

## Comparison of the Eulerian and Lagrangian methods for predicting particle transport in enclosed spaces

Z. ZHANG<sup>a</sup>, Q. CHEN<sup>a\*</sup>

<sup>a</sup> Air Transportation Center of Excellence for Airliner Cabin Environment Research (ACER), School of Mechanical Engineering, Purdue University, 585 Purdue Mall, West Lafayette, IN 47907-2088, USA

**Abstract:** The computational fluid dynamics (CFD) methods has been widely used in modeling particle transport and distribution in enclosed spaces. Generally, the particle models can be classified as either Eulerian or Lagrangian methods while each has its own pros and cons. This investigation is to compare the two modeling methods with an emphasis on their performance of predicting particle concentration distributions in ventilated spaces. Both the Eulerian and Lagrangian models under examination were performed based on the same airflow field calculated by solving the RANS equations with the k- $\epsilon$  turbulence model. The numerical results obtained with the two methods were compared with the experimental data. The comparison shows that both of the methods can well predict the steady-state particle concentration distribution, while the Lagrangian method was computationally more demanding. The two models were further compared in predicting the transient dispersion of the particles from a coughing passenger in a section of airliner cabin. In the unsteady state condition, the Lagrangian method performed better than the Eulerian method.

Keywords: Particle, Eulerian method, Lagrangian method, CFD, indoor environment, airliner cabin

### 1. Introduction

Suspended particles can cause many human health problems and are identified as a major pollutant in the air (Mølhav et al., 2000; Mendell et al., 2002; Schneider et al., 2003). When particles carried virus of infectious diseases or microorganisms traveling in the air, they can spread the diseases. The SARS outbreak in 2003 and the new threat of bird flu those days have increased our concern of infectious disease transmission in enclosed spaces, such as in buildings and transport vehicles. Meanwhile, the transport mechanism of the aerosol is complicated and not yet fully understood. Therefore, the study of particle transport and distribution in enclosed spaces has been an important topic in the field of air quality and public health studies.

As particulate matter is suspended in the air, the particle transportation and distribution are highly associated with the airflow motion and the turbulence. Hence, the computational fluid dynamics (CFD) is the most suitable modeling approach to study the spatial distributions of particles in enclosed spaces. Generally, there are two methods of

---

\* Corresponding author. Tel.: +765 496 7562; E-mail address: yanchen@purdue.edu

modeling particle transport in CFD simulations, the Eulerian and the Lagrangian method. The Eulerian method treats the particle phase as a continuum and develops its conservation equations on a control volume basis and in a similar form as that for the fluid phase. The Lagrangian method considers particles as a discrete phase and tracks the pathway of each individual particle. By studying the statistics of particle trajectories, the Lagrangian method is also able to calculate the particle concentration and other phase data. Within each kind of the particle models, there are many different models to address various characteristics of particle motion and dispersion. The development of each method, from the simplest models to the most sophisticated ones, has been described and compared throughout the literature from different perspectives (e.g., Shirolkar et al., 1996; Loth, 2000; Lakehal, 2002).

To choose the Eulerian method or the Lagrangian method for certain problem depends highly on the objective and characteristics of the problem under examination. The Eulerian method has gained its popularity on studying particle concentration distributions in indoor environments (Murakami et al., 1992; Zhao et al., 2004; Zhao et al., 2005). The Lagrangian method is mainly used to predict the overall particle dispersion pattern (Béghein et al., 2005) and the temporal development of the mean concentration (Lu et al., 1996; Zhang and Chen, 2004). But the capability of the Lagrangian method on predicting the concentration distributions of particles has not been well explored.

Recently, we have used a Lagrangian method to predict the particle concentration distributions in ventilated rooms and have compared the numerical results with experimental data (Zhang and Chen, 2006). The Lagrangian method can predict the detailed particle distributions, while it required considerable computational effort, which may limit its application. Furthermore, Loomans and Lemaire (2002) claimed that the Lagrangian method can be more precise than the Eulerian in predicting particle distribution in a room, but they did not provide sufficient evidence with experimental validation. Riddle et al. (2004) concluded that their Lagrangian method gave better results than an Eulerian one in predicting dispersion of gas pollutant around buildings. However, the two models used by Riddle et al. were not based on the same flow model, so it is very difficult to judge if and how much the advantage was brought by the flow models. The above review has posted an interesting question: if or in what situations, the Lagrangian method could perform better than the Eulerian method in predicting the particle concentration distributions in enclosed spaces? This investigation therefore aimed to compare an Eulerian and a Lagrangian method by emphasizing on their capabilities of predicting particle distributions in enclosed spaces.

## **2. Research Methodology**

The computational fluid dynamics (CFD) was used to predict both airflow fields and particle concentration distributions. This study adopted Reynolds Averaged Navier-Stokes (RANS) equations with the standard k- $\epsilon$  turbulence model (Launder and Spalding, 1972) to predict the airflow field. The popular k- $\epsilon$  model has been successfully applied to simulate indoor airflow fields (Chen and Zhang, 2005; Chen, 1995). Since the focus of this study was to compare the performance of different particle models, the turbulence

model for airflow is not detailed here. The readers can refer to Versteeg and Malalasekera (1995) about the fundamentals of CFD modeling of fluid flow and turbulence.

For particle modeling in an enclosed space, the particle volume fraction is generally low. Thus the effect of particles on the turbulent flow is negligible, and the interaction between the carrier air and the particles can be treated as one-way coupling that is from flow to particles not vice versa. In addition, the particle size is the most important control parameter for determining the particle dynamics such as deposition. In the current study, the particle diameters considered are 0.3-1  $\mu\text{m}$ , the corresponding particle deposition velocity  $V_d$  is on the order of  $10^{-5}$ - $10^{-6}$  (m/s) in ventilated chambers (Lai, 2002; Lai and Nazaroff, 2005). Considering the particle loss coefficient for deposition  $\beta$ :

$$\beta = V_d A / V \quad (1)$$

where  $A$  is the area of room inner surface and  $V$  the volume. The  $\beta$  is on the order of  $10^2$ - $10^1$  ( $\text{h}^{-1}$ ) that is about two-magnitude order lower than air exchange rate ( $\text{h}^{-1}$ ) in ventilated rooms. Therefore, the particle deposition was neglected for the particle sizes studied in this paper. When particle deposition becomes important, appropriate deposition models must be implemented. Otherwise, the numerical prediction on particle concentration distribution cannot be accurate.

The one-way coupling and the neglect of deposition have been used in both Eulerian and Lagrangian modeling for this investigation.

