Regional aerosol deposition in the human airways: The SimInhale benchmark case and a critical assessment of in silico methods

P. Koullapis, S.C. Kassinos, J. Muela, C. Perez-Segarra, J. Regola, O. Lehmkuhl, Y.Cui, M. S

January 11, 2023

Contents

1 Purpose

- Provide refined experimental data for QA of CFPD in the upper airways
- Provide critical review of different modelling approaches
- Define best practice guidelines

2 Work Done

2.1 Airway models adopted

2.1.1 Extrathoracic Airways (mouth, nose, pharynx, larynx, trachea)

2.1.2 Intrathoracic Airways (intrathoracic trachea to alveoli)

1. Conducting zone (generations 0 to 16)
2. Respiratory zone (generations 17 to 23)
   - Gas exchange takes place.
   - Not considered in this paper.

2.2 Solution of the flow field

2.2.1 Assumptions

- Particles are spherical, non-rotating and non-interacting
- Aerosol is considered a dilute suspension and modelled using a one-way coupling approach
- Effect of the particles on the flow and inter-particle interactions are neglected
- Deposition was assumed once a particle comes into contact with the airway walls
- All simulations employed a Lagrangian particle-tracking approach and assumed one-way coupling between the flow and the particles.

2.2.2 Numerical Approaches

1. RANS: Reynolds-averaged Navier-Stokes
2. LES: Large Eddy Simulation
3. DNS: Direct Numerical Simulation

2.2.3 Particle Transport Model

1. Eulerian (two-fluid approach)
2. Lagrangian (point-particles in continuous carrier phase) (not implemented)

2.2.4 Formulae

$$\begin{aligned}
\frac{d\mathbf{x}_p}{dt} &= \mathbf{u}_p \\
m_p \frac{d\mathbf{u}_p}{dt} &= \sum \mathbf{F} \\
Re_p &= \frac{\rho_f d_p |\mathbf{u}_f - \mathbf{u}_p|}{\mu_f} \\
C_D &= \frac{24}{Re_p}(1 + 0.15 Re_p^{0.687}) \\
C_C &= 1 + \frac{2\lambda}{d_p}\left(1.257 + 0.4 exp\left(-\frac{1.1 d_p}{2\lambda}\right)\right) \\
F_{Bi} &= G_i \sqrt{\frac{2k_B^2 T^2}{\tilde{D}\Delta t}}
\end{aligned}$$

$$m_p \frac{d\mathbf{u}_p}{dt} = \frac{3}{4}.\frac{\rho_f}{\rho_p}.\frac{m_p}{d_p}.\frac{C_D}{C_C}.|\mathbf{u}_f - \mathbf{u}_p|(\mathbf{u}_f - \mathbf{u}_p) + m_p g \frac{\rho_p - \rho_f}{\rho_p} + \mathbf{F}_B$$

1. Parameters Reynolds flow at inlet $= \frac{U_{in} D_{in}}{v} = 3745$ Particle diameters range: 0.5 to 10 micrometer Particle density: 914 kg/m^3 (di-ethylhexyl sebacate (DEHS))
2. Terminology

- $\mathbf{x}_p$: particle position
- $\mathbf{u}_p$: particle velocity
- m_p : particle mass
- d_p : particle diameter
- ρ_p : particle density
- μ_f : fluid viscosity
- ρ_f : fluid density
- $\mathbf{u}_f$: fluid velocity at particle location
- m_f : fluid mass displaced by particle
- Re_p : particle Reynolds number
- $\mathbf{F}_D$: drag force
- C_D : drag coeffcient
- C_C : correction factor
- λ (mean free path of air) = 0.070 micrometer
- G_i : zero mean variant Gaussian probability density function
- $T = 310$ K
- $\tilde{D}$ (brownian diffusivity) $= (k_B T C_C)/(3\pi\mu_f d_p)$
- k_B (Boltzmann constant) $= 1.3806488 \times 10^{23} J/K$
- Δt : time step

2.2.5 Observations

- As particle size increases, deposition increases significantly
- Interpolation errors in LES1c and LES2 cause higher deposition throughout the geometry
- Overprediction is observed at small particle sizes ($\mathrm{d_p} < 5$ micrometer)
- Significant variability in moutn and throat due to numerical errors for intermediate particles ($\mathrm{d_p} = 6$ micrometer)
- Prediction of flow in the upper airways is sensitive to mesh size and turbulence model, but is less influenced by the inflow conditions.

