A method to identify the point source of indoor gaseous contaminant based on limited on-site steady concentration measurements

Xinke Wang (), Wei Tao, Yuanyuan Lu, Fenghao Wang

School of Human Settlements and Civil Engineering, Xi'an Jiaotong University, Xi'an 710049, China

Abstract

Identification of potential contaminant sources in buildings is an important issue for indoor pollutant source control. In this paper, a method based on the characteristics matrix derived from the transport governing equation is proposed, and the procedure to identify the contaminant source is presented. Compared with the methods in the literature, the new method is more suitable for the identification of steady point contaminant sources because it only requires limited on-site concentration measurement data without historical information. As a demonstration case, a 2D room with a known flow field validated by the experiment in the literature is selected. A steady point source is presumed at a certain point and the concentration field is calculated by computational fluid dynamics (CFD). Then the concentration data at the specified sampling points are used to identify the source position. Without the measurement error, the method can work well when the concentration measurement data at only two sampling points are given. However, when concentration measurement errors are considered, sampling points need to be increased to improve the identification accuracy. For the simulated 2D case, nine sampling points are sufficient for acceptable accuracy when the relative measurement error is 10%. Effects of positions of the source and the sampling points, and the uncertainty of the flow field simulation on the identification results, as well as the limitation of the method are also discussed.

Keywords

source identification, indoor air quality (IAQ), steady concentration, computational fluid dynamics (CFD)

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1 Introduction

People spend more than 87% of their time indoors (Kim et al. 2001). However, since the energy crisis in 1970s, less outdoor fresh air is supplied into buildings and more air-tight measure is made in buildings for building energy saving. At the same time, more chemical products emitting lots of chemical contaminants are applied indoors. Consequently, indoor air quality (IAQ) becomes worse in the urban buildings and some significant adverse symptoms on occupants' comfort, health, productivity arise such as headaches; eye, nose, or throat irritations; heart disease and even cancer (Yang et al. 2001).

Source control is a primary and the most effective way to improve indoor air quality. However, for source control it is often difficult to identify the locations of the contaminant sources. An imaginary effective solution to find contaminant

E-mail: wangxinke@mail.xjtu.edu.cn

source is to measure the concentrations of indoor contaminants in as many positions as possible to identify the point with maximum concentration value as the position of the contaminant source. But in reality, the expense will limit the method. Therefore, some modeling methods together with limited sensors are developed. Sreedharan (2006, 2007) successfully employed Bayesian probability theory to identify the gaseous pollutant source by interpreting real-time monitoring information from the concentration sensor network. Recent years, so-called inverse modeling methods were developed rapidly for the more accurate identification of indoor contaminant sources. These inverse modeling methods were classified as forward methods, backward methods and probability methods (Liu and Zhai 2007). The forward methods employed a trial-error simulation process to find a contaminant source that can promise the best fitting between the predicted concentration and the measured

one at the specific points. However, because the methods require part of source information and are time-consuming, the applications of the methods are limited. The quasireversibility (QR) method and pseudo-reversibility (PR) method are two typical backward inverse methods. Zhang and Chen proposed a QR method (Zhang and Chen 2007a) and a PR method (Zhang and Chen 2007b) to identify the location and strength of indoor contaminant source based on the known flow field and the contaminant concentrations from several sensors or even one sensor. The results demonstrated that the methods worked well basically. Zhang et al. (2012) extended the QR method for particle tracking as the Lagrangian-reversibility (LR) method. Besides, a probability-based inverse method was introduced by Liu and Zhai (2007) for the identification of indoor contaminant sources and was developed (Liu and Zhai 2007, 2008, 2009; Zhang et al. 2012; Liu et al. 2013; Hwang et al. 2012). Zhai et al. (2011) advanced the method to identify the single contaminant source with continuously releasing based on the concentrations from the real sensor readings with about 10% relative error. And the first validation experiment for the probability-based inverse methods was also conducted. Recently, an artificial neural network-based method was proposed (Vukovic and Srebric 2007) and improved (Bastani et al. 2012) to identify the source zone. And the method required none of the source information. However, because of much training time for the artificial neural network, the method is difficult for the detailed position identification like those in the inverse CFD methods. Cai et al. (2012a,b) presented a new method for the identification of indoor contaminant sources with consideration of real sensor characteristics, which was based on the concept of the transient accessibility of the contaminant source.

