Computational Fluid Dynamic and Oxygen Transport Model of the Cardiopulmonary System

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NSF

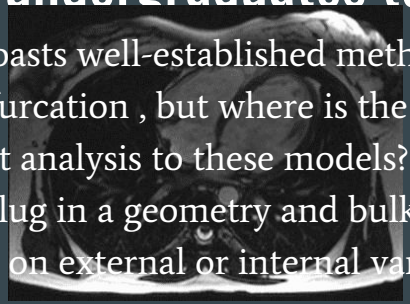
Abstract

- Goal: To create a representative model of the pulmonary system and its immediate capillaries with a focus on the bulk/intensive properties of the fluids involved.
- Results include test cases for the 1st-3rd bifurcations of the lungs and corresponding oxygen transport models.

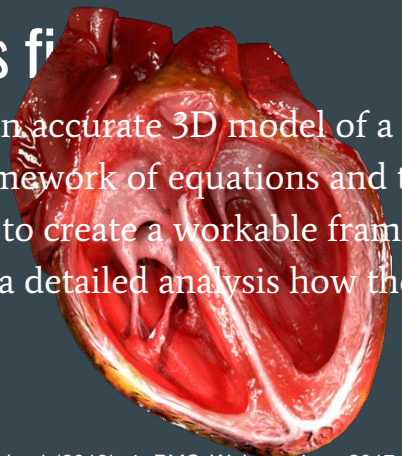
Domain Science: BioMedical CFD

Image-based CFD is the future of cardiovascular [and pulmonary] medical treatment[1]. It has only recently become a feasible option for researchers [note: not physicians], for example a December 2016 study by Virginia Commonwealth University researchers accurately modeled pulmonary drug delivery of an inhaler within 10% accuracy of clinical data[2].

W lo as undergraduates to further this fi



This particular field boasts well-established methods of obtaining an accurate 3D model of a patient's lungs down to the 3rd~5th bifurcation , but where is the plug-and-play framework of equations and test cases to properly apply finite element analysis to these models? This project aims to create a workable framework that physicians/researchers can plug in a geometry and bulk properties to get a detailed analysis how those properties will change based on external or internal variables.



[1] Pennati, Giancarlo et al. "Computational Fluid Dynamics Models and Congenital Heart Diseases." *Frontiers in Pediatrics* 1 (2013): 4. *PMC*. Web. 12 June 2017.
[2] Longest P. Worth, Tian Geng, Khajeh-Hosseini-Dalasm Navvab, and Hindle Michael. Journal of Aerosol Medicine and Pulmonary Drug Delivery. December 2016, 29(6): 461-481.

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File Edit Windows Options Tools Help

Component 1 (comp1) | Turbulent Flow, k-ω (spf) | Mesh 1 | Study 1 | Velocity (spf)

Definitions | Geometry | Materials | Physics | Mesh | Study | Results | Velocity (spf)

Model Builder

- case-f-3.8-3.801-20fps-FINEMESH-restar
  - Global Definitions
    - Parameters
    - Gaussian Pulse 1 *(gp1)*
    - Waveform 1 *(wv1)*
    - Step 1 *(step1)*
    - Materials
  - Component 1 *(comp1)*
    - Definitions
    - Geometry 1
    - Materials
      - Air *(mat1)*
    - Turbulent Flow, k-ω *(spf)*
      - Fluid Properties 1
      - Initial Values 1
      - Wall 1
      - Symmetry 1
      - Inlet 1
      - Outlet 1
    - Mesh 1
  - Study 1
    - Step 1: Time Dependent
    - Solver Configurations
      - Solution 2 *(sol2)*
      - Solution 1 *(sol1)*
  - Results
    - Data Sets
    - Derived Values
    - Tables
    - Velocity (spf)
    - Pressure (spf)
    - Wall Resolution (spf)
    - 3D Plot Group 4
    - Export
    - Reports

Settings

3D Plot Group

Plot

Label: Velocity (spf)

Data

Data set: Study 1/Solution 2 (sol2)

Time (s): 3.7

Title

Plot Settings

View: Automatic

Show hidden entities

Propagate hiding to lower dimensions

Plot data set edges

Color: Black

Frame: Spatial (x, y, z)

