Computer Methods in Biomechanics and Biomedical Engineering
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gcmb20

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Version of record first published: 26 Sep 2012.

To cite this article: T. Xiong, H. Ilmi, Y. Hoarau, P. Choquet, C. Goetz, A. Fouras, S. Dubsky, M. Braza, S. Sainlos-Brillac, F. Plouraboué & D. Lo Jacono (2012): Flow and particles deposition in anatomically realistic airways, Computer Methods in Biomechanics and Biomedical Engineering, 15:sup1, 56-58

To link to this article: http://dx.doi.org/10.1080/10255842.2012.713731

Computer Methods in Biomechanics and Biomedical Engineering
Vol. 15, No. S1, September 2012, 56–58

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Keywords: particle deposition; rat lungs; rabbit lungs; numerical simulations

1. Introduction

The aerosol particles present in our environment are identified as increasingly risk factors for the human health. In particular, small particles that reach the surface of gas exchange in the alveolar region of lungs are considered most harmful to health. Nevertheless, aerosols can also be used for diagnostic or therapeutic purposes to treat lung diseases. Inhalers, for example, are commonly used to administer drugs. In cases of lung disease, administration of medication by aerosol has the advantage of reaching the region directly affected and requires lower doses (side effects are minimized).

The morphological descriptions of the bronchial tubes of a man has appeared in literature since 1963, when Weibel (1963) introduced a physical symmetric model. The human lung is a sequence of bifurcations in two parts. It has an average of 23 generations of bifurcations which represent about 17 million of bifurcations. The last five generations are covered with cellular structures through which the exchange takes place with the blood gas (Weibel 1984).

The understanding of the flow structures and the particle transport/deposition across the human bronchial system remains a challenge to achieve because of the complexity of the geometry of human lungs.

This work relies on a strong collaboration between physicians, medical imaging researchers, fluid mechanics researcher and CFD researchers.

2. Methods

Our study focuses on the numerical modelling of the flow and particles deposition in airways using the commercial package CFD-ACE. The objective of this study was to propose a reliable and complete numerical model of transport of particles in the pulmonary flow by taking into account the full breathing cycle. For the moment, the movement of the airways imposed by the breathing is not taken into account.

This study is divided into four parts:

- First the CFD-ACE package is validated regarding flow (Zhao and Lieber 1994; Comer et al. 2001) and particles deposition in a simple model (Kim and Fisher 1999; Comer et al. 2001).
- Simple geometries derived from the Weibel model are studied.
- An anatomically realistic model of a rat lung is simulated.
- A more complex geometry of a rabbit lung is simulated.

The particle trajectories and deposition are obtained by solving a Lagrangian transport equation where only the drag force is retained. The deposition efficiency is computed as the ratio of the amount of particles stuck at the wall over the total number of released particles.

The rat geometry is obtained after an adult rat killed by IV administration of barbiturics and was infused with an iodine contrast agent (10% v/v, Visipaque320, GE Healthcare, Chalfont St Giles, UK). Imaging of the thorax was performed *ex vivo* using an X-Ray μCT scanner (eXplore Vision 120, GE Healthcare, Waukesha, USA). The protocol used involved 360 views over 360°, with one frame averages, at 100 kV, 50 mA. After reconstruction using a Feldkamp algorithm of back-projection, the imaging volume was made of cubic voxels of 49 μm × 49 μm × 49 μm. Visualisation was performed using MicroView (GE Healthcare, Waukesha, USA). After invertion of grey levels, a surface rendering (marching cubes algorithm) was applied after thresholding. The surface was then exported in stl format and prepared in *gmsh* before being meshed in *CFD-GEOM*.

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ISSN 1025-5842 print/ISSN 1476-8259 online

