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Energy Simulation Tools for Buildings: An Overview

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Validation of a Fast-Fluid-Dynamics Model for Predicting Distribution of Particles with Low Stokes Number

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SUMMARY
To design a healthy indoor environment, it is important to study airborne particle distribution indoors. As an intermediate model between multizone models and computational fluid dynamics (CFD), a fast fluid dynamics (FFD) model can be used to provide temporal and spatial information of particle dispersion in real time. This study evaluated the accuracy of the FFD for predicting transportation of particles with low Stokes number in a duct and in a room with mixed convection. The evaluation was to compare the numerical results calculated by the FFD with the corresponding experimental data and the results obtained by the CFD. The comparison showed that the FFD could capture major pattern of particle dispersion, which is missed in models with well-mixed assumptions. Although the FFD was less accurate than the CFD partially due to its simplification in numeric schemes, it was 53 times faster than the CFD.

IMPLICATIONS
This study evaluates the FFD for predicting airborne particle transportation in buildings. By quickly providing estimations of airflow motion, temperature distribution and contaminant transportation, the FFD can be useful for ventilation design and indoor environment analysis during building conceptual design.

KEYWORDS
FFD, CFD, Particle Transportation, Low Stokes Number

INTRODUCTION
Indoor airborne particles, such as cooking oil droplets, tobacco smoke particles, and microbe, are critical for occupant's health (Owen et al., 1992). To design a healthy indoor environment, it is important to know the distribution of airborne particles in different indoor conditions. The distribution information can also be used for the selection and design of ventilation system to ensure indoor air quality. Computational fluid dynamics (CFD) is often used to predict particle transportation in enclosed spaces, such as a room or an air craft cabin (Zhang and Zhao, 2007, Zhang and Chen, 2007). However, CFD simulations of particle distribution usually require a long computing time (hours or days), which may not be too time consuming for building conceptual design since it needs to quickly evaluate many different options in a short time. Thus, it is necessary to find a tool that can quickly predict particle distributions. The tool is not necessarily to be as accurate as the CFD, but it must be much faster than the CFD.

Multizone network models need little computing time and have been used to predict the contaminant concentration in buildings (Dols and Walton, 2002). However, it can only provide averaged contaminant concentration in a room due to its well-mixed assumption. Therefore, the multizone models are not appropriate for detailed analysis of indoor environment although they are fast. To fill the gap between CFD and multizone models, a fast fluid dynamics (FFD) model (Zuo and Chen, 2009) was proposed. The FFD can provide temporal and spatial information for flow velocity, temperature distribution and particle transportation. By scarifying some accuracy, the FFD can be 50 times faster than the CFD. Our previous work (Zuo and Chen, 2009, 2010) has validated the accuracy of the FFD model by comparing the predicted velocity and temperature with literature data. To apply the FFD for predicting airborne particle distributions, it is necessary to validate the FFD that is reported in this paper.

METHODS

The FFD model used in our investigation solves the continuity equation (1) for mass conservation and Navier-Stokes equation (2) for flow momentum:

(1)

(2)

where $i, j = 1, 2, 3$, U_i is the ith component of the velocity vector, P the static pressure of a flow field, and $S_{F,i}$ the ith component of the source, such as buoyancy force and other external forces. ν denotes the kinematic viscosity and ν_T tubulent kinemtic viscosity, and ρ the density of fluid. The FFD also solves an energy equation for non-isothermal flow:

(3)

where T is the temperature, α the thermal diffusivity and α_T turbulent thermal diffusivity, and S_T the heat source.

