PREDICTING TRANSIENT PARTICLE TRANSPORT IN ENCLOSED ENVIRONMENTS BASED ON MARKOV CHAIN

Chun Chen[1], Chao-Hsin Lin[2], Qingyan Chen[1,3*]
[1] School of Mechanical Engineering, Purdue University, West Lafayette, IN 47907, USA
[2] Environmental Control Systems, Boeing Commercial Airplanes, Everett, WA 98203, USA
[3] School of Environmental Science and Engineering, Tianjin University, Tianjin 300072, China

ABSTRACT

Quick information of airborne infectious disease transmission in enclosed environments is critical to reduce the risk of infection of occupants. This study developed a combined CFD and Markov chain method for quickly predicting the transient particle transport in enclosed environments. The method firstly calculated a transition probability matrix using CFD simulation. Then the Markov chain technique was applied to calculate the transient particle concentration distribution. This investigation used three cases, particle transport in an isothermal clean room, an office with Under-Floor Air-distribution system and the first-class cabin of an MD-82 airliner, to validate the combined CFD and Markov chain method. The transient particle concentration distribution predicted by the Markov chain method reasonably agreed with the CFD simulation for these cases. The proposed Markov chain method can provide faster-than-real-time information of particle transport in enclosed environments. Furthermore, for a fixed airflow field, when the source location is changed, the Markov chain method can avoid the re-calculations of the particle equations and thus reduce the computing cost.

INTRODUCTION

The transmission of airborne infectious diseases, such as tuberculosis (TB), influenza, and severe acute respiratory syndrome (SARS), has become one of the major public health concerns (Li et al., 2007). Compared with the outdoors, enclosed environments such as vehicles and buildings with low air exchange rate tend to be more susceptible to the transmission of airborne infectious diseases (Mangili and Gendreau, 2005). For instance, the outbreaks of influenza in aircrafts (Moser et al., 1979), measles in offices (Bloch et al., 1985), tuberculosis in hospitals (Menzies et al., 2000) and SARS in aircrafts (Olsen et al., 2003) and hospital wards (Li et al., 2005) have happened in the past decades. All of these outbreaks have been proven to be associated with the airflow patterns in the enclosed environments (Li et al., 2007). Exhalation activities such as breathing, coughing, talking, and sneezing by an infected person can generate particles carrying pathogen and cause the transmission of infectious diseases (Nicas et al., 2005; Morawska, 2006). Hence, it is essential to predict the transient particle transport in enclosed environments.

In recent years, Computational Fluid Dynamics (CFD) has been widely used in modeling transient particle transport in mechanical ventilated spaces. Zhao et al. (2005) applied a zero equation turbulence model with an Eulerian method to investigate the exhaled particle transport during breathing, coughing and sneezing in a ventilated room. Zhang and Chen (2007) compared the Eulerian and Lagrangian methods for predicting respiratory particle transport from a single cough in a four-row aircraft cabin. Gupta et al. (2011) and Zhang and Li (2012) used the RNG k-ε model with a Lagrangian method to calculate the droplets transport in an aircraft cabin and a fully-occupied high-speed rail cabin, respectively. Li et al. (2011) and Seepana and Lai (2012) investigated the person-to-person particle transport under various ventilation modes using an Eulerian drift flux model. Chen et al. (2013) further developed a hybrid DES-Lagrangian and RANS-Eulerian model to calculate transient particle transport in enclosed environments. These models have become more and more popular for investigating interpersonal particle transport. However, when the source location is changed, even for a fixed airflow field, all of these models require the re-calculation of the particle equations, which may consume considerable computing effort. Thus, it is worthwhile to develop an approach for quickly predicting transient particle transport in enclosed environments.

To quickly assess the transient particle transport, Nicas (2000) applied the Markov chain technique in a multi-zone model. They have shown the capability of the Markov chain technique in quickly predicting the spatial and temporal particle concentrations. However, this simple model failed to account for most of the particle dispersion mechanisms such as drag force, gravitational settling and turbulent dispersion. Since CFD simulation can easily take these influencing factors into account, it has the potential of coupling with the Markov chain technique to significantly improve the model. Therefore, this paper aims to develop and validate a combined CFD and Markov chain method for quickly predicting the transient particle transport in enclosed environments.

