Aerosol evolution and deposition in the human upper respiratory tract

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Introduction and objectives

When liquid aerosol is inhaled, the physical characteristics of particles, as well as the respiratory flow, determine the deposition profile in the human respiratory tract. The evolution of these liquid particles in the respiratory tract is temperature-driven and characterized by continuous condensation and evaporation processes within the aerosol. This impacts both the dynamics and the deposited liquid mass. We have assessed the temperature-driven size dynamics of liquid particles and their influence on deposited mass at the respiratory tract surface. Our results show that condensational growth of particles leads to a significant increase in the deposited liquid mass.

General objectives:
- Development and validation of deposition, condensation/evaporation models in the AeroSolved framework.
- 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 gradients.
- Quantification of the influence of aerosol evolution on deposition in human airways.

Methods

Open-source computational fluid dynamics (CFD) software developed in the OpenFOAM framework [1].

CFD model

Eulerian sectional approach to model the polydisperse multi-species aerosol transport, evolution, and deposition.

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

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

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

Transport of species in gas phase: $\partial_t(\rho Y_n) + \partial_j(\rho Y_n u_j) = \partial_j(Y^{-1}\gamma f_j Y_n) + S_{Y_n}$, $\quad n = 1,\dots,N-$species

Transport of species in liquid phase: $\partial_t(\rho Z_n) + \partial_j(\rho Z_n u_j) = -\partial_j(Z^{-1} f_j Z_n) + S_{Z_n}$, $\quad n = 1,\dots,N$-species

Transport of particle number density: $\partial_t(\rho M_q) + \partial_j(\rho M_q u_j) = -\partial_j(\rho M_q u^l_{j,q}) + \partial_j(\rho D_q \partial_j M_q) + S_{M_q}$, $q = 1,\dots,Q-$sections

γ	Relative vapor to liquid density	u^l	Particle drift velocity
S_Y, S_Z, S_M	Source terms for condensation/evaporation processes	f	Drift flux of particles mass

Multi-species condensation/evaporation model

Condensation rate [2]: $\frac{dm}{dt} = \rho\pi d\varepsilon_n Sh D_n H(B_n)$.

ε_n	Species specific fraction of the total condensation rate	D_n	Species mixture diffusion coefficient
Sh	Sherwood number	d	Particle diameter
$H(B_n)$	Mass transfer potential (defined in [2])	Modified Raoult's law	$X_n^{sat} = \beta_n W_n \frac{p_n^{sat}}{p}$.
		β_n	Activity coefficients

Model validation

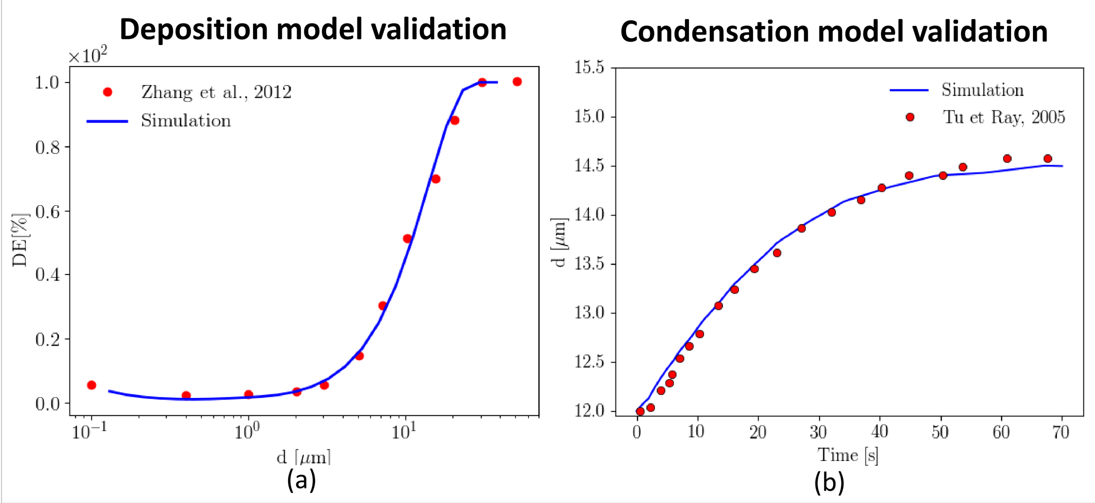


Figure 1. (a) Deposition efficiency in a human airway model. Deposition model is compared against data obtained from Lagrangian modeling [3].