### 2.1 The Eulerian method

With the one-way coupling of flow to particles, the Eulerian method used only particle concentration equations to couple with momentum and turbulence equations. This type of Eulerian method is known as single fluid model (hereafter refers as the single fluid model). The single fluid model treated the particle phase as a modified scalar species and the particle phase follows the following transport equation:

$$\frac{\partial \rho C}{\partial t} + \frac{\partial}{\partial x_i} (\rho \bar{u}_i C - \Gamma \frac{\partial C}{\partial x_i}) = S_c \quad (2)$$

where  $t$  is time,  $C$  the particle concentration,  $\rho$  the density of air,  $x_i$  ( $i=1, 2, 3$ ) the three coordinates,  $\bar{u}_i$  the averaged air velocity components in the three directions,  $\Gamma$  the effective particle diffusivity, and  $S_c$  the particle source term. The effective particle diffusivity has the form:

$$\Gamma = \rho (D + \nu_p) \quad (3)$$

where  $D$  is the Brownian diffusivity of particles,  $\nu_p$  the particle turbulent diffusion coefficient. When particle size is larger than  $0.01 \mu\text{m}$ , the Brownian diffusivity is negligible compared with turbulent diffusivity in a turbulent flow. The relationship between the particle turbulent diffusion coefficient  $\nu_p$  and the gas diffusion coefficient  $\nu_t$  has been theoretically studied by Tchen (1947). Hinze (1975) then developed a mathematical derivation of their relation. It can be stated that when the Stokes number of a particle approaches zero in a homogeneous turbulent flow,  $\nu_p$  equals to  $\nu_t$ . Although real airflows may not satisfy the homogeneous assumption used in the theory, this equality still holds as long as the Stokes number of particles kept low (Lai and Nazaroff, 2000).

When the relative motion between fluid and particle phase is significant, it can be expressed as “drift flux” terms and implemented into the source term  $S_c$  in Eq (2). Such manipulation assured the concentration equation is consistent with the general form of transport equations of the fluid so they can be solved together using the same numeric algorithm. This makes the Eulerian method easy to solve and implement. The single fluid model is thus widely used in studying indoor particle transport (Murakami et al., 1992; Holmberg and Chen, 2003; Zhao et al., 2004). Those previous studies indicated that for particles less than  $5 \mu\text{m}$ , the drift term was negligible. Thus no drift flux was considered in our study presented in this paper.

## 2.2 The Lagrangian method

The Lagrangian method usually tracks transiently a large amount of particles. The method starts from solving the transient momentum equation for each particle:

$$\frac{d\bar{u}_p}{dt} = F_D (\bar{u} - \bar{u}_p) + \frac{\bar{g}(\rho_p - \rho)}{\rho_p} + \bar{F}_a \quad (4)$$

The left hand side of the equation represents the inertial force per unit mass ( $\text{m/s}^2$ ), where  $\bar{u}_p$  is the particle velocity vector. The first term on the right hand side of Eq. (4) is the drag term, where  $F_D$  is the inverse of relaxation time ( $\text{s}^{-1}$ ) and  $\bar{u}$  the air velocity; the second term represents the gravity and the buoyancy, where  $\rho$  and  $\rho_p$  are the density of the air and the particles, respectively; and  $\bar{F}_a$  stands for additional forces (per unit mass) that may be important.

The air velocity  $\bar{u}$  consists of time averaged part  $\bar{\bar{u}}$  that is computed by solving the RANS equations with the standard  $k$ - $\epsilon$  model and the instantaneous velocity  $\bar{u}' = u'_i$  which needs modeling. Here  $u'_i$  was modeled by applying the discrete random walk model (DRW). It correlates the particle turbulent dispersion with the flow turbulent kinetic energy  $k$ :

$$u'_i = \zeta \sqrt{2k/3} \quad (5)$$

where  $\zeta$  is a Gaussian random number,  $k$  is the turbulent kinetic energy. The instantaneous air velocity accounts for particle's turbulent dispersion, and the turbulent dispersion is much more significant than the Brownian dispersion for the present study due to the particle size considered.

To compare with the Eulerian method, it is necessary to express the Lagrangian trajectory information in the form of concentration distributions. The particle concentration can be calculated by the particle source in cell (PSI-C) method as:

$$C_j = \frac{\dot{M} \sum_{i=1}^m dt_{(i,j)}}{V_j} \quad (6)$$

where  $C$  is the mean particle concentration in a cell,  $V$  is the volume of a computational cell for particles,  $dt$  is the particle residence time, and subscript  $(i, j)$  represents the  $i^{\text{th}}$  trajectory and the  $j^{\text{th}}$  cell, respectively. Zhang and Chen (2006) used the Lagrangian method with PSI-C scheme and analyzed the stability of the concentration calculation. The simulated concentration fields became statistically stable if sufficient number of trajectories were tracked.

However, in many situations, the particle number can be very limited, such as coughing from a person. In addition, the particle generation rate may not be constant. The Lagrangian method calculates new trajectories in each time step. The total number of generated trajectories,  $N_{\text{total}}$ , in the simulation is:

$$N_{\text{total}} = \sum_i n(i) dt^i \quad (7)$$

where  $n(i)$  is the number of trajectories generated in each time step  $dt^i$ , and  $i$  the  $i^{\text{th}}$  time step during particle generation. The particle concentration in a cell can be calculated by counting number of trajectories passing through the cell at the end of each time step.

### 2.3 Numerical procedures

Since the Eulerian and Lagrangian particle models developed in different frames of reference, the numerical calculation procedure is very different. In steady-state conditions, the Eulerian method needs to perform many iterations to attain a converged concentration field of particles. The Lagrangian method tracks particles in a manner of time marching and does not need iterations as long as particles are not coupled with fluid phase. While, the Lagrangian method usually tracks a huge number of particle trajectories and needs to repeat the simulation many times to obtain a stable solution. In a transient situation, the particle concentration equation in the Eulerian method was solved along with the flow equations at each time step. Iterations are necessary at each time step to ensure convergence. For the Lagrangian method, particles were tracked at the end of each time

step when the airflow computation was converged. At the same time, the particle positions were recorded and the particle concentration is computed.

Although many particle dynamics were not modeled due to the particle sizes studied here, the presented numerical methods are as framework for both Eulerian and Lagrangian methods. To extend the use of either Eulerian or Lagrangian method for a broader particle size range, it is necessary to apply appropriate ad hoc models (e.g., deposition models) to the presented work. For neutral particles, those models are mainly based on the airflow information solved by RANS equations and turbulence models. Implementing those models will not greatly increase the computational load for both Eulerian and Lagrangian methods as long as one way coupling assumption is valid. Therefore, the general conclusions derived from following discussions should be valid for a broader particle size range.

All simulations have been performed by using commercial CFD software FLUENT 6.2 (FLUENT, 2005). In addition, some user-defined functions (UDF) were developed to calculate the particle concentration distribution in both steady and unsteady states for the Lagrangian method.

### **3. Results and comparisons**

This study used the same assumptions of thermo-fluid conditions for both the Eulerian and Lagrangian methods and used the identical flow field. Thus, the differences of predicted particle distributions can reflect the performance of the two particle models. Since the numerical procedures for steady and unsteady simulation were different, this paper presents them separately in the following two subsections.

#### *3.1 Modeling particle dispersion under steady state conditions*

When particles were released at constant rate in a readily steady airflow in a room, the particle concentration distribution could reach the steady state within a certain period of time. Murakami et al. (1992) studied particle concentration distributions in a clean room under steady state conditions. Fig. 1 shows the schematics of their chamber. Two air supply openings were on the ceiling and four air exhaust outlets were on the two opposite side walls near the floor. The ventilation system supplied fresh air at a total flow rate of  $0.64 \text{ m}^3/\text{s}$ . Two particle source locations were selected in our study. Particle source 1 was just below one air supply inlet at a height of 0.8 m above the floor, and source 2 in the middle of room 0.25 m above the floor. Single sized particles with a mean diameter of  $0.31 \text{ }\mu\text{m}$  were used for both cases. In our CFD simulations, grid dependence was checked by comparing simulated air velocity, temperature and the Eulerian particle concentration from three different numbers of grids (20,000, 60,000 and 100,000) for such a simple room. The grid number of 60,000 is sufficiently fine and the corresponding results were presented. Fig. 2 gives a comparison of simulated and measured particle concentration distributions. The results of Lagrangian calculation in this figure were based on a sample size (i.e., the number of trajectories) of 100,000. The results from both Eulerian and Lagrangian methods are in reasonable agreement with the experimental data.

