$).

### 2.2.3. Relation of return air concentration and supply air concentration

In case of multiple and different outlets for the $m$th GAHU in room $n$, the concentration of each outlet can be described by Eq. (11). Assume that there are $K_m^n$ exhaust outlets for the $m$th GAHU in room $n$ and the ratio of the $k$th outlet air flow rate to the return air flow rate $Q_{Rm}^n$ of the $m$th GAHU from room $n$ is $r_{mk}^n$. Then the return air concentration of the $m$th GAHU from room $n$ is:

$$C_{Rm}^n = \sum_{m=1}^{M}\left[C_{S,m}\sum_{k=1}^{K_m^n}(r_{mk}^n A_{Sm,k}^n)\right] + \frac{S^n}{Q^n}\sum_{k=1}^{K_m^n}(r_{mk}^n A_{C,k}^n)$$
$$+ C_{od}(1 - \eta_{DF}^n)\sum_{k=1}^{K_m^n}(r_{mk}^n A_{DF,k}^n) \tag{12}$$

where $A_{Sm,k}^n$ is the accessibility of the $m$th GAHU to the $k$th outlet of the $m$th GAHU in room $n$; $A_{C,k}^n$ is the accessibility of the contaminant source to the $k$th outlet of the $m$th GAHU in room $n$. The total return air concentration of $m$th GAHU is:

$$C_{Rm}^T = \sum_{m=1}^{M}\left\{C_{S,m}\sum_{n=1}^{N}\left[R_{Rm}^n\sum_{k=1}^{K_m^n}(r_{mk}^n A_{Sm,k}^n)\right]\right\}$$
$$+ \sum_{n=1}^{N}\left\{R_{Rm}^n\left[\frac{S^n}{Q^n}\sum_{k=1}^{K_m^n}(r_{mk}^n A_{C,k}^n)\right]\right\}$$
$$+ C_{od}\sum_{n=1}^{N}\left[R_{Rm}^n(1 - \eta_{DF}^n)\sum_{k=1}^{K_m^n}(r_{mk}^n A_{DF,k}^n)\right] \tag{13}$$

where $R_{Rm}^n$ is the ratio of return air flow rate $Q_{Rm}^n$ of the $m$th GAHU from room $n$ to the total return air flow rate $Q_{Rm}$ of the $m$th GAHU, i.e.,

$$R_{Rm}^n = \frac{Q_{Rm}^n}{Q_{Rm}} \tag{14}$$

The total return air concentration of $m$th GAHU can be written simply as:

$$\begin{cases} C_{Rm}^T = \sum_{m=1}^{M}(C_{S,m}\alpha_{m,m}) + \beta_m \\ \alpha_{m,m} = \sum_{n=1}^{N}\left[R_{Rm}^n\sum_{k=1}^{K_m^n}(r_{mk}^n A_{Sm,k}^n)\right] \\ \beta_m = \sum_{n=1}^{N}\left[R_{Rm}^n\frac{S^n}{Q^n}\sum_{k=1}^{K_m^n}(r_{mk}^n A_{C,k}^n)\right] + C_{od}\sum_{n=1}^{N}\left[R_{Rm}^n(1-\eta_{DF}^n)\sum_{k=1}^{K_m^n}(r_{mk}^n A_{DF,k}^n)\right] \end{cases} \quad (15)$$

where $\alpha_{m,m}$ and $\beta_m$ are coefficients determined by the flow characteristic and contaminant source.

### 2.3. Mass balance of return air and supply air in GAHUs

For the $m$th GAHU, the fresh air ratio $f_m$ is defined as:

$$f_m = \frac{Q_{Fm}}{Q_{Sm}} = 1 - \frac{Q_{Rm}}{Q_{Sm}} \quad (16)$$

where $Q_{Fm}$ is the fresh air flow rate of the $m$th GAHU; $Q_{Sm}$ is the supply air flow rate of the $m$th GAHU.

Since return air always exists for GAHU, the range of fresh air ratio is $0 \le f_m < 1$. The contaminant concentration of supply air for the $m$th GAHU can be obtained by the mass balance of contaminant:

$$C_{s,m} = [C_{od}f_m + (1-f_m)C_{Rm}^T](1-\eta_m) \quad (17)$$

where $\eta_m$ is the cleaning efficiency of the $m$th GAHU, $0 \le \eta_m < 1$.

### 2.4. Algorithm of contaminant distribution in generic ventilation system

Substituting Eq. (15) into Eq. (17), we obtain a constraint equation for the contaminant concentration of supply air for each GAHU:

$$\begin{cases} C_{S,m} = (1-f_m)(1-\eta_m)\sum_{m=1}^{M}(C_{S,m}\alpha_{m,m}) + \delta_m \\ \delta_m = [C_{od}f_m + (1-f_m)\beta_m](1-\eta_m) \end{cases} \quad (18)$$

where $\delta_m$ is coefficient determined by the flow characteristics, contaminant source and cleaning performance.

