

Prediction Method of Steady Concentration of Passive Contaminant in Ventilation System with Air Recirculation: Contaminant released in the air duct

Yu Liu, Yemin Liu, and Xiaoliang Shao*

School of Civil and Resource Engineering, University of Science and Technology Beijing, Beijing 100083, China

Abstract. When the hazardous substances are released in the air duct of the ventilation system, they are transported into the room through the supply air inlets, causing harm to indoor personnel. In the ventilation system with air recirculation, the contaminant entering the room is recirculated to the ventilation system through the return air outlet, and then affects the contaminant concentration in supply air, making it difficult to be determined. In this work, a method is proposed to predict the steady concentration of passive contaminant when the contaminant is released in the air duct. The method is based on the fixed flow field in the room. The lumped parameter method is utilized to establish the relationship between the concentrations of contaminant in the inlet and outlet for each air duct and the air handling unit. The linear superposition relationship based on the accessibility index is adopted for the steady concentration at an arbitrary position in the room. The proposed method is compared with the prediction with the lumped parameter method in the room. It can rapidly predict the contaminant distributions in all the rooms supplied by the ventilation system with air recirculation.

1 Introduction

People spend more than 90% of their time indoors^[1,2]. They are highly vulnerable to the contaminants in the room. In addition to the formaldehyde emitted by furniture, PM2.5 and other contaminants, indoor environment is also vulnerable to toxic chemicals and biological substances, for example, the Moscow theatre hostage incident in 2002.

Li et al.^[3] proposed a numerical method to predict the steady state distribution of passive contaminant, using the concepts of accessibility of supply air and accessibility of contaminant source which can quantify the three-dimensional distribution of contaminants. The linear superposition expression of contaminant distribution in room was constructed by these two concepts, and the relationship between the concentration of supply air and return air in each room can be obtained by this expression. Combined with the mass conservation relationship, the concentration of supply air can be calculated. This method can obtain the contaminant distribution quickly and accurately by a limited number of simulations, instead of the complex modelling of the duct system and the long-term CFD (computational fluid dynamics) simulation process. In addition to the scene that the contaminant sources are indoors, the contaminant sources might also exist in the ventilation ducts. For example, terrorists might

release toxic gas in the ventilation duct during a terrorist attack. Pease et al.^[4] studied the mathematical model of contaminant concentration in rooms and ducts based on the lumped parameter method, wherein one air handling unit supplies multiple rooms. Gao et al.^[5] constructed an advection diffusion model and a node model to calculate the agent transport in the air ducts when biological or chemical agents were suddenly released into the ducts. This model helped to determine the exact time that the agent arrived at a certain location after a puff release. At present, the contaminant distribution in room under different connection forms between air handling units and rooms when contaminant sources exist in duct has not been fully studied. Most of the studies are focused on the duct, or the connected rooms are considered as well-mixed. In this study, a prediction method of the non-uniform steady concentration of passive contaminant in rooms under different connection forms when there are contaminant sources in different position of the duct was proposed. This method was compared with lumped parameter method and the results for different source locations were analyzed.

* Corresponding author: shaoxl@ustb.edu.cn

2 Prediction method of contaminant distribution in room

The proposed method was constructed based on the generic ventilation system as shown in Fig.1 [3]. The system consists of three parts: ventilated rooms, generalized air handling units (GAHUs) and duct system. GAHU is an air handling unit in which return air is handled with or without fresh air mixing. There are M GAHUs and the supplied N rooms, and different connection forms can be achieved by changing the value of M and N.

