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Large eddy simulation of particulate flow inside a differentially heated cavity

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HIGHLIGHTS

- Nuclear accident leads to airborne radioactive particles in containment atmosphere.
- Large eddy simulation with particles in differentially heated cavity is carried out.
- LES results show negligible differences with direct numerical simulation.
- Four different particle sets with diameters from 10 μm to 35 μm are tracked.
- Particle removal dominated by gravity settling and turbophoresis is negligible.

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ABSTRACT

In nuclear safety, some severe accident scenarios lead to the presence of fission products in aerosol form in the closed containment atmosphere. It is important to understand the particle depletion process to estimate the risk of a release of radioactivity to the environment should a containment break occur. As a model for the containment, we use the three-dimensional differentially heated cavity problem. The differentially heated cavity is a cubical box with a hot wall and a cold wall on vertical opposite sides. On the other walls of the cube we have adiabatic boundary conditions. For the velocity field the no-slip boundary condition is applied. The flow of the air in the cavity is described by the Boussinesq equations. The method used to simulate the turbulent flow is the large eddy simulation (LES) where the dynamics of the large eddies is resolved by the computational grid and the small eddies are modelled by the introduction of subgrid scale quantities using a filter function. Particle trajectories are computed using the Lagrangian particle tracking method, including the relevant forces (drag, gravity, thermophoresis). Four different sets with each set containing one million particles and diameters of 10 μm, 15 μm, 25 μm and 35 μm are simulated. Simulation results for the flow field and particle sizes from 15 μm to 35 μm are compared to previous results from direct numerical simulation (DNS). The integration time of the LES is three times longer and the smallest particles have been simulated only in the LES. Particle statistics in the LES and the DNS were similar and the settling rates were practically identical. It was found that for this type of flow no model was necessary for the influence of the unresolved flow scales on the particle motions. This can be explained by the dominant nature of gravity settling compared to turbophoresis which is negligible for the particle sizes of the present study.

1. Introduction

Turbulence plays a central role in many particle/fluid processes in the environment and industry. In the particular case of nuclear safety, many severe accident scenarios lead to the presence of fission products in aerosol form in the closed containment atmosphere where turbulent convection currents are dominant. How turbulence affects particle deposition rates in such a situation is very important because aerosol depletion limits the release of radioactivity to the environment if the containment is breached.

The natural circulation gas speeds in reactor containments are several orders of magnitude greater than the settling velocities of typical aerosols, and therefore, the aerosol particles will tend to be entrained by the flow rather than settle under the sole influence

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of gravity. Hence, a rigorous methodology to determine particle-turbulence interactions has to be used to get a precise description of the mechanism driving particles settling.

Experimental data related to this have highlighted some interesting phenomena of particle-turbulent flow interactions which are yet to be fully understood: for instance, it has been shown in the Phebus (Clément et al., 2003) project that particles in the containment settled at a rate which is greater than that expected under quiescent conditions. This parallels previous experimental findings (Aliseda et al., 2002) in channel flow, which found that droplets settling rates are very much enhanced when turbulence is present in the carrier gas. The Phebus data (Clément et al., 2003) also showed that the settling rate of particles displays a much weaker dependence on particle inertia than would be anticipated in the absence of turbulence. Still more recently, the ARTIST data (Güntay et al., 2004) showed the tendency of particles to deposit more readily on horizontal surface when the carrier gas velocity (i.e. turbulence level) is increased. In light of this, the coupling between the gas and turbulent fluctuations and aerosol motion needs to be carefully investigated to determine the controlling mechanism responsible for aerosol removal in the presence of turbulence within a closed cavity.

Traditional Eulerian approaches, based on statistical Fickian diffusion models, can treat particle dispersion only in a time-averaged sense and cannot predict the highly non-uniform distribution of phases giving a poor description of the true physics of the dispersion process. Time dependent, Lagrangian approaches are required for a deeper understanding of the mechanism for particle dispersion, preferential concentration and deposition mechanism.

