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Modeling transient particle transport in transient indoor airflow by fast fluid dynamics with the Markov chain method

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A B S T R A C T

It is crucial to accurately and efficiently predict transient particle transport in indoor environments to improve air distribution design and reduce health risks. For steady-state indoor airflow, fast fluid dynamics (FFD) + Markov chain model increased the calculation speed by around seven times compared to computational fluid dynamics (CFD) + Eulerian model and CFD + Lagrangian model, while achieving the same level of accuracy. However, the indoor airflow could be transient, if there were human behaviors involved like coughing or sneezing and air was supplied periodically. Therefore, this study developed an FFD + Markov chain model solver for predicting transient particle transport in transient indoor airflow. This investigation used two cases, transient particle transport in a ventilated two-zone chamber and a chamber with periodic air supplies, for validation. Case 1 had experimental data for validation and the results showed that the predicted particle concentration by FFD + Markov chain model matched well with the experimental data. Besides, it had similar accuracy as the CFD + Eulerian model. In the second case, the prediction by large eddy simulation (LES) was used for validating the FFD. The simulated particle concentrations by the Markov chain model and the Eulerian model were similar. The simulated particle concentrations by the Markov chain model and the Eulerian model were similar. The computational time of the FFD + Markov chain model was 7.8 times less than that of the CFD + Eulerian model.

1. Introduction

In recent decades, major outbreaks of airborne infectious diseases, such as severe acute respiratory syndrome (SARS) [1,2], influenza A virus subtype H1N1 (H1N1) [3], and coronavirus disease 2019 (COVID-19) [4], have occurred in indoor environments. The index person can exhale droplets containing infectious virus through coughing or sneezing [5,6]. The droplets quickly evaporate and the droplet nuclei can disperse with the air indoors [7]. These airborne infectious particles may be inhaled by the receptors and cause infection [8]. It has been proven that air distribution is strongly associated with airborne infectious particle transport indoors [9]. Therefore, it is important to calculate the particle dispersion indoors to support the ventilation design for reducing the infection risks.

Computational fluid dynamics (CFD) has been widely used in predicting indoor particle transport. For example, Chen et al. [10] used the renormalization group (RNG) k-ε model with Lagrangian tracking to calculate the patient-to-dentist particle transport in a dental clinic. Gao et al. [11] applied a similar method to investigate the lock-up phenomenon of human exhaled droplets under a displacement ventilated room. You et al. [12] used a hybrid SST k-ω and RNG k-ε turbulence model with the Eulerian approach to calculate the person-to-person contaminant transport in aircraft cabins with different air distribution systems. These studies assumed the airflow field to be steady, while the particle transport is transient. In general, the calculation of transient particle transport requires more computational time than that of the steady-state airflow field due to the large number of time steps required [13].

It is to be noted that the exhaled airflow such as a cough is also transient. Therefore, to improve the accuracy of predictions, researchers have also conducted numerical simulations for transient particle transport in transient exhaled airflow. For instance, Gupta et al. [14] investigated the exhaled droplet dispersion in an aircraft cabin by considering

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a coughed airflow profile. Chen et al. [15] numerically investigated the dispersion of exhaled particles from a single cough with various mouth covering approaches. For a single cough or sneeze, although the exhaled airflow is transient, the duration of the transient airflow is much shorter than that of the particle dispersion in the air [15]. After the local disturbance of the cough or sneeze disappears, the airflow can be regarded as steady-state for the remaining period [16]. Therefore, the extra computational time for the transient exhaled airflow may not be significant.

In recent years, unsteady airflow distribution systems have been proposed to improve the effectiveness of indoor air pollutant removal. For example, Sattari and Sandberg [17] and Fallenstein et al. [18] performed particle image velocimetry (PIV) measurements of a ventilation flow which was driven by a wall jet with a constant supply and one with a periodic velocity at 0.3, 0.4 and 0.5 Hz. Van Hooff and Blocken [19] numerically studied the impact of the frequency and amplitude of the periodic sine function for air supplies on ventilation performance. In these cases, both the airflow and contaminant transport were transient throughout the whole calculation period, which would significantly increase the computational overhead. Therefore, it is worthwhile to develop a new model for accelerating the calculations of transient particle transport in transient airflow in indoor environments.

