Wind Engineering Joint Usage/Research Center
FY2023 Research Result Report

Research Field: Indoor Environment
Research Year: FY2023
Research Number: 23232007
Research Theme: Transient contaminant transport prediction based on computational fluid dynamics and Markov chain method with application of non-uniform state size

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Budget [FY2021]: 420,000Yen

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1. Research Aim

Indoor air quality is a critical factor in human health and productivity. Studies have shown that the airborne transmission of viruses and bacteria is a major transmission route for respiratory infectious diseases. In addition to infectious particles, non-infectious particles also exist in indoor environments and can have adverse health effects. To address these issues, several studies have focused on understanding the mechanisms of particle transmission and developing effective control measures to improve system design and assist in real-time control.In recent years, the use of Markov chain technology has emerged as a promising approach for rapidly predicting spatial and temporal particle concentrations. Studies have demonstrated that the calculation speed of the Markov chain model is faster than that of the Eulerian and Lagrangian methods while maintaining the same level of computational accuracy.
The state transition matrix is a crucial factor in achieving computational accuracy in the Markov chain model. The size of the matrix depends on the resolution of the state, which in turn is determined by dividing the state into coarse and fine. Coarse state division is usually based on the size of the spatial dimension and determined by the user, without any fixed principles for division, which affects the computational accuracy. To ensure both calculation speed and acceptable prediction accuracy, a method for dividing non-uniform states based on flow field velocity is proposed in this study for the Markov chain model combined with CFD. This method obtains a coarse Markov matrix with fast calculation speed, and the non-uniform division method reduces the difference within a single state, thereby improving the calculation accuracy.

2. Research Method

2.1 Markov chain model for transient particle transport

The homogeneous Markov chain technique has been proven to describe the particle transport process in space. For a fixed flow field, its implementation is based on several assumptions:

1) The future distribution of contaminants depends only on the current state and transition matrix.
2) The transition matrix is fixed.
3) The contaminants fully follow the airflow.
4) Particles mix uniformly in each state.

Previous studies have shown that when particles are smaller than 3–5 μm in diameter, their motion is determined by passive scalar transport. To satisfy the assumption that the Markov chain is applied to particle transport, inertial effects must be ignored. However, particles larger than 3 μm are significantly impacted by inertial effects, resulting in significant errors when using the one-step homogeneous Markov chain method. Therefore, this method is primarily used for modelling particle transport for particles smaller than 3 μm in diameter and is suitable for various particles commonly found indoors, such as the rapidly evaporating droplet nuclei of human exhalation and most airborne bacteria. Assume that the domain contains n states, including n-1 spatial states and one state assigned as the extra space for the particles moving out of the computational domain. The transition matrix P_{ij} of this Markov chain model can be written as:

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

where P_{ij} is the probability that contaminants transport from state i to j within one time step Δt, and the transition probability satisfies the following property:

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

Assuming that particles do not re-enter space after being expelled,

$$p_{nj} = \begin{bmatrix} 0 & 0 & \ldots & 1 \end{bmatrix} \tag{3}$$

When the source of location is released in m state, the probability vector at time t is

$$\theta_{t,i} = \begin{cases} 1, i = m \\ 0, i \neq m \end{cases} \tag{4}$$

After one time step Δt, the probability vector of particle distribution in space is expressed as

$$\theta_{t+\Delta t} = \theta_{t,i} \cdot P_{ij} \tag{5}$$

The vector N_t represents the number of particles in each state at time t, and the number of particles $N_{t+\Delta t}$ in each state after one Δt can be expressed as a vector.

$$N_t = \begin{bmatrix} N_{t,1} & N_{t,2} & \ldots & N_{t,n} \end{bmatrix} \tag{6}$$

$$N_{t+\Delta t} = N_t \cdot P_{ij} \tag{7}$$

The number of particles in the j state can be expressed as

$$N_{t+\Delta t,j} = N_{t,1} \cdot P_{1j} + N_{t,2} \cdot P_{2j} + \ldots + N_{t,n} \cdot P_{nj} \tag{8}$$

After multiple time steps, the probability vector of particle distribution can be expressed as

$$N_{t+k\Delta t} = N_t \cdot P_{ij}^{k} \tag{9}$$

When it is a pulse source, the number of particles entering m state within every Δt time step is S, then the number of particles $S_{m,t+\Delta t}$ in m state after $k\Delta t$ time steps can be expressed as

$$S = \left(S_t, \quad S_{\Delta t}, \quad \ldots, \quad S_{k\Delta t} \right) \tag{10}$$

$$S_{m,t+k\Delta t} = S_t \theta_{t,i} \cdot P_{nm}{}^{k} + \sum_{\alpha=1}^{k} S_{\alpha\Delta t} \cdot P_{nm}{}^{k-\alpha} \tag{11}$$

The number of particles in each state can be represented by the following vectors:

$$N_{t+k\Delta t} = S_{m,t+(k-1)\Delta t}\theta_{t,i} \cdot P_{ij} \quad (12)$$

The particle concentration in the state is expressed as

$$C_{t,i} = \frac{N_{t,i}}{V_i}, \quad (13)$$

where $C_{t,i}$ is the particle concentration of state i at time t, $N_{t,i}$ is the number of particles in state i at time t, and V_i is the volume of state i.

