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DEPOSITION OF NON-SPHERICAL PARTICLES (FIBRES) IN A CHANNEL WITH SUBSEQUENT BIFURCATIONS

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Abstract. *The article presents results from the non-spherical particle deposition in a geometrical model of part of the human airways. Particle deposition in the human airways is important subject of study. The fibrous particles in this work has been modeled using assumption of high aspect ratio of length to width. The orientation of fibrous particles is following the stream according to the forces (namely torque) implied by the flow-field. The flow is simulated by large eddy simulation (LES) using dynamic Smagorinsky sgs model. Particles are assumed rigid with a density of* $1000\,{}^{kg}/_{m^3}$ *and diameter of* $1e-6\,m$ *and the length* $2, 4$ *and* $6 \times d$*. One way coupling with the continuous phase (air at standard conditions) is considered only.*

Comparing the deposition results with the spherical particles clearly shows the dependence of the fibrous deposition on the inlet boundary conditions, namely turbulence quantities. While for the computations with globular particles the velocity profile with Ornstein-Uhlenbeck fluctuation generator is sufficient, for the fibrous particles it is also the orientation of the particles that plays role. The results from this study are going to be used for the deposition calculations on extended geometry and later compared with measurements conducted at the authors' institute.

1 INTRODUCTION

The article presents results from the non-spherical particle deposition in a geometrical model of part of the human airways. Particle deposition in the human airways is important subject of study. Many papers by various authors can be found on the deposition of spherical particles[1,2]. Most of the aerosols one is exposed to are, however, not spherical. Fibrous particles are known to be more dangerous in terms of medical risk as they can penetrate deeper into the lower airways where they can cause blockage or injury of the airways tissue.

The fibrous particles in this work has been modeled using assumption of high aspect ratio of length to width. The drag force on particle has been considered with respect to the shape of the particle following the correlations by Loth[3]. The orientation of fibrous particles is following the stream according to the forces (namely torque) implied by the flow-field. The flow is simulated by large eddy simulation (LES) using dynamic Smagorinsky sgs model. Particles are assumed rigid with a density of $1000\,{}^{kg}/_{m^3}$ and diameter of $1e-6\,m$ and the length 2, 4 and $6 \times d$. One way coupling with the continuous phase (air at standard conditions) is considered only.

2 MODEL

2.1 Fibrous particles and fluid flow

The fibrous particles can be modelled in a Lagrangian framework in several ways. Taking into account fibres of aspect ratios from 2 to 8 with a typical diameter of 1 μm the following model was programmed into OpenFOAM code Lagrangian library.

Let us assume fibrous particle with a constant diameter d and length L depicted in Figure 1. The aerodynamic force on particle F can be constructed from its longitudinal and perpendicular parts F_L and F_P respectively. To calculate the forces we are using following assumptions. The perpendicular force F_P is computed assuming drag force on a infinite cylinder following slander body theory[4]:

$$F_p = \frac{1}{2} C_d \rho \left(\mathbf{U_f} - \mathbf{U_p}\right)_p^2 d_p |\mathbf{b}|, \tag{1}$$

where C_d is the drag coefficient, $(U_f - U_p)i_p$ is the relative velocity component perpendicular to the fibre axis.

The axial component of the force is computed as the friction force on a flat plate of an equivalent surface area to the cylinder[5]:

$$F_L = \frac{2.6}{Re^{1/2}} \frac{1}{2} \rho \left(\mathbf{U_f} - \mathbf{U_p}\right)_L^2, \tag{2}$$

where Re is Reynolds number of the cylinder using relative velocity, and $(\mathbf{U_f} - \mathbf{U_p})_L$ is the relative velocity component in longitudinal direction. Calculating these forces, we can model the transportation of the fibrous particles. To incorporate also the orientation and rotation of the fibers, torque must be calculated. There is only perpendicular part of the force on fiber which generates the torque:

$$\mathbf{T} = \mathbf{b} \times \mathbf{F}, \tag{3}$$

$$|\mathbf{T}| = \mathbf{F_d}|\mathbf{b}|, \tag{4}$$

where $|\mathbf{T}|$ is the module of the torque and $\mathbf{b}$ is the orientation vector.