For airflow calculations, fast fluid dynamics (FFD) has been proven to be faster than CFD with comparable accuracy [20–24]. For instance, Liu et al. [22] found that the computing cost of FFD could be 20 times less than CFD while the accuracy was still satisfactory. Note that the acceleration on the computational speed by FFD compared with CFD depends the grid size and flow features. For unsteady particle calculation, the Lagrangian model has also been proven to be faster than the Eulerian and Lagrangian models [25–29]. For example, Chen et al. [26] reported that the computing cost of the Lagrangian model was around six times less than the Eulerian and Lagrangian models. Therefore, this study aims to develop a FFD + Markov chain model solver in OpenFOAM, an open-source CFD toolbox [30], to accelerate the unsteady airflow and particle calculations. This investigation used two cases, transient particle transport in a ventilated two-zone chamber and a chamber with periodic air supply, to validate the model. The accuracy and sensitivity in regard to the time step size of the FFD + Markov chain model were compared with that of the FFD + Eulerian model to explore the pros and cons of the proposed FFD + Markov chain model.

2. Methodologies

In order to predict the transient particle transport in transient indoor airflow, in each time step, this study used FFD and Markov chain model to simulate the airflow and particle transport, respectively. This section thus briefly introduces FFD and Markov chain model and then focuses on the integration of the two methods.

2.1. Fast fluid dynamics

The FFD in this study uses a two-step, time splitting scheme to solve the momentum equations of the time-dependent Navier–Stokes equations. With the air velocity \( \mathbf{U}^n \) and pressure \( P^n \) at the current time step, FFD firstly solves the convection, diffusion, and source terms to obtain an intermediate air velocity \( \mathbf{U}^* \) in Eq. (1).

\[
\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = \frac{1}{\rho} \nabla p^n + \frac{1}{\rho} \nabla \cdot \mathbf{F}^n + \mathbf{U}^n \frac{\partial \mathbf{U}^n}{\partial t} + \mathbf{U}^n \frac{\partial \mathbf{U}^n}{\partial t} + \mathbf{F}^n
\]

where \( t \) is the time, \( \rho \) is the air density, \( F_i \) the \( i \)th body force; \( v \) the effective viscosity. By adopting a standard incremental pressure-correction (SIPC) scheme [31,32], the pressure gradient is included in the source term. The FFD then solves the pressure difference term together with the continuity equation by a pressure projection method [33] in Eq. (2) for calculating the pressure \( P^{n+1} \).

\[
\frac{\partial^2 (P^{n+1} - P^n)}{\partial x_i \partial x_i} = \frac{\rho \mathbf{U}^*}{\Delta t} \frac{\partial \mathbf{U}^*}{\partial x_i}
\]

The pressure \( P^{n+1} \) will be used to calculate the air velocity at the next time step \( \mathbf{U}^{n+1} \) by using the equation for pressure difference term in Eq. (3). The readers can refer to [22] for detailed deductions.

\[
\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = \frac{1}{\rho} \nabla (P^{n+1} - P^n) \Rightarrow \mathbf{U}^{n+1} = \mathbf{U}^n - \frac{\Delta t}{\rho} \nabla P^{n+1}
\]

2.2. Markov chain model

The Markov chain model calculates the particle transport by the principle of Lagrangian model on the Eulerian grid. With a matrix of particle transition probabilities, where \( P_{ij} \) is the probability of particle’s remaining in the current cell \( i \) and \( P_{ij} \) the probability of particle’s moving from neighboring cells \( (\text{nh}) \) to cell \( i \), the number of particles in grid cell \( (N_i) \) after a time step \( (\Delta t) \) could be calculated by:

\[
N_i((t + \Delta t) = N_i(t)P_{ij} + \sum_{\text{nh}} N_{\text{nh}} P_{\text{nh}i}
\]