As concluded by Holmberg and Li (1998), interactions between indoor particles and fluid (indoor air) can be sorted into three groups: one-way coupling from fluid to particles, two-way coupling between fluid and particles, and four-way coupling between fluid and particles, as well as particles to particles. Our FFD model uses the one-way coupling from fluid to particles since it is the simplest among the three groups. A Stokes number can be used to decide if the one-way interaction is appropriate:

(4)

where ρ_P is the particle density, d_P the particle diameter, μ_F the molecular viscosity of air, U_F the characteristic flow velocity, and L_F a length scale. When , the one-way interaction from fluid to particles is sufficient (Crowe et al., 1996). The particles can be treated as gaseous and their concentrations can be solved by using the Eulerian approach (Holmberg and Li, 1998, Zhang and Chen, 2007). These particles can be viruses, tobacco smoke, bacteriophage and cooking oil smoke (Owen et al. 1992). Note that other approaches, such as the Lagrangian method (Panton, 2005, Zhang and Chen, 2007), may be necessary if the Stokes number of the particles is large. Applying the Eulerian approach, the transport equation of the particles is:

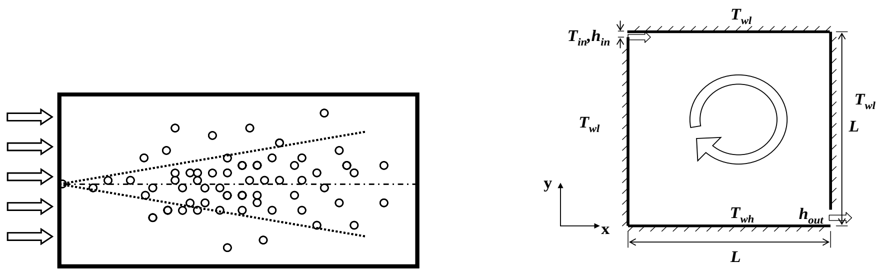
— — — (5)

where C is the concentration for specie, k_C the diffusivity of species, $k_{C,T}$ turbulent diffusivity, and S_C the source of the species.

Due to the similarity of equations (2), (3) and (5), the FFD solves them in a similar way. It first splits the equation into several simple ones by using a time splitting scheme. Then it solves the advection equation by using a semi-Lagrangian method. After that, the diffusion and source terms are solved together by using an implicit scheme. In addition, a pressure-correction method is applied to solve the continuity equation (1) together with pressure equation to ensure mass conservation. The details of FFD model can be found in our previous work (Zuo and Chen, 2010). In that paper, we also showed that the original FFD model had significant numerical viscosity due to the linear interpolation in the advection solver. A hybrid interpolation was then proposed to reduce the numerical viscosity. The results showed that the FFD simulation for laminar flows could be improved by using the hybrid interpolation. In this paper, we further added turbulent treatments to study turbulent flows. A simple approach is to assume that turbulence viscosity is constant. Since many turbulent viscosities are several hundred or a thousand times the molecular viscosity (Ilegbusi et al., 1999), we can estimate the turbulent viscosity ν_T by the following by using a constant turbulent viscosity $\nu_T = 100\ \nu$. Because the value of υ_t is a constant, no additional modeling or computing effort is necessary for this approach. However, the turbulent viscosity actually varies when the flow condition changes, such as an increase or decrease in the flow velocity. We adopted this simple but less accurate approach to make a balance between computing speed and simulation accuracy.

RESULTS

To quantitatively validate the FFD model for predicting airborne particles indoors, we selected two flows related to buildings. One is particle dispersion in a pipe flow (Figure 1a), which is similar to flow in an air duct or in a long corridor. The other is particle dispersion in a room with mixed convection (Figure 1b). This case is more complex since the flow is impacted by both inertia force from the inlet and buoyancy force from the warm floor.



(a) (b)

Figure 1 Schematic view: (a) particle dispersion in a pipe and (b) particle dispersion in a mixed convective room

Particle Dispersion in a Pipe Flow

The particle dispersion in a pipe flow is widely used to validate computer programs for particle transport (Derevich and Zdor, 2009, Snyder and Lumley, 1971) because the flow is comparably simple and high quality experimental data is available (Snyder and Lumley, 1971, Wells and Stock, 1983). Thus, our investigation also used this flow for validation. The experiment data from Snyder and Lumley (1971) was selected for reference because the data has low Stokes number (St = 0.055 for hollow glass particles).

