A Model Based on Markov Chain for Prompt Prediction of the Airborne Gaseous Pollutant Transport in Aircraft Cabins

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Abstract. Prompt prediction of the airborne gaseous pollutant transport is important to design a safe and comfortable air environment in an aircraft cabin. This paper proposes a model based on Markov chain to fulfill the task, in which the gaseous pollutant can be released from a source with an arbitrary profile. The model first obtains the airflow field by CFD to construct a transport probability matrix of the gaseous pollutant, then predicts the concentration field at each time step when an impulse is released at the known source location using the transport probability matrix. Finally, detailed trace of the pollutant released from the source with an arbitrary profile can be reproduced by linear superposition. The above strategy is applied on a two-dimensional aircraft cabin with gaseous pollutant released from one passenger for 2s. Results show that the proposed model is able to correctly predict the gaseous pollutant transport in only a few minutes. More than 90% of the computing time can be saved comparing with that from CFD without sacrificing much accuracy.

1 Introduction

The outbreak of Corona Virus Disease 2019 (COVID-19) in recent years has showed the great importance of airborne gaseous pollutant control for a safe air environment. However, conventional design methods could only monitor the pollutant concentrations by placing several sensors at typical positions in environments, in which traces of the pollutant cannot be provided. An effective method to describe the gaseous pollutant transport process is urgently required for protecting the inside occupants from infection.

Currently, computational fluid dynamics (CFD) has been widely used as a convenient tool to simulate the gaseous pollutant transport. Mora et al. [1] compared zonal model with CFD for prediction of the gaseous pollutant transport in large indoor spaces, and suggested that CFD could be an effective tool for prediction of the indoor pollutant transport in which more accurate details were required; Topp et al. [2] used CFD to observe the emission of vapors and VOCs from indoor building surfaces. Besides the above common contaminants, CFD was also used in some studies to simulate the transport of radioactive gases in indoor environments. For example, Chauhan [3] studied the transient transport of Radon in a living room by CFD, and analyzed the effect of natural ventilation on the indoor Radon distribution; Devi and Chauhan [4] observed thoron dispersion in an indoor environment by CFD, to find techniques for mitigating the exposure of indoor radioactive gases. Several studies also combined CFD with their proposed models to predict the pollutant transport. For example, Chang et al. [5] proposed to combine CFD with a multi-room pollutant transport model for simulation of the traffic-induced CO transport from outdoor to indoor; Marlow et al. [6] coupled a multidisciplinary method with CFD to obtain the indoor pollutant dispersion that considered the effects of human movements. Above studies show that CFD is able to provide detailed information of pollutant transport. However, the simulation process may take a long time, which is quite time-consuming.

To improve the computing efficiency, Zuo and Chen applied fast fluid dynamics (FFD) [7] for simulation of the airflow and contaminant dispersion in buildings. In the method, pressure and velocity were decoupled, and the advection term and the diffusion term were also solved with simple schemes different from that used in CFD; Cao et al. [8-9] proposed a linear low-dimensional ventilation model derived from the Navier-Stokes equations to rapidly reconstruct a low-dimensional pollutant concentration distribution. Current methods for fast simulation all require to solve scalar transport equations online or offline, strategies for further improvement of the computing efficiency are still expected.

In recent years, Markov chain technique has been developed for rapid prediction of the pollutant transport in indoor environments. Since no iterations are involved in the method, much computing time can be saved. Zeng et al. [10], Nicas [11] and Deng et al. [12] applied Markov chain to obtain the dynamic pollutant concentration in multi-zones. However, for these studies, the air environment can only be divided into several zones, in which details of the pollutant transport cannot be obtained. Chen et al. proposed to use Markov chain

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for characterizing the transient particle transport [13] and Mei et al. further used the technique to predict the dynamic dispersion and deposition of particles [14]. Despite their efforts, only particles from an impulse source or in a simple chamber can be predicted by the method. Few studies have predicted the airborne gaseous pollutant transport in actual complicated environments, which is essential to the control of indoor air quality. Hence, this study proposed a model based on Markov chain, which is able to promptly predict transport of the airborne gaseous pollutant released from a source with an arbitrary profile in aircraft cabins.

