Transient contaminant transport prediction based on computational fluid dynamics and Markov chain method with application of non-uniform state size

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Abstract
Markov chain technology has demonstrated great potential in predicting the transient transport of pollutants rapidly. The state transfer matrix is at the core of the Markov chain, and its size affects the computational cost, while its values directly impact the accuracy of the calculations. In order to reduce the computational cost of the Markov chain model while ensuring acceptable calculation accuracy, we propose an improved method based on velocity-based non-uniform state division for the combined model of CFD and Markov chain technology. We compared the predictive results of the improved model with experimental measurement data and CFD simulation data, and the results showed that the model's predictive performance for particle distribution concentration is good. Moreover, the prediction accuracy is higher when using the non-uniform state division method.

Highlights
• Extended bullet points in place of the keywords
• Lay emphasis on your novel methods and results
• Reach a wider audience with practical implications
• Three to five. Keep it short and precise

Introduction
The spread of pollutants in the air has always been a concern for the public. In recent times, epidemics have had increasingly serious impacts on life and production, and it has been found that the airflow pattern in indoor environments is related to the transmission of infectious disease viruses and bacteria (Li et al., 2007). As a result, there has been extensive research on the transmission of such particles in order to develop effective control measures, improve system design, and facilitate real-time control (Rayegan et al., 2023). Computational Fluid Dynamics (CFD) is a widely-used simulation tool for particle transport and distribution research, with Eulerian (F. Chen et al., 2006) and Lagrangian (Hang et al., 2014) methods being the most popular for particle transport modeling. Studies have also compared the two methods, and although both can predict particle concentration distribution well, they require significant computation time (Wang et al., 2012), making them unsuitable for real-time control needs. Given the current focus on virus transmission, it is critical to rapidly predict indoor pollutant diffusion in order to control indoor air quality. Therefore, there is a high level of concern regarding how to quickly calculate the diffusion path of pollutants, such as aerosols.

Markov chain technology has been increasingly applied in recent years for the rapid prediction of spatial and temporal particle concentration. It has been demonstrated that the Markov chain model has faster calculation speed than Eulerian and Lagrangian methods with the same accuracy requirements. Nicas (Nicas, 2000) was the first to prove the applicability of Markov chain technology in the rapid prediction of particle concentration calculation, which was subsequently verified in a multi-region model. Chen (C. Chen et al., 2014) developed a method that combines CFD and Markov chain for the rapid prediction of transient particle transport in a closed environment. Since then, Markov chain technology has been widely applied and developed in pollution propagation research. Its inverse model combined with Bayesian analysis has been used to locate pollution sources (Zeng, Gao, Lv, Zhang, Chen, et al., 2020) and optimize sensor placement (Liu et al., 2019). Fundamental research on Markov chain models has also been conducted, including the construction of transition matrices (Zeng, Gao, Lv, Zhang, Tong, et al., 2020), the comparison of different transition matrix acquisition methods for predictive performance (Hu et al., 2022), and the study of accelerated calculation methods (Mei et al., 2017). The accuracy of the Markov chain model depends on the state transition matrix, and the size of the matrix is determined by the resolution of the states. However, the number of states in the CFD data limits the granularity of the grid partition, resulting in a large number of grids and a correspondingly large order of the transition matrix. This, in turn, leads to high computational costs. When dealing with a grid of this size, the computational speed of the Markov chain model is no longer advantageous. Therefore, it cannot meet the real-time control requirements for large spaces.

To improve the accuracy of quick particle concentration prediction while ensuring fast computation, this paper proposes an improved Markov chain model combined with CFD that uses a non-uniform state grid division method based on flow field velocity. This method is a coarse grid division method, allowing for fast computation, and it reduces the velocity differences within a single state, leading to improved calculation accuracy.
The paper first introduces the Markov chain technology and the "accurate sublayer recombination algorithm" for dividing states. Next, it demonstrates the prediction effect of the non-uniform state Markov chain model and compares the results with uniform state division.

Methods

A homogeneous Markov chain is a useful technique for describing particle transport processes within a space. It is based on several assumptions, including that the distribution of pollutants in the future depends only on the current state and transition matrix, that the matrix is fixed, and that pollutants flow with the air flow. Additionally, particles mix uniformly in each state.

