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3D Modeling and Simulation of Airflow and Aerosol Deposition of 5 Years Child

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Abstract Children have special requirements in pulmonary drug delivery, as their lungs evolve continuously until they become adult. To deliver the drug to a specific area in the appropriate quantity, we need to study the deposition of particles. In our study we modelled and simulated airflow on a 5-year-old child using a CAD software to understand aerosol deposition. To design and simply the model of a child URT (Upper Respiratory Tract) on a CAD (Computer Aided Design) Software. Child specific model consist of mouth, trachea, and bronchi (left & right) with 11, 9, and 6.2 years old, respectively, was adopted. Using SolidWorks the URT model was sketched and extruded. All the simulation works were performed using software ANSYS CFX. An aerosol deposition converges at a steady-state condition for 500 iterations. A decrease in discharge was recorded as deposition transits from contraction prior to trachea at a velocity of 15 mm/s and a count of approximation of 28,000 with a time-lapse of 5 seconds. Therefore, the pressure and velocity of the particulate increases due to the contraction. Formulation particulate maximum velocity was recorded at 0.26 mm/s. Our findings suggest that a five-year-old URT model of a child has more aerosol depositions in comparison to adults and aerosol size range will evolve with age. In addition, deposition increase directly proportional to flow rate and with particle diameter.

Keywords: *aerosol deposition, 5-year-old child, upper respiratory tract, computational modelling*

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1. Introduction

To cure a pathological and unhealthy state a drug must be taken by an individual as prescribed by the physician with an appropriate suggested drug dosage amount. In addition, the specific drug should reach its precise effected region [1]. Over decades convenient and efficient methods are been studied and developed to bring into practice. The advantage of developing new and efficient manner for drug delivery approach is to reduce the unnecessary consumption of the drug and to reach the specific effected region with maximum results. Colon, intranasal, pulmonary, transdermal, transmucosal and vaginal routes are new drug delivery methods [2], instead of the traditional practice. More emphasize, working hours and monetary support are nowadays invested in establishing a successful drug delivery mechanism by pharma companies [3]. Alone in the USA annual sales for advanced drug-delivery systems is more than $10 billion with significant growth every year [4]. The cost of developing a new drug is more in comparisons to developing a new method for drug delivery [2,5,6]. However, efficient new method for drug delivery would reduce the cost and increase the recovery time of the patient [7,8,9,10]. Drug pharmacology is of vital importance in addition to the drug deposition to the effected region in case of airway dysfunction [11]. In a study lung diseases were effected by different drug delivery systems and inhalation approaches, as the deposition of aerosol in the human respiratory tract tend to change with various deposition sites [12,13]. Numerous studies and experiments were performed of the human lung during the last decade [14-17]. In addition, with the advancement of imaging techniques (radionuclide) aerosol deposition experiments for lung deposition were increased. Recently drugs can target the affected regions or sites present in a body precisely by using drug control release mechanism, it was only possible due to the development and advancement in drug delivery systems [4]. Due to the advancement in drug delivery systems it had gained influence over a short time on most of medical areas few of them are immunology, cardiology, endocrinology, oncology and pain management [4]. Drug delivery systems has conceivable upper hand on conventional approach due to desirable range of drug levels to effected region, specifically consisting targeting of the effected site and less number of dosages with decreased amount.

Drug delivery systems are real leap towards betterment in the medical field. Not only for adults but also in the case children especially for neonatal and premature babies. Over dosage of medication to children (both neonatal and

premature babies) can be fatal or can have severe other health problem later in life. Currently there are drug delivery products available in commercial market for children such as nebulizer, metered dose inhalers and spacers, and dry powder inhalers [18,19,20]. According to FDA age range of children patients start from newly born to adolescent (16-18 years, depending upon the region) [21,22,23]. Since growth in childhood is primarily dependent on region, genes, inheritance, nutrition, and environmental factors. In addition, other factors also effect the growth of children such as height, weight, and infants born with congenital diseases. Thus for our study we selected a 5 years old child airways for aerosol deposition. Thus delivery of drug to a specific area in the appropriate quantity is of significant importance to achieve optimum results in comparison to the conventional approach. With the help of recent developments increase in accuracy and with minimum drug dosage can be achieved. Developing a new drug delivery system allows you to develop faster method with lesser cost of medicine. Images obtained from CT (Computed Tomography) scans of real URT models have upper hand to an idealized model of a child, as CT images are from real human. Though, it is not possible to do experiments and research on real human especially in case of children. The idealized model of a 5 years old child can be draw on a normal computer and simulations results can be achieved. Moreover, using basic tools and changing the available parameters we can investigate the effect on the aerosol deposition according to its airflow.