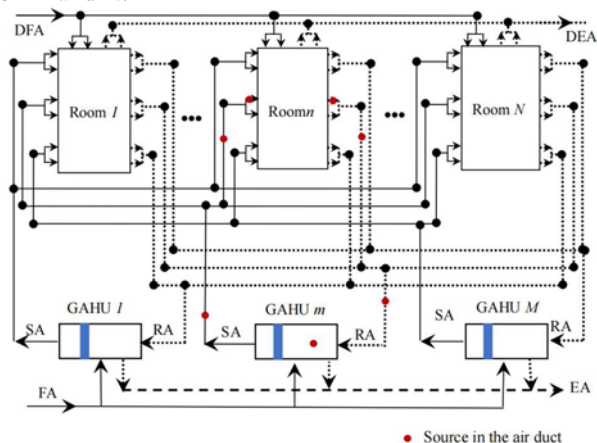


Fig. 1. Generic ventilation system [3].

2.1 Contaminant distribution in the room

In order to obtain the accurate three-dimensional passive contaminant distribution in the room, the concept of accessibility was used. The steady concentration at an arbitrary p was defined as [3]:

$$C_p = \sum_{k=1}^K [C_{S,k} A_{S,k,p}] + \sum_{i=1}^I \left[\frac{S_i}{Q} A_{Cl,p} \right] \quad (1)$$

where C_p is the contaminant concentration of point p . Then the concentration at the k th return air outlet from the m th GAHU in room n can be written as:

$$C_{Rm,k}^n = \sum_{m=1}^M \sum_{j=1}^{J_m^n} C_{Sm,j}^n A_{Sm,jk}^n + C_{od} A_{DFm,k}^n (1 - \eta_{DF}^n) \quad (2)$$

where $A_{Sm,jk}^n$ is the accessibility of the j th inlet of the m th GAHU in the n th room to the k th outlet; $A_{DFm,k}^n$ is the accessibility of the direct fresh air inlet to k th outlet of the m th GAHU in the n th room; η_{DF}^n is the cleaning efficiency of contaminant for direct fresh air supply in room n .

2.2 Relationship between supply and return air concentration in ventilation duct

Assume that there are contaminant sources in the main supply and main return air ducts, branch ducts and GAHUs of the ventilation system, as shown in Fig.1. The ventilation system is divided into five parts: return air ducts, GAHUs, main supply air ducts, supply air branch

ducts of the room, and supply air branch ducts of the supply air inlet. Assume that there are J_m^n inlets and k_m^n outlets from the m th GAHU in the n th room. For the return air duct from the outlet of the room to the GAHU after exhaust air outlet and before fresh air inlet, the mass conservation relation is:

$$C_{Rm} Q_{Rm} = \sum_{n=1}^N \sum_{k=1}^{K_m^n} C_{Rm,k}^n Q_{Rm,k}^n + \sum_{n=1}^N \sum_{k=1}^{K_m^n} S_{Rm,k}^n + \sum_{n=1}^N S_{Rm}^n + S_{Rm}^T - C_{em} Q_{em} \quad (3)$$

where $Q_{Rm,k}^n$ is the air flow rate of the k th outlet in the n th room from the m th GAHU; C_{Rm} is the inlet concentration of the m th GAHU; Q_{Rm} is the air flow rate after exhaust air and before fresh air of the m th GAHU; $C_{Rm,k}^n$ is the return air concentration of the k th outlet in the n th room from the m th GAHU; $S_{Rm,k}^n$ is the emission rate of the source in the return air branch duct of the k th outlet of the m th GAHU in the n th room; S_{Rm}^n is the emission rate of the source in the return air branch duct of the n th room; S_{Rm}^T is the emission rate of the source in the main return air duct; C_{em} and Q_{em} are the concentration and air flow rate of the exhaust air, respectively:

$$C_{em} = \frac{\sum_{n=1}^N \sum_{k=1}^{K_m^n} C_{Rm,k}^n Q_{Rm,k}^n + \sum_{n=1}^N \sum_{k=1}^{K_m^n} S_{Rm,k}^n + \sum_{n=1}^N S_{Rm}^n + S_{Rm}^T}{Q_{Rm}^T} \quad (4)$$

For the GAHUs, the mass conservation relation is:

$$C_{Sm} Q_{Sm} = (C_{Rm} Q_{Rm} + C_{od} Q_{odm} + S_m)(1 - \eta_m) \quad (5)$$

where C_{Sm} and Q_{Sm} are the outlet concentration and air flow rate of m th GAHU, respectively; C_{od} and Q_{odm} are the outdoor air concentration and fresh air flow rate of the m th GAHU; S_m is the emission rate of the source in the m th GAHU; η_m is the cleaning efficiency of the m th GAHU.