2.2 Calculation of the transition probability matrix

Methods for obtaining the transition matrix of the Markov chain model include flux-based methods, set theory methods, and Lagrangian tracking. The flux-based method calculates the transition matrix based on the airflow between CFD grids and has been used several times in Chen's studies. The set theory method helps calculate the transition matrix by tracking the transfer of edge particles and the area of intersection between them before and after a time step, which is complicated, difficult to be accurately calculated in simulations, and mainly used in two-dimensional cases. The Lagrangian tracking method is considered to be faster, has the weakest restrictions on the time step, and is suitable for three-dimensional calculations. Therefore, it was used in this study to obtain the transition matrix. Using Lagrangian random tracking to obtain the state transition matrix was first proposed by Chen et al. [23]. This method first solves the airflow field using CFD, releases a certain number of particles in each unit, and uses Lagrangian tracking and random walk models to calculate the number of particles moving from states i to j in Δt. The percentage of transferred particles to the total number of particles is taken as the transition probability. The transition probabilities $P_{i,i,t}$ and $P_{i,j,t}$ can be expressed as:

$$P_{i,i,t} = \frac{N_{i,i,t}}{N_{i,initial}}, \quad (14)$$

$$P_{i,j,t} = \frac{N_{i,j,t}}{N_{i,initial}}. \quad (15)$$

In this study, the flow field is assumed to be fixed, the particle transport is assumed to be unaffected by the flow field, and the instantaneous diffusion of particles in the chamber with time is calculated. The RNG k-ε model is used to simulate the continuous phase flow field, which achieves the best overall performance in terms of accuracy, computational efficiency, and robustness; its formulation can be found in the Fluent manual. The DPM is used to calculate the discrete phase particles, which tracks particles in the Lagrangian coordinate system by solving for Newton's second law of motion. The DPM requires only one execution throughout the computational process and is used to obtain particle transfer at one time step.

2.3 Combination of the non-uniform dividing zone and Markov chain model

According to the assumptions of the Markov chain technology currently applied to transient contaminant transport prediction, the model applied under a coarse Markov matrix to describe the particle transfer process is relatively crude. Initially, the pollutant is assumed to be uniformly distributed within the state where the pollution source is located. After one time step, the particles follow the airflow and transfer to other states, and the pollutant is assumed to be uniformly distributed in each state. In this process, the assumption that the percentage of particles transferred to other states following the airflow, known as the transition probability, remains constant and can lead to errors in each step of the calculation due to non-uniform particle distribution in each state. In reality, particles leaving state i and arriving at state j do not immediately distribute uniformly within state j as assumed. Therefore, the transition probabilities of particles in each subsequent time step may not be the same as those in the initial time step, which is one of the reasons for the deviation in the Markov chain model calculation. Chen also discussed this issue in his research, stating that owing to the unevenness of particle concentration in different states, the accuracy of the Markov chain method in different states may differ. To reduce the prediction error caused by this factor, particles should be distributed as uniformly as possible within each state, or the flow field within each state should be made as uniform as possible. However, it is difficult to distribute particles uniformly within the state because particle motion is influenced by the flow field. When the airflow in a single state is similar, particle motion within the state will also be more uniform, reducing the error caused by uneven particle distribution. Therefore, this study proposes dividing the flow field into non-uniform states and applying the Markov chain model prediction method accordingly.

The main process of this algorithm is illustrated in Fig. 1. First, the method divides the flow field into N_{sub} of sub-layers in each direction separately, with the sub-layer in one direction generated by an equal thickness criterion, and the sub-layers in each direction are merged according to the velocity to obtain the combination scheme of sub-layers in each direction. The grid classification into the corresponding sub-layer areas is performed at the coordinates of the cell centre. Finally, the layers in each direction are merged to obtain a non-uniform grid. In this study, the acquisition of non-uniform states for the Markov chain model is based on the algorithm mentioned. In fact, various methods are available for dividing the flow field. However, the main objective of this study is to explore the accuracy of the model based on non-uniform states. The focus of the study is not on the state division method itself; therefore, we only provide an example of using this method to divide the non-uniform states for the Markov chain model.

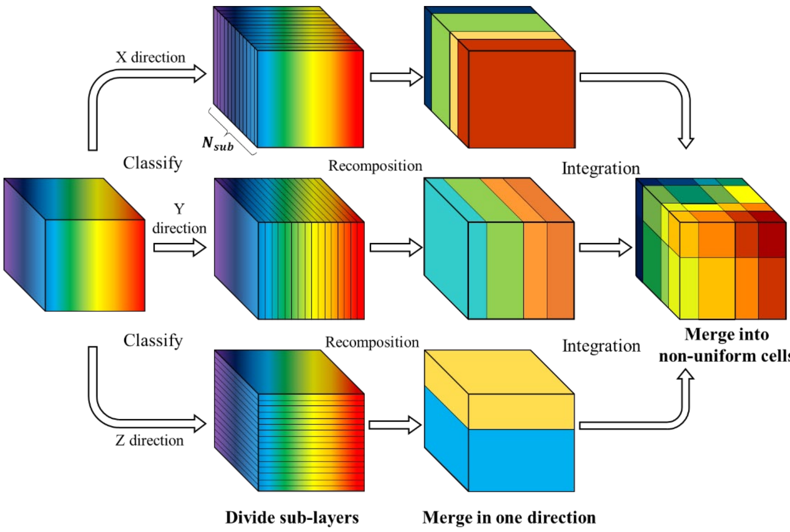

Fig. 1 Main procedure for dividing non-uniform states realized by the 'precise sub-layer recomposition' algorithm.

