Volume II

Fluid Dynamics and Computational Modeling

Maria Forest

Fluid Dynamics and Computational Modeling Volume II

Edited by **Maria Forest**

Fluid Dynamics and Computational Modeling
Volume II
Edited by Maria Forest

Fluid Dynamics and Computational Modeling

Volume II

Preface

The main aim of this book is to educate learners and enhance their research focus by presenting diverse topics covering this vast field. This is an advanced book which compiles significant studies by distinguished experts in the area of analysis. This book addresses successive solutions to the challenges arising in the area of application, along with it; the book provides scope for future developments.

This book contains updated information on topics like fluid dynamics, computational modeling and its applications. It discusses topics like: winds, building and risk prevention; multiphase flow, structures and gases; heat transfer, combustion and energy; medical and biomechanical applications; and other crucial topics. Along with all that has been mentioned, this book also gives a detailed view of computational fluid dynamics and applications, without excluding experimental and theoretical aspects.

It was a great honour to edit this book, though there were challenges, as it involved a lot of communication and networking between me and the editorial team. However, the end result was this all-inclusive book covering diverse themes in the field.

Finally, it is important to acknowledge the efforts of the contributors for their excellent chapters, through which a wide variety of issues have been addressed. I would also like to thank my colleagues for their valuable feedback during the making of this book.

Editor

Contents

Part 1

Medical and Biomechanical Applications

Surfactant Analysis of Thin Liquid Film in the Human Trachea via Application of Volume of Fluid (VOF)

Sujudran Balachandran
Bumi Armada Berhad
Malaysia/Singapore

1. Introduction

The human tracheobronchial tree is a complex branched distribution system in charge of renewing the air inside the acini which are the gas exchange units. The surfactant factor existing in the acini of the human tracheobronchial tree is exposed to thin liquid film flow where the application of volume of fluid (VOF) can significantly determine the membrane effects on the branching asymmetry. The thin film application in this chapter will focus on the breathing airway which is commonly known as the windpipe (trachea) of an adult human. The upper human airway is the primary conduit for inspiration in the breathing process. Air entering the mouth passes through pharynx and flows into the trachea via the glottal region. The air which enters the windpipe applies a surfactant pressure at the lipo-protein complex, where this complex is developed as a thin layer on the trachea (Caro et al. 2002). The surfactant is a lipo-protein complex, which is a highly surface-active material found in the fluid lining of the air-liquid interface in the trachea surface. This surfactant plays a dual function of preventing sudden collapse during the breathing cycle and protection from injuries and infections caused by foreign bodies and pathogens. The varying degrees of structure-function abnormalities of surfactant have been associated with obstructive trachea diseases, respiratory infections, respiratory distress syndromes, interstitial lung diseases, pulmonary alveolar proteinosis, cardiopulmonary bypass surgery and smoking habits. For some of the pulmonary conditions, especially respiratory distress syndrome, surfactant therapy is on the horizon. In order to understand the behaviour and relevant condition of the surfactant in the human trachea, it is important to apply the volume of fluid method on these surfaces. The phenomena that occur on the trachea will ensure that the surfactant responsibility in resolving the potential obstruction of breathing. The surfactant factor may occur with non-lateral conditions in space as well as during the inspiration of breathing in the human body. The fluid interaction in the thin surface results in serious impairment by obstructive trachea diseases as mentioned earlier. The pulmonary surfactant is essential for normal breathing, alveolar stability and as a host defence system in the lungs. The interface of surfactant films reduces the surface tension to extremely low values when it is compressed during expiration. This protects our lungs from collapse during breathing out. Thus application of the Volume of Fluid (VOF) method is introduced in this paper to study the behaviour of the pulmonary surfactant in the human trachea.

