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Prediction of particle deposition onto indoor surfaces by CFD with a modified Lagrangian method

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ABSTRACT

Accurate prediction of particle deposition indoors is important to estimate exposure risk of building occupants to particulate matter. The prediction requires accurate modeling of airflow, turbulence, and interactions between particles and eddies close to indoor surfaces. This study used a $\overline{v'^2}-f$ turbulence model with a modified Lagrangian method to predict the particle deposition in enclosed environments. The $\overline{v'^2}-f$ model can accurately calculate the normal turbulence fluctuation $\overline{v'^2}$, which mainly represents the anisotropy of turbulence near walls. Based on the predicted $\overline{v'^2}$, we proposed an anisotropic particle–eddy interaction model for the prediction of particle deposition by the Lagrangian method. The model performance was assessed by comparing the computed particle deposition onto differently oriented surfaces with the experimental data in a turbulent channel flow and in a naturally convected cavity available from the literature. The predicted particle deposition velocities agreed reasonably with the experimental data for different sizes of particles ranging from 0.01 μm to 50 μm in diameter. This study concluded that the Lagrangian method can predict indoor particle deposition with reasonable accuracy provided the near-wall turbulence and its interactions with particles are correctly modeled.

1. Introduction

Scientific studies discovered significant association between the particle pollution and people's mortality and morbidity (Pope, 2000; Long et al., 2000). A recent research found that the chance of lung cancer death increased by 8% for every 10 μg m^{-3} increase of long-term fine particle exposure in the ambient air (Pope et al., 2002). Since people spend more than 90% of their time indoors and particle concentration indoors is often higher than that outdoors (He et al., 2005), exposure to indoor particulate matter (PM) can be a major threat to our health. Good understanding of the indoor particle exposure is thus necessary and important.

Particle deposition onto indoor surfaces can greatly alter the indoor particle exposure level. According to Nazaroff (2004), particle deposition removes 10 μm particles 10 times and 2.5 μm particles 1 time as much as the ventilation does, for typical indoor environments with one air exchange rate per hour. So the accurate modeling of particle deposition is crucial in predicting the actual PM exposure level in an indoor environment.

In general, there are two methods studying the particle deposition: experimental investigations and numerical simulations. Experimental investigations provide accurate indoor particle deposition data, such as those summarized by Lai (2002) and conducted more recently by Bouilly et al. (2005) and Lai and Nazaroff (2005). Although those measured deposition rates vary with particle sizes in a similar trend, they can differ by one to two orders of magnitude between different experiments. The large variations in measurements indicate that factors other than

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particle size also influence the particle deposition rates. Those factors can be the airflow pattern, turbulence level, and properties of indoor surfaces, etc. However, it is often very difficult to measure and report all those crucial information in experiment. So those measurements may not be comparable, and the interpretation of the large variations on deposition rates can be difficult.

Alternatively, the numerical modeling approach can accurately control most of those important factors, making the comparison and interpretation between numerical results viable and meaningful. However, to develop an accurate particle deposition model is very challenging, which requires accurate modeling of airflow, turbulence, and particle–eddy interactions. Commonly used airflow and particle models may not be adequate. For example, Tian and Ahmadi (2007) compared different model predictions of particle depositions in channel flows. The predicted particle deposition velocities, based on the popular k–ε model, were higher than the measured data by one to four orders of magnitude for particles ranging 0.01–10 μm in diameters. Such errors in deposition predictions can have a major impact on the prediction accuracy of PM exposure indoors. Therefore, to develop an accurate particle deposition model along with appropriate airflow model is necessary.

In this paper, we propose a numerical model for accurate prediction of particle deposition in indoor environments. The model is validated and evaluated by quality experimental data in the literature, and is used to analyze indoor particle deposition characteristics.

