

INVERSE IDENTIFICATION OF MULTIPLE POLLUTANT SOURCES

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ABSTRACT

In case of an accidental release of indoor airborne pollutants, it is critical to know information of the pollutant sources. Current inverse modeling concentrates on identifying a single pollutant source or multiple pollutant sources in simplified puff or constant release forms. This investigation proposes an inverse model to precisely identify the multiple pollutant source number, locations and their temporal release rate profiles simultaneously. The model implements Tikhonov-based inverse matrix operation to obtain the release rate profiles for each candidate source with temporal concentrations provided by sensors. A candidate source with a solved release rate close to zero is excluded as an active source, and then the pollutant source number and locations with nonzero release rate can be determined. The above strategy was applied to identify two sources released by passengers in a three-dimensional aircraft cabin. The results show that the proposed method is able to determine the source number, locations and their temporal rate profiles correctly.

INTRODUCTION

In case of an accidental release of indoor airborne pollutants, it is critical to know the number, locations and temporal release rates of the pollutant sources. Current sensors can provide pollutant concentrations locally but cannot tell where and how the pollutants have released. To obtain the above pollutant source information, a viable method is to conduct inverse modeling, i.e., to infer the sources from certain detected consequences.

Inverse modeling in indoor environments is majorly concentrated on identification of pollutant source locations. The adopted strategies can be divided into two categories (Zhang et al., 2015), namely, directly reversing transport equations to track a source and solving forward transport equations to match a source. For example, Zhang and Chen (2007a) applied the first strategy and solved a quasi-reversibility (QR) equation to identify a single pollutant source location via directly reversing the time-marching direction of the pollutant transport equation. Bady et al. (2009) also implemented a similar reversed time-marching method in an urban environment. The QR method was further extended to locate a particulate source

after accounting for particle settling effect due to the gravity (Zhang et al., 2012). Except for reversing the time-marching direction, solving the convective pollutant transport in a reversed flow field using the so-called pseudo-reversibility method may also locate a single pollutant source (Zhang and Chen, 2007b). The first strategy does not require much priori source information assuming as known but may suffer from numerical stability.

Most researchers turn to a stable solution by applying the second strategy. If a candidate source is found providing concentration response highly comparable with a monitoring sensor, it is determined to be the source. Liu and Zhai (2008, 2009) solved the adjoint equation of pollutant source location probability to determine a single gaseous source location. Vukovic et al. (2010) and Bastani et al. (2012) applied neural network to match the pollutant source concentration to find a pollutant source. Wang et al. (2013) matched a source with the concentration response provided by the state-space matrix. The second strategy is stable but has a large computing burden in solving and matching concentration. All possible source information including the release location and temporal rate profiles must be assumed to be known in advance.

In addition to pollutant source location, some studies also addressed identification of pollutant release rates. For a gaseous source released in an instantaneous form, a linear scaling method (Zhang and Chen, 2007b) is valid for determining the total pollutant release amount. However, for a dynamically released source, identification of its rate profile is more challenging. Zhang et al. (2013) proposed a matrix inversion method to determine the temporal release rate profile of a gaseous source with the concentration monitored at a point. However, the pollutant source location must be assumed to be known before inverse identification.

For more comprehensive source information, it is necessary to identify both the pollutant source location and its temporal release rate profiles simultaneously. Sohn et al. (2002) applied a Bayesian model to predict the location and release amounts of a pollutant source. All candidate pollutant source locations, release forms and amounts were presumed to be known. Zhang et al. (2015) combined an

inverse matrix method with a Bayesian probability model to identify a single pollutant source location, temporal rate profile and the sensor alarming time. The required inputs are concentrations at two different points in a space. Cai et al. (2013) presented a model to identify locations and emission rates of multiple sources, but the sources must be in the very simple constant-release types.

To date, no inverse modeling was demonstrated to simultaneously identify the number, location and temporal release rate profiles of multiple dynamically-released pollutant sources. This investigation presents an inverse model for determination of the above source information with several temporal concentrations as inputting. A case with two sources dynamically released in a three-dimensional aircraft cabin was solved for illustrating the methodology.

