Large eddy simulation indoor airflow and contaminant concentration

Z. F. TIAN* J. Y. TU † G. H. YEOH ‡

Abstract

Computational Fluid Dynamics (CFD) has been used as a powerful tool for prediction of indoor air flow and contaminant concentration that are of significant concern to indoor air quality issues. The application of a RNG-based Large Eddy Simulation (LES) model to simulate indoor airflow and indoor contaminant particle dispersion and concentration has been investigated in two cases of ventilated rooms. The measured air phase velocity and contaminant particle concentration decay are used to validate the simulation results. It is found that RNG LES model can properly handle Low Reynolds Number (LRN) flows, which are always encountered in indoor air flows. The results also show that the particle phase boundary condition has significant effect on the concentration prediction. This suggests that more realistic particle phase boundary condition is required to improve the CFD prediction.

* School of Aerospace, Mechanical and Manufacturing Engineering
RMIT University, Bundoora Vic 3083, Australia
s3060891@student.rmit.edu.au

† School of Aerospace, Mechanical and Manufacturing Engineering
RMIT University, PO Box 71, Bundoora Vic 3083, Australia
Jiyuan.Tu@rmit.edu.au

‡ Australian Nuclear Science and Technology Organisation (ANSTO), PMB 1,
Menai, NSW 2234, Australia
ghy@ansto.gov.au

1. Introduction

Effective indoor air quality control requires detailed information of indoor ventilation airflows and contaminant particle dispersion and concentration. The experimental approach to access indoor airflows and contaminant particle transport can be rather expensive and impractical as a design tool. The zonal model approach that has been developed in past two decades gives fast approximation, but unable to provide the required detailed information. With increasing computational resources and the widespread availability of commercial codes, the computational fluid dynamics (CFD) technique is gaining in popularity as an attractive alterative tool.

However, some uncertainties of CFD approach still prevail. One is the approximation of turbulence models that requires further resolution [1]. The indoor ventilation flows are always characterised by low-Reynolds-number (LRN) turbulence. The improper handling of LRN turbulence can contribute to inaccurate calculations of airflows and consequently the contaminant particle phase since the particle dispersion is strongly affected by the turbulent fluctuations. The Large Eddy Simulation (LES) modelling approach to computing turbulent flow has seen a veritable renaissance in recent years due to the availability of faster computers and a continued desire for higher fidelity of predictive capabilities.

The first objective of this paper is to evaluate a Renormalization Group (RNG) theory Large Eddy Simulation (LES) model to predict indoor airflow for a two-zone indoor airflow environment. The calculated airflow velocities are evaluated and verified against experimental data obtained by Posner et al. [2] Then, in another two-zone ventilated room configuration, contaminant particle dispersion and distribution within the rooms are simulated using the RNG-based LES combining with a Lagragian particle tracking model. Corresponding experimental data of particle concentration decay from literature [3] are used to validate the simulation results.

2. Computational method

2.1 RNG-based LES model

A generic CFD commercial code, FLUENT [4], is utilized to predict the continuum gas phase of the velocity profiles under unsteady-state conditions through solutions to the conservation of mass and momentum. In LES models, the small eddies are separated by filters from large eddies that contain most of the energy. The resulting equations thus govern only the dynamics of large eddies and these large-scale variables can be defined by the filtering operation, $\overline{f}(x)=\frac{1}{\Delta V}\int f(x')\,dx'$. ΔV is the control volume (the finite-volume cell). Applying the filtering operation to the conservation equations, one obtains the governing equations for the large-scale variables:

$$\frac{\partial \rho^g}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho^g \bar{u}_j^g\right)=0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\rho^g \bar{u}_j^g\right)+\frac{\partial}{\partial x_j}\left(\rho^g \bar{u}_j^g \bar{u}_i^g\right)-\frac{\partial}{\partial x_j}\left(\mu_{eff}^g \frac{\partial \bar{u}_j^g}{\partial x_j}\right)=-\frac{\partial P}{\partial x_j}-\frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

