PARTICLE TRANSPORT IN A PULMONARY FLOW

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ABSTRACT

The study undertaken in this article is to develop a reliable and comprehensive numerical modelling of particle transport in pulmonary flow based on the use of CFD-ACE code of commercial calculation. This code includes a fluid solver that solves the Navier-Stokes in a finite volume formulation. The CFD-GEOM software was used to create the 3D surfaces of the generic model geometry Weibel and thereby generate the tetrahedral mesh unstructured finite volume. The air flow is assumed laminar stationary (or unsteady only in bronchial models) and incompressible, the particles of diameter 5 micrometers are spherical and non-interacting. So we have successfully modelled the flows and the transport of particles in simple configurations (Model Weibel) and realistic configuration (rat lung) and what we can say is that the simulation , although expensive in terms of computer memory and time (specially for particle deposition), does not present insurmountable difficulties. As against obtaining a realistic geometry and the associated mesh generation remains a delicate stage.

Keywords: computational fluid dynamics, particle transport, pulmonary flow, models of weibel, realistic configuration.

INTRODUCTION

Pulmonary flow is characterized by a series of bifurcations. The laminar flows in this type of bifurcations have been studied by many authors, but few researchers have focused on the efforts of the upstream turbulence. Indeed, although the flow is laminar in the bronchi (at least for normal respiration), it is turbulent in the upper airways. This turbulent appearance is paramount, as this significantly alters the transport and deposition of particles. In addition, many current research considers a steady flow at the entrance and therefore do not reproduce the cycle of breathing. These modeled air flows through an anatomically realistic system conduits and branches, are governed by contraction and expansion movements of the pulmonary system and alveolar sacs. Today, fluid dynamics (a science of everyday, but that seems very unknown) is a very active area of research with many unsolved or partially solved problems yet. She always uses numerical methods better known under the name of Computational Fluid Dynamics (CFD). In order to understand and characterize the transport of inhaled particles in human airways, many authors conducted various experimental and numerical studies that led to relevant results. We will be interested in this study to provide a reliable and comprehensive numerical modeling of particle transport in pulmonary flow without taking into account the movements imposed by breathing with the help of CFD-ACE commercial calculation code.

PARTICLE TRANSPORT EQUATIONS

For a steady laminar incompressible flow, the fluid transport equations can be written as:

Continuity

$$\nabla.\vec{v} = 0 \tag{1}$$

Momentum

$$(\vec{v}.\nabla).\vec{v} = \frac{-1}{\rho}\nabla p + \nabla.[\upsilon(\nabla\vec{v} + (\nabla\vec{v})^{tr})] \tag{2}$$

where $\vec{v}$ is the velocity vector, ρ is the fluid density, p is the pressure and υ the fluid kinematic viscosity [2].

The equation for the trajectory of the particle is obtained from the fundamental equation of fluid dynamics. In light of the small particle Reynolds numbers $\mathrm{Re}_p = \frac{\rho d_p |\vec{u} - \vec{v}_p|}{\mu} << 1$ (μ is the fluid dynamic viscosity) and a large density ratio, $\rho_p >> \rho$, the drag force is dominant , based on order-of-magnitude argument [1], [5]. These particles are relatively large, so Brownian motion can be neglected. The particulate material considered is far denser than fluid, causing terms that depend on the density ratio, such as pressure force, buoyancy force, virtual mass effect and Basset force to be very small. The lift forces in the present Stokes flow limit are negligible because of a lack of measurable particle spin (Magnus lift) and the laminar, low-level fluid shear fields (Saffman lift).

The motion of solid particles is suspension in a fluid is governed by the particle trajectory equation (Clift *et al*., 1978; Kleinstreuer, 2006) Equation. (3) where m_p is the mass of a single, spherical particle, $\vec{x}_p$ is the displacement, d_p and $\vec{v}_p$ are the diameter and the particle velocity, respectively, and C_{DP} is the drag coefficient Clift [1]:

$$m_p \frac{d^2\vec{x}_p}{dt^2} = C_{DP}\frac{\pi d_p^2}{4}\rho\frac{(\vec{v} - \vec{v}_p)|\vec{v} - \vec{v}_p|}{2} \tag{3}$$

$$C_{DP} = \frac{C_D}{C_{slip}} \quad (4)$$

$$C_D = \begin{cases} \dfrac{24}{\mathrm{Re}_p} \; pour \; 0 < \mathrm{Re}_p \le 1 \\ \dfrac{24}{\mathrm{Re}_p^{0.646}} \; pour \; 0 < \mathrm{Re}_p \le 400 \end{cases} \quad (5)$$

The correlation for the slip factor, Cslip, is also given by Clift *et al*. [1], [2], [4]. The representative Stokes number range and associated parameter values are given in Table-1.

