## Computational and theoretical models of inhaled transport in the upper airway: with applications in airborne infection mechanics and respiratory drug delivery



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## Abstract

This talk is on fluid mechanics modeling of respiratory transport in human airways, through use of experimentally validated computational and theoretical approaches. The presented material will cover:

Airway infection onset mechanics: Integrating inhaled particulate dynamics with virological and epidemiological data, can address questions like: (a) what are the hazardous particulate sizes predominantly responsible for infection onset, or (b) what might be the minimum number of virions (i.e., the infectious dose) that can launch an infection. I will present an extendable modeling framework to answer (a) and (b), with SARS-CoV-2 as an example. The work combines computational tracking of inhaled transport, with sputum assessments from hospitalized patients and prior measurements of speech ejecta sizes. For a wide range of breathing conditions modeled through Large Eddy Simulation, the regional deposition of virus-laden particulates at nasopharynx, which is the dominant initial infection site for SARS, peaks for the particulate size range of  $2 - 20 \,\mu$ m. Also, the infectious dose is projected at a remarkably low order of hundreds (~ 300), underlining high transmissibility. The results can inform disease spread modeling.

**Respiratory drug delivery:** Drug efficacy for viral infections can be enhanced by targeting the nasopharynx (initial infection trigger zone) with intranasal sprays. However, under the standard protocol ("current use" or CU), the spray nozzle enters the nose almost vertically, resulting in suboptimal drug deposition at the nasopharynx. Using Lagrangian particle transport simulations in anatomic nasal geometries, we propose an "improved use" (IU) protocol. It entails pointing the spray bottle at a shallower angle (almost horizontally), aiming slightly toward the cheeks. We have simulated the performance of this protocol for conically injected spray droplet sizes of  $1 - 24 \,\mu$ m with realistic breathing rates. The experimentally validated results show that targeted delivery via IU outperforms CU by over 2 orders of magnitude. The IU protocol is also robust to small perturbations in spray direction, underlining its practical utility.

Reduced order modeling for upper airway transport: Simulations show that  $7 - 14 \,\mu\text{m}$  particles exhibit prominent localized deposition at/near the glottis, below the narrowest cross-section of the throat. This region is marked by the strongest vortex structures observable in the respiratory flow field. We have developed a reduced-order particle transport model that mimics a slice of the physiologic system. The velocity field is approximated by a collection of point vortices embedded in a 2D potential flow, and particle motion is determined by a simplified Maxey-Riley equation. The numerical simulations and the reduced-order theoretical model agree well on the particle clustering trends, hinting at the relevance of theoretical approaches for parametric characterization of biophysical transport inside respiratory pathways.

## Biography

Dr. Saikat Basu is an Assistant Professor of Mechanical Engineering at South Dakota State University (SDSU) in the United States and directs the Biomedical and Bioinspired Fluid Dynamics Lab there. The group works on fluid mechanics of biophysical systems, with respiratory transport modeling and tumor microenvironment flow physics as focus topics. Basu's scholarly background is in theoretical and computational fluid mechanics. He received his Ph.D. in Engineering Mechanics from Virginia Tech in 2014, followed by postdoctoral stints at OIST Japan and UNC Chapel Hill School of Medicine. Basu joined SDSU in 01/2019 and his group has since been supported by grants from the US National Science Foundation and National Institutes of Health, along with industry-sponsored projects. Besides academic publications, Basu's work on intranasal therapeutics, airborne pathogenic transmissions, and bioinspired filtration has been widely reported on media outlets, e.g., NewScientist, USA Today, Newswise, NPR. Basu is also a recipient of the 2018 Fluid Dynamics Research Prize from the Japan Society of Fluid Mechanics and the 2022 – 2023 Early Career Investigator Award from SDSU's College of Engineering.