METHODOLOGY

This study addresses identification of multiple pollutant sources releasing the same gaseous pollutant dynamically in a fixed flow context. Apparently the concentration collected at a sensor is the sum of the concentrations by different sources. The governing cause-effect relation of multiple concentration responses is presented first, followed by the inverse operation principle to identify multiple source information.

Concentration responses of multiple gaseous pollutant sources

Concentration responses of multiple tracer gaseous sources can be solved from the passive scalar equation as:

$$\frac{\partial(\rho c)}{\partial t} + \text{div}(\rho \mathbf{u} c) = \text{div}(\Gamma \text{grad}(c)) + \sum_{i=1}^n q_i, \quad (1)$$

where ρ is air density, c is temporal pollutant concentration by n pollutant sources, t is time, \mathbf{u} is air velocity vector, Γ is effective mass diffusivity, and q_i is source term of the i^{th} pollutant source, i.e., the temporal rate of the i^{th} pollutant source, i is from 1 to n and n is the total number of pollutant sources. If the flow field is fixed and the mass diffusion coefficient is proportional to the effective viscosity, Eq. (1) can be decomposed into a series of concentration equations with respect to each pollutant source as:

$$\frac{\partial(\rho c_i)}{\partial t} + \text{div}(\rho \mathbf{u} c_i) = \text{div}(\Gamma \text{grad}(c_i)) + q_i, \quad (2)$$

where c_i is concentration response due to the i^{th} pollutant source, and the concentration at a sensor location can be summed together as:

$$c(t) = \sum_{i=1}^n c_i(t). \quad (3)$$

If a pollutant source location is fixed, Eq. (2) constitutes a linear system between the release rate and the concentration. Consequently, the

concentration response of an arbitrary source release rate q_i can be expressed as the convolution integral between the source release rate and the concentration response of a unit impulse release as (Zhang et al., 2013):

$$c_i(t) = \int_{-\infty}^{+\infty} q_i(\tau) F[\delta(t-\tau)] d\tau \quad (4)$$

where $F[\delta(t-\tau)]$ is the concentration response of a unit impulse release at time $t=\tau$. By discretizing Eq. (4) (Hiyama et al., 2010), the concentration response for an arbitrary source release rate q_i can be written as:

$$c_{i,t_i} = \sum_{k=0}^l q_{i,t_i-k} F_{t_k} = q_{i,t_i} F_{t_0} + \dots + q_{i,t_i-k} F_{t_k} + \dots + q_{i,t_0} F_{t_l} \quad (5)$$

where t_i is the time at the i^{th} time step.

Rewriting Eq. (5) into a matrix, it yields:

$$\mathbf{c}_i = \mathbf{A}_i \mathbf{q}_i, \quad (6)$$

where \mathbf{c}_i is a concentration vector (composed of discrete concentration at different time step) due to presence of the source release rate vector \mathbf{q}_i (composed of discrete rate at different time step), \mathbf{A}_i is the linear matrix that describes the cause-effect relation between the release rate of the i^{th} pollutant source and the exhibited pollutant concentration. The readers can refer to Zhang et al. (2013) for more details on how to extract the cause-effect matrix \mathbf{A} from the concentration response of a unit impulse release.

According to Eq. (3), the total concentration at a point in space is the sum of the component concentration by each source. The total concentration at a specific point j is:

$$\mathbf{c}^j = \sum_{i=1}^n \mathbf{A}_i^j \mathbf{q}_i, \quad (7)$$

where \mathbf{c}^j is the total concentration responses at point j by n sources, \mathbf{A}_i^j is the matrix that describes the relation between the release rate vector \mathbf{q}_i at the i^{th} pollutant source location and pollutant concentration \mathbf{c}^j at point j in space. To prevent confusion, the pollutant source index i is within the subscript, while the concentration point index j is within the superscript.