The effect of the small scales upon the resolved part of turbulence appears in the SGS stress term, $t_{ij} = r^g \overline{u_i^g u_j^g} - r^g \bar{u}_i^g \bar{u}_j^g$. Yakhot et al. [5] derive a subgrid model by applying the RNG theory to the SGS eddy viscosity. In this RNG-based SGS model, the stress is modelled according to:

$$t_{ij}-\frac{d_{ij}}{3}t_{kk}=-2m_{eff}^g \bar{S}_{ij} \tag{3}$$

Here m_{eff}^g is the SGS turbulent viscosity given as $m_{eff}^g = m^g\left[1+H(x)\right]^{1/3}$. $H(x)$ is the Heaviside function defined by $H(x)=\begin{cases} x, x\geq 0 \\ 0, x<0 \end{cases}$. The variable x equals to $\frac{m_s m_{eff}^g}{{m^g}^3}-C$ where $m_s=(C_{RNG}\Delta V^{1/3})^2\sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$. Based on the RNG theory, the constants C_{RNG} and C are given by 0.157 and 100 respectively [5].

The transport equations were discretised using the finite-volume method. The time-dependent terms were handled through an implicit second order backward differencing in time. The central-differencing spatial discretization scheme was used for all equations. The SIMPLE algorithm was used as the pressure-velocity coupling method.

2.2 Particle phase model

The contaminant particle dispersion and concentration are predicted by a Lagrangian model. The trajectory of a discrete particulate phase is determined by integrating the force balance on the particle. This force balance equates the particle inertia with the forces acting on the particle. Appropriate forces such as the drag and gravitational forces have been incorporated into the equation of motion. The equation can be written as

$$\frac{\partial u_i^p}{\partial t} = F_D\left(u_i^g - u_i^p\right) + \vec{g}\left(r^p - r^g\right) \tag{4}$$

The drag force per unit particle mass $F_D\left(u_i^g + u_i^p\right)$, and F_D is given by

$$F_D = \frac{18\rho^g}{\rho^p d_p^2}\frac{C_D d_p\left|u_i^p - u_i^g\right|}{24} \tag{5}$$

The drag coefficient, C_D, is evaluated from experimental-fitted expression of Morsi and Alexander [22]. A fourth order Runge-Kutta method is employed to predict each of the particle velocity and trajectories for the particulate phase. For LES model, u_i^g in Equation (5) is calculated by using the instantaneous gas phase velocity, $\overline{u}_i^g + \mathrm{u}_i^{g'}$, along the particle path during the integration process. Here, the resolved velocity $\overline{u}_i^g$ presents the large scale motion. The fluctuating velocity components $\mathrm{u}_i^{g'}$ that presents mall scale motion are sampled by assuming that they obey a Gaussian probability distribution: $\mathrm{u}_i^{g'} = \mathrm{I}_g\xi\left|\overline{\mathrm{u}}_i^g\right|$. I_g is the intensity of the fluctuation. ξ is a normally distributed random number satisfying $\overline{\xi} = 0$ and $\sqrt{\overline{\xi'}} = 1$. $\left|\overline{\mathrm{u}}_i^g\right|$ is the absolute value of resolved velocity $\overline{u}_i^g$. The fluid Lagrangian integral time $\mathrm{T_L}$ is equivalent to the time scale of this LES calculation.

