Numerical Assessment of Airflow and Inhaled Particles Attributes in Obstructed Pulmonary System

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Abstract— Geometry contraction algorithms are introduced in this work to implement the diverse respiratory configurations of lung related diseases associated with airways obstructions. In addition, computational fluid dynamics (CFD) techniques along with fluid particle tracing (FPT) methods are utilized to efficiently evaluate the behavior of the airflow during the inhalation period, as well as to clarify the features of the inhaled particles in terms of regional deposition. Useful deductions are drawn regarding personalized medication in obstructed conditions.

Keywords—computational fluid dynamics; fluid particle tracing; obstructive lung diseases; aerosol deposition; human airways

I. INTRODUCTION

Lung diseases, such as asthma and chronic obstructive pulmonary disease (COPD), are life-long chronic inflammatory diseases of the airways affecting over 500 million people worldwide. Several clinical tools have been utilized to assess their severity, supported by ICT infrastructure [1], [2]. Ventilation heterogeneity due to small airways dysfunction is considered an important marker of asthma disease activity, as stated by [3], whereas airborne fine water particles are among the etiological factors that induce asthma attacks in asthmatic children as presented by [4]. In this framework, the basic approach when developing severity assessment tools involves computational fluid dynamics (CFD) simulations [5], [6] accompanied by fluid particle tracing (FPT) analysis of the inhaled ambient particles [7]-[9]. In this way, the airflow characteristics, along with the density and the deposition of the particles on the respiratory airways, are discerned. As of today, various CFD models have been employed to analyze the function of the lungs in terms of inspiration and expiration [10]-[12]. Also, several approaches, based on the data acquired by the CFD analysis, introduce calculations of the particles features [13]-[16].

This work has been funded by the H2020-PHC-2014-2015 Project MyAirCoach (Grant Agreement No. 643607).
The objective of this work is focused on the accurate modelling of the airways obstructions that relate to pulmonary diseases. In addition, it aspires to provide effective evaluation of the airflow behavior in conjunction with clarification of the inhaled particle properties as an initial step of attaining personalized treatment. To pursue these goals, a geometry processing sequence is developed and utilized for the construction of several important models of the respiratory system. These discrete cases are studied by means of the finite volume method (FVM) and specifically the CFD and FPT algorithms which provide accurate deductions about airflow and deposition fraction upon several parts of the lungs. The data acquired illustrate potential use in personalized medical treatment of lung diseases by providing regional-oriented deposition information.

II. STRUCTURAL MODELING, PARAMETRIZATION AND DEFORMATION OF THE LUNG

Geometry processing approaches are developed to allow the simulation of the effects of the obstructive diseases in the 3D lung structure. This technique enables the study of the impact of any obstructions on the airflow into the lung, by using a CFD simulation. The proposed approaches are executed directly on an already available 3D model of the lung [29], extracted from CT-MRI scans, by using state-of-the-art methods. The surface of a certain part of the mesh is iteratively contracted by executing a Laplacian mesh contraction approach in the direction of the inward normal. Moreover, the lung geometry is segmented into several important components, such as the generations and the outlets, as illustrated in Fig. 1.

A. Lung Geometry contraction in the direction of the Inward Normals

In order to apply mesh contraction, we employ the Laplacian mesh processing scheme presented in [30], which have been extended in [31], allowing a unique geometry processing sequence. For the sake of self-completeness, we provide a short overview of the method. A lung 3D model is described by a mesh $(V, E)$ with vertices $V$ and edges $E$. Using cotangent weighting the Laplacian coordinates approximate the curvature-flow inward normal. Thus solving iteratively, the discrete Laplacian equation $LV = 0$ we can achieve mesh contraction or reduce the 3D model to an 1D shape. Let $L$ be the Laplacian operator and $V'$ the vertices of the final position, then we have:

$$L = \begin{cases} \cot a_{i,j} + \cot b_{i,j} & \text{if } (i,j) \in E \\ \sum_{k \in E} \omega_{i,k} & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

(1)

where $a_{i,j}, b_{i,j}$ are the angles facing the edge $(i,j)$. These angles are included to the adjacent triangles that contain the edge $(i,j)$, as depicted in Fig. 2(a). Since $L$ is singular, further constraints need to be used in order to ensure a unique solution for $V'$. Thus, we focus on solving the equation:

$$[W_L L] V' = \begin{bmatrix} W_L L & 0 \\ 0 & W_H V \end{bmatrix}$$

(2)

where $W_L$ and $W_H$ are diagonal matrices. However, by experimentation one can notice that the solution of (2) does not immediately converge to an 1D shape and that an iterative scheme has to be employed.