Then the total concentration at n different points in space due to n potential sources can be formulated into:

$$\begin{bmatrix} \mathbf{c}^1 \\ \vdots \\ \mathbf{c}^j \\ \vdots \\ \mathbf{c}^n \end{bmatrix} = \begin{bmatrix} \mathbf{A}_1^1 & \cdots & \mathbf{A}_i^1 & \cdots & \mathbf{A}_n^1 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{A}_1^j & \ddots & \mathbf{A}_i^j & \ddots & \mathbf{A}_n^j \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{A}_1^n & \cdots & \mathbf{A}_i^n & \cdots & \mathbf{A}_n^n \end{bmatrix} \begin{bmatrix} \mathbf{q}_1 \\ \vdots \\ \mathbf{q}_i \\ \vdots \\ \mathbf{q}_n \end{bmatrix} \quad (8)$$

Eq. (8) describes the concentration responses by multiple pollutant sources. The submatrix A_i^j is subject to the flow field, pollutant source location and location of a concentration monitoring point. Since A_i^j does not reply on the pollutant source release rate, the matrix can be pre-solved before inverse modeling.

Principles of inverse modeling

For demonstrating inverse principles, let us rewrite Eq. (8) into:

$$C=AQ, \quad (9)$$

where matrix $C=[c^1, \dots, c^j, \dots, c^n]^T$, matrix A represents the whole square matrix in the right hand side of Eq. (8), and $Q=[q_1, \dots, q_i, \dots, q_n]^T$.

Identification of pollutant sources should get the release rate matrix Q solved first with the input of the concentration matrix C . An intuitive strategy is conducting matrix inversion. However, matrix A is not reversible due to ill posedness of the reversed problems. A strategy is imposing the well-known Tikhonov regularization (Tikhonov and Arsenin, 1977) by adding an additional stabilized term when implementing inversion. The strategies have been proved successfully in inverting the cause-effect matrix to solve for the release rate profile for a single pollutant source (Zhang et al., 2013; 2015). It should be possible for modifying the regularized matrix inversion for identifying multiple pollutant sources.

With a regularized term added to Eq. (9), the inverse modeling is to find a matrix Q that can minimize the following objective function:

$$\text{Min } Z(Q) = \|AQ - C\|_2^2 + \lambda^2 \|LQ\|_2^2, \quad (10)$$

where Z is the objective function that describes the concentration match plus the regularized effect, $\| \cdot \|_2^2$ represents the square of the second norm of a matrix, λ is the regularized parameter that controls strength of the regularization, and L is the regularized matrix and usually taken as a second-order time derivative like format (Hansen, 1997), which is well posed for inversion. By taking derivative to Eq. (10) with respect to Q and setting the derivative equal to zero, it yields:

$$Q = (A^T A + \lambda^2 L^T L)^{-1} (A^T C). \quad (11)$$

With an appropriate λ , the matrix $(A^T A + \lambda^2 L^T L)$ can be inverted. In general, λ should be as small as possible to prevent introducing too much regularized operation to destroy the original cause-effect relation, but should still be sufficient for inverting the matrix. Eq. (11) reveals that the release rate matrix Q can be solved once provided with the concentration matrix C as the known input. The number of concentration monitoring points should be equal to the number of pollutant sources to be identified.

Because matrix A is subject to the pollutant source locations, all candidate pollutant source locations should be assumed to be known in advance. However, the number of sources that have released pollutants can be unknown. If a candidate source is identified to have zero release rate, it can be excluded to be a source. Then the number of active sources, their release locations, and the corresponding rate profiles are identified.

A DEMONSTRATION CASE

To test the proposed method, two active pollutant sources in a three-dimensional aircraft cabin, as shown in Figure 1, are identified. There are 21 passengers in a twin-aisle aircraft cabin seated in three rows. The conditioned air is supplied into the cabin by two symmetric linear slot openings on the ceiling, while the internal air is exhausted on both side walls near the floor. The total airflow rate is $0.248 \text{ m}^3/\text{s}$, with an air-supply temperature of $19.7 \text{ }^\circ\text{C}$. The passengers' surface temperature is set to $30.3 \text{ }^\circ\text{C}$, and the cabin walls are assumed approximately $24 \text{ }^\circ\text{C}$.