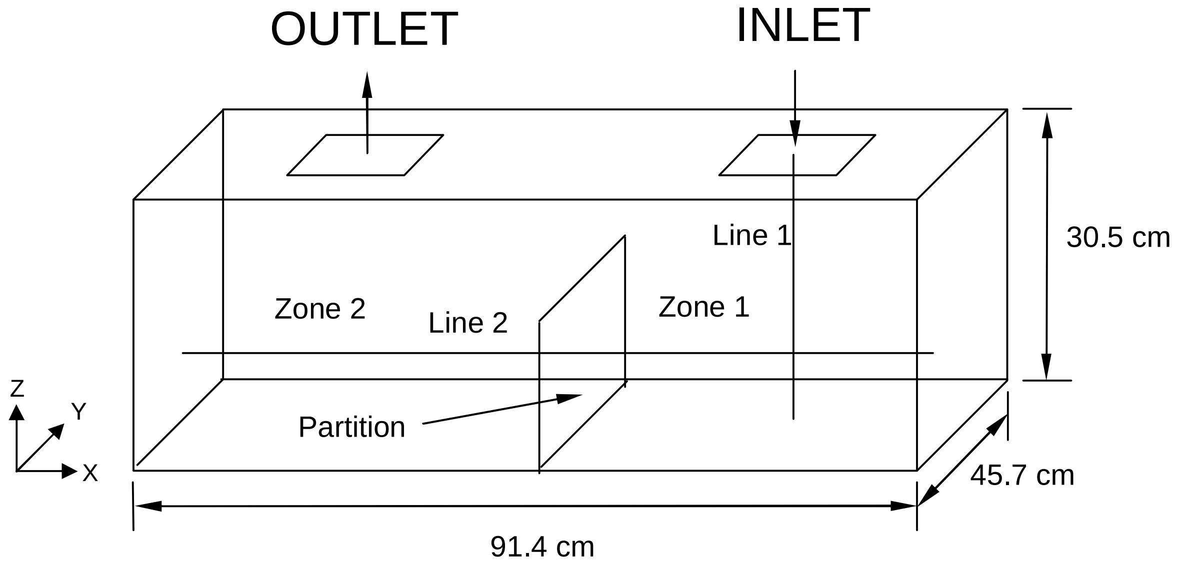

Figure 1 Configuration of ventilated room in case 1.

3. Results and discussion

In this study, the predictions of indoor airflow and contaminant particle concentration using CFD techniques are investigated in two room-ventilation cases.

Figure 1 illustrates the geometrical structure of the model room of case 1 [2]. The room is with a size of width × depth × height = 91.4 × 45.7 × 30.5 $cm^{3.}$ A partition with the height of 15 cm is located in the middle of the room. The Reynolds number of the inlet airflow was determined to be 1500, based on the vertical inlet velocity (U_{inlet}) of 0.235 m/s with a characteristic length of 0.1 m. Uniform meshes with size of 0.8 cm × 0.8 cm × 0.8 cm was generated for the whole physical domain The initial condition of the flow field in room was assumed to have a randomly perturbed velocity about the magnitude of the mean velocity U_{inlet}. A non-dimensional time step of 0.035 was used, which is defined by $t' = U_{inlet}\ t\ /\ H$ where U_{inlet} is the inlet air velocity; t is the physical time step with a value of 0.05 seconds and H is the room height. To ensure that the solution achieved sufficient statistical independence from the initial state, time-averaged results were obtained from the instantaneous values after the airflow simulation was marched for 1000 non-dimensional time steps representing 50 seconds in physical time. After this time, the instantaneous values such as the airflow velocities were averaged over 2200 non-dimensional time steps, 110 seconds in physical time.

Figure 2(a) presents the comparison of the vertical air velocity along the vertical inlet jet axis (line 1 in Figure 1) predicted through RNG LES model against the experimental data. Good agreement was seen despite marginal discrepancy at the end of the jet that could be attributed to the over-diffusion caused by the eddy-viscosity modelling. Figure 2(b) shows the comparison between the predicted and measured vertical air velocity component along the horizontal line at mid-partition height (line 2 in Figure 1). From the location $x = 0$ m to the partition, LES model yielded smooth predicted velocity profile that agree with the experiment data well. In the near-wall regions about the locations $x = 0.46$ m and $x = 0.9$ m, the RNG-based LES model successfully captured the highest positive vertical velocities. Significant under-prediction of the negative vertical velocity, found in the region right beneath the inlet, also was caused to the over-diffusion of the eddy-viscosity modelling. Generally, RNG LES model performed very well; good agreement has been achieved between the predictions and measured data and the flow trends have been successfully captured through LES model.

It is well known that the Smagorinsky SGS LES model, which is based on high Reynolds number dynamics, predicts non-zero turbulence viscosity in laminar flows. RNG-based LES model remedies this unphysical problem by introducing the function $H(x)=\begin{cases} x, x\geq 0 \\ 0, x<0 \end{cases}$. In low turbulent flow regions such as the laminar flows, the argument of the ramp function becomes negative and the effective viscosity recovers the molecular viscosity. This enables the RNG-based SGS eddy viscosity to model the LRN effects encountered in transitional, laminar flows and near-wall regions that are always encountered in indoor airflows.