1. Initialize $W_L$ and $W_H$ in the following manner:

$$W_L = k \sqrt{A}$$

(3)

$$W_H = I$$

(4)

where $I$ is a unitary matrix, $k$ a double constant and $A$ the average face area of the model.

2. Solve (2) for $V'$

3. Update $W_L$ and $W_H$ so that

$$W_L^{t+1} = s_L \cdot W_L^t$$

(5)
Fig. 3. Magnified perspective of the patient personalized model of lung geometry before and after the narrowing process.

\[ W_{H,t+1} = W_{H,t} \cdot \sqrt{A_i^0 / A_i^t} \]  \hspace{1cm} (6)

where \( s_x \) is a user defined double constant, \( A_i^0 \) is the initial one-ring area for vertex i and \( A_i^t \) is the one-ring area for vertex i at iteration t.

4. Recompute L.
5. Repeat steps 2 to 4 for a given number of iterations.

Based on the aforementioned scheme we apply mesh contraction at a certain part of the mesh in order to simulate narrowing by using stopping criteria related to the difference between the updated and the initial position. The area under contraction at a certain part of the mesh in order to simulate geometry before and after the narrowing process.

Fig. 3. Magnified perspective of the patient personalized model of lung geometry before and after the narrowing process.

Measuring the narrowing percentage

By inspecting Fig. 2 and Fig. 3, it is made obvious that the airflow has been narrowed by a significant percentage. The lung geometry topologies investigated in this work are generated by the same, CT-MRI derived, 3D respiratory model [29]. The narrowed versions of this model occur after processing the normal topology with our geometry processing algorithm. These obstructions are generated at the middle section of each respiratory branch [22] to model the lung’s contraction. In order to determine the partial obstruction of the airways, the narrowing percentage \( r \) is adopted. In this context, the airflow obstruction is measured by estimating the ratio of the initial airflow’s diameter to that produced after the geometry contraction process. The measurement of the partial obstruction is attained by using a shape diameter function based scheme (SDF) [33]. The SDF produces a scalar value for each face corresponding to the local shape diameter. Thus, by summing up the SDF values of the faces of the processed part of the mesh we derive a characteristic value for the local diameter of the processed segment. The ratio \( r \) of the sum of the SDF values before the narrowing process to the sum of the SDF values after the narrowing process corresponds to a metric of the narrowing percentage of the airway. Specifically

\[ r = \frac{\sum_{i=0}^{N} SDF(f_i^t)}{\sum_{i=0}^{N} SDF(f_i^0)} \]  \hspace{1cm} (7)

where \( f_i^t \) is the face with index i after iteration t, \( f_i^0 \) is the initial face with index i and \( N \) the number of the processed faces. In the current study the processed airways have been narrowed by a percentage of 50%.

III. METHODOLOGY OF LUNG FUNCTION ANALYSIS

The lung geometry is cleaned-up by utilizing several techniques, such as surface reconstruction, surface remeshing, triangulation, and decimation, in order to provide smoothness and facilitate the upcoming procedures of meshing and solving. Since the deformation of the airways geometry creates additional edge effects, which could affect the CFD analysis, a smoothing procedure is deemed mandatory to minimize any interactions with our studies. In addition, the previous techniques will not affect much our analysis, since the airflow into the lungs is mainly determined by the topology of the generations’ geometry rather than the surface topology of the airways.

The meshing is performed by employing the snappyHexMesh algorithm, which is part of an open source platform dedicated to CFD and FPT analyses, called OpenFoam [34]. Our analysis involves hex-dominant cells exhibiting very fine discretization near the walls of the respiratory system. In this way, the interesting properties of turbulence can be resolved, whereas the presence of particles can be accurately clarified. In particular, the domain is discretized into 5569106 cells. In order to effectively deal with the huge computational burden, ARIS, a high performance computer (HPC), was utilized to conduct the related simulations.