METHODS

Markov chain model

There are two assumptions of the first-order homogeneous Markov chain technique (Ross, 1996):

1) Any future state depends only on the present state as well as the probabilities of the state changing;

2) These probabilities of the state changing are time-independent (or fixed).

To satisfy these assumptions of Markov chain technique, an assumption of particle transport prediction has to be made. That is the inertial effect of particles is negligible, which holds well for the particles with a diameter is smaller than 3 μm (Zhao et al., 2009; Yin et al., 2011).

The first step is to divide the target enclosed environment into n-1 zones. The zone n can be assigned to represent where the particles were removed. Then the probabilities of the state changing can form an n×n transition probability matrix, p_{ij}:

$$P = (p_{ij})_{(n\times n)} = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{pmatrix} \tag{1}$$

p_{ij} is the probability of a particle moves from zone i to zone j in a certain time step, Δt. The most important property of the transition probability matrix is:

$$\sum_{j=1}^{n} p_{ij} = 1 \quad , \quad p_{ij} \geq 0 \tag{2}$$

It should be noticed that, if we assume that the removed particles cannot re-enter the space, which is corresponding to the scenario of all fresh air ventilation system, then:

$$p_{nj} = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \end{pmatrix} \tag{3}$$

For a fixed airflow field, it is expected that the transition probability matrix is also fixed since the movement of the particles is mainly determined by the airflow field.

Assuming a particle has a probability vector at the present state (state k):

$$\pi_k = \begin{pmatrix} \pi_{k,1} & \pi_{k,2} & \cdots & \pi_{k,n} \end{pmatrix} \tag{4}$$

then, after one time step (state k+1), the probability of this particle moves to zone j can be calculated by:

$$\pi_{k+1,j} = \pi_{k,1} p_{1,j} + \pi_{k,2} p_{2,j} + \cdots + \pi_{k,n} p_{n,j} \tag{5}$$

Thus, the probability vector for the particle at state k+1 can be calculated by:

$$\pi_{k+1} = \pi_k P \tag{6}$$

If the particle is initially released from zone m, the probability vector of the particle at the initial state (state 0) is:

$$\pi_{0,i} = \begin{cases} 1, & i = m \\ 0, & i \neq m \end{cases} \tag{7}$$

If we calculate the particle transport from the state 0, the probability vector of the particle at state k+1 can be calculated by:

$$\pi_{k+1} = \pi_0 P^{k+1} \tag{8}$$

The obtained probability vector versus time can be regarded as the normalized particle concentrations versus time in the zones. Therefore, the Markov chain technique can be used for predicting transient particle transport in enclosed environments. Moreover, when the source location is changed, Eq. (8) can be used with an updated π_0 to quickly calculate the updated particle concentrations versus time.

Calculating transition probability matrix using CFD

The key point of applying the Markov chain technique to indoor particle transport prediction is to obtain the transition probability matrix, p_{ij}. We first calculated the airflow field by CFD simulation. Then we uniformly released a certain amount of particles in zone i, and used the Lagrangian stochastic tracking to calculate the percentage of the particles that move from zone i to zone j for a certain time, Δt, which can be regarded as the p_{ij}. The following paragraphs detail the CFD model used in this study.

The renormalization group (RNG) k-ε model (Choudhury, 1993) was applied to calculate the airflow field. It has the best overall performance among all RANS models for enclosed environments (Zhang et al., 2007). The details of the RNG k-ε model can be found in Fluent Inc. (2005).

The Lagrangian model was adopted to calculate the particle movements in Δt. Using the momentum equation based on Newton's law, the trajectory of each particle can be calculated by:

$$\frac{d\vec{u}_p}{dt} = F_D(\vec{u}_a - \vec{u}_p) + \frac{\vec{g}(\rho_p - \rho_a)}{\rho_p} + \vec{F}_a \tag{9}$$

where $\vec{u}_p$ is the velocity vector of the particle; $\vec{u}_a$ the velocity vector of air; $\vec{g}$ the gravitational acceleration vector; ρ_p and ρ_a the particle and air density, respectively; and $\vec{F}_a$ Brownian motion and Saffman life force. The Saffman lift force was included since it may be relatively large near a room's wall for fine indoor particles (Zhao et al., 2004). The drag force is calculated by:

$$F_D(\vec{u}_a - \vec{u}_p) = \frac{18\mu}{\rho_p d_p^2}\frac{C_D \operatorname{Re}}{24}(\vec{u}_a - \vec{u}_p) \tag{10}$$

where μ is fluid viscosity, C_D the drag coefficient, Re Reynolds number, and d_p particle diameter. The transient process from a droplet to a droplet nucleus due to evaporation is negligible for the particles with a diameter smaller than 3 μm (Chen and Zhao, 2010).