The mesh topology was determined by refining the mesh until grid independence of the flow field solution was achieved. Grids consisting of about 180,000, 360,000, 700,000 and 1,000,000 cells were tested. Little variation in the parameters of interest, i.e., particle deposition efficiency and the general velocity field was observed between the two highest grid density solutions. The final mesh size of the planar and non-planar configurations was 360,000 and 394,537 cells, respectively (because the mesh 1232438 is too expensive) (Table-2).

Table-1. Numerical parameters of the steady flow.

Reynolds Number	Velocity inlet (m/s)	Stokes Number	Particle diameter, $dp(\mu m)$	Particle density, $\rho p(kg.m{-}3)$
1000	2.649	0.02-0.12	5	602 - 3612

Table-2. Data on the grid meshes configurations.

Data on the 3D model grid Weibel	In-plane model without tracheal rings	In-plane model with tracheal rings	Out-of-plane model 1	Out-of-plane model 2
Total number of nodes	81774	98786	82005	82847
Total number of triangular faces	821955	1004313	823860	822480
Total number of tetrahedral cells	393660	481987	394537	393902

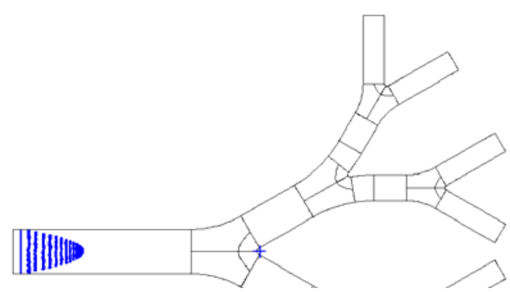
RESULTS

Our study focuses on numerical modeling of the transport and deposition of particles in a stream of airways in the lung using the CFD-ACE commercial code.

The particles, the number of 19 000 particles distributed concentrically, are released at the input of the model. The flow is stationary. Convergence time was not ensured. In what follows, we will discuss and analyze the behavior of particles carried in cylindrical pipes.

Figure-1 depicts the time evolution of particle dispersion and deposition at ($ReD1$ = 500 and St=0.02). The solid circles represent particles which have deposited while the open squares indicate moving particles. It is a mid-plane view of 3-D instantaneous particle distributions and surface depositions. Convected by the air velocity profile, a nearly parabolic volumetric particle distribution can be seen near the inlet at $t = t1 = 0.005s$ just after release. It should be noted that the particles outside the introduced bolus, which are moving slowly or have deposited were released earlier, i.e., before time $t1$. The inlet particle cloud released at $t1$ splits axisymmetrically at the first junction after only 0.075 s, and then enters first the inside second daughter tube, following the skewed flow field at t =0.08 s. At time level t =0.1 s, the inside third bifurcation has been reached, and at t =0.12 s the initial particle volume is distributed throughout the triple bifurcation airway with slowly moving particles still in the parent tube or the first daughter tube near the wall. At t = 0.15 s, almost most of the particles reached the outlet of the computational domain (see Figure-1 (f)).

Figure-2 shows a zoom on the distribution of particles observed near seemingly random duct wall-parent. The study comparing two different meshes at t = 0.1 s (see Figure-2 a) shows similar results. Dispersion is due to the unstructured cells and the difference with respect to a structured mesh is significant [2]. This dispersion is explained by the lack of smoothness of the mesh in the near-wall region. Note that the mesh refinement in the parietal regions is very delicate in unstructured and poorly managed by the mesh CFD-GEOM used here. The ideal would be to generate a structured mesh or at least cuboids near the walls but again the mesh used proved faulty.