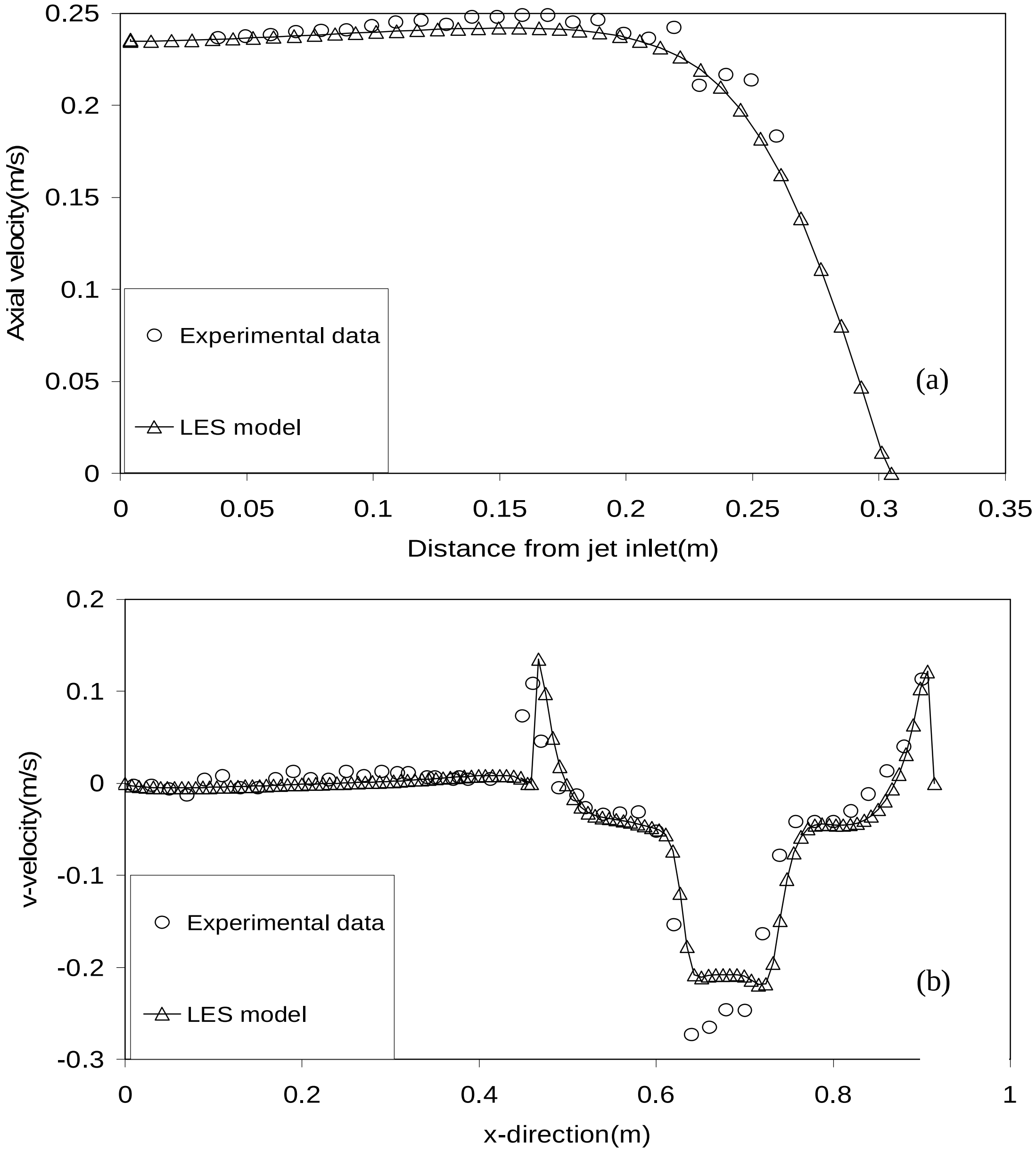

Figure 2: simulated and measured the vertical velocity component: (a) along the vertical inlet jet axis and (b) along the horizontal line at mid-partition height.

The simulated time-mean velocity fields at the mid-plane of the model room are show in Figure 3. RNG LES model predicted the recirculation structures in the region about the location x = 0.85 m and in the region beneath the outlet (x = 0.2 m, z = 0.1 m).