3. Research Result

3.1 Experimental verification

Fig. 2 shows the dimensions of the chamber room, where the inlet and outlet are located at 2.1 m and 0.3 m above the ground, respectively. Both the inlet and outlet have a size of 0.3 m × 0.3 m, and the average supply-air velocity magnitude is 0.84 m/s with an incidence angle of 10°. After the flow field became stable, particles with a size of 1 μm were injected into the chamber. After obtaining steady-state flow field data, the coordinates and velocity information of all grids were imported into the Python-based platform to construct a non-uniform state and further calculate the transition matrix. The functions performed by the platform include coordinate partitioning, sub-layer cutting, sub-layer merging, construction of the transition matrix under non-uniform states, and prediction of transient contaminant transport. In this model, the sub-layer thickness was set to 0.05 m, and the chamber was transformed into 36 zones, with the removed zones labeled as State 37, as shown in Fig. 3. Based on the flow field data and Lagrangian tracking method calculation results, a 37×37 transition probability matrix was obtained. Throughout the contaminant transport period, the particle concentration in each state was normalized based on the initial released particle number. The initial probability vector when the pollution source is located in State 20. In this experiment, the particle density at a distance of 0.9 m from the ground and at the inlet were measured using OPC with a sampling interval of 21 s. Notably, the Markov chain model can only be used calculate the transient particle transport from a pulse source. To calculate the transient distribution of the continuously released source, a certain amount of particles must be added at the source location at each time step, as shown in Eq. 11. Therefore, the inlet concentration must be divided into several pulse sources with a duration of one time step. In this study, the same setting as Zhang's study was adopted, and linear interpolation was used to calculate the inlet distribution for each time step with a time step of 1 s.

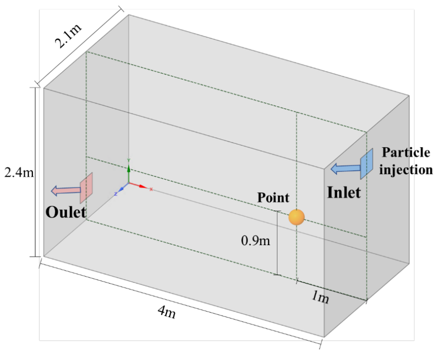

Fig. 2 Configuration of the chamber and measuring point location.

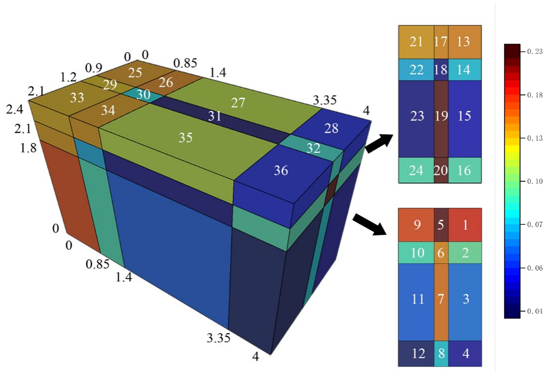

Fig. 3 States of chamber

Fig. 4 compares the numerical calculation results of transient particle concentration and the experimental measurements and displays the inlet data of the experimental measurements. The predicted results of Markov chain models with uniform and non-uniform states are also provided. The red and green lines represent the results calculated using the Markov chain model with non-uniform and uniform states, respectively. During the entire experimental measurement process, the particle density at the inlet changed rapidly during the initial period, and the peak particle concentration at the measurement point in the experiment occurred later than the concentration peak at the inlet. Both models using uniform and non-uniform state division methods showed this characteristic in their predictions. This is because the state where the measurement point was located is at a certain distance from the state at the inlet, resulting in a delayed response. The calculation results of the non-uniform state model were more similar to the experimental data before 1200 s. After the inlet conditions became relatively stable, the prediction deviation of the uniform states decreased gradually, and the prediction results of the two partition methods became better. This may be because with time, the indoor contaminant gradually diffuses in the room, and the impact of velocity differences within uniform states decreases, leading to a reduction in prediction errors in the later stages. The velocity differences within non-uniform states are small, which ensures the predictive accuracy of the model when the pollutant diffusion is insufficient. Furthermore, when the inlet particle concentration decreases and reaches a relatively stable state with periodic oscillations, the concentration predicted by the non-uniform Markov chain model also exhibits periodic oscillations, showing a trend similar to the inlet condition. Overall, the Markov chain model with non-uniform states prediction agrees with the results and trend of the experiment, and its predictive performance is better than that of the Markov chain model with uniform states.

