NUMERICAL PREDICTION OF AEROSOL DEPOSITION IN THE UPPER HUMAN AIRWAYS

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Aerosolized medicines

Aerosolized drug delivery via the pulmonary route is becoming a promising method for the treatment of diseases. Computational methods offer a valuable approach for predicting deposition characteristics. These methods can provide complementary understanding to experiments in-vivo/in-vitro. Detailed information can be obtained of local deposition patterns inside the lung geometry, showing local hot spots and regions reached less easily by the medicine at a given aerosol size.

Transport and deposition of aerosol drug can be simulated using either a Lagrangian point-particle approach, where the aerosol particles are represented as discrete entities, or the Eulerian approach in which the aerosol is considered as a continuous phase. We will compare the performance of these two methods in terms of the predicted regional aerosol deposition. Particular attention will be given to spatial resolution requirements in relation to the precise deposition – central and upwind discretization methods will be compared, with and without additional near-wall grid refinement to resolve boundary layers.

Numerical modeling – accuracy limitations

Predicting regional aerosol deposition in the upper human airways is approached on the basis of a detailed spatial model, which includes the oral cavity and the first seven generations of the tracheobronchial tree. Computational deposition predictions are compared with deposition data obtained from in-vitro measurements that also include regional deposition information.

Figure 1 shows the geometry of the upper airways along with the segments and their numbering as used in the in-vitro deposition measurements of Lizal et al. (2015). Figure 2 shows the Deposition Fractions per segment of spherical particles with a diameter of 4.3 μm during steady inhalation at an inlet flowrate of 15 lt/min. The CFD toolbox OpenFOAM was used for the simulations. Good general agreement is observed between CFD and measurements at appropriate spatial resolution and discretization of the momentum and particle transport equations.

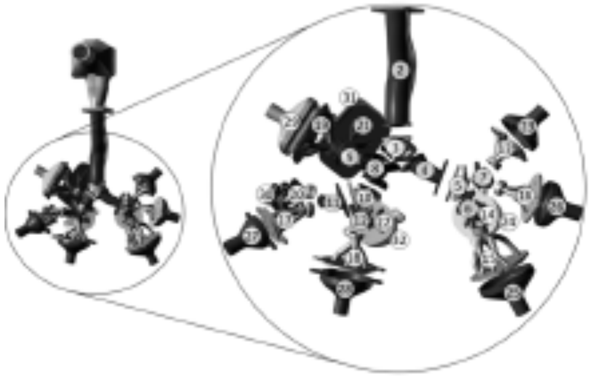

Figure 1: Geometry of the human upper airways (left) and segments with their numbering as used in the experiment (right).

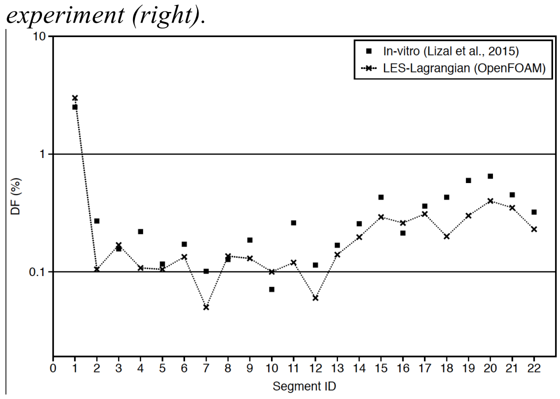

Figure 2: Deposition fraction per segment comparing CFD and in-vitro measurements of Lizal et al. (2015).

Conclusion

A detailed model of the upper human airways can be used as basis for the computational modeling of the dispersion of aerosol droplets. Both Euler-Lagrange and Euler-Euler models showed good agreement with experimental deposition data. The reliability of the predictions was found to be sensitive to the spatial resolution as well as the discretization method. Through cross-comparison between different methods of discretization (central- and upwind methods) and models, the general convergence of the results will be quantified and presented at the conference.

References

1. Lizal F., Belka M., Adam J., Jedelsky J., and Jicha M. (2015) A method for in-vitro regional aerosol deposition measurement in a model of the human tracheobronchial tree by the positron emission tomography. Proc IMechE Part H: J Engineering in Medicine, 229 (10), 750-757.