A. CFD analysis of pulmonary system

Several models can be utilized to computationally assess the lung’s behavior, such as Reynolds-averaged simulation (RAS), large eddy simulation (LES) and direct numerical simulation (DNS). Among them, RAS provides the minimum computational cost together with acceptable levels of accuracy. Therefore, RAS is efficiently employed to solve the Navier-Stokes equations and perform a steady state CFD analysis of the human pulmonary system. In particular, a kOmegaSST turbulence model is utilized to clarify the properties of the airflow. The study is conducted by means of the FVM technique, especially the SIMPLE algorithm, which is part of the OpenFoam platform. The discretization of the related equations is performed by second order schemes in time and space. In order to enable numerical stability a time step of 5 x 10^-4 s is utilized. This value is calculated by taking into account the mesh discretization, the air velocity and the Courant number as described in the CFD theoretical formulations. In this way, convergence and stability of the simulations are guaranteed. A hypothesis of a total pressure drop of -15 Pa is considered throughout the simulations of inspiratory states. Airflow velocity and pressure are calculated over the compu-
B. FPT analysis of inhaled particles

A Lagrangian approach is employed to investigate the motion of particles in fluids by solving a set of ordinary differential equations along their trajectories. The goal of fluid particle tracing is to calculate the change of particle location and the components of the particle velocity. The relevant forces acting on the particle need to be taken into account. Hence, if spherical particles are considered, the differential equations for calculating the particle location and velocity are given by Newtonian second law:

\[
\frac{dx_p}{dt} = u_p, \tag{8}
\]

\[
m_p \frac{du_p}{dt} = \sum F_i, \tag{9}
\]

\[
I_p \frac{d\omega_p}{dt} = T, \tag{10}
\]

where \(m_p = \rho_p d_p^3 \pi / 6\) is the mass of a particle (\(\rho_p\) is the particle density and \(d_p\) is the particle diameter), \(I_p = 0.1 m_p d_p^2\) is the moment of inertia for a sphere, \(F_i\) denotes the relevant forces acting on the particle, \(u_p\) is the linear velocity of a particle, \(\omega_p\) is the angular velocity of a particle and \(T\) is the torque acting on a rotating particle due to the viscous interaction with the fluid.

For small Reynolds numbers, analytical solutions are available for the different forces applied (Stokes flow). An extension to higher Reynolds numbers is usually obtained by introducing a coefficient \(C\) to be multiplied with the force,

\[
F_D = \frac{C_D}{\frac{4}{3} \rho_p d_p A_p (u_F - u_p)} |u_F - u_p|. \tag{12}
\]

where \(C\) is based on empirical correlations derived from experiments or direct numerical simulations. In most fluid-particle systems, the drag force dominates the particle’s motion. An extension to higher particle Reynolds number is based on the introduction of a drag coefficient \(C_D\), defined from

\[
C_D = \frac{F_D}{\rho_p A_p (u_F - u_p)^2}. \tag{11}
\]

where \(u_F\) is the linear velocity of a fluid, and \(A_p = d_p^2 \pi / 4\) is the cross-section of a spherical particle. The drag force can be expressed by:

\[
F_D = \frac{3}{4} \rho_p m_p C_D (u_F - u_p) |u_F - u_p|. \tag{12}
\]

The particle Reynolds number is defined as the ratio of ine-
rtial force to friction force:
\[ Re_p = \frac{\rho_d d_p |u_d - u_p|}{\mu_f}, \]
(13)

where \( \rho_d \) is the fluid density and \( \mu_f \) is the fluid dynamic viscosity. The aforementioned approach is intended to facilitate particle deposition assessment into the pulmonary system. Moreover, an investigation of the related drug delivery efficiency can be performed to mitigate asthma effects and enable dosimetry conclusions.

A transient FPT analysis is conducted to study the movement of inhaled particles through the respiratory system, as well as the deposition fraction over various areas of interest. Specifically, a one-way coupling between the flow field and the particles is considered, since the steady state field of airflow velocity acquired by the CFD simulation is utilized to calculate the position and velocity of the particles. For the purpose of our simulations, a particle density of 1000.0 kg/m³ is employed, whereas their diameter is 10 μm. A total of 54,000 particles are injected through the inlet boundary of the computational domain.