In our present we have focused and studied 3D modeling and simulation of airflow and aerosol deposition on a 5 years' old child airways. However, if the child cries, then drug delivery will be negatively affected. As the breathing pattern will change due to crying and the inspiratory flow rate will increase, that will lead to higher deposition in the airways. The most common issue medical practitioner faced today is for deciding the quantity of an adult drug when prescribing it to a child on rare occasions, due to lack clinical research. Thus is our study we modelled and simulated airflow on a 5-year-old child using a CAD (Computer Aided Design) software to understand aerosol deposition.

2. Methodology

2.1. Modeling of the URT

To design and simply the model of a child URT on a CAD software. Child specific model consist of mouth, trachea, and bronchi (left & right) with 11, 9, and 6.2 years old, respectively, was adopted. Using SolidWorks 2011 (Dassault Systèmes SolidWorks Corporation, Waltham, Massachusetts, United States, Server 25734@mimcs-pc, Serial No. 9710008817149472HBGKY3G2) the URT was sketched and extruded at the Biomedical Technology Department, College of Applied Medical Sciences, King Saud University.

We initiated the URT model without the bronchi (left & right). The diameter was kept constant and the shape was simple, numerous circles were sketched with the desired diameters to achieve the shape of a 5-year-old URT see Figure 1.

Figure 1. URT model of a 5-year old.

In the second phase, we designed the left bronchi and mirror it for right bronchi. The 3D drawing geometry from SolidWorks of the 5 years old is illustrated in Figure 2.

Figure 2. URT model with left and right bronchi

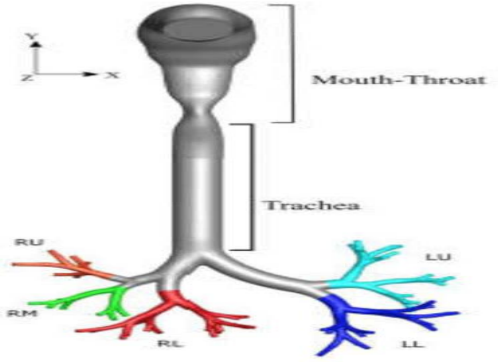

Figure 3. URT model with different color coding for different regions of the lungs

Our URT model is the idealized human model. The 64 distal outlets are grouped by their respective downstream regions of the lungs (i.e. right upper lobe, right middle lobe, left upper lobe, etc.) and are coded with different colors can be seen in Figure 3. The URT has been segmented into three regions, see Figure 3. The first region is mouth-thorat, second region is the trachea, and the third region is conducting airways.

2.2. Simulation of Airflow

In our study all the simulation works were performed at the Biomedical Technology Department, College of Applied Medical Sciences, King Saud University using software ANSYS 14.0 version (ANSYS Inc., Canonsburg, Pennsylvania, United States; License Server 1055@PC13).

The airflow simulation of the child URT was performed in the conventional approach [24]. The same airflow simulation approach can also be followed on different URT models for adults by scaling the 3D geometry of the URT model. Initially, the URT model created in SolidWorks was loaded on ANSYS (fluid flow) geometry to be simulated and meshed. The URT model had 228221, 536725, and 162474, nodes, faces and volumes respectively (Figure 4). From the setup (CFX-Pre) the propellants used in DPI's with molecular mass of approximately 137 grams per molecule with density of 41.49 grams per cubic centimeters at 28 degrees centigrade and the inlet speed was set to 0.71 meters per seconds which is the normal breathing condition at resting position of 30 liters per minute with a diameter of 2.5 centimeters. Simultaneously assuming properties of Salbutamol (i.e. approx. molecular mass: 239.31 grams per molecule with a density of 0.1 grams per centimeters cube) for the formulation particulate. The particulates diameter was selected at 10 µm as the R.M.S value for our study. However, particulates diameter has a range from 1-12 µm. We also used one way coupling between fluid and solid. The appropriate particle size range 1–5 µm diameter was selected for a 5-year-old child.

