

Evaluation of fast fluid dynamics with different solving schemes on scalar transport equation for predicting indoor contaminant concentration

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Abstract. Predicting the transport of indoor pollution can assist designer to optimize ventilation mode of room. However, the high computational cost restricts the wide implementation of computational fluid dynamics (CFD) technique to predict indoor contaminant concentration. This study evaluated three potential numerical methods with scalar transport equation to resolve this dilemma which were combine fast fluid dynamics (FFD) and different solving schemes on scalar transport equation. To test the performance of three potential numerical methods, the conventional PISO algorithm was also employed to compare. A three-dimensional ventilation case with experimental data of indoor CO₂ concentration was adopted. The results show that the FFD with iterative scheme of scalar transport equation could predicting indoor CO₂ concentration efficiently. The numerical method with semi-Lagrangian method and iterative scheme for predicting indoor air contaminant concentration could obtain satisfactory results at large time step size.

1 Introduction

Indoor air contaminant concentration is important to human comfort and health. Analysing indoor contaminant concentration can assist in the design of effective ventilation systems [1]. Nowadays, the most widely known technique for predicting indoor contaminant concentrations is computational fluid dynamics (CFD) [2], but its disadvantage is also obvious, that is, the high computational cost [3].

For improving the efficiency of solving Navier–Stokes (N-S) equations, the fast fluid dynamics (FFD) was proposed [4]. The FFD applies a time-advancement scheme to split the momentum equation into several discretized equations [5]. Those discretized equations are solved by suitable methods for improving computing speed and/or accuracy. One of methods is adopting Semi-Lagrangian method [6] to treat advection term. With some sacrifice of accuracy, the FFD was found that to be 50 times faster than conventional CFD algorithm [7]. Comparing different derivative schemes of FFD, some schemes can achieve similar accuracy as traditional CFD with half of the computation time [8]. Based on the high computing speed of FFD, many studies combine FFD with other algorithms [9]. The results of the study show that the computing speed of the models with FFD are about seven times faster than that with traditional CFD method [10,11].

Although there are many studies on FFD [12], few studies have validated the performance of the schemes which were combining FFD with scalar transport equation [13,14]. This study evaluated three potential

numerical methods which combined FFD with two schemes of solving contaminant transport equation. The accuracy of three potential numerical methods and the effect of time step size on predictions were tested by a three-dimensional ventilation case with experimental data of indoor CO₂ concentration. The objective of the study is to provide guidance for predicting indoor air contaminant transport.

2 Numerical methods

This section provides a brief introduction of FFD and describes the implementation of the three potential numerical methods in OpenFOAM.

2.1 Different methods to solve the N-S equations

2.1.1 The standard incremental pressure correction scheme (SIPC)

The SIPC scheme applies a two-step time-advancement scheme that splits the momentum equation into two equations, Eq. (1) and Eq. (2).

$$\frac{u^* - u^n}{\Delta t} = -(U^n \cdot \nabla)U^* + \nu \nabla^2 U^* + \frac{1}{\rho} F_i - \frac{1}{\rho} \nabla p^n \quad (1)$$

$$\frac{u^{n+1} - u^*}{\Delta t} = -\frac{1}{\rho} \nabla (p^{n+1} - p^n) \quad (2)$$

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The pressure gradient term of previous step is included in the source term to obtain intermediate air velocity U^* and the pressure difference term to correct the velocity field in the next sub-step would increase the accuracy. U^n and U^{n+1} represent the velocity at the previous and current time step, respectively.