As shown in Eq. (4), only were the transition probabilities of a particle staying at the current cell (one dimension) and moving to neighboring cells (six dimensions) need to be calculated in the Markov chain model. For a three-dimensional mesh with \( M \) grid cells, the size of \( P \) is thus \( 7 \times M \). According to [26], the transition probability \( P_{ij} \) is determined by solving the particle mass balance equation:

\[
P_{ij} = \exp(\sum Q_{ij}\Delta t/V_i)
\]

where \( Q_{ij} \) is the mass flux from a neighboring cell to cell \( i \) and \( V_i \) is the volume of cell \( i \). Then the transition probability \( P_{ij} \) could be determined:

\[
P_{ij} = \frac{Q_{ij}}{\sum_{\text{nh}} Q_{i,\text{nh}}(1 - P_{ij})}
\]

Once all the \( P_{ij} \) are determined, the \( P_{ab} \) are known accordingly. The Markov chain model calculates the number of particles in each grid cell, after which the particle concentration can be determined by dividing the particle number \( (N_i) \) by cell volume \( (V_i) \). The readers can refer to [26] for detailed deductions.

2.3. Integration of FFD with Markov chain model

Due to the transient airflow, the mass flux on the grid cell faces is transient, which further leads to transient particle transition probabilities. Therefore, at \( t = n\Delta t \), the FFD + Markov chain model first solves Eqs. (1), (2), and (3) in sequence to obtain the air velocity \( U^n \) as shown in Fig. 1. To calculate the turbulence, this study solves the RNG k-ε model equations. The RNG k-ε model is one of the best Reynolds-averaged Navier–Stokes (RANS) turbulence models for predicting the indoor airflow [34,35]. In solving these equations, this study used a bounded first order implicit scheme for the unsteady terms and a bounded second order upwind scheme for the convection terms.

With the predicted airflow, the combined method then constructs the matrix of particle transition probabilities by using the Eqs. (5) and (6). Finally, the particle number distribution could be calculated by Eq. (4) and the particle concentration could be further obtained by dividing \( N_i \) by cell volume \( V_i \). The solver for FFD + Markov chain model was programmed in OpenFOAM [30].

It is important to note that the matrix of particle transition probabilities needs to be calculated in each time step due to the transient indoor airflow. For steady-state airflow, the matrix of particle transition probabilities will be constructed only once after the airflow is...
predicted. Then Eq. (4) is used to obtain the particle concentration. Therefore, calculating the transient particle transport in steady-state airflow by the Markov chain model can be very efficient [24,27]. However, for predicting the transient particle transport in transient airflow, the efficiency of the Markov chain model would decrease due to solving Eqs. (5) and (6) in each time step.

3. Results

Due to the difficulty and complexity in measuring transient particle transport with transient indoor airflow, this study used two cases from literature to test the accuracy and efficiency of the FFD + Markov chain model. Case 1 was an experiment in a ventilated two-zone chamber [36] and case 2 was a room with periodic air supplies [37]. This second case had predicted airflow by sophisticated numerical tools for validating the FFD in predicting the transient airflow. This study then compared the Markov chain model with the traditional Eulerian model.

3.1. Case 1: particle transport in a two-zone ventilated chamber

Fig. 2(a) shows the geometry of a two-zone ventilated chamber with dimensions 5(L) x 2.4(H) x 3(W) m³. The two zones were separated by a partition with a sliding door (0.95 x 0.7 (y x z) m²). There was an inlet (0.5 x 1.0 (y x z) m²) located on the left wall of zone 1 and an outlet (0.5 x 1.0 (y x z) m²) located on the right wall of zone 2. Initially, the door was closed and air supply was shut off. Zone 1 was injected with smoke particles in a range of 0.5–5 μm, while there were no particles in zone 2. At t = 0, the door was opened and air supply was turned on. Zone 1 was injected with smoke particles in a range of 0.5–5 μm, while there were no particles in zone 2. The incoming air was supplied from the inlet at $U_x = 0.09216$ m/s, $U_y = 0$, and $U_z = 0$. The corresponding air change rate per hour (ACH) was 9.216 h⁻¹ or time constant was $\tau = 390$ s. The experiment measured the particle concentration at the center of each zone (green dots in Fig. 2(a)) for 26 min [36].

