Simulation of impaction filtration by a porous filter

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Abstract. We present a new numerical approach for estimating filtration through porous media from first principles. We numerically simulate particle motion as arises in a carrier gas flow. The filtration we look at occurs due to impaction of particles with obstructing surfaces that are contained in the solid filter. We consider the case when the motion of particles is governed by linear Stokes-drag, which is characterized by the particle relaxation time. The gas-particle interaction is modeled by using the Eulerian-Lagrangian approach and one-way coupling of the phases. In this case the carrier flow drags along the particles, without being affected by the motion of the particles. The gas flow is governed by Navier-Stokes equations for incompressible fluids and is calculated numerically using finite-volume discretization that is based on an energy conserving skew-symmetric discretization. We apply an immersed boundary (IB) method to capture the detailed flow in the porous filter, in which we explicitly incorporate flow around all small-scale features that make up the inner structure of the porous filter. To validate and develop our method we consider a porous medium composed of a staggered arrangement of square rods in 3D, which was already extensively considered in the literature for flow computation. This is a stepping-stone case on the way of simulating filtration of aerosol particles in complex, realistic filters. Based on results of our simulations we investigate the decay of the number of particles as a function of time. We focus on the dependence of the decay-rate on the Reynolds number of the gas and the inertial effects of the particles. For a range of particle relaxation times we observe a strong influence of the Reynolds number on filtration rate. A non-monotonic dependence of the filtration efficiency on Stokes number at different flow conditions is observed, hinting at qualitative differences in the motion of the aerosol ensemble through the structured filter.

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INTRODUCTION

Porous filters are frequently used in order to separate particulate matter from gases. The essential quantity for quantifying such porous filters is their efficiency of removal for given particle size. Several theoretical and experimental investigations of filtration mechanisms have been conducted [1]. The aim of these studies was to find a correlation for removal efficiency as a function of several material and process parameters that play a role in the filtration. In particular, the dependency of the filtration efficiency on the Reynolds number of the flow, the particle relaxation time and the porosity of the filter are key components in the regime of so-called impaction filtration, in which particles are absorbed by the filter substrate after direct collision. Such collisions arise as a result of the particle's inertia. The consequences of inertia for filtration depend on the flow conditions, e.g., expressed in terms of the shape of streamlines and the occurrence of extended separated vortical structures, and the complexity of internal structure of the porous material, e.g., quantified by its overall porosity.

The filtration efficiency of a given porous medium can be computed numerically by simulating the detailed motion of a large ensemble of particles embedded in a gas flow. In this paper we present a numerical approach for tackling this problem and discuss some simulation results. The method is based on an Euler-Lagrange description of gas-solid two-phase flow. This implies that the embedding gas-flow is obtained from a continuum description based on the incompressible Navier-Stokes equations, while the particulate phase is represented by a large number of discrete point-particles with their own dynamics [2]. The gas flow through a complex flow domain is obtained on the basis of an immersed boundary (IB) method that adopts volume penalization [3].

We investigate filtration that occurs due to inertial effects, which implies that we consider relatively heavy particles in a gas flow, e.g., an aerosol consisting of liquid droplets in air. We treat the particulate transport using the one-way coupling formulation [4], i.e., we assume that the momentum transfer between the discrete and the continuum phase, as well as the transfer due to collisions among the particles is negligible.

In a 'first principles approach' for computing filtration efficiency it is required to adopt an equation of motion for individual particles. We assume that the motion is governed by linear Stokes drag only. The numerical treatment allows to track the precise motion of particles in the porous filter. By following the trajectories of the particles we can establish collision events with the filter and, hence, whether or not any of the particles is captured in the course of its traversal in the filter.

We report on the application of direct numerical simulation to compute the porous filtration efficiency in case of flow through a structured arrangement of square rods in a staggered pattern. The IB method provides the flow that develops in full detail at different Reynolds numbers. This allows to compare the filtration efficiency for so-called ‘creeping flow’ at $Re = 1$ as well as laminar flow at much higher Re that possesses significant regions of separated flow and vortical structures. These flow structures and flow conditions will be shown to have a large influence on the filtration characteristics. Moreover, the simulations point toward qualitatively different large-scale motion of the aerosol ensemble through the porous ‘maze’, leading to a non-monotonous dependence of filtration efficiency on the Stokes relaxation time of the particles.

