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A Markov chain model for predicting transient particle transport in enclosed environments

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ABSTRACT

Obtaining information about particle dispersion in a room is crucial in reducing the risk of infectious disease transmission among occupants. This study developed a Markov chain model for quickly obtaining the information on the basis of a steady-state flow field calculated by computational fluid dynamics. When solving the particle transport equations, the Markov chain model does not require iterations in each time step, and thus it can significantly reduce the computing cost. This study used two sets of experimental data for transient particle transport to validate the model. In general, the trends in the particle concentration distributions predicted by the Markov chain model agreed reasonably well with the experimental data. This investigation also applied the model to the calculation of person-to-person particle transport in a ventilated room. The Markov chain model produced similar results to those of the Lagrangian and Eulerian models, while the speed of calculation increased by 8.0 and 6.3 times, respectively, in comparison to the latter two models.

1. Introduction

In recent decades, outbreaks of airborne infectious diseases, including influenza [1], measles [2], tuberculosis [3], and severe acute respiratory syndrome (SARS) [4], have occurred indoors. All of these outbreaks have been proven to be associated with the airflow patterns in indoor environments [5]. An infected person can exhale particles carrying pathogens through the activities of breathing, coughing, talking, and sneezing, which are transient in nature. These particles can cause the transmission of infectious diseases to other occupants in the same enclosed environment [6,7]. Hence, it is essential to predict transient particle transport in the enclosed environment in order to improve air distribution design and reduce the risk of infection.

As a powerful airflow and contaminant modeling tool, computational fluid dynamics (CFD) has been widely used in predicting transient particle transport in enclosed environments. For particle modeling, the Eulerian and Lagrangian methods are popular. For instance, Li et al. [8], Seepana and Lai [9], and Chen et al. [10] studied the effects of ventilation parameters on person-to-person particle transport using an Eulerian drift flux model. Li et al. [11] and Chen et al. [12] investigated the effectiveness of covering a cough on reducing the receptor's exposure using an Eulerian method. Hang et al. [13] used an Eulerian model to assess the influence of human walking on the transmission of airborne infectious diseases in a six-bed isolation room. Chen et al. [14], Gao et al. [15], and Zhang and Li [16] applied the RNG k-ε model with a Lagrangian method to calculate the transport of exhaled droplets in a dental clinic, an office, and a fully-occupied high-speed rail cabin. Zhang and Chen [17] compared the Eulerian and Lagrangian methods for predicting transient particle transport from a cough in a four-row aircraft cabin. Wang et al. [18] systematically compared the Eulerian and Lagrangian methods with various turbulence models and found that the Eulerian method was faster than the Lagrangian method. Both the Eulerian and Lagrangian methods can provide detailed information about transient particle concentration distributions. However, even with the Eulerian method, the unsteady-state calculation with iterations in each time step is considerably time-consuming. For instance, Wang et al. [18] reported that the computing times of the Eulerian and Lagrangian methods for calculating transient particle

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transport in a typical room were 62.2 and 84.9 h, respectively, on an eight-core cluster with two 2.5 GHz AMD quad-core processors.

Several studies have demonstrated the ability of the Markov chain technique to quickly predict spatial and temporal particle concentrations. For instance, Nicas [19] and Jones and Nicas [20,21] applied the Markov chain technique in a multi-zone model. However, this model does not inform users about particle movements between zones with respect to the required input values. Chen et al. [22] further used the CFD approach with Lagrangian particle tracking to obtain such information in order to complete the method. Since Lagrangian particle tracking is highly time-consuming, this method is suitable only for an extremely coarse grid. Therefore, a new model that not only works on a fine grid, as do the Eulerian and Lagrangian methods, but also runs faster than these two methods, is desirable. This investigation aimed to develop a Markov chain model for quickly predicting detailed transient particle concentration distributions in enclosed environments.

2. Methods

2.1. Airflow and turbulence model

This study used the renormalization group (RNG) k-ε model to calculate airflow and turbulence. This model has the best overall performance among all Reynolds-averaged Navier–Stokes (RANS) models for enclosed environments [23]. The equations for the RNG k-ε model can be found in the Fluent manual [24].

