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Shahid Bahonar University of Kerman
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Department of Mechanical Engineering

Effect of Sub-Grid Scales on Large Eddy Simulation of Particle Deposition in a Turbulent Channel Flow

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A Ph.D. Dissertation
By:
Mazyar Salmanzadeh

Supervisor:
Dr. Mohammad Rahnama

Advisor:
Dr. Goodarz Ahmadi

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استاد راهنما: آقای دکتر محمد رهنما

داور۱: آقای دکتر محمود یعقوبی

داور۲: آقای دکترسید حسین منصوری

داور۳: آقای دکتر مهران عامری

استاد مشاور پروژه: آقای دکتر گودرز احمدی گودرز احمدی

مدیر کل تحصیلات تکمیلی دانشگاه: آقای دکتر رضا نکویی

نماینده تحصیلات تکمیلی دانشکده: آقای دکتر سید عبدالرضا گنجعلیخان نسب

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presented by Mazyar Salmanzadeh, a candidate for the degree of Doctor of Philosophy, and hereby certify that it is worthy of acceptance.

Date ADVISOR Dr. Mohammad Rahnama

EXAMINING COMMITTEE

Dr. Goodarz Ahmadi (Clarkson University, Potsdam, NY, USA)

Dr. Mahmood Yaghoubi (Shiraz University, Shiraz, Iran)

Dr. Seyed Hossein Mansouri (Shahid Bahonar University of Kerman, Kerman, Iran)

Dr. Mehran Ameri (Shahid Bahonar University of Kerman, Kerman, Iran)

Dr. Mohammad Rahnama (Shahid Bahonar University of Kerman, Kerman, Iran)

Abstract

Large-Eddy Simulations (LES) of particle transport and deposition in turbulent channel flow were presented. Particular attention was given to the effect of subgrid scales on the particle dispersion and deposition processes. A computational scheme for simulating the effect of subgrid scales (SGS) turbulence fluctuation on particle motion was developed and tested for a channel flow. Large-eddy simulation of Navier-Stokes equations using a finite volume method was used for finding instantaneous filtered fluid velocity fields of the continuous phase in the channel. Selective structure function model was used to account for the subgrid-scale Reynolds stresses. It was shown that the LES was capable of capturing the turbulence near wall coherent eddy structures.

For transport and deposition of particles in the channel the Lagrangian particle tracking approach was used. The Stokes drag, lift, Brownian and gravity forces were included in the particle equation of motion. The Brownian force was simulated using a white noise stochastic process model. Effects of SGS of turbulence fluctuations on deposition rate of different size particles were studied. It was shown that the inclusion of the SGS turbulence fluctuations improves the model predictions for particle deposition rate especially for small particles. Effect of gravity on particle deposition was also investigated and it was shown that the gravity force in the stream wise direction increases the deposition rate of large particles.

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Chapter 1

Introduction

Analyzing transport and deposition of aerosols suspended in air streams has attracted considerable attention in the past two decades. Particle transport and deposition plays a major role in a number of industrial and environmental processes. Filtration and separation processes, combustion, air and water pollution, electro photography machines, targeted pharmaceutical drug delivery, and lung deposition are just a few examples. Particulate micro-contamination is also of great concern in microchip fabrication industries. With the size of feature reaching the nanometer range, small particle deposition has become the main cause of defects and loss of yield in microelectronic industries.

Extensive experimental and computational studies related to particle transport in turbulent flows have been reported in the literature (Hinze[1]; Hinds[2]; Wood[3]; Papavergos & Hedley[4]; Ahmadi[5]). Accordingly, small particles are transported by the instantaneous fluid velocity field. Thus, for computer simulation of particle transport, dispersion and deposition processes, the instantaneous flow velocity should be carefully evaluated in various fluid flow regions.

During the past decades using Reynolds averaged Navier-Stokes (RANS) equations with the aid of a turbulence model for finding the mean flow has been the most common approach, particularly for practical applications. In this approach, the instantaneous turbulent fluctuating velocity fields are simulated separately, using a stochastic method, and are added to the mean flow that are evaluated via a RANS model. This approach is inevitably inaccurate as it treats turbulence fluctuation as a Gaussian random field, and therefore, is incapable of capturing the turbulent coherence structures. The most accurate available approach for evaluating instantaneous velocities is the direct numerical simulation (DNS) of Navier-Stokes equations with a high-resolution grid that resolved the Kolmogorov scale of turbulence. Despite its accuracy, applications of the DNS method have been limited to flows in simple passages at low Reynolds numbers. This is because the sharp increase of the computation cost of DNS with flow Reynolds number. Large Eddy Simulation approach was developed because of its lower computational cost compared to DNS so that it can handle high Reynolds number flows with reasonable accuracy. In LES method, the large energy containing scales of turbulence resolved while the effect of scales of turbulence smaller than the grid size is modeled by using a so-called subgrid scale model. Thus, LES is less sensitive to modeling errors compared to RANS, since subgrid scales are contains generally much less energy compared to the large scales, and they can be estimated by relatively simple models.

