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Comparison of breathing models for determining flow and particle deposition in the lungs

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Abstract

Collection and deposition of particles in the upper airway and lungs is of considerable importance – for example, when studying chronic diseases, or when determining the efficacy of aerosol drug delivery. Modelling of particle deposition usually assumes either constant flow (typically at maximum inspiration), or oscillating flow – ignoring any effects of the lung's motion.

This paper presents a preliminary examination of the effects of ignoring mesh motion when modelling the lungs. Initially, an idealised lung model was created, corresponding to generations 0 to 3 of Weibel's morphology[14]. Simulations were then made using this geometry for steady flow, oscillating flow, and flow developed by expanding the lung. The expansion of the lung was modelled using a mesh motion library developed by the authors. This model allowed the expansion of the lung to be prescribed.

Results from the simulations show significant differences between the three modelling options – relating to both the predicted flow field, and particle deposition sites. Robustness of the moving mesh modelling technique is demonstrated on a high-resolution geometry created from CT scans of a Sprague-Dawley rat model lung.

Introduction

Simulation of the lungs is an interesting case where both biomechanics and medicine come together. Most lung research has been limited to studies of inhalation/exhalation (e.g. spirometry) and the use of medical imaging technologies (e.g. x-ray computed tomography (CT) scans). It would be exceedingly difficult to measure localised flow and pressure fields within the lungs and as such properly constructed simulations could lead to a greater understanding of lung function which could assist those in medical profession to develop medicine delivery and diagnostics.

The collection and deposition of particles in the upper airway and lungs is of considerable importance (e.g. in determining the efficacy of the delivery of inhalable medications). The flow in the lungs and upper airway is driven by the expansion and contraction of the lung, dictated chiefly by the breathing rate. While this mechanism is well-understood, modelling of the lungs in this manner is potentially complex, due to the necessity of allowing the computational domain to move and deform. To overcome these complexities, modelling of airflow in the lungs has generally focused on static models, and often using steady airflow conditions. Reasonable agreement between numerical and experimental results is claimed in the literature, though often these comparisons are made against direct experimental analogues to the numerical set-up. To date, no comparisons have been made between static lung models and those that are based on a more realistic representation of the mechanics that drive the flow in the lungs. Concerning particle deposition in particular, static analysis methods potentially incorrectly predict the regions of deposition, compared with models where the lung walls are allowed to move and stretch.

Background

A number of studies have considered the simulation of flow and particle deposition in the lungs. These have, however, all considered fixed, rigid geometries and do not consider the expansion and contraction of the lungs that occurs during breathing. Such simulations utilise either lungs models [1, 2, 5, 12] or x-ray computed tomography (CT) based lung geometries [3, 4, 8, 9]. There is perhaps some advantage in using CT-based geometries, particularly if the results are to be used to draw conclusions on breathing patterns and behaviour, however, the models are useful for developing and validating methods and are less labour intensive to prepare.

The flow fields in the studies in the literature rely on the author's choice of flow model, and on the construction of the simulation. In the simplest cases flow is allowed to exit via the extremities of the lung model, with more developed models considering flow fields based on the difference between two measured lung volumes [8]. Such models typically use Reynolds Averaged Navier Stokes (RANS) [9] or Large Eddy Simulation (LES) [8] methods to resolve the flow. Other authors have used the k-ε and k-ω turbulence models [7, 9] in the simulation of flow, which may be unnecessary as the flow in the lungs, under normal conditions, will be linear. As noted by, Walters et al. [13], there may be some areas of the exothoracic airway where the flow may be turbulent, though this should not effect the flow in the lungs, even if the whole airway and the lungs are being considered.

In terms of the simulation of particle deposition, the flow field is critical and as such needs to be accurate. Models that allow the flow to exit via the extremities of the lung are therefore unrealistic, as these do not consider the recirculation of particles in the lungs and the possible exhalation of particles. Such factors could however be considered if a 'breathing' lung model were used. The flow then would be controlled by the expansion and contraction of lungs (geometry) much like real breathing and therefore would not rely on a defined inlet flow rate.

