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TOWARDS A NUMERICAL MODEL OF BACTERIAL FILTRATION IN FIBROUS FILTERS

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A model of bacterial filtration on fibrous filter media is developed. The single fibre efficiency as well as the efficiency of the whole filter – at the onset of the process and the evolution of those quantities - are analysed. The differences between the numerical modelling of colloidal particles and bacteria are stressed in detail. The main differences are the active motion ability of bacteria and biofilm formation. The parameters of the model were identified based on the literature data.

Keywords: bacterial filtration, filtration efficiency, nonstationary filtration, biofilm formation

1. INTRODUCTION

Filtration on fibrous filters is a very important aspect of water treatment, air purification and many other techniques of liquid or gas separation. This process removes most micron- and submicron size impurities like e.g. colloidal particles, algae, bacteria etc. The filtration of colloidal (abiotic) particles has been intensively investigated experimentally as well as theoretically and today it is said to be quite well understood.

As to filtration of biotic agents like e.g. bacteria and algae, the methods elaborated for the filtration of colloidal particles are usually utilised to describe the process. Following that bacteria are treated as colloidal particles and the expressions for single fibre efficiency and re-entrainment rate are assumed to be the same as those for abiotic particles. This approach may, however, fail as there are some important differences between abiotic particles and bacteria: (i) a more complicated structure of a bacteria cell wall than the surface of common colloidal particles, (ii) the ability of bacteria to move, (iii) the tendency to form a biofilm and thus to increase the loading degree of fibres and (iv) the possibility of cell damage as a result of coming into contact with some substances (metal ions or nanoparticles).

In investigations into the filtration of colloidal particles or, more precisely, into the interactions between particles or particles and fibres the Derjaguin-Landau-Vervey- Overbeek (DLVO) theory is usually used. However, for interactions between bacteria and e.g. fibre surfaces the theory fails to provide results consistent with experiments. The reason is that bacterial cells usually contain so-called extracellular polymer substances (EPS), which may adhere to the solid substrate increasing the attractive force.

Another feature that differs bacteria (and some other biotic agents like e.g. algae or Protista) and abiotic colloidal particles is that the former possess the ability to move. The organs of motion are usually

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flagella or cells. The ability to move may result in a change of single fibre efficiency in comparison with colloidal particles of the same size and shape.

The antibacterial properties of some metal ions and nanoparticles (NPs) have been reported in many papers. The mechanism of the mortality of bacteria in such a case has not been completely investigated yet. Some proposals, however, have been put forward in the literature. Some metals, e.g. silver nanoparticles (SNPs), are believed to release metallic ions which interacting with the cellular wall give free radicals as products (Arabagi et al., 2011; Sondi and Salopek-Sondi, 2004). These react then with the cellular structures and nucleotide destroying them and finally cause the destruction of the cellular wall. All these processes lead to the death of the bacterium and destruction of its cell. Other NPs, e.g. TiO_2 or ZnO, have photocatalytic properties which result in free radical generation (Dalrymple et al., 2010). Though the kinetics of this process has also been understood very poorly, there are some models describing it. The most popular are those describing bacteria decay dynamics in a similar way as the first-order or higher-order chemical reaction (Chick, 1908; Hom, 1972).

The aim of this paper is to elaborate the base of a model of bacteria filtration in fibrous filters. In Sec. 2 we propose simple descriptions of the interactions between bacteria and fibres, the bacteria motion and the kinetics of biofilm formation and bacteria number evolution in the presence and absence of metal nanoparticles. In Section 3 we present the results of computations. The dependence of the results of modelling on the values of model parameters will be widely discussed. Finally, Section 4 contains the conclusions and proposed methods of model verification.

2. NUMERICAL DESCRIPTION OF BACTERIA BEHAVIOUR IN A FILTER

2.1. Modelling of growth and decay of bacteria colony

The growth of a bacteria colony may be modelled with various models (Baranyi and Roberts, 1994).

