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SIMULATION OF IMPACTION FILTRATION OF AEROSOL DROPLETS IN POROUS MEDIA

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Abstract. *We report on the development of a method to simulate from first principles the particle filtration efficiency of filters that are composed of structured porous media. We assume that the ratio of particle density to the fluid density is high. We concentrate on the motion of the particles in a laminar flow and quantify the role of inertial effects on the filtration of an ensemble of particles. We adopt the Euler-Lagrange approach, distinguishing a flow field in which the motion of a large number of discrete particles is simulated. We associate filtration with the deterministic collision of inertial particles with solid elements of the structured porous medium. To underpin the physical 'consistency' of deterministic particle filtration, we investigate to what extent the particle tracking algorithm ensures that mass-less test-particles will not be captured by the structured porous filter at all. This element of the algorithm is essential in order to distinguish physical filtration by inertial effects from unwanted numerical filtration, due to the finite spatial resolution of the gas flow. We consider filtration of particles whose motion is governed by Stokes drag and determine the filtration efficiency in a range of Stokes relaxation times. An exponential decay of the number of particles with time is observed.*

1 INTRODUCTION

Driven by various applications, in particular the protection from hazardous aerosol materials, a number of approaches have been developed to determine the filtration efficiency of particulate filters. The mechanisms that determine aerosol filtration consist of several elements like interception, diffusion, inertial impaction and gravitational settling[5]. In the present work, we concentrate on filtration by impaction which implies the deposition of aerosol droplets on the substrate that makes up the filter. This deposition is associated with rapid spatial changes of the direction of the gas flow, e.g., arising near sharp corners in the flow geometry. Heavy particles, which cannot follow the motion of the carrier gas, may collide with the obstructing surfaces of the filter, leading to their capturing. In general, the rate of particle capturing by the filter depends on a number of parameters, such as the Reynolds number that characterizes the flow conditions, the particle size which is a direct measure for its inertia, and the porosity of the media as a measure for the structure of the porous filter. Here, we will consider the dependency of the overall filtration efficiency on the particle size in case the particle's motion is governed by Stokes drag. Only the deterministic motion in a steady carrier gas flow will be incorporated and random motion due to Brownian effects will be neglected. This corresponds, e.g., to rather heavy aerosol droplets consisting of water, with diameters in the micrometer range, in a flow of air. From our simulations we observe an increase in the droplet uptake by the filter with increasing droplet size.

The organization of the paper is as follows. In Section 2 we describe the mathematical modeling of the two-phase flow inside a structured porous medium. We illustrate the motion and filtration of droplets that were initially uniformly positioned on a straight line. Section 3 is devoted to a discussion of the simulation results, in which we use random initial conditions and simulate the exponential decay in time of the number of droplets that are still in free flight through the porous medium. Concluding remarks are collected in Section 4 discussing the influence of the Stokes response time on the droplet capturing.

2 MATHEMATICAL MODELING OF AEROSOL FILTRATION

In this section we explain our mathematical model for the problem of deterministic aerosol filtration by impaction, stemming from inertial effects. The mathematical model that we consider is based on the Euler-Lagrange approach in which the two-phase flow of a carrying gas-flow with a large number of embedded discrete aerosol droplets is studied. We study this system as a one-way coupled two-phase flow[6]. More precisely, we assume that the fluid moves the particles and the particles do not influence the flow of the fluid. We will start with the governing equations for the gas phase. Afterwards, the physical model for the particle phase will be described. We will present the numerical approach for solving the governing system of coupled partial and ordinary differential equations.

2.1 Eulerian approach for the gas phase

In order to perform a numerical study of filtration from first principles, the motion of all particles in the gas flow through the porous medium has to be modeled and simulated. The gas flow is calculated by solving the incompressible Navier-Stokes equations[1]. The immersed boundary (IB) method[3] based on a volume penalization forcing method is applied to capture the detailed gas flow through the porous medium. The porous medium is formed by a staggered arrangement of square rods in 3D (Figure 1). This geometry facilitates the development and validation of our approach. It is a stepping stone problem toward the computational modeling of aerosol filtration in filters of a realistic complexity. We assume periodic boundary conditions and maintain a flow in this domain by imposing a mean pressure gradient over a periodic unit.