Direct numerical simulations (DNS) of particle deposition in wall-bounded turbulent flows were performed by McLaughlin[6] and Ounis, et al.[7,8] Brook et al.[9] and Pendinotti, et al.[10] employed DNS to study the vortical structures and particle transport in the turbulence wall regions. These studies were concerned with providing an understanding of particle deposition mechanisms in turbulent flows. Recently, Zhang & Ahmadi[11] studied aerosol deposition from turbulent air streams in vertical and horizontal ducts using the DNS approach. They showed that the particle-to-fluid density ratio, the shear-induced lift force, the flow direction relative to gravity, and the shear velocity affect the particle deposition rate. Furthermore, the effect of gravity and its direction on the particle deposition rate becomes more significant at low shear velocities.

LES has also been used for particle transport analysis in the last decade. In earlier applications of LES, however, just the filtered velocity that contains the resolved scale of turbulent was used for particle trajectory analysis and the contributions of subgrid scales were ignored (Vance and Squires[12], Uijttewaal and Oliemans[13], Wang and Squires[14] and Yeh and Lei[15]). Recently, however, more attention was given to the effect of subgrid scale fluctuations on particle transport. Armenio et al.[16] investigated the effect of disregard the subgrid scale fluctuation on particle motion by comparing the DNS and the LES. They observed certain differences between the DNS and LES prediction especially when a significant percentage of the fluctuation energy is in unresolved part. They also showed that inertia particles are less sensitive than tracer particles to subgrid scale fluctuations in the LES approach.

Including the effect of subgrid scale fluctuations on particle motion was addressed by a few researchers in literature. Wang and Squires[17] solved a transport equation for the SGS kinetic energy and obtained the corresponding SGS intensities using the same relative magnitudes as the resolved scale intensities. Then they generated the SGS fluctuation velocities using the computed intensities scaled by random numbers sampled from a Guassian distribution. They used the sum of the filtered velocity and the subgrid scale fluctuating velocity for computing the particle trajectory analysis. However, it is known that the use of simple scaled random numbers will lead to dispersion that will depend on the computational time scale.

Kuerten[18] and Shotorban and Mashayek[19] reconstructed the instantaneous velocities from the filtered ones by an approximate deconvolution model. Kuerten[18] studied turbophoresis process and particle velocity fluctuations near the wall in channel flow. Shotorban and Mashayek[19] showed improvement in particle–phase statistics using this method. .

The present study is concerned with developing a computational model for studying the effect of subgrid scale turbulence fluctuations on particle dispersion and deposition processes. LES of the Navier-Stokes equations in a turbulent channel flow was solved and the filtered instantaneous velocities were evaluated. Subgrid scale Reynolds stresses are modeled by using Selective Structured Function model of Métais & Lesier[20] and David.[21] The instantaneous subgrid scale velocity fluctuations were simulated using Kraichnan's[22] Gaussian random field model scaled with the appropriate SGS intensities. Transport and deposition of particles of different sizes was studied using the Lagrangian particle tracking approach. The Stokes drag, lift, Brownian and gravitational forces were included in the particle equation of motion. The Brownian excitation was simulated as a white noise process.

A series of one-way coupled simulations were performed and the deposition rate of particles in the size range of 1 to 130 μm was studied. The importance of subgrid scale fluctuations on the deposition rate of different size particles was assessed. The effect of presence of gravity on particle deposition is also studied. The simulation results show that the inclusion of subgrid scale fluctuation significantly affects the deposition rate of small particles.

Chapter 2

Introduction to Aerosoles

2-1 What is an Aerosol

Aerosol is scientific term which is a suspension of solid or liquid particles in a gas, usually air.

The term 'aerosol' applies to a very wide range of particulate systems. First there are naturally occurring aerosols such as snow storms, dust storms, sand storms, volcanic ashes, smokes (from fires), mists, fog, haze and so on. This category also includes biologically-active systems such as airborne pollens, fungi, viruses and bacteria. However, we also have man-made aerosols, resulting from a wide range of industrial activities. Such aerosols may be found either outdoors or indoors, and become important in relation to the natural aerosol background because they are usually quite in homogenous (with relatively high concentrations).

