Predicting deposition in the human airways using CFD: The SimInhale benchmark case

P. Koullapis
Computational Sciences Laboratory
University of Cyprus

The SimInhale International Conference: Current Challenges and Future Opportunities for Inhalation Therapies.
30th September – 2nd October 2019
Athens, Greece
1. Airflow - CFD & PIV measurements

2. Aerosol Deposition part - CFD & in vitro PET measurements

Relevant publications

- Lizal et al. 2015. “A method for in vitro regional aerosol deposition measurement in a model of the human tracheobronchial tree by the positron emission tomography“.
- Janke et al. 2019. “PIV measurements of the SimInhale benchmark case”.
Contributors

**PIV measurements:** K. Bauer, T. Janke (TU Bergakademie Freiberg)

**Deposition measurements:** F. Lizal, J. Jedelsky, M. Jicha (Brno University)

**Numerical simulations**

P. Koullapis, F. Stylianou, S. Kassinos (University of Cyprus)

J. Muela, C. Perez-Segarra, J. Rigola (Universitat Politècnica de Catalunya)

O. Lehmkuhl (Barcelona Supercomputing Center)

Y. Cui, O. Sgrott, M. Sommerfeld (Otto von Guericke-University Magdeburg)

J. Elcner (Brno University of Technology)

I. Saveljic, N. Filipovic (University of Kragujevac)

Laura Nicolaou (Imperial College London)
Motivation & Objective

Deposition in the human airways

→ *In vivo*: real state but exposure to radiation

→ *In vitro*: expensive equipment & manufacturing limitations
Motivation & Objective

Deposition in the human airways

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→ *In vitro*: expensive equipment & manufacturing limitations

→ **Computational Fluid Dynamics (CFD) methods**
  + Non invasive / simulations at all scales
  + Detailed information on airflow and deposition patterns
  - Limited to small regions of the lung (computational cost)
  - **Need for proper validation prior use... “Garbage in, garbage out”**

**SimInhale Benchmark case**
Airway geometry

Fusion of different patients data

Oral cavity: molded from in vivo dental impression of a living subject

(Lovelace Respiratory Research Institute – Zhou&Cheng 2005)

Trachea to G7: HRCT of adult male lung (Schmidt model)

<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>Trachea</td>
<td>Diameter (mm) Left / Right</td>
<td>Diameter (mm) Left / Right</td>
<td>Diameter (mm) Left / Right</td>
<td>Diameter (mm) Left / Right</td>
</tr>
<tr>
<td>1</td>
<td>10.2 / 12.6</td>
<td>12.2</td>
<td>12 / 11.1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>6.5 / 8.3</td>
<td>8.3</td>
<td>7.8 / 8.1</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>5.6 / 5.9</td>
<td>5.6</td>
<td>6</td>
<td>6 / 5.8</td>
</tr>
<tr>
<td>4</td>
<td>3.8 / 4.4</td>
<td>4.5</td>
<td>5</td>
<td>/ 5.2</td>
</tr>
<tr>
<td>5</td>
<td>2.8 / 3.9</td>
<td>3.5</td>
<td>3.5</td>
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</table>
PIV measurements

- Silicone model - Full optical access
- Measurement tank with water-glycerin mixture
- Flow is driven by a piston diaphragm pump – uniform outlet pressures
- Quasi-stationary inspirational flow
- Flow is seeded with neutrally buoyant polyamide particles ($d_p = 50 \, \mu m$, $\rho_p = 1060 \, \text{kg/m}^3$, $\text{Stk} \approx 0.002$)
- Flow rates that correspond to 15, 30 & 60 L/min for air
Deposition measurements

- Positron Emission Tomography (PET)
- Radioactive DEHS particles with MMAD $4.3 \pm 1.24 \mu m / \rho_p = 914 \text{ kg/m}^3$
- 10 terminal branches with flow meters - **fixed outlet flowrates**
- Air flow rates of 15 & 60 L/min.
- Measuring technique compared to optical microscopy – good agreement
CFD – Reference cases

