Matrix-Based Simulation for Patient-Specific Human Respiratory Air-Particle Flow Analysis

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Abstract—Conventional approach of simulating patient-specific human respiratory air-particle flow involves tedious steps that include solid-fluid grid generations, air-particle solutions and results visualizations. A novel approach of combining the efficient Immersed Boundary method and Finite Difference Splitting solver within a matrix-based open source programming platform achieved in this work has radically simplified the procedure especially in the pre-processing stage. Air and particle interactions are based on Eulerian-Lagrangian technique while convergence error of less than 1 x 10^-6 in all validations. Quantitative comparisons were made based on standard five percent difference. Air flow rate of 30 litre/minute was used throughout the analyses representing normal inhalation condition while a number of 10,000 and 5,000 micro particles were modeled for simplified and image-based airways respectively. Three patient-specific air-particle flow analysis showed that 42.35% of particles inhaled by female subject managed to reach the end of trachea while male subject with epiglottis blockage recorded a very minimum of 0.43%. Oversized male subject recorded merely none of complete particle inhalation. Apart from the attainment of more practical matrix-based algorithm, this work also suggests that such possible pattern analyses are crucial to facilitate medical practitioners in their diagnosis and decision making process of airway flow related diseases.

Keywords—Human Respiratory; Air-Particle Flow; Simulation

I. INTRODUCTION

Air-particle flow simulations in human airways have been around for years. Commercial software have always been the main preference for researchers around the globe since there is still no established software dedicated for such simulations. The conventional way of having the simulation done is by the use of multiple commercial software to cater all simulation stages i.e. pre-processing, simulation solver and post-processing. This is more complicated when medical image-based flow simulation is expected.

One of the earliest studies in air-particle distribution through human respiratory system was by Martonen T.B., (1993). He however only developed a model to calculate the deposition of hygroscopic aerosols in the human tracheobronchial (TB) tree. The TB airflow pattern studied is acceptable with the experimental observations and valid with the anatomical features such as the larynx and cartilaginous rings in large airways.

As the computing power is improving, researchers are able to explore more detail phenomena through simulations. The usage of computational Fluid Dynamics, CFD for human airway flow simulations are part of the revolution. Luo et al., (2007) and Li et al., (2007) were some of the researchers trying to expand the previous studies in turbulent modeling. While Zhang and Kleinsteuer, (2004), Zhang et al., (2010) and Ghalati et al., (2012) broadened the scope of air-particle distributions not only from larynx downwards but also throughout oral airways with deployment of micro and nano particles on the calculations.

Unfortunately, researchers are still depending on multiple software to come up with all the analyses. The hassle of integrating these engineering software for the sake of medical concern has left these researchers with the conventional way of software-to-software conversions. This work however proves that matrix-based algorithm is more practical in integration all three major simulations stages when it comes to medical image-based fluid-particle analysis.

Present work proposes a single matrix-based algorithm comprising the advantage of pre-processing immersed boundary method adopted from Choi et al., (1993) who proposed a general immersed boundary method that is valid at all Reynolds number with a highly accurate flow solver by Karniadakis et al., (1991). The simulation results are validated based on qualitative and quantitative comparison with previous works done with multiple software. The results similarities with far simpler methodology in achieving such establishments prove that the present work is a novel effort that demonstrates the practicality of having matrix-based algorithm for medical image-based simulation of human respiratory air-particle flows.
II. METHODOLOGY

In matrix-based algorithm, three-dimensional space is represented by a three-dimensional matrix. The size of the space is pre-defined by the distance between each adjacent matrix nodes. Matrix-based programming platform is used for all simulation stages with the aim of zero value conversion that can cause error accumulations.

Flow and non-flow regions are distinguished based on the matrix element numberings. These numberings indicate the mathematical operations dedicated for each node in the physical space. As a result, three-dimensional matrix with numberings in all the matrix element will represent a three dimensional physical space that consist of flow regions, boundaries and non-flow regions. Appropriate interpolations are performed for boundaries not at the pre-defined node positions.

A. Mathematical Preliminary

Flow solver was based on Splitting method by Karniadakis et al (1991). The method is labeled Splitting for the technique used in coupling the velocity and pressure for all fluid nodes in each time step. The time integration of the Navier-Stokes system is partly discretized using semi-implicit Splitting method, which was initially introduced by Karniadakis and then used by other researchers.