The initial velocity of the particles is considered the same as the inlet velocity of air for the CFD simulations. A stick boundary condition is applied on the wall of the lung geometry as well as on the outlets to efficiently simulate the particle’s entrapment on the wall’s surface. A transient analysis is performed utilizing the icoUncoupledKinematicParcelFoam solver, which is part of the OpenFoam platform. This algorithm assumes that the particles’ effects on turbulence are negligible, thus the flow affects the particles but the particles don’t affect the flow. Finally, the position of the particles on the respiratory airways is determined.

IV. NUMERICAL ASSESSMENT OF THE RESPIRATORY SYSTEM

Several lung models associated to different levels of obstructions have been created using the method described in section I. Each case is determined by the lung generation, after which, obstructions in the form of bottlenecks are observed. Also, an additional case, where only one lung (the right) exhibits obstructions, is modeled. For the development of these models an in-house developed software, based on the aforementioned geometry processing methods, have been employed. A CFD analysis is performed for each model, whereas the output velocity fields are utilized for the corresponding FPT studies. Then, the particles deposition is calculated for every segment of the lung’s model. In this way, deposition fractions are extracted for each generation of the respiratory system, as well as for the left/right sections.

A. CFD Analysis

The inlet velocity of the air is determined by the simulations, since a total pressure drop of \(-15\) Pa is assumed in all cases as validated by past studies of airflow into human lungs [16], [22]. For example, the normal lung exhibits an inlet velocity of \(1.475\) m/s, while the air velocity when obstructions are observed after the second generation is \(0.711\) m/s. Indicative results are presented in Figs. 4-6, where the air velocity distribution cross-sections at the sagital plane, the trachea, and main bronchi, are illustrated. As discerned from Fig. 4, the airflow is reduced at the region of the trachea, when several obstructions occur, thus decreasing
the breathing capability. If only one lung is obstructed the airflow is fairly reduced. Similar deductions can be drawn from Fig. 5. Also, Fig. 6 clarifies the airflow behavior at the region of the main bronchi. In the case of one obstructed lung, the airflow is driven at the other functional section. This observation denotes that any inhaled particles, ambient or medical oriented, will be guided mostly to the functional part of the respiratory system.

B. FPT Analysis

A transient analysis of the particles behavior is conducted for each lung model studied in the previous paragraph. The whole inhalation procedure is simulated resulting in a total duration of 2.16 sec. Several snapshots of the particles movement into the domain of the normal lung is presented in Fig. 7 for various time steps. Depending on the different conditions and obstruction topologies, the particles will stick on discrete areas of the lung, thus affecting any related diseases. A more comprehensive perspective is attained by the deposition of particles after the inhalation period is completed. Fig. 8 illustrates these depositions for three distinct cases: normal lung, as well as obstructions in both lungs and in the right one only. As observed, when obstructions occur most particles are deposited on their vicinity, in comparison to the normal lung function.

Moreover, particle deposition fraction is calculated for different generations as well as for discrete lung sections. By observing Fig. 9, a maximum deposition on the fifth generation is attained, when obstructions occur all over the respiratory system. This behavior is attributed to the size of the particles examined in this work. A diameter of 10 μm is considered, thus enabling their accumulation upon the fifth generation. Particles with diverse sizes will provide maximum deposition at different generations of the lungs as well. Thus, medical oriented particles of particular size will be deposited on identifiable areas targeting specific treatment. In addition, most particles are located on the right lung, as discerned from Fig. 10, when obstructions occur symmetrically in both lungs. On the other hand, most particles are driven on the left lung, when obstructions are present on the right section only, as expected from the CFD simulations. In this way, any medication will be guided away from the problematic obstructed area. This notice should be taken into account when designing personalized medical treatment of lung diseases. Doctors could utilize the findings of the CFD and FPT simulations of specific patients to select and provide appropriate medication according to the particle deposition capability on their lungs, thus maximizing the efficiency of personalized treatment.

V. CONCLUSIONS

The employment of contraction algorithms to model the different conditions of lung obstructions has been introduced in this paper. Furthermore, accurate CFD and FPT simulations have been utilized to effectively assess the effects of inhaled particles in a regional oriented perspective. Most particles are delivered upon the narrow areas when symmetrical obstructions occur. In addition, partial medication delivery is attained when only one lung is obstructed. This observation could be beneficial when treating lung diseases with inhaled medical substances.
ACKNOWLEDGMENT

This work was also supported by computational time granted from the Greek Research & Technology Network (GRNET) in the National HPC facility - ARIS - under project ID 004004.

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