

CRITICAL ASPECTS OF FLOW AND AEROSOL SIMULATIONS IN THE AIRWAY TRACT

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Abstract

The numerical prediction of the propagation of aerosols in airways is an area of growing interest [1, 2]. For instance, predicting the deposition patterns of particles in the mouth-throat or the inner lung pathways is needed for designing inhalers. Indeed recovering experimental deposition patterns, both in vivo and in vitro, happens to be difficult and expensive, and one often has to rely on numerical models of gas-particle flows for predicting such patterns in a cost-effective way. Two approaches are commonly used to model such multiphase flows, namely the Eulerian and Lagrangian approaches, but much of the literature on aerosols in airways rely on the Lagrangian tracking approach [1, 2]. A common justification for the use of the Lagrangian approach is that air flows in airways are internal and pulsatile, and present reverse flow regions, potentially leading to crossing particle trajectories. These arguments have been partly waived by a recent paper [3]. An Eulerian model could provide a competitive approach to compute internal dilute gas-particle flows, even in the presence of recirculations. In [4], we obtained numerical results of

gas-particle flows in a 2-D prototype airway using a FEM for an Eulerian model. We recently extended our previous Eulerian model to the aerosol propagation in 3-D patient-based geometries of the airway tract [6]. CT images of the thorax were processed to generate the geometry of the trachea and the first six bronchus generations [5]. The air flow was then obtained by solving the Navier-Stokes equations for different values of the flow dimensionless parameters. Preliminary numerical results for aerosol propagation in these geometries were obtained by coupling our Eulerian model with the previous flow solutions. Figure 1 shows the time-evolution of the aerosol density on a vertical cross-section of the airway tract. In the current paper, we investigate the critical aspects required to improve the realism of the simulations. Among these critical aspects, we consider the boundary conditions on in- and out-flow boundaries. During inspiration, the in-flow boundary is the cross-section of the trachea below the pharynx. In-flow boundary conditions requires special care as the flow is perturbed downstream of the pharynx. The out-flow boundaries includes all the cross-sections of the third to sixth generation bronchi. The out-flow boundary conditions control the global distribution of air between the right and left lungs. The general simulation strategy, as well as techniques to handle these critical aspects, will be covered in the talk.

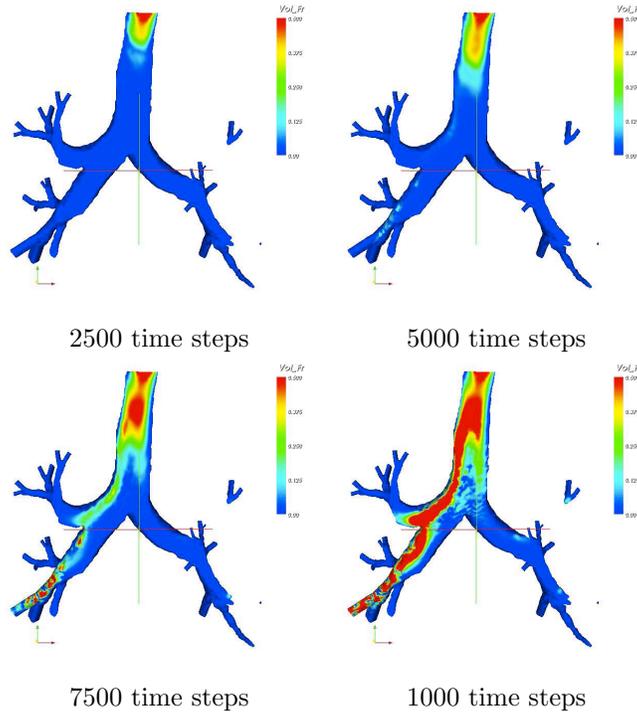


Figure 1: Volume fraction of aerosols at various times.

KeyWords: *Aerosols in airways, multi-phase flows, Eulerian model, finite element methods.*

References

- [1] Z. Zhang, C. Kleinstreuer, and C.S. Kim, *Cyclic micron-size particle inhalation and deposition in a triple bifurcation lung airway model*, J. of Aerosol Sc. **33** (2002), 257–281.
- [2] E. A. Matida, W. H. Finlay, C. F. Lange, and B. Grgic, *Improved numerical simulation of aerosol deposition in an idealized mouth-throat*, J. of Aerosol Sc. **35** (2004), 1–19.
- [3] Z.F. Tian, J.Y. Tu and G.H. Yeoh, *Numerical simulation and validation of dilute gas-particle flow over a backward-facing step*, Aerosol Sc. and Technology, **39** (2005), 319–332.
- [4] Y. Bourgault, *Computing gas-particle flows in airways with an Eulerian model*, Eur. Conf. Computational Fluid Dynamics (September, 2006), ECCOMAS CFD 2006, Egmond aan Zee, The Netherlands.
- [5] C. Fetita, S. Mancini, D. Perchet, F. Prêteux, M. Thiriet, and L. Vial. *An image-based computational model of oscillatory flow in the proximal part of tracheobronchial trees*, Comput. Meth. Biomech. Biomed. Eng. **8** (2005), no. 4, 279–293.
- [6] Y. Bourgault and M. Thiriet, *Simulation of aerosols in the airway tract with a 3-D Eulerian model*, 6th Internat. Congress on Industrial and Applied Mathematics (July, 2007), Zurich, Switzerland, pp. 16–20 .