Color Legend

Show legends

Show maximum and minimum values

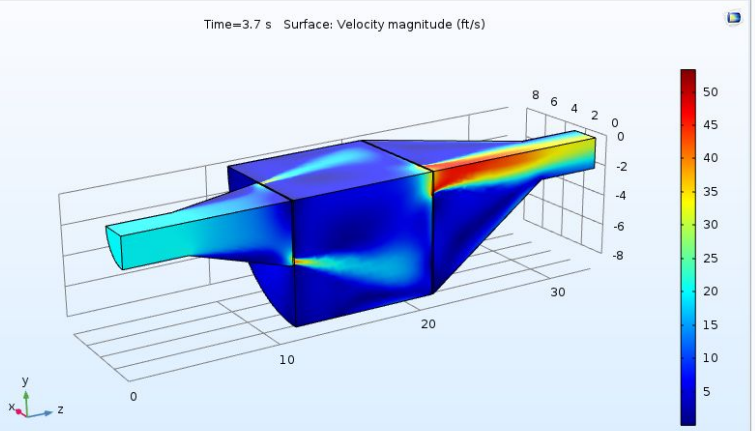
Position: Right

Text color: Black

Number Format

Window Settings

Graphics



Messages | Progress | Log | Table

x	y	z	Value
0.85437	-1.0108	0.0000	0.036590
0.62430	-0.68117	0.0000	0.036572
1.1121	-0.65894	0.0000	0.036578
1.5831	-0.67181	8.8818E-1	0.036593
1.8599	-0.45943	-2.6645E-	0.036496
2.0684	-0.74970	4.7934	0.036986
0.94058	-0.92260	1.7764E-1	0.036588
-1.7764E-	-6.1795	20.770	2.6681
3.5527E-1	-6.2938	20.791	1.9722
0.0000	-6.2319	20.829	2.0120
0.0000	-6.3269	20.838	1.8322
-1.7764E-	-6.4318	20.835	0.022614

Add to Component | Add to Selection

Search

- Recent Materials
- Built-In
- Liquids and Gases
- User-Defined Library

1.48 GB | 8.41 GB

Research Plan

What we accomplished

Geometry that shows 2-3 generations into tracheobronchial tree

Using an idealized geometry

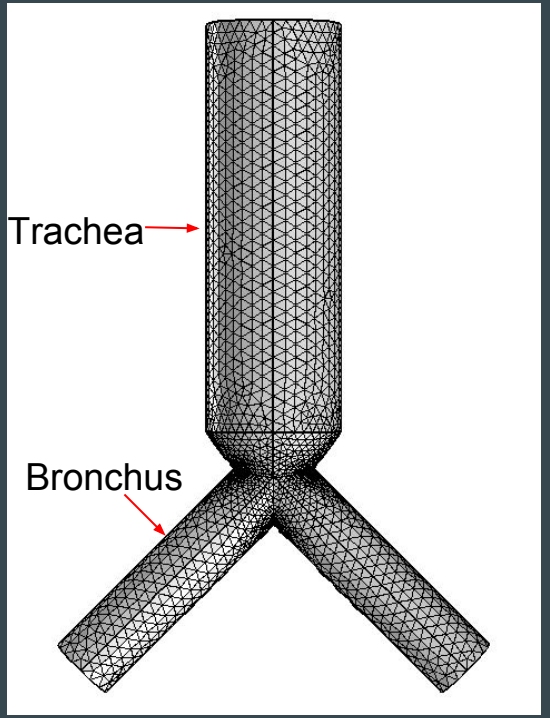
Simulate “at rest” breathing conditions in 3D and 2D

Oxygen Transport and Hemodynamic Models

Simulate the O_2 and CO_2 diffusion between alveoli at the end of the bronchial tree and the pulmonary capillaries

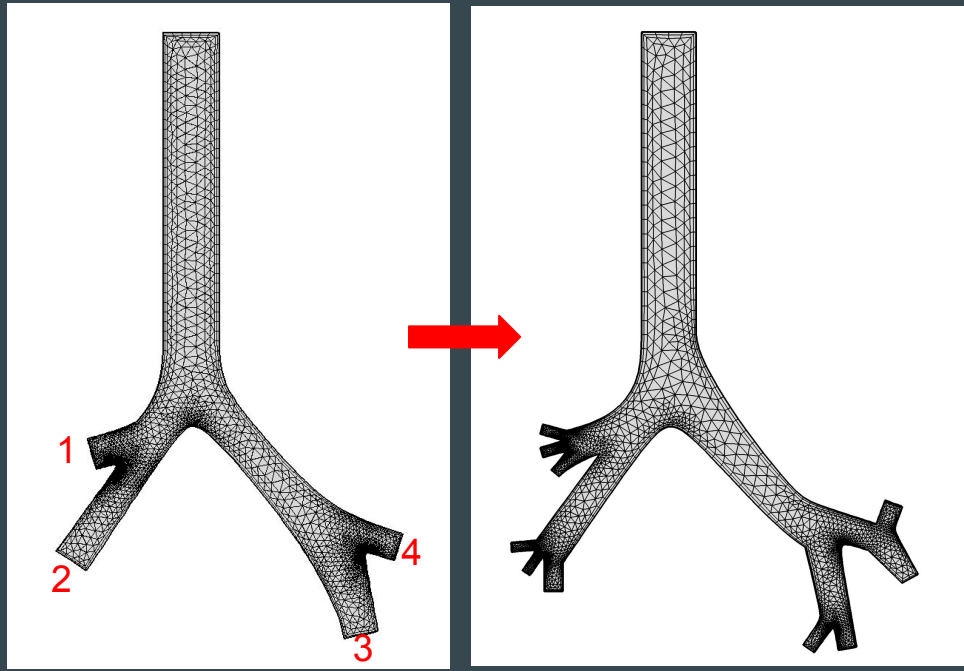
3D Pulmonary Geometry

- Created using cylinder and cone tools in Comsol
- *Very* idealized system
- 3D provided useful benchmark data to build off of in 2D