The structure of the paper is as follows. First, we present 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. Then we discuss the simulation results, in which we use random initial conditions and simulate the approximately exponential decay in time of the number of droplets that are still not captured by the porous filter. We compare findings at creeping flow conditions at $Re = 1$ and more complex flow at $Re = 100$. Concluding remarks are collected discussing the influence of the Reynolds number on the droplet filtration.

MATHEMATICAL MODELING OF PARTICLE MOTION IN GAS FLOW

In this section we will briefly describe the mathematical and computational model for gas-particle two-phase flow [4]. We distinguish a steady flow field in which the motion of a large number of particles is simulated. The mathematical model that we consider is a one-way coupled system, meaning that the gas transports the particles, while the particles have no feedback influence on the gas flow. The governing equations for both phases will be described.

Governing equations for the gas phase

The first step in simulating the filtration of particles in a porous filter is to describe the motion of the particles in the gas flow. For calculating the gas flow we use the Navier-Stokes equations for incompressible fluids [5]:

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0, \\ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\frac{1}{\rho_f} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f} \end{aligned} \tag{1}$$

This set of equations describes conservation of mass and conservation of momentum. In this formulation $\nabla \equiv (\partial/\partial x, \partial/\partial y, \partial/\partial z)^T$ 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 $\mathbf{f}$ is a body force per unit mass. The main task is to compute the flow inside the porous filter that takes the full complexity of the filter into account and imposes no-slip boundary conditions at the interface between the solid and the fluid. The latter is a challenging task in case conventional structured body-fitted grids are used to discretize the equations. Here, we follow an alternative, approximate approach that exploits the forcing term $\mathbf{f}$.

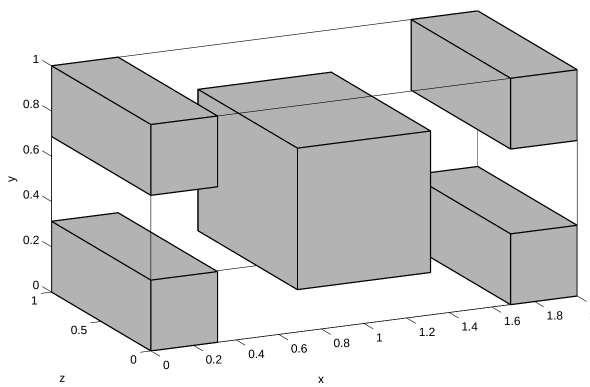

FIGURE 1. A structured porous medium is composed of the periodic arrangement of staggered square rods of which a basic unit is shown. We concentrate on a geometrical arrangement with a porosity of 3/4, denoting the open part in a representative elementary volume.

We consider a porous medium composed of the staggered arrangement of square rods in 3D as shown in Fig. 1. Periodic boundary conditions are assumed in all directions. In order to incorporate the geometrical structure of this computational domain we apply the immersed boundary (IB) method [3] based on a volume penalization forcing. This approach provides the detailed gas flow inside the porous medium. One of the advantages of using the IB method is the accurate and computationally effective representation of complex domains.

The complications related to the boundary conditions on all fluid-solid interfaces ($\mathbf{u} = 0$ no-slip condition) are handled to a close approximation by the IB method by choosing a proper forcing **f**. This issue has attracted considerable interest in literature [3] and various approaches have been put forward. In this paper we use a forcing function based on a volume-penalization strategy:

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

The phase-indicator function Γ in the definition of the forcing function has value 1 within the solid and 0 otherwise. The control parameter ε is called the sensitivity parameter and $\mathbf{u}_s$ is a prescribed solid body velocity. The use of this forcing generates a rapid adaptation of the flow velocity toward $\mathbf{u}_s$, close to the solid-fluid interface. A highly localized numerical boundary layer is formed in this approximate no-slip condition - we adopt $\varepsilon = 10^{-10}$, which implies that the numerical boundary layer is well contained within a single grid cell. To facilitate very small values of ε we adopt an implicit time-stepping for the forcing term, which avoids numerical instability.

The simulation of the flow field is based on a finite volume discretization method. This is used to discretize the governing equations of the gas phase. We adopt a discretization which preserves the positive-definite dissipative nature of the viscous fluxes and the skew-symmetry of the nonlinear convective fluxes [6]. A second order accurate method is used for calculating the fluxes and for their time integration we use explicit Adams-Bashforth method. Due to the skew-symmetric discretization it is possible to compute the flow structures in the considered case at relatively coarse spatial resolution [6]. By calculating the flow at different Reynolds numbers and by simulating the particle motion in the corresponding flow fields, we may quantify the filtration efficiency of the porous filter at a range of conditions. The aim is to correlate the decay of the number of particles with the Reynolds number and the inertia of the particles. In the following subsection we will describe in detail the particle tracking.