The simplest one is the first-order kinetic equation, which is often used to model the population growth of living organisms:

$$\frac{dN}{dt} = \mu N \tag{1}$$

where μ is the specific growth rate. This parameter depends in general on the bacteria concentration N: it is supposed to be a monotone decreasing function which vanishes when the bacteria concentration reaches the maximum possible value for the environment N_{max}. However, the concentration of bacteria deposited in a filter during the filtration of common feed solutions may be assumed to be much less than the maximum one and thus the specific growth rate is treated as independent of bacteria concentration. The value of the growth rate depends also on the conditions of the parameters of the environment, e.g. pH (Presser et al, 1997) but for the most cases it is of order of 10^{-4}-10^{-3} s^{-1} (Baranyi et al., 1996).

To take into account the effect of antimicrobial effect of NPs we should add an extra term describing the interactions between bacteria and nanoparticles. Most kinetic models assume that the inactivation rate is of the first-order with respect to bacteria concentration (Darlymple et al., 2010). Although the dependence on NPs concentration has not been investigated yet, it may be expected that the rate is of the first-order also with respect to this concentration (Wei et al., 1994). Taking these assumptions into account, we may rewrite the equation describing the evolution of bacteria number in the following form:

$$\frac{dN}{dt} = \mu N - \beta n N \tag{2}$$

where β is an additional constant, characterising the rate of bacteria decay.

2.2. Modelling of the bacterial motion

Another factor differing bacteria and abiotic particles is that the former one have the ability to move. As mentioned in Sec. 1, the organs of bacterial motion are flagella or cells. Here we concentrate on the flagella motion, which is typical of various common bacteria like Escherichia Coli and Serratia Marcescens (Arabagi et al., 2011). Each cell of these bacteria has 1-5 flagella, which may rotate clockwise or counterclockwise. A single flagellum is a long helix having a length of 10 μm, thickness of 20 nm and 0.5 μm diameter coils. Flagella rotation frequency is equal up to 100 Hz. A scheme of a bacterium cell with flagellum is presented in Fig. 1.

Fig. 1. Scheme of a bacterium cell with flagellum

The motion of such bacteria is composed of two phases (Arabagi et al., 2011). In the former, known as the run phase or run state all the flagella rotate counterclockwise and they exert a constant driving force, which causes the cell motion. During the latter, the tumble phase, the flagella start to rotate in the opposite direction. At this stage the bacterium does not exhibit the straight motion, but chaotically tumbling motion changing the direction of its axis. As a result, during the next phase of the motion the bacterium can move in a different direction than the previous one while the driving force is the same.

Similarly as Arabagi et al. (2011), we assume that the probability of transition from one phase to another per time unit is constant for both phases. This means that the probability distribution of the duration of the two phases is exponential:

$$P(t) = \frac{1}{\tau_i} \exp\left(-\frac{t}{\tau_i}\right) \qquad i = 1,2 \tag{3}$$

where τ_i is the average duration of each phase. The value of this time value is usually of the order of 0.1 - 1 s and it depends on the composition of the bacterium environment (Stryer, 2002). Generally speaking, the higher concentration of nutrients (especially glucose) the longer the run phase tends to be. In this paper, we take in general $\tau_1 = 0.1\ s$ for the tumble phase and $\tau_1 = 1.0\ s$ for the run phase (Arabagi et al., 2011). We should, however, note that the length of both phases depends on the chemical composition of the solution. As a typical value of the driving force in the run state we set

0.480 pN (Arabagi et al., 2011). We assume that during the run state the direction of the bacteria motion does not change even if it is surrounded by a flowing liquid.