2D Pulmonary Geometry

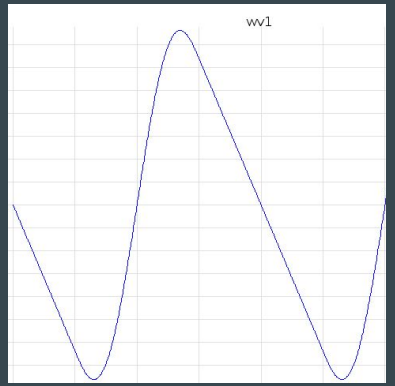
- Accomplished more accurate representation of tracheobronchial tree
- Measurements taken from a 2015 study from Weidong Mi et al
- The outlets are labeled counterclockwise from the top left outlet

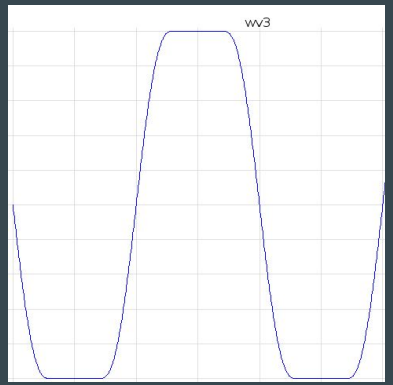


Steady State vs. Transient Simulations

- Steady state means that the system has reached total equilibrium based off of a single set of initial and boundary conditions.
- We care about this solution because it computes faster and gives a reliable snapshot of pressure and velocity.
- For example, we know that the lungs can create a pressure difference of +/- 130 Pa. However, this pressure is found in the deepest parts of the lungs, we had to conduct numerical experiments to determine a ballpark estimate for the actual pressure in the bronchus.

- Transient simulations allow us to see the flow of air over a time period
- In our transient simulations we use a mixture of square waveform and sawtooth graphs to better replicate the mechanics of inspiration and expiration





Flow Rates for Pulmonary Simulation

- At rest breathing conditions:

V=0.5L =0.0005 m3
Q = 0.0005 m3 / 2 s = 0.00025 m3/s
(2 seconds corresponds to 15 breaths per minute)

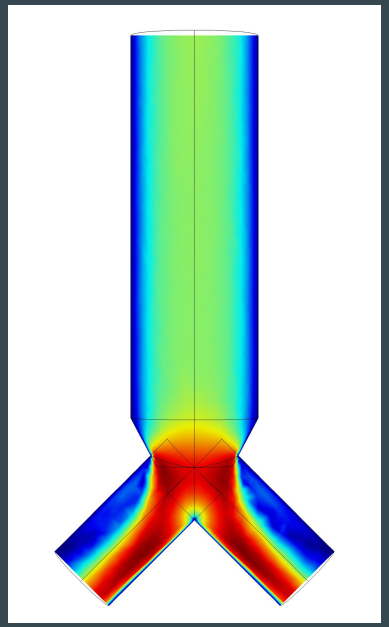
- These velocities represent the average velocity needed through a 2 second inhale or exhale

- To calculate the data in the table we used:

$$Lp(dia)=1/4\times\pi\times dia$$
$$Q=V\times d\times Lp(d)=V\times 1/4\times\pi\times d^2$$

	Diameter (m)	Volume Flow Percentage	Velocity (m/s)
Outlet 1	.0094	20	.7204
Outlet 2	.0110	35	.9208
Outlet 3	.0101	20.3	.7708
Outlet 4	.0087	24.7	.8536