Governing equations for the particle phase

The motion of particles in a gas flow in general is affected by a number of forces [2]. We concentrate here on the linear drag-force and monitor the motion of particles subjected to this force. At the beginning of a simulation, a large number of particles is injected in the gas flow. The initial velocity of a particle is taken equal to the velocity of the gas flow at the location of the particle. We approximate this using trilinear interpolation. Starting from this initial condition we compute the trajectories of the particles. This allows to identify where and when particles collide with the filter. Every collision is assumed to lead to filtration: once the trajectory of an individual particle crosses the surface of the solid filter that particle is considered as captured. The rebounding of particles is not considered in this work. We extract the number of captured particles as a function of time to quantify the efficiency of the filter.

In the equation of motion for a particle, the key parameter is the velocity response time or relaxation time τ. Considering the Stokes drag, the particle response time depends on its diameter D, the density of the particle ρ and the molecular viscosity of the carrier gas μ:

$$\tau = \frac{\rho D^2}{18\mu} = \frac{D^2}{18\nu}\,\frac{\rho}{\rho_f} \tag{3}$$

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 total description of the motion of an individual particle is given by:

$$\begin{aligned} \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} &= \mathbf{v}\,(\mathrm{t}) \\ \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} &= \frac{1}{\tau}(\mathbf{u}(\mathbf{x},t)-\mathbf{v}(t)) \end{aligned} \tag{4}$$

where $\mathbf{x}$ and $\mathbf{v}$ are the particle's position and its velocity respectively.

The motion of a particle originates from the external gas flow, which drags the particles along. This gas velocity at the particle position is represented by $\mathbf{u}(\mathbf{x},t)$. The discrete representation of the velocity field $\mathbf{u}$ is used to estimate its value at $(\mathbf{x},t)$ via interpolation. The trajectories are computed from (4) by using a combination of Euler's implicit (for $\mathbf{v}$) and explicit (for $\mathbf{x}$) first order time integration methods:

$$\begin{aligned} \mathbf{x}^{n+1} &= \mathbf{x}^n + \triangle t\mathbf{v}^n \\ \mathbf{v}^{n+1} &= \frac{\tau}{\tau+\triangle t}(\mathbf{v}^n + \frac{\triangle t}{\tau}\mathbf{u}^n) \end{aligned} \tag{5}$$

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.

Apart from the accuracy of the integration scheme, it is important that the algorithm is closely representing basic physical properties of the flow problem. An example of this is the property that mass-less particles will not be captured at all in a realistic flow. It is important to maintain this aspect to good approximation in a computational model. Theoretically, no filtration should be detected for mass-less particles. These are known to follow the flow exactly and never get captured. This means that for $\tau = 0$ there should be no decay of the number of particles. Any observed filtration for mass-less particles would be of 'numerical' nature. In contrast, for particles that are heavy enough, we expect them to deviate from the streamlines and to be captured. The following section will be devoted to a discussion of the simulation results.

