Aerosol deposition in the human upper respiratory tract with different inhalation patterns

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Introduction

Pulmonary aerosol deposition depends on a variety of factors ranging from the complex airflow in the respiratory tract to the evolving physical and chemical aerosol properties. Inhalation patterns determine the airflow space and time profile in the respiratory tract and, therefore, influence on the aerosol deposition patterns. In addition, characterization of the aerosol deposition under distinct inhalation patterns helps better estimation of the realistic delivery doses in the upper respiratory tract as an input to *in-vitro* buccal/epithelial tissue exposure experiments. In our computational study, we explore the impact of the puffing topography on the size dependent regional aerosol deposition in a realistic human respiratory tract cast. While we have restricted our study to non-evolving aerosol deposition within the initial phase of the inhalation pattern (puffing topography), we aim at extending this work to consider the condensational growth of the liquid droplets and their subsequent deposition in puffing and post-puffing diluting airflow regimes.

Methods

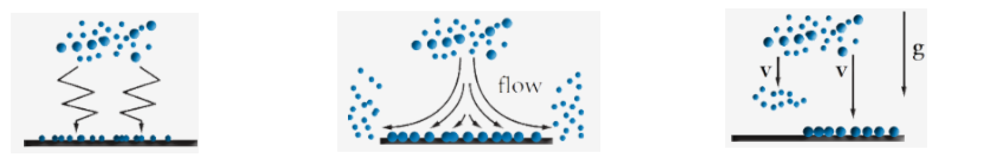
Computational platform AeroSolved[1,2] publicly available at https://www.aerosolved.com

AeroSolved

- Simulations of mass, momentum (Navier-Stokes equations) and energy conservation equations
- Eulerian internally mixed aerosol model in density coupled framework (PISO algorithm)
- Multi-species formulation for gas and liquid phases (N-species)
- Sectional discretization of the droplet size distribution function (Q-sections)
- Applied for non-evolving single species (N=1) glycerol droplets with density of 1258 kg/m^3
- The droplet size covers the range of 50nm-5μm in Q=24 segments

Deposition mechanisms (model validation in the reference[3])

- Diffusion
- Impaction
- Sedimentation



Diffusional deposition   Inertial deposition   Gravitational deposition

Equations

Mass conservation: $$\partial_t \rho + \partial_j(\rho u_j) = -\partial_j[(1-\gamma) f_j]$$

Momentum conservation: $$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = -\partial_i p + \partial_i(\mu \tau_{ij}) \qquad i = 1,\ldots,3$$

Energy conservation: $$\rho c_p(\partial_t T + u_j \partial_j T) = \partial_j(k \partial_j T) + \partial_j(\mu u_k \tau_{kj}) + \Im_h + Dp/Dt$$

Transport of compounds in gas phase: $$\partial_t(\rho Y_n) + \partial_j(\rho Y_n u_j) = \partial_j(Y^{-1} \gamma f_j Y_n) + \Im_{Y_n} \qquad n = 1,\ldots,N$$

Transport of compounds in liquid phase: $$\partial_t(\rho Z_n) + \partial_j(\rho Z_n u_j) = -\partial_j(Z^{-1} f_j Z_n) + \Im_{Z_n}$$

Transport of droplet number density: $$\partial_t(\rho M_q) + \partial_j(\rho M_q u_j) = -\partial_j(\rho M_q u^l_{j,q}) + \partial_j(\rho D_q \partial_j M_q) + \Im_{M_q} \qquad q = 1,\ldots,Q$$

Mass conservation constrain: $$\sum_{n=1}^{N}(Y_n + Z_n) = 1 \qquad Z = \sum_{q=1}^{Q} s_q M_q$$

Deposition efficiency

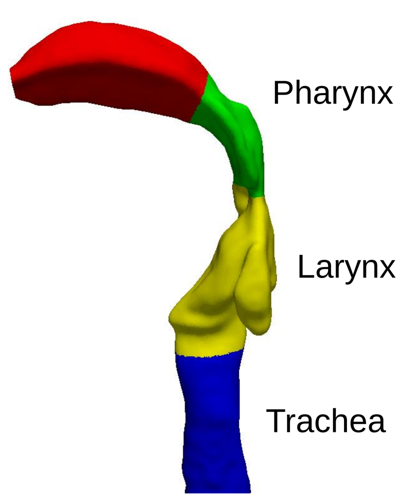
Deposition efficiency in segment (c) of the cast: $$\eta_c(S_i) = \frac{\int_t \int_{A_c} flux_i \, dA \, dt}{\int_t \int_{A_{inlet}} flux_i \, dA \, dt}$$