While both methods seem to give similar results, there are fundamental differences. The Lagrangian particle tracking method could introduce uncertainty into particle concentration calculations. When particle number is low, the predicted particle concentration may not be a stable solution due to the random factors used in the model. Fig. 3 shows that at least 100,000 particles from the source are needed to reach a statistically stable solution. Obviously, the Lagrangian method requires considerably more computing time if more particles are tracked. On the other hand, as soon as the numerical results are converged, the Eulerian solution of particle concentration became stable. Furthermore, compared with the Eulerian method, the Lagrangian method predicted higher concentration gradient near the ceiling and floor as shown in Fig. 3. For the Lagrangian method, the particles mainly followed the mean airflow while they were dispersed due to turbulence. In the region where the mean flow is more dominant than the turbulence, the dispersion became less significant as predicted by the Lagrangian method. Consequently, a relatively high concentration gradient was formed from such region to its vicinity. In contrast, the Eulerian method treated particles as a continuum, and the diffusion always smoothed out the sharp concentration gradient.

Although both methods were based on the same flow field, they made use of the flow and turbulence information differently. The two particle models can have different performance for another case with different flow and turbulence structure. In the clean room studied, the ventilation rate was very high compared with that for offices and homes. Thus it is interesting to study the performance of the two particle models with a lower ventilation rate.

The second case selected in our investigation is particle dispersion in a room with floor displacement ventilation as shown in Fig. 4, which was a case with low ventilation rate. Monodispersed particles of 0.7  $\mu\text{m}$  were released into the chamber at two source locations (S1 or S2) at 0.3 m above the floor. The total airflow rate from the two supply openings was 0.0994  $\text{m}^3/\text{s}$ . A more detailed description of experimental procedures and boundary conditions can be found in Zhang and Chen (2006). Fig. 5 shows a contour view of particle concentration distribution predicted by the two methods. The Eulerian and Lagrangian methods again predicted similar particle concentration pattern, although the Eulerian prediction was smoother.

Fig. 6 plots the predicted and measured particle concentration distribution profiles in different locations of the room. In most of the positions, the two particle models agreed well with experimental data on the particle concentration levels and gradients. Compared with the clean room case, the Eulerian and Lagrangian methods agreed better in predicting the particle concentration stratification near walls. The figure also presents a comparison of the results of Lagrangian methods from different computational grids used for calculating particle concentrations. One grid resolution was the same as that for airflow calculation used in CFD that contained 389,338 cells, the other had only 7,500 uniform-size cells. The results with the two grids are similar. The Lagrangian method seems to produce a good particle concentration distribution even when the grid resolution used for calculating particle concentration is much lower than that for airflow.

With a coarse grid resolution for calculating particle concentration, the required number of Lagrangian trajectories can be lowered, and the computational cost can hence be reduced. Taking the current case for instance, one million particles is necessary if we use the grid resolution for airflow calculation (389,338) as that for particle concentration calculation, while 10,000-50,000 trajectories are sufficient by using the coarser mesh (7,500). Since the computing time for each trajectory was about the same, the total computing time for Lagrangian method based on the coarser mesh was about only 1-5% of that based on the finer mesh. This makes the Lagrangian method more attractive for more complicated problems.

Generally, the results demonstrate that the Eulerian and Lagrangian methods have similar accuracy on predicting the particle concentration distributions in enclosed spaces. In terms of computing cost, the Eulerian method is faster than the Lagrangian method. Tracking sufficient number of particles and analyzing them in Lagrangian approach required more time than the Eulerian iterations. However, the Lagrangian method gives detailed information of individual particles that can be crucial in many applications.

### *3.2 Particle dispersion under unsteady state conditions*

In many cases, particle emission rate is not constant or even not continuous. Even if the airflow remains steady state, the particle dispersion and transport are unsteady state. For example, the droplet dispersion from a coughing person is unsteady state. The Eulerian and Lagrangian methods may not perform the same for unsteady state conditions as for the steady state situations. Thus, their performance for unsteady state conditions was examined in this section.

This investigation used coughing process as an example of unsteady state conditions and studied the particle dispersion from a coughing passenger in a section of an airliner cabin. Fig. 7 shows the geometry information of the modeled cabin, a four-row section of a Boeing 767, with periodical flow and thermal conditions in the longitudinal direction. The periodical boundary conditions imply that the cabin is infinitively long and the thermal and fluid conditions in each section are exactly the same. This study further assumed that all seats were occupied, and the index person was in the middle of the last row. Two air supply openings on the ceiling discharged air into cabin at a total flow rate of 0.28 m<sup>3</sup>/s, corresponding to 36 air changes per hour (ACH) or 10 L/s per passenger. The air exhaust outlets were on both side walls next to the floor. The airflow in the cabin was assumed to be steady until the index person started a single cough. According to Zhu et al. (2005), a single cough from a healthy person lasted about 200 ms and expelled a total of 1.7 L air from the person's mouth. The total number of particles was assumed to be 10<sup>5</sup>. The particle generation rate in our simulation was thus 5 × 10<sup>5</sup> particles/s for 0.2 s, and afterwards, it remained zero. As most of coughing droplets evaporated almost immediately (Morawska, 2005), droplets evaporation was not considered. The remaining non-evaporative nuclei were assumed to be monodisperse with a diameter of 1 μm. Although the assumption of monodispersity may not be accurate, its simplicity made the comparison of particle models more tractable.



Table 1 shows the time steps for the airflow and particle simulations used in this study. Fig. 8 illustrates the dispersion of the particles within three seconds predicted by the Eulerian and Lagrangian methods. The two methods agree each other reasonably while the Eulerian method again shows that the particles dispersed faster. As the particles dispersed further to a greater region in the cabin, the differences between the two methods become remarkable. Fig. 9 illustrates the predicted particle dispersion pattern at one minute after the cough. The Lagrangian method predicted that particles were highly dispersed and the particle concentration field was not as smooth as that predicted by the Eulerian method. Generally, the Eulerian method gave a higher particle concentration over the domain than the Lagrangian method. As no experimental data is available at present, a further discussion on the predicted particle concentration results was difficult. On the other hand, it was easier to compare the two particle models in terms of computing time for the same problem. Both Eulerian and Lagrangian methods required more computing time in the unsteady state than that in steady state conditions. For the coughing case studied here, the Lagrangian method was more cost efficient while the Eulerian method required higher computational effort.

