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# Direct numerical simulation of polydisperse aerosol particles deposition in low Reynolds number turbulent flow

Yu Li, Weiguo Gu, Dezhong Wang *, Jinpeng He

*School of Nuclear Science and Engineering, School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai 200240, China*

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ABSTRACT

Aerosol behaviors have a great effect on the evaluation of the leak rate of the coolant in the concept of Leak Before Break (LBB) in the Nuclear Power Plant (NPP) as the coolant will be released into the containment mainly in the form of aerosols if there exists a leak in the primary loop. The transportation and deposition of aerosol particles strongly affect the accuracy of evaluating the leakage source term. In this paper, direct numerical simulation coupled with Lagrangian particle tracking is proposed aiming at the transportation and deposition of polydisperse micron-sized particles in low Reynolds number turbulent horizontal flow. Results are validated by several theoretical and empirical equations. The study reveals the diffusion and deposition mechanism of particles with different sizes. It indicates that gravity plays a main role in the deposition of large particles ($d_p > 10\ \mu m$) in the low Reynolds number turbulent flow ($Re < 6000$). For small particles, deposition is mainly determined by the turbulence and Brownian motion. The size distribution of the deposited particles is different with the initial particle size distribution, which indicates that the particle size distribution in the containment may be not the same as the leaked particle size distribution.

## 1. Introduction

In recent years, aerosol dynamics have drawn many concerns in the nuclear industry. Since an accident usually begins with a discharge of coolant into the containment system, the initial containment atmosphere would contain aqueous aerosols formed by rapid evaporation of water and radionuclides. Typically, about 25% of the discharged water would be converted to steam, and as much as 50% of the water could form aerosols (Rogers, 1990). Hence, much of the emphasis in analyzing this stage of an accident has been on aerosol physics. The leakage of the reactor coolant will destroy the integrity of the reactor coolant pressure boundary (RCPB) and threaten the safe operation of a nuclear power plant (NPP). It is of great importance to detect the leak and quantify its flow rate (Zheng et al., 2016) as soon as possible.

The leaked radionuclides will be released mainly in the form of sub-micron and micron sized aerosols (Sun et al., 2017). Hence, mastering the mechanism of aerosol movement is essential for ensuring the accuracy of the evaluation of the leak rate (Li et al., 2018). To identify all credible accidents, it is of great importance to monitor the activity concentration of aerosols in the containment and reconstruct the source term. To reconstruct the source term, the aerosol behaviors should be studied, especially the removal of aerosols. At the same time, the loss of aerosol particles in the sample pipeline before the particles entering the monitor should be assessed. The aerosols will be removed from the containment atmosphere by gravitational settling, turbophoresis, thermophoresis, diffusiophoresis, and by containment leakage, and so on. When the monitoring results are available, we can obtain the source term (the leak rate) by applying the models of particle transportation and deposition to the evaluation process.

Despite the large number of published work, however, it is extremely difficult to gather a uniform and complete features of particle transport in turbulent flows or to assess the effectiveness of computer simulation models on the accuracy of predicted particle deposition rates (Marchioli et al., 2008), which significantly affect the accuracy of the evaluation of the leak rate.

The aerosol dynamic characteristics, such as diffusion, gravitational settling, thermophoresis, coagulation, and deposition, are all related to the flow field characteristics. In particular, the interaction between the particle and the flow field need to be properly accounted for. However, for turbulent flow, due to the complexity of turbulence itself, there is no completely satisfactory model for describing the gas-particle interaction in the finest scale that can be applied universally (Tian and Ahmadi, 2007). An important

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* Corresponding author.
*E-mail address:* dzwang_sjtu@sina.com (D. Wang).

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example of the effect of the flow field on the particle is particle deposition, which is called turbophoresis (Kuerten, 2005). Turbophoresis is the effect that in inhomogeneous turbulence particles migrate from a region of high turbulent velocity fluctuations to a region of low velocity fluctuations (Reeks, 1983). Some research on particle deposition in turbulent flow neglects the inhomogeneous turbulence (Mols and Oliemans, 1998). However, it is of great importance to predict the flow field accurately to ensure an accurate aerosol particle velocity prediction. Hence, the correct simulation of the flow field is one of the critical success factors to obtain the transportation, dispersion, and the deposition law of aerosol particles.

There are several methods to obtain the flow field characteristics, such as theoretical prediction, experimental measurement, and numerical simulation. Theoretical study is aiming at developing tractable mathematical models that can accurately predict the properties of turbulent flows. It is of great importance in revealing the nature of turbulence. However, due to the diversity, complexity, and nonlinearity of the turbulent flow, it is usually hard to obtain the analytical solution. Experimental study is a basic approach to learn turbulence, and it is a crucial method to verify the turbulent theory. However, due to the high cost and the limitations of experimental conditions, the numerical simulation based on Computational Fluid Dynamics (CFD) methods is widely used in the prediction of the flow field with the development of computer technology. Currently, there are three general approaches for simulating turbulent flow, Reynolds-averaged Navier-Stokes (RANS) equation method, large eddy simulation (LES), and direct numerical simulation (DNS) (Sajjadi et al., 2017). Among which, DNS can provide the most promising capability to reproduce features of turbulence up to the smallest Kolmogorov scale. In addition, DNS is able to capture the details of the turbulence eddy structures as well as the anisotropy of turbulence.

