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Biophysical Respiratory Aerosol Model (ResAM): composition and pH of exhaled aerosol and application of airborne virus inactivation

The exhaled aerosol plays a crucial role in the transmission of respiratory viruses. It has been found that the inactivation of viruses (influenza A virus and SARS-CoV-2) depends crucially on the pH value and on the salt concentration in the exhaled aerosol particles (Luo et al. 2023, Haddrell et al. 2024, Schaub et al. 2024). During exhalation, particles shrink by losing water and CO_2, interact with semi-volatile atmospheric trace gases such as HNO_3, NH_3, and organic acids, and eventually may undergo efflorescence, which changes both pH and salt concentration. Under dry conditions, the exhaled aerosol can become highly viscous, so that uptake and loss of gases from/to the ambient air via condensation and evaporation become diffusion-limited in the liquid phase.
The evolution of pH depends critically on the initial composition and size distribution of the exhaled aerosol as well as the ambient conditions (temperature, relative humidity and trace gas concentration). We have developed the biophysical Respiratory Aerosol Model ResAM to study pH and composition of the exhaled aerosol based on thermodynamic and kinetic measurements of synthetic lung fluid (SLF), and subsequently the inactivation of pathogens based on virological measurements in SLF bulk solutions (Klein et al. 2022, Luo et al. 2023, David et al. 2024, Schaub et al. 2024). Here we present a description of ReSAM and some application examples, with a focus on the pH evolution of exhaled aerosols during exhalation.
ResAM is a kinetic and thermodynamic model with spherical geometry with several shells. The main species of inorganic ions that acounted for in the model are H^+, $NH4^+$, Na^+, Mg^2+, Ca^2+, OH^-, $NO_3{}^-$, Cl^-, $HSO4^-$, $SO_4{}^{2-}$, $HCO_3{}^-$, $CO_3{}^{2-}$, $H_2PO_4{}^-$, $HPO_4{}^{2-}$.
ResAM takes the following physical and chemical processes into account:

1. Condensation/evaporation kinetics of H2O, CO2, HCl, NH3, and some organic acids such as acetic acid, lactic acid, oxalic acid.
2. Equilibrium dissociation of H2O, HCO3-, HSO4-, H3PO4, H3PO4-, and of the organic acids. Dissociation/association kinetics of CO2 from HCO3- with and without enzymatic acceleration.
3. Diffusion between shells in the liquid phase using the Ernst-Planck equation, which describes the Fickian diffusion of ions and allows to ensure charge neutrality.
4. Formation of various solids, e.g. NaCl, $CaCO_3$, MgCO3, NaHC2O4, (NH4)2C2O4
5. Activities and vapor pressures calculated using the Pitzer ion interaction model.

With this model we can analyze data collected in the laboratory on aerosols and µL-droplets. Finally, the model enables us to estimate the transmission risk under various environmental conditions using the inactivation rates of different pathogens measured in bulk solutions as a function of composition and pH can be used, towards developing a strategy to prevent airborne transmission of viruses and other pathogens.

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