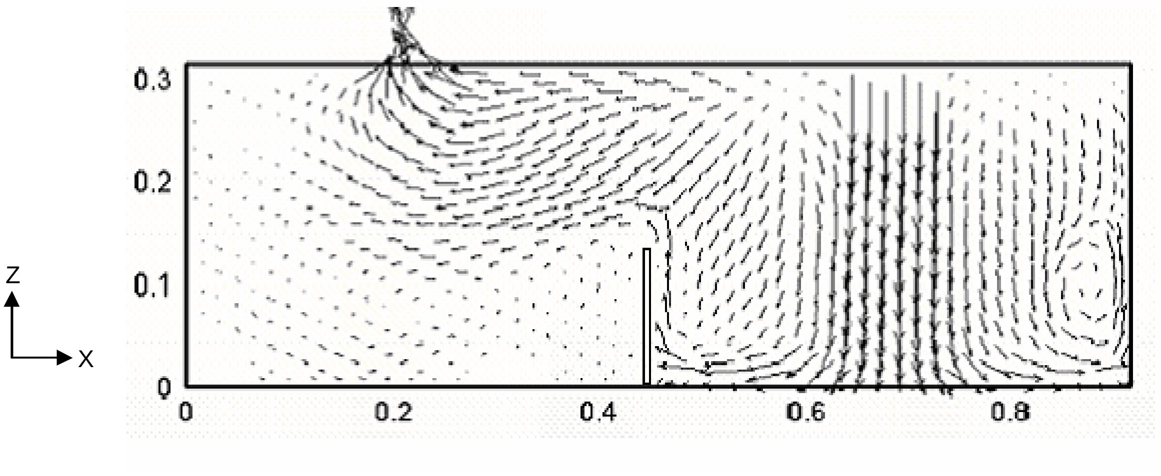

Figure 3 The predicted time-mean velocity field in the mid-plane of the room model.

In the second case of this study, contaminant particle dispersion and concentration within another two-zone ventilated room [3] is investigated using the RNG-based LES combining with the Lagragian particle tracking model. Figure 4 shows the configuration of the ventilated room in case 2. In the middle of the room, a partition with a big opening divides the room into two zones. The opening is with a size of height × width = 0.95 m × 0.70 m. A uniform mesh was generated for the whole physical domain yielding a mesh volume size of 0.08 m × 0.08 m × 0.08 m. Two air exchange rates are tested in this study: (1) air change per hour (ACH) 10.26; (2) air change per hour (ACH) 9.216. This study simulated 8000 sample particles that are equally sized from 1 to 5 µm. At the beginning of the simulation, the sample particles were injected into the whole volume of zone 1 uniformly with zero initial velocity. The particle tracking periods H is 29 minutes for the case of 10.26 ACH, while 26 minutes for 9.26 ACH. The non-dimensional time step is 0.005. The boundary conditions for particle phase are set to be the ‘reflect’ type for all the walls except the ground that is set as ‘trap’ type.

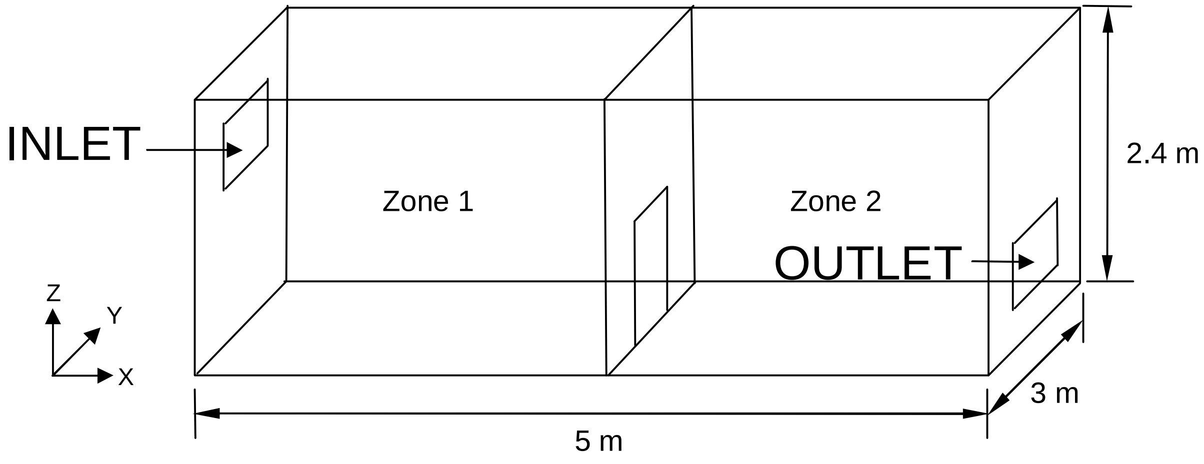

Figure 4 Configuration of ventilated room in case 2.

