Multispecies Aerosol Evolution and Deposition in the Human Respiratory Tract

Mahdi Asgari[1], Francesco Lucci[1], Arkadiusz K. Kuczaj[1,2]

[1] PMI R&D, Philip Morris Products S.A., Quai Jeanrenaud 5, CH-2000 Neuchatel, Switzerland

[2] University of Twente, Faculty EEMCS, Multiscale Modelling and Simulation, P.O. Box 217, 7500 AE Enschede, The Netherlands

Introduction and Objectives

Respiratory aerosol deposition depends on a variety of factors ranging from complex airflow in the respiratory tract to the evolving physical and chemical aerosol properties. Inhaled aerosol transported through the respiratory tract geometry experiences thermal and humidity conditions variation inducing aerosol evolution in size and liquid-gas partitioning of multispecies composition. Induced aerosol evolution consequently alters the particles deposition as a size dependent mechanism in various segments of the respiratory tract geometry. We have addressed some of the relevant questions and challenges in studying aerosol evolution and deposition in the human respiratory tract with the following objectives:

- Evaluation of mechanisms contributing to particle deposition and the effect of inhalation flow rate.
- Evaluation of aerosol size evolution in human airways under existing temperature and humidity variations.
- Quantification of the influence of aerosol evolution on deposition in human airways.

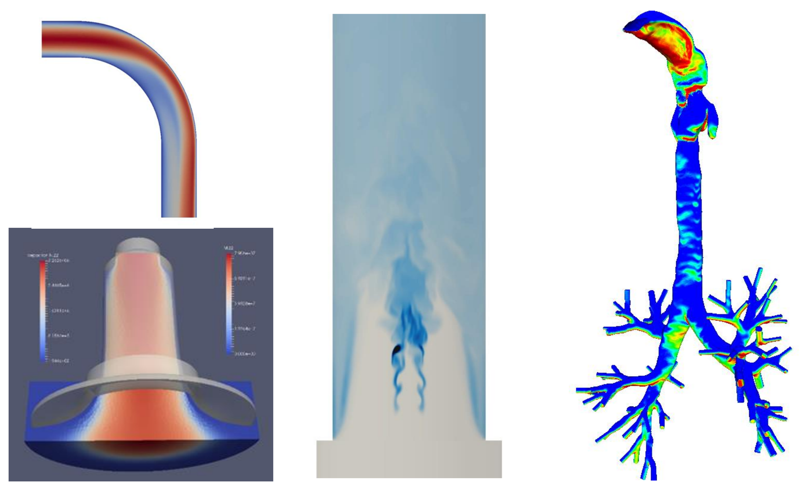
Computational Solver - AeroSolved

Computational Fluid Dynamics (CFD) code based on the OpenFOAM platform for simulations of generation, transport, evolution and deposition of multispecies aerosol.

AeroSolved

OpenSource
on GitHub:
pmpsa-cfd/aerosolved

GPL v3 Free Software — Free as in Freedom

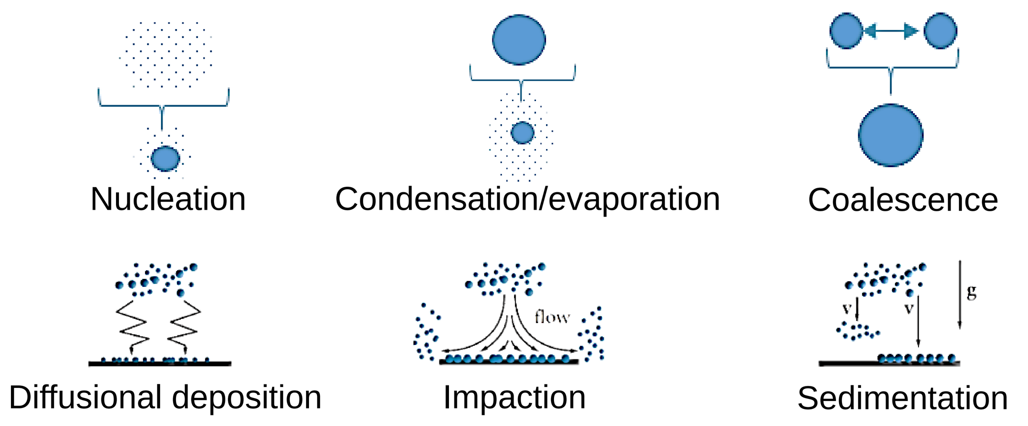


Applications

- Research on aerosol physics
- Development, characterization, and validation:
  - Inhalation devices
  - Aerosol generators
  - Aerosol delivery and exposure systems
- Wide range of applications from industrial processes such as sprays and emission reduction to environmental and atmospheric sciences