The FFD simulation of the transient airflow used exactly the boundary conditions from the experiment, except assuming the turbulence intensity of the inlet air to be 10% for calculating the inlet turbulence kinetic energy $k$ and turbulence dissipation rate $\varepsilon$, which were not provided in the experiment. Besides, this Markov chain model does not
consider the inertial force of the particles [26,38]. This investigation first conducted a grid independence test with four grid resolutions: 29,844 (mesh 1), 74,136 (mesh 2), 220,550 (mesh 3), and 472,050 (mesh 4). This study ran the FFD + Markov chain model for 2τ with a time step size Δt = 0.01 s. The time step size was the same as the value used in [36]. Fig. 3 presented the dimensionless air velocity ([U] / |U_inlet|) profiles at positions 1 and 2 after 2τ. Positions 1 and 2 were the vertical lines at the center of zone 1 and zone 2, respectively. The predictions with mesh 3 agreed well with that with mesh 4. To confirm, this study further calculated the grid-convergence index (GCI) [39] defined by:

$$GCI_{\text{mesh } 2} = F_s \frac{r^{n}|U_{\text{mesh } 1}| - |U_{\text{mesh } 4}|}{|U_{\text{inlet}}|}$$

(7)

where $r$ is the linear grid refinement factor ($r = (472,050/220,550)^{1/3} = 1.29$), $n$ the formal order of accuracy which is equal to the value of 2 since second-order discretization schemes were used. $F_s$ is a safety factor, taken to be 1.25 that was recommended by [39]. The average GCI values for mesh 3 at positions 1 and 2 were 0.043 and 0.051, respectively. Therefore, mesh 3 was able to give nearly-grid independent results, the following simulations used mesh 3 as shown in Fig. 2(b).

With mesh 3, this study ran the FFD + Markov chain model for 27 min with a time step size Δt = 0.01 s. The prediction by CFD + Eulerian model was also conducted for comparison. Due to the small particle size, the Eulerian model used a drift-flux model [40], which is a simplified Eulerian two-phase flow model. The CFD simulation used the Semi-Implicit Method for Pressure Linked Equations (SIMPLE) [41] algorithm to couple the air pressure and velocity. The other setups such as numerical schemes, time step size, boundary conditions, and turbulence model, etc. of the CFD simulation were the same with that of the FFD simulation.

Fig. 4 compares the simulated particle concentration with the experimental data in zone 1 and zone 2. To quantify the overall accuracy of the models, this study calculated the normalized root-mean-square deviation (NRMSD) between the experimental data and numerical predictions defined as:

$$\text{NRMSD} = \frac{\sum_{i=1}^{n} (C_{\text{exp},i} - C_{\text{numerical},i})^2}{C_{\text{exp,max}} - C_{\text{exp,min}}}$$

(8)

where $C_{\text{exp,max}}$ and $C_{\text{exp,min}}$ is the maximum and minimum particle concentration from the experimental data, respectively. Table 1 lists the calculated $NRMSD$s between the predictions by the three models and the experimental data. The FFD + Markov chain model had the similar accuracy to the CFD + Eulerian model in predicting the transient particle transport. Furthermore, for both zones 1 and 2, the FFD + Eulerian model predicted lower particle concentrations than the other two models, and its overall accuracy was the worst based on the $NRMSD$ results. In zone 1, all the predictions displayed minor difference and had acceptable agreement with the experimental data in the first 4 min. Afterwards, both the FFD + Markov chain model and CFD + Eulerian model overpredicted the particle concentrations in zone 1 after $t = 4$ min compared with measured data, which was consistent with the finding by an independent previous study [42]. Therefore, we suspected that there might be certain errors in the measurements and the “good performance” of the FFD + Eulerian model in this certain range was probably a coincidence.