For total $M$ number of GAHUs, there are $M$ unknown contaminant concentrations of supply air in the equations and $M$ equations available. So all the contaminant concentrations of supply air of GAHUs can be solved by the following matrix:

$$\begin{bmatrix} 1-(1-f_1)(1-\eta_1)\alpha_{1,1} & \cdots & -(1-f_1)(1-\eta_1)\alpha_{m,1} & \cdots & -(1-f_1)(1-\eta_1)\alpha_{M,1} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ -(1-f_m)(1-\eta_m)\alpha_{1,m} & \cdots & 1-(1-f_m)(1-\eta_m)\alpha_{m,m} & \cdots & -(1-f_m)(1-\eta_m)\alpha_{M,m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -(1-f_M)(1-\eta_M)\alpha_{1,M} & \cdots & -(1-f_M)(1-\eta_M)\alpha_{m,M} & \cdots & 1-(1-f_M)(1-\eta_M)\alpha_{M,M} \end{bmatrix} \begin{bmatrix} C_{S,1} \\ \vdots \\ C_{S,m} \\ \vdots \\ C_{S,M} \end{bmatrix} = \begin{bmatrix} \delta_1 \\ \vdots \\ \delta_m \\ \vdots \\ \delta_M \end{bmatrix} \quad (19)$$

When the contaminant concentrations of supply air of all GAHUs are available, the contaminant distribution in each room can be calculated using Eq. (11). The procedure for the contaminant distribution in a generic ventilation system can be described as following:

(1) Collect available information including geometry, positions and types of inlets and outlets for each GAHU, positions and types of

inlets and outlets for direct fresh air and exhaust air, positions and emission rates of contaminant sources, air flow rates etc.

(2) Calculate accessibility of each GAHU, direct fresh air and the accessibility of contaminant source to an arbitrary point in each room using Eqs. (6), (7) and (10).

(3) Calculate the contaminant concentrations of supply air of each GAHU using Eq. (19).

(4) Calculate the contaminant distribution using Eq. (11).

### 2.5. Simplified algorithm for single GAHU ventilation system

When a ventilation system has a single GAHU, Eq. (19) can be simplified as:

$$C_{S,1} = \frac{[C_{od}f_1 + (1-f_1)\beta_1](1-\eta_1)}{1-(1-f_1)(1-\eta_1)\alpha_1} \quad (20)$$

This indicates that the contaminant concentration of supply air of the GAHU can be obtained directly by calculating the accessibility of the GAHU and the accessibility of contaminant source, and the contaminant distribution can be obtained using Eq. (11).

## 3. Validation of the proposed method

The proposed method is essentially determined by two factors: the expression of concentration at an arbitrary point in each room (which is related to supply air concentration and emission rate of contaminant source), and the mass balance relationship in each AHU. No matter how complex a ventilation system with air recirculation may be, the calculation method will attribute to the two factors. Therefore, the validation of the proposed method is in nature the validations of the concentration expression in the room and the mass balance relationship in AHU. Obviously, the mass balance must be satisfied, while the expression of concentration at an arbitrary point in the room was also well validated by Yang [20]. Therefore, the reliability of these two expressions should make the proposed method reliable.

To further verify the proposed method based on the above analysis, we conducted both experimental validation and numerical validation of ventilation system with air recirculation. Experimental validation was conducted in a generic ventilation system, while numerical validation was made in a more complex ventilation system.

### 3.1. Experimental validation

A contaminant dispersion experiment was conducted to validate the proposed method. The ventilation system with recirculation consists of a single chamber airspace, an AHU and ductwork

(Fig. 3). The dimension of the chamber is 4 m ($X$) × 2.5 m ($Y$) × 3 m ($Z$). There is only one air inlet (0.2 m × 0.2 m) and one air outlet (0.3 m × 0.2 m) in the chamber. The coordinates of the center points of the inlet and outlet are (0, 2.3, 1.5) and (4, 0.3, 1.5), respectively. A Ping-Pong ball with uniform holes on the surface was adopted as a contaminant source to release $CO_2$ to the room. There was no heat source inside the chamber and all the walls were well insulated during the experiment.
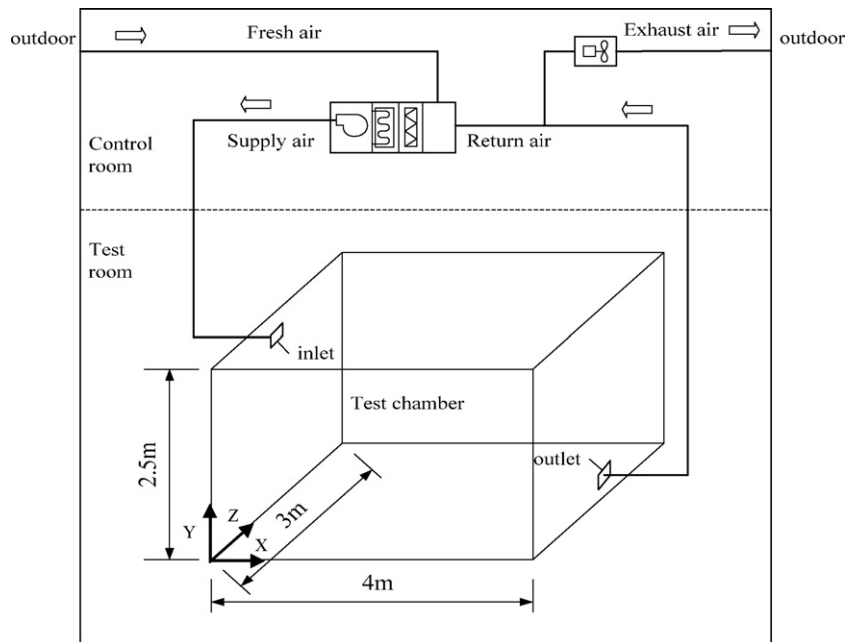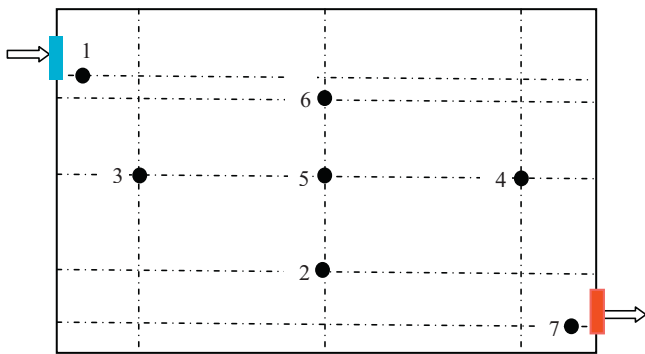
**Fig. 3.** System sketch of measurement.