In the turbulent flow field, the turbulent diffusion of particles by instantaneous flow fluctuations, together with Brownian diffusion and gravitational sedimentation, are the main mechanism for particle dispersion and deposition (Tian and Ahmadi, 2007). Although particle deposition in the near-wall region is understood in terms of the physical principles involved, the precise mechanisms responsible for deposition and the role played by near-wall flow structures are less well understood (Yao and Fairweather, 2012). Till now, there are still some divergences in the mechanism of turbulent deposition. The most faithful coupling solution of the turbulent flow and the particle motion is only possible by the DNS. Hence, DNS coupled with Lagrangian Particle Tracking (LPT) has been widely used to study the dispersion and deposition (Brooke et al., 1992) of particles in turbulent flows. Different with the most widely concerned particle deposition in the high Reynolds number (Re > 10,000) turbulent flow field, in the application of Leak Before Break (LBB), the deposition loss of aerosol particles in the low Reynolds number (Re < 6000) turbulent flow field should be considered. In addition, the previous study of turbulent deposition always focuses on the fully developed vertical flow (Vreman, 2007) which ignores the effect of gravity, or just model the deposition in the horizontal flow as the combined process of turbulent diffusion and gravitational settling fluxes. Since there are many horizontal walls in the containment, the turbulent deposition that affected by gravity should be considered (Guha, 2008) and the coupling effect of the turbulence and gravity should also be revealed. In order to simplify the approach, monodisperse distribution is mainly considered in the previous work. However, the distribution of particles is usually polydisperse in the containment when there exists a leak in the primary loop (Almenas and Marchello, 1979). To conclude, the deposition loss of polydisperse aerosol particles caused by turbulence and gravity, as well as the Brownian motion (especially for small particles), will significantly affect the accuracy of the evaluation of the leak rate in the primary loop.

In this paper, the transportation and deposition of polydisperse aerosol particles in low Reynolds number horizontal turbulent flow are investigated by direct numerical simulation of the turbulence with simultaneous Lagrangian tracking of the particles. This paper attempts to increase the understanding of the diffusion and deposition mechanism of particles moving in a horizontal turbulent flow by investigating and analyzing the flow field and the particles characteristics. The results are discussed and validated by several empirical equations.

## 2. Methodology

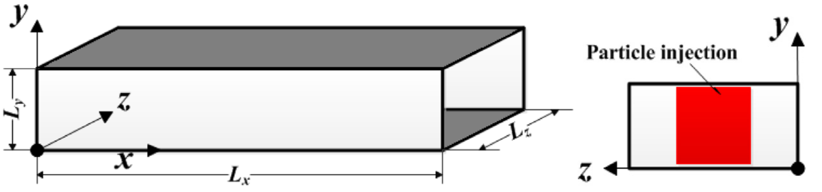
When aerosol particles move in the air flow field, the interactions between particles and the surrounding air fluid determine the velocity and direction of the aerosol particles. Direct numerical simulation of low Reynolds number turbulent transportation and deposition of polydisperse aerosol particles in a horizontal rectangular channel is proposed in this paper. The geometric model of the computational domain is shown in Fig. 1, where $L_x = 0.5$ m, $L_y = 0.1$ m, $L_z = 0.2$ m. The injection surface of the aerosol particles is shown in Fig. 1(b). Periodic boundary conditions are applied to both streamwise ($x$) and spanwise ($z$) directions, and the non-slip condition is applied to the wall normal ($y$) direction. The computation applies a mesh system of 64 × 128 × 64 grids, which is proved dense enough to sustain the turbulence. Uniform grids are used in the streamwise and spanwise directions, non-uniform grids are used in the wall-normal direction with denser mesh near the wall to resolve the small eddies. A transformation is used as

$$y_j = \frac{L_y}{2}\cdot\left[1+\frac{1}{a}\tanh\left(\frac{1}{2}\varsigma_j \ln\frac{1+a}{1-a}\right)\right]$$

where $y_j$ is the $y$-coordinate of the $j$-th gird, $j$ is the node number. $a$ is an adjustable parameter of the transformation with a constant value of 0.96.

$$\varsigma_j = -1 + 2j/Ny$$

where $N_y$ is the total number of grids in the $y$-direction. Fig. 2 is the non-uniform mesh in the $x$-$y$ plane. The grid spacing in wall units



（a）Computational domain （b）particle injection surface

**Fig. 1.** The geometric model in DNS.