Numerical modeling and experimental investigation of fine particle coagulation and dispersion in dilute flows

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Abstract

In this work, a numerical model will be developed to study the behavior of fine and ultrafine particles under conditions typical for air pollution problems. The particles considered are much heavier than the surrounding fluid, and can have sizes ranging from 5 *nm* to 10 *μm*. Effects of inter-particle collisions and coagulation will be included in the model.

For the fluid model, the Finite Element Method implemented in COOLFluiD will be used [1], with LES for turbulence modeling. The particle model will use either an Eulerian approach, based on kinetic particle PDF equations, or a Lagrangian approach.

During model development, validation will happen using small-scale experiments and literature data. In a final phase, the developed model will be tested in two industrial problems.

Keywords: Multiphase flow, Disperse flow, coagulation, LES, nanoparticles

1. Introduction

One of the major factors in determining air quality is the level of pollution in the form of particles. In general, particles with an aerodynamic diameter inferior to 10 *μm* can penetrate into the human body, and constitute a potential health risk [2]. Recently, the additional risks of nanoparticles have received much attention [3], so we will study particles in a range from about 5 *nm* to 10 *μm*. The goal of the present work is to arrive at a contribution to the numerical modeling of particle-laden flow, where the behavior of ultrafine particles is taken into account, as well as inter-particle collision and coagulation. This will be done in two phases: a model development phase, followed by an application phase. The target applications include flows in confined spaces that can be modeled using CFD. Particle loading should be such that the flow can be considered dilute, i.e. particle dynamics are dominated by the flow rather than inter-particle collisions.

2. Numerical model

The developed model must be able to capture both the flow and the particle behavior. In the class of problems studied here, the instantaneous fluid velocity is a major factor in determining particle behavior, so the accuracy of the fluid model will have a great impact on the results.

2.1. Fluid model

The fluid will be modeled by discretizing the incompressible Navier-Stokes equations using the Finite Element Method, as implemented in COOLFluiD

[1]. The resulting method is of second order accuracy. In order to obtain a reliable velocity input for the particle equations, LES is used for the turbulence modeling. There is some discussion in the literature on the validity of using the LES results as instantaneous velocity input for the particle equation of motion. Some authors suggest that neglecting the small scales of turbulence may influence the results for the particle quantities [4]. They attempt to remedy this by applying an approximate deconvolution method, as described in i.e. [5]. The added complexity of implementing such a method is considered to be beyond the scope of the current work, however, so we will attempt to work with LES solutions that are sufficiently resolved.

2.2. Particle model

When modeling the behavior of the particles, a choice needs to be made between an Eulerian or a Lagrangian approach. Of the many Eulerian methods, the approach presented by Simonin [6] seems most applicable to the current problem, especially since it has been extended to include collision effects [7; 8].

The Lagrangian approach seems more intuitive, as the particle equation of motion is solved directly, while different forces acting upon the particle can be modeled easily. The challenge is that from a computational point of view, it is impossible to track all particles, so statistical methods need to be used. The inclusion of collision effects further complicates matters: since not all particles are tracked directly, collisions can not be deduced directly either. Some approaches to these problems are presented in e.g. [9; 10].

A challenging aspect of the particle model is the inclusion of nanoparticles, which - due to their small size- may need special care in the treatment of the forces acting on the particles. Furthermore, because nanoparticles commonly are produced in very high number concentrations, there is a high probability of inter-particle collisions and particle coagulation [11], which will in turn affect the particle size distribution. This effect can be accounted for by solving a population balance equation. A possible candidate seems to be the method presented by Silva et al. [12], since it is shown to be usable when coupled with CFD simulations.

3. Model validation

During the development of the model, it will be validated against simple test cases, using both literature data and small-scale experiments. As a validation of the fluid model, the classic DNS data for channel flows [13] will of course be used. Channel flow data with dispersed particles is also widely available [14; 15; 16] and can be used for validation of the model including particles.

3.1. Experimental setup

A first experiment that is being developed is designed to measure concentration variations and the effect of particle coagulation in a flow field that should be reproducible using numerical simulation. Flow will enter a cubic chamber through a narrow slot near the top, and exit near the bottom of the opposite wall (see Fig. 1). The particle injection will happen in a short burst near the center of the expected circulation zone.

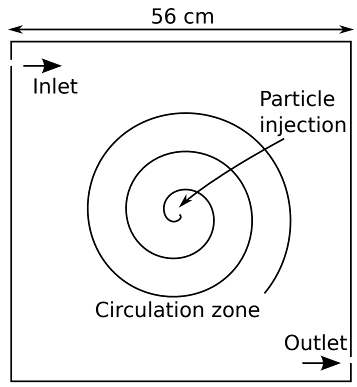

Figure 1: Schematic of the experimental test chamber.

In order to get a reproducible result, the inlet conditions will be controlled using a device similar to the inlet section of a subsonic wind tunnel, as shown in Fig. 2

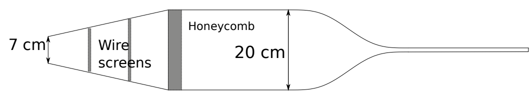

Figure 2: Conditioning of the test chamber inlet.

In a first step, the flow field will be measured using PIV in order to validate the numerical simulation of the flow itself.

It is expected that a circulation zone will appear inside the box, and in a second phase particles will be injected near the center of this zone. The evolution of the particle size distribution will then be monitored over time, and in case of coagulation a shift towards larger and larger particles should be observed. This evolution will then be compared to predictions made by the particle model.

4. Applications

The final phase of the work consists of an application to industrial problems. Two cases will be considered: the acoustic agglomeration of industrial gases, and the evolution of particles through a turbine.

4.1. Acoustic agglomeration

Acoustic agglomeration is a technique used in the treatment of industrial waste [17], where powerful acoustic waves interact with particulate matter. The particle response to these waves depends on their size, resulting in an enhanced relative motion between particles, and ultimately a higher collision rate. This allows larger particles to "scavenge" smaller particles, making subsequent filtering much easier.

4.2. Turbine

In this application, an attempt will be made to study the behavior of particles downstream the combustion chamber in a gas turbine. This could play a role in the determination of the final properties of the emissions. The effect has previously been studied by Dakhel [18], who concluded that the effect of coagulation is negligible. The study was based on time-scale arguments, however, so it would be interesting to see if it is confirmed by a more detailed simulation.

5. Conclusion

The objective of the current work is to provide a meaningful contribution to the numerical modeling of dispersed phase flow. The inclusion of nanoparticles and coagulation effects constitute new challenges, and should extend the applicability of the method. Areas of application include for example indoor air quality or risk assessment when considering the behavior of chemical or biological agents, as well as the study of pollutant aggregation in close proximity to the source.

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