Figure 5(a) and(b) present the simulated and measured zone-averaged particles concentration decay in zone1 and zone 2 respectively, for the case of 10.216 ACH. In zone 1, the LES model predicted marginally lower contaminant particles concentration than the experiment data from about 3rd minute to about 15th minute. Then from 15th minute to 26th minute, very good agreement is achieved. After 26th minute, the LES gave marginally higher concentration. In zone 2, the LES model prediction is lower than the experiment data from 2nd minute to 7th minute, and very good agreement after 7th minute. Similar comparison results for 9.26 ACH can be found in figure 5(c) and 5(d). Overall, the LES model combining with the Lagrangian model provides reasonable good prediction of the zone-averaged contaminant particle concentration decay.

Several facts may lead to the marginal discrepancies between the predicted and measured data. When applying the CFD method to flows, the simplified assumption of flows properties may be different from the actual flows. For instance, the assumption that the particles are within size of 1-5 μm equally is not true for the experiment.

The simple particle phase boundary condition that evaluates the particle-wall surface interaction also contributes to the discrepancies. When reaching a wall surface, contaminant particles either deposit on the surface or rebound. In this study, all particles reaching a particular wall surface are assumed to have the same particle-wall interaction pattern. That is not the case in experiments. The influence of particle phase boundary condition on the particle concentration is investigated here. In the case of 10.26 ACH, the predicted concentration decays with two different particle phase boundary conditions are compared. In the first boundary condition, particles are assumed to deposit when reaching the room ground and to rebound when reaching other walls. The second boundary condition is that particle phase is set to rebound on all surfaces including the room ground. Figure 5(e) and 5(f) show the comparison of the predicted results with the measured data. The numerical concentration of boundary condition 2 is obviously higher than the measured one after 10th minute in zone 1. The results show that the particle phase boundary condition has significant effect on the concentration prediction. This suggests that more realistic particle phase boundary condition will improve the CFD prediction. However, to the best of the authors' knowledge, there is no such literature about the realistic particle phase boundary condition for CFD approach to predict indoor contaminant particle concentration though researches have been done for the zonal model [7].

