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Eulerian modeling of inertial and diffusional aerosol deposition in bent pipes

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ABSTRACT

This paper presents a sectional Eulerian aerosol model for size-dependent droplet deposition at walls of the domain, driven by both diffusion and inertia. The model is based on the internally mixed assumption and employs the formulation for compressible aerosols. It is validated in a bent pipe geometry against models and experimental and numerical data from literature. Good agreement is found in both the diffusion and inertial deposition regimes. To improve the overprediction of inertial deposition by a boundary treatment that adopts zero-gradient droplet wall velocity, we use a corrected wall velocity, based on an analytical solution of the droplet motion near the wall. In the bent pipe setting the corrected wall velocity is found to reduce the overprediction of deposition and is less sensitive to grid refinement. We also show that refining the computational mesh near the pipe wall improves the predicted deposition efficiency, significantly. Finally, we present a parameter study varying the Reynolds number and the bend curvature. The deposition efficiency curve is recorded for droplet diameters ranging from the nanometer scale to beyond the micrometer scale, which is a unique contribution of this paper. The complete size range is simulated in only one simulation, due to the sectional approach. In the diffusion-dominated regime an increase in Reynolds number leads to a gradual enhancement of deposition. In the inertial regime, where droplet drift dominates deposition, a much stronger dependence on the Reynolds number is found. The dependence of the deposition on the bend curvature is less pronounced. The results shown in this paper establish the role of Eulerian simulation in predicting deposition of aerosol droplets and are useful for understanding size-dependent aerosol deposition in other more complex confined geometries.

1. Introduction

Two of the main mechanisms of aerosol deposition are inertial impaction and diffusion [1]. Both processes are strongly size dependent; small aerosol droplets deposit due to high diffusivity, large droplets due to large momentum and intermediately-sized droplets deposit more scarcely. In a setting where the Reynolds number is sufficiently high so that gravitational settling becomes negligible, this leads to the well-known deposition efficiency curve which has a characteristic 'V' shape. This was observed in many kinds of geometry that involve aerosol deposition, e.g., in respiratory flow [2–4] or flow around an object [5,6]. The exact shape of this deposition curve characterizes the filtration efficiency of an object or geometry, and is very useful for understanding aerosol deposition.

A common way to study aerosol deposition is to consider aerosol flow through a bent pipe. The bent pipe geometry offers a simple setting in which the mechanisms behind aerosol deposition can be systematically studied. In fact, the bent pipe can be used as a highly idealized mouth–throat model to emulate aerosol droplet deposition in the human airways, see [7]. By studying the bent pipe a qualitative impression can be formed of both the flow and aerosol deposition patterns.

The bent pipe problem has been studied by many authors and therefore offers a reliable and well-understood point of reference. Earlier theoretical works studied particle trajectories in the bent pipe given an approximate flow field [8–10]. More recently, many

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authors have published CFD simulations of particle deposition in bends using Lagrangian (e.g., [11–14]) or Eulerian methods (e.g., [15–20]). Others have studied aerosol deposition in pipe bends experimentally, e.g., [7,12,21,22]. The seminal work of Pui et al. [21] is key in the literature concerning bent pipe aerosol deposition efficiency and a clear source for validation. For example, Pilou et al. [15] found good agreement for Reynolds numbers $Re = 100$ and $Re = 1000$ and Vasquez et al. [20] found good agreement for $Re = 1000$ while an overprediction of the deposition efficiency for $Re = 100$ was observed.

Most bent pipe studies focused on the 'inertial deposition regime', looking at aerosol droplets or particles with a Stokes number typically larger than 0.01. For these droplets it is their inertia that leads to a collision with a geometry wall. However, as noted before, sufficiently small droplets may also deposit by diffusion. In fact, in many applications the aerosol droplet size is such that droplet diffusion and inertia are two important effects, e.g., see [2,23,24]. In this paper, we consider aerosol deposition in a bent pipe for droplet sizes ranging from the nanometer scale to beyond the micrometer scale.

Recently, we developed an Eulerian, sectional, internally-mixed aerosol model [25,26] capable of predicting the evolution of the droplet size distribution undergoing nucleation, condensation, evaporation and coagulation. We formulated a compressible model in which the mixture density is constituted by a number of chemical species, either present as vapor or in the form of liquid droplets. Building on that foundation, in this paper we extend this model to include droplet drift, diffusion and wall deposition. The main objective of this paper is to present the model and to validate our Eulerian approach against data from literature, in both the diffusion and the inertial regime. Moreover, we study how predictions depend on the chosen grid and boundary treatment for the droplet velocity.