3D Pulmonary Test Cases



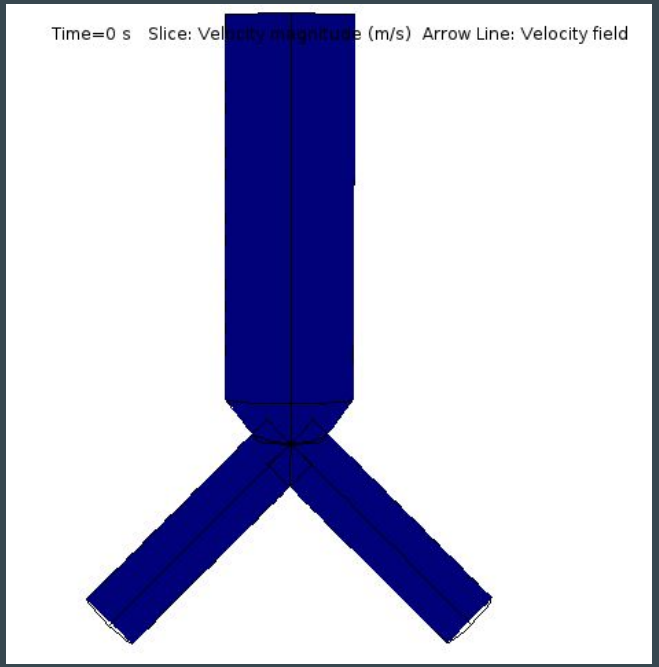
Steady State

Set Conditions:
Inlet Pressure= 0 Pa

Outlet Pressure=
-.1776 Pa

Results:
Inlet Velocity= .2057 m/s

Outlet Velocity= .2886 m/s



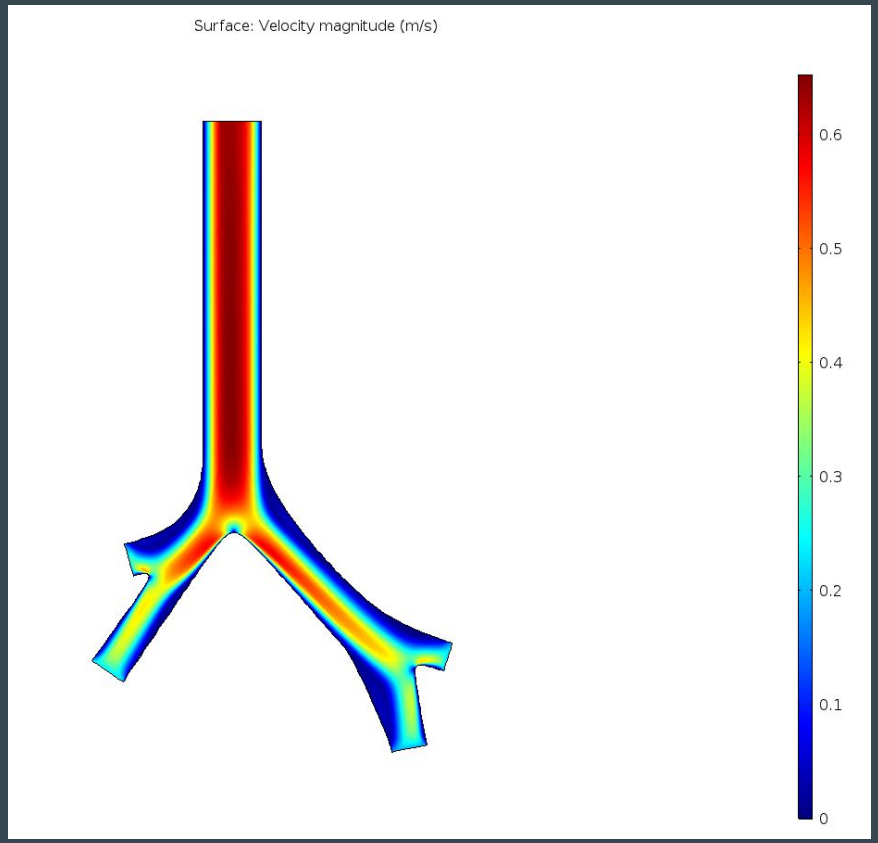
Transient

Set Conditions:
Inlet Pressure used waveform graph

Outlet Pressure= 0 Pa

- Only analyzed max inlet and outlet velocity to check if representative

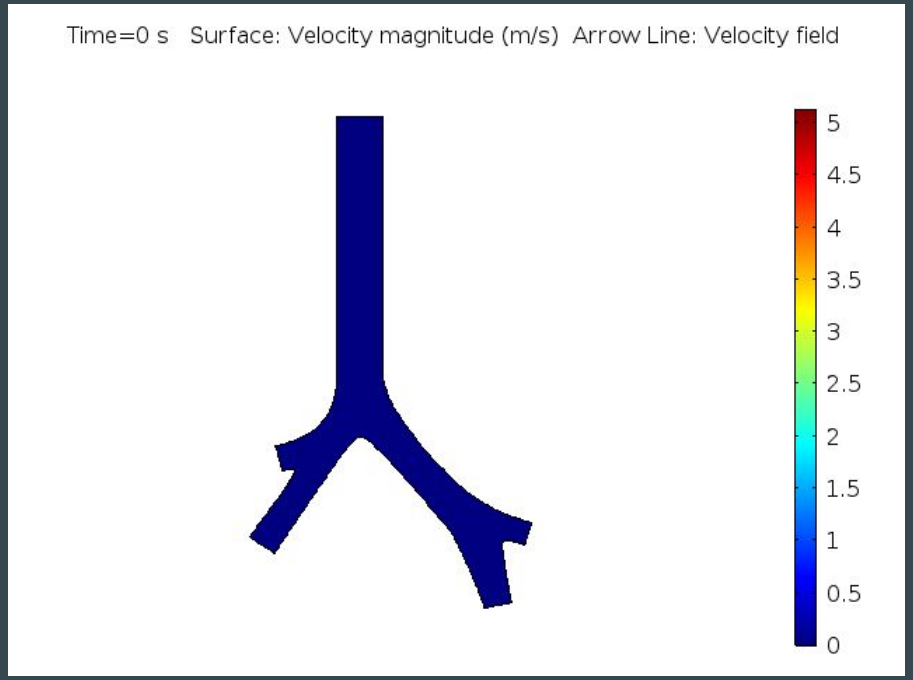
2D Pulmonary Test Case: Steady State



- Crucial step in testing flow rates calculated
- Results:

  Outlet P_{total}= 0.1435 Pa
  Inlet Velocity=..4745 m/s
- Pressure difference observed in simulation served as a benchmark for transient simulations