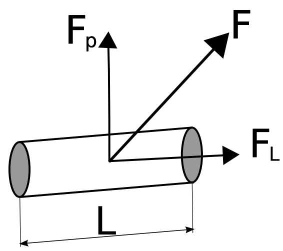

Figure 1: Forces on fiber

The fibrous particles are modelled as inert, without any influence on the air flow, and without any influence on the turbulence on the subgrid level.

The continuous medium is modelled as incompressible air using large eddy simulation LES employing dynamic Smagorinsky model for subgrid scales. The velocity fluctuations are induced at the inlet using artificial force in the momentum equations employing Ornstein-Uhlenbeck process.

The mesh is unstructured tetragonal with a typical grid size of 1×10^{-4} m. The time step of 1×10^{-4} m is used to keep the mean Courant number below 0.2. For time differencing Crank-Nicholson scheme was used and for convection terms central-difference scheme with a small amount of upwind to stabilize the solution with high Peclet numbers. The set of equations is solved using PISO algorithm with Geometric Multigrid model.

3 RESULTS

The results presented here are computed on a smooth channel of diameter 8 mm with 2 bifurcations resulting in a non-symmetrical configuration following the geometry of the 3rd to 5th generation of the real human airways we have available from a CT-scan. The outlets of the geometry has diameter of 6 mm. The geometry is depicted in Figure 2.

The asymmetry in geometry together with the flow field induced by a subsequent bifurcation brings also asymmetry in mass fluxes of the air as well as particles. This is clearly shown in Table 3, where also the difference with a mass fluxes in the realistic geometry is shown for two different Reynolds numbers.

This difference is given namely by the flow field pattern which develops in the airways. While in the real geometry the conical tubes and non-regular bifurcation geometry makes

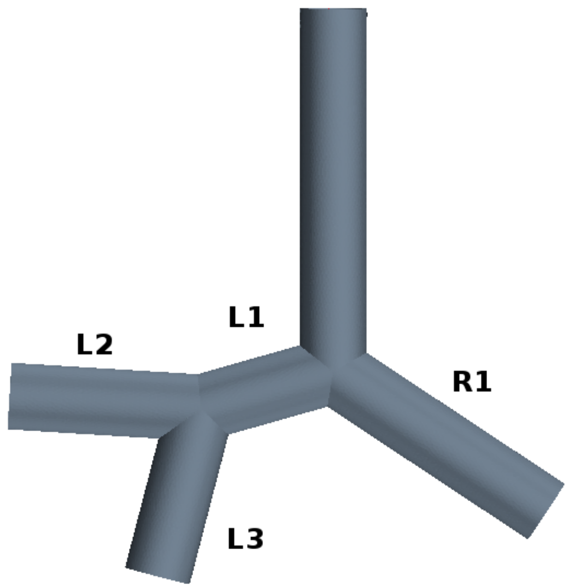

Figure 2: Geometry of the bifurcated channel

	Re = 100		Re = 1000	
outlet	real geo	idealised geo.	real geo	idealised geo.
R1	20.2	51.1	29.4	55.3
L2	39.8	24.5	42.5	22.5
L3	39.8	24.5	28.1	22.2

Table 1: Mass flux at different outlets (averaged values from LES computations)

the flow more regular in case of a smooth tube geometry the variation are larger as was seen during the transient LES simulation.

Figure 3 shows the fibers in the channel in time 0.4 seconds. Figure shows various orientations of the fibers (scaled in size). The Stokes number of the particles (based on the diameter rather than on the length) is 1×10^{-3}, For the low Stokes number particles the deposition was only 0.85 per cent for flow with $Re = 100$ and 0.48 per cent for $Re = 1000$ respectively. Previous computations shows much higher deposition for higher Stokes number particles. Further more detailed analysis of the flow as well as comparison with the spherical particles is currently in progress.