In zone 2, there were no particles at the beginning. Once the ventilation was on and the door was opened, the airflow brought particles to zone 2. In the first 2.5 min, a “wave” of airflow carrying particles came across the cells at the center of zone 2. Therefore, the particle concentration increased rapidly in the first minute due to the “wave”, but then dropped in the next minute because the “wave” was gone. From $t = 2.5$ min to around $t = 10$ min, the particle concentration increased again because the airflow in zone 2 became steady and the particles dispersed to the whole space due to diffusion. Afterwards, the particle concentration decreased gradually due to the particle removal by ventilation. Compared with the experimental data, all the simulations overpredicted the drop of particle concentration at around $t = 2.5$ min. However, this drop might not be captured by the experiment. The experiment in [36] used an infrared particle counter to measure the particle concentrations. The relatively long sampling time (1 min) would hide the possible significant drop of the particle concentration observed by the numerical simulations at around $t = 2.5$ min. Furthermore, the Markov chain model predicted a more significant drop of particle concentrations in the first 2.5 min in zone 2 than the Eulerian model. This was partially because the Markov chain model was less diffuse than the Eulerian model as observed in the previous study [26]. Namely, the “wave” was less diffusive in the Markov chain model so that the particle concentration was lower when the “wave” was gone. Moreover, after $t = 5$ min, the predicted particle concentration by CFD + Eulerian model and FFD + Markov chain model were very similar and agreed reasonably well with the experimental data (on average 20.6% difference ($\frac{|C_{\text{numerical}} - C_{\text{exp}}|}{C_{\text{exp}}}$)) between $t = 5$ min and $t = 20$ min). In contrast, the FFD + Eulerian model significantly underpredicted particle concentrations after $t = 5.0$ min.

This study further investigated the influence of time step size on the accuracy of the predictions with the extra four time steps: $\Delta t = 0.1, 1.0, 2.0$, and 5.0 s. The corresponding mean and maximum Courant numbers ($C_0$) were provided in Table 2. This study did not test time step sizes greater than 5.0 s since the $C_0_{\text{max}}$ for $\Delta t = 5.0$ s was much greater than one. If the Courant number is greater than one, fluid particles move through more than one cells at each time step.
and this can affect convergence negatively. Fig. 5 shows the particle concentration vs. physical flow time for FFD + Markov chain model. One can notice the almost identical predictions with $\Delta t = 0.01, 0.1$, and 1.0 s, which could be regarded as time-step-size independent. The prediction with $\Delta t = 2.0$ s showed some differences with those predicted with smaller $\Delta t$. With $\Delta t = 5.0$ s, the FFD + Markov chain model was unable to predict the correct particle concentrations. Therefore, the most suitable time step size for case 1 was $\Delta t = 1.0$ s.

![Fig. 3. Grid independence test for case 1.](image)

![Fig. 4. Particle concentrations vs. time in the center of zone 1 and zone 2 for case 1.](image)

Table 1

| Location       | FFD + Eulerian | FFD + Markov | CFD + Eulerian |
|----------------|---------------|--------------|----------------|
| Zone 1         | 10.8%         | 6.3%         | 7.0%           |
| Zone 2         | 16.0%         | 8.9%         | 8.9%           |
| Zones 1&2      | 13.6%         | 7.7%         | 8.0%           |

to further identify the reason for the wrong predictions with $\Delta t = 5.0$ s, Fig. 6 compares the predicted airflow by FFD with different time step sizes in the vertical mid-section of the room. Since this case was iso-thermal, the inlet jet flowed horizontally to the partition wall and then flowed downward to the door. After the door, the air flowed along the floor to the exhaust. It is clear that the flow fields changed a lot in the beginning and the greater the time step size, the more diffusive the predicted airflow in the first 50 s. With $\Delta t = 5.0$ s, the predicted airflow in the first 50 s was not sufficiently accurate for predicting the particle transport. However, at $t = 100$ s and $t = 200$ s, the predicted airflow with $\Delta t = 5.0$ s agreed well with those predicted with smaller time step sizes.