Computational domain and aerosol inhalation topography

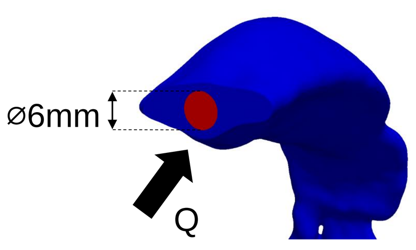
Computational domain

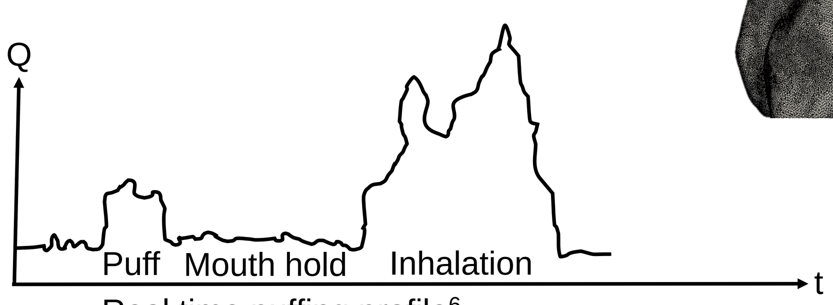
- Realistic geometry of the human upper respiratory tract[4]
- The geometry is segmented into four parts to evaluate the regional deposition
  - Mouth cavity: 23.9ml
  - Pharynx: 8.1ml
  - Larynx: 16.8ml

  } Throat: 48.8ml
  - Trachea: 31.3ml
  - Total volume: 125ml



- Computational grid generated with 1.1M cells (grid independence tested)
- The flow inlet of 6mm representing the aerosol generator connection

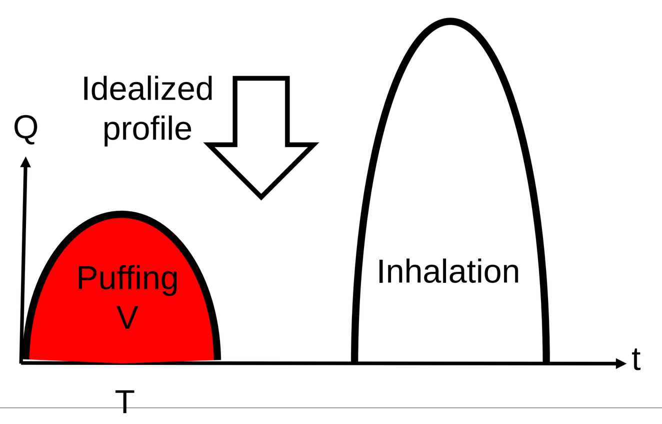


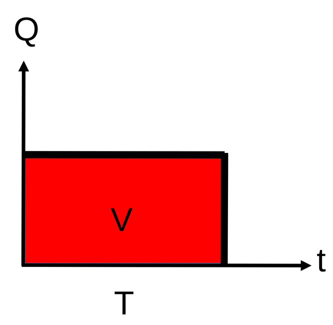


Real time puffing profile[6]

Inhalation pattern

- Idealized puffing profile shapes
  - Sinusoidal profile
  - Square profile
- Puffing characteristics
  - Intake volume[5] (V) : 50-150ml
  - Puffing period (T): 2 seconds