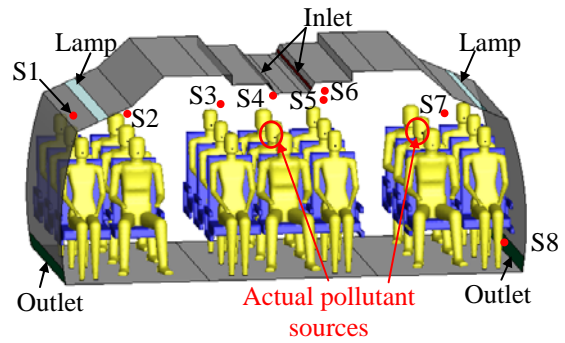


Figure 1 Geometric model of an aircraft cabin for identification of multiple pollutant sources

Suppose that the passengers seated in the second row are the seven potential pollutant sources (PPSs), namely, PPS1 to PPS7 from left to right based on Figure 1. The actual two pollutant sources are PPS 4 and PPS 6, releasing pollutant from the passengers' mouths. There are seven sensors, S1 to S7, near the seven PPSs to record the temporal concentrations. The eighth sensor near the right outlet, S8, is applied for evaluating accuracy of the inverse identification. The predicted concentration at S8 location based on the inversely identified sources is to be compared with the concentration from sensor monitoring.

Figure 2(a) shows the temporal release rate profiles of the two active pollutant sources (APSs). The APS1 or PPS4 released pollutant following an intermittent sinusoidal wave, while APS2 or PPS6 released pollutant constantly for 10 seconds. The peak value of the sinusoidal profile is 0.95 L/min , and the constant rate at APS2 is 0.71 L/min .

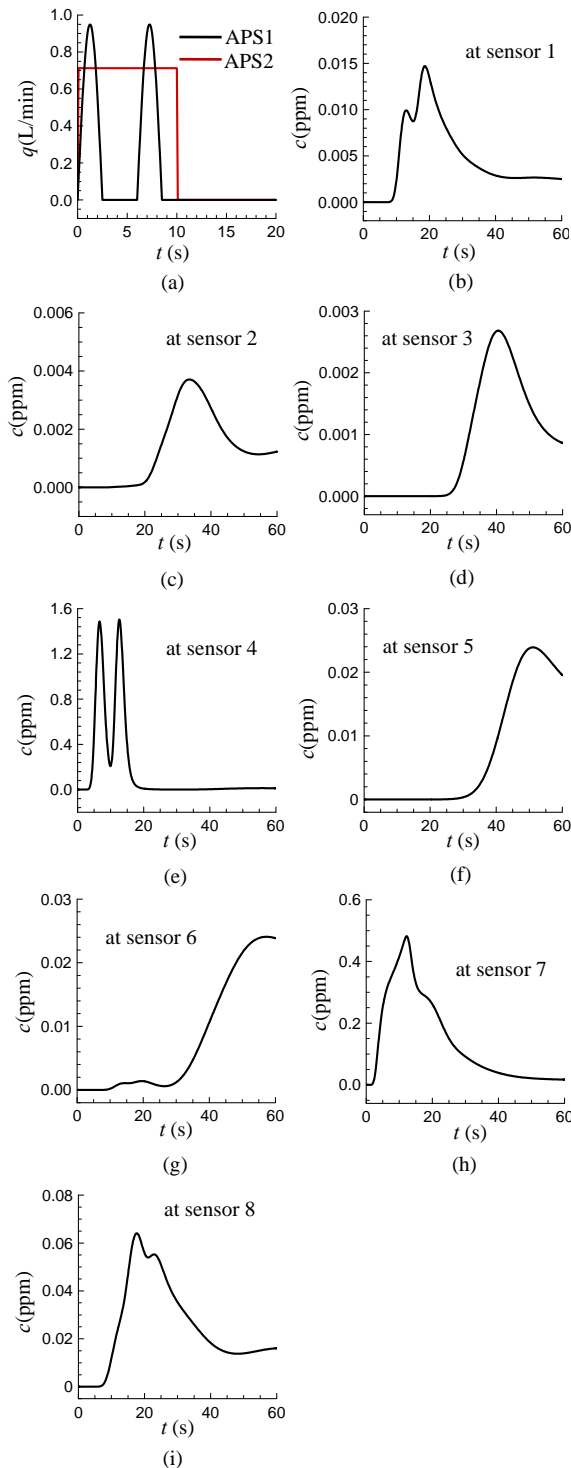


Figure 2 Actual pollutant source release rate profile and simulated sensor monitored concentrations: (a) temporal release rate profiles of the two actual pollutant sources (APSs), (b) to (i) simulated temporal concentrations at sensors 1 to 8, respectively

Assume that all sensors can record concentrations simultaneously with the pollutant release. Figure 2 (b) to (i) show the CFD simulated concentration responses at eight sensor locations. Because sensor 4 is near APS1, the concentration is much larger and

two peaks can be detected. Similarly, sensor 7 is close to APS2, so the recorded concentration is also relatively larger than the others. The rest sensors can capture only one peak and the concentration values are much smaller due to the dilution effect.