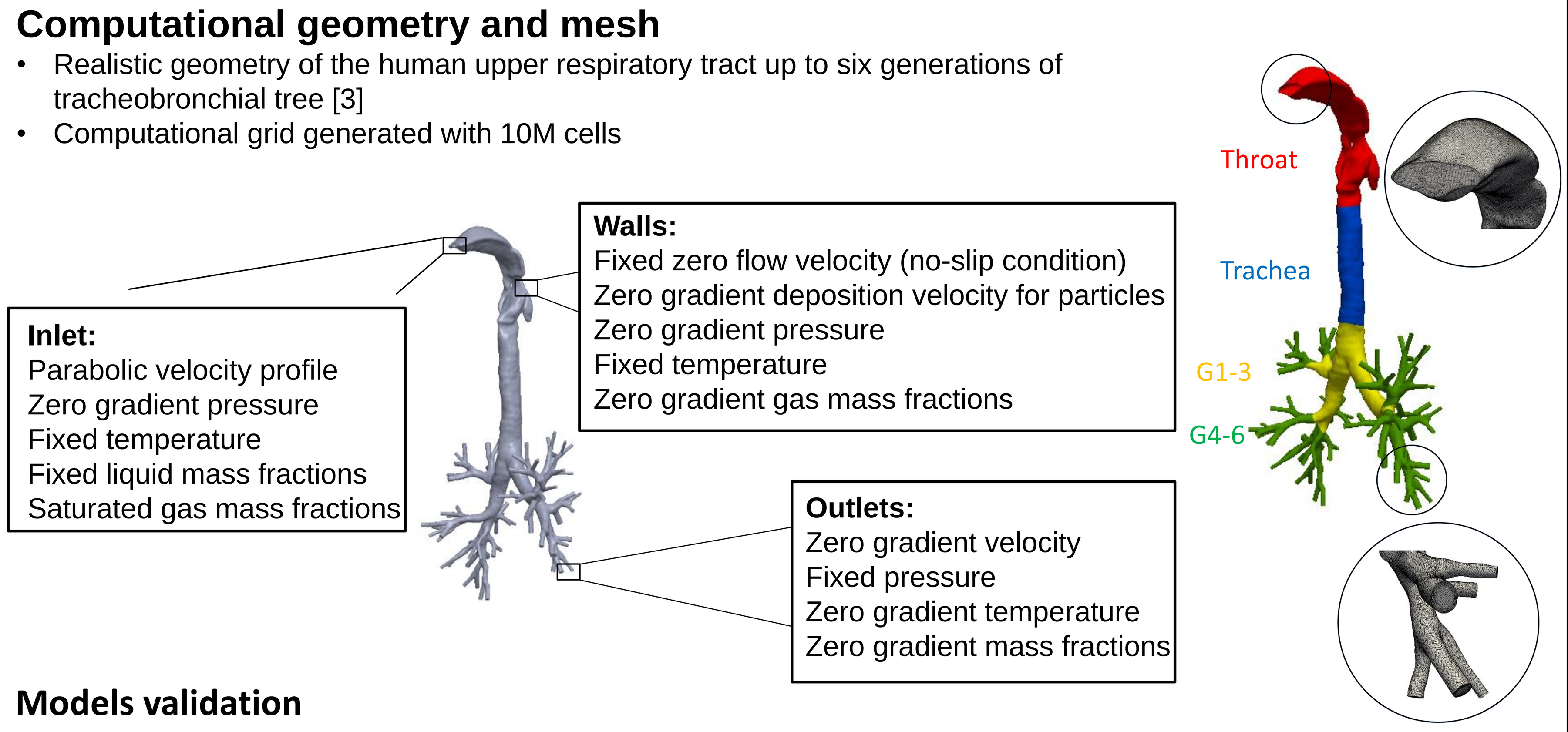
Aerosol processes

- Aerosol evolution
  - Condensation/evaporation
  - Nucleation
  - Coalescence
- Particles deposition
  - Diffusion
  - Impaction
  - Sedimentation



Computational geometry and mesh

- Realistic geometry of the human upper respiratory tract up to six generations of tracheobronchial tree [3]
- Computational grid generated with 10M cells