For the main supply air duct, the mass conservation relation is:

$$C_{Sm} Q_{Sm} + S_{Sm}^T = C_{Sm}^T Q_{Sm} \quad (6)$$

where S_{Sm}^T is the emission rate of the contaminant source in the main supply air duct of the m th GAHU; C_{Sm}^T and Q_{Sm} are the concentration and air flow rate of the main supply air duct of the m th GAHU, respectively.

For the n th supply air branch duct of the m th GAHU, the mass conservation relation is:

$$C_{Sm}^T Q_{Sm}^n + S_{Sm}^n = C_{Sm}^n Q_{Sm}^n \quad (7)$$

where C_{Sm}^n and Q_{Sm}^n are the concentration and air flow rate of the supply air branch duct, respectively.

For the j th supply air branch duct of the n th room, the mass conservation relation is:

$$C_{Sm}^n Q_{Sm,j}^n + S_{Sm,j}^n = C_{Sm,j}^n Q_{Sm,j}^n \quad (8)$$

where $C_{Sm,j}^n$ and $Q_{Sm,j}^n$ are the concentration and the air flow rate of the supply air branch duct, respectively. Substituting Eq. (3) – Eq. (7) to Eq. (8), the relation of supply and return air concentration can be obtained by Eq. (9):

$$C_{Sm,j}^n = \left[\sum_{n=1}^N \sum_{k=1}^{K_m^n} C_{Rm,k}^n r_{Rm,k}^n (1-f_m) + \frac{\sum_{n=1}^N \sum_{k=1}^{K_m^n} S_{Rm,k}^n}{Q_{Rm}^T} (1-f_m) + \frac{\sum_{n=1}^N S_{Rm}^n}{Q_{Rm}^T} (1-f_m) + \frac{S_{Rm}^T}{Q_{Rm}^T} (1-f_m) + C_{od} f_m + \frac{S_m}{Q_{Sm}} \right] (1-\eta_m) + \frac{S_{Sm}^T}{Q_{Sm}} + \frac{S_{Sm}^n}{Q_{Sm}^n} + \frac{S_{Sm,j}^n}{Q_{Sm,j}^n} \quad (9)$$

The return air concentration can be obtained by Eq. (2). Substituting Eq. (2) to Eq. (9), the constraint equation for the contaminant concentration of supply air for each inlet

can be obtained by Eq. (10), and all the unknown supply air concentrations can be solved by the following matrix (Eq. (11)):

$$C_{Sm,j}^n = (1-f_m)(1-\eta_m) \sum_{n=1}^N \sum_{p=1}^M \sum_{j=1}^{J_m^n} (C_{Sp,j}^n \alpha_{mp,j}^n) + \delta_{m,j}^n$$

$$\left\{ \begin{aligned} \alpha_{mp,j}^n &= \sum_{k=1}^{K_m^n} r_{Rp,k}^n A_{Sp,jk}^n \\ \delta_{m,j}^n &= \left[\sum_{n=1}^N \sum_{k=1}^{K_m^n} C_{od} A_{DFm,k}^n (1-\eta_{DF}) r_{Rm,k}^n + \frac{\sum_{n=1}^N \sum_{k=1}^{K_m^n} S_{Rm,k}^n}{Q_{Rm}^T} + \frac{\sum_{n=1}^N S_{Rm}^n}{Q_{Rm}^T} + \frac{S_{Rm}^T}{Q_{Rm}^T} \right] (1-f_m)(1-\eta_m) + \\ &C_{od} f_m (1-\eta_m) + \frac{S_m}{Q_{Sm}} (1-\eta_m) + \frac{S_{Sm}^T}{Q_{Sm}} + \frac{S_{Sm}^n}{Q_{Sm}^n} + \frac{S_{Sm,j}^n}{Q_{Sm,j}^n} \end{aligned} \right. \quad (10)$$