The Discrete Random Walk (DRW) model (Fluent Inc., 2005) is used to calculate the turbulence dispersion:

$$u_i' = \zeta_i\sqrt{2k/3} \tag{11}$$

where ξ_i is a normal random number.

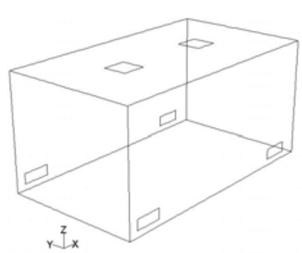
Note that the time step of the Markov chain, Δt, is an important parameter that needs to be determined based on the ventilation rate of the space and the size of the divided zones. The Δt can be neither too short nor too long. If the Δt is too short, the particles may have no chance to "escape" from the current zone. If the Δt is too long, some significant information of the particle movements may be missing. Thus, the Δt should allow the particles move to only the adjacent zones.

VALIDATION

This study used three cases, particle transport in an isothermal clean room (Murakami et al., 1992), a room with Under-Floor Air-distribution (UFAD) system (Zhang and Chen, 2006) and the first-class cabin of an MD-82 airliner (Liu et al., 2013; Chen et al., 2013), to validate the combined CFD and Markov chain method.

Particle transport in an isothermal clean room

The first study selected the particle transport case in a ventilated clean room by Murakami et al. (1992). Figure 1(a) shows the configuration of the clean room with two ceiling supply diffusers and four exhausts located at the lower walls of the room. The total air exchange rate was 40 ACH. As shown in Figure 1(b), we divided the room into 6 zones and set the "removal zone" as zone 7.



(a)

2	4	6
1	3	5

Removed: 7

(b)

Figure 1 (a) Configuration of the clean room studied by Murakami et al. (1992); (b) divided zones from the bird view of the clean room.

Based on the calculated airflow field and Lagrangian particle tracking, the transition probability matrix can be obtained:

$$P = \begin{pmatrix} 0.61 & 0.01 & 0.07 & 0.00 & 0.00 & 0.00 & 0.31 \\ 0.04 & 0.63 & 0.00 & 0.01 & 0.00 & 0.00 & 0.32 \\ 0.08 & 0.00 & 0.69 & 0.10 & 0.13 & 0.00 & 0.00 \\ 0.00 & 0.15 & 0.04 & 0.70 & 0.00 & 0.10 & 0.00 \\ 0.00 & 0.00 & 0.03 & 0.00 & 0.70 & 0.02 & 0.25 \\ 0.00 & 0.00 & 0.00 & 0.03 & 0.02 & 0.67 & 0.27 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 \end{pmatrix} \tag{12}$$

The time step of the Markov chain, Δt, was set as 15 s for this case, which can ensure the particles moving to only the adjacent zones within the Δt. Two scenarios, the particle source was located in zone 3 and 6, respectively, were used to validate the Markov chain method. The initial probability vector was:

$$\begin{aligned} \pi_0 &= \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \textit{source in zone } 3 \\ \pi_0 &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \textit{source in zone } 6 \end{aligned} \tag{13}$$

Using Eq. (8), the probability vectors versus time of the particle transport can be calculated.

Although the airflow field and steady-state particle dispersion has been validated by the experimental data for this case (Wang et al., 2012), the experimental data of transient particle concentrations were unavailable. Thus, this study used the calculated particle concentrations versus time by RNG k-ε – Eulerian drift flux model as a bench mark.

