An Offline Inverse Model for Identification of Multiple Pollutant Sources in Aircraft Cabins

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Abstract. Gaseous pollutant source identification is important to protect passengers from infectious agents in aircraft cabins. Current identification method may either suffer from numerical instability or require extensive prior knowledge. This paper proposes an offline inverse model, which needs no iterations to identify the locations and release profiles of multiple gaseous pollutant sources. The model first uses airflow field in the domain to construct a transport probability matrix by Markov chain, which contains the probability of pollutant transports through faces in each cell. Then the transient concentration responses at the monitoring points of a unit impulse releases from each candidate source can quickly be predicted by the transport probability matrix, to construct another matrix describes the relation between the source releases and the monitored concentrations. Finally, Tikhonov regularization is used to inverse the matrix for identification. The above model was applied on a two-dimensional aircraft cabin with gaseous pollutant released from two passengers. Results showed that the proposed model could correctly reproduce the detailed travel path of pollutant transport, as well as identify the locations and release profiles of multiple pollutant sources. More than 90% decrease of the computing time as compared with the conventional CFD method showed that the proposed model had high efficiency.

Keywords: Markov chain · Tikhonov regularization · Offline inverse model

1 Introduction

The outbreak of Corona Virus Disease 2019 (COVID-19) in recent years increases the demand for gaseous pollutant source identification in aircraft cabins, to protect inside passengers from being infected. Pollutant source identification is an inverse problem that determines causal information from certain consequences, since outcomes such as continuing pollutant concentrations at the monitoring points, are always known as prior information to determine the pollutant sources.

Currently, a number of CFD based inverse models have concentrated on indoor gaseous pollutant source identification, which can be divided into forward methods and backward methods. Forward methods construct a number of candidate sources to find the one that makes the pollutant concentrations at typical points coincide best with that

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from the actual sensors, while backward methods directly reverse the flow to determine the source, by solving the N-S equations with a negative time step or a reversed airflow field. For the first strategy, Azimi and Daneshgar [1] proposed an inverse zonal method to optimize a defined objective function by iterations; Sohn et al. [2] applied Bayesian approach, which first builds numbers of scenarios contained hypothetical pollutant sources in the pre-event stage, then compares concentrations between the model simulations and actual sensor monitoring data by Bayesian statistics to determine the actual source in the second stage. Similar methods such as Neural Network [3], probability-based adjoint method [4] and that proposed by Cai et al. [5] were also used to identify the sources. Generally, forward methods have moderate computing efficiency, since all the candidate source locations and release strengths as well as the corresponding monitored concentrations are required to be known before the identification.

To further increase the source identification speed, some researchers turn to the backward method. For example, Zhang and Chen proposed quasi-reversibility (QR) method [6] and pseudo-reversibility (PR) method [7] for pollutant source identification. The former method reverses the time-marching direction of the pollutant transport equation, while the latter one reverses the airflow instead. Results showed that although PR method had less prior knowledge and was more stable, the accuracy was slightly worse than QR method. To balance the computing efficiency and stability, we raised an inverse model to identify multiple sources in indoor environments, which builds a matrix that describes the relation between the release rates of all the candidate sources and the monitored concentrations for inversion [8, 9]. However, to construct the matrix, a large number of pollutant transport equations need to be solved by CFD for preparation.

Several methods were also proposed to accelerate the solution speed for pollutant transport equations, such as FFD [10], which approximately replaces the diffusion and advection terms in N-S equations with other schemes that can decouple the pressure and velocity in CFD iterations to improve the computing efficiency. But the method still needs online iterations to obtain a convergent solution. Markov chain model has developed in indoor environment recently. The method constructs a transport probability matrix by determining the possibility of pollutant transports through faces in each cell, then the pollutant movement can be predicted by the matrix without iterations. Nicas [11] used the method to describe the gaseous pollutant dispersion in an indoor environment; Chen et al. [12] further applied the method on transient particle transport prediction. However, currently few studies have concentrated the method on inverse identification of the indoor pollutant sources. Although Zeng et al. [13] proposed a Markov-chain-based inverse modeling to identify the location and release rate of a pollutant source, the study only identified a single pollutant source, and the identification was applied in a multi-zone model, in which the detailed travel path of pollutant could not be obtained. This paper proposes a model that combined Markov chain and Tikhonov regularization, which is capable of reproducing the detailed travel path of pollutant transport, as well as identify the locations and release profiles of multiple pollutant sources in aircraft cabins. Solution speed and accuracy will be discussed in the paper for evaluation of the proposed model.