Methodology

Geometry

We constructed a four-branch model of a lung bifurcating lung, described by the bifurcation angle, branch diameters, and branch lengths corresponding with generations 0 to 3 from Weibel [14].

The geometry and surface mesh is indicated in Figure 1.

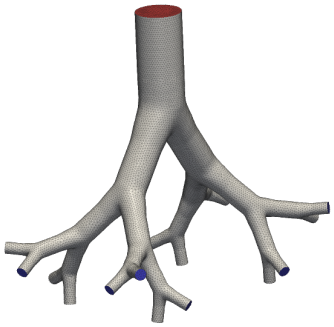


Figure 1: Mesh and boundary locations

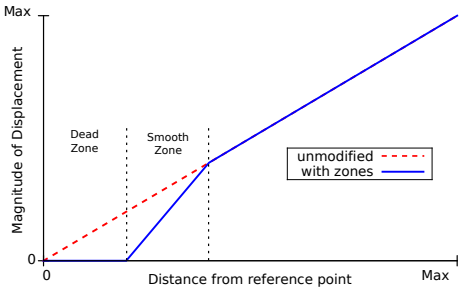
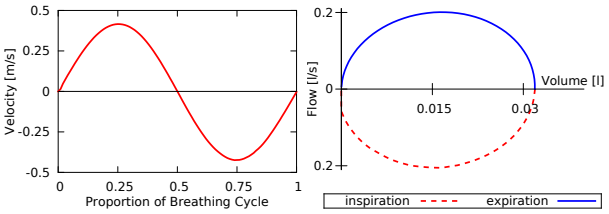


Figure 2: Motion zones



(a) Inlet velocity (b) Spirogram

Figure 3: Breathing Parameters

Computational Fluid Dynamics

Flow simulations were conducted using the OPENFOAM suite of CFD applications and solvers[11]. For particle modelling, the Lagrangian particle simulation code and methodology of the authors was used[6]. OPENFOAM implements very robust mesh motion routines, and these were used to deform the lung model for the moving mesh simulations. Details of the mesh motion code are given in the following section.

Lung Motion Model

A prescribed lung motion model was developed in OPENFOAM to account for expansion of the lungs, and to drive the flow. To achieve this the boundary of the mesh was expanded relative to a fixed reference point, with the ability to adjust the expansion in along each axis separately. The overall expansion of the lung e, in addition to the relative expansion along each axis (as ratios, $e_x : e_y : e_z$), became the key input parameters for the simulations. These parameters were used to solve for scaling parameters s_x, s_y and s_z such that

$$s_x s_y s_z = e \tag{1}$$

These scaling parameters defined the scaling of the lung surface at the maximum expansion point, relative to the fixed reference point. To account for the unsteady motion of the lungs an additional time dependent scale s_t was used, where

$$0 < s_t(t) < 1 \tag{2}$$

This scale allows the lung motion to be adjusted to give a specific spirometry.

Mesh quality

In the case where the moving lung boundary connects to a non-moving boundary, such as the trachea, the mesh can deform such that poor quality cells are present at the join. To overcome this our motion model includes a 'dead-zone' where no mesh motion occurs. A second 'smoothing' zone is also included, to blend the zero-motion zone to the full-motion zone. These zones are kept as small as practical so the desired expansion rate is not changed, while still maintaining the cell quality. The displacement modification is shown in Figure 2.

Comparison Cases

Three cases were set-up with changes to the flow condition and mesh motions to represent modelling approaches for particle deposition in the lungs. The breathing parameters for the simulations as shown in Figure 3 (Figure 3(a) showing the time varying inlet velocity profile and Figure 3(b) showing the resulting spirogram). The three flow conditions simulated were: steady flow, oscillating flow on a static mesh, and oscillating flow on a moving mesh. For the static mesh case, the flowrate was set to the maximum inspiration (from Figure 3(a)).

Boundary Conditions

For the inlet boundary, a prescribed velocity was applied (discussed above), while the pressure was found as part of the solution. For the outlet boundary (at the extent of the branches), a total pressure boundary was used, while the flow velocity was determined from the pressure field. For the lung surface a zero slip condition was used. For the deforming mesh cases this was enforced relative to the motion of the mesh.