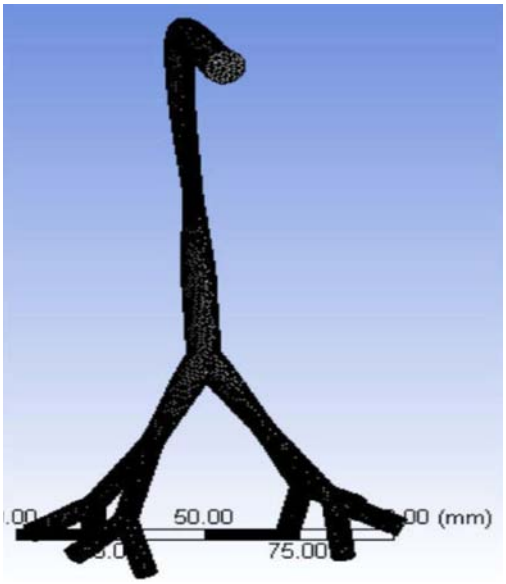

Figure 4. Meshing of the URT model

2.3. Boundary Condition

Setting the boundary condition of the URT (Figure 5), we set the mass flow rate at 0.5680 kilograms per second. Further, the left lower and upper lobe is distributed at 15% and 31% respectively.

The computation of outlet mass in the left lobe was considered average (i.e. 23% of inlet mass flow rate) 0.13064 kg/s. Correspondingly, mass distribution of the right lower, right middle & right upper lobe was set to 33 %, 7% & 31% respectively. Hence outlet mass distribution rate in the right lobe was considered average (i.e. 18% of inlet mass flow rate)0.10224 kg/s. The turbulent Eddy Dissipation and turbulence kinetic energy (TKE) accounts for 0.9 m^2/s^2 and 0.02 m^2/s^3, respectively. The diameters discharge and further computation velocity accounts to 3.395 X 10^4mm/s. for the Formulation particulates injected from a conical geometry at the inlet domain an actuator nozzles diameter range from 0.20-0.30mm, hence we consider nozzle diameter of 0.25 mm with a cone angle of 25° for defining the geometry of inlet domain.

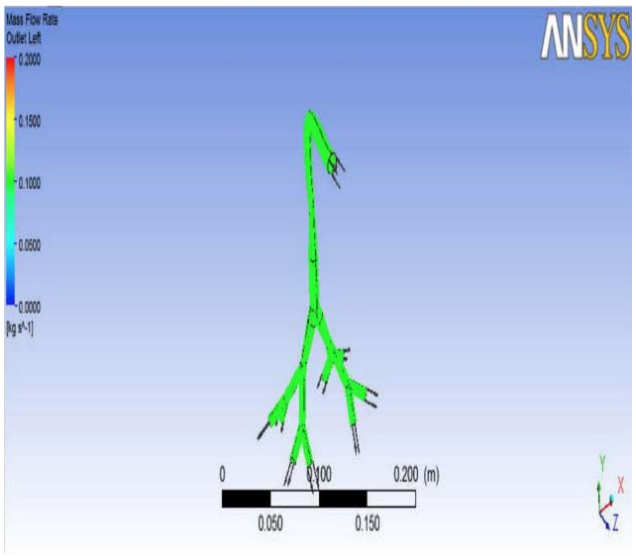

Figure 5. URT model with its boundary conditions.

3. Results and Discussion

One URT model of a five-year-old child was analyzed and simulated for airflow and aerosol deposition using CAD software.

An aerosol deposition converges at a steady-state condition for 500 iterations. Hence the simulation is more accurate and reliable in comparison to transient simulation. The velocity in the Figure 6 with the red curve is the transient simulation which decomposes. It shows the kinetic energy of the formulation particulates from the mouth gets dissipated simultaneously losing all of its energy inside the lobes same as earlier study by Ahmad and Proctor [25]. More accurate and reliable data could be calculated in transient simulation by distributing a multi-zone mesh for all 4 different cross-sections i.e. left lobe, right lobe, mouth, and trachea.