The most accurate method for the understanding of turbulence is the direct numerical simulation (DNS) which involves the solution of the full, transient, non-linear Navier–Stokes equations. Recently, accurate solutions of the differentially heated cavity including particles have been computed by Puragliesi et al. in two (Puragliesi et al., 2011) and three dimensions (Puragliesi, 2010). The computational cost of a DNS increases with the Rayleigh number like $Ra^{3/2}$ and therefore, this method is only applicable for low to moderate levels of turbulence. On the other hand, the large eddy simulation (LES), where the dynamics of the large eddies is resolved by the computational grid and the small eddies are modelled by the introduction of a subgrid scale tensor and a subgrid heat flux vector, is a compromise which can provide reasonably accurate turbulence data for complex flows and higher levels of turbulence than can be achieved with DNS. In the present work, the method used to simulate the turbulent flow is the LES. The major limitation of LES is that the range of scales in turbulent flows increases rapidly with the Reynolds number (for forced flows) and Rayleigh number (for buoyancy driven flows) so that LES calculations are time-consuming and require powerful computational resources. As a result, most practical engineering problems have a too wide range of scales to be directly computed using LES. Therefore, idealisations have to be made in the geometry of the problem in order for LES computations to be tractable. Judicious use of dimensional analysis and scaling will be needed to complement basic LES studies and arrive at practical estimates for containment geometries. Hence this estimation uses the so-called differentially heated cavity as a model of a closed volume. The differentially heated cavity is a three-dimensional (3D) cubical domain, where the two opposite vertical walls are kept isothermal at different temperatures whereas all the other walls are insulated.

In LES with Lagrangian particle tracking, a subgrid error is introduced in the particle equation because only the filtered fluid velocity and temperature fields are available. Previous LES applications to the problem of particle dispersion in turbulent bounded flows have shown that LES tends to underestimate turbophoresis if the effect of the filtered subgrid scales on particle dynamics is not taken into account (Marchioli et al., 2008a). Turbophoresis (Reeks, 1983) is an effect of inhomogeneous turbulence that tends to drive particles from high to low turbulence regions. Therefore closure models for the Lagrangian particle tracking are usually needed. Two different ideas can be found in the literature: fractal interpolation (Salvetti et al., 2006) and approximate deconvolution of the filtered field (Kuerten and Vreman, 2005; Shotorban and Mashayek, 2005; Shotorban et al., 2007). A comparison of the two methods has been done by Marchioli et al. (2008b). One objective of the present work is to investigate the influence of the removal of subgrid scales for the particle dynamics in the differentially heated cavity and develop closure models if necessary.

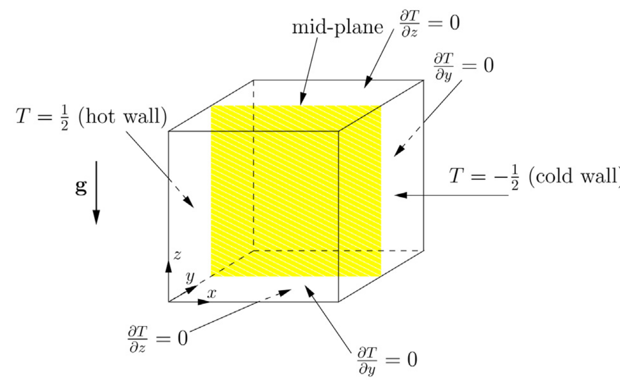

Fig. 1. Differentially heated cavity.

Experiments by Kalilainen et al. (2013) in the DIANA facility (DIfferentially heated cavity with Aerosol in turbulent NAtural convection) will complement the numerical simulations. DIANA consists of two heated/cooled aluminium side walls. The other walls are made of glass which allows optical access. In DIANA, the flow field and the particle depletion are measured by Particle Image Velocimetry (PIV). In addition, Condensation Particle Counter (CPC) and Tapered Element Oscillating Microbalance (TEOM) will be used to determine the change of particle concentration in time.

The paper is organised as follows: In Section 2.1 the governing equations, the non-dimensionalisation and the properties of the continuous and the particle phases are presented. Section 2.2 reviews the LES method and the numerical discretisation. The second part of the paper, Section 3 shows numerical results. First the basic flow features of the continuous phase are described briefly in Section 3.1. Section 3.2 investigates the particle settling process for the four different particle sizes. Results are also compared to DNS reference solution. In Section 3.3 particle segregation is investigated by computing the correlation dimension. Some information about parallel computing and the required CPU time is given in Section 3.4. Finally, in Section 4 we draw some conclusions.

2. Physical problem and methodology

2.1. Particle-laden differentially heated cavity flow

The differentially heated cavity problem is one of the classical heat and mass transfer problems with significance for fundamental fluid mechanics, as well as for engineering and geophysical applications. A fluid is confined in a three-dimensional cavity bounded by rigid and impermeable walls. The fluid in the cavity is heated over one vertical wall and cooled on the opposite wall at equal rates. All other walls are adiabatic (see Fig. 1). Complex flow patterns develop and the flow characteristics depend on the Rayleigh (Ra) and the Prandtl (Pr) numbers. The Rayleigh number of the differentially heated cavity problem is computed with the temperature