(b) Particle size growth due to condensation of water vapor on a single glycerine particle in a closed chamber. The condensation model is validated against [4].

Results

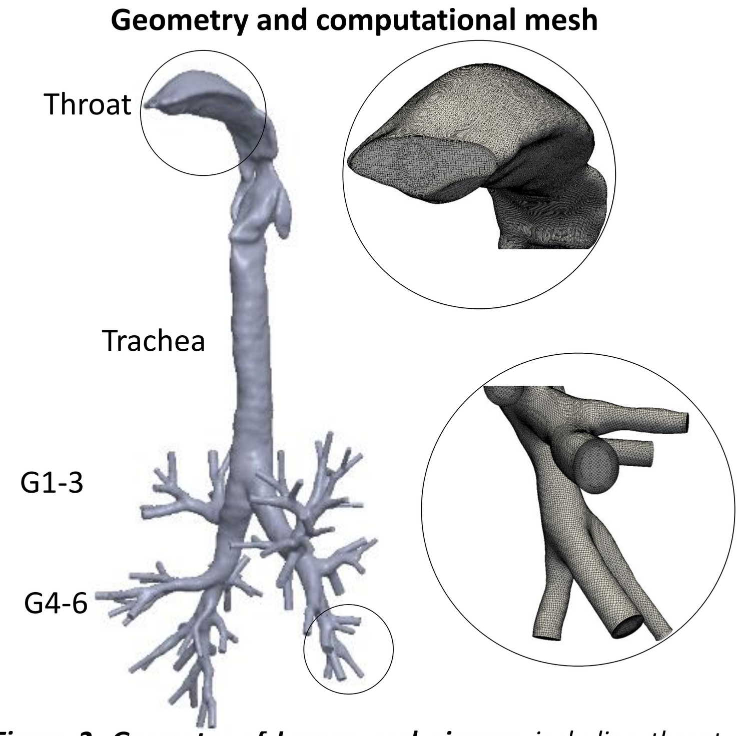


Figure 2. *Geometry of human oral airways including throat, trachea, generations 1-3 (G1-3), and generations 4-6 (G4-6) of the tracheobronchial system obtained from [3].*

- Computational **mesh resolution**: between **50 µm and 360 µm.**

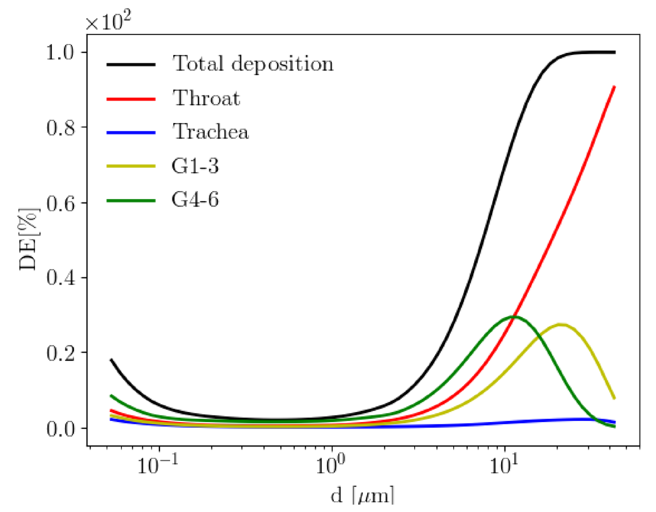


Figure 3. *Regional particle deposition efficiency calculated for flow rate of 1.5 L/min (steady flow representing puffing flow of 50 ml in 2 seconds).*

- Regional deposition efficiency **highly depends on the particle size.**
- **Particle filtration** in the upper respiratory tract is **dominant for > 10 µm.**