Figure 2 and 3 compares the trends of the normalized particle concentrations versus time by Markov chain method and CFD simulations with a source in zone 3 and 6, respectively. The CFD simulation results were obtained by averaging the particle concentrations in each zone. Furthermore, all the particle concentrations were normalized by the maximum concentration appears in the room. Figure 2 shows that both the Markov chain and CFD method predicted higher particle concentrations in zone 1, 4 and 5 compared with that in zone 2 and 6. That was because zone 1, 4 and 5 were adjacent to zone 3 where the source located. Comparing Figure 2 with 3, both the Markov chain and CFD method predicted higher particle concentrations with a source in zone 3 than that with a source in zone 6. The results make sense since a large portion of particles were directly removed through the exhaust located in zone 6 and resulted in low concentrations in other zones for the latter case. In general, the trends of transient particle transport predicted by the Markov chain method agreed well with the results by CFD simulation.

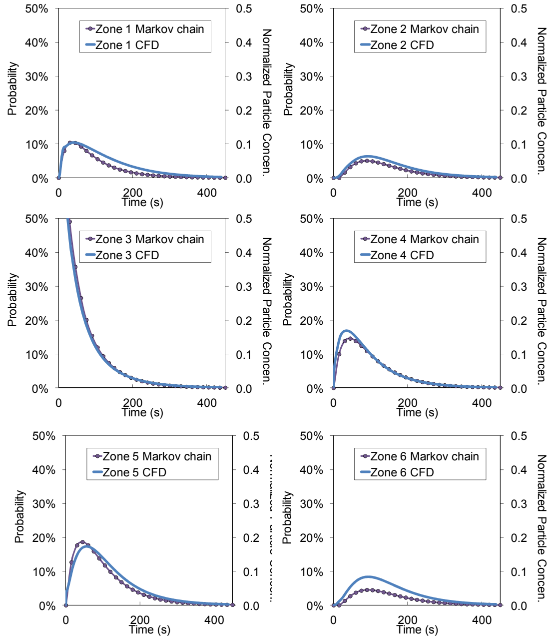


Figure 2. Comparison of the trends of the normalized particle concentrations versus time by Markov chain method and CFD simulation with a source in zone 3 for the isothermal clean room.

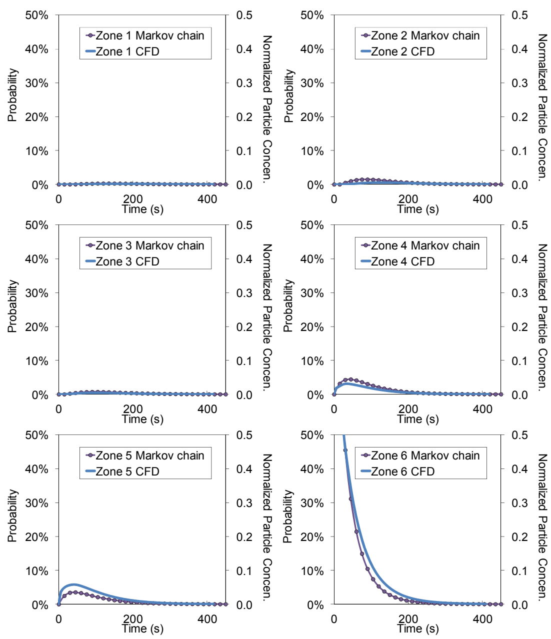
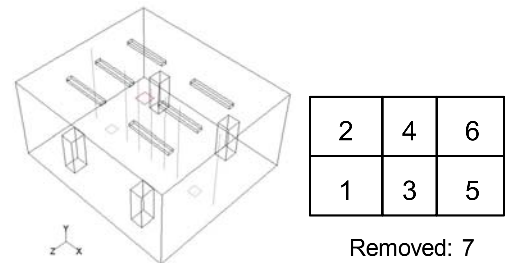


Figure 3. Comparison of the trends of the normalized particle concentrations versus time by Markov chain method and CFD simulation with a source in zone 6 for the isothermal clean room.

Particle transport in a room with UFAD system

The investigation chose the second case as a room with Under-Floor Air-Distribution (UFAD) system, as shown in Figure 4(a) (Zhang and Chen, 2006). Four heated boxes were used to simulate occupants in the room. The air supplied from the two floor inlets, and was exhausted from the exhaust at the ceiling. The total air exchange rate was 5.5 ACH. As shown in Figure 4(b), we divided the room into 6 zones and set the "removal zone" as zone 7.