(a)

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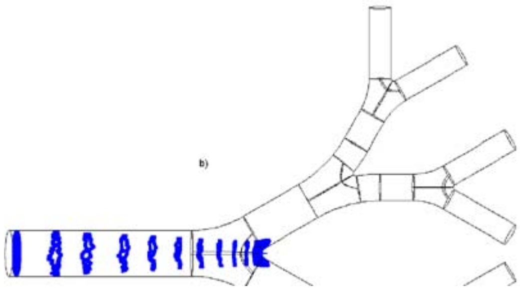

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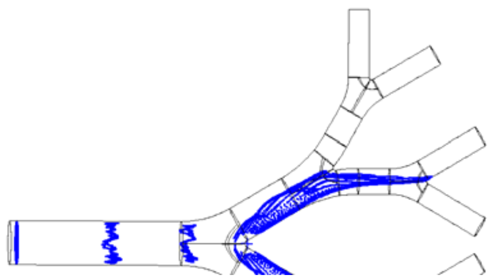

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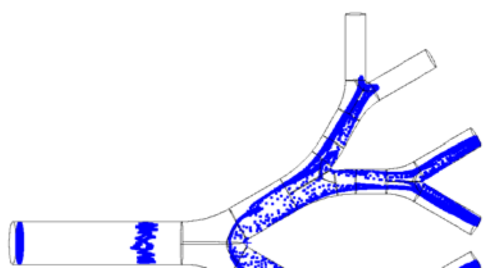

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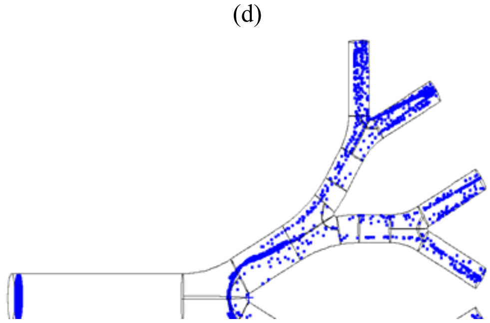

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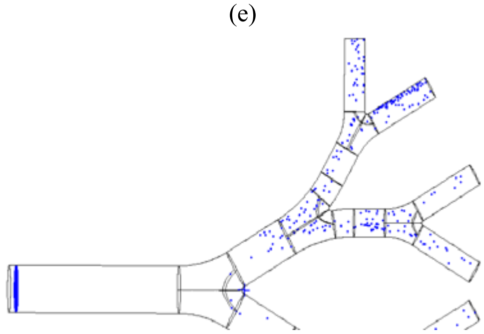
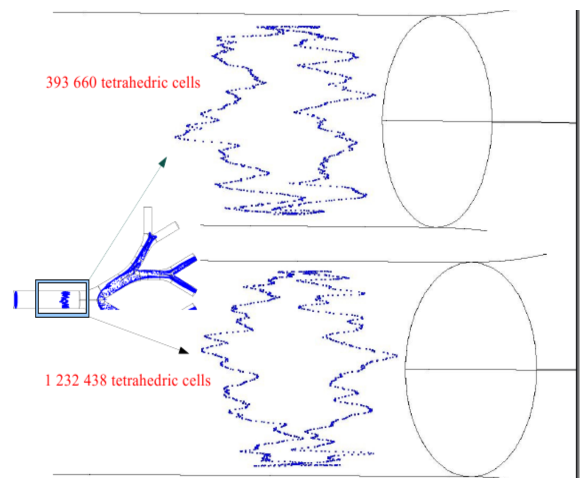


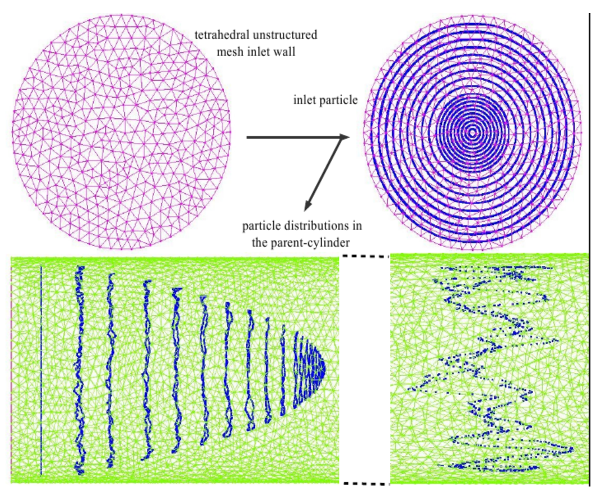
(f)

Figure-1. Particle positions at different instants of time during the inspiratory flow.

We validated the model of deposition for different four generations model defined by Weibel [9] for both steady and unsteady flows: two planar axes geometries (with and without tracheal rings) and two off-planar geometries obtained by a 30 degrees rotation at each bifurcation. The results are found in a very good agreement with existing bibliography [2], [3].