2. Research methods

2.1. Brief review of modeling methods of predicting indoor particle deposition

There are two modeling methods in predicting particle deposition: the Eulerian and Lagrangian methods. The Eulerian method treats particles as continuum and correlates particle deposition to airflow properties inside the concentration boundary layer. The airflow properties are input parameters of the deposition model and can be obtained analytically by assuming ideal airflow conditions and by fitting with experimental data. For example, Lai and Nazaroff (2000) developed an indoor particle deposition model that represents the state-of-the-art of such Eulerian method. By presuming an airflow parameter (i.e., the friction velocity) their model prediction agreed reasonably well with the experimental data by Cheng (1997). However, the model prediction was less satisfactory in predicting particle deposition in another enclosed environment (Lai and Nazaroff, 2005). Such Eulerian deposition model is semi-empirical, and relies on the assumptions of the flow features inside the boundary layer. Due to the complexity of the indoor airflow, those assumptions could fail, and the performance and robustness of the Eulerian method can be affected.

Alternatively, the Lagrangian method tracks each particle directly based on the predicted airflow field by computational fluid dynamics (CFD), and avoids presuming flow conditions inside the boundary layer. However, the performance of the Lagrangian method is very sensitive to the accuracy of the predicted mean flow and turbulence, particularly near walls. The strict requirement on near-wall flow and turbulence modeling challenges the modeling capacity of many Reynolds-averaged-Navier-Stokes (RANS) models (Zhao et al., 2004; Zhang and Chen, 2006).

Effective near-wall treatment for the Lagrangian method is therefore necessary to the accurate prediction of particle deposition. Li and Ahmadi (1992) developed a near-wall model using DNS analysis of simple flows to quantify the wall-normal turbulent fluctuation within the viscous layer near a wall. Tian and Ahmadi (2007) successfully applied the near-wall model with a Reynolds stress model (RSM) to predict particle depositions in channel flows. Lai and Chen (2007) adopted a similar method with the RNG k–ε turbulence model to predict indoor particle dispersion and deposition. The Lagrangian prediction of deposition fractions agreed with their Eulerian simulations. However, the deposition prediction was not further validated experimentally due to the lack of directly measured deposition data. Bouilly et al. (2005) conducted both Lagrangian simulations and experimental measurements of particle deposition rates in an indoor environment. They used large eddy simulation to predict the airflow and turbulence. The predicted deposition rates of coarse particles (5 μm and 10 μm in diameters) agreed well with their measured data. Measured deposition rates for finer particles were reported, but no corresponding numerical results were provided. They indicated that further validation, especially for finer particles, was still necessary. More efforts need to be made in developing an accurate Lagrangian particle deposition model for both fine and coarse particles for indoor environments. This requires both suitable airflow and particle–eddy interaction models.

2.2. Modeling of airflow and turbulence features by CFD

Accurate prediction of airflow and turbulence is crucial to the success of modeling the particle deposition onto surfaces (Tian and Ahmadi, 2007). Zhai et al. (2007) and Zhang et al. (2007) evaluated a large variety of turbulence models in predicting airflow and turbulence in enclosed environments. These models covered a wide range of CFD approaches including RANS, detached eddy simulation, and large eddy simulation. Among these models, a modified $\overline{v'^2}-f$ model (Lien and Kalitzin, 2001; Davidson et al., 2003) had the best accuracy in predicting the mean flow and the turbulence. This study thus applied the $\overline{v'^2}-f$ model (hereafter v2f-dav model) in predicting the airflows. The model formulation has the general form:

$$\rho\frac{\partial\overline{\phi}}{\partial t}+\rho\overline{u}_j\frac{\partial\overline{\phi}}{\partial x_j}-\frac{\partial}{\partial x_j}\left[\Gamma_{\phi,\mathrm{eff}}\frac{\partial\overline{\phi}}{\partial x_j}\right] = S_\phi, \tag{1}$$

where ϕ represents independent flow variables, $\Gamma_{\phi,\mathrm{eff}}$ the effective diffusion coefficient, S_ϕ the source term of an equation, and the over bars denote the Reynolds averaging. Table 1 summarizes the mathematical form of each transport equation of the v2f-dav model. In Table 1, u_i is the velocity component in i direction, T air temperature, k the kinetic energy of turbulence, ε the dissipation rate of turbulent kinetic energy, $\overline{v'^2}$ the wall-normal turbulence fluctuation, p air pressure, H air enthalpy, μ_t eddy viscosity,