Numerical Simulation of Particle Transport and Simulation in a Rhythmically Expanding Sac: Toward Deciphering the Inhaled Particle Journey in the Deep Lung

Khaled Talaat and Jinxiang Xi
School of Engineering and Technology
Central Michigan University
Mt Pleasant, MI, 48859
Email: talaa1ka@cmich.edu, xi1j@cmich.edu

Background: Due to inaccessibility of alveoli in human deep lungs, little is known about the behavior and fate of inhaled particles in the end alveolar (sac). Current imaging techniques (micro-CT) still fall short of visualizing the particle motions in such small structures. Numerical simulations

Objective: This study aims to develop a numerical model to simulating airflow and particle motions in a rhythmically expanding sac. The second aim is study the effects of various affecting factors on aerosol transport and deposition in a rhythmically expanding sac-like structure. Such factors include sac geometry, respiration rate, breath holding time, and sac orientation.

Methods: ANSYS Fluent was used to simulate the flow and particle motions. User-defined functions were used to control the dynamic mesh motion and to capture particle data. One thousand particles with defined distribution were injected during inhalation at a fixed release time relative to the breathing cycle through an inlet cylindrical duct connected to the sac. The effect of expansion mode was studied in order to determine the effect of sac symmetry on particle deposition. A 1:1:1 sac expansion model was compared with a 1:1:0.375 model. The effect of respiration rate was also studied by comparing particle deposition at different tidal volumes. Four tidal volumes were simulated namely 1 TD, 2 TD, 4 TD, and 8 TD. The effect of breath holding was also studied by adding a breath holding period between each breathing cycle. The effects of the five different breath holding periods (0.5s, 1s, 2s, 4s, 8s) were studied. The effect of sac orientation relative to the direction of gravitational pull was also explored by comparing a horizontal orientation of the alveoli with a vertical one. Furthermore, the effect of particle size was explored for 1 µm, 2 µm, and 3 µm particles.

Results and Conclusion: The sac expansion mode at the ratios compared had little to no effect on particle deposition. On the contrast, larger tidal volumes were found to be associated with higher particle deposition. The deposition rate for the 8 TD expansion was 7.6% higher than the deposition rate for the 1 TD expansion. The larger the tidal volume, the faster the particles deposited onto the sac walls due to higher particle speed. The particle speed increment ratio caused by increasing the tidal volume decreases as the tidal volume increases. Breath holding was found to enhance the particle depositions depending on the particle size. For 1 micron aerosol particles, breath holding for 0.5, 1, 2, 4, 8 seconds resulted in 0.4%, 0.6%, 0.8%, 0.8%, 1.3% increase in particle deposition, respectively. For 2 micron particles, however, breath holding didn't affect particle deposition. The likely explanation for the small effect of breath holding is the fact that the majority of particles that exit the sac do so in the first cycle of particle release. Breath holding would be more effective if particles entered the sac during breath holding instead of during inhalation. It is worthy to mention that breath holding significantly affected the trajectory of the particles without strongly affecting the average particle speed. The orientation of the sac relative to the direction of gravitational pull was found to be a significant factor in particle deposition. Although particles deposited faster on the horizontally oriented sac compared to the vertically oriented one, less particles actually deposited as particles were closer to the inlet which also served as an outlet during contraction of the sac; 69.1% of particles deposited in the vertically oriented one vs. 50.9% and 48.5% on

the horizontally oriented one. Particle size was also found to be a significant factor in particle deposition. The deposition rates for 1 µm, 2 µm, and 3 µm particles were 69.1%, 93.9%, and 97.0% respectively. Particles were also deposited faster as their diameter increased.