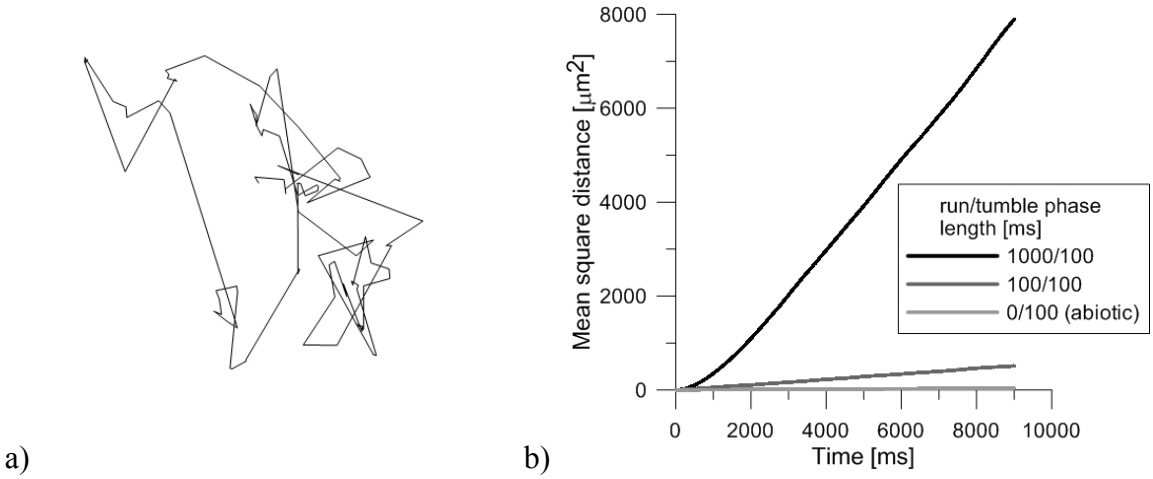


Fig. 2. Sample trajectory of bacterium (a) and the dependence of mean square distance of the bacteria on time for different values of run and tumble phase length (b)

A sample trajectory of bacterial motion as described above is presented in Fig. 2a. We may recognise that it is similar to the trajectory of a Brownian particle. This hypothesis is confirmed when we plot the dependence of mean square displacement of bacteria as a function of time. This dependence is presented in Fig. 2b. The mean square displacement is proportional to the time - just as in the case of a Brownian particle. That allows us to introduce the effective diffusion coefficient which describes the motion of bacteria in the same manner as that of Brownian particles. The coefficient for bacteria is about three orders of magnitude greater than the diffusion coefficient of the abiotic particles in the same size. This circumstance may have a significant influence on the efficiency of bacteria removal on fibrous filters.

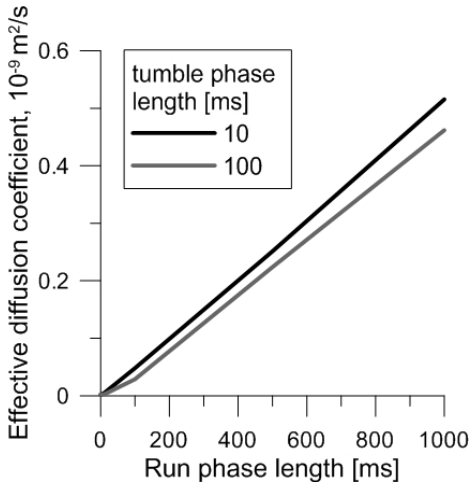


Fig. 3. Dependence of effective diffusion coefficient on the length of run and tumble phase

2.3. Modelling of bacteria/fibre interactions

The mathematical description of the interactions between bacteria cells and fibres is crucial for predicting the efficiency of collisions (i.e. if a collision results in bacterium deposition or not) and the re-entrainment rate. In most papers, the interactions between bacteria and solids are described with the

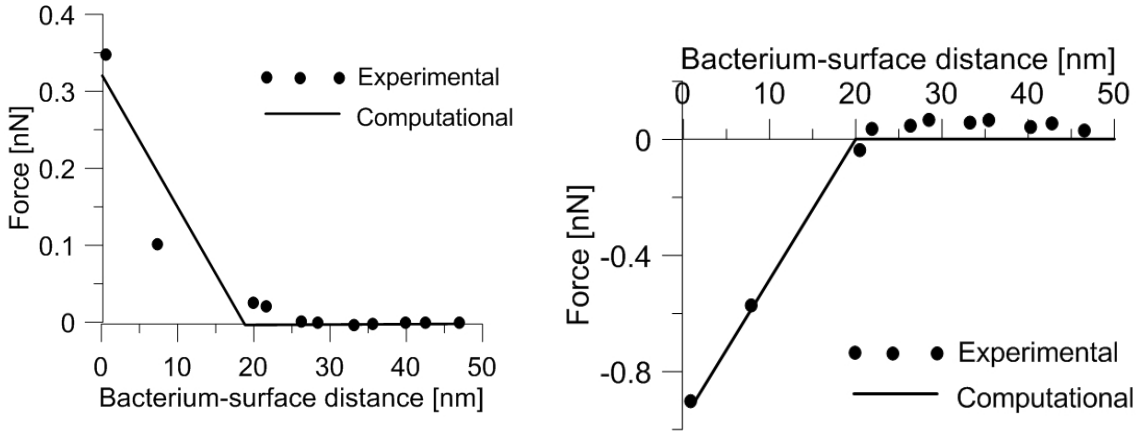
DLVO/XDLVO model (Derjaguin and Landau, 1941; Ruggiero et al., 1999; Verwey and Overbeek, 1948). However, findings (obtained with the model) were repeatedly reported to have failed to agree with experimental data. That is the reason why a new model of these interactions seems to be required.