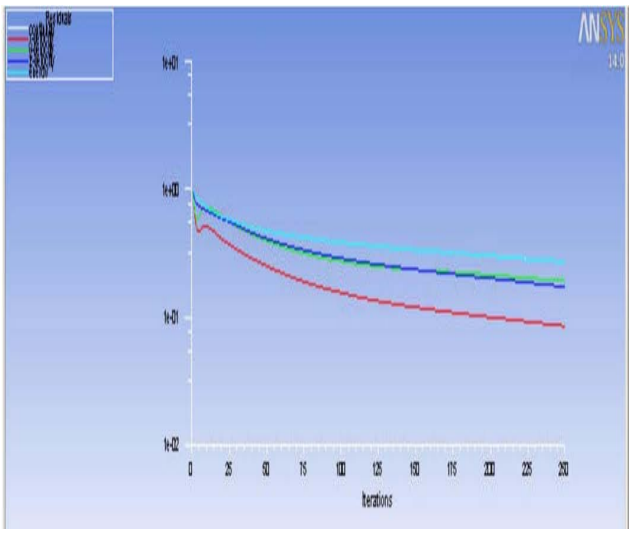

Figure 6. Simulation results of aerosol deposition on the URT model

Both, right and left lobes are experiencing negative velocity due to the reverse flow producing turbulence which may aid in the process of breaking down the formulated particulate. Thus paving the way for more deposition of particulate.

A decrease in discharge was recorded as deposition transits from contraction prior to trachea at a velocity of 15 mm/s and a count of approximation of 28,000 with a time-lapse of 5 seconds. Therefore, the pressure and velocity of the particulate increases due to the contraction. Formulation particulate maximum velocity was recorded at 0.26 mm/s, see Figure 7.

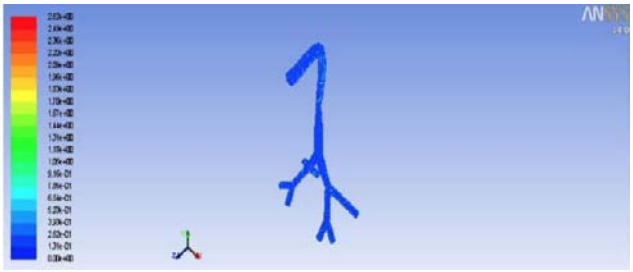

Figure 7. Recording of the particulate maximum velocity

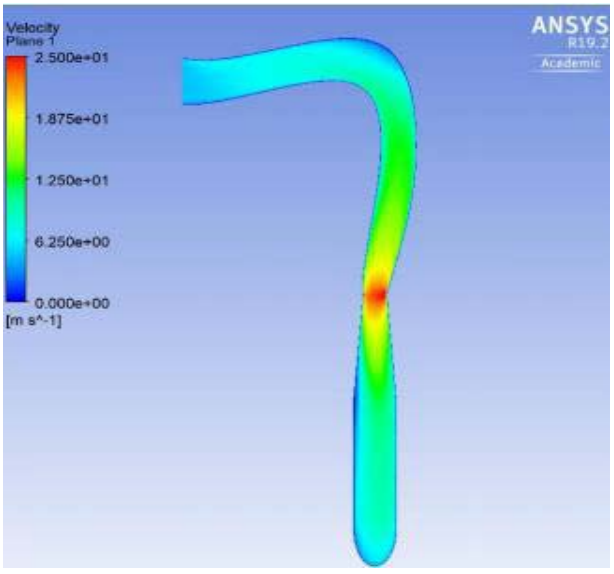

Figure 8. Diameter increase in the middle

Figure 8, shows the particle diameters increase in the middle as the model is narrow and tight at that particular area.

Our findings suggest that a five-year-old URT model of a child has more aerosol depositions in comparison to adults and aerosol size range will evolve with age. In addition, deposition increase directly proportional to flow rate and with particle diameter.

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