The SIPC scheme solves the pressure-velocity coupling problem using the pressure projection method, which substitutes Eq. (2) into continuity equation deriving Poisson equation Eq. (3) for calculating the pressure difference term. Finally, the velocity at current time step is obtained by solving Eq. (2).

$$\nabla^2(p^{n+1} - p^n) = \frac{\rho}{\Delta t} \nabla \cdot U^* \quad (3)$$

2.1.2 The standard incremental pressure-correction scheme with the semi-Lagrangian method (SLSIPC)

The SLSIPC scheme splits the momentum equation into three discretized equations, Eq. (4), Eq. (5), and Eq. (6).

$$\frac{U^* - U^n}{\Delta t} = -(\mathbf{U}^n \cdot \nabla)U^* \quad (4)$$

$$\frac{U^{**} - U^*}{\Delta t} = \nu \nabla^2 U^{**} + \frac{1}{\rho} F_i - \frac{1}{\rho} \nabla p^n \quad (5)$$

$$\frac{U^{n+1} - U^{**}}{\Delta t} = -\frac{1}{\rho} \nabla(p^{n+1} - p^n) \quad (6)$$

The SLSIPC scheme first solves Eq. (4) with SL method to obtain intermediate air velocity U^* . U^{**} is the intermediate air velocity which was calculated by Eq. (5). The next procedure is similar to the SIPC method. The Poisson equation is given by Eq. (7). Finally, the velocity at current time step is obtained by solving Eq. (6).

$$\nabla^2(p^{n+1} - p^n) = \frac{\rho}{\Delta t} \nabla \cdot U^{**} \quad (7)$$

2.2 Different methods to solve the scalar transport equation

There are two schemes for predicting indoor contaminant concentration, which are iterative scheme and split scheme.

2.2.1 Iterative scheme

The iterative scheme calculates the indoor contaminant concentration after obtained the current velocity field. The equation for predicting indoor contaminant concentration is:

$$\frac{C^{n+1} - C^n}{\Delta t} = -(\mathbf{U}^{n+1} \cdot \nabla)C^{n+1} + \Gamma \nabla^2 C^{n+1} + S \quad (8)$$

where C is the indoor contaminant concentration, Γ is the mass diffusive coefficient, and S is the source term.

2.2.2 Split scheme

The split scheme splits the scalar transport equation into two discretized equations, Eq. (9) and Eq. (10). C^* represent the intermediate contaminant concentration.

$$\frac{C^* - C^n}{\Delta t} = -(\mathbf{U}^n \cdot \nabla)C^* \quad (9)$$

$$\frac{C^{n+1} - C^*}{\Delta t} = \Gamma \nabla^2 C^{n+1} + S \quad (10)$$

First, the SL method calculates the intermediate contaminant concentration and intermediate velocity simultaneously and then Eq. (10) is solved iteratively for indoor air contaminant concentration after obtained the current velocity field.

2.3 Research methods to predict indoor contaminant concentration

The basic FFD method have described above. It is uneconomic that using SL method to predict intermediate scalar transport only because the procedure of SL method is depending on the parameters of the velocity field. So, the potential numerical methods with different combinations to predict indoor contaminant concentration was listed in table 1. The SL method used the cellPoint scheme in OpenFOAM for interpolation. The conventional PISO algorithm with iterative scheme was also employed for comparison.

Table 1 Three potential numerical methods

| Methods | N-S equation | Scalar transport equation |
|-------------|---------------|---------------------------|
| Scheme S+I | SIPC scheme | Iterative scheme |
| Scheme SL+I | SLSIPC scheme | Iterative scheme |
| Scheme SL+S | SLSIPC scheme | Split scheme |

3 Comparison of the numerical methods

To test the different numerical methods, this study used a ventilation case in environment chamber with experimental data from Chung and Hsu [15]. As shown in Fig.1(a), the size of the chamber was 400×300×250 cm³. Inlet and outlet had the same size of 40 cm×40 cm. The coordinates of the central points of inlet and outlet were (0, 120, 150) and (400, 120, 240), respectively. The inlet air velocity was 0.68 m/s and the CO₂ concentration level of supply air was 350 ppm. The initial uniform CO₂ concentration in the chamber was of around 2000ppm. The kinematic viscosity of indoor air was 1.85×10⁻⁵ m²/s at air temperature 27 °C. There was an isothermal condition and no heat source in the experimental chamber. The turbulent Schmidt number, which was defined as the ratio of the turbulent momentum diffusivity and the turbulent mass diffusivity, was set to 0.7 in this study[16]. A grid size of 21×26×31 was used for simulation.

