Modeling transport and evolution of aerosols for accurate predictions of local deposition in an in-vitro exposure system

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Introduction
Understanding the physical conditions governing deposition of aerosol droplets and its influence on the cell functioning is a key step towards the ultimate goal to relate the exposure of inhaled and deposited aerosols to health outcomes. This is important two-fold, i.e., the same physical mechanisms are acting in much more complex geometries (e.g., human airways), and simultaneously acquired knowledge allows for improved in-vitro inhalation toxicology experiments. Evaluation of flow and aerosol dynamics together with aerosol deposition in the in-vitro exposure system is presented here.

Validation of computational approach
Developed compressible low-Mach Navier-Stokes aerosol drift-flux OpenFOAM® solver ([1, 3]) validated for pipe geometry flow by comparison with DNS results (boundary Reynolds number Reτ = 180).

Extruded polyhedral mesh and snapshot of velocity magnitude:

Comparison of in-house results with Direct Numerical Simulations by Kasagi [2] for the mean flow and r.m.s. velocity fluctuations:

Flow rate [mL/min]
Deposition [%]

¯\(d\) = 0.2µm - impaction+settling
¯\(d\) = 0.2µm - impaction
¯\(d\) = 0.4µm - impaction+settling
¯\(d\) = 0.4µm - impaction

Deposition of two different aerosol mean particle sizes \(d\) taking into account impaction and gravitational settling for four various flow rates

Conclusions
• Aerosol mixing and uniformity in the exposure system can be controlled via proper adjustments of flow rates
• Developed computational framework allows for accurate computations of aerosol flow and deposition in exposure systems
• Future: application of developed platform for complete evaluation of in-vitro exposure studies

References


Acknowledgements: The research presented in this poster was financially supported by Philip Morris Products S.A. The authors wish to thank Vitrocell® Systems GmbH for delivering geometry of the exposure system.