4 CONCLUSIONS

Comparing the deposition results with the spherical particles clearly shows the dependence of the fibrous deposition on the inlet boundary conditions, namely turbulence quantities. While for the computations with globular particles the velocity profile with Ornstein-Uhlenbeck fluctuation generator is sufficient, for the fibrous particles it is also

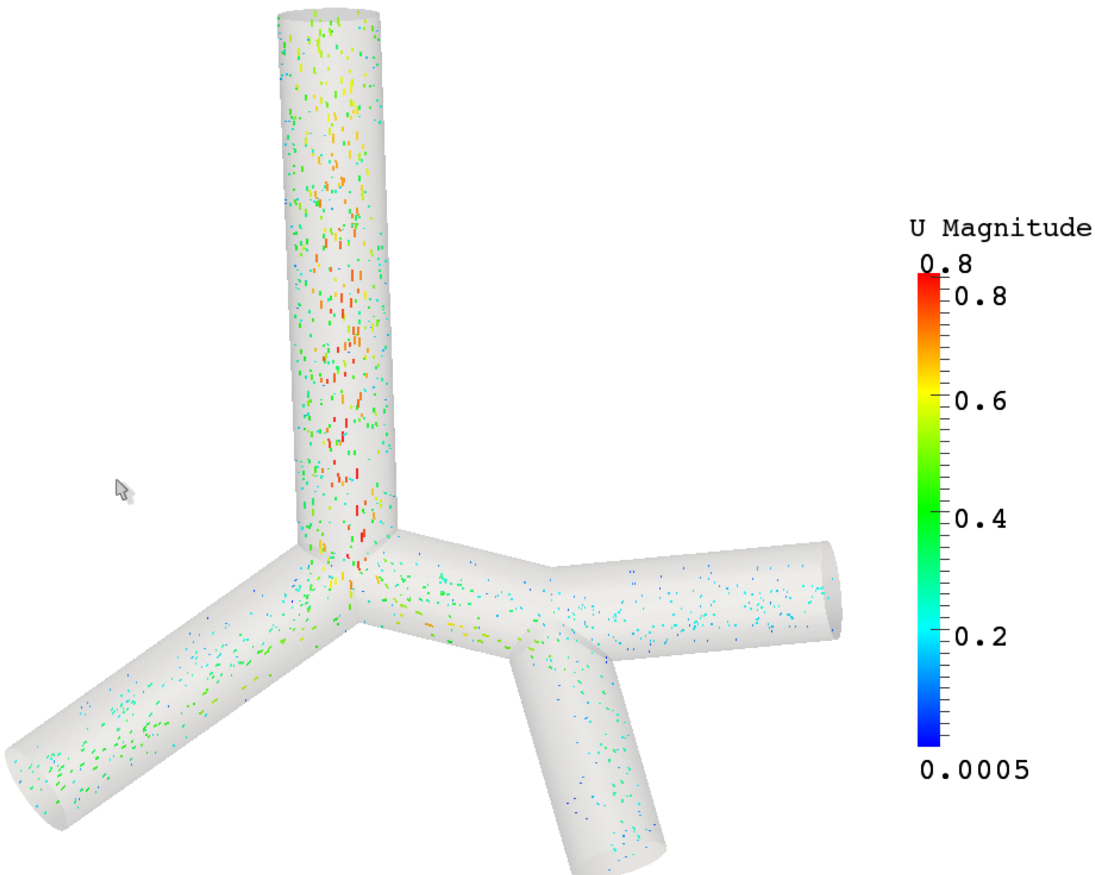

Figure 3: Fibers of length 6 and 4 times the diameter at time 0.4 second colored by velocity magnitude

the orientation of the particles that plays role. For that reason longer inlet part (trachea) had to been modelled including the epiglottis which influence the flow field significantly as has been shown by e.g. Forman [2]. The local distribution of the deposition defined by Deposition Enhancement Factor is different to the one of the spherical particles. The results from this study are going to be used for the deposition calculations on extended geometry and later compared with measurements conducted at the authors' institute.

5 ACKNOWLEDGEMENT

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