**LES 1: Large Eddy Simulations (LES)**
- Dynamic Smagorinsky subgrid scale model
- Finite volume method in OpenFOAM
- Lagrangian tracking for spherical-rigid particles
- One-way coupling
- Sphere Drag, gravity & Brownian force

**RANS 1: Reynolds-Averaged Navier-Stokes (RANS)**
- $k$-$\omega$ SST turbulence model
- Finite volume method in OpenFOAM
- Lagrangian tracking for spherical-rigid particles
- One-way coupling
- Sphere Drag, gravity, Saffman Lift & Brownian force
Airflow: PIV vs CFD (60L/min)
Airflow: PIV vs CFD (60L/min)
Deposition: In vitro vs CFD

Overall

15 L/min, $d_p=4.3\mu m$

60 L/min, $d_p=4.3\mu m$
Variability across different CFD methods
- LES vs RANS
## LES & RANS details - Airflow

<table>
<thead>
<tr>
<th></th>
<th>LES1 *</th>
<th>LES2</th>
<th>LES3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Flow solver</strong></td>
<td>OpenFoam (FVM)</td>
<td>Termofluids (FVM)</td>
<td>Alya (FEM) (Vázquez et al., 2016)</td>
</tr>
<tr>
<td><strong>Turbulence model</strong></td>
<td>LES dynamic Smagorinsky (Lilly, 1992)</td>
<td>LES variational multiscale (Hughes et al., 2000)</td>
<td>LES WALE (Nicoud and Ducros, 1999)</td>
</tr>
<tr>
<td><strong>Inlet boundary conditions</strong></td>
<td>Atmospheric pressure, turbulent (mapped inlet)</td>
<td>Atmospheric pressure, turbulent (mapped inlet)</td>
<td>Atmospheric pressure, extrapolated velocity</td>
</tr>
<tr>
<td><strong>Outlet boundary conditions</strong></td>
<td>Zero-gradient pressure, specified flow rates</td>
<td>Zero-gradient pressure, specified flow rates</td>
<td>Zero-gradient pressure, specified flow rates</td>
</tr>
<tr>
<td><strong>Mesh size</strong></td>
<td>50 M</td>
<td>10 M</td>
<td>7 M</td>
</tr>
<tr>
<td><strong>Mesh type</strong></td>
<td>Tetrahedral, 3–5 wall prism layers</td>
<td>Tetrahedral, 3 wall prism layers</td>
<td>Tetrahedral, 3 wall prism layers</td>
</tr>
<tr>
<td><strong>Time step</strong></td>
<td>$2.5 \times 10^{-6}$ s</td>
<td>$4.55 \times 10^{-7}$ s</td>
<td>$1.3 \times 10^{-5}$ s</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>RANS1 *</th>
<th>RANS2</th>
<th>RANS3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Flow solver</strong></td>
<td>OpenFoam (FVM)</td>
<td>CD-Adapco Star-CCM+ (FVM)</td>
<td>PAKF solver (FEM)</td>
</tr>
<tr>
<td><strong>Turbulence model</strong></td>
<td>RANS k-ω-SST (Menter, 1994)</td>
<td>RANS low-Re k-ω-SST (Menter, 1994)</td>
<td>RANS k-ε model (Lauder and Spalding, 1974)</td>
</tr>
<tr>
<td><strong>Inlet boundary conditions</strong></td>
<td>Atmospheric pressure, turbulent inlet</td>
<td>Atmospheric pressure, uniform velocity</td>
<td>Atmospheric pressure, uniform velocity</td>
</tr>
<tr>
<td><strong>Outlet boundary conditions</strong></td>
<td>Zero-gradient pressure, specified flow rates</td>
<td>Zero-gradient pressure, specified flow rates</td>
<td>Zero-gradient pressure, specified flow rates</td>
</tr>
<tr>
<td><strong>Mesh size</strong></td>
<td>12 M</td>
<td>6.3 M</td>
<td>1.3 M</td>
</tr>
<tr>
<td><strong>Mesh type</strong></td>
<td>Tetrahedral, no wall prism layers</td>
<td>Polyhedral, 8 wall prism layers</td>
<td>Tetrahedral, no wall prism layers</td>
</tr>
<tr>
<td><strong>Time step</strong></td>
<td>$1 \times 10^{-5}$ s</td>
<td>$2.5 \times 10^{-4}$ s</td>
<td>$1 \times 10^{-5}$ s</td>
</tr>
</tbody>
</table>

*LES1, RANS1: reference cases

Q=60 L/min
Variability across different CFD methods - Airflow
## LES & RANS details - particles

Computational details of the Lagrangian particle-tracking schemes.