With $\Delta t = 1.0$ s, Fig. 7 shows the predicted transient particle concentration distributions by the Markov chain model and Eulerian model in the vertical mid-section of the room. The particles in zone 1 moved along the airflow to zone 2. Both the Markov chain model and Eulerian model were able to predict the residual particles above the inlet in zone 1 and the recirculated particles in zone 2. In general, the two models had similar performance in capturing the major features of the transient particle transport.

3.2. Case 2: particle transport in a ventilated room with periodic air supplies

The second case was particle transport in a ventilated room ($9 \times 3 \times 3$ m$^3$) with two inlets and two outlets [37]. As shown in Fig. 8(a), the air was supplied by two inlets ($0.168 \times 3$ m$^3$) oppositely located in the upper part of the side walls. Accordingly, the
Fig. 5. Effect of the time step size for FFD + Markov chain model in case 1.

Fig. 6. Predicted airflow (dimensionless velocity magnitude; $|U|/|U_{inlet}|$) by FFD with different time step sizes in the mid-section of the room in case 1.

The air was exhausted by two outlets ($0.48 \times 3 \text{ m}^2 (y \times z)$) oppositely located in the floor level of the side walls. The air supply velocities for the left and right inlets were:

$$U_{left \text{ inlet},x}(t) = U_0(1 + \sin(2\pi t/T))$$  \hspace{1cm} (9)

$$U_{right \text{ inlet},x}(t) = U_0(1 - \sin(2\pi t/T))$$  \hspace{1cm} (10)

where the period was $T = 0.4\tau$ with the room time constant $\tau = 160.71 \text{ s}$ and $U_0 = 0.5 \text{ m/s}$. According to [37], the turbulence intensity ($TT$) and turbulent viscosity ratio $\frac{\mu_t}{\mu}$ of the inlet jets were assumed to be 10% and 10, respectively. Then the inlet $k$ and $\epsilon$ could be calculated by:

$$k = \frac{3}{2}(U_{inlet,x}(t)/TT)^2$$  \hspace{1cm} (11)

$$\epsilon = \rho C_{\mu} \frac{k^2}{\mu} \left( \frac{\mu_t}{\mu} \right)^{-1}$$  \hspace{1cm} (12)

where $C_{\mu}$ is an empirical constant. For the RNG $k-\epsilon$ model used in this study, the value of $C_{\mu}$ was 0.0845.

Due to complex air supply conditions in this case, this study first validated FFD in predicting the airflow. The validation used the numerical results by unsteady Reynolds-averaged Navier–Stokes (URANS) CFD simulations using the RNG $k-\epsilon$ turbulence model and large-eddy simulation (LES) using the dynamic Smagorinsky subgrid-scale model from [37]. Accordingly, the FFD simulation used the same mesh (505,760 hexahedral cells) as shown in Fig. 8(b) and time step size ($\Delta t = 0.1 \text{ s}$) with those used by the URANS simulations. The time
The size of the particles was assumed to be 3 μm. The particles were released between \( x = H \) and \( y = 1 \) m, in the vertical center plane, where \( H = 3 \) m is the room height. The mean air velocity was calculated from the predicted velocity, while the Markov chain model is faster than the Eulerian model in capturing the airflow. Therefore, discrepancies still exist between the two particle transport models.}