$$\begin{bmatrix} 1-(1-f_1)(1-\eta_1)\alpha_{11,1}^1 & \cdots & -(1-f_1)(1-\eta_1)\alpha_{m1,j}^n & \cdots & -(1-f_1)(1-\eta_1)\alpha_{M1,J_M^N}^N \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ -(1-f_m)(1-\eta_m)\alpha_{1p,1}^1 & \cdots & 1-(1-f_m)(1-\eta_m)\alpha_{mp,j}^n & \cdots & -(1-f_m)(1-\eta_m)\alpha_{Mp,J_M^N}^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -(1-f_M)(1-\eta_M)\alpha_{1M,1}^1 & \cdots & -(1-f_M)(1-\eta_M)\alpha_{mM,j}^n & \cdots & 1-(1-f_M)(1-\eta_M)\alpha_{MM,J_M^N}^N \end{bmatrix} \begin{bmatrix} C_{S1,1}^1 \\ \vdots \\ C_{Sm,j}^n \\ \vdots \\ C_{SM,J_M^N}^N \end{bmatrix} = \begin{bmatrix} \delta_{1,1}^1 \\ \vdots \\ \delta_{m,j}^n \\ \vdots \\ \delta_{M,J_M^N}^N \end{bmatrix} \quad (11)$$

where f_m is the fresh air ratio of the m th GAHU, $f_m = \frac{Q_{odm}}{Q_{Sm}}$; $r_{Rm,k}^n$ is the ratio of return air flow rate $Q_{Rm,k}^n$ to the total return air flow rate Q_{Rm}^T , $r_{Rm,k}^n = \frac{Q_{Rm,k}^n}{Q_{Rm}^T}$.

When lumped parameter method is used in both ventilation ducts and rooms, the supply air concentration can be solved by the following matrix (Eq. (12)):

$$\begin{bmatrix} 1-(1-f_1)(1-\eta_1)r_{S1,1}^1 & \cdots & -(1-f_1)(1-\eta_1)r_{Sm,j}^n & \cdots & -(1-f_1)(1-\eta_1)r_{SM,J_M^N}^N \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ -(1-f_m)(1-\eta_m)r_{S1,1}^1 & \cdots & 1-(1-f_m)(1-\eta_m)r_{Sm,j}^n & \cdots & -(1-f_m)(1-\eta_m)r_{SM,J_M^N}^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -(1-f_M)(1-\eta_M)r_{S1,1}^1 & \cdots & -(1-f_M)(1-\eta_M)r_{Sm,j}^n & \cdots & 1-(1-f_M)(1-\eta_M)r_{SM,J_M^N}^N \end{bmatrix} \begin{bmatrix} C_{S1,1}^1 \\ \vdots \\ C_{Sm,j}^n \\ \vdots \\ C_{SM,J_M^N}^N \end{bmatrix} = \begin{bmatrix} \delta_{1,1}^1 \\ \vdots \\ \delta_{m,j}^n \\ \vdots \\ \delta_{M,J_M^N}^N \end{bmatrix} \quad (12)$$

where:

$$\left\{ \begin{aligned} \delta_{m,j}^n &= \left[\sum_{n=1}^N C_{od} (1-\eta_{DF}) + \frac{\sum_{n=1}^N \sum_{k=1}^{K_m^n} S_{Rm,k}^n}{Q_{Rm}^T} + \frac{\sum_{n=1}^N S_{Rm}^n}{Q_{Rm}^T} + \frac{S_{Rm}^T}{Q_{Rm}^T} \right] (1-f_m)(1-\eta_m) + C_{od} f_m (1-\eta_m) + \frac{S_m}{Q_{Sm}} (1-\eta_m) + \frac{S_{Sm}^T}{Q_{Sm}} + \frac{S_{Sm}^n}{Q_{Sm}^n} + \frac{S_{Sm,j}^n}{Q_{Sm,j}^n} \\ r_{Sm,j}^n &= \frac{Q_{Sm,j}^n}{Q_{Sm}} \end{aligned} \right.$$