In the present work we propose a model similar to that developed for ligand-receptor interactions. The particles of EPS are treated as springs with a given spring constant and maximum length (Gupta, 2012). According to this model, the interactions of bacteria and between bacteria and materials can be treated as harmonic interactions and chemical bonding as Hooke springs. Hence the force F_b acting on the binding of a single molecule can be given by:

$$F_b = \sigma\left(x(t) - \lambda\right) \tag{4}$$

In fact, the ligand-receptor binding is often built by more than one molecule of EPS (more than one spring). However, in this work we limit ourselves to modelling these interactions with one spring only.

The results based on the ligand-receptor binding model are very satisfactory as it has been presented in Fig. 4.



a) b)

Fig. 4. Comparison of experimental and ligand-receptor binding model based numerical results for interactions between E. Coli D21 bacteria with polystyrene (a) and mica (b) surface

We can see that the typical values of forces acting between bacteria and surface of various materials are of the order of 0.1-1 nN. It is approximately a 100 times higher value than the typical force generated by the flagellum during the run phase. Thus, the re-entrainment of bacteria as an effect of flagellum dynamics may be neglected.

Another important fact is that between the bacteria and some materials there exist force which is repelling independently of the distance, like e.g. between bacteria E. coli D21 and mica (see Fig. 4b). The deposition of bacteria on surfaces of such materials is, of course, impossible.

3. RESULTS OF THE MODELLING

3.1. Bacterial colony growth and decay during filtration

Now, let us consider a filter with metal NPs present at the surface of fibres. To describe the evolution of the number of bacteria during filtration of the solution, Equation (2) can be used. Both the constants,

μ, and β, may be obtained from experimental results. We expect that they are different for different kinds of bacteria or even for the same bacteria but in different process conditions, e.g. temperature.

In the present work, we do not relate to the specific experimental results but we would like to give a quantitative description of the influence of metal NPs on the bacterial removal efficiency. Thus, we are not interested in determining the precise value of both constants of the model. Instead, we are going to find the order of magnitude of these values. That will give us a broad picture of the relation between the characteristic time of bacterial growth and/or decay and other characteristic time scales of the process. The values of the parameters are calculated based on the experimental results presented by Xu et al. (2006) who investigated the antibacterial effect of SNPs placed in the poly(L-lactide) fibres. The value of μ for the experimental conditions reported in that work is equal to 0.66 h^{-1} for *E. coli* and 0.64 h^{-1} for *S. aureus* bacteria. The value of β cannot be computed based on the reported results since the concentration of silver NPs was not known. In fact, it is very difficult to estimate the concentration of NPs deposited on fibres. However, based on the results presented by Xu et al. (2006), we may estimate the product of βn as equal to 0.24 h^{-1} for *E. coli* and 0.35 h^{-1} *for S. aureus*.

Fig. 5 presents the long-time results of the bacteria number evolution in the absence and presence of silver NPs for *E. coli* (the results of *S. aureus* look very similar). The concentration of NPs is assumed to be equal to that analysed by Xu et al. (2006). We recognise that although the presence of SNP in such a concentration does not prevent the growth of bacteria number, it slows down this growth. To stop the growth of bacteria number the SNP concentration should be about three times greater.

The concentration of SNP at which the bacteria number stop to increase is dependent on many factors, among others the diameter of single nanoparticle, the shape of nanoparticles and the method of immobilization of SNP on fibers. This problem calls for further investigations. The results of these investigations will be presented in forthcoming papers.

3.2. Single fibre efficiency

To compute the initial single fibre efficiency (SEF) (i.e. the efficiency of an unloaded fibre) we apply a similar formula to that used for colloidal abiotic particles. The only difference is that we should use, instead of diffusion coefficient, the effective diffusion coefficient as discussed in Section 2.2.