The fixed thermo-flow field, the concentrations monitored by sensors 1 to 7, and locations of the seven potential pollutant sources are the known inputs for the inverse identification.

RESULTS AND DISCUSSION

Figure 3 compares the inversely solved release rate profiles with the corresponding actual release rate profiles at the seven potential pollutant source (PPS) locations. The adopted regularized parameter λ is 0.001. At PPS4 or APS1 as shown in Figure 3(d), a sinusoidal profile with two peaks is well captured. However, there are fluctuations in the rate profile after each peak. At PPS6 or APS2, the constant release lasting 10 seconds is also well reproduced except for the rate fluctuations at $t < 15$ s, as shown in Figure 3(f). The release rates are nearly zero at other locations, though some small amplitude fluctuations exist. The rate fluctuations are ascribed to the tailored cause-effect relationship by the regularized operation. On the one hand, the regularized operation is necessary to modify the original ill-posed concentration response matrix to make inversion viable. But on the other hand, it also results adverse impacts by interrupting the originally accurate cause-effect relationship. The inverse modelling just presents an effort trying to obtain an approximate solution matching with the inputting concentration profiles. Nevertheless, it can still be clearly seen that there are two active sources in this case, and the corresponding rate profiles are well identified.

To further quantify the inverse identification errors between the inversely solved release rate profiles and the actual ones, the following relative error is defined:

$$\text{Error} = \frac{|q_{\text{calculated}} - q_{\text{actual}}|}{q_{\text{peak}}} \quad (12)$$

where $q_{\text{calculated}}$ is the inversely solved temporal rate, q_{actual} is the actual release rate, and q_{peak} is the peak release rate of the actual profile. In this investigation, $q_{\text{peak}} = 0.95$ L/min was adopted, which corresponds to the peak value of the sinusoidal release at APS1.

Figure 4 shows the relative identification errors for the release rate profiles versus time at the seven PPS positions. The relative identification errors are smaller than 15% at all PPS locations, except near $t = 10$ s at PPS6. As shown in Figure 3(f), the actual release suddenly stops at $t = 10$ s, but the inversely solved rate has difficulty in responding such sudden change in the rates. The relative errors are also a little bit larger at PPS4 before and after the two peaks. It can thus conclude that the proposed model has difficulty in capturing sharp changes of the release rates.

Figure 5 compares the reconstructed concentration (RC) based on the identified temporal release rates at the seven PPS locations with the actual concentration (AC) monitored by sensor 8. The reconstructed concentration profile is in good agreement with the actual one except for slight deviations from $t=20$ s to $t=25$ s and $t>50$ s. It again attests that the proposed inverse method has good accuracy in identifying the pollutant sources.