INERTIAL PARTICLE FILTRATION IN STRUCTURED GEOMETRY

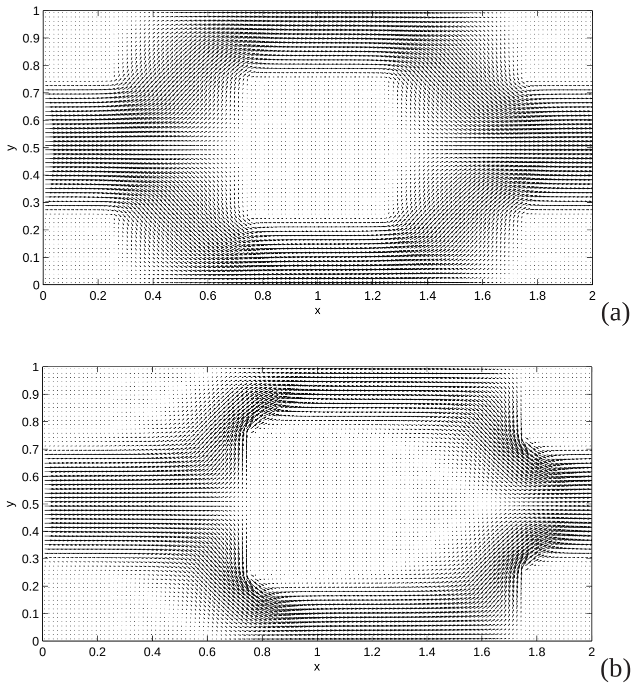

FIGURE 2. Flow through an arrangement of staggered square rods. The flow is characterized by a Reynolds numbers $Re = 1$ (a) and $Re = 100$ (b), based on the mass flow-rate, the length of the side of a square and the viscosity of air.

In this section we will present the results of simulations of particle motion inside the structured porous medium as shown in Fig. 1. In order to investigate the dependence of the filtration rate on the Reynolds number, we simulated the flow of particles for two Reynolds numbers, $Re = 1$ and $Re = 100$. The simulated flow through the considered porous medium is given in Fig. 2. The resolution we used is 128×64 in the cross-section shown, and 4 in the direction normal to the figure. With this choice of resolution we can capture the development of vortical structures that occur in the relatively complex flow at $Re = 100$. In the latter case, we detect separation of the main flow at the sharp corners of the square rods and observe that a considerable part of the domain is occupied by separated vortical structures. These vortices are missing at creeping flow conditions $Re = 1$. We are interested in the consequences of such flow structures on the filtration - as we do not include random diffusive motion, the presence of a steady vortex near a solid implies a partial 'shielding' of the filter to capture particles, and hence affect the efficiency of the filter.

The particle motion depends on the Stokes relaxation time, which implies a natural variation in the sensitivity of the particle motion to details in the flow structure. If particles are light enough then they nearly follow the streamlines while if the particles are heavy enough, they deviate strongly from the local gas flow and may be captured due to the inertial effect. We illustrate this in Fig. 3, where we consider particle trajectories emanating from a line of initial particle positions, chosen on the left of the domain. Each curve corresponds to the location of all these particles at a particular moment in time. We observe that particles with relaxation time $\tau = 0.05$ behave effectively as mass-less particles in a smooth $Re = 1$ flow: they are seen to follow the streamlines precisely, without being captured; all particles are shown with an asterisk, indicating their position as well as the property that they did not (yet) collide with the filter. On the other hand, in case of $Re = 100$ the same particles are seen to 'become heavy', i.e., they express their inertia because of the increased accelerations in the gas flow. Correspondingly, some of the particles are trapped by the filter: this is indicated by marking the particles that get captured with circles.

The qualitative differences in particle motion that were observed in Fig. 3 have strong effects on the filtration efficiency. To quantify this, we simulated the motion of particles at three different Stokes relaxation times: $\tau = 0.05, 0.1$ and 1. The initial positions of the particles were generated at random in the open fluid part of the domain: we included 10^4 particles initially. The decay of E, defined as the ratio of number of particles that at certain time t are not yet captured and the initial number of particles, is presented in Fig. 4. For all cases we observe an approximately exponential decay of the number of unfiltered particles, after a short initial transient. There is considerable fluctuation in the individual curves - a more precise impression of the filtration efficiency can be obtained by repeating such simulations, starting from a number of statistically independent random initial conditions. This is currently not available - hence we restrict to observations based on single realizations of the initial condition.

The filtration efficiency obtained at $\tau = 0.05$ is seen to confirm the qualitative impression as seen in case of the structured initial positions on a line. For creeping flow the filtration is virtually absent while at a stronger curved flow at $Re = 100$ the inertia of particles at $\tau = 0.05$ is expressed strongly enough for them to get filtrated. We notice that filtration by impaction is not merely a matter of Stokes relaxation time, but also of flow conditions.