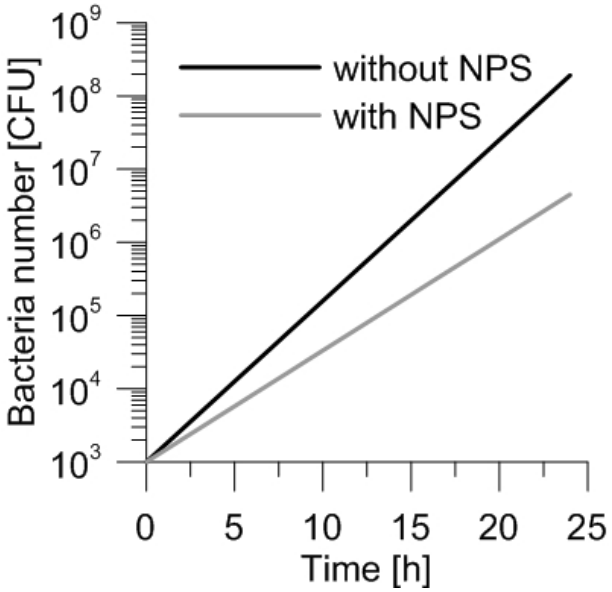


Fig. 5. Evolution of the deposited bacteria number in the filter in the absence (black line) and the presence of SNP (grey line)

According to the method, SEF may be expressed as a sum of terms describing various mechanisms of bacterial (particle) deposition: diffusion, inertial impaction and direct interception efficiency. In the literature one can find many various formulae describing these efficiencies. In this paper we use those developed by Li and Liu (1982) as they are reported as providing the good consistency with experimental results and have a good theoretical justification. The interception efficiency can be given by:

$$\eta_I = \frac{Stk^3}{Stk^3 + 0.77Stk^2 + 0.22} \tag{5}$$

The inertial impaction efficiency can be expressed in the following form:

$$\eta_R = \frac{(1-\alpha)\left(\frac{d_p}{d_f}\right)^2}{Ku\left(1+\frac{d_p}{d_f}\right)} \tag{6}$$

The diffusion term can be expressed as:

$$\eta_D = 2.9\left(\frac{1-\alpha}{Ku}\right)^{1/3} Pe^{-2/3} \tag{7}$$

where the Péclet number (Pe) is calculated in respect to the effective diffusion coefficient. The coefficient, however, depends on the length of the run phase (which depends, on the other hand, on the concentration of glucose in the feed solution) as discussed in Section 2.2. Fig. 6 presents the dependence of SEF on the run phase length for three values of water velocity. For the run phase length equal to 0 (i.e. abiotic particles or dead bacteria), the value of SEF is nearly independent of that velocity, while the main mechanism governing particle deposition is the inertial impaction. However, when the run phase length increases, the significant increase of SEF is observed while the diffusive mechanism becomes dominant.

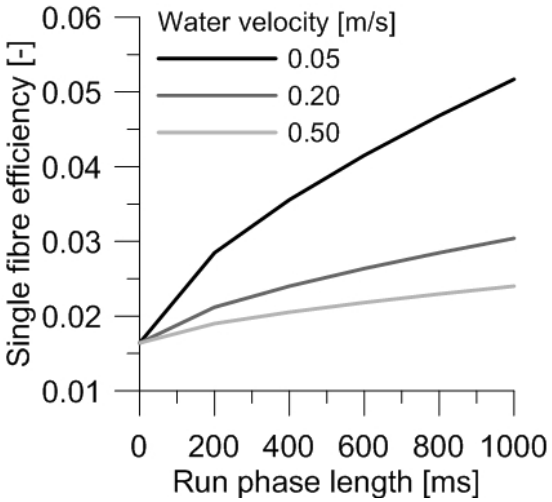


Fig. 6. Dependence of the initial single fibre efficiency on the mean run phase length for three values of water velocity

During the filtration process, the number of deposited bacteria changes. One reason is the deposition of successive bacterial cells and their potential re-entrainment, so the same mechanisms as in the case of colloidal particles. On the other hand, the number of bacteria may increase as an effect of biofilm formation or decrease as a result of the interactions with metal ions.