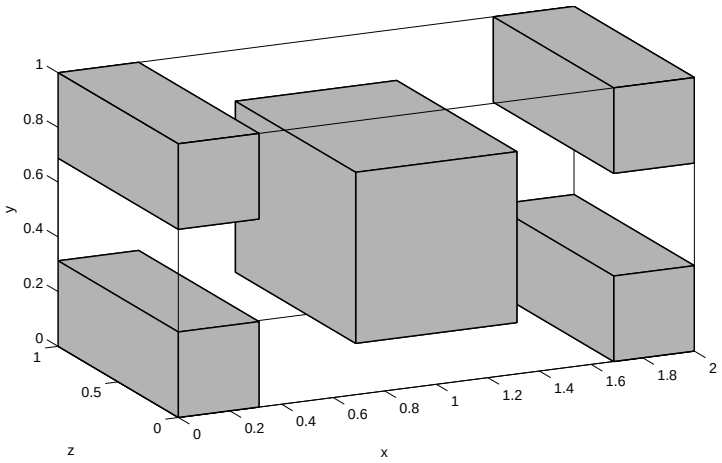

Figure 1: A structured porous medium is composed of periodic arrangements of staggered square rods. We concentrate on a geometrical arrangement with a porosity of 3/4, denoting the open part in a representative elementary volume.

The fluid phase is characterized by conservation equations for mass (1a) and momentum (1b), i.e. the Navier-Stokes equations[1] for incompressible fluids:

$$\nabla \cdot \mathbf{u} = 0 \tag{1a}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho_f} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}. \tag{1b}$$

The notation $\nabla \equiv (\partial/\partial x, \partial/\partial y, \partial/\partial z)^T$ represents the vector differential operator and $\nabla^2 \equiv \nabla \cdot \nabla$ the Laplace operator. Here $\mathbf{u} = (u, v, w)^T$ is the fluid velocity, ρ_f the fluid mass density, p is the pressure and ν is the kinematic viscosity. The term $\mathbf{f}$ on the right hand side of the equation of conservation of momentum is a body force per unit mass. For all fluid-solid interfaces the no-slip boundary condition $\mathbf{u} = 0$ has to be satisfied. In case of the IB method this is done with the help of a so-called forcing function. For complex

geometries this approach helps to avoid complications with meshing and corresponding inaccuracies in the numerical solution. By introducing a phase-indicator function Γ, which has value 1 within the solid and 0 otherwise, we employ the following forcing:

$$\mathbf{f} \equiv -\frac{1}{\epsilon}\Gamma(\mathbf{u} - \mathbf{u}_s), \qquad \epsilon \ll 1 \tag{2}$$

where ϵ is called the sensitivity parameter and $\mathbf{u}_s$ is a prescribed solid body velocity. Such form of forcing is called volume-penalization form, which provides a continuous description of the velocity vector $\mathbf{u}$ in the whole computational domain.

In order to solve the resulting system of equations we use a finite volume discretization method that preserves the positive-definite dissipative nature of the viscous fluxes and the skew-symmetry of the nonlinear convective fluxes[2]. The fluxes are computed on a staggered grid using a second order accurate method. For time integration of the fluxes we used an explicit Adams-Bashforth method. In order to avoid instability, related to small values of ϵ, the forcing term $\mathbf{f}$ is integrated implicitly in time.

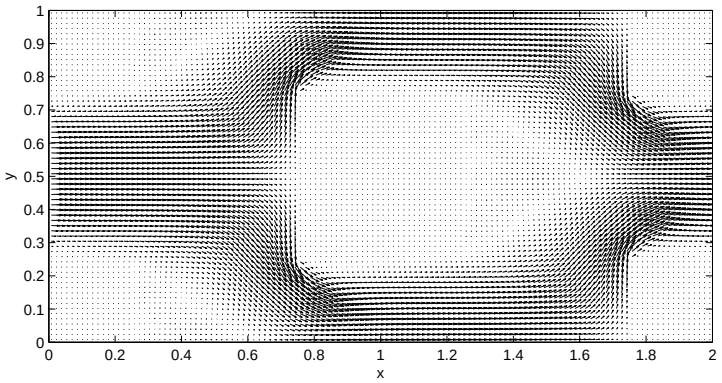

Figure 2: Flow through an arrangement of staggered square rods. The flow is characterized by a Reynolds number $Re = 100$, based on the volume-averaged velocity, the length of the side of a square and the kinematic viscosity.

