The effect of Cartilaginous rings on Deposition by Convection, Brownian Diffusion and Electrostatics.

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Abstract: This paper presents a numerical study of the deposition of spherical charged nanoparticles caused by convection and Brownian diffusion in a pipe with a cartilaginous ring structure(fig.1). The model is supposed to describe deposition of charged particles in the upper generations of the tracheobronchial tree of the human lung. The upper airways are characterized by a certain wall structure called cartilaginous rings which are believed to increase the particle deposition when compared to an airway with a smooth wall. The problem is defined by solving Navier-Stokes equations in combination with a convective diffusion equation and Gauss law for electrostatics. Three non-dimensional parameters describe the problem, the Peclet number $Pe = \bar{U}2a/D$, the Reynolds number $\mathrm{Re} = \bar{U}2a/\nu$ and an electrostatic parameter $\alpha = a^2 c_0 q^2/(4\varepsilon_0 \kappa T)$. Here $\bar{U}$ is the mean velocity, a the pipe radius and D is the diffusion coefficient due to Brownian diffusion given by $D = \kappa T Cu/(3\pi\mu d)$, where Cu is the Cunningham-factor $Cu = 1 + \lambda/d(2.34 + 1.05\exp(-\frac{0.39d}{\lambda})$. Here d is the particle diameter and λ is the mean free path of the air molecules.
Results are provided for generation 4 of the human airway and for normal breathing conditions with a Reynolds number of 450 and a Peclet number of 100000, corresponding to a pipe radius of 2.25mm and a particle radius of 10nm. The electrostatic parameter is varied to model different concentrations c_0 and charge number q.

Keywords: Charged nanoparticles, Brownian diffusion, Electrostatics, Deposition, Human respiratory airways.

1. Introduction

Use of Carbon-nanotubes in material design enables the development of new materials with superior properties. A drawback of this development is that these particles when inhaled may be toxic and can cause substantial health risks of the human lung[1]. In experiments these particles are known to be electrically charged which probably leads to an increase in particle deposition in the lung.

In this paper we analyze how nanoparticles are deposited in the human lung airways and especially we consider the effects caused by charged nanoparticles. We also include a wall structure called cartilaginous rings, located in the upper airways of the lung.

To find the transport and deposition in a general flow geometries there are essentially two methods. One method is to solve the equations of motion of the particles in the flow field which is generated by solutions of Navier-Stokes equation Högberg et al.[2]. To get statistical measures of the deposition a large number of particles (*N*) need to be simulated with an error of the order $O(N^{-1/2})$.This approach is difficult if we wish to find the electric field from a concentration of particles.

An alternative method is to more directly consider the equation that describe the probability density of the particles, i e. the Fokker-Planck equation[3] or a convective diffusion equation for the concentration[4].

In the present paper we consider this latter approach of solving the convective-diffusion equation for the concentration combined with Navier-Stokes equations for the fluid flow and Poisson's equation for the electrostatic field.

Studies of the deposition of charged particles in a cylindrical tube have been performed earlier by Yu[5], Yu and Chandra[6] and Ingham[7]. These authors assume fully developed fluid flow. This is a good approximation for the higher generations of the human lung, but for the upper lower generation airways, the effect of a developing fluid flow is important. In this paper where we consider generation 4 we therefore assume the fluid to develop from uniform velocity at entry.

2. Governing equations

Each generation of the human airways is supposed to be described by a pipe with a smooth surface or a pipe with a cartilaginous ring structure, see figure 1. For the individual airways of each generation we assume axial symmetry. The following set of equations describes the physics of the problem.

$$(\mathbf{u}\cdot\nabla)c+\frac{1}{Pe}\nabla\phi\cdot\nabla c-4\alpha\frac{c^2}{Pe}=\frac{1}{Pe}\nabla^2 c \quad (2.1)$$

$$(\mathbf{u}\cdot\nabla)\mathbf{u}=-\nabla p+\frac{1}{Re}\nabla^2\mathbf{u} \quad (2.2)$$

$$\nabla^2\phi=-4\alpha c \quad (2.3)$$

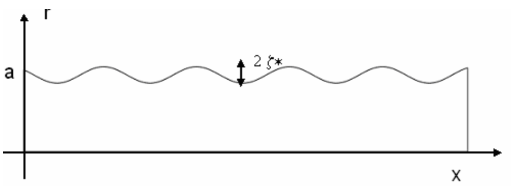

Figure 1. Axisymmetric pipe geometry with a wall structure given by $r=a+\varsigma * g(x)$ where ζ^* is an amplitude of the wall structure.

