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PREDICTION OF PARTICLE TRANSPORT IN ENCLOSED ENVIRONMENT

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Abstract Prediction of particle transport in enclosed environment is crucial to the welfare of its occupants. The prediction requires not only a reliable particle model but also an accurate flow model. This paper introduces two categories of flow models – Reynolds Averaged Navier-Stokes equation modeling (RANS modeling) and Large Eddy Simulation (LES); as well as two popular particle models – Lagrangian and Eulerian methods. The computed distributions of air velocity, air temperature, and tracer-gas concentration in a ventilated room by the RANS modeling and LES agreed reasonably with the experimental data from the literature. The two flow models gave similar prediction accuracy. Both the Lagrangian and Eulerian methods were applied to predict particle transport in a room. Again, the computed results were in reasonable agreement with the experimental data obtained in an environmental chamber. The performance of the two methods was nearly identical. Finally the flow and particle models were applied to study particle dispersion in a Boeing 767 cabin and in a small building with six rooms. The computed results look plausible.

Keywords computational fluid dynamics, Lagrangian method, Eulerian method

1. Introduction

In developed countries, people spend more than 90% of their time in enclosed environments, such as buildings and transportation vehicles. The air quality in the enclosed environments is therefore an important factor of their welfare. The air quality is determined by the level of air contaminants, such as materials used for internal furnishings, equipment, and cleaning, personal activities, environmental tobacco smoke, pesticide, furnaces, soil emissions, and combustion products from cooking, as well as those from outdoors due to infiltration, such as traffic pollutants, pollen, dusts, etc. Many of the pollutants are suspended particles in air, such as dusts, smoke, fumes, and mists (ASHRAE, 2005). Wallace (1996) showed that people who were exposed to micron-sized particulate matter was related to these environments. In addition, the terrorist attacks on September 11, 2001 and the following anthrax dispersion by mails have spawned concerns about various possible forms of terrorism, including airborne/aerosolized chemical and biological warfare agent attacks. The study of particle transport in enclosed environments has thus received more attention at present.

The study of particle transport in enclosed environments can be performed by experimental measurements and computer simulations. Experimental measurements that are often regarded as reliable are expensive and sometimes can be dangerous, such as for SARS, bird influenza, and anthrax transport. Computer simulations are a good alternative. Since many approximations are used in the computer models, experimental validation of the simulated results is necessary. This paper provides a general overview of using computer models to simulate micron-sized particle transport in enclosed environment and the assessment of the model performance through a few examples.

2. Computer Models

The most popular computer model for studying particle dispersion in enclosed environment is computational fluid dynamics (CFD). CFD has become an indispensable tool for gathering information to be used for design, control and optimization of enclosed environments. To accurately predict micro-sized particle transport, the first step is to determine the airflow pattern with acceptable precision.

CFD can be divided into direct numerical simulation, Large Eddy Simulation (LES), and the Reynolds Averaged Navier-Stokes equations with turbulence models (RANS modeling). Direct numerical simulation would require a fast computer that does not currently exist, and would take years of computing time for predicting air distributions in enclosed environment. Only LES and RANS modeling are appropriate for studying airflow in enclosed environment.

2.1 RANS modeling

RANS modeling separate all spatial parameters, such as velocity and temperature, into their mean and fluctuating components and the fluctuating components are only predicted with time-averaged root-mean-square (rms) values. Thus, RANS modeling solves only the mean components. For time-averaged and incompressible buoyant flow, the basic RANS equations are

(a) Continuity equation:

$$\frac{\partial(\rho U_i)}{\partial x_i} = 0 . \tag{1}$$

(b) Momentum equations:

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial(\rho U_j U_i)}{\partial x_j} = \frac{\partial}{\partial x_j}(\nu_{\mathrm{eff}} \frac{\partial U_i}{\partial x_j}) + S_{U_i} , \tag{2}$$

where S_{ui} is the source term and ν_{eff} the effective viscosity. ν_{eff} has the form:

$$\nu_{\mathrm{eff}} = \nu_t + \nu , \tag{3}$$

where ν_t is the eddy (turbulent) viscosity. In the standard k-ε model (Launder & Spalding, 1974) that is most popular, the eddy viscosity is obtained from

$$\nu_t = C_\mu \frac{k^2}{\varepsilon}. \quad (4)$$

Then we need two extra transport equations to solve turbulent kinetic energy, k, and its dissipation rate, ε.