2.2.6 Geometry and Results (as Figures)

1. Schematic of the respiratory system (Figure 01)
2. Geometry of respiratory airways (Figure 02)
   (a) Original realistic airway geometry (a)
   (b) Geometry adopted for the benchmark case (b)
   (c) Physical segmented model for deposition measurements (c)
3. Schematic of the experimental set up (Figure 03)
4. Contours of mean velocity magnitude and turbulent kinetic energy (Figure 04, 06, 08, 09, 11)
   (a) Mean velocity magnitude
      i. Central sagittal plane of extrathoracic airways and trachea (4a)
      ii. Carina (6a)
      iii. Left main bronchus (6b)
      iv. Right main bronchus (6c)
      v. Segment 5 (left lung) (9a)
      vi. Segment 9 (right lung) (9b)
      vii. Segment 7 (left lung) (9c)
      viii. Segment 12 (right lung) (9d)
   (b) Mean turbulent kinetic energy
      i. Central sagittal plane of extrathoracic airways and trachea (4b)
      ii. Carina (8a)
      iii. Left main bronchus (8b)
      iv. Right main bronchus (8c)
      v. Segment 5 (left lung) (11a)
      vi. Segment 9 (right lung) (11b)
      vii. Segment 7 (left lung) (11c)
      viii. Segment 12 (right lung) (11d)
5. Profiles of mean velocity magnitude and turbulent kinetic energy (Figure 05, 07, 08, 10, 11)
   (a) Cross-section: A1-A2 (5a)

(b) Cross-section: A1-A2 (5b)
(c) Cross-section: A1-A2 (5c)
(d) Cross-section: A1-A2 (5d)
(e) Cross-section: A1-A2 (5e)
(f) Cross-section: A1-A2 (5f)
(g) Cross-section: G1-G2 (7a, 8a (carina))
(h) Cross-section: H1-H2 (7b, 8b (left main bronchus))
(i) Cross-section: J1-J2 (7c, 8c (right main bronchus))
(j) Cross-section: M1-M2 (10a, 11a (segment 5))
(k) Cross-section: P1-P2 (10b, 11b (segment 9))
(l) Cross-section: U1-U2 (10c, 11c (segment 7))
(m) Cross-section: Y1-Y2 (10d, 11d (segment 12))

6. Deposition patterns (Figure 14, 15, 16)

   Fig 14: Particle Diameter (d_p = 1.0 micrometer) **Fig 15**: Particle Diameter (d_p = 4.3 micrometer) **Fig 16**: Particle Diameter (d_p = 8.0 micrometer)

   (a) Sagittal view of extrathoracic airways (14a, 15a, 16a)
   (b) Posterior view of extrathoracic airways (14b, 15b, 16b)
   (c) Anterior view of trachea and major bronchial airways (14c, 15c, 16c)
   (d) Posterior view of trachea and major bronchial airways (14d, 15d, 16d)

7. Deposition fractions vs particle size (Figure 12, 13)

   Graph: Deposition fraction (%) vs particle size (d_p (0.5 to 10 micrometer))

   (a) Entire airway geometry (12a (15,30,60L/min LES1), 13a (60L/min))

   (b) Mouth-throat region (12b (15,30,60L/min LES1), 13b (60L/min))

   (c) Tracheobronchial tree (12c (15,30,60L/min LES1), 13c (60L/min))

8. Deposition fractions vs segment (Figure 17, 18, 19)

   Graph: Deposition fraction (%) vs segments of airway geometry (segment 1 to segment 22)

   (a) Particle size (d_p) = 0.5 micrometer (19a (RANS1))
   (b) Particle size (d_p) = 1.0 micrometer (17a (LES))
   (c) Particle size (d_p) = 2.5 micrometer (17b (LES), 18a (RANS))
   (d) Particle size (d_p) = 4.3 micrometer (17c (LES), 18b (RANS), 19b (RANS1))
   (e) Particle size (d_p) = 6.0 micrometer (17d (LES))
   (f) Particle size (d_p) = 8.0 micrometer (17e (LES), 18c (RANS)
   (g) Particle size (d_p) = 10.0 micrometer (17f (LES), 18d (RANS))

2.3 Aerosol physics included in the models

3 Limitations

- 3D CFPD studies of extra-thoracic and upper conducting airways
- Anatomically accurate models are limited to the first 6 or 7 generations due to imaging resolution
- Lack of detaield experimental data sets for validation of regional deposition results

4 Further reading

- Broader overview: Kleinstreuer and Zhang (2010) and Longest and Holbrook (2012)
- Effect of condensation of cigarette smoke particles: Longest and Xi (2008)

5 Glossary

- CFPD: Computational Fluid Particle Dynamics
- CT: Computed Tomography

- HRCT: High Resolution Computed Tomography
- MRI: Magnetic Resonance Imaging
- STL: Stereolithography files
- PET: Positron Emission Tomography
- in vitro, in vivo
- Saffman lift: Transverse lift force experienced by particles in shear flow