This work however has both semi-implicit Splitting method and fully explicit Splitting method solely based on current computational limitations on more consuming implicit formulations. Splitting method is a continuum flow solver based on the Navier-Stokes expression below,

\[ \frac{\partial \vec{v}}{\partial t} + \vec{N}(\vec{v}) = - \nabla p + \frac{1}{\Re} \vec{L}(\vec{v}) \]  

(1)

The linear term, \( \vec{L} \) and non-linear term, \( \vec{N} \) above stand for standard derivatives as follow,

\[ \vec{L}(\vec{v}) = \nabla^2 \vec{v}, \]
\[ \vec{N}(\vec{v}) = \vec{v} \cdot \nabla \vec{v} \]  

(2)

These terms are handled by taking the divergence of (1) and use the continuity equation to obtain the Poisson’s equation for pressure,

\[ \nabla^2 \vec{p}^{k+1} = \nabla \cdot \left( \frac{\vec{v}}{\Delta t} \right) \]  

(3)

For the particle distributions, Mechanics of sphere solid particle motions are used in attaining the particle trajectory. Consider a particle of mass \( m \) moving through a fluid under the action of an external force \( F_E \). Let the velocity of the particle relative to the fluid be \( u \), the buoyant force on the particle be \( F_B \) and the drag be \( F_D \), then we have,

\[ m \frac{du}{dt} = F_E - F_B - F_D \]  

(4)

Considering gravity as the external force together with both buoyant and drag forces, (4) can be expressed as,

\[ \frac{du}{dt} = g \frac{\rho_p - \rho}{\rho_p} - C_D A_p \rho \frac{u^2}{2m} \]  

(5)

Where \( C_D \) is the drag coefficient, \( A_p \) is the projected area of the particle in the plane perpendicular to the flow direction and \( g \) is the gravitational acceleration. The particle Reynolds number is denoted as,

\[ N_{Re,p} = \frac{uD_p \rho}{\mu} \]  

(6)

Where \( u \) is the velocity of approaching stream, \( D_p \) is the diameter of the particle, \( \rho \) is the density of fluid and \( \mu \) is the viscosity of fluid. Stokes’ law applies for particle Reynolds number less than 1.0. The drag coefficient is simply,

\[ C_D = \frac{24}{N_{Re,p}} \]  

(7)

The three-dimensional integrated algorithm is based on the fundamental formulation described above.

B. Simulation Parameter

The in-house algorithm was developed non-dimensionally. Fluid, particles and algorithm parameters were relatively integrated in dimensionless forms. Fluid properties were represented by the Reynolds numbers where the only variable was its velocity while the others were kept constant. The range of breathing flow velocity was generalized in terms of Reynolds number equivalent to 100, 500, 1000, 1500 and 2000. The particle size was set to exhibit common inhaler micro-particle characteristics relative to the actual airway size. The algorithm on the other hand was developed specifically for the said application where sub-time increment for the Lagrangian particle dynamics was implemented apart from the overall Eulerian fluid dynamics time increment.
Another significant difference of this code parameter was the use of a single Successive Over-Relaxation, SOR iteration in every time increment to enhance the convergence rate. It was found that the use of higher number of SOR iteration does not improve the convergence rate significantly.

C. Validations

The robustness and validity of the developed algorithm was tested by comparing a complete air-particle simulation in a simplified airway flow with results by Zhang et al., (2002). The case study was chosen for the fact that it simulated the most identical environment to the one to be analyzed in this work which was meant for actual airway flows. Geometrical complexity, rapid flow characteristics and air-particle interactions were the critical points to be validated where failure to cater any of the criteria would lead to wrong simulation results.

D. Human Airways Flow Simulation

All Digital Imaging and Communications in Medicine (DICOM) CT-scan data represented in this work were courtesy of Department of Radiology, Hospital Universiti Sains Malaysia, Kubang Kerian. Three patients from different physical groups were chosen for this work. 34 years old female, 35 years old male and 38 years old oversized male were selected to represent three human airways with different geometrical characteristics. Figure 1 shows all three reconstructed three-dimensional images of normal female, normal male and oversized male involved in this work.

Air and particle flow distributions were tabulated in contour slices and temporal locations respectively. The air velocity contours were scaled in an identical range for more apparent qualitative assessments. Each particle distribution on the other hand was represented in a form of a single point in three-dimensional space regardless of the actual size of the particle.

III. RESULTS AND DISCUSSIONS

A. Algorithm Validations

Qualitative comparison between the velocity contour and particle distribution results at steady state by Zhang et al., (2002) and the current results at time 2.5001 can be found in Figure 2 and Figure 3 respectively. Even though the exact match of the contour values at all nodes were not possible due to the slight variations on the model construction, solver degree of accuracy and even the grid intensity deviations, the flow patterns as shown in Figure 2 were comparably of the same pattern.

Fig. 1. Three-dimensional upper airway reconstructed images of normal female, normal male and oversized male.

Fig. 2. Velocity contour comparison between Zhang et al., (2002) at left and current work at right for flow rate equivalent to 30 l/min.