4. Discussions

4.1. Computing speed

This investigation ran the numerical simulations in case 1 and the FFD simulations in case 2 with an Intel Xeon platinum 8179M processor with the frequency of 3.0 GHz. All the FFD simulations were run with one core. Since the CFD simulation was time-consuming, this study ran the CFD simulations for case 1 with eight cores and the computational time was 0.7 h for the time step size of 1.0 s. To compare the computational time, our test found that using eight cores would speed up the computation by 6.2 times for case 1. Therefore, the computational time of CFD simulation for case 1 with one core was estimated to be 4.52 h. Fig. 13 shows the computational time for predicting airflow and particle transport. In terms of simulating the air distribution, the FFD was 9.2 times faster than the CFD. For both cases, the Markov chain model consumes twice the computational time of the Eulerian model. Further, in case 1, the computational time with FFD + Markov chain model was 7.8 times less than with the CFD + Eulerian model. Since the computational time of predicting the particle transport was one order of magnitude less than that of predicting the airflow, further acceleration of the computational speed should focus on accelerating the prediction of the airflow.

A previous study [28] proposed the following equation to determine the ideal time step size for the Markov chain model:

\[ \Delta t_{\text{ideal}} = \frac{3}{4} \frac{h}{|U_t|} \]  

According to Eq. (13), the ideal time step sizes for cases 1 and 2 were 1.25 s and 0.2 s, respectively. Therefore, the calculated ideal time step sizes were in the same magnitude as that identified in this study, i.e. 1.0 s and 0.1 s for cases 1 and 2, respectively. Although Eq. (13) correctly estimated the suitable magnitude of the time step sizes, careful tests on the time step sizes were still needed to ensure the accuracy of predictions. Besides, our tests indicated that the performance of the Markov chain model was dependent on the input accuracy of airflow. As long as the FFD simulations were able to give the accurate airflow, further acceleration of the computational speed should focus on accelerating the prediction of the airflow.

4.2. Limitations and prospects

Theoretically, FFD is faster than CFD for airflow simulations since it does not have external iterations for coupling the pressure and velocity, while the Markov chain model is faster than the Eulerian model. However, it is important to note that this speedup is achieved at the cost of reduced accuracy, especially in complex geometries. Therefore, the choice of simulation methodology should be based on the specific requirements of the study.
model for transient particle transport calculations since it does not require iterations in each time step. The advantages of both the FFD and Markov chain model in terms of computing speed prompted us to develop the FFD + Markov chain model solver in OpenFOAM. Indeed, the results showed that the FFD + Markov chain model was even slightly lower than FFD + Eulerian model. This can be explained by the fact that the transition probabilities in the Markov chain model need to be calculated in every time step, the computational cost of which overwhelmed the model's advantage of not requiring iteration. Therefore, to accelerate the Markov chain model, one option is to pre-calculate the transition probabilities under different airflow distributions to form an off-line database. Although the transient airflow fields are case dependent, the acceleration using the offline–online approach should be applicable for all the cases. Note that, for a given space, the offline calculations of airflow fields would be the same for the FFD + Markov chain model and the existing FFD + Eulerian model, no matter how complex the space is. However, for the online transient particle transport calculations, the Markov chain model does not require any iteration, while the Eulerian model needs to solve the scalar transport equation with iteration. Since the Markov chain model was at least five times faster than the Eulerian model [24], the
acceleration using the offline–online approach should be applicable for the cases. Another potential issue for the offline–online approach is the storage of the database. However, please note that the approach does not require to store the full airflow field information, but only the transition probabilities. Therefore, the required storage space is less than that for the full airflow fields. Furthermore, the offline–online approach is especially suitable for the periodic ventilation cases, such as case 2 in this study, because the airflow fields are periodic so that the transition probabilities to be stored are relatively limited. In addition, in terms of the searching and matching process, since the transient transition probabilities are time-series data, it is easy to match with the transient particle transport calculations. This offline–online approach deserves further investigation in the future.