The significant increase of computing time of the Eulerian method was mainly due to the associated numerical procedure. Under an unsteady state situation, particle concentration in all cells could fluctuate greatly. The Eulerian method implicitly solved the particle concentration equation together with momentum and energy equations and assumed the concentration unchanged within a time step. To accurately reflect the frequent change of the particle concentration, the time step must remain sufficiently small. In order to control the truncation error caused by time discretization, it is also necessary to use small time steps. In contrast, the Lagrangian method tracks discrete particles by time marching in both transient and steady state calculations. Thus the Lagrangian particle tracking did not increase the computing time in unsteady state conditions. The increased computing effort mainly came from the calculation of unsteady state airflow and turbulence. Taking the present case for instance, when a steady airflow was restored from the coughing effect after about 30 seconds, the Lagrangian calculation became as efficient as that in the steady state condition. Therefore, the Lagrangian method was more suitable than the Eulerian method for such unsteady state problems.

Nevertheless, the Lagrangian method produced a highly scattered particle concentration field based on a high resolution mesh when the coughing particles were highly dispersed. The finer of the grid resolution used in the particle trajectory calculation, the more scattered the results look like. In order to reduce the scattering and fluctuating concentration field associated with fine meshes, this investigation used three coarser grid resolutions, i.e. 46,080, 5,760, and 720 cells for the four-row cabin that corresponds to a grid size of 0.1 m, 0.2 m, and 0.4 m, respectively. As a reference, the mean particle concentration for each row was also calculated. Fig. 10 illustrates the differences of particle concentration patterns with different grid resolutions. The results of mesh size 0.2 and 0.4 m were sufficiently stable, while other results looked either too scattered or too bulky. A grid size of 0.2 - 0.4 m seems the best. Fig. 11 shows the particle concentration distributions over time computed with 0.2 m mesh resolution. Four minutes after the

cough, 10,000 particles out of 100,000 were still in the domain. The number of trajectories was larger than the grid number, which was necessary to ensure a statistical stability of concentration simulation as discussed in Fig. 3.

Although no experimental data is available for the validation of the numerical results, the proposed Lagrangian method has shown to be more plausible in modeling particle transportation under unsteady state conditions.

#### **4. Conclusions**

This study compared the modeling performance of an Eulerian and a Lagrangian method in predicting particle concentration distributions in enclosed spaces. This investigation studied steady-state particle dispersion in a clean room with a high ventilation rate and in a room with underfloor displacement ventilation with a low ventilation rate, as well as unsteady particle dispersion in a section of an aircraft cabin with a coughing passenger. The comparison focused on accuracy and reliability of particle concentration simulation and the computing efficiency. Based on identical airflow fields, the performance of the Eulerian and Lagrangian models for calculating particle dispersion were evaluated and the following conclusion can be drawn.

Under steady state conditions, the particle phase behaved more like a continuum. Both the methods were able to predict the particle concentration distributions in enclosed spaces and the results agree reasonably with the experimental data. The Eulerian method needs less computing time than the Lagrangian method, because the latter needs to track the development of each particle and the particle number needs to be sufficiently large to ensure statistical stability.

For unsteady particle dispersion and transport with limited amount of particles, the Eulerian method requires small time steps and needs hundreds iterations per step to ensure a good convergence. It turned out that the application of the Eulerian method in predicting the particle dispersion of a coughing process over a long time was very difficult. On the contrary, the Lagrangian method was more computationally efficient. The particle tracking process does not significantly increase the computing time compared with that under a steady state condition. The calculation of unsteady state airflow and turbulence was the main reason for the increased computing time with the Lagrangian method. When the steady airflow was restored from the transient state, the computing time under an unsteady state condition will be similar to that under a steady state situation. As particles can be highly scattered in the air, it is practical to reduce the resolution of particle concentration simulation to predict particle dispersion over a long time. This in turn can further reduce the computational cost for the Lagrangian method. The Lagrangian method is more capable in modeling particle transportation under unsteady state conditions and it is thus recommended for future applications.

#### **Acknowledgement**

This project is funded by the U.S. Federal Aviation Administration (FAA) Office of Aerospace Medicine through the Air Transportation Center of Excellence for Airliner Cabin Environment Research, Cooperative Agreement 04-C-ACE-PU-002. Although the FAA has sponsored this project, it neither endorses nor rejects the findings of this research.

## References

- Béghein, C., Jiang, Y., and Chen, Q.Y., 2005, "Using large eddy simulation to study particle motions in a room," *Indoor Air*, Vol. 15, pp. 281-290.
- Chen, Q., 1995, "Comparison of different k- $\epsilon$  models for indoor airflow computations," *Numerical Heat Transfer, Part B: Fundamentals*, Vol. 28, pp. 353-369.
- Chen, Q. and Zhang, Z., 2005. "Prediction of particle transport in enclosed environment," *China Particuology*, Vol. 3(6), pp. 364-372.
- FLUENT, 2005, *Fluent 6.2 User's guide*, Fluent Inc., Lebanon, NH.
- Hinze, J.O., 1975, *Turbulence*, 2<sup>nd</sup> Edition, pp. 460-471, New York: McGraw-Hill.
- Holmberg, S. and Chen, Q., 2003, "Air flow and particle control with different ventilation systems in a classroom," *Indoor Air*, Vol. 13, pp. 200-204.
- Lai, A.C.K. and Nazaroff, W.W., 2000, "Modeling indoor particle deposition from turbulent flow onto smooth surfaces," *Journal of Aerosol Science*, Vol. 31, No. 4, pp. 463-476.
- Lai, A.C.K., 2002, "Particle deposition indoors: a review," *Indoor Air*, Vol. 12, pp. 211-214.
- Lai, A.C.K. and Nazaroff, W.W., 2005, "Supermicron particle deposition from turbulent flow onto vertical surfaces with varying roughness," *Atmospheric Environment*, Vol. 39, pp. 4893-4900.
- Lakehal, D., 2002, "On the modelling of multiphase turbulent flows for environmental and hydrodynamic applications," *International Journal of Multiphase Flow*, Vol. 28, pp. 823-863.
- Launder, B.E. and Spalding, D. B., 1972, *Lectures in Mathematical Models of Turbulence*, Academic Press, London, England.
- Loomans, M., and Lemaire, T., 2002, "Particle concentration calculations using cfd-a comparison," *Proceedings of Indoor Air 2002*, pp. 153-156, Edinburgh, Scotland.
- Loth, E., 2000, "Numerical approaches for motion of dispersed particles, droplets, and bubbles," *Progress in Energy and Combustion Science*, Vol. 26, pp. 161-223.
- Lu, W., Howarth, A.T., Adam, N., and Rifat, S.B., 1996, "Modelling and measurement of airflow and aerosol particle distribution in a ventilated two-zone chamber," *Building and Environment*, Vol. 31 (5), pp. 417-423.
- Mendell, M.J., Fisk, W.J., Petersen, M.R., Hines, C.J., Dong, M., Faulkner, D., Deddens, J.A., Ruder, A.M., Sullivan, D., and Boeniger, M.F., 2002, "Indoor particles and

symptoms among office workers: results from a double-blind cross-over study,” *Epidemiology*, Vol. 13, pp. 296-304.

Møhlave, L., Kjærgaard, S.K., and Attermann, J., 2000, “Sensory and other neurogenic effects of exposures to airborne office dust,” *Atmospheric Environment*, Vol. 34, pp. 4755–4766.

Morawska, L., 2005, “Droplet fate in indoor environments, or can we prevent the spread of infection?” *Proceedings of Indoor Air 2005*, pp. 9-23, Beijing, China.