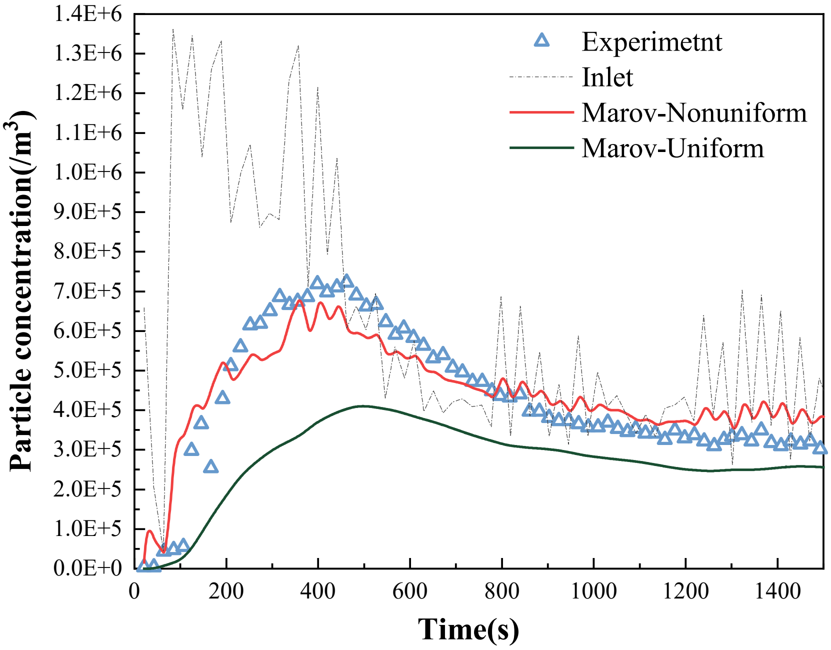

Fig. 4 Comparison between the numerical results for transient particle concentration of the Markov chain model and the experimental data at 0.9 m.

3.2 Application of different flow fields

The Markov chain model with non-uniform state partitioning is applicable to different flow fields and has higher prediction accuracy. For Case A, the time step of the Markov chain model is set to 10 s, and the comparison of particle transfer results over a period of time is shown in Fig. 5. Owing to the slanting direction of the air flow and the diffusion of particles outside the jet axis, the concentration of particles in States 3 and 11, located on both sides of the source in the downward direction, increases rapidly and to a higher level. Compared to the CFD simulation results, the Markov chain model slightly underpredicts the peak concentration but still accurately predicts the trend of particle concentration and captures the state where the peak occurs. Overall, the prediction of the model is reliable.

Fig. 6 shows the size of the cleanroom of case B. There were two air supply ports on the ceiling, which vertically supply air at a velocity of 1.0 m/s. Regarding Case B, the time step of the Markov chain model was set to 5 s. Figs. 7 and 8, respectively, show the variation of particle concentration in each state over time when the source is located in States 3 and 7. The blue lines represent the predicted probability by the Markov chain model, and the grey lines represent the normalized particle concentration obtained by CFD. When the source is located in State 3, the particles follow the airflow to move to States 2 and 6, and then the pollutant in State 6 moves to State 9. Fig. 7 shows that the peak of State 9 is significantly later than those of States 2 and 6. When the source is located in State 7, a similar situation is observed where particles first reach the adjacent States 4 and 10, and approximately 10 s later, States 1 and 13 reach the peak concentration. When the source is located in State 7, the particle concentration in the vast majority of states is generally higher than when the source is located in State 3, which is due to some particles being directly exhausted from the exhaust port at State 3. Overall, the predicted results of the model are in good agreement.