Contribution of deposition mechanisms

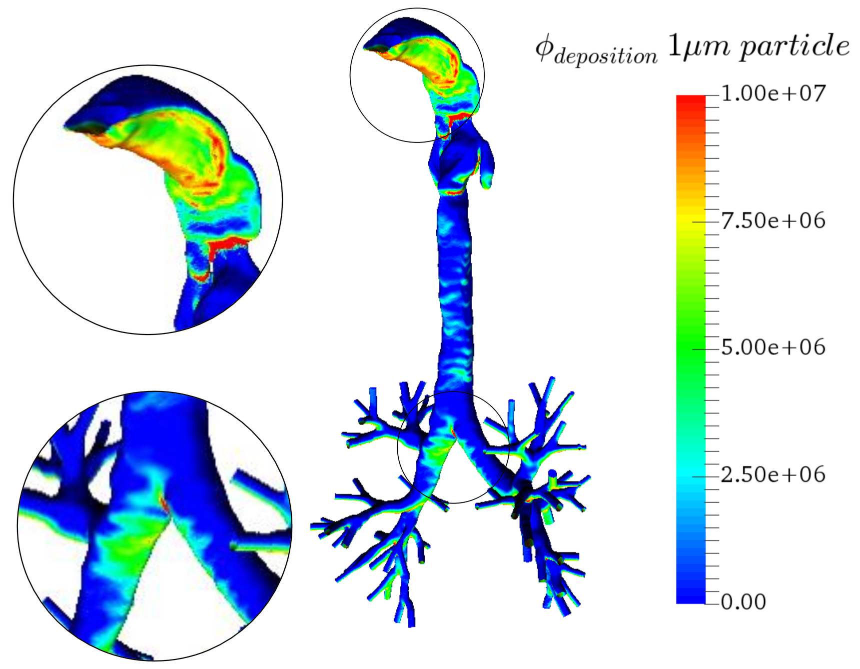


Figure 4. *Deposition flux of 1 µm particles in the human airways geometry for flow rate of 1.5 L/min.*

- Sedimentation is the **dominant deposition mechanism.**
- **Hot spots of deposition** in throat and bifurcations are clearly captured and shown.

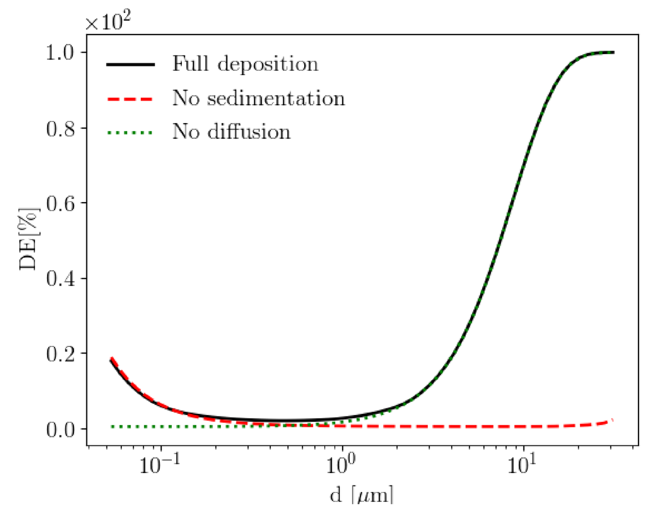


Figure 5. *Deposition efficiency versus particle size shown for various deposition mechanisms.*

- **Sedimentation** governs deposition of **large particles** > 2 µm.
- **Diffusion** rules deposition of **small particles** < 2 µm.

Effect of flow rate variation on deposition

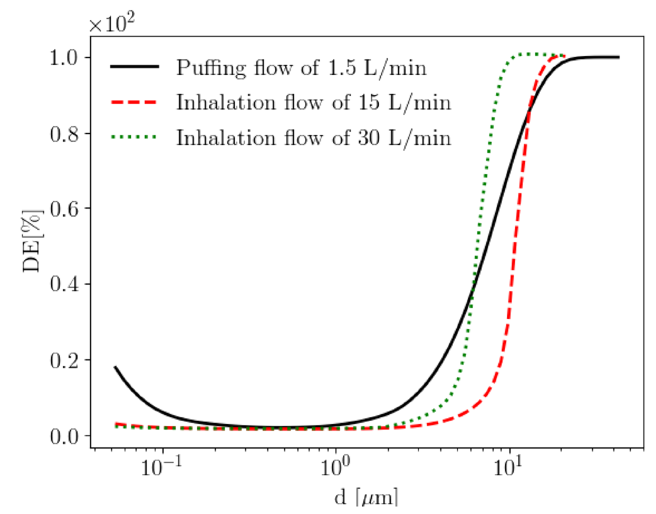


Figure 6. *Deposition efficiency versus particle size and its sensitivity to flow rate for typical steady puffing and post-puffing inhalation flow rates.*

- **Diffusional deposition efficiency is reduced** for increased flow rate due to decreased particle residence time.
- **Inertial deposition (impaction) efficiency increases** with increased flow rate.
- **Increased flow rate shifts** the deposition efficiency curve **toward smaller particle size.**

Results (cont.)