Murakami, S., Kato, S., Nagano, S., and Tanaka, S., 1992, “Diffusion characteristics of airborne particles with gravitational settling in a convection-dominant indoor flow field,” *ASHRAE Transactions*, Vol. 98, part 1, pp. 82-97.

Riddle, A., Carruthers, D., Sharpe, A., McHugh, C. and Stocker, J., 2004, “Comparisons between FLUENT and ADMS for atmospheric dispersion modeling,” *Atmospheric Environment*, Vol. 38, pp. 1029–1038.

Shirolkar, J.S., Coimbra, C.F.M., and McQuay, M.Q., 1996, “Fundamental aspects of modeling turbulent particle dispersion in dilute flows,” *Progress in Energy and Combustion Science*, Vol. 22, pp. 363-399.

Schneider, T., Sundell, J., Bischof, W., Bohgard, M., Cherrie, J.W., Clausen, P.A., Dreborg, S., Kildesø, J., Kjærgaard, S.K., Løvik, M., Pasanen, P., and Skyberg, K., 2003, “‘EUROPART’. Airborne particles in the indoor environment. A European interdisciplinary review of scientific evidence on associations between exposure to particles in buildings and health effects”, *Indoor Air*, Vol. 13, pp. 38–48.

Tchen, C.M., 1947, Mean value and correlation problems connected with the motion of small particles suspended in a turbulent fluid, Ph. D. thesis, Delft.

Versteeg, H.K. and Malalasekera, W., 1995, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*, McGraw-Hill, Loughborough University.

Zhang, Z. and Chen, Q., 2004, “Numerical analysis of particle behaviors in indoor air using Lagrangian method,” *Roomvent Proceedings 2004*, Coimbra, Portugal.

Zhang, Z. and Chen, Q., 2006, "Experimental measurements and numerical simulations of particle transport and distribution in ventilated rooms," *Atmospheric Environment*, 40(18), 3396-3408.

Zhao, B., Zhang, Z., Li, X., and Huang, D., 2004, “Comparison of diffusion characteristics of aerosol particles in different ventilated rooms by numerical method,” *ASHRAE Transactions*, Vol. 110, pp. 88-95.

Zhao, B., Zhang, Z., and Li, X., 2005, "Numerical study of the transport of droplets or particles generated by respiratory system indoors," *Building and Environment*, Vol. 40, pp. 1032-1039.

Zhu, S., Kato, S., and Yang, J.H., 2005, "Study on transport characteristics of saliva droplets produced by coughing in a calm indoor environment," *Building and Environment*, In Press.

Table 1. Time steps used in the simulation of unsteady state airflow and particle concentration in the cabin

Time (s)		0 - 0.2	0.2 - 5	5 - 60	> 60
Time steps					
Flow time steps (s)		0.002	0.02	0.05	1
Concentration time steps (s)	Eulerian method	0.002	0.02	0.05	-
	Lagrangian method	0.001	0.001	0.001	0.001

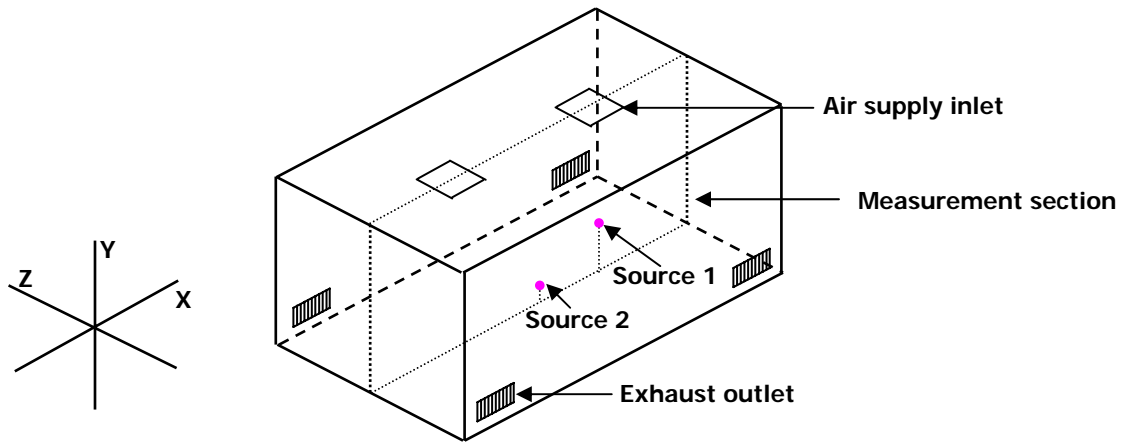


Fig. 1. A schematic view of the clean room used by Murakami et al. (1992). The rectangle in dotted lines shows the measurement section.