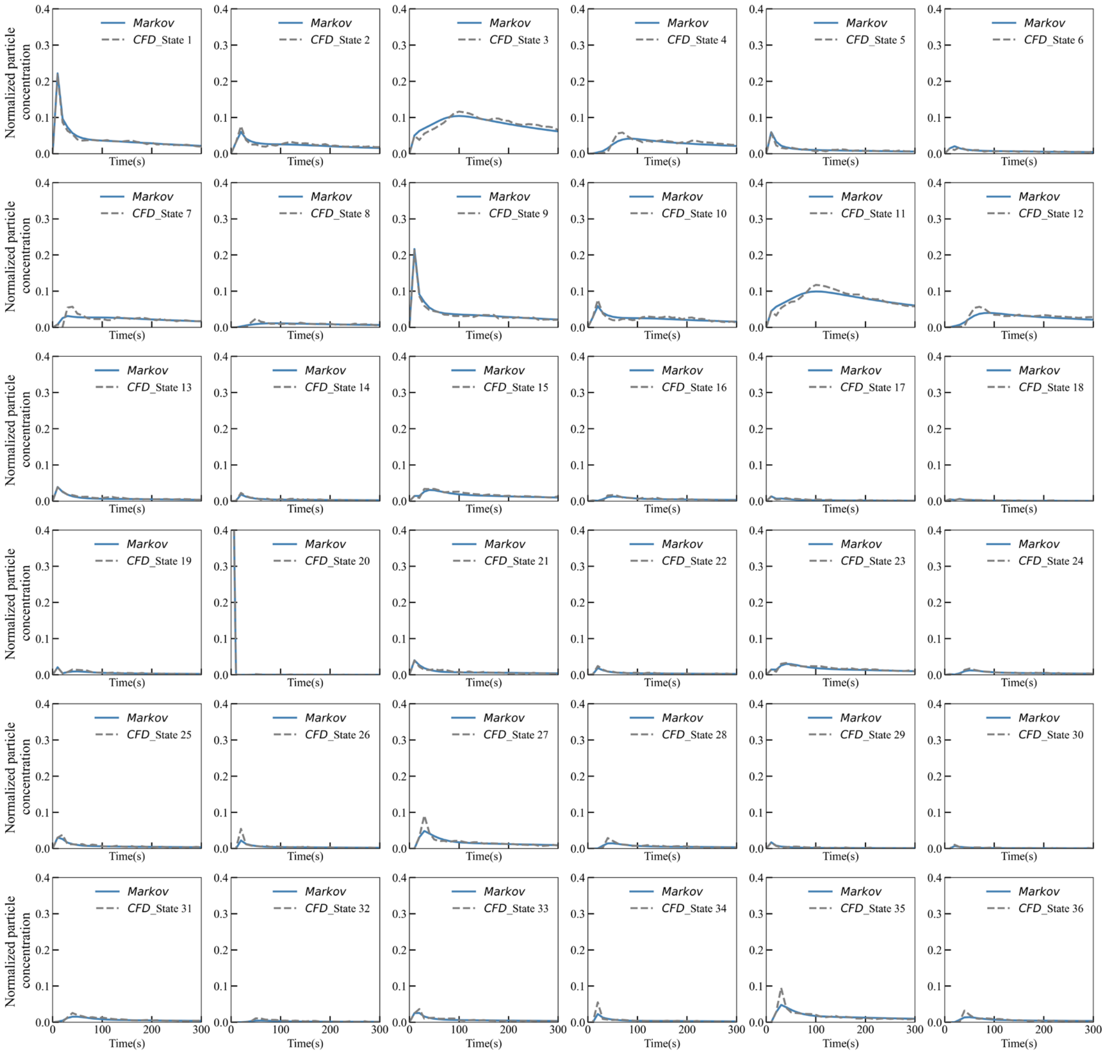

Fig. 5 Comparison of trends of particle concentration versus time with a pulsed particle source in state 20.

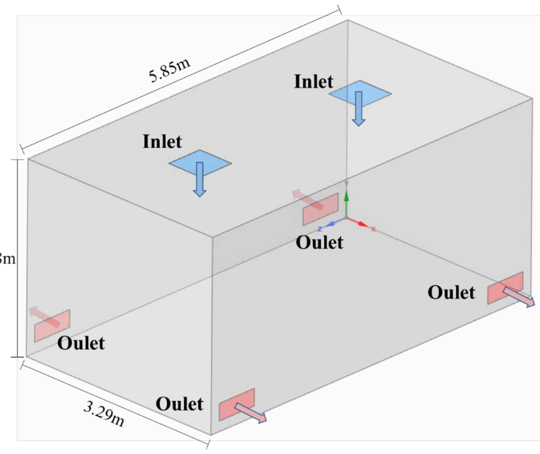

Fig. 2 Configuration of the ventilated chamber of case B.

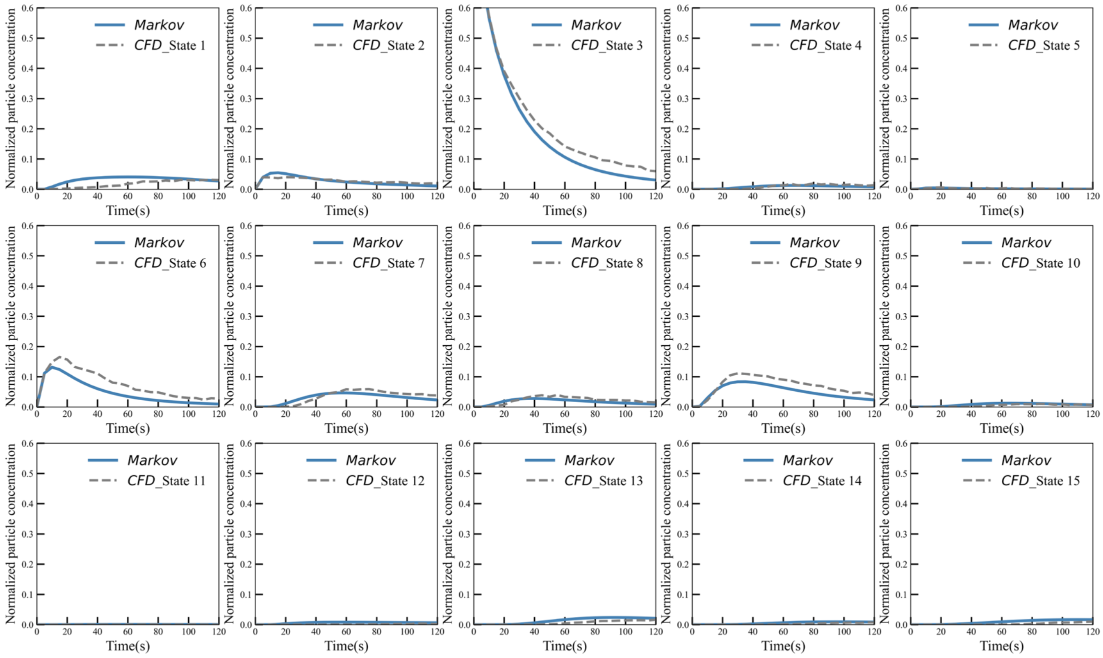

Fig. 7 Comparison of the trends of the normalized particle concentrations vs. time as obtained by the Markov chain model and CFD simulation with a source in State 3.