3 Case demonstration

3.1 Case setup

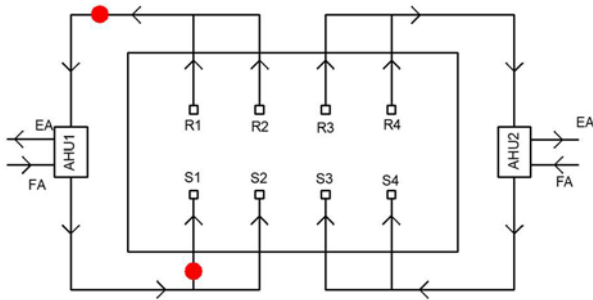


Fig. 2. System sketch of two cases.

The contaminant distribution in the ventilation system with air recirculation was calculated using the proposed method (method 1) and the lumped parameter method (method 2), respectively. The dimension of the ventilated room was 3m (height) × 6m (width) × 10m (length), as shown in Fig. 2. The room was supplied by two AHUs (air handling units) and each AHU had two supply air inlets (S1, S2, and S3, S4) and two return air outlets (R1, R2, and R3, R4) in the room. The size of each inlet and outlet was 0.25m × 0.25m. The air change rate of the room was 6 ACH. There was no contaminant source in the room. All the walls were well insulated. The location of inlets and outlets are listed in Table1 and the detailed parameters used in the two methods are listed in Table2.

Two different source locations were studied under two methods: return air main duct (Case 1) and supply air branch duct of the supply air inlet S1 (Case 2).

Table 1. Locations of inlets and outlets.

Object	Start Point			End Point		
	X(m)	Y(m)	Z(m)	X(m)	Y(m)	Z(m)
S1	1.875	1.60	3.00	2.125	1.85	3.00
S2	3.875	1.60	3.00	4.125	1.85	3.00
S3	5.875	1.60	3.00	6.125	1.85	3.00
S4	7.875	1.60	3.00	8.125	1.85	3.00
R1	1.875	4.15	3.00	2.125	4.40	3.00
R2	3.875	4.15	3.00	4.125	4.40	3.00
R3	5.875	4.15	3.00	6.125	4.40	3.00
R4	7.875	4.15	3.00	8.125	4.40	3.00

Table 2. Detail parameters of the ventilation system.

Emission rate (mg/s)	Source 1	5
	Source 2	5
Cleaning Efficiency	AHU 1	0.4
	AHU 2	0.4
Fresh Air Ratio	AHU 1	0.3
	AHU 2	0.2
Outdoor air concentration (mg/kg)		5

3.2 Contaminant source in the main return air duct

The calculation process of method 1 was as follows: (1) simulate the accessibility distribution of each air supply inlet to obtain the accessibility of supply air at each outlet; (2) use Eq. (11) to calculate the supply air concentration; and (3) calculate the contaminant distribution using Eq. (2). Fluent was employed to calculate the accessibility

using pressure-based solver type. The Reynolds Averaged Navier-stokes (RANS) equations with the standard k-epsilon model were used as the turbulence model. When the contaminant source was located in the main return air duct (Source 1), the supply air concentration of each air supply inlet is listed in Table 3.

Table 3. Supply air concentration for Case 1 using method 1.

Object	Supply Air Concentration (mg/kg)
S1	19.33
S2	19.33
S3	5.34
S4	5.34

As the lumped parameter method was used in the ventilation duct, the supply air concentration of inlets from one GAHU was the same when the contaminant source was in the main return air duct. The contaminant distribution in the room is shown in Fig. 3 and the average concentrations of different methods are shown in Fig. 4.