2. Model selection

Figure 1 shows the three-dimensional model of the lung. Detailed geometries of this model were extracted from the anatomical model by Schmidt et al. (2004). This explicit human lung was derived from High-Resolution Computed Tomography (HRCT) imaging of an in vitro preparation. This model was a selection of data extracted from the anatomy of a healthy human lung of an adult male. This lung model is free from pathological alteration (Gemci et al. 2008). In Figure 2, an isometric view of the human lung is presented. The notation of G0, G1, G2 and G3 are the cross-sectional gate to facilitate the model drawn for indication segments. This model was selected based on the actual structure of the human lung. No additional tissue configuration was created due to investigation which only focused on the airway blockage area. At each generation, the branching is essentially dichotomous; each airway being divided into two smaller daughter airways (Farkas et al. 2007). The tree starts at the trachea (G0-G0) whose average diameter and length are respectively D0 = 1.8 cm and L0 = 12 cm in the healthy human adult (Allen et al. 2004), and ends in the terminal bronchioles. From the trachea to terminal bronchioles, this element is located on average in generation G1-G1, these airways are purely conducting pipes. Two important features have
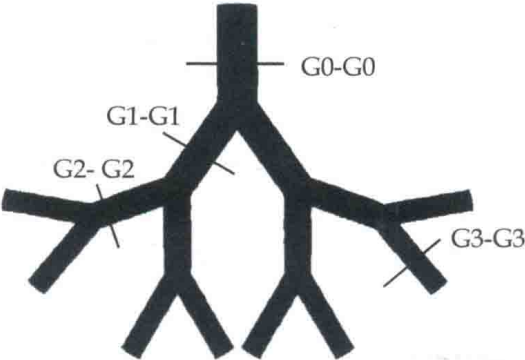
Fig. 1. General three-dimensional lung airway model

Fig. 2. Isometric view of lung airway

been included. First, the airway dimensions at the first generations (G0-G0 and G1-G1) are specific to the human anatomy and they are essentially independent of physiological variability (Martonen et al. 2003). Second, for higher generations (G2-G2 and G3-G3), a systematic branching asymmetry has been modelled in the different tree bifurcations.

Figure 3a and 3b illustrate the overall mesh of the model selected. The meshes are generated using a tetrahedral unstructured mesh format. The total number of grids generated is approximately 0.62 million. Concentrated mesh is applied near the branches of the bifurcation to increase the result interpretation. The flow details are critical as the effect of the boundary layer becomes significant in this region.
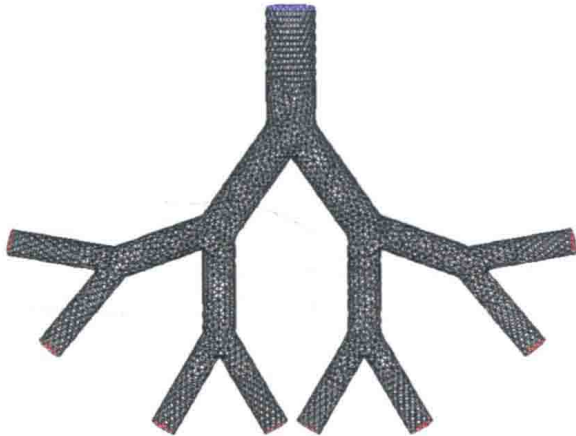
Fig. 3a. Mesh concentration on lung model

Fig. 3b. Mesh concentration on lung model (isometric view)

3. CFD simulation

The categorization of the anatomy of tracheobronchial tree airways constitutes the first step in the examination of the respiratory flow field and surfactant impact with volume of fluid

(VOF). The intention of this study is to understand the behaviour of the membrane which acts as a thin liquid film and the role of the surfactant on the model. In this study, the homogenous airflow is a comprehensive digital reference model with a maximum of four sections of pulmonary airway tree computed using the commercial CFD code FLUENT® (version 6.2). The computational mesh was generated using the FLUENT mesh generation code GAMBIT®. FLUENT employs a finite-volume method to solve the Navier-Stokes and continuity equations on an arbitrarily shaped flow domain with appropriate boundary conditions. The steady-state solution of the flow fields assumed converged when the residuals reduced to less than 10^{-4}. A typical run time was approximately 38 hours on a normal processor. In this CFD study of surfactant in the human pulmonary tree model, computations were performed at 28.3 L/min for a quasi steady-state volumetric adult inhalation flow rate for pulmonary surfactant.

3.1 Volume of Fluid (VOF) method in Fluent 6.2
The Volume of Fluid (VOF) model has been widely used in many research fields and commercial software. Known for its wide range of usage, implementation of this model in commercial code has been popular and FLUENT 6.2 is one of the software where their codes have been implemented. Isothermal VOF formulation was considered in this project with heat transfer and is assumed negligible due to analysis being based on surface interface. Formulation of laminar flow is presented here. For the turbulence effect, it can be done by averaging the Navier Stokes equation and detailed formulation can be found in Versteeg and Malalsekera (1995).

3.1.1 The basic of VOF for interface development
The VOF model is based on a volume fraction denoted by α where this volume of fraction is using a two fluids mixture in a fixed computational grid. The transport of the two fluids results in solving the multiphase fluid equation using the α values and interface location is reconstructed from the volume fraction field. The following procedures are used in solving the VOF model:

i.   Initial interface shape is modelled in computation domain.
ii. From the existing interface in the model, volume of fraction is obtained. (Truncated volumes calculation was done at each interfacial cell, this discrete volume fraction is used instead of the exact interface information.)
iii. The volume fraction field is adverted. (Transport of fluid.)
iv. Finally, the interface geometry and location are obtained using the new volume fraction.

All these steps are repeated until a convergence criterion is achieved. In VOF, especially in FLUENT 6.2, one can conduct a simulation for two different fluids without mixing the respective fluids. There will be an interface region between the both liquids and for each region α_q of 1 and 0 values will be given.

α_q = 0: the cell is empty
α_q = 1: the cell is full
$0 < \alpha_q < 1$: the cell contains the interface between the qth fluid and one or more other fluids.
Using the same momentum equation, both fluids shared the same velocity field and it is solved throughout their domain. The tracking interface between both phases is accomplished by the solution of a continuity equation for the volume fraction of one of the phases. The equation is:

$$\frac{\partial \alpha_q}{\partial t} + \vec{v}.\nabla \alpha_q = \frac{S_{\alpha_q}}{\rho_q} \tag{1}$$

The primary phase of the fluid will not be solved by the volume fraction equation, but will be computed through the following constrains:

$$\sum_{q=1}^{n} \alpha_q = 1 \tag{2}$$

For each of the phases, the properties will be presented in control volume of the respective component phase. For the two phase system, for example, if the phases are represented by the subscripts 1 and 2, and if the volume fraction of these is being tracked, the density in each cell is given by:

$$\rho = \alpha_2 \, \rho_2 + (1 - \alpha_2)\rho_1 , \tag{3}$$

and for every n – phase system , the volume fraction averaged density takes on the following form:

$$\rho = \sum \alpha_q \rho_q \tag{4}$$

3.1.2 The momentum equation
As mentioned earlier, both fluids will share the same momentum equation throughout the domain. The momentum equation is:

$$\frac{\partial}{\partial t}\rho u_j + \rho u_i \frac{\partial u_j}{\partial u_i} = -\frac{\partial P}{\partial x_j} + \mu \frac{\partial}{\partial x_i}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \rho g_j + B_j , \tag{5}$$

Velocity component and direction denoted by u_j and x_j in j direction and t is the time. The summation of convention is applied when an index is repeated and i, j = 1, 2 for this problem. Pressure and gravitational acceleration are denoted by P and g respectively and B is a source term due to any additional force applied (per unit volume). This momentum equation dependant on the volume fraction α_q where in this case q = 1, 2 of the phases through the density ρ and viscosity μ. The computational domain is calculated through the following equation:

$$\frac{D\alpha_2}{Dt} = \frac{\partial \alpha_2}{\partial t} + u_i \frac{\partial \alpha_2}{\partial x_i} = 0 \tag{6}$$

The value of α_1 for the first phase is not solved directly at any stage, but it is solved based on the volume condition $\alpha_2 + \alpha_1 = 1$. By applying the properties of density ρ and viscosity μ, the following equations are obtained since ρ and μ depend on the volume fraction values:

$$\rho = \alpha_2 \rho_2 + \alpha_1 \rho_1 , \tag{7}$$

$$\mu = \alpha_2 \mu_2 + \alpha_1 \mu_1 \tag{8}$$

The volume transport equation then, yields an updated volume fraction field with discrete values in computational cell. The values will later be used in reconstructing the new interface location.

