Investigation of the effect of material’s cell size with the fixed porosity on the efficiency of aerosol particle deposition

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Abstract. In this work, numerical simulation of the motion of dusty gas in the open cell foam material (filter’s model) is carried out. The geometry of the porous material is created by a set of intersecting spheres arranged randomly in the space. Simulation of the gas flow in a porous medium without the use of averaged models is of great interest to scientists, and it is a detailed numerical simulation that takes into account the features of the internal structure. The studies were carried out for three characteristic pore sizes of 4, 5 and 6 mm of the filter cell to determine the size that is most preferable for the creation and use of porous filters operating at a given flow rate. Calculations have shown that a filter with the cell size of 4 mm has the highest quality factor, whereas a change in the deposition efficiency and the filter quality parameter for a casing with pore sizes of 5 mm and 6 mm differ insignificantly and much less than the parameters of the first case. The calculations performed are in good agreement with the semiempirical dependence of other authors.

1. Introduction
The growth of pollutant emissions in industrial plants, the reduction in the size of hazardous particles, the difficulty in their capturing, and the appearance of new materials support the researcher's interest of a detailed study of the filtration process.

In [1], experimental and analytical studies of the aerosol flow with a highly porous cellular material were carried out for the first time, taking into account the permeability, thermal conductivity of the material, and inertia of the particles, using the "pores per inch" (PPI) parameter as the main one, which indirectly characterizes the porosity of the medium. The authors of [2] and [3] presented experimental results of the value of the air pressure drop for flow through an open cell foam material for various values of the porosity of the medium. In accordance with the Darcy-Forchheimer equation, the value of the pressure drop was significantly less for a material with a higher parameter of porosity. The use of a particular flow model in a porous medium affects the correctness of the calculation. In [4], a

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comparison is made between the Brinkman and Darcy models for a flow passing through the porous cylinder. However, a detailed numerical simulation of the gas flow in a porous medium consisting of an ordered set of intersecting spheres was carried out in [5, 6], however, in order to calculate the particle deposition efficiency, the use of an ordered model is inadequate because of the presence of transparency in the porous structure. In this paper, a structure is constructed with a random arrangement of spheres in space that repeats the actual porous structure. We determine the main flow parameters, the efficiency of particle deposition, the effect of the cell size of the porous medium on these parameters, and the quality of the filter material as a whole. The problems of increasing of the particle deposition efficiency are discussed in [7, 8], but the complex structure of porous media, which affects air movement and the trajectory of particles, keeps the filtration theme actual nowadays.

2. Problem formulation and numerical simulation

2.1. An open cell foam geometry
In this paper, three geometric models were constructed to estimate the effect of the pore size on the fixed porosity of a medium consisting of a set of intersecting spheres arranged randomly in space. The porosity of the media remained constant and was equal to $\varepsilon = 0.54$, while the diameters of the pores (spheres) were $d_1 = 4$ mm, $d_2 = 5$ mm, $d_3 = 6$ mm (see Figure 1 – a, b, c, respectively). The computational domain is a cube, with linear dimension of 2 cm.

![Figure 1. Geometric models of a porous medium with different pore diameters.](image)

2.2. Mesh quality
The number of mesh elements was an average of 9 million, which ensured a sufficient accuracy of the calculation. Figure 2 shows a part of the mesh.

![Figure 2. Mesh used for calculations.](image)
2.3. Boundary conditions
The mass flow rate at the inlet and the value of the atmospheric pressure at the outlet, as well as the symmetry conditions on the other 4 boundaries, are set on two opposite boundaries of the calculation areas. The assumption of symmetry condition is acceptable if the walls of the real object are at a considerable distance from the boundaries of the calculation area, where the wall effect is insignificant, and the calculation model is an element cut out of the porous medium.

Hydrodynamic calculations were carried out on the basis of the Navier-Stokes equations in the CFD package ANSYS Fluent using the finite volume method. The calculation is made in accordance with the model of laminar flow of a viscous incompressible gas.

3. Results and discussion

3.1. Numerical simulation of the gas flow. Calculation of the value of pressure drop
The complex geometry and porosity of the medium provide a non-linear change in the pressure drop, depending on the average filtration velocity, which is shown in Figure 3. Detailed simulation of the gas movement in a porous medium taking into account the morphology of the surface is performed. In the case of using the averaged gas flow model, the Forchheimer model is used with allowance for nonlinearity. To use this model, the value of the permeability coefficient of the medium, which can be obtained from experimental data, must be known in advance.