2 Methods

2.1 Construction of a Pollutant Transport Probability Matrix

The proposed model first uses Markov chain to construct a pollutant transport probability matrix for source identification. With a known airflow field, the probability of pollutant remains in the current cell can be obtained as [12]:

$$p_{i,i} = \exp\left(-\frac{\sum Q_{i,nbhd}}{V_i}\Delta t\right) \tag{1}$$

where $p_{i,i}$ is the probability of pollutant remains in the current ith cell, $\sum Q_{i,nbhd}$ is the sum of the airflow rate from the ith cell to the neighboring cells, which can be obtained from the airflow field in the domain, V_i is the cell volume, Δt is the time step. Equation (1) can be derived from a mass balance equation that describes variation of the pollutant amount in one cell in a certain time step must be equal to the sum of amount of pollutant that transports to other cells in this time step. Suppose that the probability of pollutant transports from one cell to another is proportional to the airflow rate through the corresponding adjacent face, then the probability of pollutant transports from the ith cell to the jth, denoted by $p_{i,j}$ in this study, can be solved as [12]:

$$p_{i,j} = \frac{Q_{i,j}}{\sum Q_{i,nbhd}}\left(1 - p_{i,i}\right) \tag{2}$$

where $Q_{i,j}$ means the airflow rate from the ith cell to the jth cell.

With the known $p_{i,i}$ and $p_{i,j}$, the transport probability matrix can be constructed, in which $p_{i,j}$ is the element in the ith line and jth column. Totally nn elements are contained, where n is the cell number in the domain used by CFD.

2.2 Identification of Multiple Pollutant Sources

The matrix P contains the probability of pollutant both remains in the current cell and transports to the adjacent cells, hence the pollutant amount field after k time steps M_k can easily be obtained by the matrix as:

$$M_k = M_0 P^k \tag{3}$$

where M_0 represents the initial pollutant amount field, which can be obtained by multiplying the initial pollutant concentration in each cell and the corresponding cell volume.

With Eq. (3), the concentration responses at the monitoring points of a unit impulse that releases from each candidate source can be predicted. For a candidate source, concentrations at a monitoring point that are contributed by this source can be written as:

$$\begin{bmatrix} c^j_{0,i} \\ c^j_{1,i} \\ \vdots \\ c^j_{k,i} \end{bmatrix} = \begin{bmatrix} c^j_{p,0,i} & 0 & \cdots & 0 \\ c^j_{p,1,i} & c^j_{p,0,i} & \ddots & \cdots \\ \vdots & \ddots & \ddots & 0 \\ c^j_{p,k,i} & \cdots & c^j_{p,1,i} & c^j_{p,0,i} \end{bmatrix} \begin{bmatrix} s_{0,i} \\ s_{1,i} \\ \vdots \\ s_{k,i} \end{bmatrix}, \text{ or } \mathbf{c}^j_i = \mathbf{A}^j_i \mathbf{s}_i, \tag{4}$$

where $c_{k,i}^{j}$ in the vector $\mathbf{c}_i^j$ on the left hand side of Eq. (4) represents the contributed concentrations at the jth monitoring point of the ith source at the kth time step, $c_{p,k,i}^{j}$ in the matrix $\mathbf{A}_i^j$ means the concentration responses at the jth monitoring point of a unit impulse that releases from the ith source at the kth time step, $s_{k,i}$ in the vector $\mathbf{s}_i$ means the release strength of the ith source at the kth time step. For all the candidate sources, the monitored concentrations at the jth point can be derived as:

$$\mathbf{c}^j = \sum_{i=1}^{m} \mathbf{c}_i^j = \sum_{i=1}^{m} \mathbf{A}_i^j \mathbf{s}_i \tag{5}$$

where $\mathbf{c}^j$ is the concentration responses at the jth point due to all the m candidate sources. To make all the matrices $\mathbf{A}_i^j$ construct a square matrix, concentrations of m monitoring points should be known, then Eq. (5) can be formulated into:

$$\mathbf{C} = \mathbf{AS} \tag{6}$$

where $\mathbf{C} = [\mathbf{c}^1, \cdots, \mathbf{c}^j, \cdots, \mathbf{c}^m]^{\mathrm{T}}$, which contains concentrations at m monitoring points, $\mathbf{S} = [\mathbf{s}_1, \cdots, \mathbf{s}_i, \cdots, \mathbf{s}_m]^{\mathrm{T}}$, which contains release strengths of m sources, $\mathbf{A}$ represents the whole square matrix on the right hand side of Eq. (5). Equation (6) illustrates that the monitoring points number should be equal to the candidate sources number for dimension balance.