There are a few models describing the changes of single fibre efficiency in respect to the amount of particles deposited on it (Kasper et al., 2009). Most of them have been elaborated for aerosol filtration i.e. the case when gas is the continuous phase. One may, however, expect that similar formulae should be valid also for colloid filtration. Indeed, the only difference between these two cases (besides the values of physicochemical parameters of gas and liquid: viscosity and density) is the different nature of interactions between particles and fibres. The models of aerosol filtration assume that at typical filtration conditions every collision between a particle and a fibre results in deposition and the re-entrainment of particles may be neglected at least at the early stage of filtration. In Section 2.3 we have demonstrated that these assumptions remain equally valid for the filtration of bacteria.

The model presented in this work assumes the growth of effective fibre diameter as an effect of bacterial deposition and biofilm formation. If every bacterium cell has the same diameter and thus the same volume, the effective fibre diameter may be expressed as a function of the number of deposited bacteria in the following form:

$$d_{f,eff} = \sqrt{d_{f,0}^2 + \frac{2}{3} N d_p^3} \tag{8}$$

where N denotes the number of deposited bacteria per length of a single fibre.

When the thickness of biofilm exceeds the critical value, the re-entrainment should commence. The value of critical thickness depends on some biofilm properties. It is expected that it also depends on water velocity. In the present work we treat this value as a control parameter.

Fig. 7 presents single fibre efficiency as a function of the number of deposited bacteria obtained by means of the model described above for three values of fibre diameter. Initially, we observed the slight decrease of SEF while the dominant mechanism of deposition was diffusive. It is well-known that the diffusive term of SEF decreases when the porosity of the filter decreases and the fibre diameter increases. Finally, when this term is no longer dominant, we observe the increase of SEF with the number of bacteria deposited as it is the case for abiotic micron-size particles. An interesting result of the model is that SEF in the case of bacterial filtration grows more slowly than in the case of abiotic colloidal particles. Increase the bacteria number from 0 to 10^{12} cells per 1 mm of fibre length results in 2.5-fold increase of SEF. The same growth of the concentration of deposited colloidal particles results in 4.5-fold increase of SEF. In fact, this increase is even greater while the dendrite-like structures start to form. Taking that into account we may conclude that the bacterial filtration may be considered as more “stationary” than the colloidal filtration.

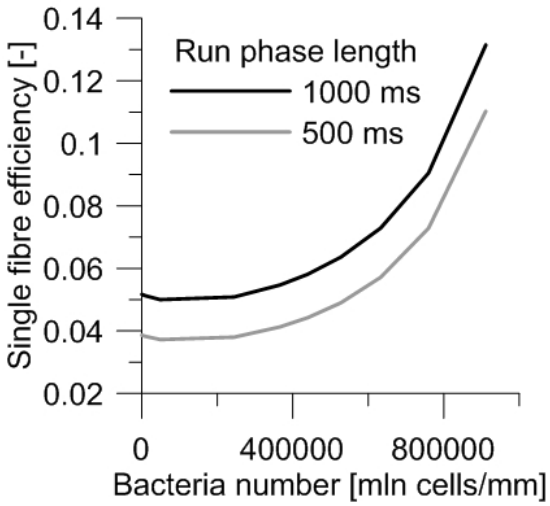


Fig. 7. Single fibre efficiency as a function of number of deposited bacteria for two run phase length.

3.3. Filtration efficiency of fibrous filters

In the classical filtration theory the efficiency of the fibrous filter (or the fibrous layer) may be expressed in terms of single fibre efficiency:

$$E = 1 - \exp\left(-\frac{4\alpha\eta\Delta x}{\pi(1-\alpha)d_f} \right) \tag{9}$$

where η denotes SEF. In the first approximation we may assume that the same formula is valid for bacterial filtration. The only difference is the different value of SEF for bacteria and abiotic particles with the same diameter, as shown in previous section.

The efficiency of the filter – in the same manner, as the efficiency of a single fibre – does not change significantly with the number of bacteria deposited unless this number is large enough to increase the porosity about three-four times. However, such amount of bacteria seems to be nonphysical – the biofilm structure would earlier break down as an effect of crowding of bacteria. The dynamics of this process has not been recognised yet. However, from the practical point of view, the filter should be exchanged before such an amount of bacteria will be collected in its structure.