Results

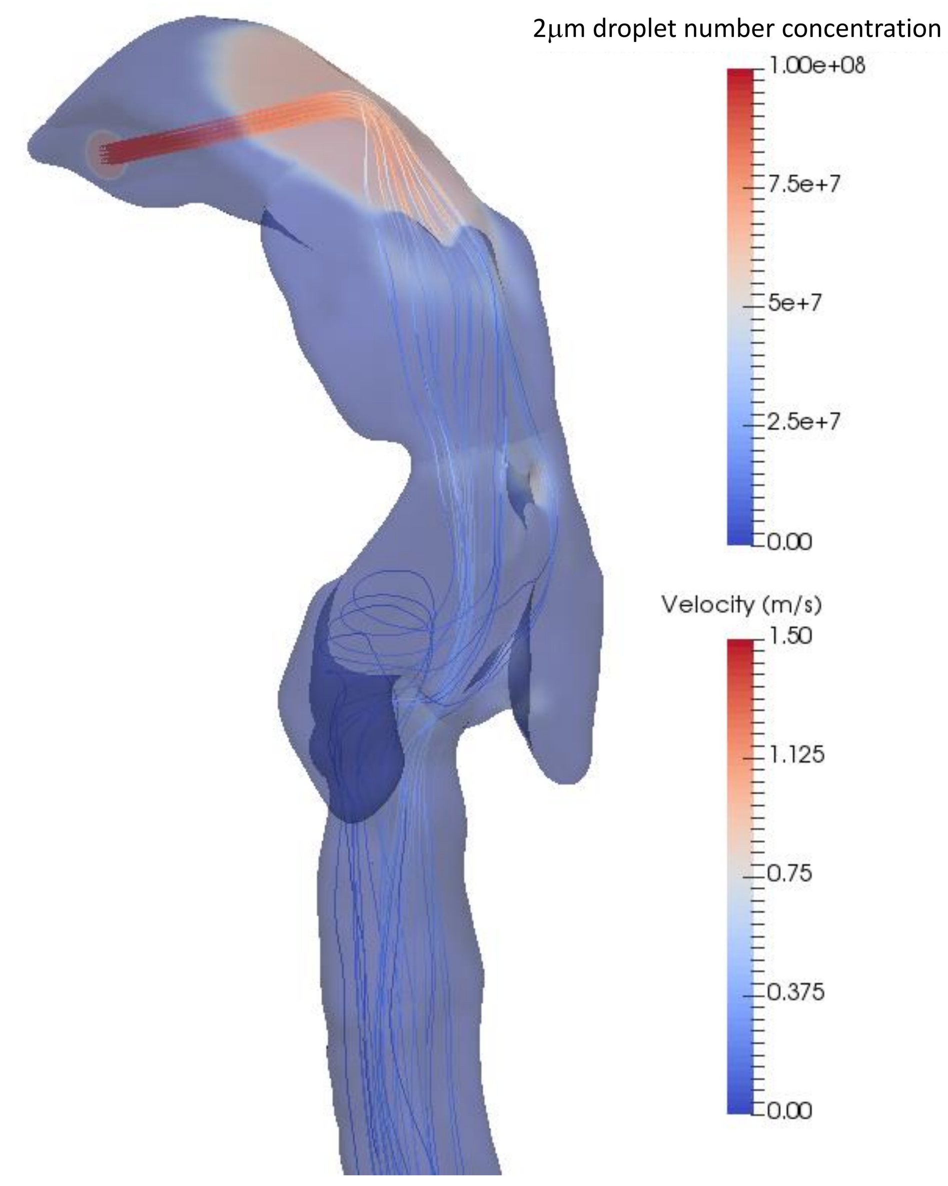
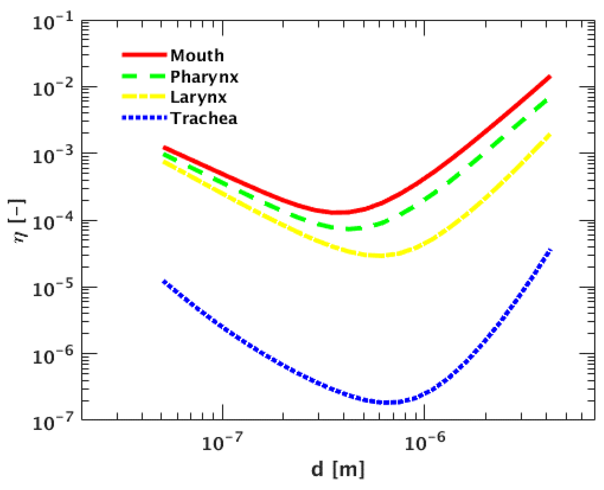


Figure 1: Snapshot of the flow and 2μm droplet number concentration at t=1s with the sinusoidal profile. The intake volume (V) and duration (T) are 50ml and 2 seconds. The high particle concentration in the mouth cavity indicates dominancy of the inertial deposition in this region.