For most of these methods, part of the historical information such as historic concentrations, release time is necessary. However, when conducting an IAQ problem diagnosis for a building, lack of history of concentration is usual and only on-site measured concentration data in some positions can be obtained for the location and strength identification of indoor contaminant sources. Besides, usually the release of indoor contaminant from the sources varies with time slowly such as indoor VOC (volatile organic compounds) pollutants from dry building materials (Xu and Zhang 2003) so that available historical information is also scarce. Thus, it is a difficult problem for the mentioned methods to find the contaminant source when the source and the concentration field are almost steady and only very limited on-site concentration measurements can be conducted. This research attempts to propose a simple method to identify the position and strength of indoor steady contaminant point source based on some limited on-site concentration measurement data.

2 Principle

The method is based on understanding the characteristics of transportation of indoor gaseous contaminants. When the source of indoor contaminants is invariable, the steady concentration field of indoor contaminants is governed by Eq. (1):

$$
\nabla \cdot (\rho \mathbf{U} C) - \nabla \cdot (\Gamma_c \nabla (\rho C)) = S \tag{1}
$$

where, ρ is the density of indoor air, U is the velocity vector, *C* is the concentration of the target pollutant, $Γ_c$ is the effective diffusion coefficient of indoor pollutant and *S* is the intensity function of the pollutant source.

After the flow field and information of the source are known, the concentration field can be obtained by numerically solving Eq. (1) with boundary conditions, which are so-called direct problems.

Equation (1) can be discretized numerically as Eq.(2) (Minkowycz et al. 2006) with the following assumptions: (1) the contaminant transport depends on the flow field but does not affect the flow field; (2) the contaminant concentration is so low that the density of the air does not change with the contaminant concentration. Obviously, for indoor air pollution, the assumptions are reasonable.

$$
AC = S \tag{2}
$$

here, *C* is the concentration vector with the dimension $N \times 1$ (*N* is the number of the discretized space grids) comprising the concentration at every discrete grid; *S* is the source vector with the dimension $N \times 1$ comprising the source intensity at every grid; and *A* is the coefficient matrix with the dimension $N \times N$, which is derived from the discretized convection and diffusion terms in Eq. (1) and is dependent of discretization scheme (Minkowycz et al. 2006). Because the concentration field is unique, the coefficient matrix *A* is invertible and the inverse matrix *B* can be obtained by numerical methods such as Gaussian elimination method (Fletcher 1988). Then Eq.(3) can be obtained.

$$
C = BS \tag{3}
$$

which has another expression as Eq. (4):

$$
c_i = b_{i,1}s_1 + b_{i,2}s_2 + \dots + b_{i,j}s_j + \dots + b_{i,N}s_N = \sum_{j=1}^N b_{i,j}s_j
$$
 (4)

here *ci* is the steady concentration of the pollutant at the *i*-th point, $b_{i,j}$ is the element in the row *i* and the column *j*, and *sj* is the intensity of the pollutant source at the *j-*th point.

Equation (4) indicates that the element $b_{i,j}$ quantifies the impact of the source at the grid *j* on the contaminant concentration at the grid *i*. Therefore, $b_{i,j}$ is named as Spatial Flow Impact Factor by Zhang et al. (2006). Because the matrix *A* is independent of the contaminant source, the derived inverse matrix *B* is also independent of the contaminant source.

When the only point source is located at the grid with the unknown index *m*, then the concentration at the grid *i* can be obtained through Eq. (4) as:

$$
c_i = b_{i,m} s_m \tag{5}
$$

If the concentrations at the grids *i* and *j* are measured without error, then the equation $c_i/c_j = b_{i,m}/b_{j,m}$ should exist. By searching the elements in the rows *i* and *j* of the matrix *B*, if the ratio of $b_{i,m}$ and $b_{j,m}$ is equal to the ratio of c_i and *cj*, the point with the index *m* will be identified as the point source. After the source location is identified, i.e. the element $b_{i,m}$ is determined, the strength of the source is also obtained through the measured concentration at sampling point *i* and the determined corresponding element $b_{i,m}$ by Eq. (6):

$$
s_m = c_i / b_{i,m} \tag{6}
$$

However, in practice, because of the error in the concentration measurement and the determination of matrix *B*, Eq. (5) is not strictly true. When the error is tiny (no more than 1%), the concentration measurements at two points are enough for the identification and the point with the minimum value of the criterion function $\varepsilon = (c_i/c_i$ $b_{i,m}/b_{i,m}$) + $(c_i/c_i - b_{i,m}/b_{i,m})$ can be identified as the source. But when the error is larger (more than 1% but less than 15%), the concentration measurements at more than two points are needed. In this case, the point with the minimum

value of the function
$$
\varepsilon(m) = \sum_{k=1}^{M-1} (c_{i(k)}/c_{i(k+1)} - b_{i(k),m}/b_{i(k+1),m}) +
$$

 $(c_{i(M)}/c_{i(1)} - b_{i(M),m}/b_{i(1),m})$ (here, *M* is the number of the measurement points, *i*(*k*) is the index of the *k-*th sampling point, *m*=1,2,…, *N*) is suggested as the criterion for the source identification. If the error is no less than 15%, the method may fail.