An example of simulated flow through our model porous medium is shown in Fig. 2, corresponding to a Reynolds number of $Re = 100$, which is defined based on the volume-averaged velocity, the length of the side of a square and the kinematic viscosity. We clearly observe the development of vortical structures where the main flow separates from the square rods at sharp corners. The use of a skew-symmetric discretization allows to capture reliably the flow structures at relatively coarse spatial resolution[2]; here we used a resolution of 128×64 in the cross-section shown, and 4 in the direction normal to the figure. We will investigate filtration efficiency in this reference geometry to quantify the consequences of the pronounced flow separation on the droplet capturing. We present the particle-tracking in the next section.

2.2 Lagrangian approach for the particle phase

The particle phase is simulated numerically by tracking all individual trajectories of a large number of particles embedded in the flow. By computing the trajectories of particles and monitoring possible collisions of these particles with solid parts of the filter material, we investigate the filtration properties. Once the trajectories intersect with the surface of solid material that makes up the filter, the particles are assumed to be captured - we do not include a probabilistic aspect that would also allow for rebounding droplets. The number of captured particles as a function of time quantifies the filtration efficiency and is the key component that we want to extract from the simulations.

The motion of particles is governed by a variety of forces[4]. Here, we focus on the dominant drag-force that is characterized by a single Stokes relaxation time. The dynamics of the ensemble of particles quantifies the filtration efficiency. In detail, we assume that the motion of the particle is governed by Stokes' law:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}\ (\mathrm{t}) \tag{3a}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{1}{\tau}(\mathbf{u}(\mathbf{x},t) - \mathbf{v}(t)) \tag{3b}$$

where $\mathbf{x}$ and $\mathbf{v}$ are the particle's position and its velocity, respectively. The acceleration of a particle originates from the external gas flow, at the location of the particle. This is represented by $\mathbf{u}(\mathbf{x},t)$. In order to evaluate this contribution, the discrete representation of the velocity field $\mathbf{u}$ is used to estimate its value at $(\mathbf{x},t)$ via interpolation. The parameter τ is referred to as the velocity response time or relaxation time. The particle response time depends on its diameter D, the density of the particle ρ and the molecular viscosity of the carrier gas μ:

$$\tau = \frac{\rho D^2}{18\mu} = \frac{D^2}{18\nu}\ \frac{\rho}{\rho_f} \tag{4}$$

where in the latter expression we emphasize the dependence on the ratio of the particle and fluid mass density, in terms of the kinematic viscosity ν. We consider situations in which $\rho \gg \rho_f$.

The trajectories of the particles are calculated by integrating (3a) and (3b) using a combination of Euler's explicit (for $\mathbf{x}$) and implicit (for $\mathbf{v}$) first order methods:

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \triangle t \mathbf{v}^n \tag{5a}$$

$$\mathbf{v}^{n+1} = \frac{\tau}{\tau + \triangle t}(\mathbf{v}^n + \frac{\triangle t}{\tau}\mathbf{u}^n) \tag{5b}$$

Here $\mathbf{u}^n$ is the velocity of the gas at the particle position. We use trilinear interpolation in order to get the flow field at the particle position. Interpolation is based on staggered grid cells where the velocities of the gas in $\{x, y, z\}$ directions are defined.