The dimensionless parameters of the problem are the Reynolds number, the Peclet-number and an electrostatic parameter

$$\mathrm{Re}=\frac{\bar{U}2a}{\nu}$$

$$Pe=\frac{\bar{U}2a}{D}$$

$$\alpha=\frac{1}{4}\frac{c_0 q^2 a^2}{\varepsilon_0\kappa T}.$$

Here $\bar{U}$ is the mean uniform velocity at inlet and a is the pipe radius, ν is the kinematic viscosity of air and D is the Brownian diffusion constant defined as

$$D=\frac{\kappa T\, Cu}{3\pi\mu d},$$

$$Cu=1+\frac{\lambda}{d}(2.34+1.05\exp(-0.39\frac{d}{\lambda}))$$

where Cu is the Cunningham factor which is a correction factor needed to bridge the gap between the continuum limit and the free molecular limit for the flow past a sphere. Here λ is the collision mean free path and d is the particle diameter. κ is Boltzmanns constant, T is the absolute temperature and μ is the dynamic viscosity of the air.

Equation (2.1) is an equation describing the evolution of the concentration c, which is an equation of convective-diffusion type with an extra source-term including the effects from the electric field. Equation (2.2) is the Navier-Stokes equation describing the evolution of the fluid flow and equation (2.3) is Poisson's equation which gives the link between the charged particles and the electric field.

3. Use of COMSOL Multiphysics

The set of equations (2.1-2.3) needs to be solved together as a system and using Comsol Multiphysics 3.5a or 4.0a greatly facilitates the solution of the problem. The application modes that have been used are Fluid dynamics, stationary Navier-Stokes, stationary Diffusion-convection and Electrostatics. The boundary conditions for the fluid flow are no slip on the pipe wall. At the inlet x=0 a uniform velocity is chosen and at x=L outlet conditions are applied. On the x-axis axial symmetry is chosen.

For the application of the diffusion-convection mode, the concentration at the inlet is uniform $c=c_0$. The boundary condition of the absorbing wall is $c=0$ and at the outlet convective flux is chosen. For the electrostatics mode, zero charge/symmetry is chosen at the inlet and outlet. Since the wall of the respiratory airways consists of a so called mucus-layer including mainly water, the wall is treated as a good conductor so the wall potential is chosen as zero. For the meshing adaptive mesh is applied and for the finest mesh the number of degrees of freedom are about 1000000.

4. Numerical Results

The morphology of the respiratory airways of the human lung is represented by a system of pipes where each pipe belongs to a certain generation. The first generation is a single pipe called trachea. After the trachea the pipe bifurcates into two pipes of generation 2. After these two pipes one more bifurcation takes place so that we end up with 4 branches of pipes in generation 3. This pattern is repeated until generation 16, after which further bifurcations follow, with the difference that now the so called alveoli appear which provide with the necessary gas exchange with the blood-vessel system.
In the upper airway generations another feature is present. The walls of the pipe have a so called cartilaginous ring structure, see figure 1-2. These rings can cause separation of the fluid flow and also modify particle deposition to the wall[4].

We have chosen to provide results from generation 4 for which the airway has a ring structure with an amplitude of 0.1 diameter. For light breathing conditions in generation 4 we have a mean velocity of 1.75 m/s. The radius is 2.25mm and the length of the pipe is 12.375 mm. The Reynolds number is then $\mathrm{Re} = 450$. The reason for choosing generation 4 is that here one can consider the flow as laminar in contrast with lower generations N=1-3 which are usually characterized by turbulent flow. To determine the Peclet number the size of the particles is important. We have chosen a particle with a diameter of 5nm, which gives a Peclet-number of Pe=100000.

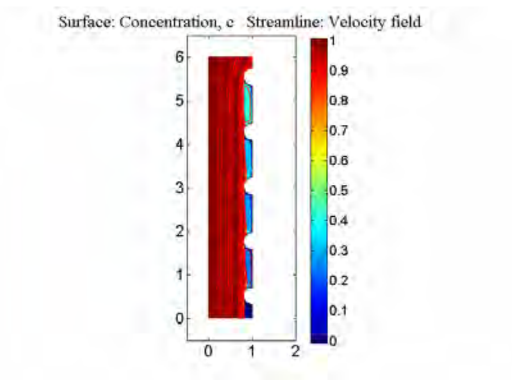

Figure 2. A pipe with a cartilaginous ring structure

We first consider results for uncharged particles. More results from this case is presented by Åkerstedt et al. (2010)[4]. In figure 3 the deposition is calculated for a smooth pipe and with a pipe with a cartilaginous structure with five rings.