'Aerosol science' in general covers all aspects of airborne particulate matter. Many aerosols are considered to be good as they make positive contributions to the earth and to man. For example, a balanced climate requires cloud and droplet formation in the atmosphere. Many industrial processes require aerosols as components vital to their effectiveness such as photo reproduction, chemical reactors, materials synthesis and etc. Many medicines need to be aerosolized before they may be delivered to the site in the body where they can be effective (e.g. inhalers for the treatment of respiratory complaints such as asthma and etc.). Industry usefully employs sprays for the efficient delivery of paints and etc. There is clearly plenty of scope for aerosol science to continue to make direct positive contributions to the earth's environment and ecology and to man's health and industrial activities. Modern aerosol research is therefore increasingly motivated in these directions.

There is a wide range of aerosols which are clearly perceived as 'bad'. An unwanted aerosol is, by definition, a pollutant and may be difficult to recapture. One aspect which is growing in importance in terms of its potential cost to industry is the problem of the contamination of products (e.g. electronics components, pharmaceuticals, food, etc.) by unwanted particle deposition. A whole branch of aerosol science has grown out of this need for 'clean technology'. However, the area where interest has consistently remained high since the birth of aerosol science is that concerned with the health that can arise from the human exposure to aerosols by inhalation, whether it is in the home, in the outdoor environment, in public buildings, or in the workplace. Such exposure needs to be eliminated or, at least kept to within limits considered to be safe.

It is clear from the introductory remarks that aerosols feature very widely in nature and in human experience. So it is not surprising to find that the study of aerosols has grown into a major field of scientific enquiry, touching on many individual disciplines, including physics, chemistry, mathematics, engineering, biology and medicine.

Aerosol particles are found in different shapes and different sizes. For irregular shaped particles, different equivalent diameters are defined. Examples of equivalent diameters are:

- Equivalent area diameter
- Feret's diameter (maximum distance edge to edge)
- Stoke's diameter (diameter of a sphere with the same density and the same velocity as the particle);
- Aerodynamic diameter (diameter of a sphere with the density of water and the same velocity as the particle).

The range of diameters of common aerosol particles is between 0.01 and 100 μm. The lower limit of 10 nm roughly corresponds to the transition from molecule to particle. Particles larger than 100 μm normally do not remain suspended in air for a sufficient amount of time.

2-2 Aerosol Motion

Analyzing the diffusion, transport and deposition of aerosols suspended in air streams can be done in two different approaches called Euilerian and Lagrangian.

2-2-1 Particle Brownian Diffusion and Euilerian Approach

Particle distributions in fluids could be assumed as a specie in the fluid with defined concentration, c. These particles always tend to move from regions of high concentration to regions of low concentration, and then there will always be a tendency for aerosols to migrate to walls or other surfaces where the concentration, because of deposition, is essentially zero.

Small particles suspended in a fluid undergo random translational motion due to molecular collisions. This phenomenon is referred to as the Brownian motion. The Brownian motion leads to diffusion of particles in accordance with Fick's law.

$$J = -D\frac{dc}{dx} \tag{1}$$

where J is the flux and D is the diffusion coefficient. When the effect of particle inertia is negligible, using (1) in the equation of conservation of mass for particles leads to

$$\frac{\partial c}{\partial t} + V\nabla c = D\nabla^2 c \tag{2}$$

where V is the fluid velocity vector. This is the general convective diffusion equation for particles in an isothermal gas when the particles are not subjected to any forces other than the convective motion of the gas ($V\nabla c$) and the molecular motion of the gas molecules ($D\nabla^2 c$).

2-2-2 Particle kinetics and Lagrangian Approach

When particles are transported by air currents different forces are acting on each particle and cause the particle to accelerate or decelerate. To see the effect of all forces acting on the particles on their motions and investigate their fate in a flow, Lagrangian approach that's tracking of all particles one by one can be used.

When air carrying particles suddenly changes direction, the particles because of their inertia, tend to continue along their original paths. If the change in air direction is caused by an object placed in the air stream, particles with sufficient inertia will strike the object. This process is known as *impaction* . It is the mechanism by which many large particles are removed from the atmosphere, it is one of the important mechanisms for removal of particles by lungs, and it is important in air cleaning as well as aerosol sampling. The process of impaction can be modeled by using the equation of motion of an aerosol particle that's a Lagrangian approach.

Consider an aerosol particle in fluid flow as shown in Figure 1. By applying the Newton's second law on the particle of mass m, the equation of motion is given as

$$m\frac{du^p}{dt}=\sum F \qquad (3)$$

where F could be any force exerted on the particle such as drag, lift, gravity, buoyancy, Brownian and….. and u^p is the particle velocity. Different forces can be considered in this motion based on the nature of the problem. Drag, Lift, Brownian forces are explained in the next session and other forces such as Thermoforetic, electric and … can be found in Parker[23] and Ahmadi[24].