To identify $\mathbf{S}$ in Eq. (6) with a known $\mathbf{C}$, $\mathbf{A}$ should be inversed. However, $\mathbf{A}$ is proved to be an ill-conditioned matrix for pollutant source identification. So, Tikhonov regularization is introduced to stabilize the ill-conditioned matrix inversion as [9]:

$$\mathbf{S} = \left(\mathbf{A}^{\mathrm{T}}\mathbf{A} + \lambda^2 \mathbf{L}^{\mathrm{T}}\mathbf{L}\right)^{-1}\left(\mathbf{A}^{\mathrm{T}}\mathbf{C}\right) \tag{7}$$

where λ is the regularized parameter and L is the regularized matrix, both used to adjust the strength of regularization. Finally, locations and release strengths of the actual sources can be obtained by excluding the candidate sources that are determined to have approximate zeros of release strengths. With the monitored concentrations at several points and the airflow field as prior knowledge, no iterations are involved both in the transport probability matrix construction process and in the source identification process, hence the proposed model is an offline model.

3 Case Description

The proposed model was applied on half of a full-scale aircraft cabin for validation, as shown in Fig. 1a. The model has an inlet on the side wall near the ceiling, and an outlet near the floor, with three passengers seated inside. Three small circles above the passengers represent their nasal orifices, which are all supposed to be the candidate sources, denoted by S1, S2 and S3 from left. S1 and S2 are two actual sources, their release strengths are: S1 releases constantly with 100 ppmkg/(m^2s) for 2.5 s from the beginning, and S2 releases a sinusoidal wave for 2.5s with the peak value of 200 ppmkg/(m^2s) from the beginning. Both locations and release strengths of the actual sources are unknown before identification.

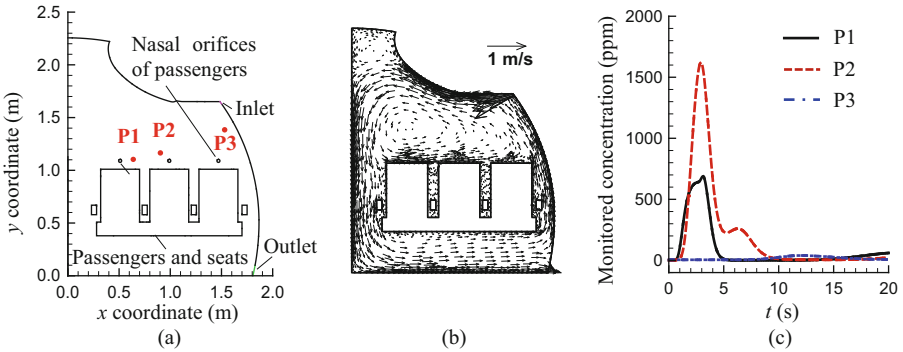

Fig. 1. Configuration of the cabin and prior knowledge for the proposed model: **a** the cabin; **b** the airflow field obtained by CFD; **c** the monitored concentrations at P1, P2 and P3.

Table 1. Boundary conditions for the aircraft cabin.

Item	Value (°C)	Item	Value
Ceiling temperature	22	Passenger surface temperature	30.3 °C
Side wall temperature	22	Air supply velocity	1.2 m/s
Luggage surface temperature	21	Air supply temperature	19.5 °C
Floor temperature	23	Turbulence intensity	10%

Prior knowledge for identification by the proposed model is the airflow field in the cabin and concentrations at the monitoring points whose number is equal to the candidate sources number, both were obtained by CFD in this study. Totally 5596 quadrilateral grids were generated in the cabin model, which has been verified by the grid independence. Boundary conditions are listed in Table 1, consistent with our previous study [14]. The turbulent flows were resolved with the renormalization group (RNG) *k-e* model with enhanced wall treatment, since y + for almost all the cells is less than 5. To solve the N-S equations, SIMPLE was selected as the pressure-velocity coupling algorithm, and PRESTO was selected for discretization of the pressure, Power Law for the momentum, while second-order upwind scheme was used for other variables. In addition, a time step size of 0.01 s was set to capture the transient features of pollutant transport with appropriate convergence criterion.

Figure 1b shows the airflow field obtained. The air supplies from the inlet, flows along the ceiling with the effect of thermal plume on passengers, then goes into the central seating region, and finally flows to the outlet. Monitored concentrations at three typical points are shown in Fig. 1c, and the monitored positions are marked in Fig. 1a with P1, P2 and P3, respectively.