We look at the trajectories of the particles that are injected in the flow and study the decay of the number of particles as a function of time. For the limiting case of mass-less particles we can be guided by the basic property that these test-particles follow the flow exactly. This implies that theoretically particles at $\tau = 0$ should not be filtrated at all - any residual filtration would originate from inaccuracies in the numerical method. On the other hand, if the particles are big enough, then as the particles move they deviate from the streamlines and their trajectories may intersect with the filter surface. A large number of particles can be released uniformly in the flow, with locations chosen either at random or uniformly distributed, and initial velocities equal to the local interpolated velocity of the gas flow. In Figure 3(a) we illustrate the fact that mass-less particles do follow the streamlines and hence do not get captured by the filter, while the effect of inertia associated with heavy particles is shown in Figure 3(b), clearly indicating that these particles may collide with the filter and hence get captured. In the next section we quantify this general impression in terms of the actual filtration efficiency that is observed in simulations.

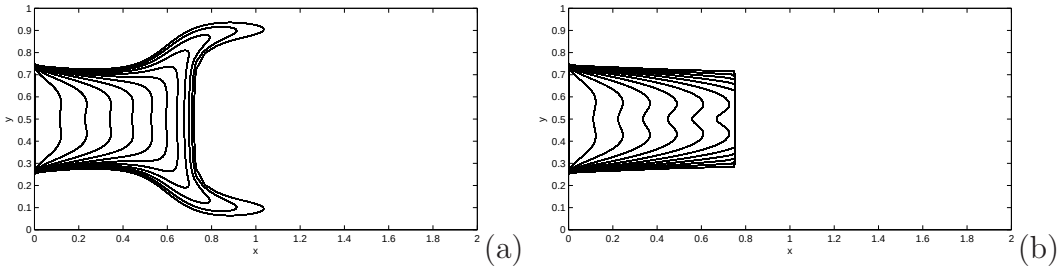

Figure 3: Particle trajectories emanating from a line of initial particle positions. Each curve corresponds to a particular moment in time, connecting particle positions that originated from a straight line of initial conditions at $z = 0$. In (a) mass-less particles are considered while in (b) we simulated heavy particles with $\tau = 1$.

3 INERTIAL PARTICLE FILTRATION IN STRUCTURED GEOMETRY

In this section we will present the results of filtration efficiency for a range of particle sizes. We consider the reference geometry and flow as presented earlier in Fig. 2, i.e., using Reynolds number 100 and porosity 0.75. The embedded particles are assumed to have a fixed diameter which we vary to investigate the effect of particle size on evolution of the number of unfiltered particles E. This is defined as the ratio of the number of particles that have not been captured to the initial number of particles.

In Figure 4 we present the decay of the fraction of particles still in free flight, for five values of the Stokes relaxation time, i.e., $\tau = 0, \tau = 0.05, \tau = 0.1, \tau = 0.5$ and $\tau = 1$. We plot E on a logarithmic scale with respect to time. Initial positions of the particles were generated at random. In order to better appreciate the decay of E it is good to know that a particle travels through the computational box roughly in $t = 2.5$ dimensionless

time units. The behavior of $\log(E)$ as a function of time displays some fluctuations about an otherwise smooth decay - these fluctuations are associated with the randomness of the initial condition. In order to obtain reliable statistical data on the filtration of very large number of particles, the numerical experiments need to be repeated starting from a sufficiently large number of independently generated initial conditions. This is currently being analyzed and will be presented elsewhere.

As can be seen from the figure, for $\tau = 0$ only a small fraction of particles gets captured. This implies that the tracking algorithm is capable of delivering reliable filtration results in case the Stokes response time is sufficiently large. The asymptotic range of very small Stokes relaxation times needs to be reconsidered and a truly 'non-leaking' algorithm needs to be devised. The decay of particles due to the numerical method is, however, acceptably low for us to draw conclusions for sufficiently heavy particles, beyond $\tau \approx 1/20$. The larger particles, which correspond to Stokes relaxation time $\tau = 0.5$ and $\tau = 1$ are captured rapidly and already after traveling once through the computational domain almost 90% of the particles is filtrated. Approximately after traveling 4 times through the domain all the particles with $\tau = 1$ are seen to be captured. We also notice that particles with $\tau = 0.5$ and $\tau = 1$ are captured more or less with the same rate; apparently, these relaxation times denote an asymptotic range with quite similar filtration characteristics. The decay rate of number of particles with $\tau = 0.1$ and $\tau = 0.05$ is considerably smaller than for $\tau = 0.5$ and $\tau = 1$. In all cases a strong indication of exponential decay of E with time is observed.