(c) Turbulent kinetic energy equation:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho U_j k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho \frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right) + \rho(G_k + G_b - \varepsilon). \quad (5)$$

(d) Dissipation rate of turbulent kinetic energy equation:

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial(\rho U_j \varepsilon)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho\left(\nu + \frac{\nu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right) + \rho\frac{\varepsilon}{k}\left(C_{1\varepsilon}G_k + C_{1\varepsilon}C_{3\varepsilon}G_b - C_{2\varepsilon}\varepsilon\right), \quad (6)$$

where the shear production term is defined by

$$G_k = \nu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\frac{\partial U_i}{\partial x_j}, \quad (7)$$

and, if heat transfer is involved, for ideal gas, the buoyant production term by

$$G_b = -\frac{\nu_t g_i}{\rho \sigma_T}\frac{\partial \rho}{\partial x_i}. \quad (8)$$

2.2 Large eddy simulation

LES is based on Navier-Stokes and mass continuity equations. LES assumes that flow motion can be separated by large and small scale eddies through a filter. The larger scale eddies are directly solved in LES, while the smaller scales are modeled. Since larger scale eddies carry the majority of the energy, they are more important. The smaller scales have been found to be more universal, and hence are more easily modeled. By filtering Navier-Stokes and mass continuity equations, one would obtain the governing equations for the large-eddy motions as

(a) Continuity equation:

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0. \quad (9)$$

(b) Momentum equations:

$$\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial}{\partial x_j}(\overline{u_i}\cdot\overline{u_j}) = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu\frac{\partial^2 \overline{u_i}}{\partial x_i \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}. \quad (10)$$

The bar represents grid filtering. For example, a onedimensional filtered velocity can be obtained from

$$\overline{u_i} = \int G(x,x')\, u_i(x)\, \mathrm{d}x', \quad (11)$$

where $G(x, x')$, the filter kernel, is a localized function. $G(x, x')$ is large only when $(x-x')$ is less than a length scale or a filter width. The length scale is a length over which averaging is performed. Flow eddies larger than the length scale are "large eddies", and those smaller than the length scale are "small eddies". If a box filter is used, then

$$G(x_i) = \begin{cases} \dfrac{1}{\Delta_i} & \left(|x_i| \le \dfrac{\Delta_i}{2}\right) \\ 0 & \left(|x_i| > \dfrac{\Delta_i}{2}\right) \end{cases}, \quad (12)$$

where Δ_i is the filter width.

The subgrid-scale Reynolds stresses in Eq. (10),

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \cdot \overline{u}_j, \quad (13)$$

are unknown and must be modeled. The simplest but also most popular one uses the Smagorinsky subgrid-scale model (Smagorinsky, 1963) to model the subgrid-scale Reynolds stresses. The model has been widely used since the pioneer work by Deardorff (1970). The Smagorinsky model assumes that the subgrid-scale Reynolds stresses, τ_{ij}, are proportional to the strain rate of the tensor, $\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right)$, namely

$$\tau_{ij} = -2\upsilon_{SGS}\overline{S_{ij}}, \quad (14)$$

where υ_{SGS} is the subgrid-scale eddy viscosity defined as

$$\upsilon_{SGS} = (C_{SGS}\Delta)^2(2\overline{S_{ij}}\cdot\overline{S_{ij}})^{\frac{1}{2}}, \quad (15)$$

where C_{SGS}=0.1−0.2 is the Smagorinsky constant, which varies according to flow type. The Smagorinsky model actually adopts the mixing length model of RANS modeling to the subgrid-scale model of LES.

LES has been a very useful tool in simulating flow in multiple scales. It was developed for application in meteorology. In the early 1970s, the grid resolution was as large as 100 km. Today, the same application is with a grid resolution as fine as one kilometer. At the other end of the spectrum, LES has no limitation on the size of small scales. When LES has a scale that can catch the smallest size of turbulent flow, it turns to direct numerical simulation. On the other hand, RANS modeling is applicable to certain scales. Different turbulent models should be used for different scales of flow. It is also possible to mix the LES and RANS modelings together.

Regardless if RANS modeling or LES is employed, a particle model must be used to calculate particle transport. There are two generic approaches for the numerical simulation of particle transport in airflows: the Lagrangian method and the Eulerian method. In the Lagrangian method (Loth, 2000), the velocity, mass, and temperature history of each particle in the cloud are calculated. The local cumulative motion and state of each particle in the cloud represent the spatial properties of the cloud. In the Eulerian approach, the cloud of particles is considered to be a second fluid that behaves like a continuum, and equations are developed for the average properties of the particles in the cloud (Crowe et al., 1998). Either approach has its advantages and disadvantages depending on the nature of the flow. Compared to the Eulerian method, the main drawback of the Lagrangian approach is that a large amount of particles must be injected into the flow field in order to obtain statistically independent results. However, the Lagrangian method does not need a diffusion coefficient of the particles. The following two sections will briefly describe the two methods normally used in enclosed environments.

2.3 Lagrangian method

In most cases, the particle concentration in enclosed