2 Methods

2.1 Principles of the proposed model based on Markov chain

The proposed model first obtains the airflow field in the air domain by CFD to solve the airflow rate through faces of each cell. Then Markov chain technique is introduced to predict the pollutant transport from sources with the fixed airflow field. Probability of the gaseous pollutant transport is a main thread runs through the method, which can be solved based on the corresponding airflow rate ratios as:

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

where $p_{i,j}$ means the probability of pollutant transporting from the i^{th} cell to the j^{th} cell in the next time step, $p_{i,i}$ means the probability of pollutant remaining in the current i^{th} cell, $Q_{i,j}$ means the airflow rate from the i^{th} cell to the j^{th} cell, and $\sum Q_{i,nbhd}$ means the sum of the airflow rate from the i^{th} cell to other cells. Pollutant in the current cell can only flow to the neighbouring cells or remain in the current cell in the next time step, so the airflow rates from the i^{th} cell to other cells that are not adjacent to it are zeros.

In Eq. (1), $p_{i,i}$ can be obtained from the mass conservation law as:

$$p_{i,i} = \exp\left(-\frac{\sum Q_{i,nbhd}}{V_i}\Delta t\right) \tag{2}$$

where V_i is the volume of the i^{th} cell.

With $p_{i,i}$ and $p_{i,j}$ obtained from Eqs. (1) and (2), a transport probability matrix can be constructed as:

$$P = \begin{pmatrix} p_{1,1} & p_{1,2} & \cdots & p_{1,n} \\ p_{2,1} & p_{2,2} & \cdots & p_{2,n} \\ \cdots & \cdots & p_{i,i} & \cdots \\ p_{n,1} & p_{n,2} & \cdots & p_{n,n} \end{pmatrix} \tag{3}$$

where the subscript n represents the total number of cells used in CFD.

The initial pollutant concentration field when an impulse is released at the known source location, denoted as C_0, can be directly obtained once the source location is known, and the initial pollutant amount field can be solved as:

$$M_{0,i} = C_{0,i}V_i \tag{4}$$

where $C_{0,i}$ means the initial concentration in the i^{th} cell, while $M_{0,i}$ means the corresponding initial pollutant amount field. Then the pollutant amount field of the impulse release after k time steps M_k can be obtained as:

$$M_k = M_0 P^k \tag{5}$$

With Eq. (5), the concentration field at the k^{th} time step when an impulse is released at the known source location can be obtained by dividing the volume into M_k for each cell. Finally, transport of the pollutant released from the source with an arbitrary profile can be predicted, by using linear superposition upon the concentration fields at the corresponding time steps. Since no iterations are involved, the prediction process can be very fast.

2.2 Solution procedure for the proposed model

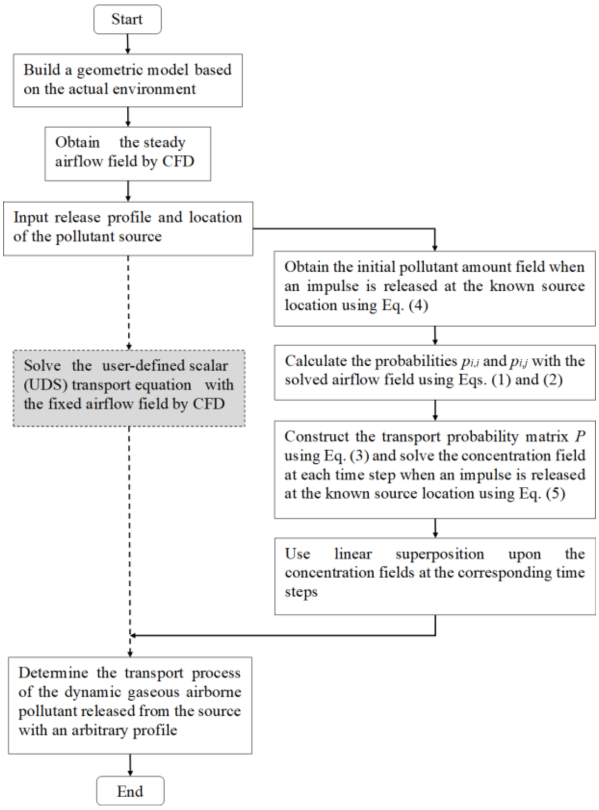


Fig. 1. Solution procedure for the proposed model based on Markov chain to predict the airborne gaseous pollutant transport, and its comparison with the conventional CFD method (the grey box and the dotted lines represent the CFD process that is replaced by the proposed model)

Fig. 1 shows the solution procedure for the proposed model to predict transport of the airborne gaseous pollutant releases from a source. Iterations in each time step when solving the UDS transport equation with the fixed airflow field for the conventional CFD method are replaced by simple multiplications and linear superposition for the proposed model, so much time can be saved.