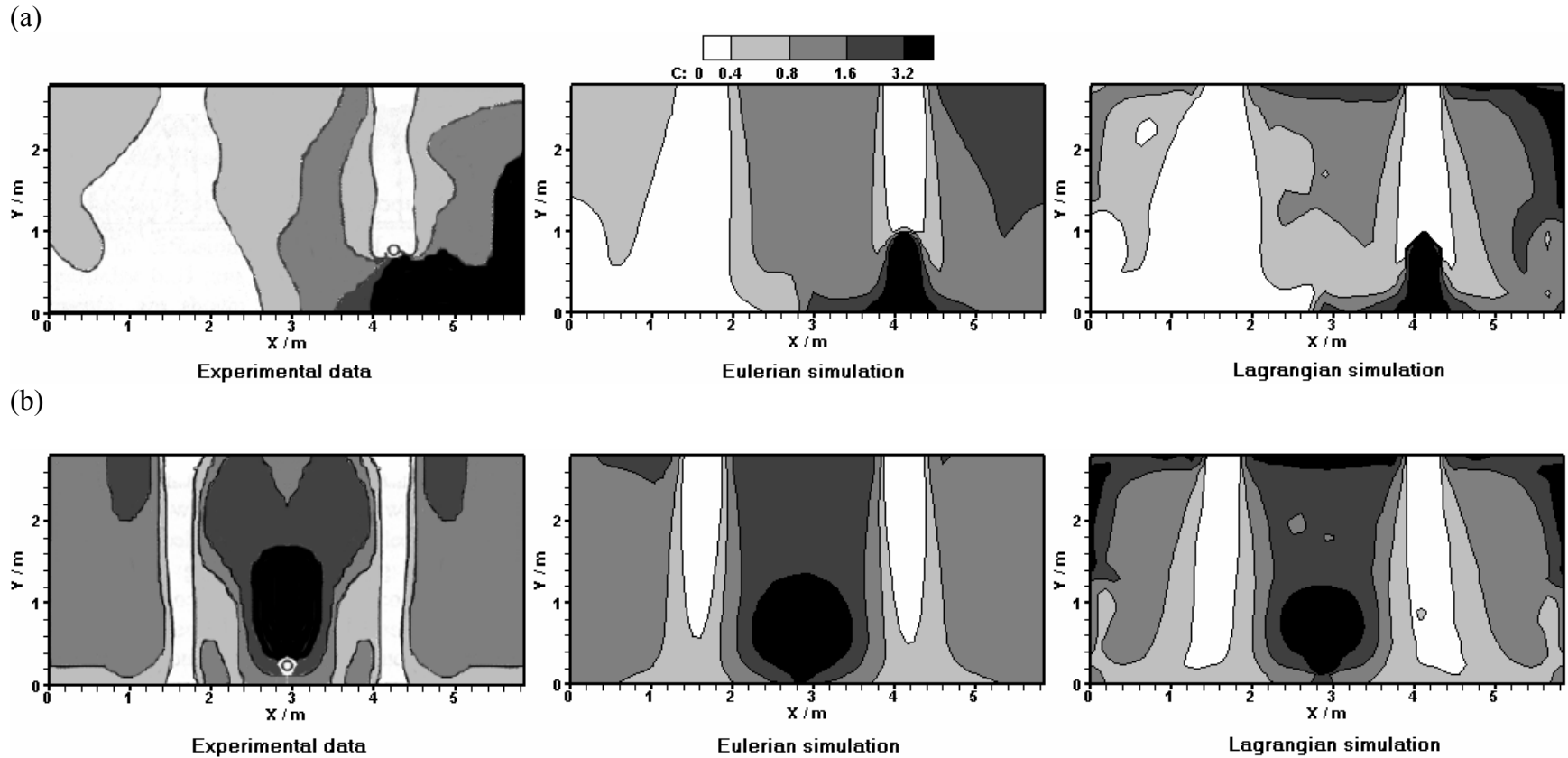


Fig. 2. A comparison of simulated particle concentration distributions by Eulerian and Lagrangian methods with experimental data in the measurement section. (a) Source 1: particle source below the right air supply. (b) Source 2: particle source above the floor at the center.

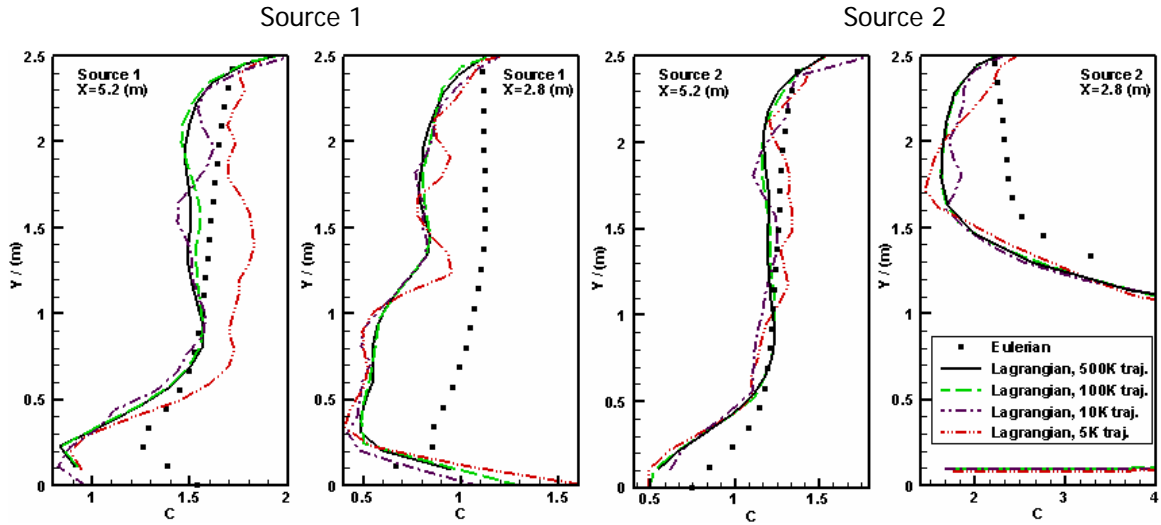


Fig. 3. Particle concentration profiles at two poles in center of the room for the two source positions. Measurement data were extracted from the original work by Murakami et al. (1992).

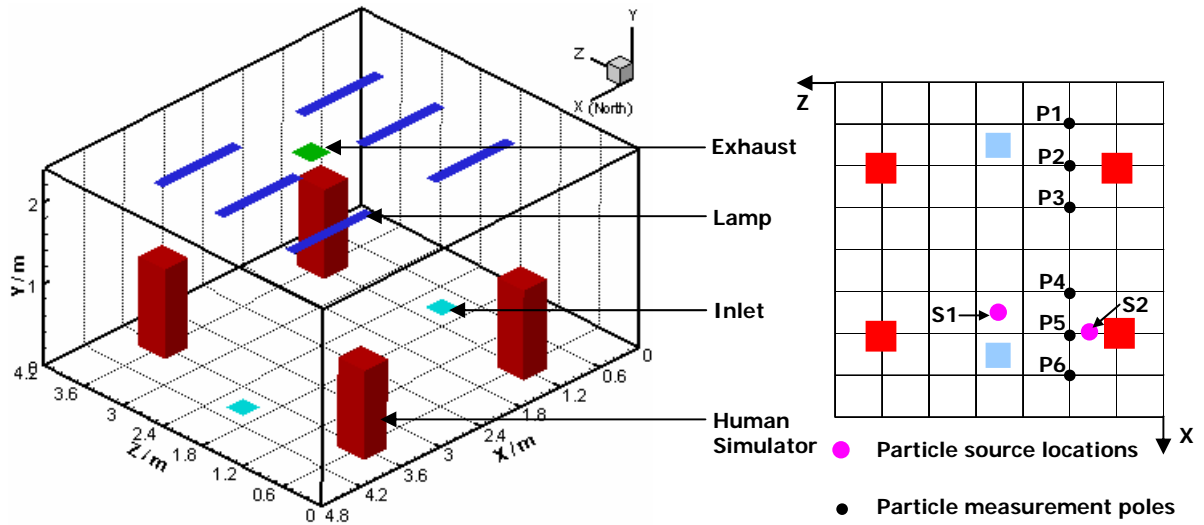


Fig. 4. A sketch of the room with displacement ventilation and particle measurement locations.