Mesh Motion

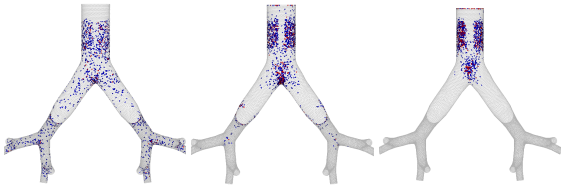
The expansion parameters for the lung were determined such that the volume of inspired air was consistent with the volume of the modelled lung. This resulted in zero net-flow across the outlets of each branch. To satisfy this condition a lung expansion value of 1.4 was used in conjunction with directional expansion ratios of 1:1:2, meaning the domain expanded in the z-direction (along the main branch) twice as much as the other directions.

Particle Injection & Capture

Particles were injected into the domain in a spherical region with the same diameter as the largest branch, located one diameter downstream from the inlet to the domain. Particles were captured by all surfaces, and their number and locations recorded during the simulation. This allowed the regions where particles collected to be compared between all three simulation types. The tracking algorithm, requirements for capture, and validation results are presented in King et al. [6] and Mead-Hunter [10].

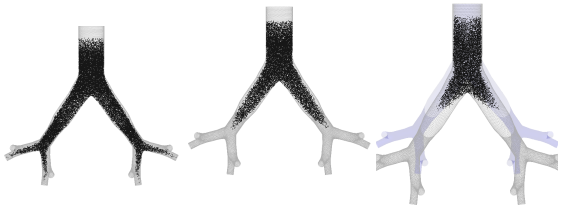
Results - Idealised Geometry

Figure 4 shows the relative flow at various cross sections for the steady flow, oscillating flow and moving mesh cases. The difference in profiles is particularly pronounced when compar-



(a) Steady Flow (b) Oscillating Flow (c) Moving Mesh

Figure 5: Particle deposition locations after 5s



(a) Steady Flow (b) Oscillating Flow (c) Moving Mesh

Figure 6: Particle ingress after 0.25s

ing the moving mesh case to the steady and oscillating flow cases. For the steady and oscillating flow cases large velocities are observed in the smaller branches, whereas for the moving mesh case the velocity decreases as along the branches, such that there is no flow at the outlets. For the steady and oscillating flow cases the velocity is determined by the flow rate and total cross-sectional area of the branches only. However for the moving mesh case expansion of the lung itself accounts for the inspiration, and contraction for the expiration. As expected, this results in the lower velocities observed in the moving mesh case.

Particle deposition

Figure 5 shows locations of collected particles at the end of the simulation (5 seconds) for the steady flow, oscillating flow and moving mesh cases. For all of the cases a number of particles are collected near the injection zone, with a higher number observed for the unsteady cases due to the effects of the oscillating flow. Of more importance is the collection of particles in the branches, and the extent of particle ingress. For the steady flow case, the particles are somewhat uniformly distributed along the flow paths, including a large rate of collection at the outlets of the branches. In the oscillating flow case there are no particles collected at the outlets, and the remainder of the collected particles are concentrated at the cusps of the bifurcations, with a small number of particles collected at the third split. The moving mesh case has a still smaller number of particles collected around the first bifurcation, with no particles collected beyond this point. In all cases, the particles preferentially collect in the cusp of the bifurcations, with significantly lower deposition in the straight branch sections, this, however, is less evident in the steady flow case.

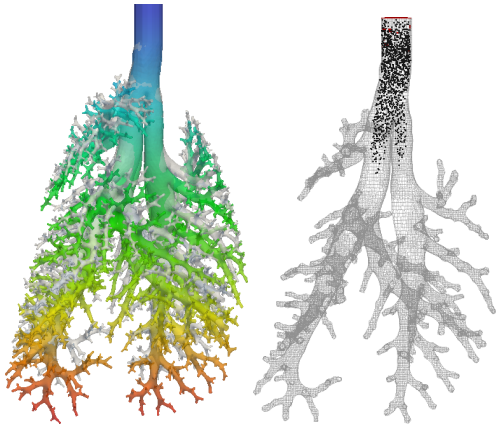
Figure 6 shows particle ingress for each of the cases after 0.25 seconds (maximum expansion), and Figure 7 shows the ingress after 5s.