3 A demonstration case

A two-dimensional aircraft cabin model is used for validation of the proposed model, whose width is 4.6 m on the floor level and height is 2.07 m in the maximum, as shown in Fig. 2(a). Frames in the cabin represent legs of 7 seated passengers and part of seats, while 7 circles in the central region represent nostrils of the passengers. Two nostrils of each passenger are simplified as one circle shown in the figure. The airborne gaseous pollutant is supposed to be released from nostril of the 7th passenger from left for 2s with 100 ppm, and one sensor is placed to monitor the dynamic pollutant concentration, whose position is shown in the figure. The air supply openings are installed on the ceiling, with 1.54 m/s and 19.7 °C of the air supply velocity and temperature, while the exhausts are on the two sides near the floor for outflows of the mixed air. Surface temperatures of floor and lamps are set as 24.5 °C and 25.6 °C, respectively, and passengers are 30.3 °C, while others are all set as 24.2 °C, which are consistent with our previous studies [15].

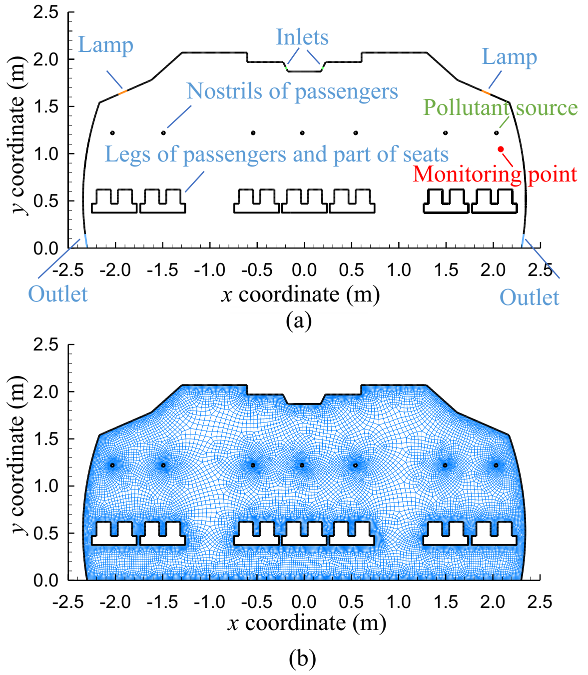


Fig. 2. A vertical section of an aircraft cabin used for validation of the proposed model on pollutant transport prediction: (a) sketch of the cabin; (b) meshes generated in the domain.

To obtain the steady airflow field in the cabin model by CFD, meshes should be generated in the air domain first. With comparison of the solved thermo-flow fluids in three cell numbers, 8731, 24348, and 48946, respectively, the middle size with totally 24348 grids is finally used in the paper to satisfy the grid independence, as shown in Fig. 2(b), in which the grids near boundaries are much smaller than that in the central region.

For CFD settings, the pressure staggering option (PRESTO) scheme is selected for discretization of the pressure term in the Navier-Stokes equations, and the second-order upwind scheme is applied for other terms. Semi-implicit pressure linked equation (SIMPLE) scheme which couples the pressure and velocity in iterations is also adopted to obtain the solution. In addition, the renormalization group (RNG) k-ε model plus enhanced wall treatment are used for turbulence flows, since airflows in the aircraft cabin have low Reynolds number and y+ for almost all the near-wall cells in the domain are less than 5.

4 Results

4.1 Steady airflow field

Fig. 3 shows the steady airflow field obtained by CFD. The air supplies from the two inlets on the ceiling, then flows to the side walls, and finally forms two big vortices near the passengers.

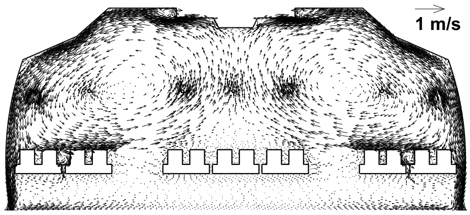


Fig. 3. Airflow field in the cabin model obtained by CFD

4.2 Prediction of the pollutant transport

Fig. 4 shows the obtained airborne gaseous pollutant concentrations at the monitoring point per second for 10 s by the proposed method and its comparison with that by CFD. The pollutant is released from the source at 0 s, and a time step size of 0.01s was set for both methods to capture the transient features. Results show that the profiles obtained by the two methods have identical trends, although there are slight differences on values, which may be due to the fact that diffusion is almost ignored for the current proposed model. The difference is largest near the peak, so below we further compare the concentration fields at 2.5 s, 3s and 5s by the two methods, as shown in Figs. 5, 6 and 7.

