Chapter 1
Introduction

1.1 Background and objectives

Turbulent gas-particle flows are commonly found in many engineering applications. Some typical examples include indoor airflow and contaminant particle transport in buildings (Fogarty and Nelson, 2003), flue gas and flue ash flows in pulverized coal-fired boilers (Tu et al., 1997), and medicine particles delivered in inhalers (Tang et al., 2004). The research, optimal design and malfunction diagnose of these engineering systems require a fundamental understanding and detailed information of both the gas and particle phases.

With the increase of computer power and advancement of commercial modeling software, computational fluid dynamics (CFD) technique to study turbulent gas-particle flow problems is gradually becoming an attractive investigative tool. CFD has the capacity of providing the “microscopic” or “local” information, for instance, the maximum and minimum gas and particle velocity, local particle concentration, individual particle trajectory, and particle-wall collision procedure. It can also give the “macroscopic” or “global” parameters such as mean gas and particle velocity, turbulence intensity, and total mass flow rate. In most situations, CFD is more cost effective and time efficient than the physical model testing approach. Another feature of CFD approach is the graphical presentation of the flow geometry, velocity, pressure and particle concentration fields. These features facilitate scientists and engineers to gain more insights into the gas-particle behaviors in the many engineering applications.

Currently, there are two basic CFD approaches, the Eulerian-Eulerian model and the Eulerian-Lagrangian model, which are used to predict the gas-particle flows. In the Eulerian-Eulerian model, both the gas and particle flows are treated as continuous fluid flow and regarded as interacting with each other. This enhances the ease of implementation of the approach in CFD codes. It can be handled efficiently through current state-of-the-art solvers resulting in a relatively less computational time of mean parameters for the particle flow. However, the Eulerian-Eulerian model has some inherent limitations in modelling the turbulent gas-particle flows. The current Eulerian formulation is still deficient in correctly describing the aerodynamics drag force on the particle phase in the vicinity of a solid wall. Another problem with the Eulerian-Eulerian model is the justification of the continuum assumption as the particle equilibrates with neither local fluid nor other particles when flowing through the flow field (Shirolkar et al., 1996). The Eulerian model describes the averaged local particle parameters instead of the individual particle trajectory. This introduces the problem of "crossing trajectories" (Slater et al., 2001), and the lost of the particle properties could be significant when considering the local reaction rate of a particle that is essential for reacting flow systems (Shirolkar et al., 1996).

In Eulerian-Lagrangian approach, the Eulerian equations of the gas phase are solved and the Lagrangian equations of particle motion are integrated by tracking individual particle through the flow field. For Eulerian-Lagrangian approach, the large computational expense may be experienced because of the requirement to track substantial number of the particles to successfully attain good statistical information of the particle phase. Lengthy computational times have prevented the use of the Eulerian-Lagrangian model in the past. With the progress of computer speeds, the time expense has been significantly reduced and this makes the Eulerian-Lagrangian model an affordable tool to predict the turbulent gas-particle flows.

Although encouraging simulations of turbulent gas-particle flows by both the Eulerian-Eulerian model and the Eulerian-Lagrangian model have been reported in literature, no in-depth investigations have been performed on the comparison of their performance with measurements on benchmark problems such as gas-particle flow over a backward facing step and gas-particle flow through a 90-degree bend.

Furthermore, some uncertainties of CFD approach for turbulent gas-particle flows still prevail in particular the approximation of turbulence models for gas phase that requires further resolution. Turbulence models play a significant role in accurately predicting both the gas and particle flows. It has been found that standard k-ε model, which is the most used turbulence model in simulation of engineering applications, to be inadequate in a variety of flows. For instance, standard k-ε model is not able to accurately predict the indoor air flows that are characterized by low-Reynolds-number (LRN) turbulence. The improper handle of LRN flows and turbulence can contribute to inaccurate calculations of the indoor airflows and consequently the contaminant particle concentration, since the particle concentration is strongly affected by the air phase velocity and turbulent fluctuations.

Many variants of k-ε models including Renormalization Group (RNG) k-ε model and realizable k-ε model have been developed to improve the performance of the standard k-ε model. In addition, the Large Eddy Simulation (LES) 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. Nevertheless, evaluation and validation of these turbulence models for gas-particle flows in particular engineering applications are lacking. For example, no literature has been found reporting the prediction of the indoor contaminant particle transport by LES model.