3.1.3 Interface reconstruction

Reconstruction of new interface needs formulation from the discrete values of volume fraction inside the domain. In FLUENT 6.2, there are four interface reconstruction schemes, which are geometric reconstruction, donor-acceptor, Euler explicit and Euler implicit. Both Euler explicit and Euler implicit schemes treat cells that lie near the interface using the same interpolation as other cells. Meanwhile, the geometric reconstruction and the donor acceptor scheme treat the interfaces in an advanced interpolation. Full description of these schemes can be found in the FLUENT 6.2 User Manual (2002). A brief explanation on geometric reconstruction is explained here as it is recommended in FLUENT 6.2.

In the FLUENT 6.2 User Manual, the geometric reconstruction scheme approach standard interpolation to obtain face fluxes as the cell fills with one phase or another. Only at the cell near the interface between two phases is this method widely applied. This method is generalized for unstructured meshes and obtained from the work of Young (Piecewise linear 1982). It is assumed that for the calculation of the advection of fluid through the cell faces, the interface between two fluids has a linear slope within each cell. The following are the procedures of reconstruction on interface using geometric reconstruction scheme:

i.   First, calculation of position of the linear interface relative to the centre or each partial cell is done based on values of volume fraction.
ii. Second, the advection amount of fluid through each face is calculated using computed interface representation. Normal and tangential velocity distribution on the faces is also used as information in calculating the advection of fluid.
iii. Finally, each cell of volume fraction is calculated by computing the balance fluxes from the previous step.

Aside from the steady state problem, the geometric reconstruction scheme also available for transient cases. User defined functions can be used in order to obtain the desired solution of interest.

3.1.4 Effect of surface tension in volume of fraction

In VOF, attraction between the molecules in a fluid causes the rises of surface tension effect. This surface tension is a force only acting on the surface. The surface tension model in FLUENT is the continuum surface force (CSF) model proposed by Brackbill et al. 1992. In this model, the addition of surface tension to the VOF calculation results in a source term in the momentum equation. The pressure drop across the surface depends upon the surface tension coefficient and the surface curvature as measured by two radii in an orthogonal direction, R1 and R2:

$$\Delta p = p_2 - p_1 = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \tag{9}$$

where,

$$\kappa = \left(\frac{1}{R_1} + \frac{1}{R_2} \right), \tag{10}$$

hence, $$\Delta p = \sigma \kappa \tag{11}$$

In equation $\Delta = p$ is the pressure drop across the surface, σ is the surface tension and κ is the mean curvature.

The formulation of CSF model is used in surface curvature computation and it is located from the local gradient in the surface normal at the interface. For example, let n be the surface normal and the gradient is α_q. Then, the volume fraction will be:

$$n = \nabla \alpha_q \tag{12}$$

And the curvature represented by divergence of the unit normal, $\hat{n}$ $\kappa = \nabla . \hat{n}$

where $$\hat{n} = \frac{n}{|n|} \tag{13}$$

With this equation, the pressure variation across the interface is assumed linear and given by:

$$p_2 = p_1 + \sigma \kappa (\Delta \alpha_q) \tag{14}$$

The force at the surface can be expressed as a volume force using divergence theorem:

$$F_{vol} = \sum_{pairsij, i<j} \sigma_{ij} \frac{\alpha_i \rho_i \kappa_j \nabla \alpha_j + \alpha_j \rho_j \kappa_i \nabla \alpha_i}{\frac{1}{2}(\rho_i + \rho_j)} \tag{15}$$

And if only two phases are present in a cell, then $\kappa_i = -\kappa_j$ and $\nabla \alpha_i = -\nabla \alpha_j$, this equation can simplified to:

$$F_{vol} = \sigma_{ij} \frac{\rho \kappa_i \nabla \alpha_i}{\frac{1}{2}(\rho_i + \rho_j)} \tag{16}$$

ρ is the volume averaged density computed using Equation 4. The simplified volume force shows that the surface tension source term for a cell is proportional to the average density in the cell.

3.2 Boundary conditions

The liquid was considered Newtonian with viscosity μ, density ρ and surface tension α flows in the region. The film thicknesses were obtained from the lipo lipid thickness in the human airway and it was set to be constant from the entrance of the tracheobronchial tree and uniform to its outlet. The membranes were patched with a similar thickness of the film, in order to reduce the computation period. A very fine mesh was created at the edge of the lung walls. The number of cells used was 198200 and a finer grid was placed near the thin film where the location of the interface was used. Two velocities inlets and a pressure outlet were used as boundary condition inputs. Inlet velocities were separated into two parts; small inlet and big inlet. The small inlet was selected for the thin film boundary condition and the flows maintained at 0.0001 m/s. Meanwhile the big inlet was set to 0.001 m/s to develop consistent laminar flows throughout the geometry.
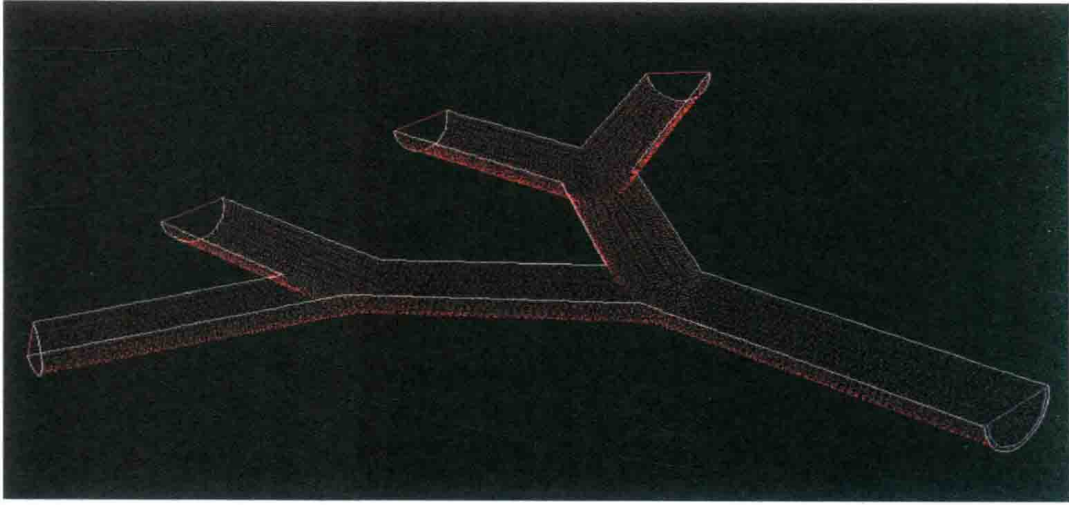
Fig. 4. Patch region in the semi symmetrical airway model

These velocities were applied as the Reynolds number for thin films considered to be ≈ 1. The density of water and viscosity of the lipo liquid was fixed to be 1023 kg/m3 and 0.00093 kg/ms and for air the density was 1.225 kg/m3 and viscosity 1.7894 x 10-5 kg/ms. The calculations were performed transiently using FLUENT 6.2 until the steady state system was reached. Initial the study was done to anticipate that the solution could be run in a steady state so as to avoid time consuming transient calculations, but for better results for the interface it was run under transient mode. A grid dependency study was done until it was found that the location of the interface was not changing with the grid refinement. The time step was set to be 0.001s and simulation was done until 6750 iteration for the solution to converge. Later the iteration was reduced to 4600 iteration as the convergence residual was achieved sooner than expected. After total time of 38 hours, all the simulations reached convergence state. In order to achieve the state of convergence, severe computational time step needed to be selected. Initially time step was set to be 0.00001s and it not only prolonged the state of convergence, but also required more computational time. An assumption was made to set the time step to be 0.001s after 2500 iterations with results not showing prominent converging state of residuals. It was important to select the correct values of velocity based on thin film liquid flow. As per the initial guesses done with different velocity magnitude, the results show the region of multiphase fluids washed by the greater velocity of air. Based on several recalculations, attempts were made to maintain the thin film velocity to be as low as 1 (Reynolds number) in order to achieve the desired profile.

4. Results and discussion

The simulations on lipo lipid with interface were done with two different selections of velocity intake based on nominal inhalation in the human body. To obtain more detailed studies on each of these cases, the effect of surface tension were also included later to the simulation to provide better understandings of the membrane function of the pulmonary surfactant (lipo lipid in the human airway). A contour plot of lipid air volume fraction is