Particle size growth

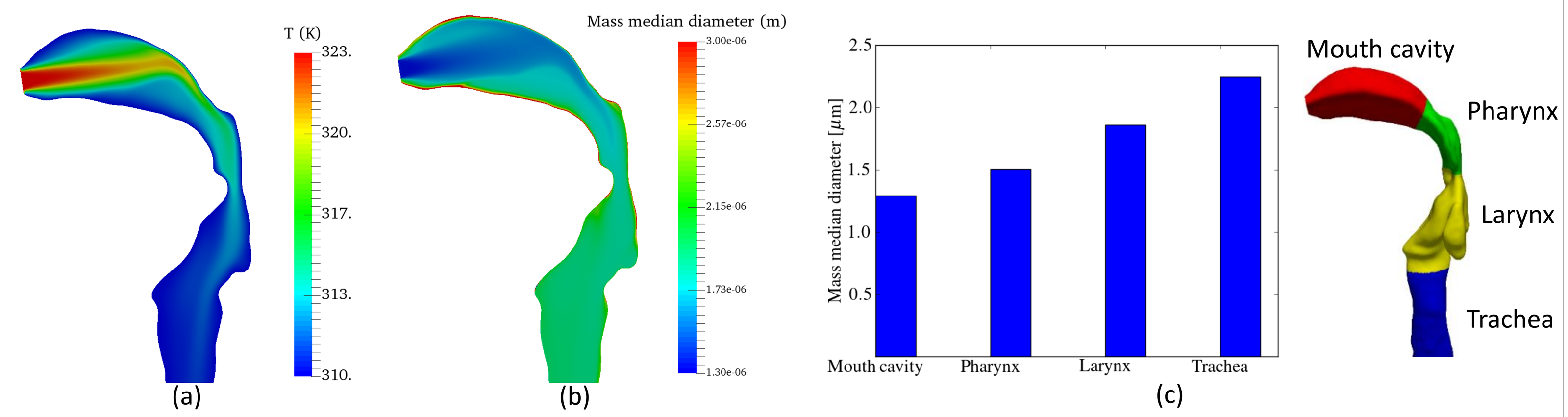
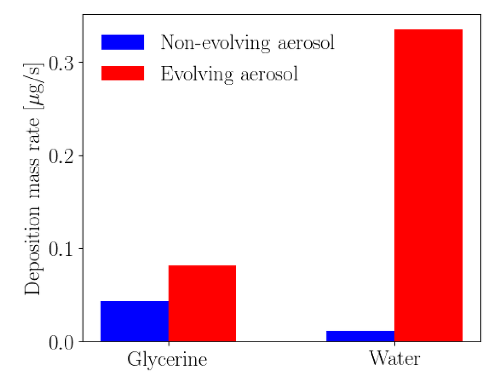


Figure 7. *Particle size growth under a temperature change in the human respiratory tract. (a) Temperature field. (b) Mass median diameter (MMD) field. (c) Average particle MMD in different segments of the geometry.*

- **Rapid particle growth** in the **boundary layer** due to heat transfer with the walls.
- Particles reach **equilibrium size in trachea.**
- **65% particle size growth** from mouth cavity to trachea.

Effect of particle evolution on deposition



- Increased (> 7 times) total deposition rate for evolving aerosol due to increased deposition efficiency of the large particles in the throat region.
- Increased deposition rate of species in evolving aerosol: glycerine (> 2 times) and water (> 30 times).
- Increased deposited mass is mainly attributed to water in our simulated conditions. Change in delivered mass of each species depends on the thermophysical properties of the species.

Figure 8. *(a) Total deposition rate for simulations of non-evolving and evolving aerosols. (b) Species-specific deposition rate for non-evolving and evolving cases. Initial composition of simulated aerosol in both cases is 80%-20% glycerine-water.*

Concluding remarks

- Computational models were validated for deposition and evolution of particles in comparison with the available literature data.
- Contribution of deposition mechanisms 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 intertial impaction is dominant.
- We showed that mass deposition flux of the particles in the respiratory tract can be highly dependent on the temperature along the aerosol transport streamlines.
- Temperature decrease inside the cast for an initially saturated mixture led to oversaturation near the cast surface, resulting in particle growth and subsequent increased liquid mass (aerosol) deposition.
- Species-specific deposition rate depends on the thermophysical and chemical properties of the species.
- Future work is devoted to the development of temperature- and humidity-controlled *in vitro* cast models enabling experimental exploration of aerosol size evolution and deposition [5].

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