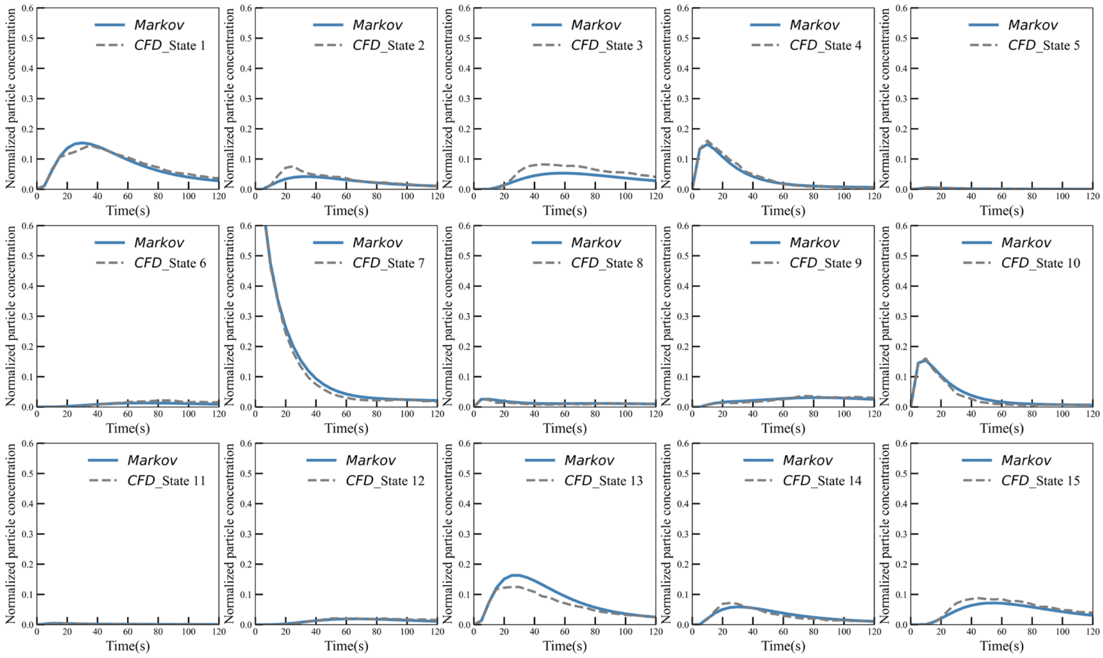

Fig. 8 Comparison of the trends of the normalized particle concentrations vs. time as obtained by the Markov chain model and CFD simulation with a source in State 7.

Additionally, the prediction performance of the Markov chain model with non-uniform and uniform states was compared, and the normalized root mean square deviation (NRMSD) was used to quantify the difference between the two, as defined using Eq. 17. To avoid the randomness of setting a single source, this study conducted a comprehensive comparison. Taking Case B as an example, each state was set as the source location, and 15 calculations were performed. The calculation results of each time step were compared, as shown in Fig. 9. The horizontal axis represents the running time, and the vertical axis represents the state where the source is located. Each scatter represents the NRMSD of the concentration of particles in the entire room between the Markov chain model and CFD. The blue and grey scatters represent the calculation deviation of the model under uniform and non-uniform states, respectively. In each time step, the scatters with a smaller area are always located above the others. Only one colour of scatter indicates that there is almost no difference in the calculation accuracy between the two methods. Evidently, for most time steps, the grey scatters are bigger than the blue ones, indicating that the non-uniform method has better calculation results. When the source is located in States 1, 3, 13, and 15, the non-uniform model performs better in the early stages. This is because these four states are located in the corners of the room, and when the particles first start to transfer, some of them are directly exhausted from the exhaust port, whereas others are left in the current state owing to the eddy current phenomenon of the flow field, resulting to an increased proportion of absorbed states. The division of non-uniform states distinguishes this part. For all calculation conditions, the average NRMSDs of the models for uniform and non-uniform states were 2.4% and 1.9%, respectively. Using the non-uniform state method reduced the NRMSD by 20%, indicating that it resulted in better prediction performance. Notably, previous studies assumed that particles were uniformly distributed within the source state, which results in the volumes filled by particles in uniform and non-uniform states not being completely identical, making the comparison insufficiently rigorous. However, although there were slight differences in the initial conditions of the sources after dividing them into different states, both datasets are compared based on their respective CFD calculation results as the true value. Therefore, comparing the NRMSDs of the two groups can reflect the difference in their prediction accuracy. Thus, we believe that this comparison method is feasible and effective.

$$NRMSD = \frac{\sqrt{(\sum_{i=1}^{n}(C_{CFD,i} - C_{Markov,i})^2)/n}}{C_{CFD,\max} - C_{CFD,\min}} \tag{16}$$