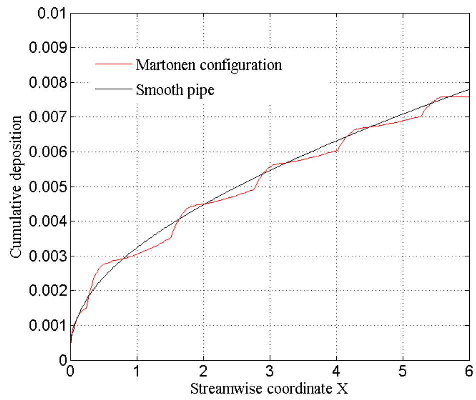

Figure 3. Cumulative deposition rate for a smooth pipe and a pipe with cartilaginous rings.

The local deposition is calculated as the local normal diffusion flux divided by the inlet convective flux. Figure 3 shows the cumulative deposition after a length X. In figure 2 the distribution of concentration and the streamlines are shown. It is to be noted that the flow separates in a region between the rings. The local maximum diffusion flux is found in the region close to the reattachment of the flow.

In general the local flux is smaller in the region between the rings. This means that the distance between the rings is of importance in the overall diffusion flux of the pipe.

Next consider the effect of charged particles. The dimensionless parameter that describes all electrostatic effects is then

$$\alpha = \frac{1}{4}\frac{c_0 q^2 a^2}{\varepsilon_0 \kappa T}$$

Here c_0 is the concentration of particles at the inlet and q is the charge of the particles.
As an example for generation 4 and particles that carry 10 elementary charges and where the particle concentration at inlet is $c_0=10^{10}$ particles/m^3 the electrostatic parameter is α=3.4.

First we give some results for a smooth pipe of generation 4 for different values of α. In figure 4 the concentration and the electric field is plotted. Since we consider positively charged particles the electric field is in the radial direction. Note also the very thin concentration boundary layer, which is expected for the large values of the Pe-number. For larger Pe-numbers this leads to numerical difficulties. In figure 5 the evolution of the concentration boundary layers is shown.

In figure 6 the total deposition after a length of 5.5 pipe radii is plotted for different values of the electrostatic parameter. It is seen that increasing α from 0 to 90 the deposition rate increases by a factor of 65%.

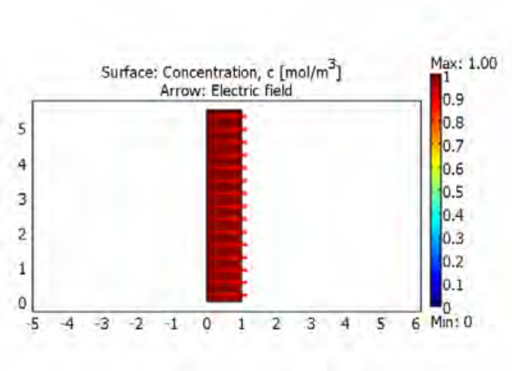

Figure 4. Concentration and electric field arrows for a smooth pipe.

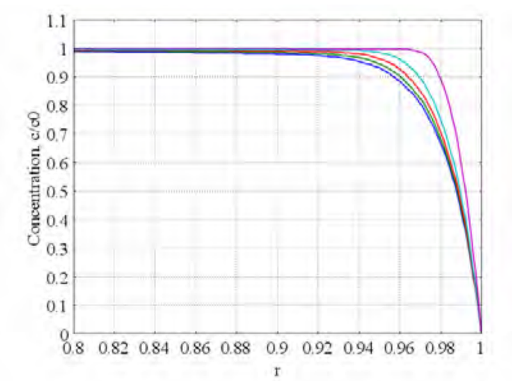

Figure 5. Evolution of concentration boundary layer for a smooth pipe.

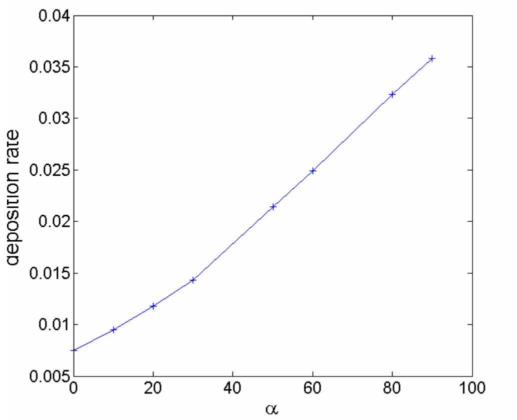

Figure 6. Smooth pipe deposition rate for different values of the electrostatic parameter α .