![Figure 3](https://example.com/figure3.png)

**Figure 3.** The change in pressure drop on the filtration velocity for three cases of the pore diameter of the porous structure: 1 - \( d_c = 5 \) mm, 2 - \( d_c = 6 \) mm, 3 - \( d_c = 4 \) mm.

| \( Q_m \), kg/s | \( u_1 \), m/s | \( \Delta p_1 \), Pa | \( u_2 \), m/s | \( \Delta p_2 \), Pa | \( u_3 \), m/s | \( \Delta p_3 \), Pa |
|-----------------|--------------|----------------|--------------|----------------|--------------|----------------|
| \( 5 \times 10^{-7} \) | 0.00246 | 3.22E-10 | 0.02122 | 2.529E-9 | 0.00214 | 1.45E-4 |
| \( 5 \times 10^{-6} \) | 0.0246 | 5.604E-9 | 0.04243 | 6.288E-8 | 0.02138 | 8.208E-5 |
| \( 1 \times 10^{-6} \) | 0.0492 | 1.731E-7 | 0.21216 | 4.371E-5 | 0.04276 | 8.208E-5 |
| \( 5 \times 10^{-5} \) | 0.24602 | 7.534E-5 | 0.42432 | 4.111E-4 | 0.21381 | 2.47E-4 |
| \( 1 \times 10^{-4} \) | 0.49204 | 3.99E-4 | 0.84865 | 0.00207 | 0.42761 | 8.63E-4 |
| \( 2 \times 10^{-4} \) | 0.98408 | 0.00278 | 1.27297 | 0.0066 | 0.85522 | 0.00481 |
| \( 3 \times 10^{-4} \) | 1.47612 | 0.01144 | 1.69729 | 0.01085 | 1.28283 | 0.01387 |
| \( 4 \times 10^{-4} \) | 1.96816 | 0.03512 | 2.12162 | 0.02763 | 1.71045 | 0.02917 |
| \( 5 \times 10^{-4} \) | 2.4602 | 0.05952 | 2.54594 | 0.05619 | 2.13806 | 0.04914 |
| \( 6 \times 10^{-4} \) | 2.95223 | 0.12755 | 3.39459 | 0.13201 | 2.56567 | 0.14052 |
3.2. Calculation of the efficiency of particle deposition

In view of the smallness of the aerosol particles concentration, the trajectories were determined in the gas velocity field found, the particle deposition efficiency was calculated as the ratio of the settled particles quantitative value to the started particles quantitative value and for three cases of the pore diameters for a fixed inlet mass flow rate $Q=10^{-3}$ m$^3$/s is shown in figure 4. Calculations were carried out for various values of the Stokes number determining the measure of particle inertia:

$$\text{St} = \frac{d^2 \rho_p u_0}{18 \mu d_c},$$

(1)

where $d_p$, $\rho_p$ is the diameter and density of the aerosol particle, respectively, $u_0$ is the velocity of the undisturbed gas flow, $\mu$ is the viscosity of the gas, $d_c$ is the diameter of the cell of the porous medium.

![Figure 4. Comparison of the dependences of the deposition efficiency on the Stokes number by numerical simulation for three cases of the pore diameter: 1 - $d_c = 4$ mm, 2 - $d_c = 5$ mm, 3 - $d_c = 6$ mm.](image)

The results of the calculations demonstrate that the particle deposition efficiency for a model with a smaller pore diameter ($d_c = 4$ mm) is significantly higher for all values of Stokes number, which is explained by the large surface area in the model.

For highly inertial particles, the values of the efficiency curves for the cell diameters of 4 mm and 5 mm practically coincide, this indicates that when filters are used at high gas flow rates or for large inertial particles, it is not necessary to use a porous material with a smaller cell diameter.

The deposition efficiency curves differ slightly for the diameters $d_c = 5$ mm and $d_c = 6$ mm in the case of small particles, however, with an increase in particle inertia, the use of a model with smaller pore diameters is preferred.

3.3. Comparison of the results of numerical simulation with experimental data

The authors of [5] carried out an experimental study of the dusty gas flow in the open cell foam material and proposed semiempirical dependence of the deposition efficiency of aerosol particles as a function of the thickness of the filter material, the diameter of the filtering fiber (the width of the septum in a porous medium), the Stokes number, which, neglecting gravity affects the particles, will be written in the form:

$$E = 1 - \exp \left( -\frac{t}{d_f} \cdot 5.486 \text{St}^{2.382} \right),$$

(2)
where \( t \) is the thickness of the porous material, \( d_f \) is the diameter of the fiber (partitions of the porous material).

In the calculation model, the thickness of the media was 2 cm, the diameter of the fiber in \( d_c = 4 \) mm, \( d_c = 5 \) mm, \( d_f = 6 \) mm are \( d_f = 0.0975 \) mm, \( d_f = 1.2 \) mm and \( d_f = 1.5 \) mm, respectively.