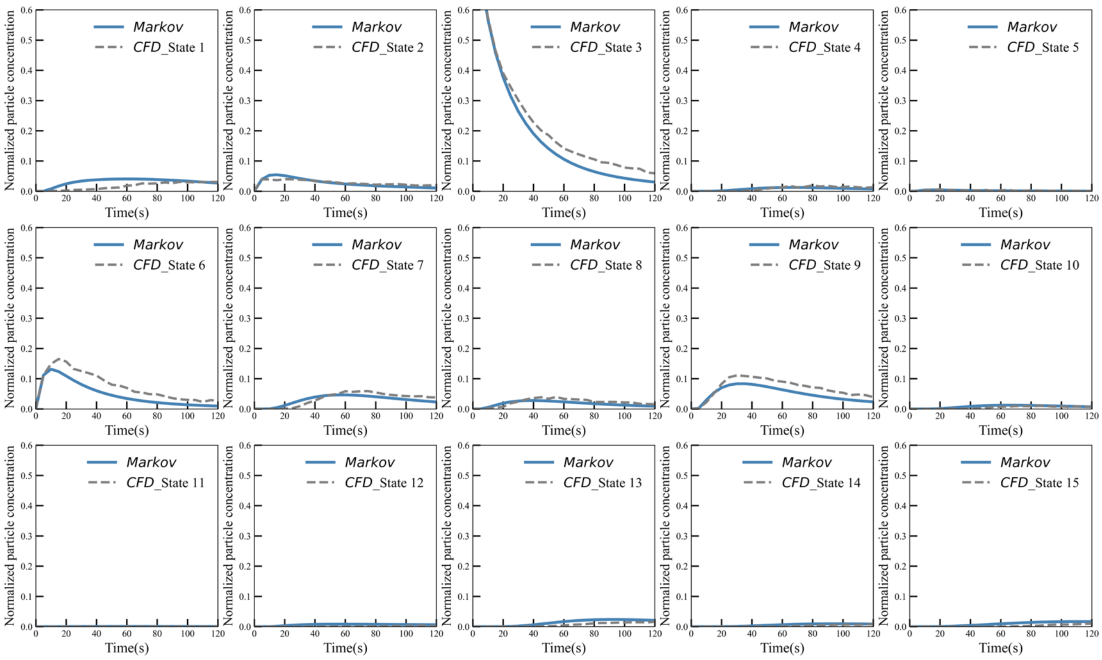

Fig. 3 Comparison of the trends of the normalized particle concentrations vs. time as obtained by the Markov chain model and CFD simulation with a source in State 3.

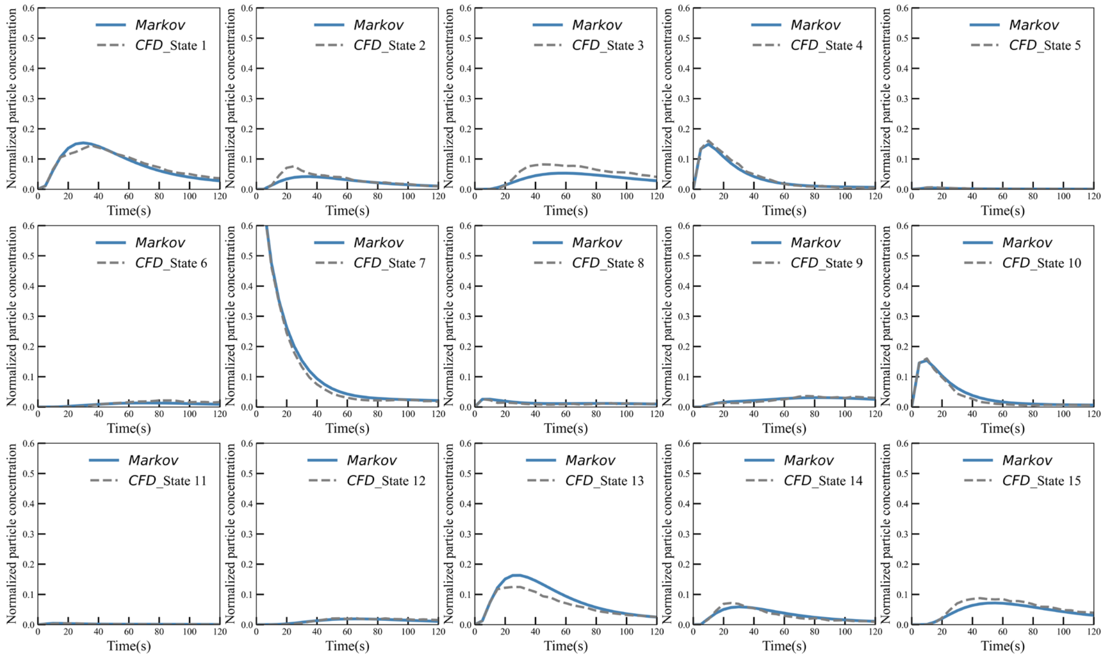

Fig. 4 Comparison of the trends of the normalized particle concentrations vs. time as obtained by the Markov chain model and CFD simulation with a source in State 7.

