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.

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**Methods**

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

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

Mass conservation:
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

Momentum conservation:
\[ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla \cdot \mathbf{p} + \rho \mathbf{g} + \nabla \cdot \mathbf{T} \]

Energy conservation:
\[ \frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) = -\nabla \cdot (\mathbf{e} \mathbf{u}) + \mathbf{S}_p \]

Transport of species in gas phase:
\[ \frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y) = \nabla \cdot (\rho D \nabla Y) + \rho S_Y \]

Transport of particles in liquid phase:
\[ \frac{\partial (\rho N)}{\partial t} + \nabla \cdot (\rho \mathbf{u} N) = \nabla \cdot (\rho D_N \nabla N) + \rho S_N \]

Transport of particle number density:
\[ \frac{\partial (\rho n)}{\partial t} + \nabla \cdot (\rho \mathbf{u} n) = \nabla \cdot (\rho D_n \nabla n) + \rho S_n \]

**Multi-species condensation/evaporation model**

Condensation rate [2]:
\[ \frac{\partial C}{\partial t} = \rho \beta \phi \exp \left( \frac{T_0 - T}{T_0} \right) \]

\( C \) Condensation rate
\( \rho \) Mass density
\( \beta \) Activity coefficients
\( \phi \) Relative vapor to liquid density
\( T \) Temperature along the aerosol transport streamlines

\( H(B) \) Mass transfer potential (defined in [2])

\( S_p \) Source terms for condensation/evaporation processes

\( f \) Drift flux of particles mass

\( d \) Particle diameter

**Results**

**Concluding remarks**

Effect of particle evolution on deposition

- Increased (> 7 times) total deposition rate for aerosol due to increased deposition efficiency of the large particles in the throat region.
- Increased deposition rate of species in aerosol: glyceral (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 thermophilic properties of the species.

- 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 inertial 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 thermophilic and chemical properties of the species.
- Future work is devoted to the development of temperature- and humidity-controlled in vivo test models enabling experimental exploration of aerosol size evolution and deposition (5).

- Particle size growth in the boundary layer due to heat transfer with the walls.
- Inertial deposition is the characteristic of particles with significant mass.
- Increased particle growth in the boundary layer due to heat transfer with the walls.
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