Another uncertainty with regard to the Eulerian-Lagrangian approach is the particle-wall collision model, especially when particles are relatively large. The accurate descriptions of particle-wall interaction are fundamental to correctly understanding and predicting the gas-particle flows. Despite the many experimental and computational investigations, the success in properly modeling the particle-wall collision process remains elusive due to its complex nature. The particle-wall collision model should take into consideration of several physical parameters that govern the particle-wall collision process. Among these parameters are the particle incident velocity, particle initial angular velocity, incident angle, diameter and shape of the particle as well as its material properties. The particle-wall collision model should also consider the wall roughness and the resulting stochastic nature of the process, since experimental investigations (Grand and Tabakoff, 1975; Govan et al., 1989) have found that the particle restitution coefficient is subject to some scatter due to wall roughness and non-spherical particles (Sommerfeld, 1992).

Three main objectives were accomplished in the thesis. Firstly, this research aimed to perform the model validation through the numerical studies of the gas-particle flow over backward facing step and in a 90-degree bend using both an Eulerian-Lagrangian model in a generic CFD code FLUENT and an Eulerian-Eulerian model in an in-house code. Secondly, the performance of different turbulence models and the Eulerian-Lagrangian model was evaluated in the indoor air and contaminant particle flows in two room configurations. The FLUENT code was used to assess the performance of standard k-ε model, RNG k-ε model and a RNG-based LES model. The influences from the turbulence models and particle-wall collision model to the particle phase prediction were also investigated. Thirdly, two particle-wall collision models that account for the effects of particle incident velocity, initial angular velocity and wall roughness on the particle-wall collision procedure was developed and validated. The algebraic particle-wall collision model of Brach and Dunn (1992, 1998) and the stochastic wall roughness model of Sommerfeld (1992) were combined and implemented into the Eulerian-Lagrangian model in FLUENT code via the User-defined subroutines. This allows the flexibility for extending the collision model to handle complex engineering flows. The new Eulerian-Lagrangian model was employed to investigate gas-particle flow through an in-line tube bank. Also, the effects of wall roughness on a gas-particle flow in a two-dimensional 90-degree bend were studied via another particle-wall collision model developed by Sommerfeld (1992) and the stochastic wall roughness model.

1.2 Outline of this thesis

The contents of the remaining six chapters are as follows:

In Chapter 2, the basic concepts of turbulent gas-particle flows are reviewed, followed by the review of the two numerical approaches for gas-particle flow, i.e. the Eulerian-Eulerian model and Eulerian-Lagrangian model. The literature review of turbulence models and the particle-wall collision model then follow.

Chapter 3 addresses the mathematical and numerical methodology. Standard k-ε model, RNG k-ε model, realizable k-ε model, and a RNG-based LES model are firstly described and discussed. Then, the numerical details of the Eulerian-Eulerian model and the Eulerian-Lagrangian model used in this thesis are given. The third part of this chapter is mathematical description of the particle-wall collision models used in this thesis.

Chapter 4 covers the numerical simulations of the gas-particle flow over the backward facing step and in a three-dimensional 90-degree bend. The performance of both the

Eulerian-Eulerian model and the Eulerian-Lagrangian model is validated, compared and discussed.

In chapter 5, the indoor airflow and contaminant particle concentration in two geometrically different rooms are investigated using the Eulerian-Lagrangian model. For the first room configuration, the performances of three turbulence models for simulating indoor airflow are evaluated and validated against the measured air phase velocity data obtained by Posner et al. (2003). In the other two-zone ventilated room configuration (Lu et al., 1996), contaminant particle concentration decay within the zones are simulated and validated using the RNG-based LES model together with a Lagrangian particle tracking model. The influences from the turbulence models and particle-wall collision model to the particle phase prediction are also discussed.

In chapter 6, the physical characteristics of gas-particle flow in an in-line tube bank are firstly numerically investigated. The algebraic particle-wall collision model (Brach and Dunn, 1992, 1998) and the stochastic wall roughness model (Sommerfeld, 1992) are implemented into the FLUENT code via the User-defined subroutines. The predicted mean flow fields for both gas and particle phase are validated against experimental data of Tu et al. (1998). Then, the effects of wall roughness on the gas-particle flow in a two-dimensional 90-degree bend are simulated using the particle-wall collision model and the stochastic wall roughness model.

Finally, the conclusion and recommendations are made in Chapter 7. Further research direction is also suggested.