Another option is that the Markov chain model could use a time step size larger than that of FFD to save the computing time without sacrificing the accuracy as the flow field could be quasi-constant within a short time period. Using adaptive time step sizes to re-calculate the transition probabilities only when the flow changes drastically could also accelerate the calculations. For example, this study further ran case 1 using FFD with $\Delta t_{FFD} = 1.0$ s and Markov chain model with $\Delta t_{Markov} = 2.0$ s (larger than $\Delta t_{FFD}$) after $t = 390.0$ s (one time constant). Fig. 14 compares the predicted particle concentrations by the FFD ($\Delta t_{FFD} = 1.0$ s) + Markov chain ($\Delta t_{Markov} = 2.0$ s) model with the original model ($\Delta t_{FFD} = \Delta t_{Markov} = 1.0$ s). The results with the larger time step size agreed well with that from the original model, but the computing time was reduced by 26.2%. This example demonstrated that the calculations can be accelerated by using a time step size for Markov chain model greater than that for FFD. Besides, running FFD on graphic processing unit (GPU) would speed up the simulations because a GPU could have hundreds of cores. One can always accelerate the computational speed by parallel computing. Some previous studies have shown the improvement of computing speed by implementing FFD codes on GPU [43,44]. These potential algorithms can be further implemented into the FFD + Markov chain model solver in OpenFOAM developed in this study to overcome the identified challenges and show the theoretical advantages in the computing speed. Therefore, we believe that this work is still meaningful for the advancement of fast predictions of transient particle transport in transient flows.
lead to the following conclusions:

In case 1, the FFD had similar accuracy with CFD in predicting transient airflow, because Markov chain model is faster than Eulerian model. The results from this study well prove this hypothesis; in case 2, the FFD had similar accuracy with CFD in predicting transient airflow, because FFD is faster than CFD and Markov chain model is faster than Eulerian model. The results from this study well prove this hypothesis;

• Before this study, it was hypothesized that the FFD + Markov chain model would be faster than the FFD + Eulerian model for transient airflow, because FFD is faster than CFD and Markov chain model is faster than Eulerian model. The results from this study well prove this hypothesis;

• Before this study, it was hypothesized that the FFD + Markov chain model would be faster than the FFD + Eulerian model for transient airflow, because Markov chain model is faster than Eulerian model. However, the results and analysis from this study show that this hypothesis is not necessarily correct. Since the transition probabilities in the Markov chain model need to be calculated in every time step, the FFD + Markov chain model is even slightly slower than the FFD + Eulerian model.

5. Conclusions

This study integrated the FFD and Markov chain model and programmed the solver in OpenFOAM for predicting the transient particle transport with transient indoor airflow. The developed solver was validated by the airflow and particle transport in a ventilated two-zone room and a ventilated room with periodic air supplies. Not only the performance in predicting the transient particle transport, but also the performance in predicting the transient airflow was tested. The results lead to the following conclusions:

• The FFD + Markov chain model had a similar accuracy with the CFD + Eulerian model in predicting the particle transport;

• In case 1, the FFD had similar accuracy with CFD in predicting the complex transient indoor airflow and it could be 9.2 times faster, while the computational time with FFD + Markov chain model is calculated in every time step, the FFD + Markov chain model is 9.2 times faster, while the computational time with FFD + Markov chain model is 9.2 times slower than the original model (\(\Delta t_{\text{FFD}} = 1.0 \text{s} \), \(\Delta t_{\text{Markov}} = 2.0 \text{s} \)).

• In case 2, the FFD had similar accuracy with CFD in predicting the transient particle transport in SARS-CoV-2 in two Wuhan hospitals, Nature (2020) http://dx.doi.org/10.1038/s41586-020-2271-3.

• Before this study, it was hypothesized that the FFD + Markov chain model would be faster than the CFD + Eulerian model for transient airflow, because FFD is faster than CFD and Markov chain model is faster than Eulerian model. The results from this study well prove this hypothesis;

• Before this study, it was hypothesized that the FFD + Markov chain model would be faster than the FFD + Eulerian model for transient airflow, because Markov chain model is faster than Eulerian model. However, the results and analysis from this study show that this hypothesis is not necessarily correct. Since the transition probabilities in the Markov chain model need to be calculated in every time step, the FFD + Markov chain model is even slightly slower than the FFD + Eulerian model.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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