(a) (b)

Figure 4. (a) Configuration of the room with UFAD system studied by Zhang and Chen. (2006); (b) divided zones from the bird view of the room.

Based on the calculated airflow field and the Lagrangian particle tracking, the transition probability matrix can be obtained:

$$P = \begin{pmatrix} 0.85 & 0.04 & 0.11 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.05 & 0.82 & 0.00 & 0.13 & 0.00 & 0.00 & 0.00 \\ 0.15 & 0.00 & 0.78 & 0.07 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.15 & 0.00 & 0.73 & 0.00 & 0.00 & 0.12 \\ 0.00 & 0.00 & 0.14 & 0.00 & 0.77 & 0.09 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.09 & 0.07 & 0.84 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 \end{pmatrix} \tag{14}$$

The time step of the Markov chain, Δt, was set as 25 s for this case. Two scenarios, the source located in zone 4 and 6, respectively, were used to validate the Markov chain method. The initial probability vector was:

$$\begin{aligned} \pi_0 &= (0\ 0\ 0\ 1\ 0\ 0\ 0), \quad \textit{source in zone}\ 4 \\ \pi_0 &= (0\ 0\ 0\ 0\ 0\ 1\ 0), \quad \textit{source in zone}\ 6 \end{aligned} \tag{15}$$

Due to the lack of the experimental data of transient particle concentrations, this study again used the CFD results as a bench mark for this study. Figure 5 and 6 compares the trends of the normalized particle concentrations versus time by Markov chain method and CFD simulation with a source in zone 4 and 6, respectively. The CFD simulation results were again obtained by averaging the particle concentrations in each zone. Comparing Figure 5 with 6, both methods predicted lower concentrations for the case with a source in zone 4. That was because a considerable portion of particles released from zone 4 tended to be directly removed by the exhaust located in zone 4. Generally speaking, the trends of the normalized particle concentrations predicted by Markov chain method again agreed well with the CFD simulation. However, since this case is more complicated than the isothermal clean room case, the agreement tends to be somewhat worse than the clean room case.

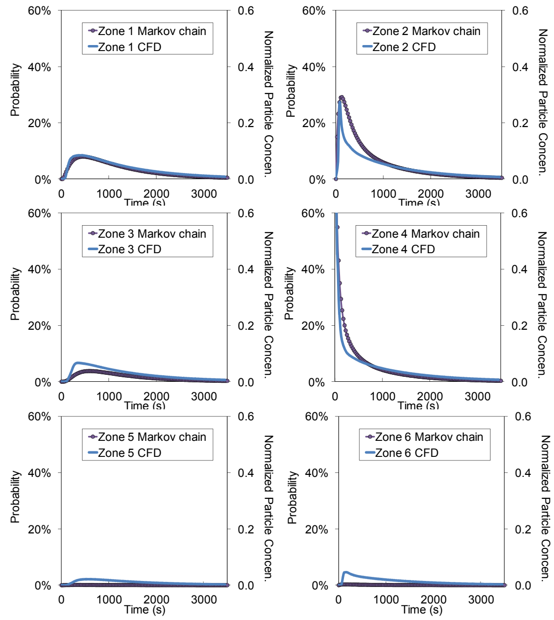


Figure 5. Comparison of the trends of the normalized particle concentrations versus time by Markov chain method and CFD simulation with a source in zone 4 for the room with UFAD system.