**Fig. 4.** Test points in the chamber (sectional view).

Two validation cases (Case 1 and Case 2) were conducted at two different contaminant source (the Ping-Pong ball) locations (Table 1). Seven $CO_2$ sensors (No. 1–7, ranging 0–5000 ppm; accuracy ±3%) were placed at different locations in the chamber, and one $CO_2$ sensor (No. 8) was placed at the fresh air inlet (Fig. 4 and Table 2). Prior to the release of $CO_2$ source, the background concentrations are measured for the eight sensors, which will be subtracted from the measured steady state concentrations to obtain the net concentration values caused by the contaminant source. A hot-bulb anemometer (ranging 0–20 m/s; accuracy ±3%) was used to measure the velocity of supply air. A nozzle flow meter in the supply air duct was used to verify the measurement results of the hot-bulb anemometer. The measurement results are shown in Table 3. It can be found that the relative error between two

measurements was 4.75%, indicating a good agreement with each other.

A validated CFD program STACH–3 developed by Li [22] was used as the simulation tool. An indoor zero-equation turbulence model [23] was used to account for the turbulent flow in a room. The Reynolds Averaged Navier-Stokes (RANS) equations, together with averaged energy and mass conservation equations, were discretized using a finite volume method (FVM). The difference scheme is a power law scheme. A SIMPLE algorithm was adopted while momentum equations were solved on non-uniform staggered grids [24]. Through the grid-independence study, the room was discretized by 14,352 structured hexahedral meshes with an average mesh size of around 0.13 m. Based on the experiment information including the room dimension, locations of inlet, outlet and contaminant source and wall insulation, the flow field, the ASA and ACS distributions were simulated by STACH-3. Then the contaminant distribution was calculated based on the proposed method.

**Table 2**
Coordinates of the $CO_2$ sensors.

| Sensor | Coordinates | | |
|---|---|---|---|
| | $X$ (m) | $Y$ (m) | $Z$ (m) |
| 1 | 0.18 | 2.21 | 1.43 |
| 2 | 2.02 | 0.45 | 0.70 |
| 3 | 1.20 | 1.23 | 0.70 |
| 4 | 2.80 | 1.18 | 0.72 |
| 5 | 2.02 | 1.23 | 0.71 |
| 6 | 1.97 | 1.96 | 0.70 |
| 7 | 3.75 | 0.24 | 1.40 |

**Table 1**
The contaminant source for two cases.

| Case | Coordinate of Contaminant Source Center | | | Intensity (L/min) |
|---|---|---|---|---|
| | $X$ (m) | $Y$ (m) | $Z$ (m) | |
| 1 | 1.47 | 0.85 | 1.63 | 2.6 |
| 2 | 2.12 | 0.98 | 2.49 | 2.6 |

**Table 3**
Measurement of air flow rate.

| Air Flow Rate (Hot-bulb Anemometer) | Supply Air (m³/h) | 323.20 |
|---|---|---|
| | Return Air (m³/h) | 353.52 |
| | Fresh Air (m³/h) | 102.40 |
| Air Flow Rate (Nozzle Flowmeter) | Supply Air (m³/h) | 307.84 |
| Relative Error (%) | | 4.75 |
| Fresh Air Ratio (ratio of fresh air flow rate to supply air flow rate) (%) | | 31.68 |

**Table 4**
Relative errors between measurement and proposed method.

| Case | Sensor | Measurement (ppm) | Proposed Method (ppm) | Relative Error (%) | Uncertainty (ppm) |
|---|---|---|---|---|---|
| 1 | 1 | 1146.46 | 1213.56 | 5.85 | 28.50 |
| | 2 | 1488.34 | 1538.43 | 3.37 | 33.91 |
| | 3 | 1821.86 | 1552.52 | (14.78 | 40.40 |
| | 4 | 1524.40 | 1537.09 | 0.83 | 35.61 |
| | 5 | 1636.93 | 1535.74 | (6.18 | 38.63 |
| | 6 | 1572.36 | 1555.21 | (1.09 | 35.33 |
| | 7 | 1579.86 | 1633.07 | 3.37 | 36.41 |
| 2 | 1 | 1021.32 | 1126.30 | 10.28 | 26.52 |
| | 2 | 1451.93 | 1450.50 | (0.10 | 33.21 |
| | 3 | 1557.66 | 1494.13 | (4.08 | 35.96 |
| | 4 | 1452.26 | 1437.74 | (1.00 | 33.30 |
| | 5 | 1567.64 | 1443.79 | (7.90 | 37.21 |
| | 6 | 1479.56 | 1465.94 | (0.92 | 32.54 |
| | 7 | 1455.15 | 1655.22 | 13.75 | 34.16 |