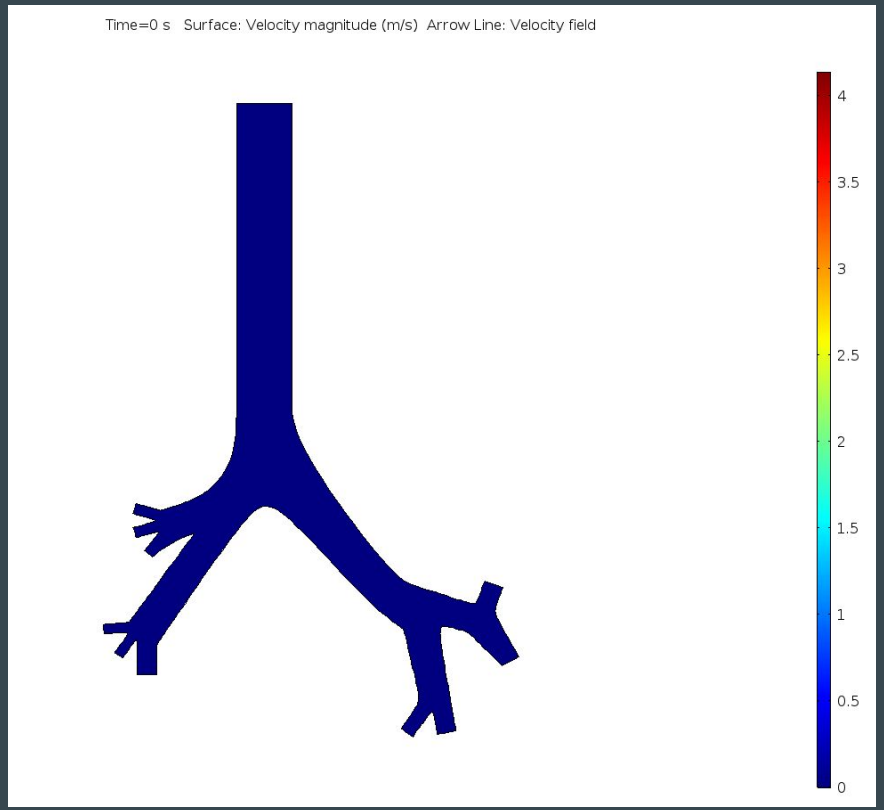
2D Pulmonary Test Case: 2nd Generation



Right upper Segmental Bronchial (Outlet 1)

Time (s)	Velocity magnitude (m/s)	Volume Flow Rate (m^3/s)
0	0	0
0.1	0.104030746	2.8878E-05
0.2	0.166598297	4.62462E-05
0.3	0.179480588	4.98222E-05
0.4	0.179306368	4.97739E-05
0.5	0.179306368	4.97739E-05

2D Pulmonary Test Case: 3rd Generation



Inhale inlet	Line Integration (m^2/s)		Volume Inhaled
0	0		0.0002194
0.1	0.011406		
0.2	0.018263		
0.3	0.019659		
0.4	0.019658		
0.5	0.019658		

Outlet 1 Data

Hemodynamic Simulations

Our ultimate goal is to create an interface between the lungs and the blood. This group of simulations starts from simple flow of blood through a cylinder and ends with a representative model of the blood/lung system.

The following simulations were ran to benchmark the fluid and diffusion behavior...

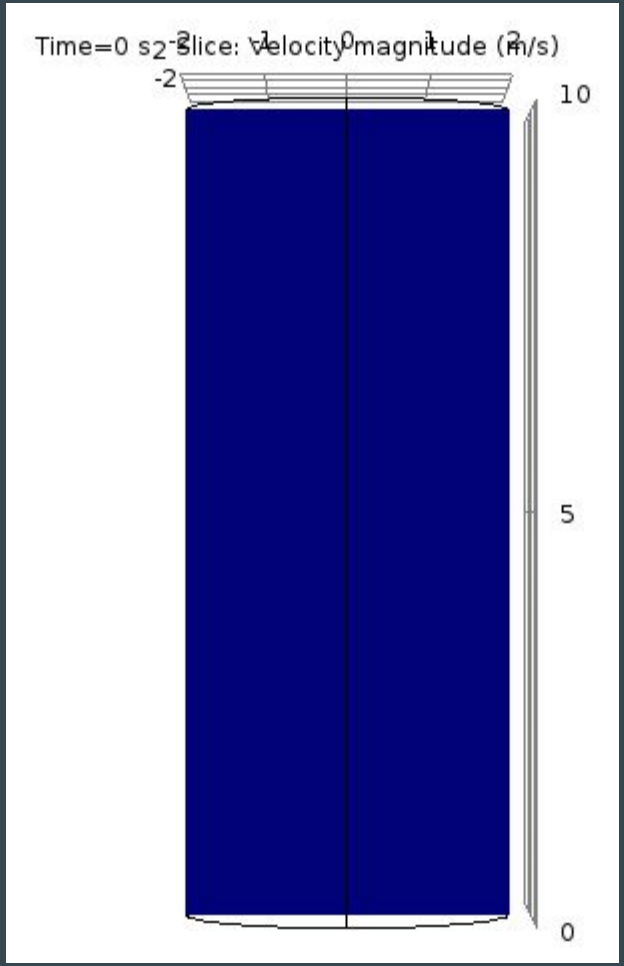
1. 3D Pulsatile Duct Flow
2. 3D Pulsatile Curved Duct Flow
3. Axisymmetric Mesh Expansion/Contraction
4. Closed Loop System
5. Diffusion from Alveoli into Blood
6. Bulk Blood/Lung System

3D Pulsatile Duct Flow

We used this as a basis for our blood flow in our other simulations. The inlet velocity is a function of cardiac output, heart bpm and time.

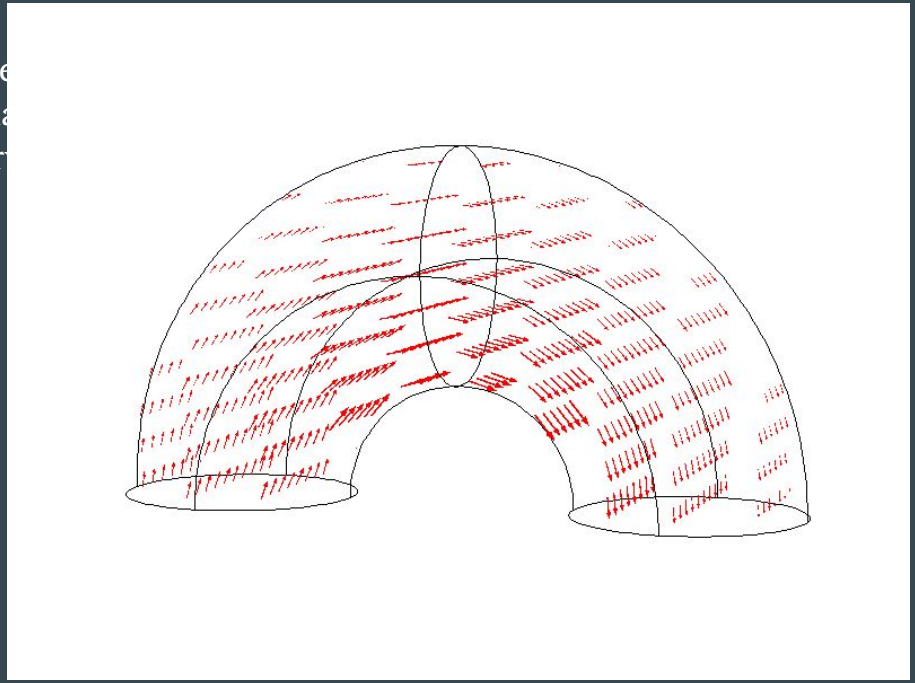
Average Cardiac Output:

5.0L/min = 8.33E-5 m^3/s



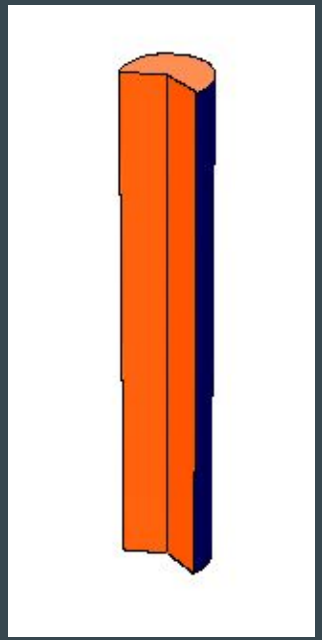
3D Curved Duct Flow

We wanted our mode
the terminal pulmona
would have to be cur



Should the blood vessel walls deform?

Ideally, yes. But we lack the structural mechanics module of Comsol and it was decided that the structural deformation of such vessels are of secondary interest.

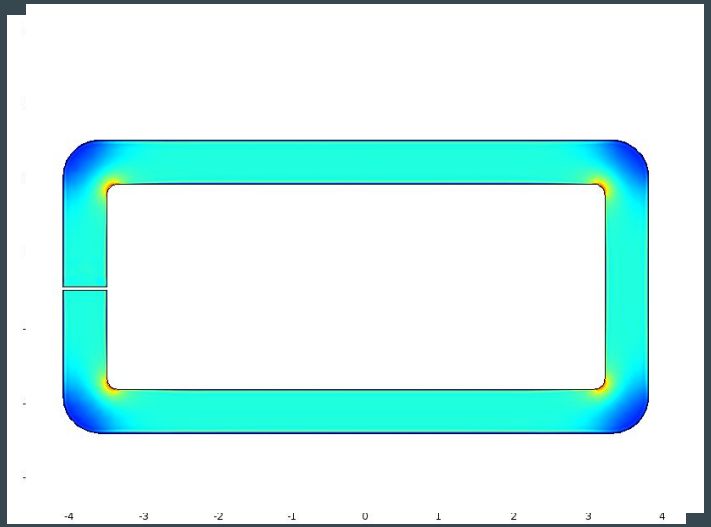


In reality, the pulmonary capillaries are interwoven into the alveolar capillary bed meshwork (ACM) that forms a near-continuous sheet of blood.

The implications of this deformation are negligible for the bulk characteristics that we are focusing on. Any potential increase in blood pressure that can be accounted for with the inlet/outlet velocities for the blood.

Closed loop system

When our model simulates oxygen diffusion, how would we treat the system as a bulk? Our first idea was to incorporate some type of “closed loop” system...



We couldn’t find a way to relate the outlet and the inlet.
Diffusion of oxygen out of the blood was difficult to simulate.