Next consider the influence of the cartilaginous rings on the deposition of charged particles. In figure 7 the concentration distribution and electric field arrows are shown for α=45. In figure 8 the deposition is plotted versus the elctrostatic parameter and for comparison the corresponding deposition for a smooth pipe is shown. Remarkably the deposition rate for charged particles is lower than the corresponding values for a smooth pipe. The reason for this is that in the separated regions the concentration is lower than in the main stream (see figure 9). Therefore the charge-density in the separated regions is lower and from this it follows that the electric field (see figure 10) and deposition become smaller.

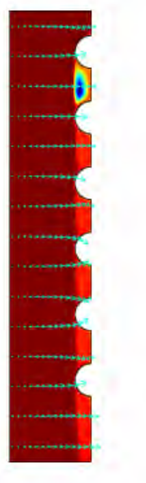

Figure 7. Concentration and electric field arrows for α=45

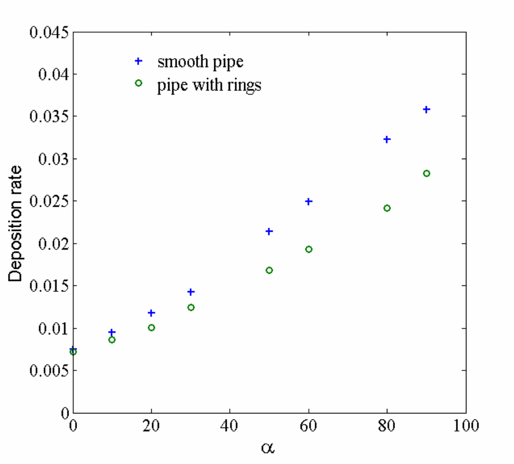

Figure 8. Comparison of deposition rates for a pipe with a Cartilaginous ring structure and a smooth pipe.

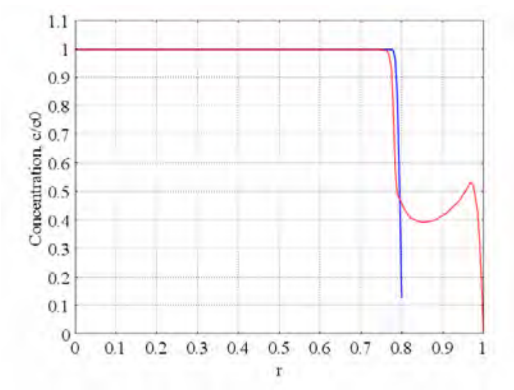

Figure 9. Concentration versus r along a line of separated flow(red) and along a line of no separation(blue).

4. Conclusions and discussion

The deposition of nano-sized charged spherical particles on the walls of cylindrical tube with a periodically spaced cartilaginous ring structure is investigated. The model includes convective and Brownian diffusion transport as well as effects from the electric field created by the charged particles.

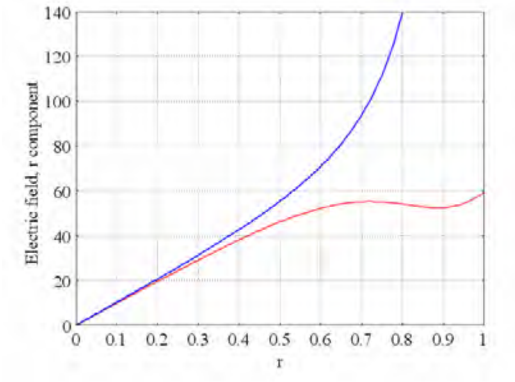

Figure 10. Electrical field, r component versus r along a line of separated flow(red) and along a line of no separation(blue).

The influence of the cartilaginous ring on the flow is to create a separated flow in the regions between the rings. This causes a difference in the concentration in the separated regions and the main stream, where the concentration in the separated regions is about one half of the concentration in the main stream.

We consider deposition of particles in generation 4 for light breathing conditions. The first case studied is the deposition due to the electric field caused by charged nano-particles for the case of a smooth pipe. The effects of the electric field can be described by one single dimensionless parameter; the electrostatic parameter α. Increasing α from zero to 90 the deposition is increased by 65%.

Next the effect of the cartilaginous rings is introduced with amplitude of the rings equal to 0.1 diameters. Comparison with the smooth pipe case the effect of the rings is to decrease the deposition rate. An explanation of this result is that the concentration in the separated regions (see figure 9) is lower, causing a smaller electric field (see figure 10) and smaller deposition.

Future work involves other generations, both higher and lower generations. For the lower generations N=1-3 the flow may be turbulent and the modification needed is to use a low-Re turbulent model for the flow, which also modifies the convective-diffusion equation.

For higher generations N>4 the effect of the cartilaginous rings is smaller. An interesting application of the present theory is to investigate the possibility of designing aerosols for optimized delivery of drugs via pharmaceutical charged aerosols.

5. References

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