Realistic Geometries

In addition to the idealised lung geometry presented above, the numerical method was applied to a high resolution scan of a Sprague-Dawley rat model lung. Due the large number of small

(a) Steady Flow (b) Oscillating Flow (c) Moving Mesh

Figure 7: Particle ingress after 5s



(a) Expanded lung (b) Particle tracking

Figure 8: Imposed mesh motion, and particle tracking inside the lung of high resolution Sprague-Dawley rat model. In (a) Colours indicate maximum displacement, and the grey boundary the undeformed mesh, in (b) particle locations are indicated in black.

branches in the geometry, the mesh required over 8×10^6 cells, to resolve the geometry while maintaining suitable mesh quality. Figure 8(a) shows the imposed maximum displacement of the lung superimposed on the undeformed lung, while Figure 8(b) shows the particle locations after 0.125s (maximum inspiration).

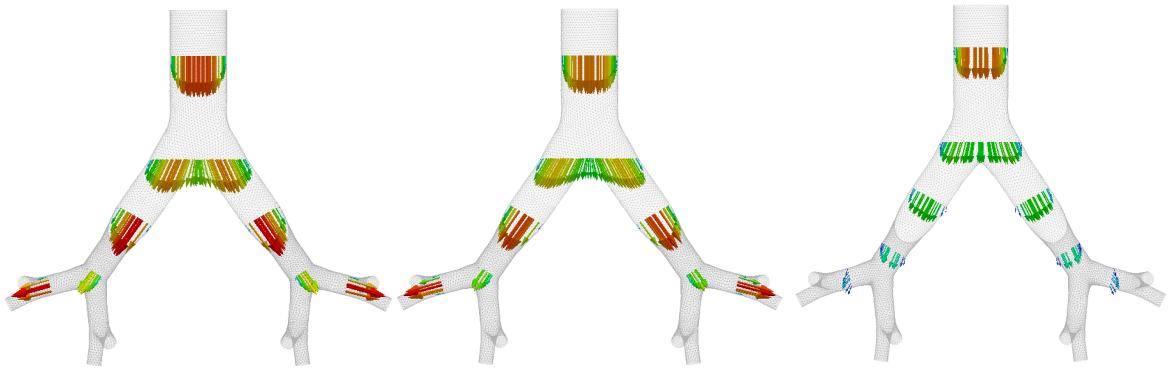
Discussion

The results shown in Figures 5, 6 & 7 demonstrate that the particle deposition is highly dependent on the nature of the simulation. This indicates that previously used models may be unable to accurately resolve particle deposition. The results presented here create flow in the lungs through expansion only, or oscillating flow. In reality, the ideal situation is most-likely somewhere in between, and is dependent on the resolution of the lung geometry used (in terms of levels of resolved branches). By combining mesh motion with suitable oscillating outlet and inlet flow conditions, accurate spirometry can be created, while correctly accounting for the motion of the lung walls.

Finally, the mesh motion model presented in this paper is robust and is successfully used in combination with an accurate particle tracking method. This has allowed simulation of a highly resolved rat-lung geometry to be simulated for both flow and particle capture.

Conclusions

This paper has shown that considerably different flow fields are observed in a simple lung geometry, depending on the mod-



(a) Steady Flow (b) Oscillating Flow (c) Moving Mesh, Oscillating Flow

Figure 4: Velocity at various cross-sections at maximum inspiration.

elling method used. Large differences exist between an expanding mesh model, where the flow is induced through unsteady motion of the lung walls, and a static lung model, where the flow is explicitly provided using an unsteady velocity profile at the inlet. These results are significant as the majority of computational work published to date has made use of static meshes. This work has shown that this approach is likely not accurate in all cases, and will tend to over-predict particle deposition. Future work will investigate the effects of a combined flow and motion model, and determine the correct combinations to achieve a prescribed spirometry.

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