Models validation

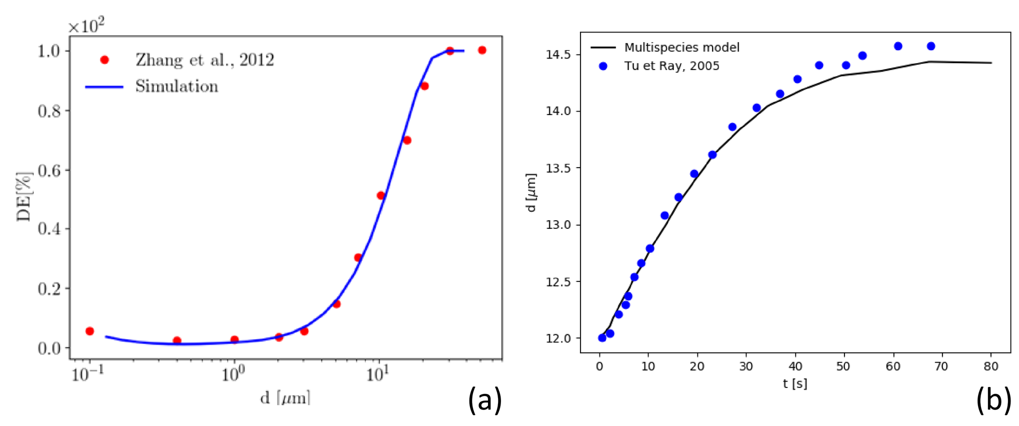
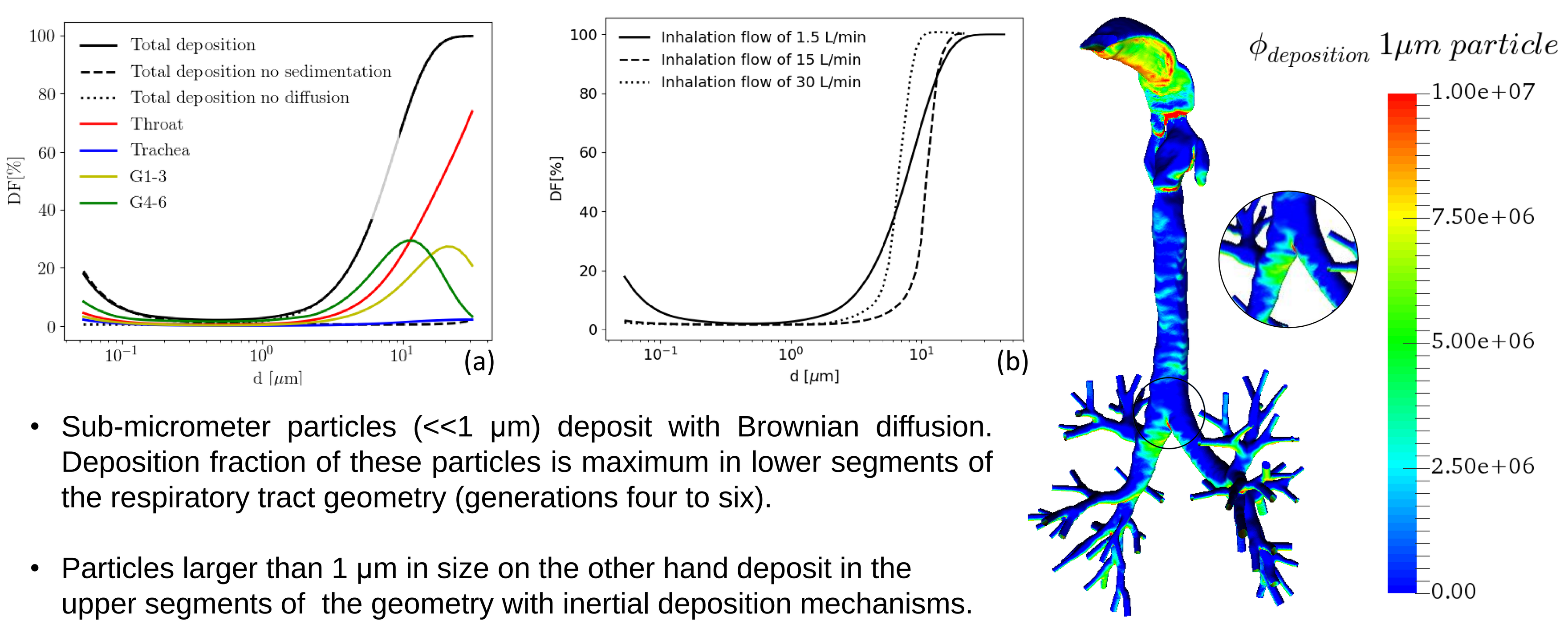


Figure 1:
(a) Deposition fraction versus particle size diameter in a human airways model. Deposition model is compared against data obtained from Lagrangian modeling [3].
(b) Particle size growth due to condensation of water vapor on a single glycerol particle in a closed chamber. The condensation model [4] is validated with experimental data [5].

