Bioaerosol inhalation models considering COVID-19 aerosol transmission

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Task 7, Subgroup 5 Inhalation: Meet the team

- Dr Nader Karimi, Queen Mary University of London
  - Multiphase Flows
  - Computational Fluid Dynamics
  - Low Order Models

- Dr Andrea Cammarano, University of Glasgow
  - Low-Order Modelling
  - Fluid-Structure Interaction
  - Non-Linear Dynamics

- Prof Darragh Murnane, University of Hertfordshire
  - Pharmaceutical Aerosol Science
  - Targeted Pulmonary Deposition
  - Formulation Modelling

- Dr Andrea Coraddu, University of Strathclyde
  - Data-Driven methods
  - Artificial Intelligence
  - Machine Learning

- Dr David Sykes, AEROS-Consultancy
  - Bioaerosol Science
  - Microbiology
  - Project Management

- Dr Xizhong Chen, University of Cambridge
  - Particle technology
  - Multiphase modelling
  - Data analytics

- Prof James Elliott, University of Cambridge
  - Multiscale Modelling
  - Particle Technology
  - Atomistic Simulations

- Dr Angela Busse, University of Glasgow
  - Computational Fluid Dynamics
  - High Performance Computing
  - Turbulent Diffusion and Dispersion

- Prof Alison McMillan, Wrexham Glyndwr University
  - Computational Mechanics
  - Geometry Flaws & Features
  - Synthetic Experiments

- Dr Hossein Zare-Behtash, University of Glasgow
  - Experimental Fluid Mechanics
  - Data Reconciliation
  - Fluid-Structure Interaction

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Aerosols inhaled with wide size range (0.1-100 μm)

- ‘Absorption’ into epithelium
- Ventilation – Deposition – Clearance from epithelium
- Exhalation clearance

Duration of exposure and inhalation parameters
- Must consider concentration of particles of exposure
- Must consider size specific virion concentration
- Must consider size-specific virion viability
The ICRP anatomical description of the respiratory tract where each of the abbreviations ET1, ET2, BB, bb, and Al constitutes a filter in the ICRP filter-in series model.

Aerosol exposure dosimetry assessment

This model can be thought of as a series of filters where each filter corresponds anatomically to regions of the respiratory tract.

https://journals.sagepub.com/doi/pdf/10.1177/ANIB_24_1-3
Hofmann compared the five different models described in the size range 1 nm to 10 μm for nasal inhalation under sitting breathing conditions. It was found that the total (i.e. entire respiratory tract) deposition fraction of all models lie within ± 10% with typical U-shaped form.
Bioaerosol enhancement of ICRP (Guha, 2014)

- For purified monodispersed bioaerosols – flu, anthrax, toxins, etc
- Enabling non-spherical and narrow normal distribution particle ranges
- Valuable in evaluating exposure risk for different populations with confidence limits on prediction

https://doi.org/10.1080/02786826.2014.975334
Shortcomings of existing dosimetry tools for Covid-19 pandemic

- Virion clearance/absorption mechanisms differ substantially compared to radiochemical aerosols.
- Different aerosol size fractions respond differently to ambient humidity (atmosphere & within lung).
- Highly polydisperse, multi-modal size populations.
- SARS-CoV-2 shows a gradient infectivity from the proximal to distal (high to low) respiratory tract (see Figure).

https://doi.org/10.1016/j.cell.2020.05.042
The challenges of CFD models for bioaerosol deposition: Upper respiratory tract

3D CFD using CT scan images for laminar flows

Particles are often assumed to be solid and surfaces are smooth and rigid, questionable assumptions!

3D CFD in simplified configuration for turbulent flows

Huang and Zhang 2011

Ghalati et al. 2012
The “elastic bag” problem
The LRT is not a static cylinder
• Pressure change rather than bulk flow
• Laminar flow driven by wall flexing
• Wall geometric features interacting with the gas

Modelling challenges
• This is a Fluid/Structure Interaction (FSI) problem: a coupled problem requiring elastic solid (FEA) and fluid modelling (CFD)
• Large deformation of airways: Elastic analysis is geometrically nonlinear
• Biological materials: hence the material characteristic is nonlinear
• Conventional Navier-Stokes based CFD will struggle with grid and boundary definitions: a Lattice Boltzmann based CFD might be more appropriate
Development of bioaerosol inhalation model

- Provide high level (low-fi), rapid information for potential respiratory exposure following measurements of ambient aerosols
  - Airway-by-airway dosimetry for multi-modal, polydisperse aerosols spanning several orders of magnitude
  - Take into account hygroscopic growth, surface area dose, and lung penetration depths of aerosol boluses
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• Be suitable for high-fi, detailed information on changes to deposition behaviour as a result of PPE or individual inspiratory airflow mechanics, and clearance mechanisms

• Provide detailed information to virologists and immunologists of the regional dosimetry of viral aerosol to characterise disease mechanisms

Employ CFD experimentation to develop the in-silico deposition data to compose an enhanced bioaerosol dosimetry tool, which can be cross-validated against publicly available deposition data.
Gray Box Models allow exploiting both the mechanistic knowledge of the underlying physical principles and available experiments.
Web-based assessment toolkit: surrogate model from high fidelity simulations

Interactive GUI tool for real time assessment and immediate summary report

Demo web link: https://public.jmp.com/packages/RAMP-predictive-tool-demo/js-p/8wHTZmLLdmBYwxIFg3R1b
• There is clear information that respiratory exposure to SARS-CoV-2-containing bioaerosols is important for disease transmission

• Respiratory exposure to SARS-CoV-2-containing bioaerosols occurs for both large droplet aerosols and dry nanoparticle aerosol, and can occur throughout the respiratory system

• There is a need for inhalation dosimetry assessment tools that address the physiological exposure routes to infectious bioaerosols that can be used in pandemic risk assessment, as well as for studying infection processes.