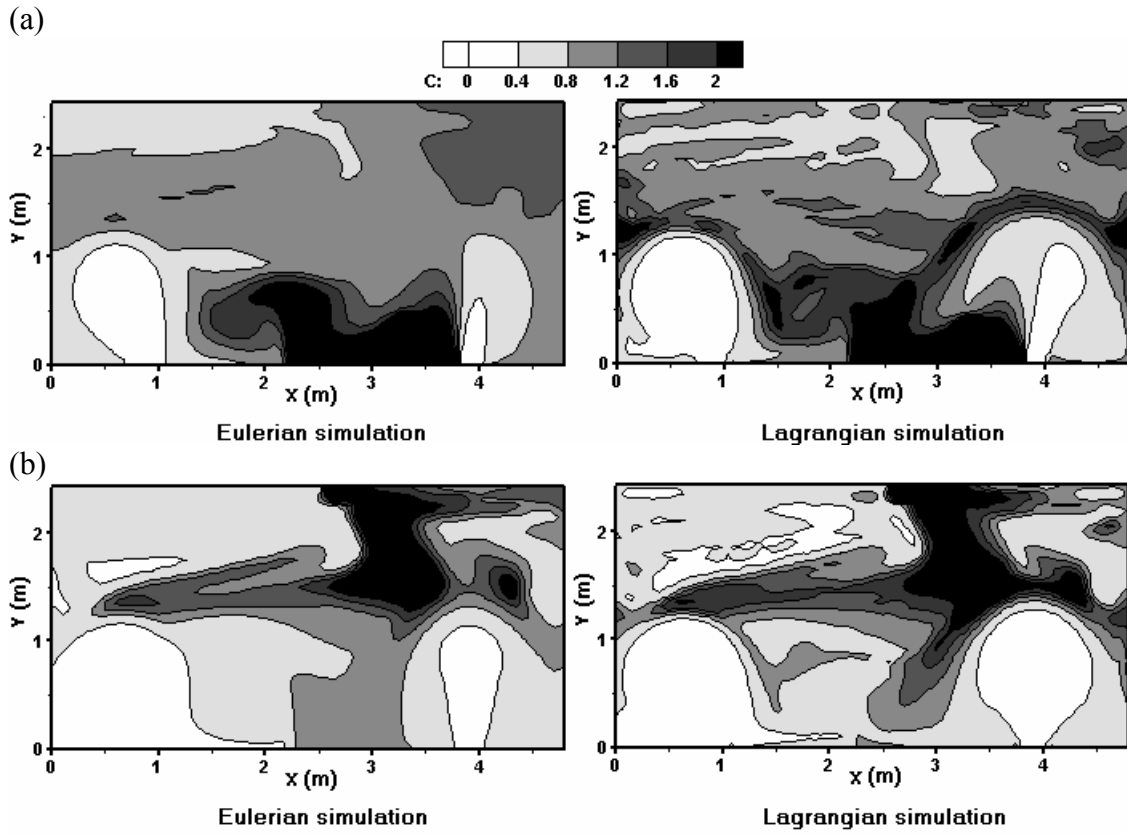


Fig. 5. A contour plot of predicted particle concentration distributions in  $Z=2.1$  m plane. (a) particle source at S1; (b) particle source at S2.

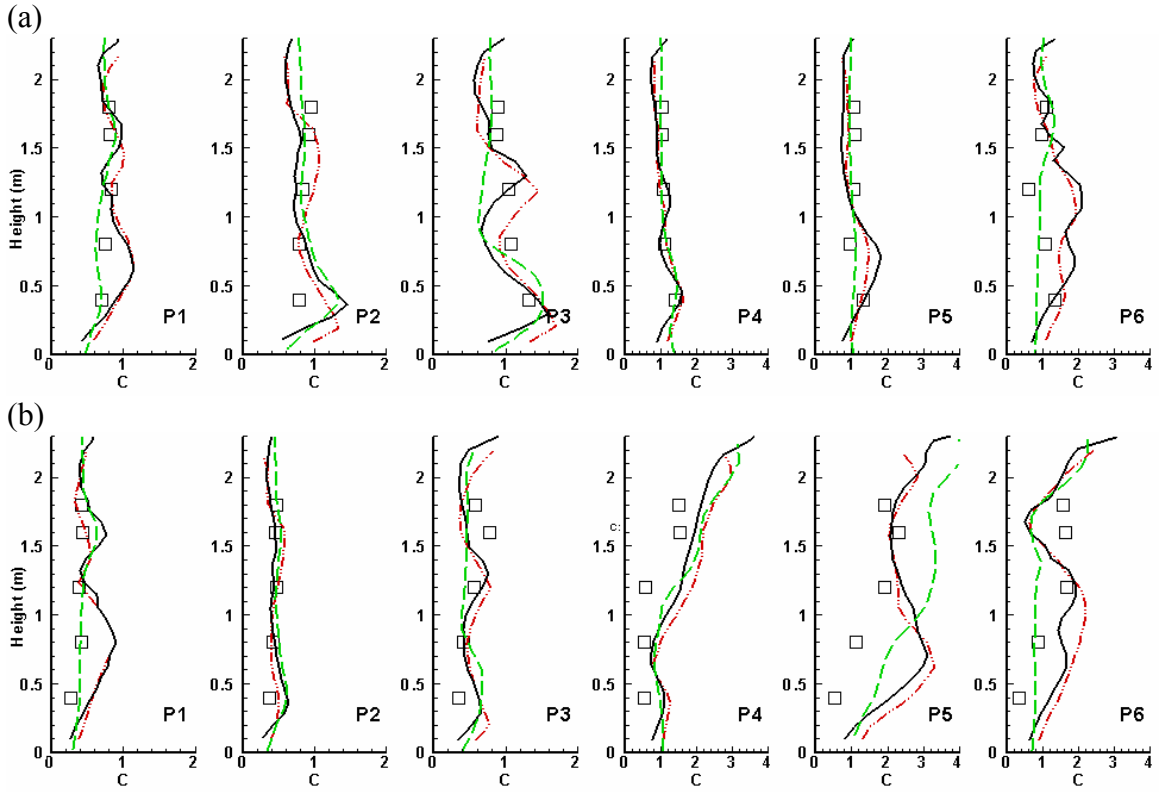


Fig. 6. A comparison of measured and predicted particle concentration profiles in poles P1 through P6. (a) particle source at S1 near an air supply inlet; (b) particle source at S2 near an occupant. (Square symbols: measurement data; dash lines: Eulerian prediction; solid lines: Lagrangian prediction based on finer meshes; dash dot-dot lines: Lagrangian prediction based on coarser meshes.)

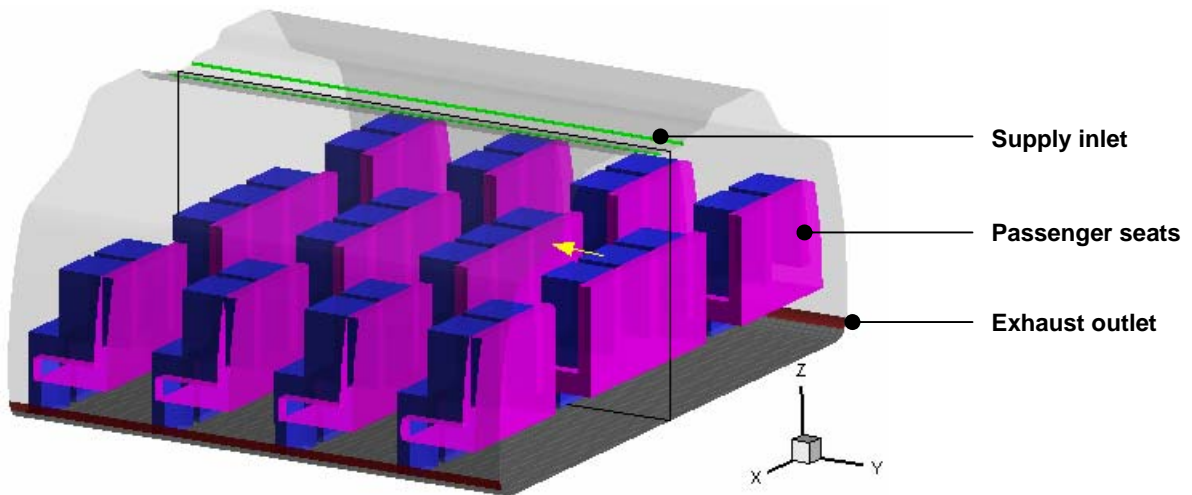


Fig. 7. The geometry of a Boeing 767 section. The cabin is symmetric about the  $X=0$  plane shown as a black rectangle. The arrow indicates the index coughing person and coughing direction.