Results

Contribution of deposition mechanisms to regional aerosol deposition

Figure 2: (a) Regional deposition fraction calculated for various particle size diameters for non-evolving glycerol particles. This figure shows the change in total deposition fraction neglecting respectively sedimentation and Brownian diffusion mechanisms. (b) Total deposition fraction for various inhalation flow rates of 1.5, 15, and 30 L/min.

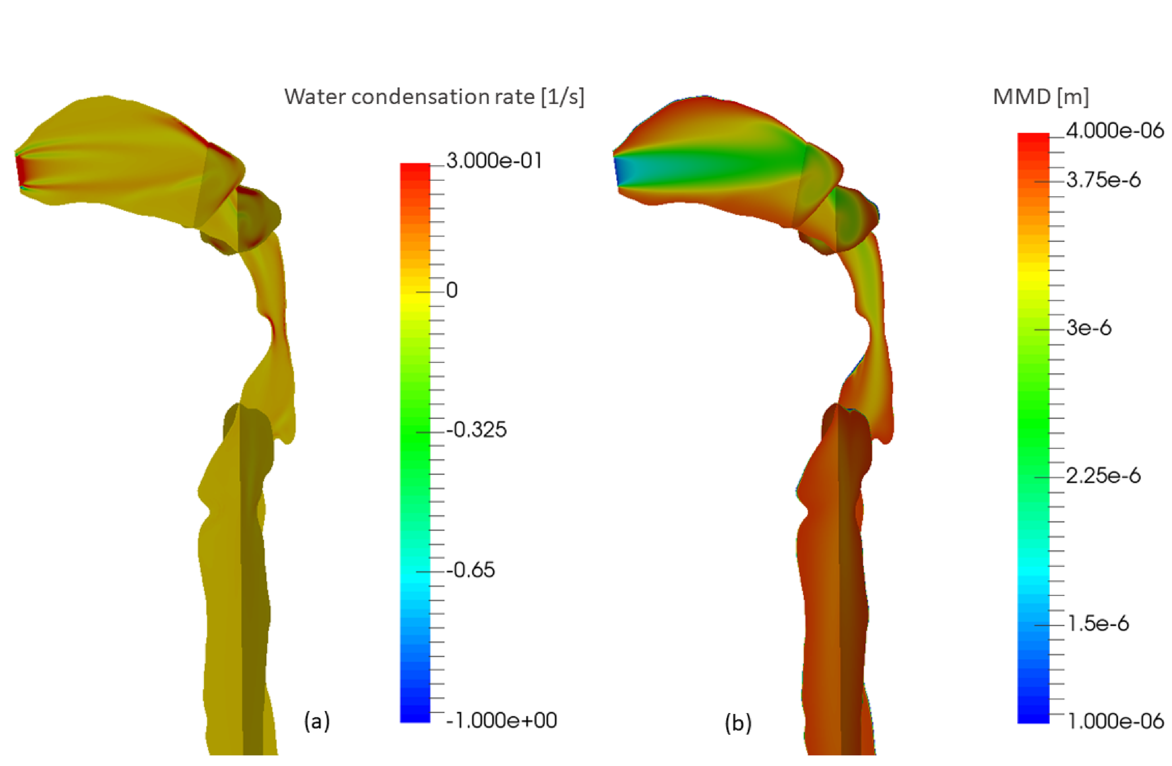


Particles number deposition flux captured on the respiratory tract surface.

- Sub-micrometer particles (<<1 μm) deposit with Brownian diffusion. Deposition fraction of these particles is maximum in lower segments of the respiratory tract geometry (generations four to six).
- Particles larger than 1 μm in size on the other hand deposit in the upper segments of the geometry with inertial deposition mechanisms.
- Filtration of these particles in the upper respiratory tract geometry does not allow the aerosol delivery to lower respiratory tract.