Based upon the theory, the identification of indoor contaminant sources will be fulfilled by the method as described in Fig. 1.

3 Demonstration case

For simplification, a 2D case is selected for demonstration. Ito et al. (2000) conducted a ventilation experiment as schematically shown in Fig. 2. And the discretized grids are also indexed from 1 to 1485 as shown in Fig. 2. Computational fluid dynamics (CFD) is employed to obtain the flow field with the numerical conditions listed in Table 1.

Fig. 1 Procedure of the proposed method

Fig. 2 Schematic show of the experiment by Ito et al. (2000) and mesh index

Table 1 Numeric conditions for the 2D validation case by the CFD method

Number of grid points for the room	$45(L=4.5 \text{ m}) \times 33(H=3.0 \text{ m})$
Number of grid points for the inlet	$3(0.06 \text{ m})$
Velocity of air at the inlet U_0	0.1 m/s
Air density	1.225 kg/m ³
Viscosity	1.79×10^{-5} kg/(m·s)
Turbulence model	RNG k - ε model

The calculated results are shown in Fig. 3, and are compared with the measured results by Ito et al. (2000). From Fig. 3, a good agreement between the calculated and experimental results has been observed, which proves the reliability of the calculated flow field. Based on the calculated flow field information, the matrix *A* is obtained, and the corresponding inverse matrix *B* is derived.

Fig. 3 2D flow field validation: (a) the flow field calculated by CFD method; (b) comparison of the horizontal distribution of velocity at *y*=1.5 m between CFD and experimental results; (c) comparison of the vertical distribution of velocity at *x*=2.25 m between CFD and experimental results

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4 Results and discussion

A source with the intensity $0.5 \text{ mg/(m}^3 \text{·s})$ is presumed to locate at the grid 780. Using CFD method, the steady concentration field is simulated. The two grids with the indexes 300 and 900 are selected as measurement points and the steady concentrations without the measurement errors, i.e. 1.710 and 0.885 mg/m³ respectively, are obtained from the simulated results. Then the related two row elements with the row indexes 300 and 900 (i.e. $b_{300,i}$ and $b_{900,i}$, *j*=1,2,…, 1485) of the matrix *B* are picked out. Based on the data, the criterion function $\varepsilon(j) = (c_{300}/c_{900} - b_{300,j}/b_{900,j}) +$ $(c_{900}/c_{300} - b_{900,j}/b_{300,j})$ is calculated for each point of the whole room and the contour of log_ε is plotted as shown in Fig. 4. From that, it is found that *ε* with the index *j*=780 is the smallest and is nearly equal to zero. Therefore, the source is found out at the grid 780, which agrees with the presupposition. That demonstrates the present method is successful. However, in reality, some factors affect the identification such as the measurement error of the concentration, the error of the flow field information, the position of the sampling points, and so forth. To provide more solid validation, some factors are discussed as follows.

4.1 Effect of the error in concentration measurements

The previous result is based on accuracy of the concentration measurements. However, the measurement error cannot be avoided and will affect the calculation of log ε. Therefore, the effect of the measurement error on the identification result should be taken into account. Random errors of $\pm 1\%$ and $\pm 5\%$ respectively in the two cases are added to the predicted concentration at the points with the indexes 300 and 900 as the real measurement results. Figure 5 shows the identification results. From that it can be seen that the concentration measurement error of 1% can be accepted for the source identification by the concentration measurement at the two points but the one of 5% will result in a wrong identification.

Fig. 4 The contour of logε without the concentration measurement error when the source is located at the point with the index 780

Fig. 5 The contour of log ε with concentration measurement error of (a) 1% and (b) 5% using the two sampling points when the source is located at the point with the index 780

An idea to improve the identification is increasing the sampling points to obtain more information. Five points are selected as the sampling points as schematically shown in Fig. 6 and the contour of log *ε* is also plotted. Figure 6 shows a smaller derivation between the identification result and the presumed source position than that using two sampling points. For the measurement error of 10%, the average distance for 20 times between the identified position using 5, 7 and 9 sampling points and the presumed source

Fig. 6 The contour of $\log \varepsilon$ with the concentration measurement error of 5% using five sampling points when the source is located at the point with the index 780

position is investigated respectively and the statistical results are shown in Fig. 7. And a smaller average distance is observed when the sampling points are increased.

