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Computational Fluid Dynamics in Small Airway Models of the Human Lung

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Abstract

The promise of gene replacement therapy for cystic fibrosis, the administration of drugs via inhalation therapy, and the deposition location of man-made airborne particulates all involve a more complete understanding of the fluid dynamics in the human lung. Flow in the larger airways may be measured through life-sized models directly, but the airways in the peripheral lung are too small and the flows are too complex to be studied in this manner. Computational models can be developed which will accurately represent both the geometric nature of the central airways and the fluid dynamics within them.

Two-dimensional and three-dimensional models of central lung airway bifurcations were developed based on morphometry. These models were used as the spatial basis upon which the differential equations that describe incompressible flow, the Navier Stokes equations, are solved. Flow solutions have been computed at Reynolds numbers from 1000 down to 100. Solutions for single and double bifurcations agree with the experimental data for flow in a branching tube. These studies are being extended to multiple bifurcations in three dimensions.

Introduction

Scientific investigation of fluid flow within the human lung is important in the understanding of the transportation of particulates in gasses. The human lung is comprised of a series of 16 Y-shaped branches which divide the flow into ever smaller branches terminating in the aveolei. Because the lung does not have an 'outlet', there is no flow at the aveolei. The necessary exchange of oxygen and carbon dioxide at the terminus of the lung is driven solely by diffusion, so the geometry produced mixing of gasses within the lung is of utmost importance. The geometry of the lung consists of a single symmetric primary branch while the remaining branches (bifurcations) are asymmetric. A generalized symmetrical and asymmetrical model has been developed from morphometry of samples of small human airways and is the geometry used in this study (Hammersley and Olsen, 1992).

Physical models can be used only to investigate the flow of simple geometries since complex three dimensional models are difficult to manufacture, and the transduction elements actually interfere with the slow flows

found in the central airways. Grid generation techniques are more suitable to model complex geometries of multiple bifurcations and accurately represent the flows found in them.

Materials and Methods

Numerical Simulation.—Numerical simulation of physical phenomenon can be performed by many methodologies. One of the oldest methods involves the use of the iterative solution of governing partial differential equations (PDEs) expressed in an appropriate coordinate system. For example, the Navier-Stokes equations may be cast in the different form in cylindrical coordinates and used to determine the steady-state flow of a fluid in a cylinder. The geometry thus obtained is a 'grid' of points described by a points axial and radial values as well as some angular indicia. Boundary values, initial conditions, the present value of neighboring points and the last iterated values of the point in question are all applied at a point on the geometry to solve the difference equation at

that point. The solution then marches to another point until solutions at all points of the entire volume are generated. The solutions of the previous iteration are then used in subsequent iterations until some predefined minimum between previous and present solutions is reached, this limit is known as the convergence criteria for the solution. Convergence criteria may be also based on the first or even the second derivatives of solutions differences. Solutions to partial differential equations by this method are useful for simple geometries, but are not applicable to more interesting and practical problems. The generation of complex geometrical grids may be performed by developing a boundary-conforming coordinate system. The boundary-conforming coordinate system may then be transformed with transformational matrices into a cubic computational grid where the PDE system is more readily solved.

Small Airway Grid Generation.--The generation of internal geometry points (field values) for a boundary-conforming coordinate system can be obtained by interpolation between the boundaries or by solving the boundary value problem. Algebraic interpolation produces a grid which reduces computational time, but the grid can have non-uniform variations in first and second order spatial derivatives, which can cause the solution to diverge. Solution of the boundary-conforming coordinate system that has smooth variations in spatial derivatives by maximizing grid surface orthogonality (Thompson, et. al. 1982).

An elliptic boundary-conforming coordinate system grid generation program developed for the U.S. Air Force known as EAGLE (Eglin Arbitrary Geometry Implicit Euler) has been used to develop the small airway models for this project (Thompson, 1988; Thompson and Gatlin 1988a, b). The program requires the boundary values of the geometry in question to be input in the form of points used to generate space curves, which are in turn linked to produce surfaces, which are assembled to produce grid volumes. Since solution of the flow equation is calculated on a computational cube, the grid volumes (blocks) generated must have a total of six four-sided surfaces. The complex geometry of the airway models is divided into multiple blocks which reduces the grid generation time as well as reducing the size of the computational matrices for the solution (Thompson, 1986; Steinberner and Chawner, 1988). Continuity for the solution is provided between blocks by overlapping the blocks along mutual faces by a point in depth, this allows a derivative to be calculated between the blocks which aids in the solution convergence.

Flow Solution.--The form of the Navier-Stokes equations used to obtain the results in this research is an implicit incompressible algorithm described by Taylor and Whitfield (1991). Finite-volume mass conservation

maintains accuracy while an artificial compressibility term (Chorin, 1967) added to the mass conservation term couples pressure and velocity. The resulting algorithm allows the incompressible equations to be solved as time-marching compressible equations. The viscous diffusion terms are center differenced while the convection terms are upwind differenced. The code is written to allow almost any arrangement of arbitrarily sized blocks (Arabshahi, 1989). This allows the flow solver to operate on the complex geometrics created by the boundary-conforming coordinate system.

