

Computational simulations of inhaled ultrafine aerosols in the distal regions of the lung

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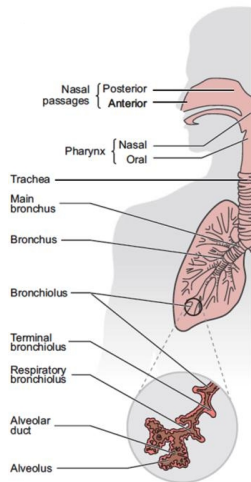
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Introduction

Simulation of inhaled ultrafine particles

- Realistic 3D geometries from morphometric models or reconstructed imaging data
- Transient particle simulation including sedimentation, convection & diffusion
- Fluid-structure interaction (FSI) to mimic physiological breathing motion



Fluid & particle properties

Fluid - Air

- Characteristic length $D_{ch} \sim 100 \mu m$
- Reynolds number regime $Re \leq 1$
- Womersely number $Wo \leq 1$
- Flow induced by domain deformation

Particles

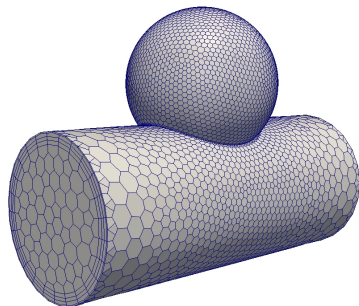
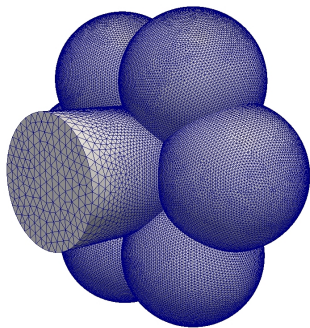
- Diameter $0.05 \mu m \leq D \leq 5 \mu m$
- Peclet number $Pe \leq 1$
- Concentration $C_{Particle} \ll 1 \text{ vol.}\%$

CFD - OpenFOAM

Version	2.1.1
Solver	pimpleDyM & icoUncoupledKinematicParcel
Spacial discretisation	linear / upwind
Temporal discretisation	fully implicit
Mesh motion	kinematic, self-similar & sinusoidal
Fluid-Particle coupling	one-way coupled
Particle forces	standard gravity & drag, working on Brownian motion

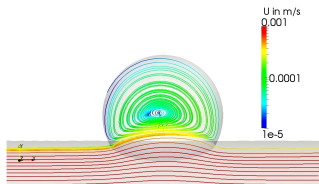
Mesh generation

Software: Gambit (Ansys) and polyDualMesh (OF)



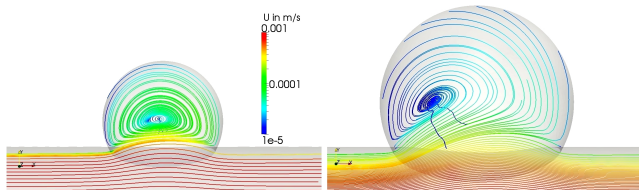
Single alveoli

Characteristic flow patterns with increasing depth of the lung



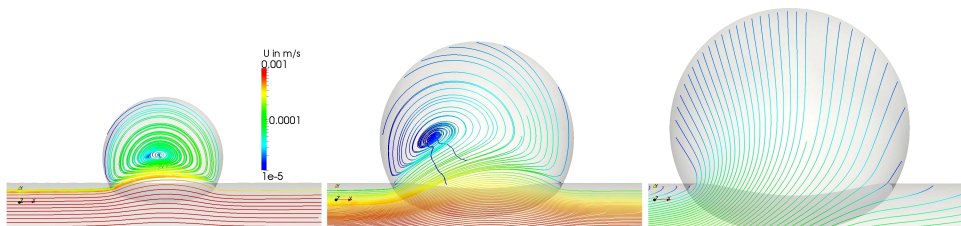
Single alveoli

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Single alveoli

Characteristic flow patterns with increasing depth of the lung



Particle simulations

Video.

Particle deposition in acinus ($d = 1 \mu m$), at $\sim 0.5x$

Future work

- Implement and test a Brownian motion model (random walk)
- Build geometries with increasing complexity and test different morphometric models
- Implement a FSI solver (possible: icoFsiFoam)

**Thank you for listening.
Any questions?**