Fig. 8 demonstrates the distribution of the mass of deposited bacteria in the filter after a relatively long time of filtration. We recognise that the highest mass is deposited near the inlet of the filter – on the left hand side. However, we further recognise that the difference between the mass deposited near the inlet and near the outlet is very low and reaches five per cent of the mean value. This result confirms that the bacterial filtration may be modelled as a stationary process.

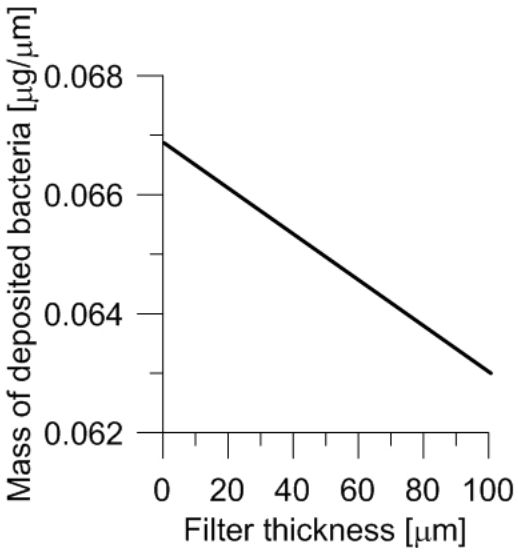


Fig. 8. Distribution of the mass of bacteria deposited inside the filter. Inlet – on the left hand side

4. CONCLUSIONS

In this paper the proposal of a numerical model of bacterial filtration was developed. We analysed the possibility of using the existing filtration models developed for abiotic colloidal particles. We pointed out the differences between the numerical description of the filtration of abiotic particles and bacteria. The main property considered here was the ability of bacteria to move. This feature of bacteria has been taken into account by introducing the "effective diffusion coefficient". This coefficient is usually much higher than the diffusion coefficient of the abiotic particles with a similar diameter. As a result, the dominant mechanism of bacterial filtration is "diffusion-like" instead of inertial impaction mechanism,

typical from micron-size particles. It resulted in a greater value of single fibre efficiency in comparison with abiotic particles of the same diameter.

Also, the efficiency of bacterial removal there was affected by bacterial mortality following contact with metal nanoparticles. The results of preliminary computations showed that metal nanoparticles inhibited biofilm formation while their influence on bacterial removal efficiency could be neglected while the single fibre efficiency is very weakly dependent on the biofilm thickness. The inhibition of biofilm formation is dependent on the specific interactions between bacteria and metal nanoparticles, characterised by the bacteria decay rate constant β. Nowadays, it is not known which parameters influence the value of β and this problem calls for further investigations.

The most interesting result is that the value of a single fibre efficiency as well as the efficiency of the whole filter changes more slowly than the filtration efficiency of the colloidal abiotic particles. This is an effect of domination of diffusion mechanism of bacteria filtration. The efficiency of this mechanism is very weakly dependent on the amount of bacteria deposited. This result allows us modelling bacterial filtration as a stationary process.

There are some aspects of bacterial filtration which may not be included into the model before experimental studies are conducted. They are: biofilm breakdown as an effect of crowding followed by the re-entrainment of biofilm fragments and spore formation by the certain species of bacteria. These phenomena are now under investigation.

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SYMBOLS

d_f	fibre diameter, µm
$d_{f,eff}$	effective fibre diameter, µm
d_p	particle/bacteria diameter, µm
F_b	force between bacteria and fibre, nN
Ku	Kuwabara factor
N	number of deposited bacteria per fibre length, mm^{-1}
n	number of nanoparticles per fibre length, mm^{-1}
Pe	Peclet number
Stk	Stokes number
t	time, s

Greek symbols

$\acute{\alpha}$	packing density
β	constant characterising the bacteria decay in contact with nanoparticles, mm
η	single fibre efficiency
η_D	diffusion single fibre efficiency
η_I	inertial impaction single fibre efficiency
η_R	interception single fibre efficiency
λ	constant characterising the force between bacteria and fibre, nm
μ	specific growth rate
σ	constant characterising the force between bacteria and fibre, N/m
τ_1, τ_l	run/tumble phase length, s

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