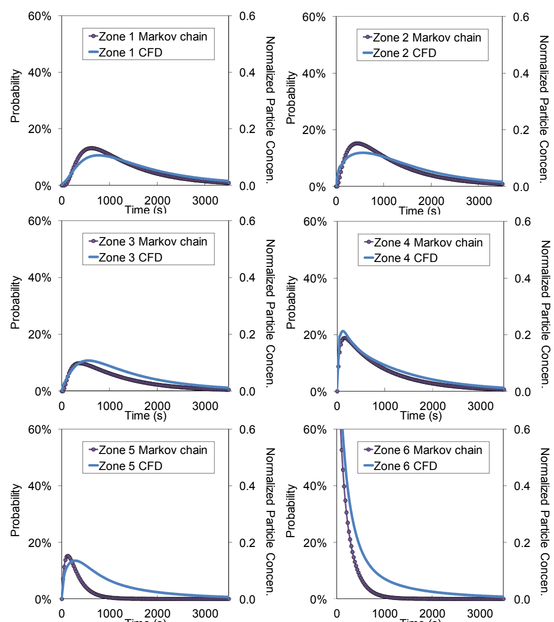
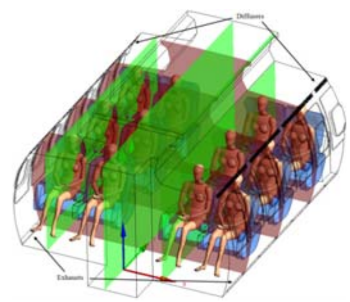


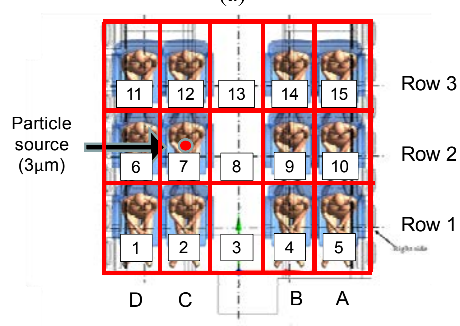
Figure 6. Comparison of the trends of the normalized particle concentrations versus time by Markov chain method and CFD simulation with a source in zone 6 for the room with UFAD system.

Particle transport in an MD-82 aircraft cabin

The study used the third case as the first-class cabin of a functional MD-82 commercial airliner, as shown in Figure 7(a) (Liu et al., 2013). The cabin had three rows of seats, and each row contained four seats as numbered in Figure 7(b). The sensible heat production of the heated manikin was 75 W. The airflow and thermal boundary conditions of the first-class cabin were measured previously by Liu et al. (2013). At the mouth of the manikin 2C, particles with a diameter of 3 μm were released to the cabin air for 20 s. The particle concentrations versus time at the breathing zones were measured in front of each passenger's mouth. A detailed description of the experimental procedure and data analysis can be found in Chen et al. (2013). Both the experimental data and CFD simulation were used to validate the Markov chain method. As shown in Figure 7(b), we divided the room into 15 zones and set the "removal zone" as zone 16.



(a)



(b)

Figure 7. (a) Configuration of the aircraft cabin (Liu et al., 2013); (b) divided zones from the bird view of the cabin.

Based on the calculated airflow field and the Lagrangian particle tracking, the transition probability matrix can be obtained. The time step of the Markov chain, Δt, was set as 4 s for this case. To better match the experimental setup, in zone 7 where the source located, the particles were released only from the month of the manikin instead of the whole space of zone 7.

Figure 8 compares the trends of the normalized particle concentrations versus time by the Markov chain method, CFD simulation and experimental data. The Markov chain method correctly predicted relatively high peak concentrations at 1B and 1C and low concentrations at most of the other locations. However, the Markov chain method over-predicted the concentrations at 1D and 2D. We suspected that the discrepancies were mainly attributed to two reasons. First, the differences between the modeled and measured airflow fields were significant, which might result in the discrepancies of particle concentrations (Chen et al., 2013). Second, the Markov chain method calculated the average particle concentrations in each zone, while the experimental data only represented the concentrations at the breathing zones. To validate this hypothesis, we calculated the average particle concentrations in each zone by CFD simulation as shown in Figure 8. It can be seen that the CFD simulation also over-predicted the concentrations at 1D and 2D. Generally speaking, the Markov chain method can predict the transient particle concentration distribution with reasonable accuracy for engineering applications.