In this model, each state in a space with n states (including n-1 empty states and one state from which the particle is released) represents a state in the Markov chain. The transfer matrix for this model can be expressed as:

\[
P_{ij} = \begin{bmatrix}
P_{11} & p_{12} & \cdots & p_{1n} \\
p_{21} & p_{22} & \cdots & p_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
p_{n1} & p_{n2} & \cdots & p_{nn}
\end{bmatrix}
\]

Where \( P_{ij} \) is the probability that a particle will move from state i to state j within a time step of \( \Delta t \). The transition probability satisfies the following properties:

\[
\sum_{j=1}^{n} P_{ij} = 1, \quad P_{ij} > 0
\]

The probability vector representing the particle distribution within the space at time step \( \Delta t \) is:

\[
\theta_{i+\Delta t} = \theta_{i,t} \cdot P_{ij}
\]

The concentration of particles in a state is represented as:

\[
C_{i,t} = \frac{N_{i,t}}{V_i}
\]

To obtain the transition matrix, this paper employs a Lagrangian-based tracking method. This technique, which was first introduced by Chen et al., involves using Lagrangian random tracking to calculate the number of particles that move from one state to another in a given time interval. To begin, the airflow field is solved using CFD. A set number of particles are then released in each state, and the Lagrangian tracking and random walk models are used to determine the particle movement between states i and j during \( \Delta t \). The percentage of particles that move from one state to another is considered as the transition probability. The transition probabilities \( P_{ij,t} \) and \( P_{ij,t} \) are expressed as:

\[
P_{i,j,t} = \frac{N_{i,j,t}}{N_{i,initial}}
\]

To simulate the continuous phase flow field, this study employs the RNG k-\( \varepsilon \) model. The equation for this model can be found in the Fluent manual. It is assumed that the flow field is fixed throughout the study. The discrete phase particles are calculated using the DPM model. The flow field data and particle information are exported to a Python-built platform. The particles are then classified and gridded based on their IDs and coordinates, which are exported from the computational fluid dynamics (CFD) software. The Markov chain model's transition matrix is obtained through this platform and is used for subsequent prediction calculations.

One of the factors that may cause prediction errors in the Markov chain model is the assumption that particles are uniformly distributed in each state, which may not align with the actual particle movement. Chen's study notes that the accuracy of the model may vary in different regions due to differences in particle concentration uniformity. To reduce this source of error, efforts should be made to achieve a more uniform particle distribution within each state or to ensure a consistent flow field in each state. However, since particle movement is affected by the flow field, achieving uniform particle distribution is challenging.

To address this issue, the present study proposes to partition non-uniform states based on the flow field and apply the Markov chain model for prediction. When the airflow in a single state is consistent, the particle movement within that state is also more consistent, which to some extent mitigates the errors caused by non-uniform particle distribution.

Results

To validate the proposed method of non-uniform partitioning of state grids, two cases were selected from the literature, namely particle transport in side-supply and top-supply ventilation rooms, which have large flow field differences. The method was validated by combining CFD with a platform built using Python.

- Case A
  
  The first study was a transient particle transport experiment conducted by Zhang (Zhang et al., 2010). Figure 1(a) shows the dimensions of the experimental room, with the supply and exhaust vents located at 2.1 m and 0.3 m above the ground, respectively. The size of the vents was 0.3 m * 0.3 m, and the average supply-air velocity magnitude was 0.84 m/s with an incident angle of 10°. When the flow field reached steady state, particles with a size of 1 \( \mu \)m were injected into the chamber. According to previous studies, a resolution of 18009 is sufficient to capture indoor turbulence and meet grid independence. In this validation case, a resolution of 480162 was used for the calculation, and the reliability of the model was verified by comparing the
experimental results with the CFD simulation results. The validation results of the fixed flow field are reliable.

(a) Configuration of the chamber and measuring point location

(b) The states of chamber.

*Figure 1 Model of the chamber studied by Zhang et al (Zhang et al., 2010).*

*Figure 2 Comparison of trends of particle concentration versus time with a pulsed particle source in State 20 (Case A).*
After obtaining the steady-state flow field, the Python platform was used to construct a non-uniform state grid by importing the coordinates and velocity components of each grid. The platform’s functions include grid coordinate partitioning, sub-layering, sub-layer merging, constructing a transition matrix under non-uniform states, and particle transfer calculation. The sub-layer thickness in this model was set to 0.05 m, and the grid was divided into 36 regions. The removal region was labelled as State 37, as shown in Figure 1(b), and a $37 \times 37$ transition probability matrix was obtained based on the flow field and Lagrangian tracking. During the entire particle propagation cycle, the ion concentration in each state was normalized based on the initial released particle number. The time step of the Markov chain model was set to 5 seconds, and when the pollution source was located in State 20, the initial probability vector was defined as in Equation 7. Figure 2 shows a comparison of the particle transfer results during one cycle. Due to the inclined air supply and air diffusion, the concentration in States 3 and 11 below and on both sides of the pollution source increases rapidly, and the concentration is relatively high. Although the peak value predicted by the Markov chain model is slightly inadequate compared to the CFD calculation results, the capture of the concentration trend and the peak value state is still accurate, and the overall prediction is reliable.

$$\theta_{ij} = \begin{cases} 1, & i = 20 \\ 0, & i \neq 20 \end{cases}$$  \hspace{1cm} (7)

- Case B

The second study was a particle transmission experiment conducted by Murakami et al. (Murakami S et al., n.d.), which has also been adopted multiple times in the study of particle transmission using the Markov chain model. Figure 3(a) shows the dimensions of the clean room. Two air supply outlets are located on the ceiling, delivering air vertically downwards at a velocity of 1.0 m/s, and four exhaust outlets are located on the four side walls, forming two relatively parallel downward jets in the space, qualitatively compared with references (Mei et al., 2017). In the simulation, the particle diameter was 1 μm, and particle deposition and re-suspension were negligible. The flow field was spatially non-uniformly divided using an accurate sub-layer recombination algorithm, and the room was divided into 15 states, with the removal area marked as State 16, as shown in Figure 3(b). Based on the calculated airflow field and Lagrangian tracking, a transition probability matrix of $16 \times 16$ could be obtained.