Results

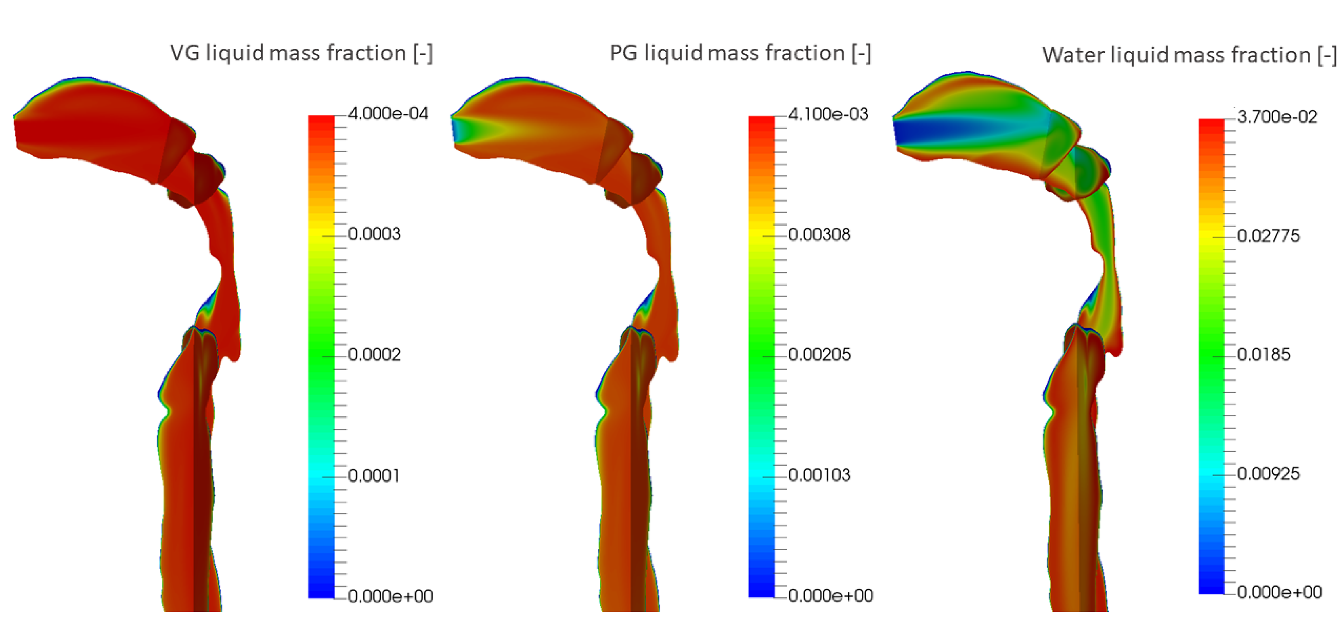
Multispecies aerosol evolution



- Aerosol was simulated for a warm mixture 50 ℃ at the inlet cooling down to human body temperature 37 ℃ at the respiratory tract walls.
- Relative humidity at the walls of the geometry was kept at 100 % to consider the saturation condition for the water vapor released from wet surfaces of the respiratory tissue.
- Mass median diameter of the particles grows from 1 μm at the inlet to the maximum size of 4 μm in the regions close to the walls due to thermal and hygroscopic effects.
- Particles achieve equilibrium size in throat and trachea region and there in no major condensation in lower respiratory tract. Major condensation zone occurs in close-to-inlet region.

Figure 3: (a) Water condensation rate for a multispecies aerosol with initial mixture of glycerol (VG), propylene glycol (PG), Water with 40-40-20 % mass fractions in liquid phase. (b) Mass median diameter of the particles inhaled with steady flow rate of 1.5 L/min.

Species specific condensation



- Aerosol gains the largest liquid mass fraction of water compared to the other species in the mixture. This is explained with the large condensation rates of water and high relative humidity in the respiratory tract.
- Propylene glycol (PG) is a semi-volatile species and condensates in large values due to thermal conditions of the respiratory flow.
- Glycerol (VG) is a non-volatile species in the range of considered temperatures 37-50 ℃ and does not undergo condensation process.

Figure 4: Liquid mass fractions of each species of multispecies aerosol with initial mixture of VG, PG, Water with 40-40-20 % mass fractions. Aerosol is inhaled with steady inhalation flow rate of 1.5 L/min. Thermal and humidity conditions were kept the same as in Figure 3.