2: Deposition efficiency calculated for the puffing period (T) with volume (V) of 50ml in 2 seconds. The deposition efficiency is shown in nt regions of the upper respiratory tract: mouth cavity, pharynx, and trachea. Deposition in general is much lower in the trachea red with the throat regions.

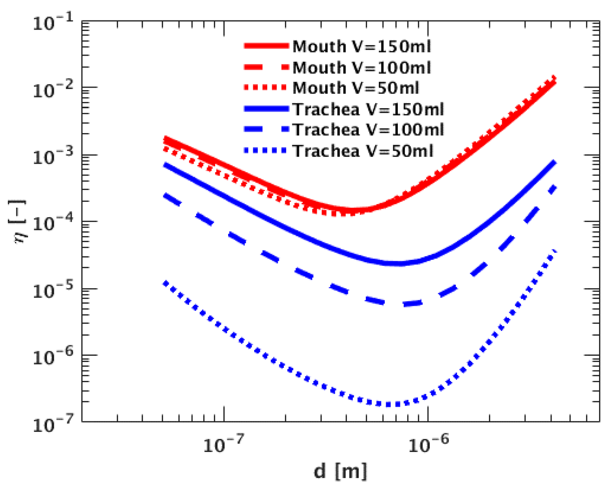


Figure 3: Deposition efficiency calculated for the puffing period (T) with intake volume (V) of 50 and 150ml in 2 seconds. While the deposition is similar in the mouth cavity with different intake volumes, there is a large difference seen in the trachea. With the small intake volume, particles do not reach the lower parts of the respiratory tract and deposition happens only in the throat for full range of particle size.

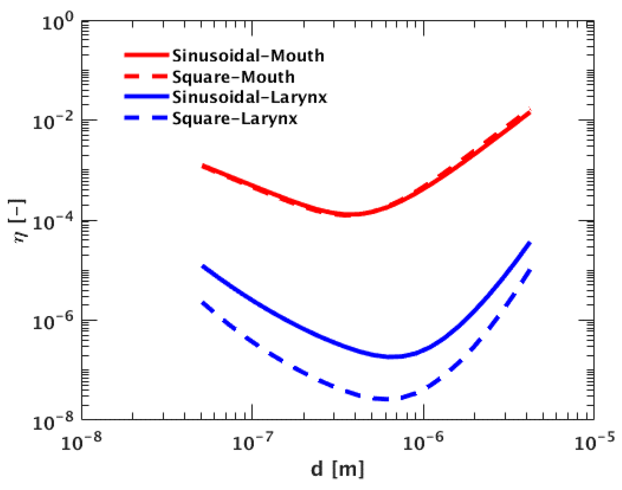


Figure 4: Deposition efficiency calculated for the puffing period (T) with sinusoidal and square profile shapes. Intake volume (V) and time are respectively 50ml and 2 seconds. While deposition is similar in the mouth cavity with two profiles, there is a difference seen in the trachea. With the sinusoidal profile, the peak velocity allows the particles to reach the lower region of the upper respiratory tract.

Concluding remarks

- Deposition of non-evolving polydisperse liquid aerosol is simulated in the realistic geometry of the human upper respiratory tract. The calculated deposition efficiency diagrams follow the common deposition profile. This profile shows the dominancy of the diffusional deposition for the small particles and inertial/ gravitational deposition for the large particles (d>0.8um).
- Large droplets (d>1um) deposit in the throat region due to their impaction at the mouth cavity surface.
- Aerosol inhalation characteristics such as intake volume (in our investigated range) affects the deposition efficiency in the lower segments of the upper respiratory tract such as trachea but it does not have a considerable impact on the deposition efficiency in the throat. This behavior might be explained regarding the volume of the upper respiratory tract which is 125ml. Larger intake volumes (>50ml) allow the particles to reach the lower regions.
- The same effect can be seen comparing the two puffing profile shapes: Sinusoidal profile with the larger peak velocity compared with the square profile is able to trigger the particles to reach the lower regions of the upper respiratory tract.
- We estimated the regional deposition for various inhalation patterns with the outlook of our computational study to consider evolving liquid droplets and characterize their condensational growth and subsequent deposition both in puffing and inhalation airflow regimes.

References

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Competing Financial Interest

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