In this study, the unsteady RANS simulation employed the RNG k-ε model to predict the turbulent airflow[17]. To ensure stable calculation, the time step was 0.2 s according to the Courant-Friedrichs-Lewy (CFL)

condition. Fig.1(b) shows the six measurement points in the experiment. For evaluation and comparison of different methods, the CO₂ concentration at P1 and P6 were selected.

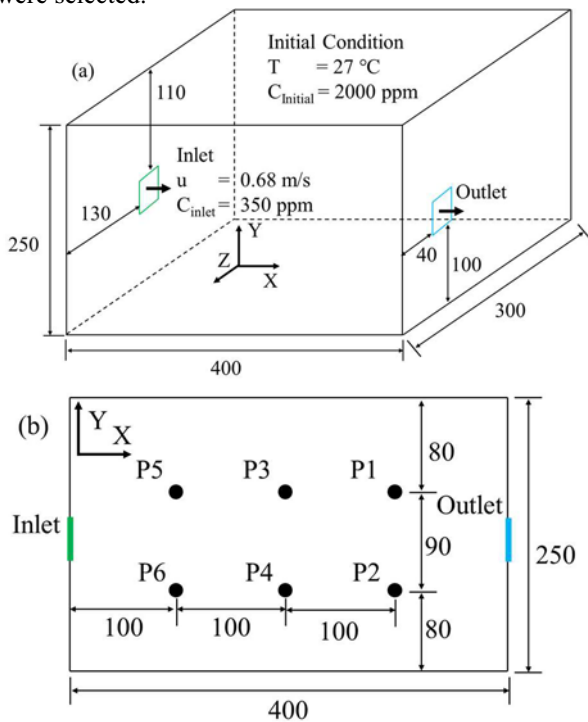


Fig.1. Schematic of the validation model room and the measurement positions in the experiment

3.1 The accuracy of three potential numerical methods

As shown in Fig.2, in comparison with the experimental data, the scheme SL+S shows the poor performance of predicting indoor CO₂ concentration with a mean absolute percentage error (MAPE) of 47%. The prediction results of scheme S+I and scheme P+I show similar decay curve of indoor CO₂ concentration. The MAPEs of scheme S+I and scheme P+I are 9% and 11%, respectively. The scheme SL+I has the best performance with a MAPE of 5%. At the beginning of the simulation process, there are some differences in prediction results of indoor CO₂ concentration. As the indoor CO₂ concentration decay with the development of airflow, the differences among scheme S+I, scheme P+I, and scheme SL+I was gradually decreased and finally close to experiment data. The reason for better performance of methods with iterative scheme than with split scheme is solving scalar transport equation with iteratively ensuring the mass conservation of the indoor CO₂ concentration. The CO₂ concentration of schemes S + I and P + I have fluctuation with the development of flow due to the fluctuation of air velocity predicted by schemes S + I and P + I and the specific reasons of fluctuation at measurement points in steady state need further study.

