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A grid-merging operation to accelerate the Markov chain model in predicting steady-state and transient transmission of airborne particles

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ABSTRACT

To accelerate the process of obtaining the faster-than-real-time information for both steady-state and transient particle transmission in the indoor or local atmospheric environment, a grid-merging operation has been developed as applying the Computational Fluid Dynamics (CFD) combined Markov chain model. A steady-state flow field was calculated in advance, and then the flow rate data were exported into MATLAB platform and preprocessed with matrixing process. The grid-merging operation combined Markov chain model therefore was realized in a computational resource saving way. Two particle transmission cases including both a constant particle releasing source and a pulsed particle releasing source were used to validate the simulation results, and the general trends of the particle concentration distributions agreed reasonably well with the experimental data. In addition, the computing time costs after the grid-merging operation can remarkably be reduced while maintaining an acceptable accuracy. Besides, it is crucial for the overall computing accuracy to select one appropriate time step size Δt for as many cells as possible within the whole computational domain.

1. Introduction

Infectious disease transmission has been treated as a threat to the public's health, and airborne particles have been playing a crucial role in the corresponding transmission process in both enclosed spaces and local atmospheric environment [1–3]. For instance, the PM2.5 problems have become increasingly serious in China, the distributions of fine particles ($PM_{2.5}$), coarse particles ($PM_{2.5\text{-}10}$) and total suspended particulate (TSP) were experimentally measured by groups of researchers [4–6] to find out effective control measures. Particularly in the indoor environment, those behaviors of airborne particles, which may serve as carriers of infectious disease related viruses and bacteria, were widely investigated [7]. For decades, numerous researches have focused mainly on the mechanism of such behaviors mentioned above, including deposition [8–11], re-suspension [12,13], penetration [14,15] and most importantly transmission [16–20].

Commonly adopted methods of modeling particle transmission can generally be classified into two basic categories, namely, the Eulerian method and the Lagrangian method. The former method treats the particle phase as a continuous phase, and such primary models can only be used to investigate the transmission of gaseous contaminant or sub-micro particles. Since the gravitational settling was taken into consideration by adding a particle settling velocity to the convective term of the momentum equation, the so-called drift-flux model has been widely adopted to predict the transmission of coarse particles [21–24]. The other method acquires the particle trajectory by solving the force balance equations of each single particle. The effect of various forces such as the gravity force and thermophoretic force therefore can be accurately predicted. To figure out the advantages and disadvantages, comparative investigations [25,26] between Eulerian and Lagrangian models were extensively conducted. However, both the Eulerian and Lagrangian methods require numerous computational costs. But in emergency cases, fast and precise prediction of airborne particle distributions with a constant releasing source and dynamic decay process with a pulsed releasing source is crucial.

Markov chain is one of the fast, precise tools in simulating spatial and temporal particle concentrations. The so-called Markov chain model is a popular statistic/stochastic model which can be used to simulate a specified transfer process from one state to

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another [27]. The Markov chain model has already been implemented to simulate the electricity consumption for a better energy demand management [28], the collective process of particulate systems [29] and the production of annual weather data [30]. But in the indoor environment, the Markov chain model was first proposed to solve the contaminant concentration by Nicas [31]. In Nicas' research, both single-zone and two-zone well-mixed rooms were cast as the Markov chain models, and the variability in exposure intensity as well as infection risk was also estimated. Some researches further combined the Markov chain model with CFD software to quickly obtain the particle concentration distributions [32]. Due to the lack of iterations in each time step, the calculation speed of the Markov chain model was 8.0 and 6.3 times faster than the conventional Eulerian and Lagrangian methods, respectively [33]. Besides, the Markov chain model was sensitive to some dominant parameters such as the time step size and the grid resolution, which have been partially analyzed and verified [34].

Nevertheless, for a problem/case with a necessarily high grid resolution to satisfy the grid independency when solving a fixed flow field, the Markov chain model would require a large amount of computer memory. And the calculation speed could still be relatively low, which would not be satisfied for real-time or even faster-than-real-time prediction. For instance, the computational resource requirements of predicting city-scale contaminant (PM2.5/PM10/TSP) transmission are extremely high. Further acceleration of the Markov chain model therefore is needed. Besides, a user-defined function (UDF) has usually been implemented to realize the Markov chain model when combined with the CFD software [33]. However, the flow rate data on grid faces within the calculation domain would be more suitable to be processed and stored in matrix forms, which would consequently increase the flexibility and execution speed of the original code.