4 Results

The transport probability matrix constructed in this case contains 5596 × 5596 elements, and the sum of elements in each line is verified to be 1, since the pollutant in each cell could only transport to other cells or remain in the current cell. With the obtained matrix, concentration responses at the monitoring points of a unit impulse that releases from each candidate source can be determined. Figure 2a shows the concentration responses at P2 of a unit impulse releases from S2 obtained by the proposed model and by CFD. The two profiles have quite similar trends, although the profile obtained by the proposed model seems to be a little behind that by CFD. The difference probably since that diffusion is not considered in construction of the transport probability matrix for the proposed model. Concentration fields at 5 s of the impulse releases from S2 determined by the two methods are further shown in Fig. 2b and c. Similar distributions can be seen, which shows that the high accuracy of the proposed model on prediction of the concentration responses of a unit impulse releases from the candidate sources.

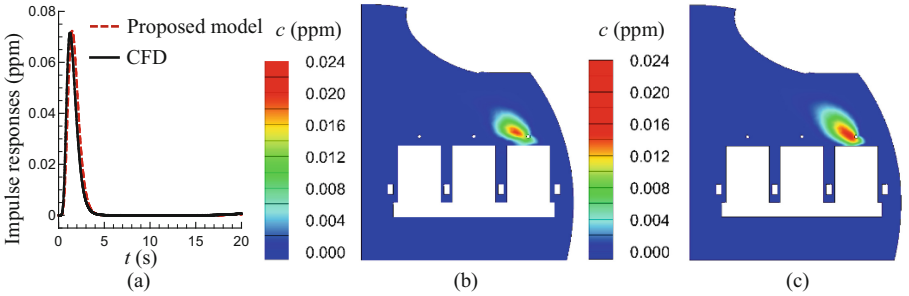

Fig. 2. Concentration responses of a unit impulse releases from S2: **a** concentration profiles at P2 obtained by the proposed model and by CFD; **b** the concentration field obtained by the proposed model at 5 s; **c** the concentration field obtained by CFD at 5 s.

Concentration responses for 20 s at 3 monitoring points of a unit impulse that releases from each candidate source were used to construct the matrix **A** in Eq. (6), which contains 3◊2000 lines and 3◊2000 columns for this case, since the time step size was set as 0.01 s. Then Tikhonov regularization in Eq. (7) was used for the matrix inversion, in which l is set as 80 to relieve the ill-condition of the matrix **A**, who has a huge condition number of 8.5210^{29}. Finally the release profiles of all the candidate sources can be determined, as shown in Fig. 3. S1 and S2 have obvious strengths, while S3 is almost zero, illustrates that S1 and S2 are two sources identified by our model. Source locations identified are consistent with the actual ones. Moreover, only slight differences can be observed when comparing the release profiles with the actual ones, shows that the proposed model could correctly identify the release strengths of multiple sources.

Computing time for the proposed model depends on the cells generated in the domain and the memory of the computer. For the validation case with 5596 cells worked on a computer with 3.7 GHz of CPU and 32 GB of memory, only less than one minute is required to construct the transport probability matrix as well as identify the multiple

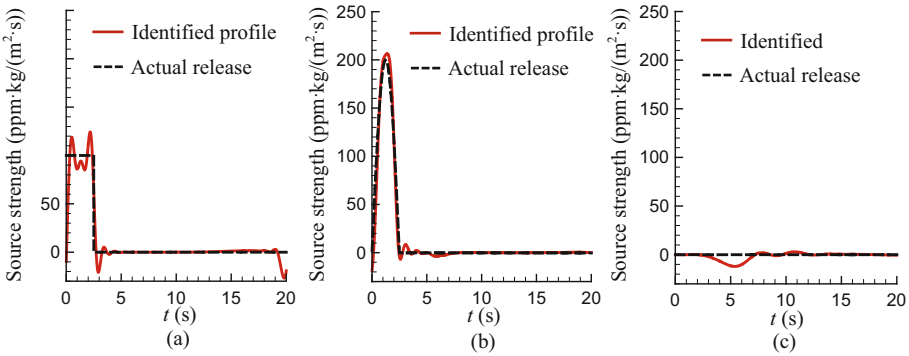

Fig. 3. Source strengths determined by the proposed model and its comparison with the actual release profiles: **a** S1; **b** S2; **c** S3.

sources. However, a few hours are required for CFD only to obtain the concentration responses of a unit impulse releases from each source, let alone the multiple sources identification. More than 90% of the computing time can be saved, which shows the high efficiency of the proposed model.

5 Conclusions

This study proposed an offline method combines Markov chain and Tikhonov regularization to rapidly and correctly identify multiple sources in aircraft cabins. By applying the model on an aircraft cabin, it is proved that the proposed model is capable of identifying the locations and release strengths of multiple sources, with the airflow field and concentrations at several monitored positions as prior knowledge. In addition, more than 90% of the computing time can be saved by the proposed model in comparison with the conventional CFD method, which shows its high efficiency.

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