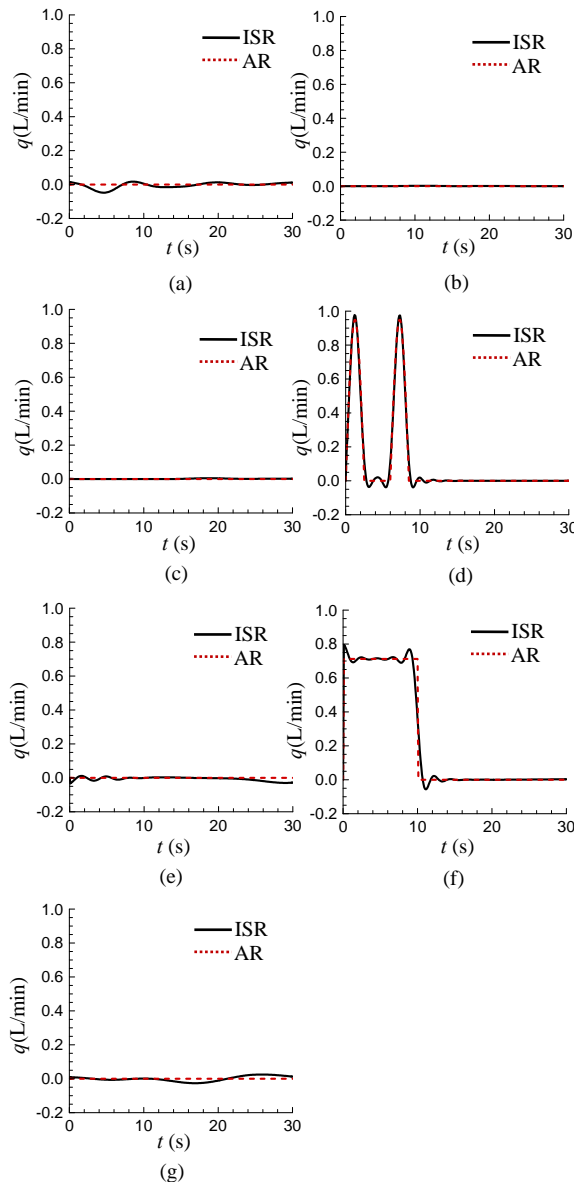


Figure 3 Comparison of the inversely solved release rate (ISR) profiles with the actual release (AR) rate profiles at: (a) PPS1, (b) PPS2, (c) PPS3, (d) PPS4 (APPS1), (e) PPS5, (f) PPS6 (APPS2), (g) PPS7

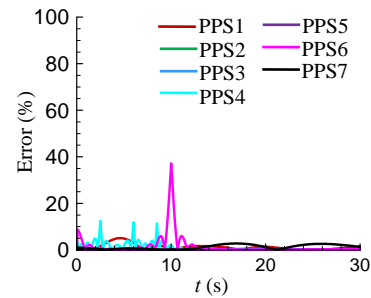


Figure 4 Relative identification errors of the release rate profiles versus time at seven potential pollutant source (PPS) locations

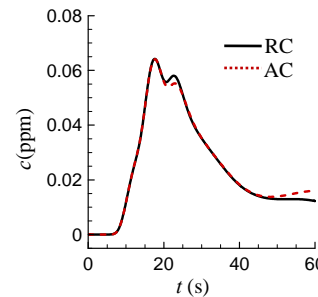


Figure 5 Comparison between the reconstructed concentration (RC) based on the inversely identified temporal release rate profiles and the actual concentration (AC) monitored by sensor 8

CONCLUSIONS

This investigation proposes an inverse model to identify multiple pollutant sources including the source number, locations and temporal release rate profiles simultaneously. By adopting the model to identify two active sources in a three-dimensional cabin, it shows that the method can correctly determine the pollutant source number and locations. The inversely identified release rate profiles are also in good agreement with the actual release rate profiles. The identification errors between the inversely solved release rates and the actual rates are generally smaller than 15%. The known conditions inputting into the inverse model include a steady flow field and the valid temporal concentrations in the same number of the potential pollutant sources.

ACKNOWLEDGEMENTS

The work was supported by the National Key Basic Research and Development Program of China (the 973 Program, Grant No.: 2012CB720100) and the Distinguished Young Scholar Program of Liaoning Province (Grant No.: LJQ2013004).

NOMENCLATURE

- i = index of pollutant source location
- j = index of sensor location
- k = index of time step

l	=	total number of time steps
ρ	=	air density
A	=	linear matrix that describes the cause-effect relation between the release rate and the exhibited pollutant concentration
c	=	temporal pollutant concentration
\mathbf{c}	=	concentration vector
C	=	concentration matrix
F	=	concentration response of a unit impulse release or response factor
L	=	regularized matrix
n	=	total number of pollutant sources
q	=	temporal release rate of the pollutant source
\mathbf{q}	=	temporal release rate vector
Q	=	temporal release rate matrix
t	=	time
\mathbf{u}	=	air velocity vector
Z	=	objective function that describes the concentration match
$\delta(t-\tau)$	=	unit impulse release at time $t=\tau$
Γ	=	effective mass diffusivity
λ	=	regularized parameter
τ	=	time

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