At 3 s, as shown in Fig. 6, the concentrations near the source obtained by the proposed model are slightly lower than that by CFD, while in other figures, almost no difference can be observed, showing that the pollutant concentrations obtained by the proposed model agree very well with that by the conventional CFD method. In addition, the transport trends obtained by the two methods shown in Figs. 5, 6 and 7 are consistent with the airflow field shown in Fig. 3, in which the airborne gaseous pollutant gathers near the source at the beginning, then goes down due to the gravity, and finally disperses into the central seating region with the effect of thermal plume. Profiles in Fig. 4 also prove this point, in which the concentrations at the monitoring point near the 7th passenger increase first and then decrease.

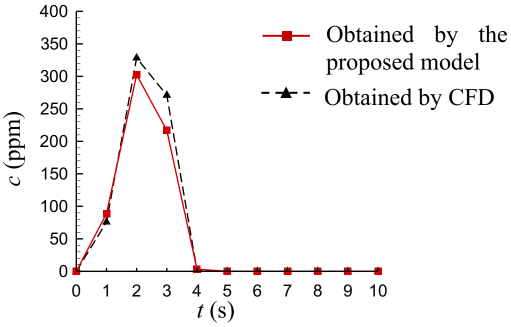
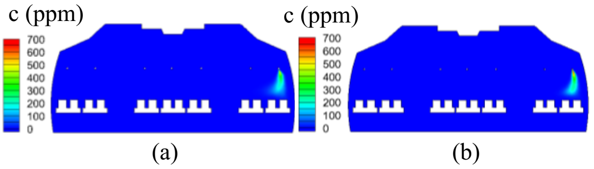


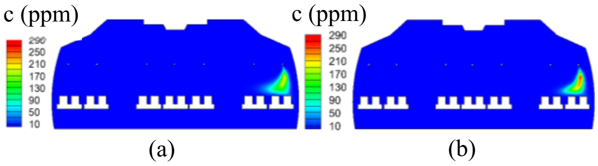
Fig. 4. Comparison of the pollutant concentrations at the monitoring point per second for 10 s obtained by the proposed model and by CFD

For the computing time, only a few minutes are required by our proposed model to construct the transport probability matrix as well as to obtain the dynamic pollutant transport from an arbitrary source. However, for CFD simulation, a few hours at least are required to fulfill the task. More than 90% of the time can be saved by the proposed model without sacrificing much accuracy, since iterations involved in the CFD simulation are replaced by superposition and simple multiplications between vectors and matrices.



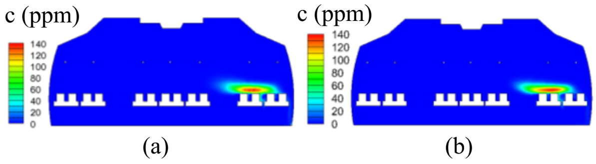
(a) (b)

Fig. 5. Comparison of the concentration field in the cabin at 2.5 s: (a) by the proposed model; (b) by CFD



(a) (b)

Fig. 6. Comparison of the concentration field in the cabin at 3.0 s: (a) by the proposed model; (b) by CFD



(a) (b)

Fig. 7. Comparison of the concentration field in the cabin at 5.0 s: (a) by the proposed model; (b) by CFD

5 Discussion

In the validation case, 0.01 s was used as the time step size for the proposed model, which was in keeping with the CFD setting, and we found that larger time step sizes for the proposed model may reduce the solution accuracy although more computing time could be saved. So proper time step size is a key factor for balance between the solution accuracy and efficiency, which will be researched in future. Pollutant diffusion will also be added into the model in future to further improve the prediction accuracy. In addition, Experiments for validation of the CFD accuracy and extension of the proposed model on transport prediction of multiple sources may be the main direction of the future work as well.

6 Conclusions

This paper proposes a model based on Markov chain, which solves the airflow field by CFD first, and then constructs the transport probability matrix to reproduce the pollutant transport process. Validation of the proposed model on a two-dimensional aircraft cabin shows that the proposed model can correctly predict the airborne gaseous pollutant with more than 90% of the computing time be saved.

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