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Comparison between Lagrangian and Eulerian approaches in predicting motion of micron-sized particles in laminar flows

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HIGHLIGHTS

- This study compares the results of two approaches of Lagrangian and Eulerian.
- In low concentration of particles, the results of two approaches are different.
- Lagrangian model converge to the Eulerian one by increasing simulation time.

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ABSTRACT

Modeling the behavior of suspended particles in gaseous phase is important for diverse reasons; e.g. aerosol is usually the main subject of CFD simulations in clean rooms. Additionally, to determine the rate and sites of deposition of particles suspended in inhaled air, the motion of the particles should be predicted in lung airways. Meanwhile there are two basically different approaches to simulate the behavior of particles suspension, Lagrangian and Eulerian approaches. This study compares the results of these two approaches on simulating the same problem. An in-house particle tracking code was developed to simulate the motion of particles with Lagrangian approach. In order to simulate the same problem with Eulerian approach, the solution to the transport equation with appropriate initial and boundary conditions was used. In the first case study, diffusion of particles, initially positioned homogeneously on an infinite plane was modeled with both approaches and the results were compared and the mismatch between Lagrangian and Eulerian approaches was analyzed for different concentrations. In the second case study, airflow with parabolic velocity profile moving between two parallel plates was modeled with two approaches. The airflow initially contained a homogeneous suspension of particles and the plates were maintained at zero concentration. The concentration along the plates was compared between the two approaches and the differences in the performance of each approach were investigated, again for different initial concentrations. The overall results confirm that as particle concentration falls below a minimum amount, approximately 10^5 m^{-2}, the results of the two approaches deviate considerably from each other and hence the Eulerian approach cannot be taken as an alternative for Lagrangian approach for low concentrations. For the third problem, we investigated the 3D particle flow in an expanding lung alveolus. It is shown that when the number of total released particles increases, the results of Eulerian approach can be used as an alternative to Lagrangian simulation. Since the number of particles existing in the lung alveolus in normal condition is much lower than this value, we concluded that Eulerian method cannot be applied to problems involving low concentration of particles. Although, the results of the Lagrangian problem may converge to the Eulerian one by increasing simulation time, but it is a hypothetical situation which not really exist in short time scale problems such as third case study in this paper.

1. Introduction

The atmosphere where we all breathe in is in fact a suspension of a wide variety of fine particles. Studying the behavior of fine particles in a gas suspension is crucial to human being. Hence, this subject is becoming increasingly attractive to scientists. As an

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example, one of the areas where study of aerosol behavior is significant is simulation of clean rooms. Any clean room is designed to accommodate a manufacturing or scientific task in which even a limited number of aerosols may play a destructive role and result in erroneous results. Therefore, there is a vast pool of modern studies on simulation of aerosol motion in clean rooms among which one can point to numerical modeling in Sznitman et al. (2009), Gao and Zhang (2010) and combined numerical and experimental investigations in Shih et al. (2011), Whyte et al. (2010).

The industry of clean rooms is not the only field where studying the behavior of fine particles seems necessary. Also airways of human lung, both acinar and conducting ones, are where transport and deposition of fine particles should be modeled and analyzed. Drug delivery would be much more efficient if drug particles were delivered straight to the intended tissue (Langers, 1998; Brain and Valberg, 1979). The drug injected in the cardiovascular system may have to pass from different organs like kidney, liver, etc. before arriving at the intended tissue. So the possibility of administering drugs via acinar airways of the lung can contribute a great deal to an efficient method of drug delivery. In order to fulfill such a task, a given drug should be first aerosolized and its resulting physical and pharmaceutical characteristics should then be determined. The next step is to determine the dynamics of the inhaled aerosol all the way to the deepest parts of respiratory system. This approach is, however, not an easy task to achieve mainly due to lack of adequate in-vivo measuring techniques. Therefore the numerical simulations can be the only way to predict the behavior of particles in acinar airways.

In addition to drug delivery, the increasing rate of mortality and morbidity because of inhaling fine particulates in the environment reported in Schwartz and Dockery (1992), Wilson and Spengler (1996) and the increasing threats of bio-terrorism reported in Harrington et al. (2006) are other issues which add to the importance of the subject.