Results and Discussion

Two Dimensional Solutions.--The two dimensional symmetrical and asymmetrical single bifurcation multi-block grids produced using the EAGLE grid generation program appear in Fig. 1. From the figure, it may be seen that the grids possess a high degree of orthogonality at the coordinate boundaries. Additionally, a tight grid spacing is maintained at the boundary while the spacing in the interior is larger. This aids in solution convergence, and yields more information at the flow boundaries where the pressure and velocity derivatives are larger, while reducing the amount of computation in the interior. The blocking structure for the single asymmetric bifurcation is shown in Fig. 2. The inset in Fig. 2 shows a small radius at the flow divider (carina) which simulates the structure of the airway in that region.

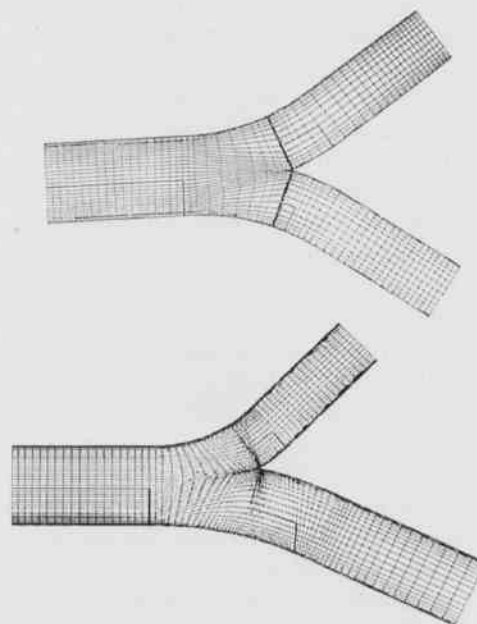


Fig. 1. Two dimensional symmetric and asymmetric double outlet lung bifurcation grid.

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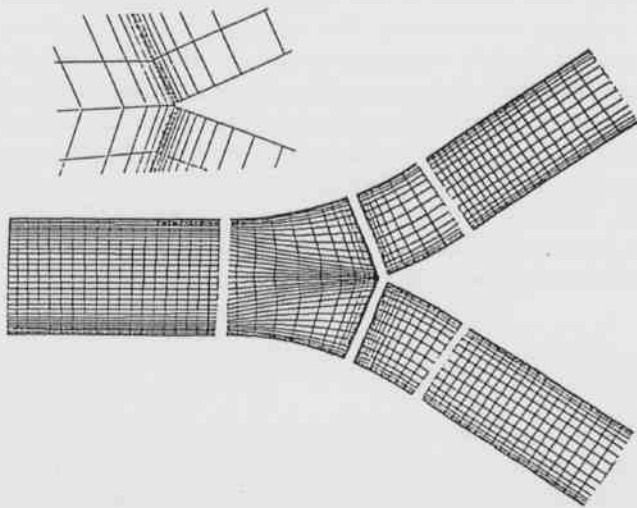


Fig. 2. Blocking structure for two dimensional symmetric model. Inset is grid at flow divider.

Velocity vectors which are normalized with the central inlet velocity are shown in Fig. 3. Flat inlet profile is seen which develops into a parabolic profile as the flow proceeds down the inlet tube. At the carina, the flow divides equally but the maximum velocity vectors are shifted towards the proximal surfaces of the bifurcation which thins the boundary layer at the flow divider. This is due to the momentum of the flow which resists the change in direction as the two daughter tubes sweep away from each other. Velocity vectors on the distal surfaces just past the carina are slightly negative indicating flow separation at that location, flow solutions at higher Reynolds numbers indicate a greater degree of separation at higher Reynolds numbers. For the asymmetrical bifurcation, the majority of the flow divides into the larger branch, but the smaller branch shows a strong skew from parabolic flow towards the proximal surface. Clinically the surfaces just past the carina are the major sites of inhaled particle deposition, in spite of the high velocities found there. Figure 4 shows a two dimensional asymmetric double-outlet bifurcation produced by dimensional scaling, translation and radial point reduction of the original single bifurcation. Radial point reduction matches the inlet points of the second (daughter) bifurcation with the outlet of the first (parent) bifurcation. For the four outlet bifurcations the majority of the flow is concentrated along the bifurcations which parallel the parent tube. The flow is not equally divided at the outlet as was thought by pulmonary researchers. Flow separation in these two dimensional models does not agree with closed form solutions for simple flow dividers and are now being compared with 3D solutions.