4.2 The effect of the measurement positions

The identification for the presumed source with the index 780 using another group of five sampling points different from that in Fig. 6 is conducted and the result is shown in Fig. 8. The present identification result deviates from the presumed source farther than that in Fig. 6. A reason is that the source has a larger impact on the sampling points in Fig. 6 than those in Fig. 8. The element $b_{i,j}$ can be used to express the impact of the source *j* on the sampling point *i*. Figure 9 pictures the element $b_{i,j}$ for the two groups of sampling points and an obvious difference is observed. However, when identifying the source in practice, the impact of the source on the sampling points cannot be prejudged. Therefore, the representative points just like those in Fig. 6 will be available selections as the sampling points.

Fig. 7 The statistical distance for 20 times between the identified positions and the presumed source position using 5, 7 and 9 sampling points with the concentration measurement error of 10%

Fig. 8 The contour of log ε with the concentration measurement error of 5% using five sampling points different from ones in Fig. 6

Fig. 9 The impact of the presumed source on the two groups of sampling points

4.3 The effect of the point source position

Because the source could exist everywhere in the room, it should be discussed whether the source can be found out when it is located at indoor various points. Four typical points including a corner point (Grid 1), a boundary point (Grid 675), a central point (Grid 700) and air inlet (Grid 1306) are presumed as the source locations in different cases. For the four cases, the sampling points are the same as those in Fig. 6. And the concentrations with the measurement error of 5% are adopted for the identification. The identification results are shown in Fig. 10. From that, it is revealed that the accuracy of the identification is very different when the source is located at different position. When the source is located in the middle zone, the identification result is closer to the presumed source position. Especially, when the source is located in the boundary or the air supply inlet, the identification provides only a rough zone of the source position.

4.4 The effect of the uncertainty of the flow field information

From Eq. (5), the identification will be affected by the elements of the matrix *B*, which is derived from the flow field information**.** Because the flow field is obtained by CFD method, the uncertainty of simulation in the flow field will affect the identification. In common, the uncertainty is influenced by some factors such as boundary condition settings, discretization schemes, and turbulence model selections (Zhang et al. 2007). In Section 3, the RNG *k*-*ε* turbulence model was adopted in the flow field simulation and a good agreement between the simulated results and experimental results was observed. Hence, this simulated flow field is assumed reasonably accurate. The standard *k*-*ε*

Fig. 10 Results of the source identification based on the contour of log *ε* when the source is located at different points: (a) a corner point; (b) a point neighbour to a boundary wall; (c) a point in the middle; (d) a point neighbour to the air supply inlet

turbulence model is employed for CFD simulation in a comparison case and a deviation in the flow field is expected to bring out. Obvious difference is observed between the velocity-based two turbulence models as shown in Fig. 11. Based on the deviated flow field information from the standard *k*-*ε* (SKE) turbulence model and the accurate concentrations at five sampling points from the RNG *k*-*ε* turbulence model, the identification of the source location is made as shown in Fig. 12. It proves that the uncertainty

Fig. 11 Comparison of the flow fields obtained by RNG turbulence model and standard *k*-*ε* turbulence model: (a) horizontal distribution of velocity at *y*=1.5 m; (b) vertical distribution of velocity at the *x*=2.25 m

Fig. 12 The identified result based on the contour of $\log \varepsilon$ in the flow field with a deviation

in the flow field affects the precision with no doubt, but an acceptable identification can still be provided.

5 Conclusions

This paper proposed a method to identify the quasi-steady indoor contaminant point source using some limited steady measured concentration data. In an illustrative case, the identification was fulfilled successfully and was validated with the presumed source position when the concentration can be obtained without measurement error. However, when the measurement error is considered, the method needs to be improved for accuracy by increasing the number of the concentration measurement points. The calculated cases show that nine sampling points may be enough for the identification when the concentration measurement error is 10%. Besides, the identified results based on the different sampling point arrangements suggest obvious different accuracy. And the sampling points at representative zones are available selections for practical applications. The study also indicates that the source position affects the accuracy of the identification and the identification is more accurate when the source is located at a middle zone.

Certainly, because of the principle limitation, the method for some special ventilation systems such as well mixing ventilation or piston flow is not applicable. Besides, as a preliminary study, the illustrative case is simple. Therefore the further study needs to be conducted for the improvement of the robustness and reliability including: (1) the application for real buildings with complex ventilation modes and flow fields; (2) the application for the non-point source; (3) experimental verification for the method and so forth.

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