The numerical simulations used in the above mentioned references follow two main separate approaches called Lagrangian and Eulerian. Lagrangian approach deals with individual particles and calculates the trajectory of each particle separately, whereas the Eulerian approach deals with concentration of particles and calculates the overall diffusion and convection of a number of particles. It is evident that when handling the same question, the calculations in Lagrangian approach are quite more time consuming than Eulerian approach since in Eulerian approach, an average behavior of particles is investigated instead of the behavior of each existing particle.

Hu et al. (2002) applied CFD simulation for particle dispersion in clean rooms and Zhao and Wu (2005) applied Eulerian approach to study if the particles could be treated as passive gas pollutants. Zhao and Wu (2005) have modeled clean rooms using a well-known derivation of Eulerian approach called drift-flux model has been used in simulation of indoor particle dispersion (Gao and Zhang, 2010).

Although when discussing why Eulerian method has been preferred over Lagrangian one, it is mostly argued that because: 1) Eulerian method has less computational cost in comparison with Lagrangian one and 2) instead of positions of particles, Eulerian method works with concentration of particles which is more appropriate for engineering applications. However, the question is that for what conditions the results of the two approaches are equivalent and when the two methods are different. Although much has been written on using these methods, less has been written on the answer to this question in the area of aerosols.

Zhang and Chen (2007) compared Lagrangian and Eulerian approaches for two special geometries. However the shortcoming is that modeling and analyzing two special cases on two special geometries will not raise an overall rule for the mismatch between the results of Lagrangian and Eulerian approaches for other studies and geometries. Zhao et al. (2008) evaluated particle dispersion in ventilated rooms by three different approaches of Lagrangian, drift flux and mixture models. They concluded that Lagrangian models agreed well with experimental data. The drift flux model is more accurate near the wall while mixture model yield unacceptable results for particle concentration. Although the result of drift flux model agreed well with Lagrangian and experimental model, but they did not report number of tracked particles and simulation time in their Lagrangian model which is the purpose of this article.

Zhao et al. (2010) found penetration coefficient through a single crack in a building envelope by three different approaches; Analytical, Eulerian and Lagrangian. They used Fluent software for Lagrangian simulation which independent results is obtained by increasing number of particles. They according to Aliabadia and Rogaka (2011), Zhao et al. (2011) concluded that Fluent Lagrangian method cannot be used to model Brownian motion of fine particles correctly.

Most of these studies are constricted to the steady state problems and they did not discuss the differences between the results of two approaches in unsteady problems. Moreover, there is no discussion on the dependency of this mismatch with concentration of particles; although it is expected that for high concentrations the results of Lagrangian and Eulerian calculations may be the same and as gradually the concentration is reduced, this mismatch should also become more significant. Therefore there is a need to bring up a quantitative comparison between Lagrangian and Eulerian results for different particle concentrations and simulation time.

It should be remarked that numerous studies such as Chibbaro and Minier (2011), Sanjose et al. (2011) have compared Lagrangian and Eulerian approaches for multiphase flow of bubbles in liquids, but these studies cannot be related to aerosols, as different mechanisms play role in the motion of bubbles in liquids compared with the motion of particles in atmosphere.

In current work, we investigate three case studies to compare the difference between the results of Lagrangian and Eulerian approaches. The basic mechanism in these two case studies which makes particles move is Brownian motion of particles; or diffusion of group of particles.

2. Methods

2.1. Lagrangian approach

A particle tracking code was developed to analyze the motion of particles in atmosphere, capable of taking into account the effects of diverse forces such as Brownian, Saffman, Drag and gravity force. If the fluid flow domain is steady and simple and if flow velocity components can be defined by simple functions, this code uses these functions to obtain the velocity of fluid at the position of particle; whereas if flow domain is rather complicated or if fluid flow is unsteady, this code can be used in conjunction with fluid flow solvers. Hence, at each time step of fluid flow this code interacts with flow properties computed by the solver and particle positions will be advanced in time. This code solves the following equation to obtain the particle trajectories:

$$\frac{du_p}{dt} = F_D + g\left(1 - \frac{\rho}{\rho_p}\right) + F_p + F_m + F_{Ba} + F_b + F_s \qquad (1)$$

In which the right hand side of this equation is the summation of forces on the particle including drag F_D, gravity, pressure gradient force F_P, virtual mass F_m and Basset force F_{Ba}, Brownian force F_b, and