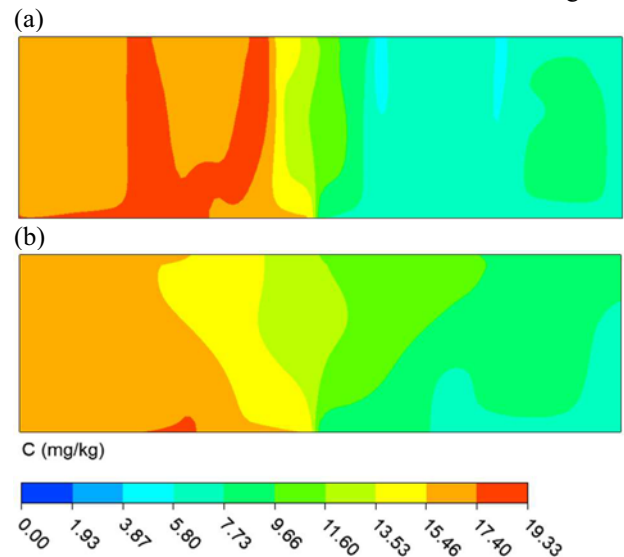


Fig. 3. Contaminant distribution for Case 1 at (a) Y=1.725m (b) Y=4.275m.

The contaminant was transported to the room by the supply air duct of AHU1, and then entered two AHUs through the outlets and polluted AHU2. The supply air concentration of S1 and S2 was higher than that of S3 and S4, as the contaminant source was close to AHU1. In addition to the contaminant source, the return air concentration of AHU1 was higher than that of AHU2 (Fig.3 (b)). Contaminant was accumulated in the left part of the room. The average contaminant concentration of the left and right part of the room was 16.22 mg/kg and 8.33 mg/kg, respectively. If there were personnel in the room, the exposure level of the personnel in the left part was higher. For method 2, the contaminant concentration was uniform in the room, and the supply air concentration of each inlet is listed in Table 4.

Table 4. Supply air concentration for Case 1 using method 2.

Object	Supply Air Concentration (mg/kg)
S1	17.59
S2	17.59
S3	6.34
S4	6.34

The calculated concentration was 11.97mg/kg, which was different from the average contaminant concentration of 12.26 mg/kg for the proposed method. Moreover, method 2 was unable to reflect the non-uniform characteristics of the contaminant distribution in the room.

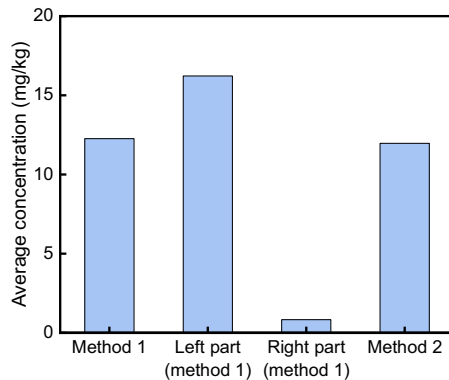


Fig. 4. Average concentration for Case 1.

3.3 Contaminant source in the supply air branch duct

When the contaminant source was in the branch supply air duct of inlet S1 (Source 2), the supply air concentration of each inlet is listed in Table 5. The contaminant distribution in the room is shown in Fig. 5 and the average concentrations of different methods are shown in Fig.6.

Table 5. Supply air concentration for Case 2 using method 1.