**Table 5**
Coordinates of room air openings in the numerical validation case.

| Object | | Start Point | | | End Point | | |
|---|---|---|---|---|---|---|---|
| | | $X$ (m) | $Y$ (m) | $Z$ (m) | $X$ (m) | $Y$ (m) | $Z$ (m) |
| Inlet | S1 | 1.4 | 3 | 1.4 | 1.6 | 3 | 1.6 |
| | S2 | 4.4 | 3 | 1.4 | 4.6 | 3 | 1.6 |
| | S3 | 7.4 | 3 | 1.4 | 7.6 | 3 | 1.6 |
| | S4 | 10.4 | 3 | 1.4 | 10.6 | 3 | 1.6 |
| Outlet | R1 | 1.4 | 3 | 4.4 | 1.6 | 3 | 4.6 |
| | R2 | 4.4 | 3 | 4.4 | 4.6 | 3 | 4.6 |
| | R3 | 7.4 | 3 | 4.4 | 7.6 | 3 | 4.6 |
| | R4 | 10.4 | 3 | 4.4 | 10.6 | 3 | 4.6 |

**Table 6**
System parameters of the numerical validation case.

| | | |
|---|---|---|
| Emission Rate (mg/s) | Source 1 | 5 |
| | Source 2 | 5 |
| Fresh Air Ratio | AHU 1 | 0.2 |
| | AHU 2 | 0.3 |
| | AHU 3 | 0.4 |
| Efficiency of Fresh Air Cleaner | | 0.4 |
| Efficiency of Each AHU Cleaner | | 0.4 |
| Concentration of Outdoor Air (mg/kg) | | 5 |

The validation details of the simulated velocity field using STACH-3 can be found in references [25,26]. The following is the comparison results of concentration distribution (Table 4).

Case 1 and Case 2 are different in both experiment and simulation. The main reason is that the contaminant source locations are different in the two cases, which causes different effect of source on the concentration at each sensor position. From the results comparison, It can be found that for Case 1, the relative difference of test points with maximum absolute is −14.78% and 0.83% for minimum absolute; while for Case 2, the relative difference of test points with maximum absolute is 13.75% and −0.10% for minimum absolute. The averaged absolute of relative differences for the two cases are 5.02% and 5.43% respectively, which indicates an acceptable agreement between two approaches for the ventilation system in this experiment.

### 3.2. Numerical validation

The numerical simulation validation is based on the system shown in Fig. 5. The dimension of the room is $12\,\text{m}$ $(L) \times 3\,\text{m}$ $(H) \times 6\,\text{m}$ $(W)$. All the walls were well insulated. The air change rate was 5.33 ACH. Two contaminant sources were located in the room with the positions (3,1,3) and (9,1,3) respectively. The coordinates of the inlets and outlets are shown in Table 5 and the detailed parameters used in the simulation are shown in Table 6.

The numerical iteration method was adopted [27], which goes through the following steps: First, set the initial concentrations of supply air (generally set zero) and conduct the CFD simulations for each room in the ventilation system to obtain the return air concentrations; Second, in each AHU, use the mass balance relationship among return air, fresh air and supply air to solve the supply air concentrations. Until now, the first iteration including CFD simulations and calculation of supply air concentration has been finished. Then update the initial values of supply air concentration by the newly obtained values and again conduct the CFD simulations to obtain the new supply air concentration values for the next iteration. After
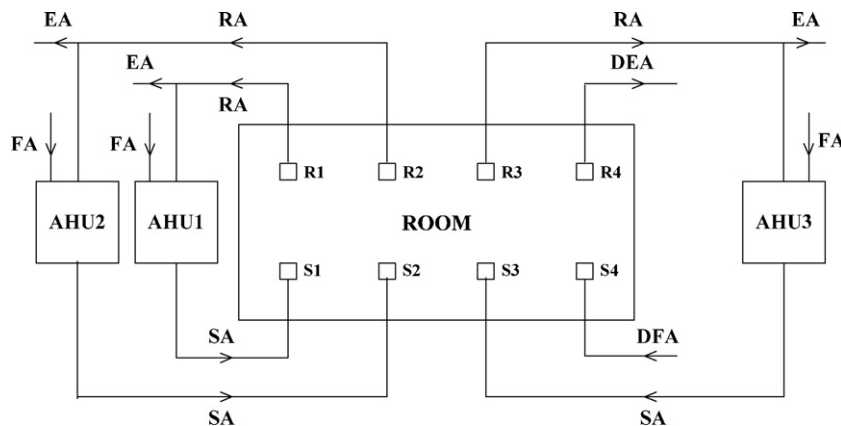


**Fig. 5.** System sketch of the numerical validation case.

**Table 7**
Comparison of concentrations calculated by proposed method and iteration method.

| Method | Concentration of Supply Air (mg/kg) | | | Volume-averaged concentration (mg/kg) |
|---|---|---|---|---|
| | AHU1 | AHU2 | AHU3 | |
| Proposed Method | 25.2409 | 17.9281 | 13.9760 | 35.84 |
| Iteration Method | 25.2336 | 17.9268 | 13.9764 | 35.84 |
| Relative Error (%) | 0.02892 | 0.00725 | 0.00286 | 0.00 |

a certain number of iterations, the supply air concentrations for each room will converge to the final contaminant distribution values.