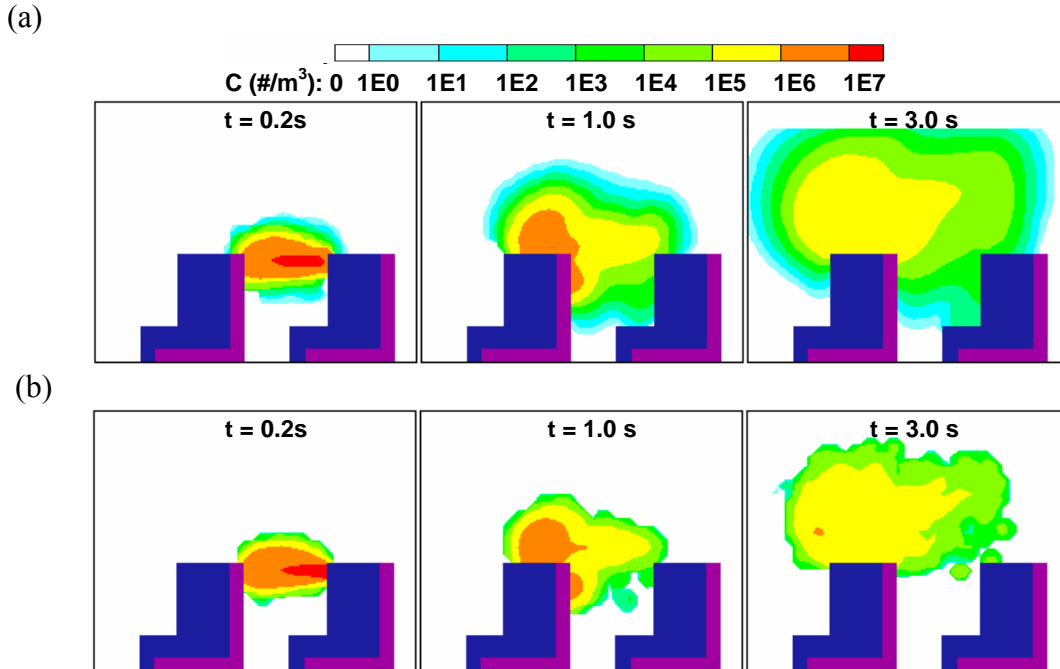


Fig. 8. A comparison of simulated temporal concentration development of the particles in the cabin within three seconds after coughing. (a) by the Eulerian method and (b) by the Lagrangian method.

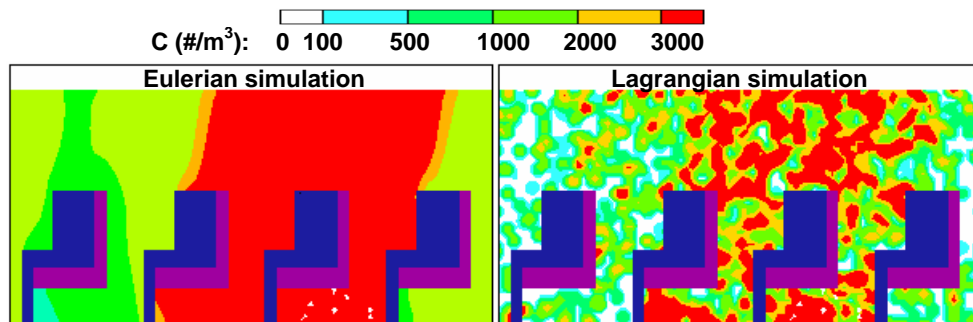


Fig. 9. A comparison of simulated temporal particle concentration development at time  $t=1.0$  min by the Eulerian and Lagrangian methods.

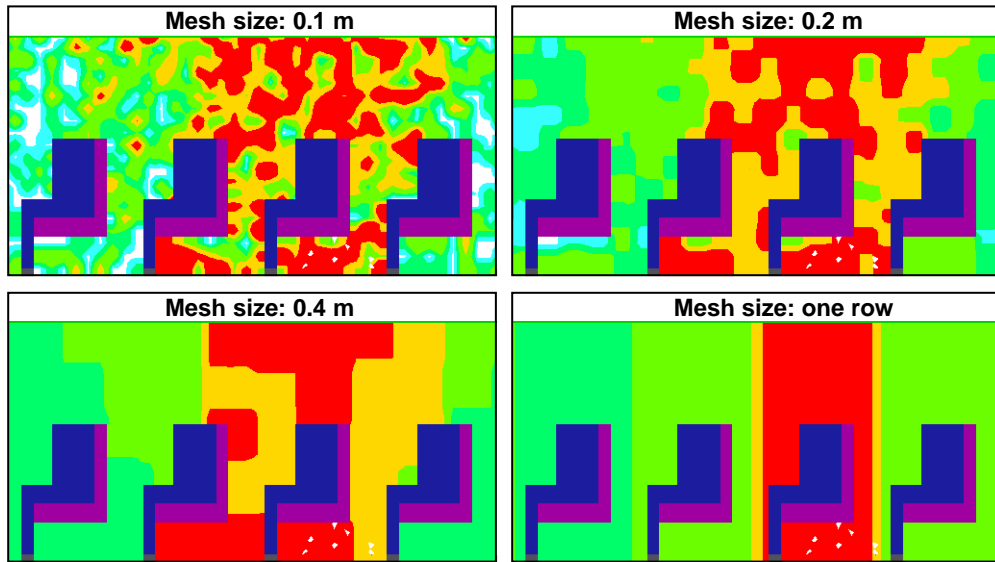


Fig. 10. A comparison of predicted particle concentration distribution at  $t = 1$  minute with different mesh resolutions.

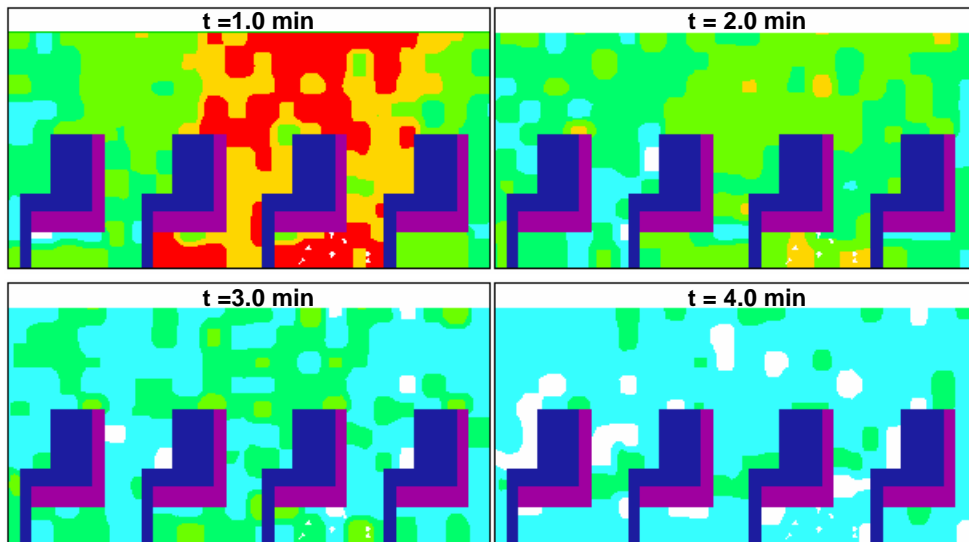


Fig. 11. The predicted particle dispersions over time by the Lagrangian method with a 0.2 m mesh resolution.