Parameters

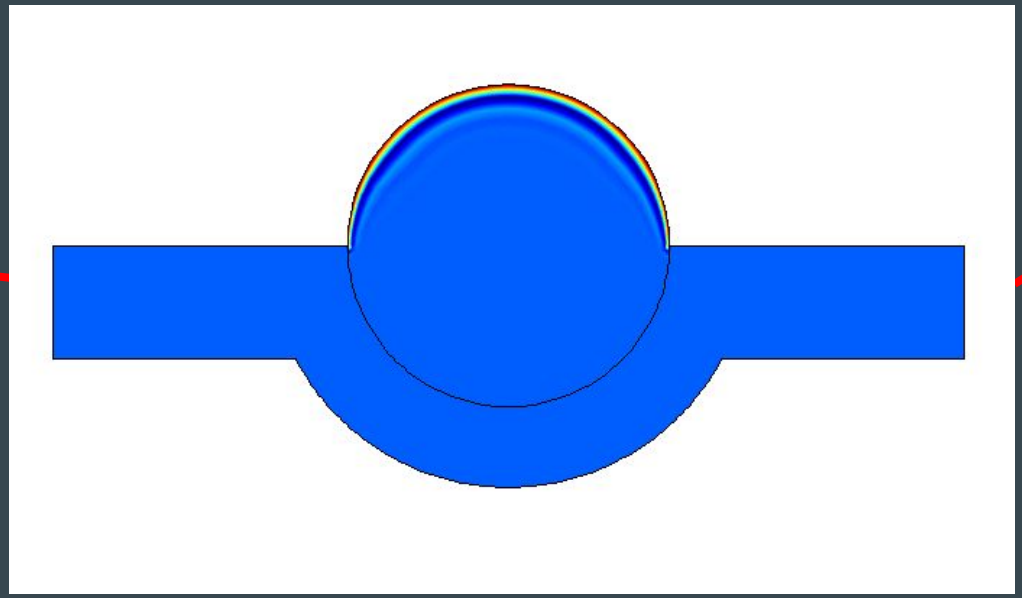
The simulations up until this point have used a variety of parameters, most have gone into the making of the following diffusion models, they are summarized below:

Parameter	Value	Units	Reference
Blood Flow	4.5	L/min	
Inlet Velocity	1	m/s	
Inlet Diameter	1	cm	
Mixed Venous Content of Oxygen	15	mL/dL (%)	[1]
Inlet Oxygen by Mass Flow	1.61E-05	kg/s	
Arterial Content of Oxygen	20	mL/dL (%)	[1]
Outlet Oxygen by Mass Flow	2.14E-05	kg/s	
Target Oxygen Into System	5.36E- 6	kg/s	
	160	mL/min	[1]
Mass Fraction Oxygen in Alveolar Air	13.16	%	
[1] - Hlastala and Berger Appendix B			

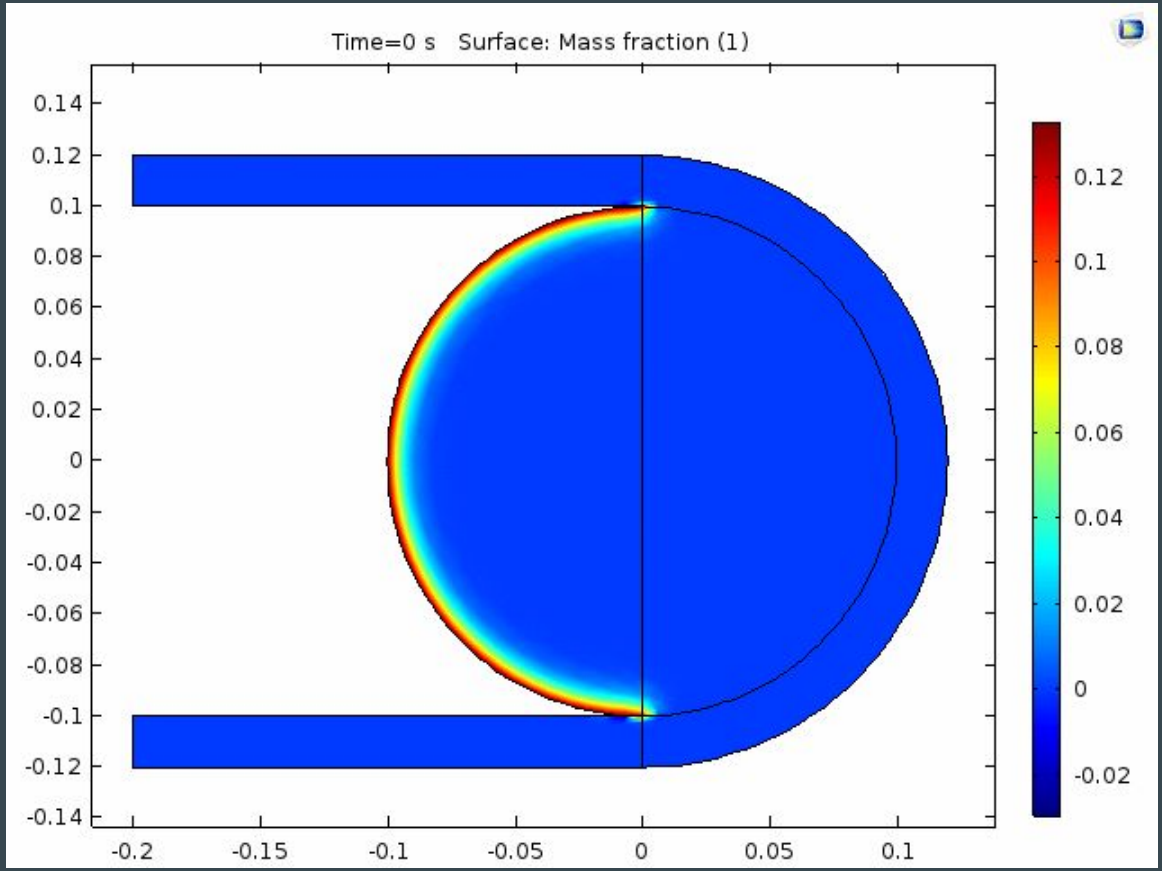
The variable we manipulated to get the target oxygen consumption was solely the Maxwell-Stefan diffusivity matrix for each of the two fluids. (and in a minor way, inlet diameter)