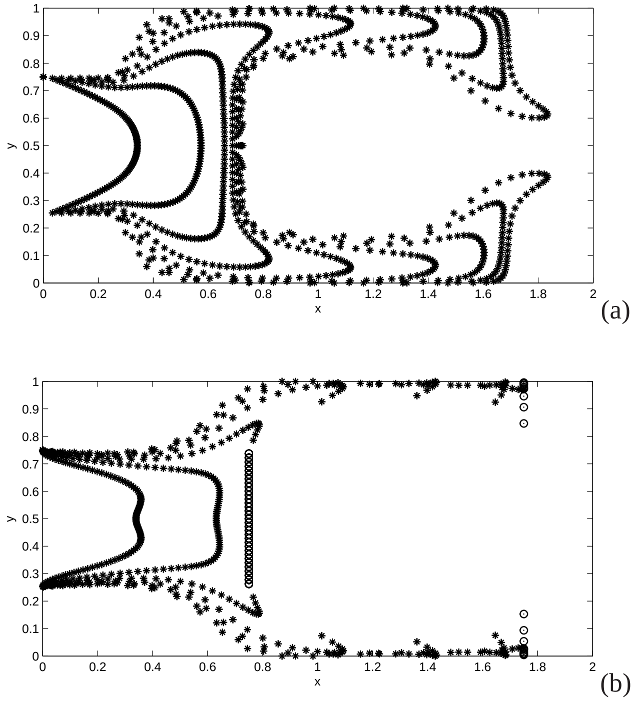

FIGURE 3. Particle trajectories emanating from a line of initial particle positions. Each curve corresponds to a particular moment in time. The particle positions originate from a straight line of initial conditions on the left side of the figure. The flow is characterized by $Re = 1$ (a) and $Re = 100$ (b). We simulated the motion of particles with $\tau = 0.05$. Unfiltered particles are denoted by $(*)$ and particles that hit an object by $(\circ)$.

This complicates a clear distinction of impaction filtration and diffusive filtration. In case of heavier particles at $\tau = 1$ the ensemble of particles basically has an analogous filtration efficiency in case of $Re = 1$ and $Re = 100$. In this case the evolution of the number of unfiltered particles is quite similar in dimensionless time. Remarkably, for the intermediate value of Stokes relaxation time $\tau = 0.1$ we observe a qualitatively different behavior. We notice that at this relaxation time particles get filtrated less effectively at the higher Reynolds number. At first instance this appears counter-intuitive as a flow at higher *Re* would favor inertial effects to express themselves in an enhanced filtration efficiency. However, the reverse is observed and filtration at the higher *Re* is seen to be less effective at this relaxation time than in the case of low *Re*. This hints at a qualitative difference in the motion of the ensemble of particles. An explanation for this could be the presence of recirculation zones for complex flow at $Re = 100$. A particle that starts its motion in one of these recirculation zones stays there for some time till it eventually 'escapes' to a faster flowing part of the flow, because of it being swirled out of a recirculation zone by its inertia. How long the particle stays in such a zone

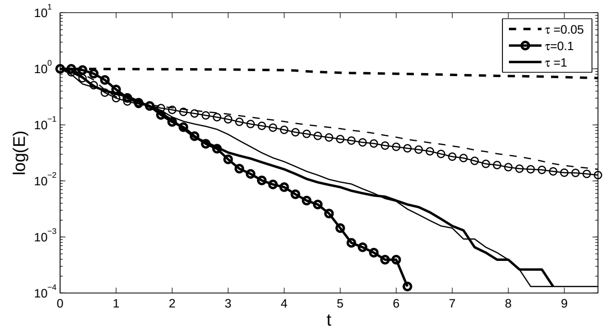

FIGURE 4. Decay of the fraction of unfiltered aerosol droplets with time at different Stokes numbers for $Re = 1$ (thick line) and $Re = 100$ (thin line): $\tau = 0.05$, $\tau = 0.1$ and $\tau = 1$ shown with dashed, solid with $\circ$ and solid lines, respectively.

depends, among others, on the size of the particle: if the particle is heavy then it will spend less time in a recirculation zone, while small particles can be held up for a significant time. This suggests that for a range of particle sizes, that are likely to remain 'trapped' in a recirculation zone, filtration will be faster for less complex flows, i.e., flow without recirculation zones. To check this we simulated the motion of particles with $\tau = 0.1$ that are positioned in a structured way as in the case of Figure 3. This time we made sure that they are not near the corners of the obstacles, where recirculation can occur. For the geometry considered this can give us an insight into the dynamics. The corresponding results are presented in Figure 5. We observe that for the flow at $Re = 100$ all the particles get captured after traveling only once through the computational box. On the other hand, in case $Re = 1$, only a fraction of the particles gets filtrated after one flow-through time. If a particle does not start its motion in a recirculation zone, then it is unlikely to enter it quickly; in that case a higher Reynolds number implies a more rapid particle deposition on the surface of the filter. Conversely, if the particle emerges in a recirculation zone, e.g., due to processes such as nucleation or condensation, then the particle will be held up for a certain time before it escapes to a flowing part of the domain and gets filtrated. This suggests that for complex flows, related to the geometry of the porous medium and the intensity of the gas flow, filtration efficiency is a subject that requires a more fundamental analysis.