The validation case was calculated by both iteration method and proposed method and the results are shown in Fig. 6. It can be seen that the concentration distributions are almost the same. Table 7 further compares the concentrations of three AHUs and room mean
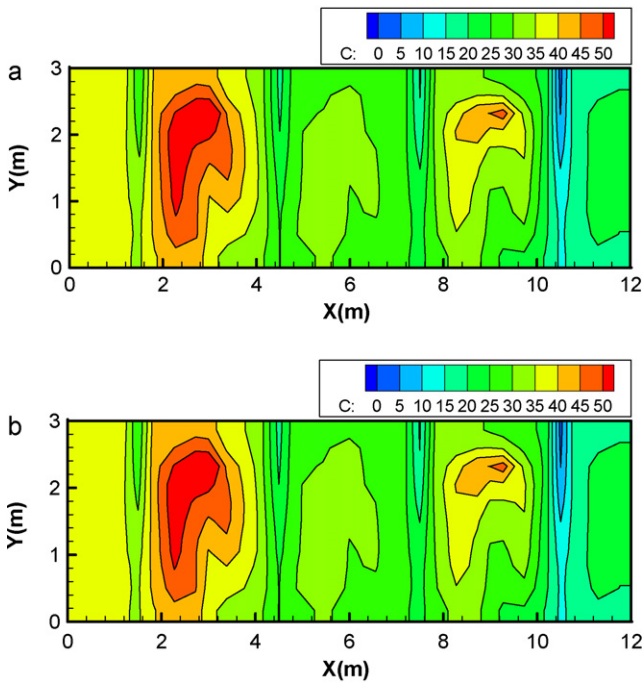


**Fig. 6.** Contaminant distribution at plane Z = 1.5 m: (a) by proposed method, (b) by iteration method.
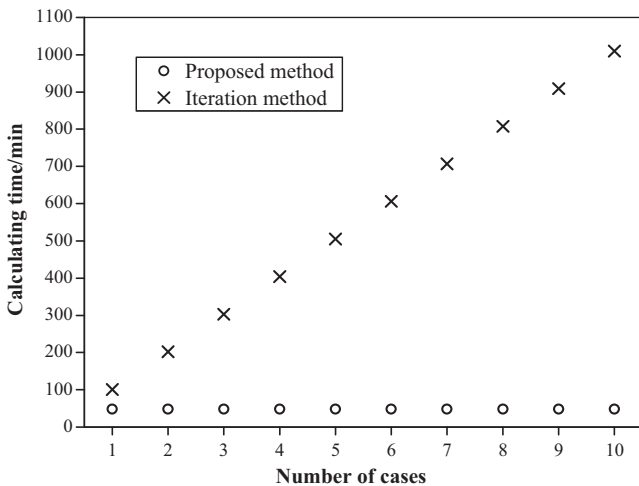


**Fig. 7.** Comparison of the time consuming between proposed method and iteration method.

**Table 8**
Concentrations of all the supply air inlets for each iteration step by iteration method.

| Step | Start Concentration (mg/kg) | | | End Concentration (mg/kg) | | |
|---|---|---|---|---|---|---|
| | $C_{S1}$ | $C_{S2}$ | $C_{S3}$ | $C_{S1}$ | $C_{S2}$ | $C_{S3}$ |
| 1 | 0 | 0 | 0 | 14.827 | 10.778 | 9.296 |
| 2 | 14.827 | 10.778 | 9.296 | 21.019 | 15.138 | 12.230 |
| 3 | 21.019 | 15.138 | 12.230 | 23.544 | 16.831 | 13.300 |
| 4 | 23.544 | 16.831 | 13.300 | 24.562 | 17.494 | 13.710 |
| 5 | 24.562 | 17.494 | 13.710 | 24.965 | 17.755 | 13.872 |
| 6 | 24.965 | 17.755 | 13.872 | 25.128 | 17.860 | 13.933 |
| 7 | 25.128 | 17.860 | 13.933 | 25.190 | 17.902 | 13.958 |
| 8 | 25.190 | 17.902 | 13.958 | 25.214 | 17.914 | 13.969 |
| 9 | 25.214 | 17.914 | 13.969 | 25.224 | 17.923 | 13.973 |
| 10 | 25.224 | 17.923 | 13.973 | 25.229 | 17.923 | 13.973 |
| 11 | 25.229 | 17.923 | 13.973 | 25.234 | 17.927 | 13.973 |
| 12 | 25.234 | 17.927 | 13.973 | 25.234 | 17.927 | 13.976 |
| 13 | 25.234 | 17.927 | 13.976 | 25.234 | 17.927 | 13.976 |

**Table 9**
System parameters of the ventilation system illustrated in Fig. 8.

| Emission Rate (mg/s) | Room 1 | Source 1 | 5 |
|---|---|---|---|
| | | Source 2 | 5 |
| | Room 2 | Source 1 | 2.5 |
| | | Source 2 | 2.5 |
| Fresh Air Ratio of AHU | | | 0.3 |
| Efficiency of Each Fresh Air Cleaner | | | 0.4 |
| Efficiency of AHU Cleaner | | | 0.4 |
| Concentration of Outdoor Air (mg/kg) | | | 5 |

concentration. The relative differences between the two methods are nearly zero, which indicates that the proposed method has the same accuracy as the iteration method.

From the theoretical analysis and further validations, it can be concluded that the proposed method is reliable in predicting the contaminant distribution in complex ventilation system with recirculation.