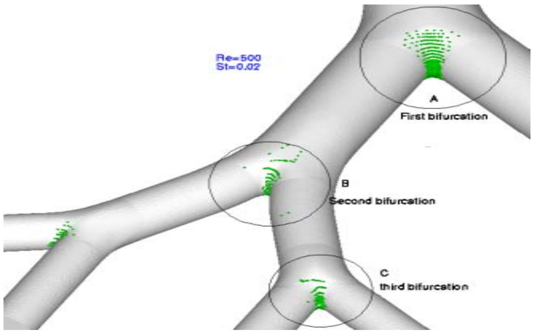
(a)



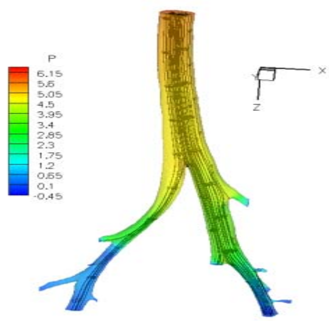
(b)

Figure-2. Behavior of particles observed near mesh wall unstructured tetrahedral.

The so obtained model is applied to the simulation of flow and particle deposition in a realistic geometry of rat lungs which is generated by a μ-CT reconstruction of a real animal provided by biophysicists of nuclear medicine, CHU Hautepierre, Strasbourg (cf. Figure-3 (b)). The figure (cf. Figure-3 (a) and (c)) represents the particle deposit and the flow at the end of the numerical simulation. Massive deposits occur only in bifurcations and they decrease from generation to generation.



(a)



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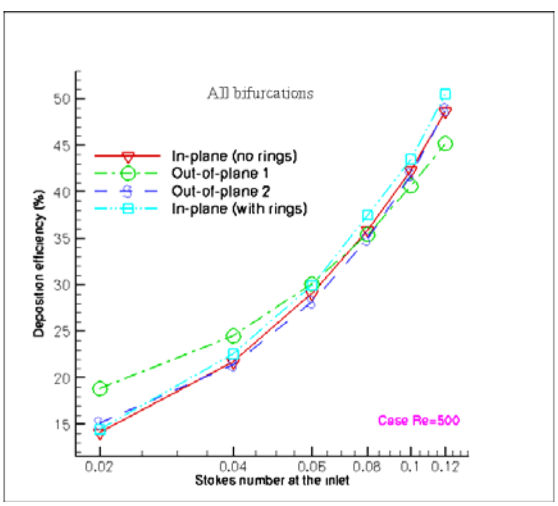

(c)

Figure-3. a) Three-dimensional view of local particle deposition patterns under steady inhalation, b) Wall pressure and streaklines for the rat model and c) Particle deposition efficiencies of the triple bifurcation models.

CONCLUSIONS

The major difficulty that highlights this study is to generate the mesh. To have a good mesh must be found suitable mesh and learn to master it. If one is interested in moving geometries to follow the deformations caused by breathing, mesh quality is even more problematic. One possible solution would be to turn to the technique of submerged Borders (Immersed Boundary Methods) where the geometry is superimposed on a Cartesian grid and imposed on the flow through the terms of forcing. Thus, it is much easier to deform the geometry because the mesh is fixed. A study of this method is in progress in the team instabilities, turbulence, two phases (ITD) of the ICube Laboratory (France) to write an unstructured solver, Cartesian, and massively parallel based on the IBM method (see Figure-4). In addition, this solver incorporates an automatic mesh refinement so that the mesh automatically adapts to the flow and geometry. This solver therefore requires more initial mesh as it adapts itself to the configuration and will facilitate all the biomechanical studies.

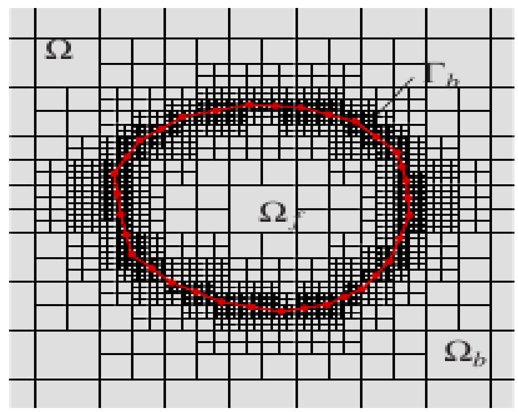

Figure-4. Principle of IBM methods: digital fine mesh $\Omega = \Omega_b + \Omega_f$; immersed surface mesh Γ_b ; non-fluid region Ω_b and fluid region Ω_f .

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