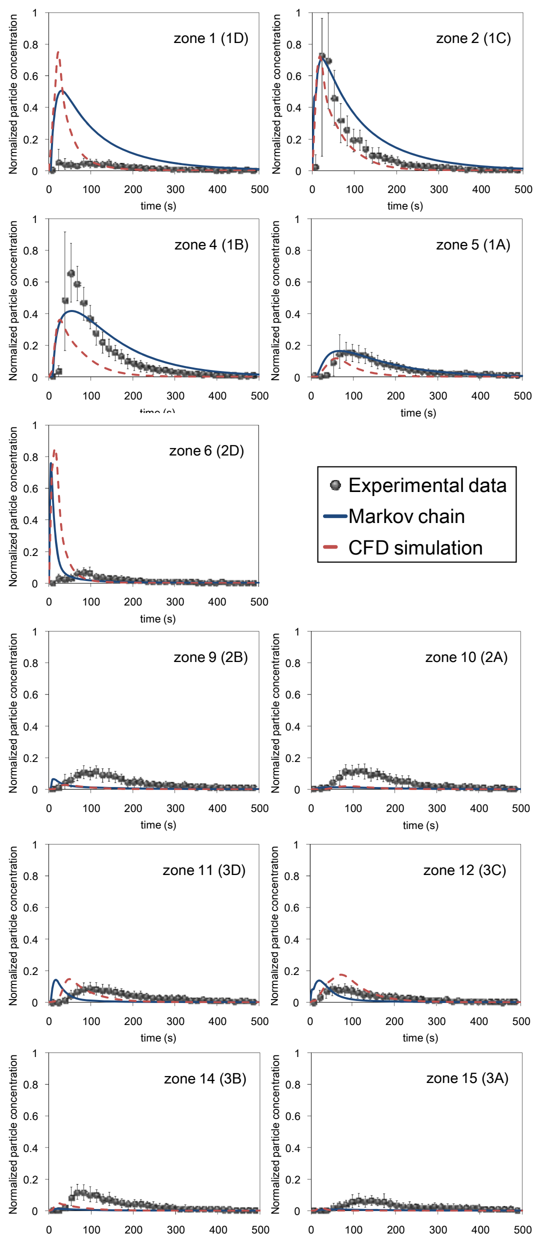


Figure 8. Comparison of the trends of the normalized particle concentrations versus time by Markov chain method, CFD simulation and experimental data (Chen et al., 2013) for the aircraft cabin.

DISCUSSION

Quick information of airborne infectious disease transmission in enclosed environments is crucial to reduce the risk of infection of occupants. The Markov chain method can provide faster-than-real-time information of particle transport in enclosed environments, since Eq. (8) only requires simple matrix multiplications. Furthermore, for a fixed airflow field, when the index patient or the source location is changed, Eq. (8) can still be used with an updated initial probability vector. That can avoid the re-calculations of particle equations and thus reduce the computing cost.

Currently, either deterministic or probabilistic approaches can be used for risk assessment of airborne infectious disease transmission (Gupta et al., 2012). For the deterministic approaches, the risk or the probability of getting infected cannot be quantified. For the probabilistic approaches, since the quanta exhaled cannot be directly determined, people have debated about their accuracy (Sze To and Chao, 2010). The Markov chain method predicts the probability of a particle appears in a zone at a certain time point. Since the movements of the indoor particles tend to be independent, the calculated probabilities should be independent probabilities. Through simple calculations of the joint probability and the probability of either event occurring, we can calculate the probability of a certain number of particles appear in the breathing zone of the receptor. For instance, if the index patient exhales 100 particles, we can calculate the probability that 10 out of these 100 particles appear in the breathing zone. Thus, the Markov chain with probability calculations has the potential of accounting for both deterministic and probabilistic information.

In addition, the Markov chain method also has the potential of accounting other influencing factors of infectious disease transmission. For instance, through slightly modifying the transition probability matrix, the effect of contaminated return air and filter can be easily assessed using the Markov chain method. The effectiveness of wearing masks and the effect of temperature/humidity on virus survival can also be investigated using the similar approach. The detailed methods and demonstrations of risk assessment using Markov chain method will be presented in a companion paper.

CONCLUSIONS

This paper developed a combined CFD and Markov chain method for predicting the transient particle transport in enclosed environments. From the results presented in this paper, the following conclusions can be drawn:

(1) The proposed combined CFD and Markov chain method can predict the transient particle transport in enclosed environments with reasonable accuracy.

(2) The Markov chain method can provide faster-than-real-time information of particle transport in enclosed environments.

(3) For a fixed airflow field, when the source location is changed, the Markov chain method can be used to avoid the re-calculations of the particle equations and thus reduce the computing cost.

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