**Figure 5.** The efficiency of particle deposition by numerical calculation and semi-empirical formula (2) for a porous medium with the cell diameter and fiber diameter, respectively:

- a – \( d_c = 4 \) mm, \( d_f = 0.0975 \) mm;
- b – \( d_c = 5 \) mm, \( d_f = 1.2 \) mm;
- c – \( d_c = 6 \) mm, \( d_f = 1.5 \) mm.
Figures 5 (a, b, c) demonstrate a good agreement between the numerical simulation results and the semiempirical dependence of the authors Hellmann A., et. al. [5]. Some discrepancy between the curves is due to the "floating" value of the fiber, which on average varies from 0.6 to 1.8 for random packing of spheres, and also depends on the cell diameter and the porosity of the medium.

3.4. Determination of the filter quality factor

The main characteristic of the filtering porous material is the filter quality parameter, which is determined by the ratio of the particle deposition efficiency to the pressure drop value:

$$QF = \frac{E}{\Delta p}.$$  \hspace{1cm} (3)

Table 2. The calculated parameters and filter quality values for the fixed input mass flow rate $Q = 10^{-5}$ m$^3$/s for three cases of the cell diameter, indices 1, 2 and 3 correspond to the cell sizes specified above.

| $\Delta p_1$, Pa | $E$ | $FQ_1$, 1/Pa | $\Delta p_2$, Pa | $E$ | $FQ_2$, 1/Pa | $\Delta p_3$, Pa | $E$ | $FQ_3$, 1/Pa |
|------------------|-----|--------------|------------------|-----|--------------|------------------|-----|--------------|
| 1.731E-07        | 3.1988E-4 | 1847.92 | 6.288E-08       | 4.8119E-08 | 0.76525 | 8.208E-08       | 4.8943E-08 | 0.59628 |

Figure 6. Values of the filter quality parameter at the same mass flow rate for three cases of the pore diameter of the porous structure: 1 – $d_c = 5$ mm, 2 – $d_c = 6$ mm, 3 – $d_c = 4$ mm.

Analysis of the tabular data 2 shows that at low flow velocities, the change in the pressure drop is insignificant compared to the change in the deposition efficiency of the particles. Therefore, for filters operating at lower flow rates, preference is given to increasing the total surface area due to the dimensions. Values of the quality parameters of filters with cells of 5 and 6 mm in diameter are small, whereas for a filter with a cell diameter of 4 mm, the value of this parameter is greater by orders of magnitude. Studies have shown that increasing the cell size of the porous material to reduce the filter resistance is impractical at low flow rates. Further studies in this area can reveal the threshold value of the size of the filter cell, and also determine a set of optimum values of the diameter, depending on the filtration velocity and inertia of the particles.

4. Conclusion

Numerical simulation of the motion of dusty gas in the open cell foam is carried out. Calculations were carried out for three values of pore diameters: 4 mm, 5 mm and 6 mm, which are average cell sizes in widely used domestic and industrial filters. The results of the study showed that for filtration
problems at low flow velocities, it is advisable to use material with the smallest pore size, which is 4 mm, parameters of calculation for media with two other diameters do not differ much.

In conclusion, it should be noted that, due to the random construction of geometries of porous media, more detailed studies are needed, such as, for example, a set of sphere packages for version with the fixed pore size to create a representative sample.

The possibilities of modern three-dimensional printing of full-scale objects allow us to carry out not only numerical, but also experimental studies based on models of created porous media and it is the goal of our further research.

The conducted researches show that a detailed study of the cell size material’s effect on the hydrodynamic calculation and the efficiency of particle deposition using computer simulations makes possible the creation of aerosol filter samples with improved characteristics.

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References
[1] Bhattacharya A, Calmidi V V and Mahajan R L 2002 *Int. J Heat Mass Transfer.* **45**(5) 1017
[2] Wang M and Pan N 2008 *Int. J. Heat Mass Transfer.* **51** 1325
[3] Dukhan N 2006 *Exp. Fluids.* **41**(4) 665
[4] Mardanov R F, Soloveva O V and Zaripov SK 2016 *IOP Conf. Series: Materials Sci. Eng.* **158** 012065
[5] Hellmann A, Pitz M, Schmidt K, Haller F and Ripperger S 2015 *Aerosol Sci. Technol.* **49** 16
[6] Dmitriev A V, Madyshew I N and Dmitrieva O S 2018 *Ecology Ind. Rus.* **22**(6) 10
[7] Soloveva O V, Solovev S A, Khusainov R R, Popkova O S and Panenko D O 2018 *J. Phys.: Conf. Ser.* **944**(1) 012113
[8] Solovev S A, Soloveva O V and Popkova O S 2018 *Rus. J. Phys. Chem. A.* **92**(3) 603