## 4. Discussion

### 4.1. Computing speed of the proposed method

A main advantage of the proposed method is the reduction in computing time. Here the computing speed of the proposed method is compared with the iteration method, which is also based on the case in Fig. 5. In this case, the proposed method only needs 48 min (CPU: Intel Pentium(R) Dual, 3.00 GHz) and 5 simulations: accessibility distribution of AHU 1, accessibility distribution of AHU 2, accessibility distribution of AHU3, accessibility distribution of direct fresh air and accessibility distribution of whole contaminant source. While the iteration method will need 101 min CPU time and 12 simulations (Table 8). Fig. 7 shows the computing time consumption change with case number. As the case number increases (e.g. changes of emission rate of contaminant source, concentration of direct fresh air or the ratio of fresh air), the proposed method will still only need 5 simulations to obtain the accessibility indices and consume the same 48 minutes. The following calculation of sup-
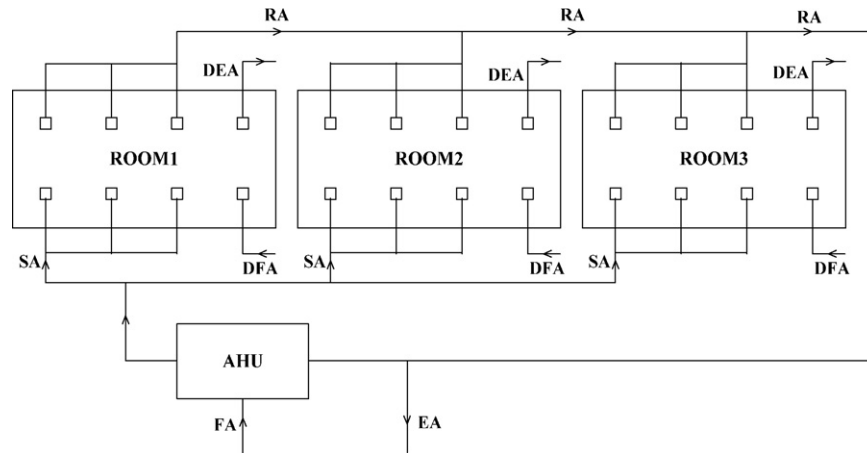
Fig. 8. System sketch of one AHU for multiple rooms.

ply air concentration and final concentration distribution (by Eqs. (19) and (11)) will hardly need time. But for the iteration method, the computing time will increase in proportion with the increase of case number, because it is necessary to do the CFD simulations repeatedly when boundary condition changes. Since it is inevitable to do a large number of case simulations when contaminant dispersion features are studied in a complex building, the proposed method can be much more efficient than the iteration method.
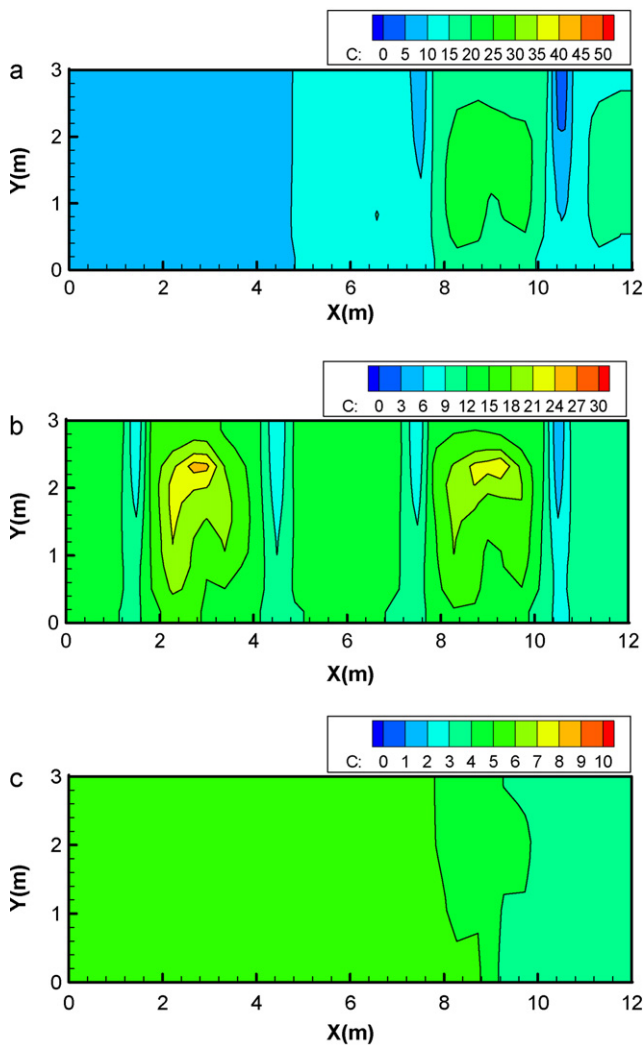


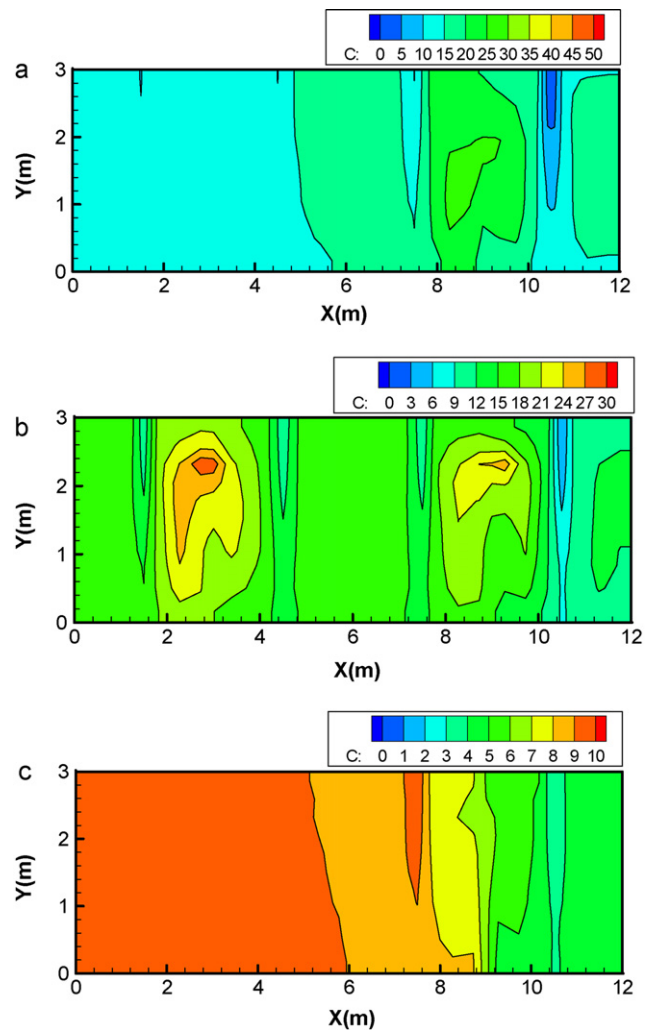Fig. 9. Contaminant distribution by proposed method ($Z = 1.5$ m): (a) Room 1, (b) Room 2, (c) Room 3.