In this paper, to accelerate the speed of predicting particle transmission and save the computational resources while maintaining an acceptable computational accuracy, the CFD combined Markov chain model was modified with a proposed grid-merging operation. A steady-state flow field was solved in advance, and the corresponding flow rates (or velocity components) on grid faces were exported to the MATLAB platform to realize the modified Markov chain model. The influences of grid-merging rate as well as the time step size were also tested and analyzed.

2. Methods

2.1. Basic concept of Markov chain model

Once an enclosed area or space was divided into several cells as shown in Fig. 1, particles can move from one cell i to another j randomly during a specified time step size Δt. Then the transmission process from state t to state $t+\Delta t$ can be described via a certain transfer probability P_{ij} under a steady-state flow field.

For the first-order homogeneous Markov chain model implemented in particle transmission under a steady-state flow field, several assumptions are claimed as follows:

(1) A future state is merely determined by the present state.
(2) The state transfer probability is fixed.
(3) Particles are assumed to be well mixed within each subspace.
(4) Particles are assumed to have relatively good following behaviors.

In order to satisfy these assumptions, the tracked particles were statically released by the particle source(s) and the gravitational settling effect was ignored or transferred to vertical downward flow rate.

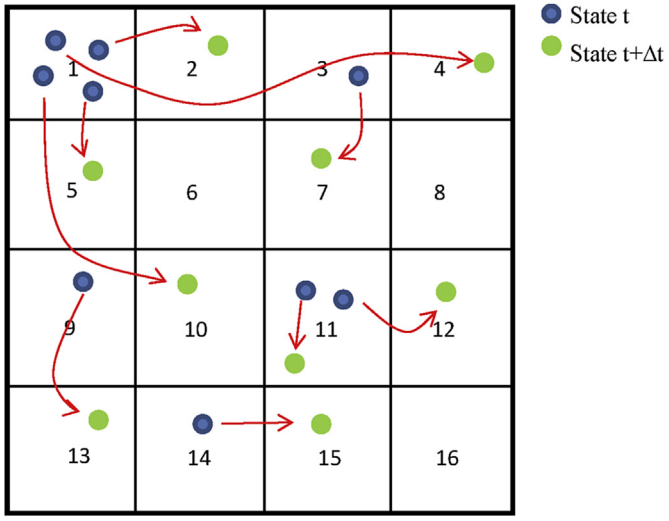

Fig. 1. A sketch map of particle transmission in an enclosed space.

Assuming that the target CFD computational domain has n cells, and the additional cell n+1 can be assigned as the extra space for the particles moving out of the computational domain. In the computational domain, the State Transfer Matrix P can be constructed by arranging each probability P_{ij} to its corresponding position [32]:

$$P = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{bmatrix} \tag{1}$$

Outside the computational domain, the transfer probability between the inner cells and cell n+1 can be calculated as:

$$p_{in+1} = 1 - \sum_{j=1}^{n} p_{ij} \tag{2}$$

$$p_{n+1n+1} = 1 \tag{3}$$

Then the complete State Transfer Matrix P can be rewritten as Eq (4), but most components of which are generally equivalent to zero:

$$P = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} & p_{1n+1} \\ p_{21} & p_{22} & \cdots & p_{2n} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ p_{n1} & \cdots & \cdots & p_{nn} & \cdots \\ \cdots & \cdots & \cdots & \cdots & p_{n+1n+1} \end{bmatrix} \tag{4}$$

For a first-order homogenous Markov chain model related State Transfer Matrix P, the following properties should be satisfied:

$$\sum_{j=1}^{n} p_{ij} = 1 \tag{5}$$

$$p_{ij} \geq 0 \tag{6}$$

The vector S_t denotes the present state of how many particles are in each cell at the present time t:

$$S_t = \begin{bmatrix} S_{t,1} & S_{t,2} & \cdots & S_{t,n} & S_{t,n+1} \end{bmatrix} \tag{7}$$

And the vector $S_{t+\Delta t}$ shows the objective state of how many particles are in each cell after a certain time step size Δt: