STUDY OF PARTICLES TRANSPORT ALONG SECOND AND THIRD GENERATION OF HUMAN AIRWAYS USING CFD

MOHD QHAIRUL BIN MOHD BOKHARI

Report submitted in partial fulfillment of the requirement
for the award of the degree of
Bachelor of Mechanical Engineering

Faculty of Mechanical Engineering
UNIVERSITY MALAYSIA PAHANG

DECEMBER 2010

UNIVERSITI MALAYSIA PAHANG
FACULTY OF MECHANICAL ENGINEERING

We certify that the project entitled *"Study of Particles Transport along Second and Third Generation of Human Airways Using CFD"* is written by *Mohd Qhairul Bin Mohd Bokhari*. We have examined the final copy of this project and in our opinion; it is fully adequate in terms of scope and quality for the award of the degree of Bachelor of Engineering. We herewith recommend that it be accepted in partial fulfillment of the requirements for the degree of Bachelor of Mechanical Engineering.

(Mr. Muhammad Ammar Bin Nik Mu'tasim)
Examiner Signature

SUPERVISOR'S DECLARATION

I hereby declare that I have checked this project and in my opinion, this project is adequate in terms of scope and quality for the award of the degree of Bachelor of Mechanical Engineering.

Signature
Name of Supervisor: Mr. Muhamad Zuhairi Bin Sulaiman
Position: Lecture
Date: 6th December 2010

STUDENT'S DECLARATION

I hereby declare that the work in this project is my own except for quotations and summaries which have been duly acknowledged. The project has not been accepted for any degree and is not concurrently submitted for award of other degree.

Signature
Name: Mohd Qhairul Bin Mohd Bokhari
ID Number: MA07017
Date: 6th December 2010

ACKNOWLEDGEMENTS

I am grateful and would like to express my sincere gratitude to my supervisor Mr. Muhamad Zuhairi Bin Sulaiman for his germinal ideas, invaluable guidance, continuous encouragement and constant support in making this thesis possible. He has always impressed me with his outstanding professional conduct and advices which gave inspiration in accomplishing my final year project. I also sincerely thanks for the time spent proofreading and correcting my many mistakes.

Special thanks to University Malaysia Pahang for supporting and providing equipment and information sources that assisted my studies and projects.

My sincere appreciation to the lecturers of Faculty of Mechanical Engineering who have put in effort to the lectures and always nurture and guide us with precious advices. Thank you for sharing those experiences.

To all my lovely current and ex roommates and friends who always willingly assist and support me throughout my journey of education, you all deserve my wholehearted appreciation. Many thanks.

I acknowledge my sincere indebtedness and gratitude to my parents for their love, dream and sacrifice throughout my life. I cannot find the appropriate words that could properly describe my appreciation for their devotion, support and faith in my ability to attain my goals.

ABSTRACT

This thesis deals with simulation of particles transport along human airways to predict the particles deposition pattern with different inhalation flow rate and particles size. Realistic human airways model base on study by Kleinstreuer et al. (2007) was been used. The simulation has been done by two different Reynolds numbers with laminar and turbulent flow. Commercial CFD software, ANSYS FLUENT 12.1 was used. $Re = 1883$ ($Q_{in} = 20\, l/min$) and $Re = 4710$ ($Q_{in} = 50\, l/m$) are used for boundary condition. Laminar model was used for laminar flow and k-ω turbulent model was used for turbulent flow in the simulation. The results of this thesis show that flow behavior of both micro- and nano- particles vary measurably. However the deposition patterns are much more uniform for nano particle.

ABSTRAK

Tesis ini adalah mengenai simulasi pengangkutan zarah sepanjang saluran nafas manusia untuk menjangka pola pengendapan zarah dengan aliran penafasan pada tahap yang berbeza dan saiz zarah yang berbeza. Realistik saluran nafas manusia model berdasarkan kajian et al Kleinstreuer. (2007) yang telah digunakan. Simulasi telah dilakukan oleh dua bilangan Reynolds yang berbeza dengan laminar dan aliran turbulen. Komersial perisian CFD, ANSYS 12.1 FLUENT digunakan. $Re = 1883$ ($Q_{in} = 20\,l/min$) and $Re = 4710$ ($Q_{in} = 50\,l/m$) digunakan untuk ketetapan sempadan. Model laminar digunakan untuk aliran laminar dan model turbulen k-ω digunakan untuk aliran turbulen dalam simulasi. Keputusan kajian tesis ini menunjukkan bahawa kelakuan aliran kedua-dua zarah mikro- dan nano- adalah berbeza. Namun pola pengendapan jauh lebih seragam untuk nano partikel.

TABLE OF CONTENTS

LIST OF TABLE

LIST OF FIGURE

LIST OF SYMBOLS

IP	Inertial impaction
Q	Proportional to the air flow rate
d_p	Particle diameter
C_{slip}	Cunningham slip correction factor
ρ_p	Particle density
U	Air velocity
D	Length scale
m_p	Mass of the particle
F_D	Drag force
$F_i^{gravity}$	Gravity
D_{nano}	Nano particle diffusivity
Y	Mass fraction
σ_Y	Turbulence Schmidt number
A_i	Area of the local wall cell
n	Number of wall cells
Q_{in}	Inhalation flow rate

LIST OF ABREVIATIONS

CFD	Computational fluid dynamics
COPD	Chronic obstructive pulmonary diseases
DEF	Deposition enhancement factor
DF	Local deposition fraction

CHAPTER 1

INTRODUCTION

1.1 INTRODUCTION

Computational simulation of particles transport along human airways is quiet challenging because of the complex airways geometries. Simulation of human airways can be done to predict the particles deposition pattern in human airways. Many studies are discussed about the particles deposition in the human airways and its effect on health. It shows that particles deposition is an important study for improve human health (Kleinstreuer et al., 2005). These simulation studies are useful for toxicologists and healthcare providers to improve research in health effects of inhaled toxic particles and also to determine drug aerosol targeting in human airways to improve its effect.

The development of 3D simulation of particles transport along human airways has many applications. This simulation can be apply in inhalation toxicology, where the knowledge of deposition patterns of inhaled pollutants in the respiratory system can assist in risk assessment protocols. This simulation also can be apply in aerosol therapy, where the delivery of inhaled drugs can be targeted to specific regions of the respiratory system to optimum therapeutic effects.

1.2 PROJECT BACKGROUND

A lot of particles are encountered in the ambient air and these airborne particles are inhaled through the airways region. A certain percentage of the particles may deposit by touching the wall of the airways.

In order to predict the particles deposition, a simulation of particles transport along human airways is done. CFD software becomes a good option for particles prediction due to its powerful and often indispensible tool for stimulates particles transport in complicated geometry. It's also capable to give effective and detail result. The model of human airways is design by using SOLIDWORK. Then, by using GAMBIT, volume meshing is applied to the model and its boundary type is defined. After that, the model is export to ANSYS FLUENT to decide other parameters before run the simulation.

1.3 PROBLEM STATEMENT

Although the study of particles transport along human airways may be done by using clinical experimental, however it is difficult to be done because of the complicated procedures and also many precautions need to take during the experiment. It is also cannot be done for small diameter of airways and difficulties in visualization result. The clinical experimental also expensive because require a lot of equipments. Therefore, by using CFD software to stimulate particles transport along human airways, it can provide approximate result of particles trajectory and deposition pattern in human airways for different inlet flow rates and particles sizes. It's also cost-effective because not require a lot of equipments.

Since drug-aerosols for the treatment of lung and other diseases is becoming a preferred option compared to injection or oral intake. The drug-aerosols effectiveness is very important to make sure it can provide systematic hopefully effect. Therefore, this simulation study can be use as a prediction to increase the deposition efficiencies and drug delivery target.

1.4 OBJECTIVE OF THE RESEARCH

The objectives of this project are to predict the particles trajectory along human airways and also to observe flow behavior and particles deposition pattern in human airways with different inlet air flow and sizes of particles.

1.5 SCOPE OF STUDIES

The specific scope of this project is to make prediction of particles trajectory along human airways and also to observe the flow behavior and particles deposition pattern in second and third generation of human airways with 3 different sizes of particles, *5μm, 50nm and 100nm*. Laminar flow and turbulent flow are considered in this simulation study and the temperature is assume to remain constant (Isothermal process) with Reynolds number 1883 (laminar) for low-level breathing and Reynolds number 4710 (turbulent) for high-level breathing. Lagrangian frame of reference for the particles trajectory computation of the particles was employed (dilute particles suspensions and negligible particles rotation).

CHAPTER 2

LITERATURE REVIEW

2.1 INTRODUCTION

This chapter will discuss about the type of inhalation particle and its particle size effect. This chapter also will explain about drug-aerosol targeting, designing human airways model, inhaled air flow and also particle deposition transportation for micro and nano particle size.

2.2 TOXIC PARTICLE MATTER INHALATION

A lot of particles are encountered in the ambient air and at the workplace or are generated by inhalers as drug aerosols for therapeutic purposes. These airborne particles or drug aerosols are inhaled through the extra thoracic and trachea bronchial airways down into the alveolar region. A certain percentage may deposit by touching the moist airway surfaces in various lung regions and hence are available for interactions with pulmonary tissue. As a result, toxic particles may induce pulmonary and other diseases, while drug aerosols may be absorbed to combat diseases.

In past studies, the creation and analysis of human airways have been done in variety of methods. These methods typically used to construct idealized models of either a symmetric or asymmetric nature (Kleinstreuer et al., 2008). Idealized models have the advantage of being widely used and well understood, but it has limited realism and flexibility. The result from analysis that done to their model also limited and don't have visualization result.

Toxic material in vapor, liquid droplet and solid particle forms is being inhaled, as it appears indoors or outdoors in all shapes and sizes, typically ranging from nanometers (10^{-9}m) to micrometers (10^{-6}m) (Kleinstreuer et al., 2008). Most severely affected by polluted air may be the children and the elderly. So, it is important to predict how much toxic particle deposited in human airways under realistic breathing conditions. The results are of great interest to toxicologists, epidemiologists, health-care providers, and regulators of air pollution standards. Toxic material dynamics are described in two size-dependent categories because the transport mechanism. Transport mechanism for nano particle is diffusion dominant while for micron particles are impaction and possibly gravitation dominant.

2.2.1 Toxic nano particle

Nanotechnology and related manufacture of nano-scale materials are major growth industries (Roco, 2006). Clearly at the stages of nano material production, handling and use, nano particles become airborne and inhaled. Hence, the serious health problems may cause from inhalation of such toxic (metal, metal-oxide, carbon-based and synthetic nano materials) that are may contain in nano particle. After nano particle inhalation, tissue absorption and transport to extra-pulmonary organs, nano particle may target the central nervous system and immune system (Bang and Murr, 2002). It is not just the level of toxicity of some nano particle which poses potential respiratory and other health risks, but also their size, shape and surface distribution which turns out to be even more toxic than inhaled micron particles of the same material. Also, other toxins could bind with nano particles and piggyback their way into the body. In summary, the enhanced toxicity of nano particle can be attributed to:

(i) The greater surface reactivity of nano particles due to high curvatures as well as the larger surface area relative to the nano particle mass.
(ii) The prolonged retention time and decreasing fraction of clearance for nano particles.
(iii) An almost uniform coating of the airway surfaces by nano particles.
(iv) Larger deposition fractions (DF) of nano particle in deeper parts of the lung, including the alveolar region.

So far, there are relatively few investigations of (spherical) nano particle deposition in the human airways, primarily because of the difficulty of nano particle generation for experimental measurements and accurate predictions with CFD simulations. In a series of papers, Cheng et al.(1988, 1995, 1996, 1997a,b) and Smith et al. (2001) published their measurements of mass transfer and deposition of nano particles ($3.6nm < d_p < 150nm$) in casts of human nasal, oral and upper trachea bronchial (TB) airways, Cohen et al. (1990) reported their experimental work on nano particle deposition in an upper trachea bronchial airway cast and measured the nasal deposition efficiencies of nano particles with diameter between $5\ to\ 150nm$, Daigle et al. (2003) and Kim and Jaques (2004) measured total respiratory tract deposition fraction of nano particles (8–100 nm) in healthy adults.

2.2.2 Toxic micron particle

While the potential health hazards of nano particle has been very recently acknowledged, inhaled micron particle depositions for dosimetry and health risk assessments have been studied for decades (Heyder, 2004). Clearly, the experimental and computational contributions reviewed deal with spherical micron particles that are completely neutral concerning toxic or therapeutic effects.

For example, Schlesinger et al. (1982), Gurman et al. (1984) and Kim and Garcia (1991) showed that cyclic inhalation generates higher particle deposition efficiencies than steady inhalation at the mean Reynolds number of the inlet flow waveform. The deposition efficiencies at each generation were usually measured in these studies for different combinations of particle size and inspiratory flow rate. However, detailed particle transport phenomena as well as particle deposition patterns in human airways are difficult to obtain experimentally.

2.3 MECHANICAL DRUG-AEROSOL TARGETING

Inhalation of drug aerosols, typically in the effective diameter range of $3 - 10\mu m$ (Kleinstreuer et al., 2008), is a standard procedure for treating respiratory ailments, especially chronic obstructive pulmonary diseases (COPD) and asthma. The

nasal and oral pathways are now also being used as portals to deliver medicine for pain management and to combat systemic diseases, respectively, where oral inhalation of insulin for diabetes patients is one modern example. However, to be successful and cost-effective, drug-aerosol delivery has to be targeted. Obviously, maximum deposition of suitable therapeutic solid particles (or droplets or vapors) at predetermined sites, which are related to specific diseases, minimizes potential side-effects in case of aggressive drugs and reduces health-care cost with the increased efficacy. “Targeting” is here understood as a mechanical goal to bring drug aerosols from their release points (the inhaler exit) to a desired landing area in the respiratory system for maximum medical effectiveness. In order to achieve that goal, future inhaler devices have to operate based on a targeting methodology featuring optimal:

(i) particle characteristics
(ii) inhalation waveform
(iii) particle-release positions
(iv) concentration range

This mechanistic approach different from drug targeting via special design of molecular, carrier and controlled-release properties which cause selective distribution characteristics and pharmacokinetic behavior leading to improved therapy.

Several aspects of drug-aerosol delivery have been recently reviewed in the books edited by Gradon and Marijnissen (2003) as well as Hickey (2004). The book by Finlay (2001) and the volume edited by Bissgard et al. (2002) also discuss pertinent elements of drug delivery to the lungs.

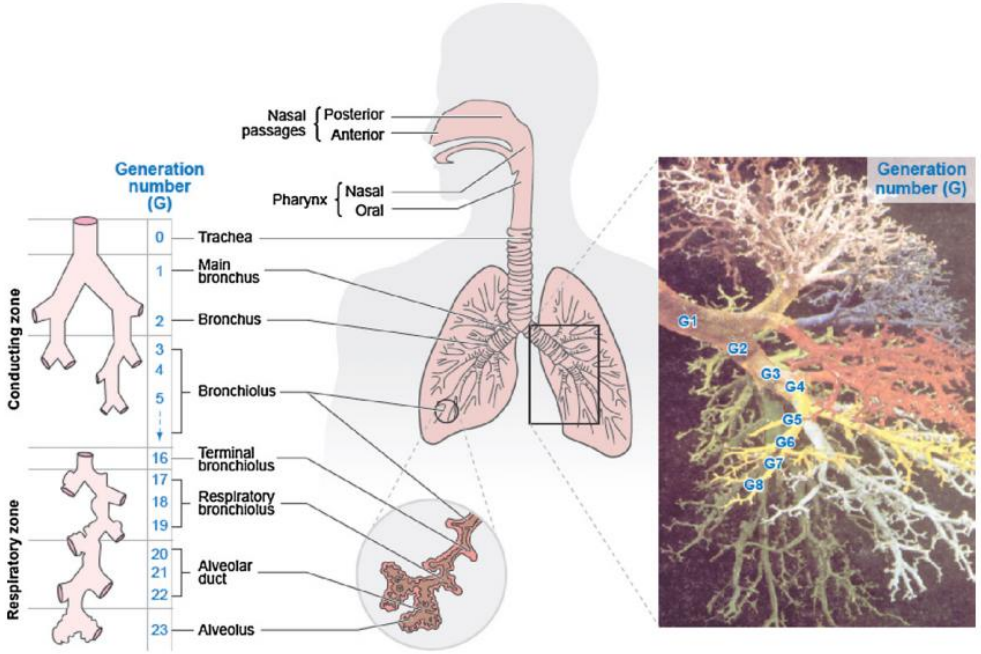

Figure 2.1: Schematics of human respiratory system and image of actual airways

Source: Kleinstreuer et al., 2008

2.4 DESIGN OF HUMAN AIRWAYS

Accurate and realistic airway models are the most important criteria for experimental or computational particle transport along human airways. Once a comprehensive, flexible and experimentally validated computer simulation model has been developed, particles deposition analysis for optimal drug-aerosol targeting can be determined.

2.5 INHALED AIR FLOW

The understanding of air flow structures in the human airways underlies the basis for analyzing particle transport and deposition. Steady and transient inspired air flows in the human airways have been reviewed by Pedley (1977) and Grotberg (1994, 2001). The detailed investigations, both experimentally and theoretically were recently provided by Lieber and Zhao (1998). Effects of geometric airway to air flow are important factor that may affect particles transport in human airways. So far,

experimental and computational analyses focused mainly on isolated sections of the human airways and only for laminar airflows. However, at high breathing rates, the air flow from the larynx to generation G3 is transitional to turbulent which may complicate flow structures as well as aerosol transport and deposition (Zhang and Kleinstreuer, 2004).

Usually, the turbulent intensity in the oral airway rises rapidly after the constriction caused by the soft palate, and then decreases until the disturbance is activated again by the throat (glottis) (Lin et al., 2007).

Turbulence levels, in terms of kinetic energy, k seem to increase quickly through the strong varying diameter-zone after the glottis, and then decay approaching an asymptotic level of approximately 0.2–0.3 k/μin^2 at six-diameter station from the throat (Corcoran and Chigier, 2000). The flow instabilities may be induced again at the bifurcation region due to the great geometric transition from the parent tube to two daughter tubes (Zhang and Kleinstreuer, 2004). Then, turbulence decays rapidly in the straight segments of the bifurcating tubes. Generally, turbulence which occurs after the throat can propagate to at least a few generations even at a low local Reynolds number (say, Re =700) because of the enhancement of flow instabilities just upstream of the flow divider (Olson et al., 1973; Zhang and Kleinstreuer, 2004).

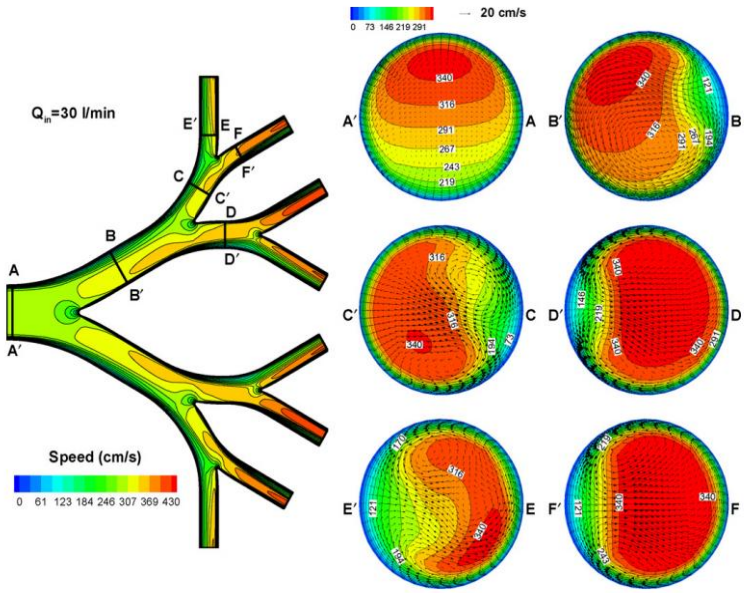

Figure 2.2: Velocity profiles in the bifurcation airway model at steady inhalation with $Q_{in} = 30\ l/min$. The left panel exhibits mid-plane speed contours. The right panel shows the axial velocity contours and secondary velocity vectors at different cross sections

Source: Clement Kleinstreuer, 2008

Typical inspiratory airflow patterns in bifurcating airways are shown in Figure 2. The essential flow characteristic includes:

(i) The air stream splits at the flow dividers and new boundary layers are generated at the inner walls of daughter tubes.

(ii) The velocity patterns vary with the development of upstream flows and the generation of the new boundary layers near the inner walls at the dividers.

(iii) The skewed profile with a maximum axial velocity near the inner wall may be observed just after the flow divider so that different tubes may experience different airflow rates.

(iv) Strong secondary vortices appear inside the branch tubes.

2.6 PARTICLES DEPOSITION

In general, both transport and deposition of inhaled particle matter are definitely base on the size of the particle. Typically, nano material dispersion is due to diffusion and convection, while micron particles are transported via convection. Specifically, micron particle deposition in the human airways occurs mainly by impaction, including secondary airflow converting particles to the airway walls, as well as diffusion or gravitational effects. Clearly, inertial impaction (*IP*) is proportional to the air flow rate (Q_{in}) and the (aerodynamic) particle diameter (d_p) squared, as expressed with the impaction parameter.

$$IP = Q d_q^2 \tag{2.1}$$