Figure 1a shows the schematic view of the experiment. A grid generated homogeneous turbulent flow was given at the inlet of a circular pipe. The diameter of the pipe is 0.2m and the length is 4 m. The inlet velocity of the flow is 6.65 m/s. Particles were released at the center of the pipe inlet. Then they were dispersed due to the turbulent flow motion. The flow pattern and particle dispersion were axially symmetric so that they could be simulated by using a two-dimensional code. This study tested grid independence by using three different meshes and found that the mesh with 100 × 41 grids was sufficient.

To simulate the particle dispersion using Eulerian approach, this study assumed $k_C = \nu$. The experiment measured averaged displacement of particles on an axial surface at a certain position. The displacement data was given by using a mean square average:

(6)

where r_i is the shortest distance of particle i to the axis and N is the total number of particles on the surface. Although the Eulerian approach does not have individual particle information, one can still calculate the displacement d^2 by using particle concentration:

(7)

where $C(r)$ is particle concentration at a location with distance r to the axis and R is the radius of the pipe.

Figure 2 compares the simulated displacement with the experimental data. The particle displacement increases from the inlet (x = 0m) to the downstream. The FFD simulation successfully captured this trend. Although there is difference between the FFD prediction and experimental data, the FFD prediction is better than a uniform distribution by models with well-mixed assumption.

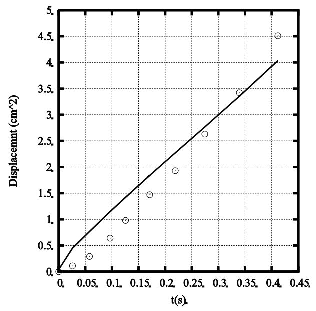


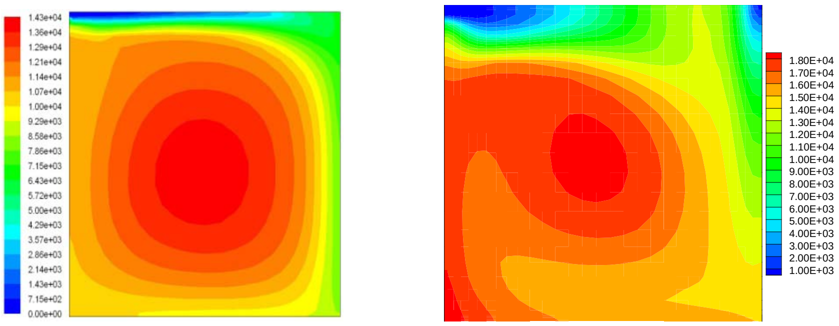
Figure 2 Comparison of particle displacement predicted by the FFD with experimental data.

Dispersion of Particles with Small Stokes Number in a Room with Mixed Convection

The flow in a room with mixed convection is based on the experiment from Blay et al. (1992). As shown in Figure 1b, the cold air, which was injected from the upper-left corner, was mixed with warm air heated by the floor. The experiment measured the air velocity and temperature, but not particles distributions. This paper assumed that the Stokes number of studied particles was much small than one so that their behaviour was similar as tracer gas, such as CO_2, in the

Eulerian approach. As a result, we could use CO_2 concentration to represent the particle distribution. We added CO_2 in this study by releasing it homogenously in the room air at a rate of mg/m^{3}s. A commercial CFD code FLUENT (www.ansys.com) with RNG k-ε model was used to provide reference data. The CFD code was validated to ensure that it could precisely calculate the velocity and temperature. Then it generated reference data for CO_2 concentration by using Eulerian approach. A grid of 32 x 32 was used in the FFD simulation. The time step size was 0.1s and a time-averaged solution was obtained for both simulations for comparison.

As shown in Figure 3, the FFD predicted the highest concentration in the center of the room and the lowest concentration near the inlet. It also captures the decreasing of concentration from the center to the wall. Due to simplification in the FFD scheme and the limitation of constant turbulent viscosity assumption, the flow predicted by the FFD is not as the same as the one by CFD. We compared the computing time for both FFD and CFD simulations. The computing time required by the CFD is 54.12 times of that by the FFD. This is consistent with our previous finding (Zuo and Chen, 2009) that the FFD was about 50 times faster than the CFD.