Open Loop System

The difficulties presented with the Closed Loop system were solved by simply creating an open loop, with the inlet blood concentration being another parameter you must set (rather than the outlet conditions dictating the inlet condition).



Series of Diffusion Simulations



Scale

The simulation on the last slide had an average of 1E-6 kg/s into the system (target: 5E-6).

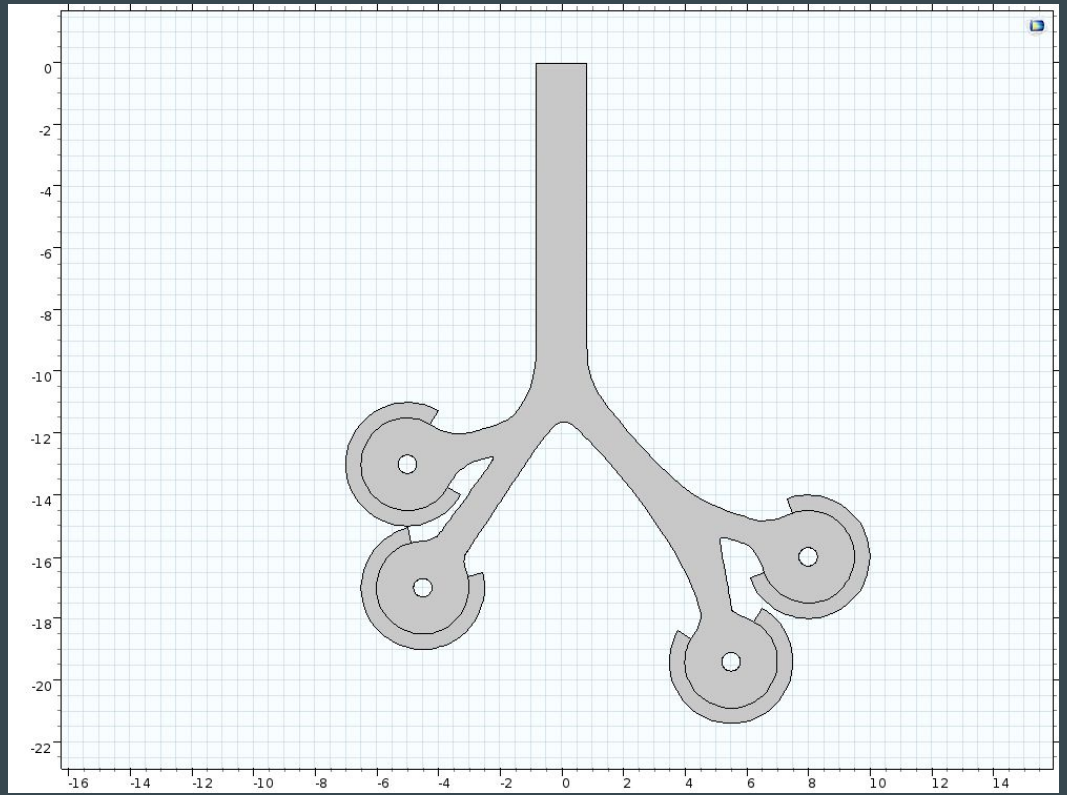
We manipulate the diffusion coefficients further, but the oxygen will “diffuse” up the bloodstream. Even with the diffusion coefficients reach such a level, the best we can get out of the model is only within a factor of 5.

One possible solution is changing the parametric length, from imitating a duct to something like a deep rectangle. Another solution is that splitting the model into smaller divisions will give us more (parameterized) surface area to diffuse through.

Coupling the Systems

This model represents the current state of our project. Work continues, but challenges include...

- Outlets? Periodic condition?
- Numerical error when oxygen meets a wall
- Evenly distributing oxygen



Continuing Work...

We hope to smooth and further bifurcate our 2D pulmonary model.

Finish the 2nd bifurcation diffusion model (previous slide) and apply to the 3rd bifurcation model (ten outlets/“terminal units”).

Apply different breathing, altitude, heart rate conditions to test the robustness of our model.

Questions?

“To raise new questions, new possibilities, to regard old problems from a new angle, requires creative imagination and marks real advance in science.”