Fig. 3. Particle deposition comparison between Zhang et al., (2002) at left and current work at right for flow rate equivalent to 30 l/min and Stokes number 0.08.
Locations where supposedly at maximum, minimum and main streamline velocities were all matched with superbly indistinguishable velocity ratio values. Looking at the particle distributions in Figure 3, similar hypothesis could be confirmed as both results agreed that the most depositions were found prior to all constricted locations where velocities were minimized.

The current result however recorded that the most deposited region at the innermost region of the mouth cavity while the previous result concluded that the particle deposition was mostly occurred at the pharynx region. The variation could be the outcome of the different nature of the particle introduction between the two results. The previously employed simulation was carried out with the particle introduction on the steady state flow condition while the current result was based on the transient response both fluid and particles started from the same initial time at zero.

**B. Air-Particle Flow in Image-Based Three-Dimensional Human Upper Airway**

A noble analysis successfully performed with the use of this integrated algorithm was the analysis of air-particle distributions in airways of the three different subjects. The aim was to estimate the percentage of particles that reach the end of trachea region. In order to have the best visualization of particles during actual breathing condition, simultaneous fluid-particle coupling was implemented with particle sub-time iterations introduces within the flow time calculations.

The fluid-particle flow simulation results are illustrated in Figure 4 at 1.2 non-dimensional time. Prior to the illustrated results at time 0.2, more particles initially located outside the female subject nose entrance had started to move toward the entrance followed by the male subject. Oversized male subject recorded the least particles moving at this instance as compared to the other subjects. This was due to the fact that the air velocity at this location was higher for the female subject and actuated more particles to the entrance. Fewer particles were in motion at this instance for the oversized subject as the air flow was yet to fully develop due to the obstruction effect.

Similar pattern was also observed for time = 0.4 as the particles entering the nasal cavity with different mean velocities depending in the air velocity profiles. Particles were found more diverse entering the male subject as compared to the female subject. This might be caused by the geometrical complexity difference and the air velocity between the subjects. Particles were still at the nose opening of the oversized subject during this instance as smaller air velocity was observed earlier. The particles seemed to diverse similar to the male subject case at time = 0.6.

At times equal to 0.8 and 1.0, some particles had reached the trachea end of the female subject while the movements were obstructed by the epiglottis of male subject. For the oversized male, small amount of particles were seen rushed into the narrow pharyngeal cavity before it deposited at the acute surface.

No particle was still in motion at time = 1.2 as shown in Figure 4. For the same flow rate of 30 l/min of air with 5,000 micro particle introduced at the nose entrance, 42.35 percent of the total particles were manage to reach the bottom of the female subject trachea. This numerically countable figure was far better than that of male subject as the epiglottis obstruction severely reduced the percentage down to only 0.43 percent.

![Fig. 4. Inhaled particle distributions for image-based three-dimensional upper airway of female subject (top), male subject (center) and oversized male subject (bottom) at time = 1.2.](image-url)
subject for this simulation setup of micro sized particles inhaled with 30 l/min air flow rate.

The overall result of this analysis suggested that further analyses on variable flow rates, particle sizes, grid resolutions, numerical time increments and even particle initial velocities are required to determine the optimum to acquire the maximum particle delivery throughout the air passageways.

IV. CONCLUSIONS

This work is considered as a successful novel attempt to comprehensively integrate the overall procedure of simulating time-dependent air-particle flow behavior through three-dimensional medical image-based upper human airway system in single in-house software. This all-in-one biomechanics dedicated software has been proven to be viable to substitute the conventional procedure involving expensive, non-dedicated pre-processing software. As a dedicated integration of in-house medical image-based segmentation, fluid flow, particle distribution and volume visualization solvers for biomechanics application, this software was built with the aim of minimizing the difficulties of implementing engineering based software on biomechanics applications.

The integrated algorithm underneath the full blown software was successfully developed from the initial idea of maintaining the original medical image data structure throughout the code with the employment of fluid solver, particle analyzer and volume visualization approach that suit the overall algorithm architecture. The selection of array-based programming language was also proven to be beneficial as the code is flexible enough to be used both under open source and commercial algorithm platform.

The fully validated software was also successful in emulating the actual air-particle behavior in actual image-based three-dimensional upper human airway system as shown earlier with three reconstructed airways of normal female, normal male and oversized male subjects. The simple yet convincing mock analysis concluded that patient-specific air-particle flow studies are essential in order to have accurate pattern of the actual situation when dealing with specific diagnosis.

The common generalized human airway flow patterns are not practical to be used in patient-specific diagnosis since it was proven in this work that there are significant differences in each case. As the common practice of attaining an actual simulation of any single air-particle distribution in a specific subject acquires multi-software skill and considerably huge amount of time, this all-in-one complete integrated software is definitely a handy alternative for medical practitioners and researchers.

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