Fig. 10. Contaminant distribution by lumped parameter model ($Z = 1.5$ m): (a) Room 1, (b) Room 2, (c) Room 3.

## 4.2. Comparison with the lumped parameter model

In calculating contaminant distribution in ventilation systems with recirculation, lumped parameter model [28] is often used to build up the relationship between return air concentration and boundary conditions of supply air inlets and sources, which can be used to solve the unknown supply air concentration integrated with the mass balance of return air, fresh air and supply air in GAHUs. After obtaining the supply air concentrations of all GAHUs, all the boundary conditions are known for each room, so the final contaminant distributions of all the rooms can be simulated. However, the real indoor environment is not fully mixed and the real concentration of return air or exhaust air is different from the average concentration in the room, which may result in discrepancy between the calculated supply air concentration and the real value and further influence the finally simulated results. One comparison case is conducted between the proposed method and the lumped parameter model (Fig. 8). Each room in this case has the same structure as that in Fig. 5. There are two contaminant sources in Room 2 with the same locations as those in Fig. 5. While in Room 1 the coordinates of the two sources are (10.5, 2.85, 4.5) and (9, 1, 3), respectively. No contaminant source exists in Room 3. The detailed parameters are listed in Table 9.

Contaminant distributions are calculated using both the proposed method and lumped parameter model. The obtained supply air concentrations are 9.9713 and 5.8868 mg/kg, respectively. The final contaminant distributions from both methods are illustrated in Figs. 9 and 10. It can be seen that the contaminant distribution by the lumped parameter model is different from that by the proposed method, especially the distributions in Room 1 and Room 3. In Room 1 both two sources are located in the right area, so they have relatively smaller influence on the left area. In this situation, the effect of supply air concentrations on the concentration distribution of the left area is dominant. While in Room 3, no contaminant source exists and the only pollution factor is the supply air concentration. Therefore, different results in Room 1 and Room 3 show the difference of calculated supply air concentrations between proposed method and lumped parameter model.

From this case, it indicates that sometimes the calculation by the lumped parameter model may cause large discrepancy and the result can be impractical. A primary reason for the large discrepancy is that the lumped parameter method supposes the concentrations in all return air outlets in one room are the same, but real return air concentrations are different because of the non-uniform feature in the room. The deviation in the assumption of return air concentration from the real situation will cause different calculated supply air concentrations, and further result in large discrepancy between the proposed method and lumped parameter model. Therefore, it is suggested that lumped parameter model be not employed unless the users are sure that the discrepancy between lumped parameter model and proposed method is small enough.

The objective of this proposed method is to solve the incapability or low speed of traditional CFD method in calculating complex ventilation systems with air recirculation. The assumptions of steady flow field and passive contaminant constitute the applicable conditions (and limitations) of the proposed method. In most HVAC systems the airflow doesn't fluctuate dramatically and can be considered as steady-state, and the contaminant concentration is usually low enough to be treated as passive contaminant. Therefore, the proposed method can have a large application potential.

The accuracy of the proposed method depends on two parts. The first part is the accuracy of the proposed method with respect to the traditional CFD method. This is determined by the satisfaction level of the real case to the assumptions of the proposed method. No matter what kind of ventilation system is calculated, the differ-ence between the proposed method and CFD method will be small enough if the assumptions can be well satisfied (as in the validation case). The second part is the accuracy of the CFD method with respect to the real case. Since the crucial indices such as ASA and ACS in the proposed method are calculated using the CFD method, the accuracy of CFD simulation will influence the accuracy of the proposed method. The accuracy of CFD method is influenced by the simplification degree of each kind of boundary condition and the accuracy of the adopted turbulence model, which are the problems to solve for the CFD method itself. The higher the accuracy of CFD method is, the higher the accuracy of the proposed method will be.

## 5. Conclusion

A numerical method to calculate the contaminant distribution at steady state is developed based on generic ventilation system. The steady state distribution of contaminant concentration is determined for each room based on the ASA of each GAHU and ACS of the whole contaminant source. The return air concentration of each GAHU is then related to the supply air concentrations of GAHUs. With the mass balance of contaminant in each GAHU, there are $M$ constraint equations for $M$ supply air concentrations of GAHUs. All the supply air concentrations of GAHUs can be obtained with linear equations and the distribution of contaminant concentration can be determined with the ASA of each GAHU and ACS of the whole contaminant source.