<table>
<thead>
<tr>
<th></th>
<th>LES1*</th>
<th>LES2</th>
<th>LES3 (Houzeaux et al., 2016)</th>
<th>RANS1*</th>
<th>RANS2</th>
<th>RANS3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Time integration scheme</strong></td>
<td>Implicit Euler</td>
<td>Explicit second-order</td>
<td>(implicit) Newmark</td>
<td>Implicit Euler</td>
<td>Implicit Euler</td>
<td>(implicit) trapezoidal</td>
</tr>
<tr>
<td><strong>Forces on particles</strong></td>
<td>Drag, gravity, Brownian</td>
<td>Drag, gravity, Brownian</td>
<td>Drag, gravity</td>
<td>Drag, gravity</td>
<td>Drag, gravity</td>
<td>Drag, gravity</td>
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<tr>
<td><strong>Cunningham correction factor ($C_C$)</strong></td>
<td>Davies (1945)</td>
<td>Davies (1945)</td>
<td>1.0</td>
<td>Davies (1945)</td>
<td>1.0</td>
<td>1.0</td>
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<tr>
<td><strong>Turbulent dispersion</strong></td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>Continuous random walk</td>
<td>Eddy interaction model</td>
<td>Mean-flow tracking</td>
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<tr>
<td><strong>Number of particles per size</strong></td>
<td>100,000</td>
<td>100,000</td>
<td>300,000</td>
<td>100,000</td>
<td>10,000</td>
<td>30,000</td>
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<tr>
<td><strong>Release time of particles</strong></td>
<td>0.025 s</td>
<td>0.025 s</td>
<td>0.3 s</td>
<td>0.025 s</td>
<td>0.1 s</td>
<td>0.08 s</td>
</tr>
</tbody>
</table>

*LES1, RANS1: reference cases
Variability across different CFD methods - Deposition

Mouth-throat

\[ d_{p} (\mu m) \]

\[ 10 \mu m \]

\[ 4.3 \mu m \]

\[ 2.5 \mu m \]

\[ 17/22 \]
Variability across different LES methods – Deposition

Coarse mesh
10M cells

Fine mesh
50M cells

In-vitro
LES1 - coarse
LES2 - coarse

In-vitro
LES1 - fine
LES2 - fine
Variability across different RANS methods - Deposition

Mouth-throat

- $2.5 \mu m$
- $4.3 \mu m$
- $10 \mu m$

Segments 1 to 22

Graphs showing deposition efficiency (%) vs. diameter ($d_p$) for different methods:

- LES1
- RANS1
- RANS2
- RANS3
- In-vitro
Variability across different CFD methods – Deposition patterns (4.3μm)
Variability across different LES methods – Deposition
Conclusions

**CFD vs Experiments**

- LES1 & RANS1 show good agreement to measurements (almost)

**Variability across different CFD methods**

- **Airflow**
  - LES: good agreement for the mean airflow (even on coarse meshes)
  - RANS: larger deviations - more setup parameters (modeling)

- **Deposition**
  - LES: Convergence for larger particles - sensitivity on mesh for smaller particles
    - proper mesh resolution is essential
  - RANS: Larger discrepancies - more uncertainties (modeling)

We get what we pay… LES → more consistent / accurate (~days)
  - RANS → difficult fine tuning (~hours)
ERCOFTAC APPLICATION CHALLENGE → new Application Area - Biomedical Flows

1. Deposition part (CFD & in vitro measurements)

2. Airflow part (CFD & PIV measurements)

(http://www.kbwiki.ercoftac.org/w/index.php/Application_Areas)
Thank you