Object	Supply Air Concentration (mg/kg)
S1	72.50
S2	25.08
S3	11.42
S4	11.42

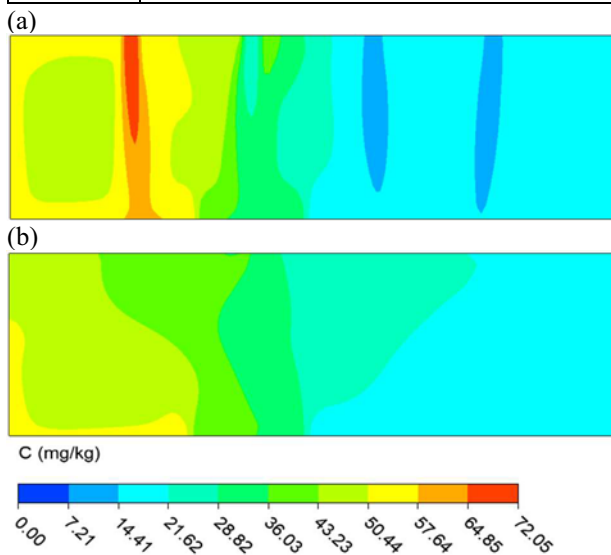


Fig. 5. Contaminant distribution for Case 2 at (a) Y=1.725m (b) Y=4.275m.

The average concentration of the room was higher than that in Case 1 because the contaminant of the source was directly transported into the room through the supply air duct without purification, and the air flow rate of

supply air branch duct was smaller than that of main return air duct.

As the contaminant source was in the branch supply air duct of inlet S1, the supply air concentration of S1 was higher than the other inlets, which caused the contaminant to accumulate in the left part of the room. The average contaminant concentration of the left and right part of the room was 44.43 mg/kg and 18.43 mg/kg, respectively. For method 2, the contaminant concentration is uniform in the room, and the supply air concentration of each inlet was listed in Table 6.

Table 6. Supply air concentration for Case 2 using method 2.

Object	Supply Air Concentration (mg/kg)
S1	69.13
S2	21.71
S3	15.13
S4	15.13

The concentration of the room was 30.28 mg/kg, which was close to the average contaminant concentration of 31.33 mg/kg using the proposed method. However, the zonal pollution level cannot be evaluated using method 2.

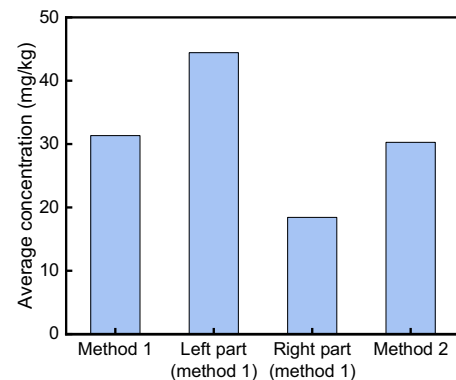


Fig. 6. Average concentration for Case 2.

In this study, the prediction method for the steady distribution of passive contaminants in the ventilation system with air recirculation was proposed with the lumped parameter method assumed for the air duct section. The assumption of lumped parameter method makes it unnecessary to consider the complex duct network in detail, and therefore the calculation process can be greatly simplified. However, the contaminant distribution in the actual duct system and the outlet section of each air duct is non-uniform. The non-uniformity of the upstream air duct outlet will further affect the non-uniformity of the inlet and outlet of the downstream air duct. That will make the uniformity assumption of each section of the lumped parameter method deviate from the real situation. The deviation level depends on the well-mixing length of the contaminants in the air duct. When the contaminants can be well-mixed before the inlet of the downstream air duct, the deviation using the lumped parameter method will be small. On the contrary, the deviation may be large. Studies on the specific deviation level will be carried out in the follow-up work.

4 Conclusion

A prediction method of steady concentration of passive contaminant in ventilation system with air recirculation was proposed with the contaminant source located in the air duct. The relation of supply air and return air concentration was calculated by mass conservation, and the concentration distribution in room was obtained by the concept of accessibility. The different source locations in the air duct resulted in significantly different supply air concentrations and contaminant distribution in the ventilated room. The proposed method was compared with the lumped parameter method for the contaminant concentration in the room. The concentration calculated by lumped parameter method was lower in the left part and higher in the right part compared to proposed method. The proposed method can reflect the contaminant distribution in room with air recirculation.

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