http://dx.doi.org/10.1080/10255842.2012.713731
http://www.tandfonline.com

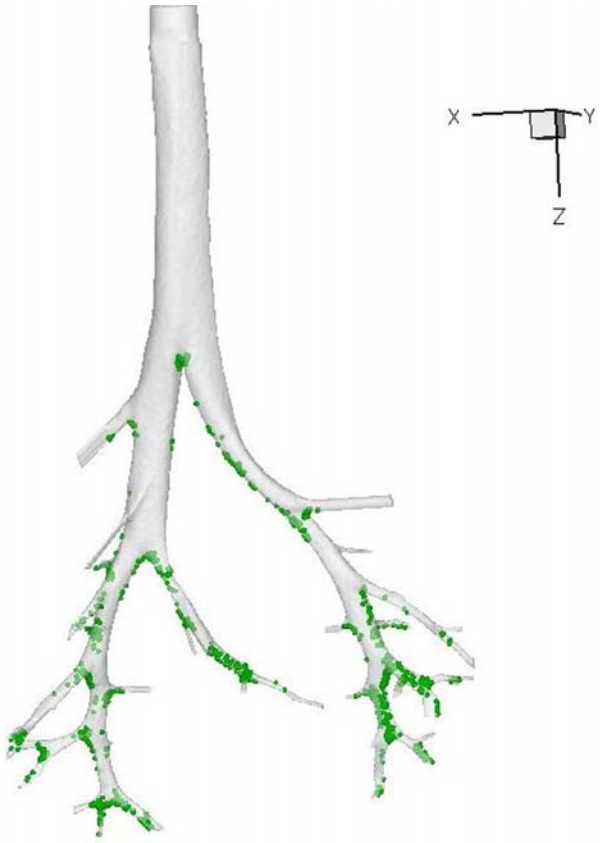

Figure 1. Deposition in rat lungs.

The rabbit geometry was obtained using synchrotron-based dynamic computed tomography. Details of the experimental technique and segmentation protocol are provided elsewhere (Dubsky et al. 2012). Briefly, newborn rabbit pups are ventilated and imaged using propagation-based phase-contrast imaging. The lungs are an ideal sample for phase-contrast imaging, as they exhibit large phase boundaries at air–tissue interface. This technology can provide rapid imaging of the lungs without contrast agent (Fouras et al. 2012). By synchronising the image acquisition with the ventilation and by rotating the sample, 4D (4D = 3D + time) images of the bronchial tree can be achieved. Again, one stl geometry was prepared in *gmsh* before being meshed in CFD-GEOM.

Most of this work was performed by Ilmi (2012) during the thesis preparation; the remaining part was studied by T. Xiong during her master 2 internship.

3. Results and discussion

Concerning the Weibel's generic models, the solutions generated by the solver CFD-ACE were in very good agreement with the literature, and we evidenced the importance of the Dean vortices on both the flow and the particles deposition. The deposition is essentially of inertial type and the deposition efficiency increases with both the Stokes and the Reynolds numbers. The deposition occurs mainly at the bifurcations. We have simulated different geometries where the successive bifurcations were rotated by 90°, and we observed a strong influence of the geometry: at the first bifurcation, the Dean vortices are properly split in each bifurcation, and the flow rate in the inner tube is much higher, but at the second bifurcation the Dean vortices are broken and the flow is more chaotic, the particle deposition is also significantly higher.

The simulations of the rat and the rabbit lungs raised the major difficulty of this study: the appropriate grid generation. Very fine grids were necessary to obtain grid convergence on the particles' deposition and such grids are very difficult to obtain in these kinds of complex geometries.

The rat geometry is quite linear and no recirculations were found. The particles deposition is again mainly inertial, increases with the Stokes number and occurs in the lower bifurcations (Figure 1) because they are pushed towards the wall after each bifurcation.

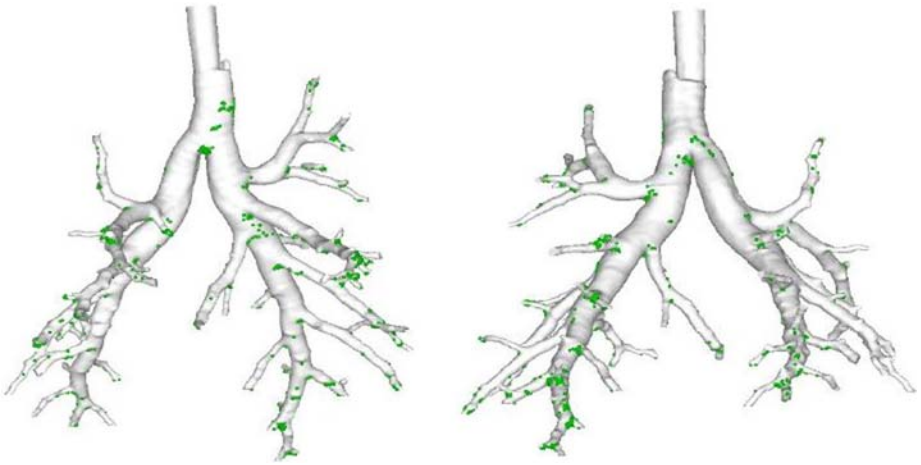

Figure 2. Deposition in rabbit lungs.

The rabbit geometry is much more complex and a large and strong vortex appears near the inlet because of the intubation which causes abnormal particle deposition at the inlet (Figure 2). Dean vortices were evidenced in few bifurcations. The deposition occurs at the bifurcations in the lower part of the airway and again it increases with the Stokes number which is characteristic of the inertial process.

4. Conclusions

After a validation phase, we have simulated the flow and the particle deposition in many of Weibel's generic models and in anatomically realistic geometries of rat and rabbit coming from medical imaging. The particle deposition is mainly inertial and increases with the Stokes number and the Reynolds number. One of the major difficulties of this study is the generation of the appropriate mesh for the realistic geometries.

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