(a) (b)

Figure 3 CO_2 concentration predicted by (a) CFD and (b) FFD

DISCUSSION

Current FFD model only considers the one-way coupling between the flow and particles with small Stokes number. Thus, the Eulerian approach seems sufficient. To study particle with large Stokes number, a Lagrangian approach would be necessary. To track each individual particle, the accuracy of Lagrangian approach highly depends on the flow field predicted. However, our previous studies have shown that the predicted velocity by using FFD was not very accurate. Thus, it is necessary to use CFD if two-way or four-way coupling is needed.

The principle of FFD model is to achieve high speed by scarifying accuracy. As an intermediate model, the FFD is not to take place of CFD or nodal models, but rather to fill the gap between these two approaches. Thus, the FFD can be useful when one expects a simulation with speed and accuracy between multizone model and CFD. For instance, during the conceptual design of ventilation system and indoor environment, a designer can use FFD to try various configurations in a relatively short time. Then he/she can select the most promising candidates for more accurate simulation using the CFD.

CONCLUSIONS

This study validated an FFD model for predicting particle transportation in buildings by applying it to the particle dispersion in a duct and particle dispersion in a room with mixed convection. The results show that the FFD model can capture the major pattern of the particle dispersion, but there is difference between prediction and reference data. By scarifying some accuracy, the FFD can be 50 times faster than CFD. Being able to quickly providing general information for flow and particles distribution, the FFD can be used as a pre-screen tool for the conceptual design of indoor environment before detailed CFD study is applied.

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REFERENCES

Blay, D., Mergui, S., and Niculae, C. (1992) "Confined turbulent mixed convection in the presence of horizontal buoyant wall jet", *Fundamentals of Mixed Convection,* **213**, 65-72.

Chen, Q. and Xu, W. (1998) "A zero-equation turbulence model for indoor airflow simulation", *Energy and Buildings,* **28**, 137-144.

Crowe, C.T., Troutt, T.R., and Chung, J.N. (1996) "Numerical models for two-phase turbulent flows", *Annual Review of Fluid Mechanics,* **28**, 11-43.

Derevich, I.V. and Zdor, A.G. (2009) "A closed model of fluctuating particle motion in a turbulent flow", *Fluid Dynamics,* **44**, 55-67.

Dols, W.S. and Walton, G.N. 2002. Contamw 2.0 user manual, multizone airflow and contaminant transport analysis software (No. NISTIR 6921). Gaithersburg, MD, USA: National Institute of Standards and Technology.

Holmberg, S. and Li, Y.G. (1998) "Modelling of the indoor environment - particle dispersion and deposition", *Indoor Air,* **8**, 113-122.

Ilegbusi, O.J., Iguchi, M., and Wahnsiedler, W. (1999) "Mathematical and Physical Modeling of Materials Processing Operations," Boca Raton, CRC Press.

Owen, M.K., Ensor, D.S., and Sparks, L.E. (1992) "Airborne particle sizes and sources found in indoor air", *Atmospheric Environment Part a-General Topics,* **26**, 2149-2162.

Panton, R.L. (2005) *Incompressible flow* (3rd ed.), Hoboken, N.J., J. Wiley.

Snyder, W.H. and Lumley, J.L. (1971) "Some measurements of particle velocity autocorrelation functions in a turbulent flow", *J. Fluid Mechanics,* **48**, 41-71.

Wells, M.R. and Stock, D.E. (1983) "The effects of crossing trajectories on the dispersion of particles in a turbulent flow", *Journal of Fluid Mechanics,* **136**, 31-62.

Zhang, Y. and Zhao, B. (2007) "Simulation and health risk assessment of residential particle pollution by coal combustion in china", *Building and Environment,* **42**, 614-622.

Zhang, Z. and Chen, Q. (2007) "Comparison of the eulerian and lagrangian methods for predicting particle transport in enclosed spaces", *Atmospheric Environment,* **41**, 5236-5248.

Zuo, W. and Chen, Q. (2009) "Real-time or faster-than-real-time simulation of airflow in buildings", *Indoor Air,* **19**, 33-44.

Zuo, W. and Chen, Q. (2010) "Simulations of air distribution in buildings by FFD on GPU", *HVAC&R Research,* **16**, 783-796.