The time step of the Markov chain model was set to 5 seconds, and the Markov chain model was verified using two scenarios where the pollutant source was located in States 3 and 7, respectively. The initial probability vector was:

$$\phi_0 = [0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0]$$  \hspace{1cm} \text{source at State 37}

It is worth noting that while the RANS-Lagrangian model has been validated in previous studies for predicting steady-state airflow fields and pollutant distributions, its predictability for transient particle distributions is not necessarily guaranteed. However, since the transient particle distribution is controlled by the same physical quantities as the steady-state particle distribution, the RANS-Lagrangian model can still be used to generate transient particle distributions for verifying the Markov chain model under non-uniform states, as was done in this study.

Figures 5 and 6 show the comparison between the concentration predicted by the Markov chain model and the normalized concentration of particles obtained by CFD simulation over time, when the pollution source is located in States 3 and 7, respectively. The results show that when the pollution source is in State 3, the pollutants move to States 2 and 6 following the airflow, and then the pollutants from State 6 move to State 9. The peak value in State 9 is obviously later than in States 2 and 6. When the pollution source is in State 7, a similar pattern is observed. Pollutants first reach adjacent States 4 and 10, and about 10 seconds later, States 1 and 13 reach their peak concentration. In general, the Markov chain model predictions agree well with the experimental results.

In this study, we compared the prediction performance of Markov chain models under non-uniform and uniform states. We used the normalized root-mean-square deviation to quantify the difference between the two, as shown in Equation 8. To ensure a comprehensive comparison, we conducted 15 calculations for each state to avoid testing a single pollution source. We then compared the results for each time step, as shown in Figure 6, where the horizontal axis represents the running time, the vertical axis represents the state where the pollution source is located, and the scatter plot represents the root-mean-square deviation of the concentration of pollutants in the entire space calculated by the Markov chain model and CFD. The green and red colours respectively represent the calculation deviation under uniform state and non-uniform state. We observed that the majority of green scatter plots were larger than red ones.

$$\text{NRMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (C_{\text{CFD}} - C_{\text{Measurement}})^2 / n}$$

When States 1, 3, 13, and 15 serve as pollution sources, the model under the non-uniform state performed better in the early stage. This is because these four states are distributed in the indoor corners, where particles start to transfer. Some are directly exhausted from the exhaust port, while others have a larger absorption ratio due to the presence of obvious eddies. The non-uniform state distinguishes the eddy effect of this part. For all calculation conditions, the average root-mean-square deviation of the uniform and non-uniform state models
was 2.4% and 1.9%, respectively. Thus, the calculation accuracy improved by 0.5% with non-uniform state division, indicating better prediction performance.

(a) Configuration of the ventilated chamber.
(b) The states of chamber.

Figure 3 Model of the chamber studied by Murakami et al. (Murakami S et al., n.d.).

Figure 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 3.

Figure 5 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.
Previous studies assumed that pollutants are uniformly distributed in the source states, which led to the fact that the volume of the source states filled with pollutants under uniform and non-uniform states is not exactly the same, making the comparison not rigorous enough. Although the initial conditions of the pollution source are slightly different after different state divisions, both groups of data were compared based on their respective CFD calculation results as the true value. Therefore, comparing the root-mean-square errors of the two groups can still reflect the difference in their prediction accuracy. We believe that this comparison method is feasible and effective.

![Figure 6 Comparison of prediction ability between non-uniform and uniform state division.](image)

Conclusion

Fast and accurate prediction of indoor pollutant diffusion is crucial, and coarse-grained Markov chain models have been proven to have the advantage of low computational cost. However, their prediction accuracy needs improvement. In this study, we propose an improved method for Markov chain models to enhance their prediction accuracy using coarse-grained grids. By dividing non-uniform states based on flow field velocity, we reduce the variability within a single state, thus reducing computational bias. We verified the model using experimental data and CFD simulation data. The results show that the Markov chain model based on non-uniform states effectively predicts particle transport in steady flow fields and has higher prediction accuracy for target area pollutant concentration than the model based on uniform states.

The proposed improvement method in this study can improve computational accuracy, save computational resources, and can be used for subsequent high-precision real-time prediction and control services.

References