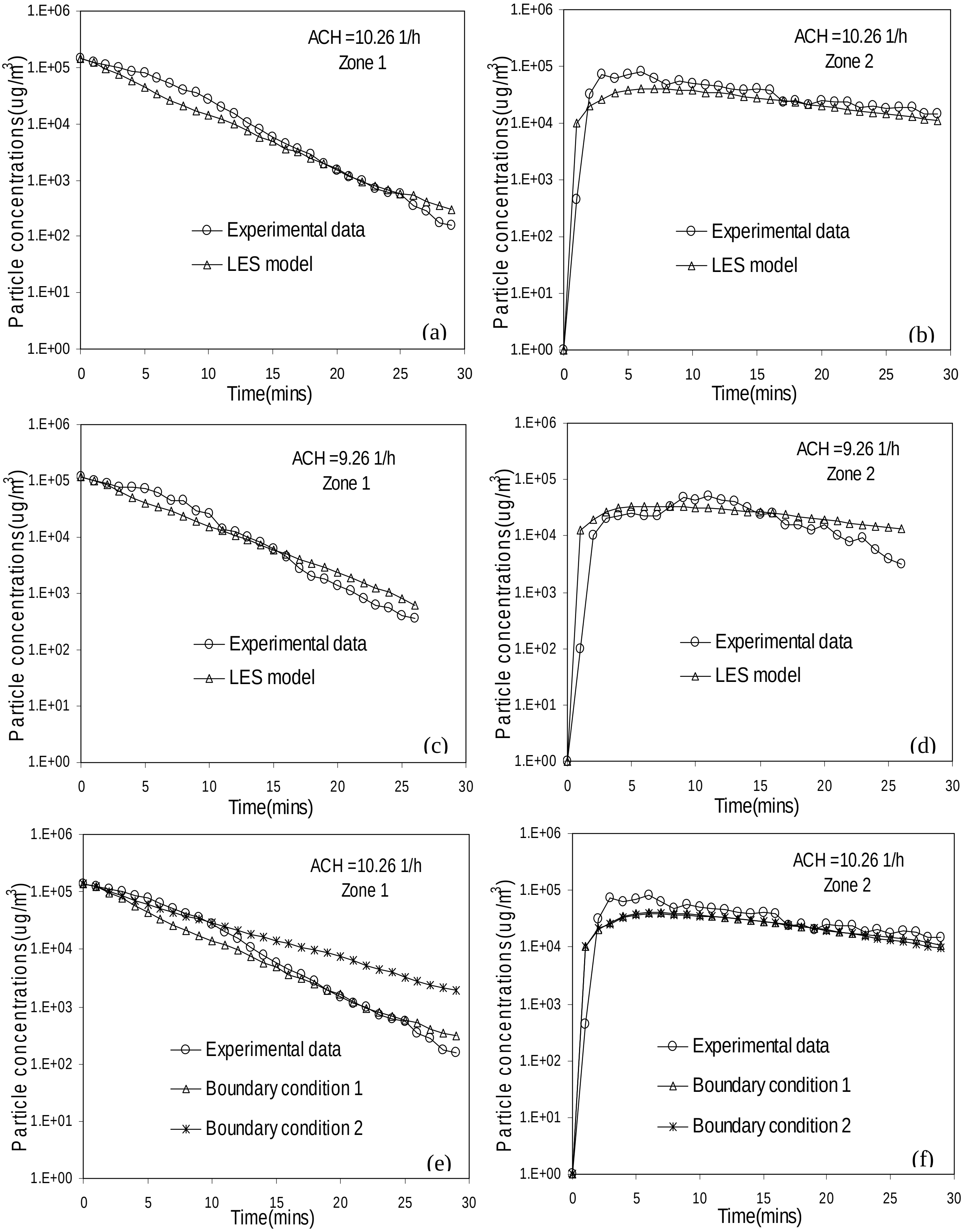

Figure 5 The predicted and measured zone-averaged particle concentration decay.

4. Conclusion

This paper investigates the application of Renormalization Group (RNG) theory Large Eddy Simulation (LES) to predict indoor airflow in a ventilated two-zone model room. Corresponding experimental data from literature [2] are used to validate the simulation results. It is found that RNG LES model can properly handle Low Reynolds Number (LRN) flows, which are always encountered in indoor air flows. Then the RNG LES model combing with a Lagrangian model is applied to predict the contaminant particle concentration in another ventilated room [3]. The results are also validated with the measured data from literature. The boundary condition for particle phase and the sample number size of particle affecting the concentration prediction are investigated and analysed. The boundary condition for particle phase has significant effect on the concentration prediction. This suggests that more realistic particle phase boundary condition is required to improve the CFD prediction.

References

[1] Chen Q. Computational fluid dynamics for HAVC: successes and failures. ASHRAE Transactions, 1997;103(1):178-187.

[2] Posner JD, Buchanan CR, Dunn-Rankin D. Measurement and prediction of indoor air flow in a model room. Energy and Buildings 2003;35:515-5.

[3] Lu W, Howarth A, Adam N, Riffat S. Modeling and measurement of airflow and aerosol particle distribution in a ventilated two-zone chamber. Building and environment. 1996;31;417-423

[4] FLUENT User’s Guide, Version 6.0 FLUENT Incorporated, Lebanon, NH, 2001.

[5] Yakhot A, Orszag SA, Yakhot V, Israeli M. Renormalization group formulation of large-eddy simulation. Journal of Scientific Computing. 1989;4:139-158.

[6] Morsi SA, Alexander AJ. 1972. Investigation of particle trajectories in 2-phase flow systems. Journal of Fluid Mechanics 1972;55:193-208.

[7] Lai.A.C.K. Particle deposition indoors: a review. Indoor air 2002; 12: 211-214.