Effect of aerosol evolution on regional deposition

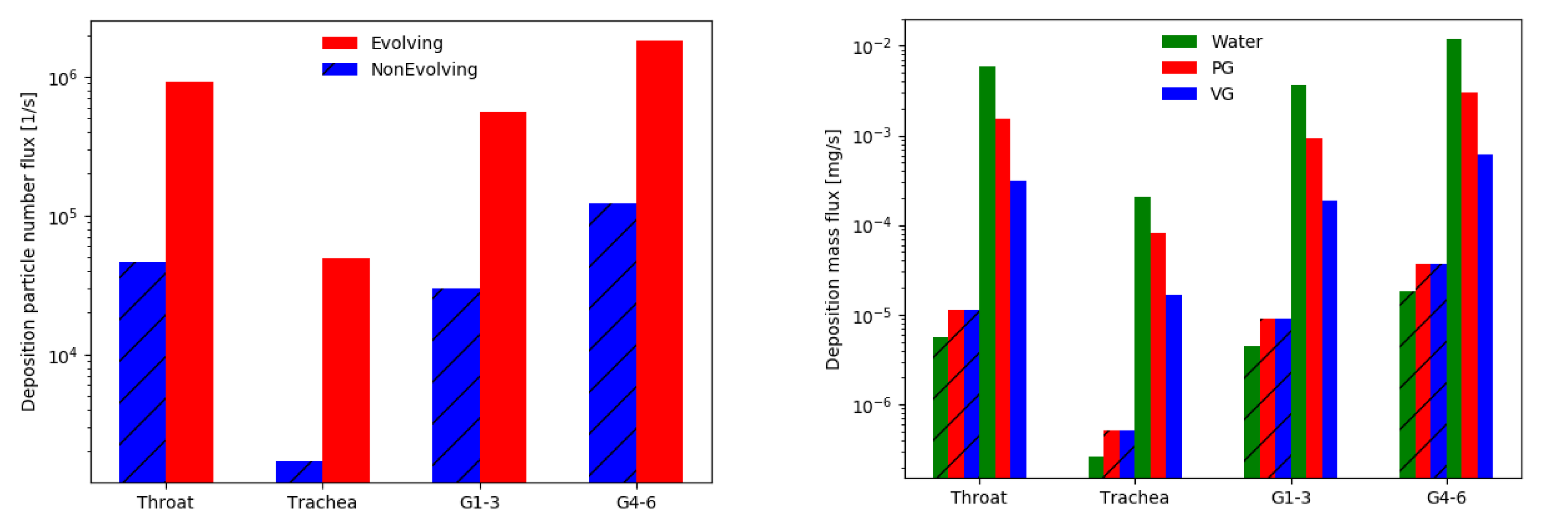


Figure 5: (a) Particle number flux deposition in various segments of the cast geometry compared for non-evolving (hashed bar) and evolving (solid filled bar) aerosol simulations with similar initial mixture and thermal properties. (b) Regional mass deposition flux of each species compared for non-evolving and evolving aerosol simulations.

- Particles number deposition flux increases ~15 times in all segments of the respiratory tract geometry due to increased inertial deposition of grown particles.
- The extent of increased deposited mass in evolving case correlates with the volatility of the species.
- Deposited mass of non-volatile glycerol species increases due to increased particles number deposition flux driven by hygroscopic growth of the particles.

Concluding remarks

- Contribution of deposition mechanisms to particles deposition in various inhalation flow rates were evaluated and quantified. For low inhalation flow rates (puffing regime), our results indicated that the dominant deposition mechanism for micron-size particles is sedimentation. For higher inhalation flow rates, contribution of inertial impaction is dominant.
- Multispecies aerosol evolution and deposition was simulated for an initially warm mixture entering the respiratory tract geometry. Our results showed that the simulated aerosol achieves equilibrium in size and multispecies composition in throat region and there is no major condensation happening in the lower segments of the respiratory tract for the considered inhalation flow rates.
- We showed that mass deposition flux of the particles in the respiratory tract is highly dependent on the temperature and humidity along the aerosol transport streamlines.
- Temperature decrease inside the cast for an initially saturated mixture led to oversaturation near the cast surface, resulting in particles growth and subsequent increased liquid mass deposition.
- Species-specific deposition rate depends on thermophysical and chemical properties of the species. There is a significant increased liquid deposition for volatile species such as PG and water due to large condensation rates of these species. Deposition of non-volatile glycerol species is also increased due to increased particles number deposition flux.
- Future work is devoted to development of temperature- and humidity-controlled *in vitro* cast models enabling experimental exploration of aerosol size and composition evolution and deposition [6].

Concluding remarks

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