This investigation assumed that the airflow field was fixed. It could be problematic if the source was able to change the airflow pattern, as in the case of a powerful cough without covering the mouth. Therefore, this study assumed that the mouth was effectively covered when a person was coughing and that, as a result, the influence of the initial momentum from the cough on the receptor's exposure was minimized [12]. Thus, the assumption of a fixed airflow field should be valid in most cases.

2.2. Markov chain model for transient particle transport

This study used the first-order homogenous Markov chain technique [25] to calculate transient particle transport. This Markov chain technique is effective for particles with a diameter smaller than 3 μm, which have negligible inertial effects [22]. Assuming that the CFD grid has n-1 cells, the additional cell n can be assigned to represent the space to which the particles are removed. Then the probabilities of the state's changing of a particle can form an n × n transition probability matrix, p_{ij}:

$$P = \left(p_{i,j}\right)_{(n\times n)} = \begin{pmatrix} p_{1,1} & p_{1,2} & \cdots & p_{1,n} \\ p_{2,1} & p_{2,2} & \cdots & p_{2,n} \\ \vdots & \vdots & & \vdots \\ p_{n,1} & p_{n,2} & \cdots & p_{n,n} \end{pmatrix} \tag{1}$$

where $p_{i,j}$ is the probability of a particle's moving from cell i to cell j in a certain time step, Δt. The transition probability matrix has the following property:

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

This property can be regarded as the constraint of mass balance for the whole domain. Since the movement of the particles normally does not have a major impact on the airflow field, the transition probability matrix is fixed.

The particle number vector at the present time (state k) is assumed to be:

$$N_k = \left(N_{k,1} \;\; N_{k,2} \;\; \cdots \;\; N_{k,n}\right) \tag{3}$$

where $N_{k,i}$ represents the number of particles in cell i at time k. Then, after one time step (time k+1), the number of particles in cell i can be calculated by:

$$N_{k+1,i} = N_{k,1}p_{1,i} + N_{k,2}p_{2,i} + \cdots + N_{k,n}p_{n,i} \tag{4}$$

Thus, the particle number vector at time k+1 can be calculated by:

$$N_{k+1} = N_k P \tag{5}$$

If one calculates the particle transport from time zero, the particle number vector at time k can be calculated by:

$$N_k = N_{\text{int}} P^k \tag{6}$$

where N_{int} is the initial particle number vector. The particle number concentration in cell i at time k can be calculated by:

$$C_{k,i} = \frac{N_{k,i}}{V_i} \tag{7}$$

where V_i is the volume of the cell.

The transition probability matrix can require a considerably large storage memory for a normal CFD grid. To reduce the size of the matrix, Eq. (4) was rewritten as:

$$N_{k+1,i} = N_{k,i}p_{i,i} + \sum_{nb} N_{k,nb}p_{nb,i} \tag{8}$$

where the subscript nb represents the neighboring cells or boundaries. Eq. (8) shows that the Markov chain model does not require iterations in each time step. Therefore, this model has the potential to reduce the computing cost.

2.3. Transition probabilities

The key operation in applying the Markov chain technique to the calculation of transient particle transport is to obtain the transition probabilities, p_{ij}. Again, p_{ij} is the probability of a particle's moving from cell i to cell j in a certain time step, Δt. The first step is to calculate the probability of a particle's remaining in the current cell in Δt, p_{ii}. It is assumed that there are N_0 particles present in cell i at time zero and that these particles can be removed only by the flow of air. The particle mass balance equation for this cell is [19]:

$$\frac{dN(t)}{dt} = -\frac{N(t)}{V_i}\sum_{nb} Q_{i,nb} \tag{9}$$

where $Q_{i,nb}$ is the airflow rate from cell i to the neighboring cell. Solving Eq. (9) leads to the following equation [19]:

$$N(\Delta t) = N_0 \exp\left(-\sum_{nb}\frac{Q_{i,nb}}{V_i}\Delta t\right) \tag{10}$$

Therefore, after a certain time step, Δt, N(Δt) particles remain in this cell. Thus, the probability of a particle's remaining in the current cell in Δt can be expressed as [19]:

$$p_{i,i} = \exp\left(-\sum_{nb}\frac{Q_{i,nb}}{V_i}\Delta t\right) \tag{11}$$