The sectional Eulerian model retains a compressible formulation in which the mixture density is composed of both vapors and liquids, mitigating a passive scalar approach as is done in many other works, e.g., [15,23]. This couples the aerosol processes, such as droplet drift and diffusion but also nucleation and condensation (see [25,26]) to the transport equations for mass, momentum and energy. This may be relevant in cases where mixture compressibility is important, or where temperature changes are large. However, also in systems not exhibiting these features the compressible fluid framework is beneficial for obtaining general and accurate models as reliable constitutive relations can be formulated explicitly. In combination with a pressure-based approach [27] this combines consistency in the physical model with computational efficiency. We develop a scheme which, by construction, implements two constraint equations ensuring (1) that species mass fractions always add up to unity and (2) that the first moment of the size distribution is also reflected in the liquid mass concentration solution.

For large droplets we compare the predictions of our model against aforementioned experimental and numerical bent pipe studies. For small droplets we compare against the analytical straight pipe diffusional deposition model of Ingham [28]. In both regimes we find good agreement, provided sufficient spatial resolution of the solution is adopted.

In this paper we present a detailed numerical study of our model for droplet diffusion, drift and subsequent deposition. We study the two cases presented by Pui et al. [21], for Reynolds number $Re = 100$ and $Re = 1000$, on five different meshes in which we compare results obtained with or without grid refinement near the wall. We use two boundary treatments for the droplet velocity at the wall, i.e., a 'zero-gradient' boundary condition, keeping the droplet velocity from cell center to the wall constant, and a corrected boundary condition as proposed in [23], employing the analytical solution of the droplet equation of motion near the wall in a linearized flow field. The corrected boundary condition is shown to decrease the overestimation of the deposition efficiency, and generally is less resolution sensitive. We show that the wall grid-refined meshes improve the predictions of the deposition curve significantly. We also present a parameter study for the dependence of the deposition efficiency on the Reynolds number and the bend curvature. An enhancement of both diffusion and inertial deposition is shown for increasing Reynolds number whereas the dependence on the bend curvature is small.

In the model validation presented in this paper, we consider aerosol deposition in a bent pipe for droplet sizes ranging from the nanometer scale to beyond the micrometer scale. This enormous size-range is the unique feature of our model: within one formulation the corresponding deposition efficiency curve spanning the complete size domain is predicted. Moreover, the sectional formulation spanning many decades in droplet sizes allows for a straight-forward extension to include aerosol processes such as nucleation, condensation, evaporation and coagulation or break-up, as was done before (see [25,26,29]). The combination of these capabilities forms a unique and quite complete aerosol model.

The layout of this paper is as follows. In Section 2 we will, starting from the equation of motion for the droplet size distribution, construct a set of equations describing a compressible 'internally mixed' [30] multi-species aerosol in an Eulerian way, including a new drift flux term. Next, in Section 3, we will adopt a finite volume method and discretize the transport equations accordingly. Again, special attention is paid to retaining the consistency among the equations, also in their discrete forms. Two boundary treatments for the droplet velocity at the wall are discussed. In Section 4.1 we present the bend pipe geometry and in Section 4.2 the fluid velocity solution is validated against data from [15]. Next, in Section 4.3 the grid sensitivity of the solution is shown using both the corrected and uncorrected wall treatments. We validate the inertial and diffusion regime of the deposition curve in Sections 4.4 and 4.5, respectively. Finally, in Section 4.6 we present a parameter study.

2. An internally mixed Eulerian aerosol model with droplet drift and diffusion

In this section, we will discuss the 'internally mixed' multi-species Eulerian model that we adopt for the description of the evolution of an aerosol mixture. Subsequently, we extend it to incorporate drift flux and diffusion terms, based on a size-dependent drift velocity and Brownian diffusivity. The considerations taken in arriving at the drift flux model will be discussed here.

2.1. Mass and droplet concentration transport equations

Let us consider a volume in which we have $\mathcal{N}$ species, present as vapor and liquid, where the liquid phase is contained in dispersed droplets. With respect to the total mass in this volume, the jth species has a mass fraction Y_j present as vapor and Z_j present as liquid. By definition, we have

$$\sum_j (Y_j + Z_j) = 1. \tag{1}$$

Vapors are assumed to be ideal gases and liquids are assumed to be incompressible. Using Amagat's law [31], the mixture density ρ can be related to the species-specific vapor compressibility ratios, species-specific liquid densities, pressure and temperature, giving an equation of state in the form of

$$\rho = \psi(p, T)p, \tag{2}$$