CONCLUSION

In this contribution, we reported on the development and testing of a numerical method for simulating the detailed motion of particles in structured porous geometries. The key element to be extracted from the simulations is the

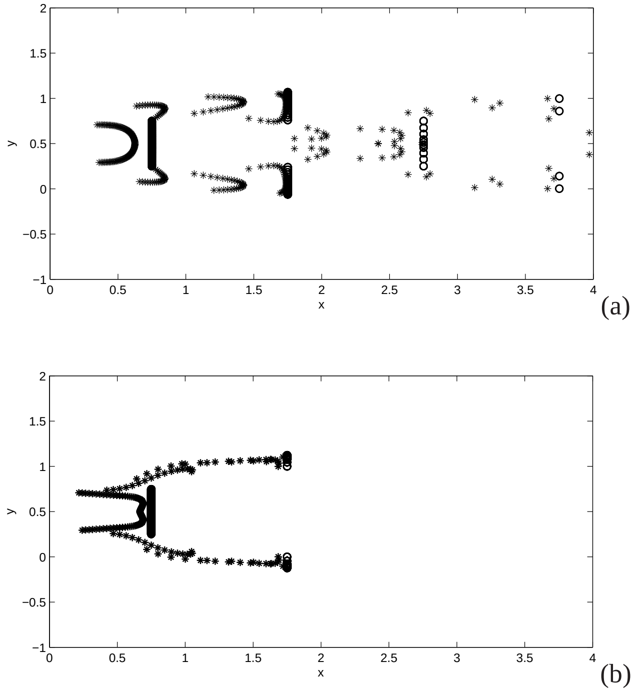

FIGURE 5. Particle trajectories emanating from a line of initial particle positions, which are not in the recirculation zones. Each curve corresponds to a particular moment in time. The particle positions originate from a straight line of initial conditions on the left side of the figure. The flow is characterized by $Re = 1$ (a) and $Re = 100$ (b). We simulated the motion of particles with $\tau = 0.1$, deposited particles are shown by ($\circ$) and particles that are still in motion are shown with ($*$).

dependency of the removal efficiency of porous filters on the flow condition, expressed by the Reynolds number. The suggested approach provides detailed microscopic information about the behavior of particles inside the filter, as well as yields the macroscopic consequences in terms of the overall filtration efficiency. The IB resolution of the flow allows to have a close look at the flow structures that develop and relate this to the particle dynamics inside the filter. We considered two cases at Reynolds numbers $Re = 1$ and $Re = 100$. For a range of particle relaxation times we detect that in a smoother flow field the particles act as mass-less and are hardly filtrated. In a relatively complex flow at $Re = 100$ there are more local regions of high acceleration and the particles express a richer dynamics, actually being trapped by the filter. Hence, particles with the same relaxation time can behave as nearly mass-less or heavy, depending on the flow conditions. For particles that have high inertia, such as particles with $\tau = 1$, we observe a high rate of filtration for both flow conditions. An interesting 'transition' is observed for particles with relaxation time $\tau = 0.1$ in this flow. It was shown that an increased inertial effect does not necessarily lead to a higher filtration - this shows that also the precise inner geometry of the filter is of importance to the total effect. We conclude that the presence of recirculation zones in the complex flows represents the possibility that a certain fraction of the particles is 'retained' for some time, leading to their later capturing. For a range of relaxation times, the 'residence time' in the recirculation zones is long enough to result in much slower filtration rates. As a whole, the particles that are heavy enough, get completely filtrated for both values of Reynolds numbers considered here, at a decay rate that depends on *Re*. Further investigations will be done to underpin the obtained results. This is particularly aimed at identifying the relevance of all three influences on particle filtration: Stokes relaxation time, Reynolds number and the structure of the flow inside the domain. Apparently, filtration is not just determined by the Stokes relaxation time of the particles that quantifies to what extent the particle would be able to follow the streamlines. The Reynolds number, expressing the acceleration, and the inner complexity of the porous structure imply qualitatively different filtration characteristics. We will publish this elsewhere.

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