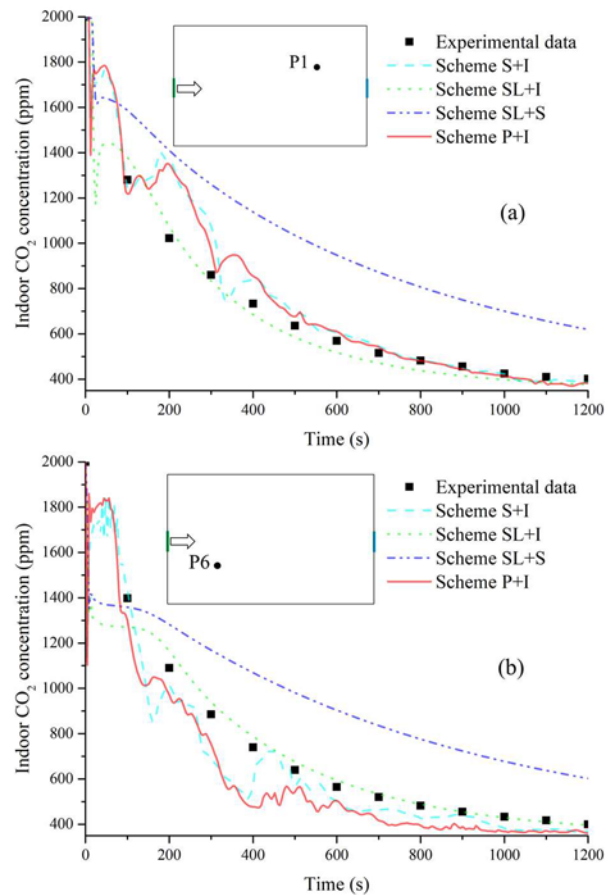
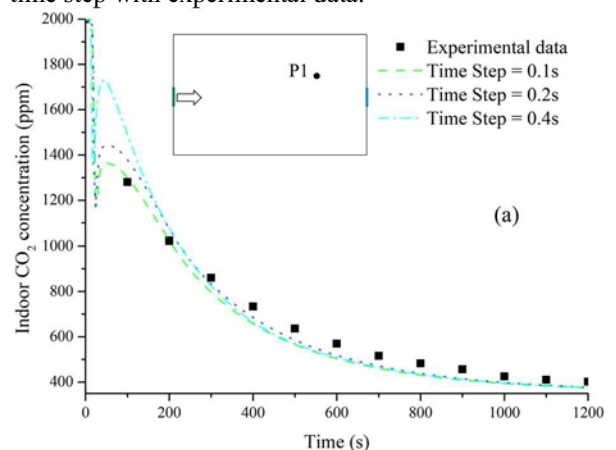


Fig.2. Comparison of indoor CO₂ concentration, predicted by different methods, to the experimental data

3.2 Compare the accuracy of numerical method on different time step sizes

The numerical methods with iterative scheme of scalar transport equation show good agreement with the experimental data. Considering the method of solving N-S equation with SL method remain stable at large time steps. To test the effect of time step size on the prediction results, the time step size of 0.1 s, 0.2 s, 0.4 s are selected. When time step size was 0.4s, the corresponding maximum CFL number was larger than 1. Fig. 3 shows the prediction results of scheme SL+I at different time step sizes. There are some differences of prediction results at the beginning. After 400 s, the prediction results of scheme SL+I agree well at different time step with experimental data.



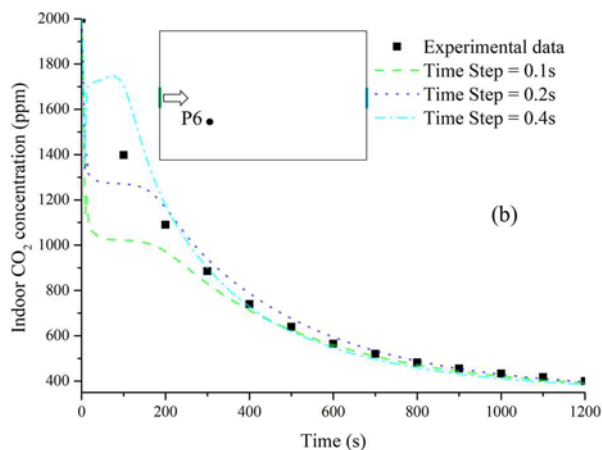


Fig.3. Comparison of indoor CO₂ concentration, predicted by scheme SL+I with different time steps, to the experimental data

4 Results

This study evaluated the performance of three potential numerical methods, by applying them to a ventilation case, to predict indoor CO₂ concentration. The study led to the following conclusions:

- The numerical method with iterative scheme of scalar transport equation could predict indoor CO₂ concentration efficiently.
- Split scheme with SL method of the scalar transport equation will overpredict the indoor CO₂ concentration.
- The numerical method with semi-Lagrangian method and iterative scheme also obtain satisfactory results in predicting indoor air contaminant concentration when the CFL number is larger than one.

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