The proposed method is validated by both experimental and numerical methods. It is shown that the proposed method has comparable accuracy with the experiment and numerical simulation to predict the contaminant distribution in ventilation systems with recirculation at steady state.

The proposed method is also compared with the iteration method and the lumped parameter model. It is shown that the proposed method may be much more time-saving even for one case calculation. As the number of cases to be calculated under the same flow field increases, the proposed method will save more computing time. The lumped parameter model does not take the information of the source location and flow pattern into account, so it may cause large discrepancy with the real values. The advantages of the proposed method in terms of accuracy, speed and versatility make it possible to be widely applied for complex ventilation systems with recirculation.

## References

[1] L. Wallace, Indoor particles: a review, J. Air Waste Manage. 46 (1996) 98–126.
[2] J.D. Spengler, K. Sexton, Indoor air pollution: a public health perspective, Science 221 (4605) (1983) 9–17.
[3] Y. Chen, J. Wen, Sensor system design for building indoor air protection, Build. Environ. 43 (7) (2008) 1278–1285.
[4] P. Heiselberg, Room air and contaminant distribution in mixing ventilation, ASHRAE Trans. 102 (2) (1996) 332–339.
[5] A.K. Melikov, R. Cermak, M. Majar, Personalized ventilation: evaluation of different air terminal devices, Energy Build. 34 (8) (2002) 829–836.
[6] R. Cermak, M. Majar, A.K. Melikov, Improved quality of inhaled air with personalized ventilation, in: Proceedings of Indoor Air 2002, Monterey, CA, 2002, pp. 1054–1059.
[7] N. Kobayashi, Q. Chen, Floor-supply displacement ventilation in a small office, Indoor Built Environ. 12 (4) (2003) 281–292.
[8] X. Yang, S. Jelena, X. Li, G. He, Performance of three air distribution systems in VOC removal from an area source, Build. Environ. 39 (11) (2004) 1289–1299.

[9] H. Brohus, P.V. Nielsen, Contaminant distribution around persons in rooms ventilated by displacement ventilation, in: Roomvent 94: Air Distribution in Rooms, 1994, pp. 294–312.

[10] T. Hayashi, Y. Ishizu, S. Kato, S. Murakami, CFD analysis on characteristics of contaminated indoor air ventilation and its application in the evaluation of the effects of contaminant inhalation by a human occupant, Build. Environ. 37 (3) (2002) 219–230.

[11] Q. Chen, L. Glicksman, System performance evaluation and design guidelines for displacement ventilation, in: ASHRAE, Atlanta GA, 2003.

[12] Annex 23, Multizone air flow modelling, COMIS 3.0 with IISiBat User Manual, 31st October, IEAECBCS Annex 23, 1997.

[13] W.S. Dols, G.N. Walton, CONTAMW 1.0 User Manual, NISTIR 6476, in: National Institute of Standards and Technology, 2000.

[14] E.F. Helmut, COMIS—an international multizone air-flow and contaminant transport model, LBNL-42182, 1998.

[15] J.R. Waters, M.W. Simon, The effect of recirculation on ventilation effectiveness parameters, in: Roomvent 2000: Air Distribution in Rooms, 2000, pp. 913–918.

[16] X. Li, B. Meng, J. Yang, B. Zhao, Distribution of the contaminant concentration in rooms with fan-coil units and fresh air supplies, J. Tsinghua Univ. (Sci. Technol.) 44 (6) (2004) 770–773 (in Chinese).

[17] J. Yang, X. Li, B. Meng, B. Zhao, Algorithm for quickly calculating the pollutant distribution in central ventilation systems, J. Tsinghua Univ. (Sci. Technol.) 44 (6) (2004) 774–777 (in Chinese).

[18] K. Hiyama, Y. Ishida, S. Kato, Coupling 3d transient pollutant transport in a room into a flow network model with concentration response factor method, ASHRAE Trans. 114 (Part 2) (2008) 119–129.

[19] X. Li, H. Cai, R. Li, Y. Zhao, X. Ma, X. Shao, A theoretical model to calculate the distribution of air age in general ventilation system, Build. Serv. Eng. Res. T., in press.

[20] J. Yang, X. Li, B. Zhao, Prediction of transient contaminant dispersion and ventilation performance using the concept of accessibility, Energy Build. 36 (2004) 293–299.

[21] X. Li, B. Zhao, Accessibility: a new concept to evaluate the ventilation performance in a finite period of time, Indoor Built Environ. 13 (4) (2004) 287–293.

[22] X. Li, The application of CFD method in HVAC, Master thesis, Tsinghua University, China, 1995 (in Chinese).

[23] Q. Chen, W. Xu, A zero-equation turbulence model for indoor air flow simulation, Energy Build. 28 (1998) 137–144.

[24] B.E. Launder, D.B. Spalding, The numerical computation of turbulent flows, Comput. Method. Appl. Math. 3 (1974) 269–289.

[25] B. Zhao, X. Li, Q. Yan, A simplified system for indoor airflow simulation, Build. Environ. 38 (4) (2003) 543–552.

[26] J. Chen, Study on contaminant dispersion in ventilated space and its application in emergency ventilation, Ph.D. thesis, Tsinghua University, China, 2007 (in Chinese).

[27] J. Yang, Study on indoor air supply effectiveness and contaminant dispersion characteristics, Ph.D. thesis, Tsinghua University, China, 2004 (in Chinese).

[28] Y. Zhu, Y. Zhang, X. Li, Y. Qin, Q. Zhan, Built Environment, second ed., China Machine Press, Beijing, 2005 (in Chinese).