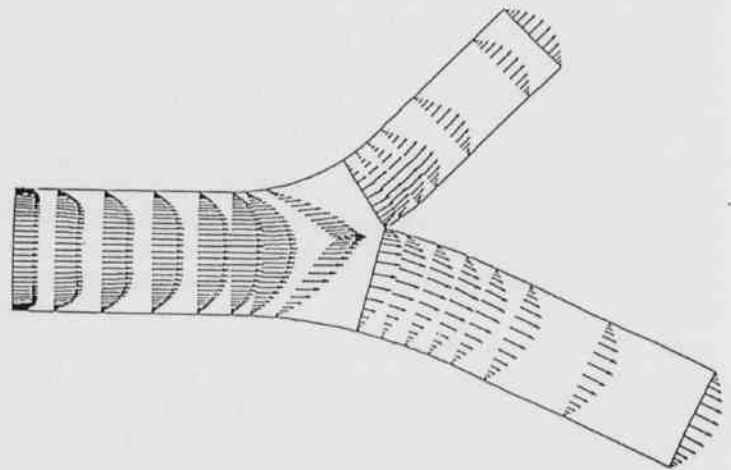
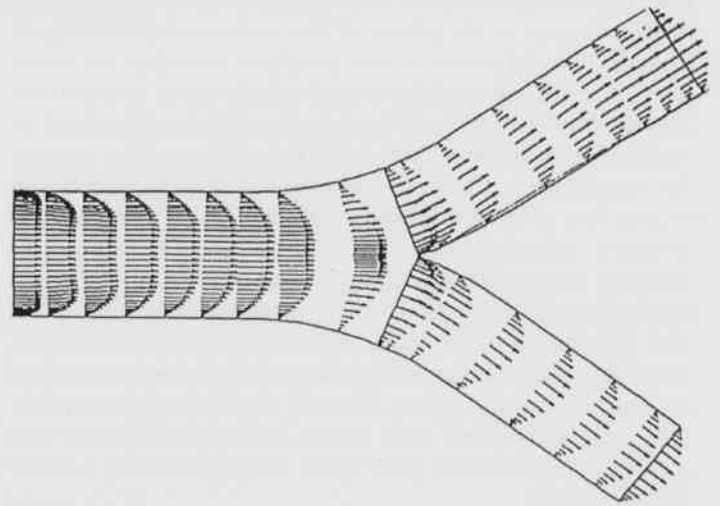
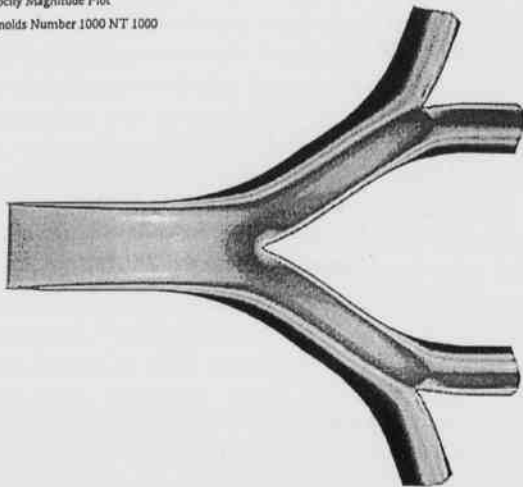


Fig. 3. Velocity vectors for double outlet grid. Flow is skewed towards flow divider.

Small Airway Symmetrical Double Bifurcation Model
Velocity Magnitude Plot
Reynolds Number 1000 NT 1000



Small Airway Asymmetrical Double Bifurcation Model
Velocity Magnitude Plot
Reynolds Number 1000 NT 1000

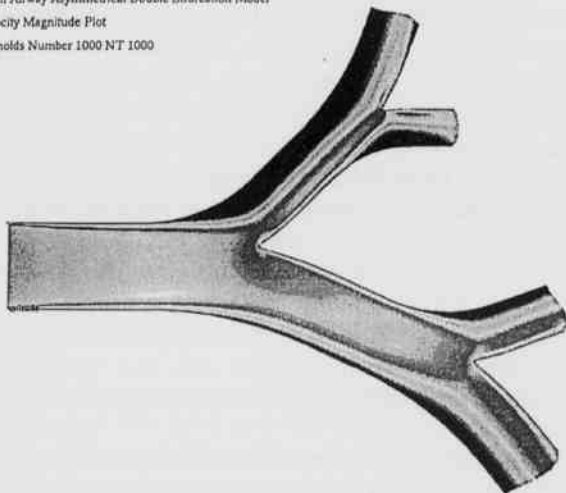


Fig. 4. Velocity magnitude for four outlet grids. Negative values indicate flow separation.

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Velocity Magnitude

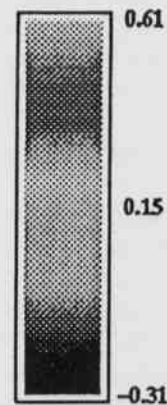


Fig. 4. (continued).