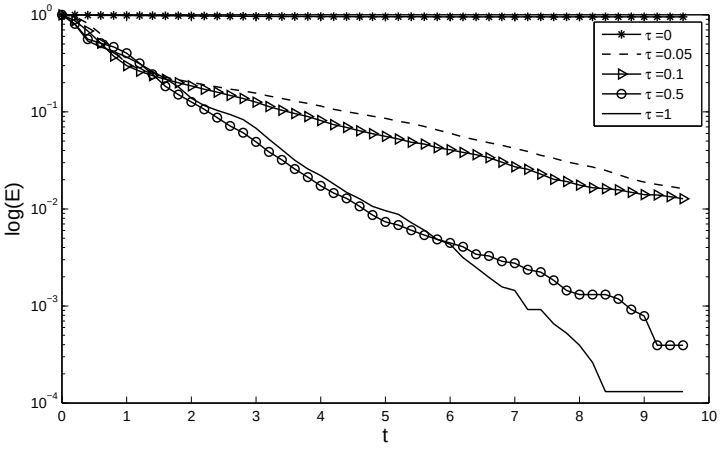

Figure 4: Decay of the fraction of unfiltered aerosol droplets with time at different Stokes numbers: $\tau = 0$ (*), $\tau = 0.05$ (- -), $\tau = 0.1$ ($\triangleright$), $\tau = 0.5$ ($\circ$) and $\tau = 1$ (-). The general decay follows an exponential trend.

We note that the rate of decay basically does not strongly depend on the initial positions of the particles. In order to illustrate this we have simulated the filtration for four different cases with randomly generated initial positions. The results are shown in Figure 5.

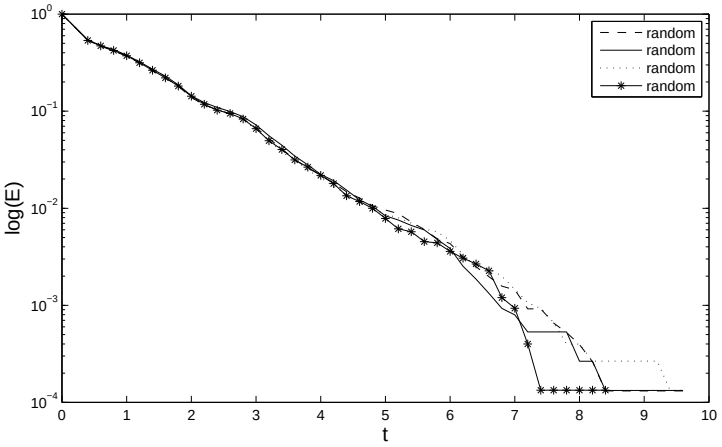

Figure 5: Decay of the fraction of unfiltered aerosol droplets with time at Stokes number $\tau = 1$ for four different random initial positions

4 CONCLUSIONS

In this study, emphasis was given to the development and testing of a numerical method for the detailed motion of particles in structured porous geometries. Through simulation we were able to directly compute the filtration of particles by a complex solid surface. This 'first principles' approach allows to relate directly microscopic parameters such as the Stokes relaxation time of individual particles to macroscopic properties such as the overall particle removal efficiency. The latter is of direct importance to engineering applications and allows a direct comparison with experimental data on realistic porous media filters. We have shown that our numerical approach allows us to closely look at the behavior of particles in flow fields in which dominant separated flow structures express their influence through extended vortices. Lagrangian tracking of particles, in combination with IB resolution of the flow field, provides detailed information about when and where the particles are being captured in the filter. We observe for large particles exponential decay of the number of particles with an increased particle capturing in case the Stokes number increases. We also detected a small residual of unwanted numerical filtration for mass-less particles. Further investigation will be done to avoid this numerical filtration for small particles, in order to estimate the natural physical filtration also for very small particles in the lower Stokes relaxation time regime. The latter category is particularly important for a number of applications.

5 ACKNOWLEDGMENTS

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