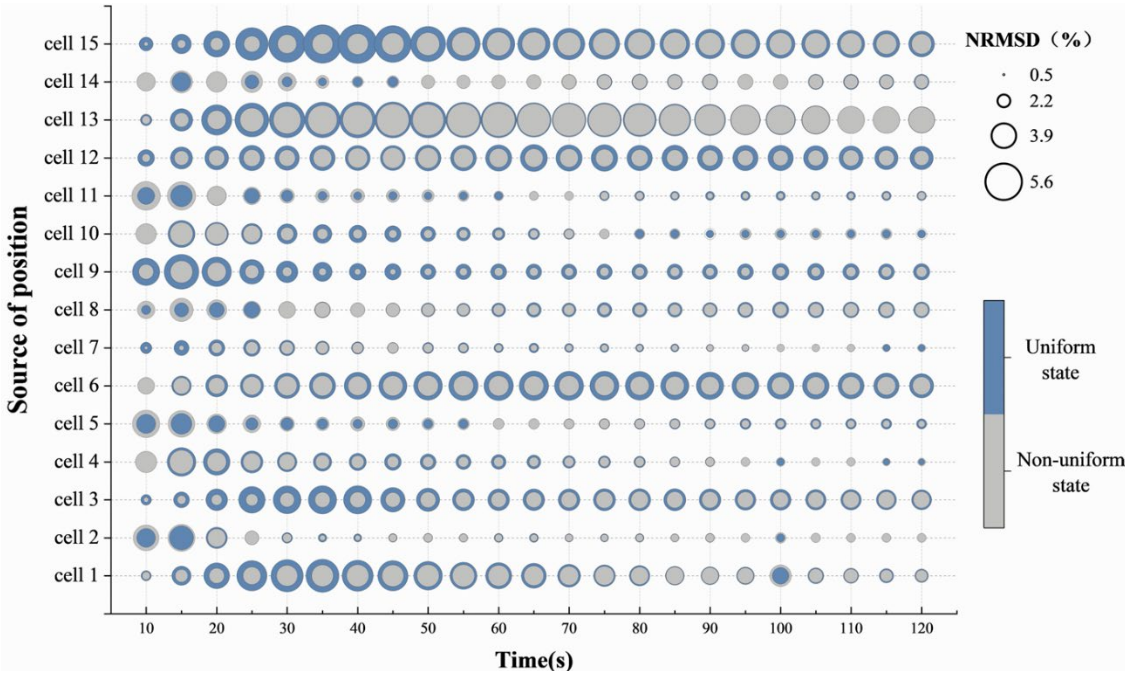

Fig. 9 Comparison of prediction ability between non-uniform and uniform state division.

4. Published Paper etc.

[Underline the representative researcher and collaborate researchers]

[Published papers]

1.H. Zhang, X. Ding, W. Zhang, W. Zhang, Y. Xuan, Optimising multi-vent module-based adaptive ventilation using a novel parameter for improved indoor air quality and health protection, Build Simul. (2023).

2.X. Ding, H. Zhang, W. Zhang, Y. Xuan, Non-uniform state-based Markov chain model to

improve the accuracy of transient contaminant transport prediction, Build Environ. 245 (2023).
3.W. Zhang, W. Zhang, H. Zhang, Y. Xuan, Effective improvement of a local thermal environment using multi-vent module-based adaptive ventilation. Build. Simul. (2023)

[Presentations at academic societies]
1.The 11th International Conference on Sustainable Development in Building and Environment (SuDBE2023): Optimising multi-vent module-based adaptive ventilation using a novel parameter for improved indoor air quality and health protection.
2.The 11th international conference on indoor air quality, ventilation & energy conservation in buildings: Study on the multi-energy supply framework for office building.
3.The 23rd China Conference on Heating, Ventilation, Air-Conditioning & Refrigeration: A new attempt to address the challenge of indoor contaminant diffusion - Multi-vent Module-based Adaptive Ventilation and its optimal design method.
4.The 18th IBPSA International Conference and Exhibition Building Simulation 2023.
5.The 23rd National Ventilation Technology Academic Annual Conference (2023):
Transient contaminant transport prediction based on computational fluid dynamics and Markov chain method with application of non-uniform state size.

[Published books]
1.
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[Other]
Intellectual property rights, Homepage etc.

5. Research Group
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2. Xiaoxiao Ding, Beijing University of Technology, PhD Student
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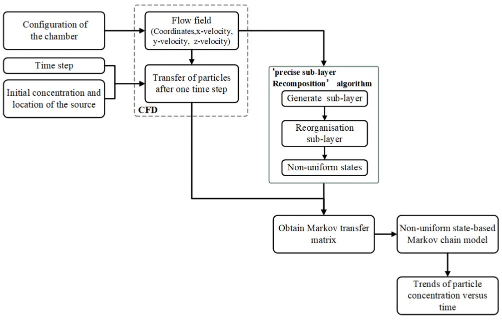
6. Abstract (half page)

Research Theme: Transient contaminant transport prediction based on computational fluid dynamics and Markov chain method with application of non-uniform state size
Representative Researcher (Affiliation): Weirong Zhang (BJUT)

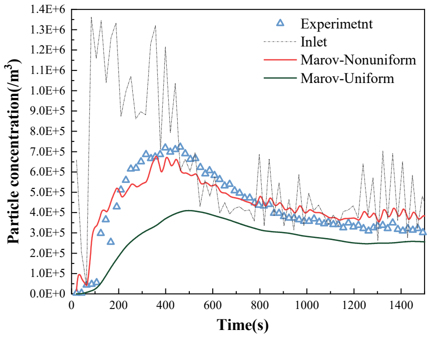
Summary・Figures

Rapid and accurate prediction of the transient transport of contaminants is crucial. The use of coarse matrices for Markov chain models has a low computational cost. However, the coarse Markov states lack a method of partitioning. This study proposed a method of partitioning Markov chain states to improve the prediction accuracy of models. By dividing the non-uniform states based on the flow field velocity, the differences within individual states were reduced, thereby reducing computational bias. The method was validated using both experimental data and CFD simulation data. The results show that:

1) The Markov chain model based on non-uniform states effectively predicts transient particle transport in steady-state flow fields. The acceptability of the Markov chain model with non-uniform states for predicting the concentration of contaminants in the target area was demonstrated using experimental data on transient contaminants.
2) Compared to the model with uniform states, the Markov chain model with non-uniform states has higher prediction accuracy. A Markov chain model with non-uniform states has been demonstrated to be closer to experimental results. Furthermore, comparison with CFD simulation data has shown that the accuracy of the non-uniform state model in predicting contaminant transport is acceptable under different flow fields.
3) Refining the states around the source helps improve the prediction accuracy of contaminant distribution. When focusing on the early transfer of contaminants, the states near the source should be refined.
4) The transfer matrix obtained under different time steps is affected by the brief concentration peak within the state, which affects the model's prediction results. The time step and state size should be adjusted according to the application requirements.



Procedures for obtaining non-uniform state-based Markov chain model and for simulating particle transport with the model.



Comparison between the numerical results for transient particle concentration of the Markov chain model and the experimental data at 0.9 m