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Simulating Microbubble Flows Using COMSOL Mutiphysics

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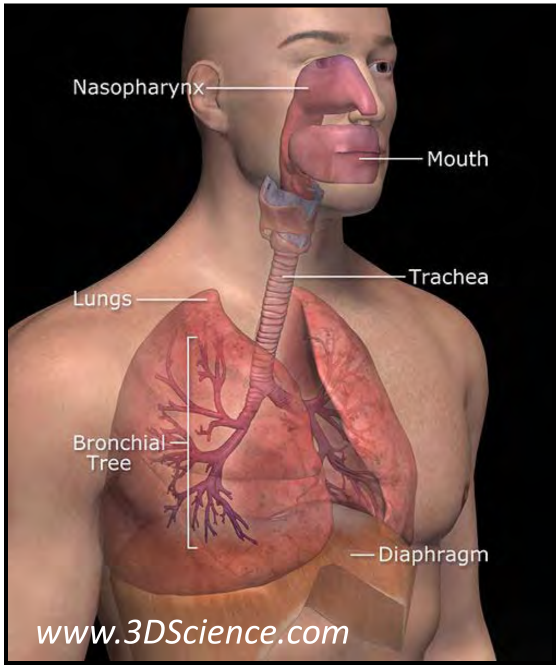
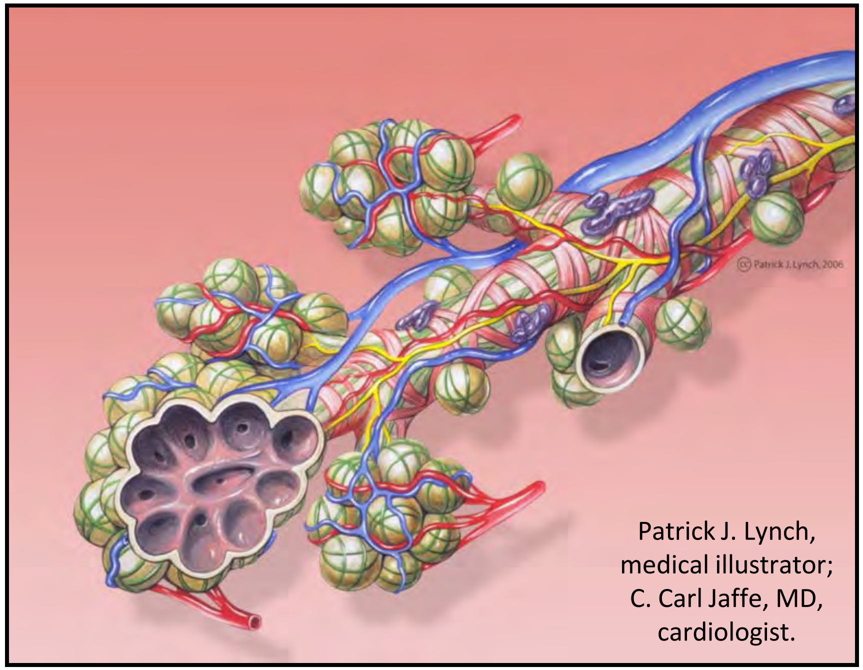
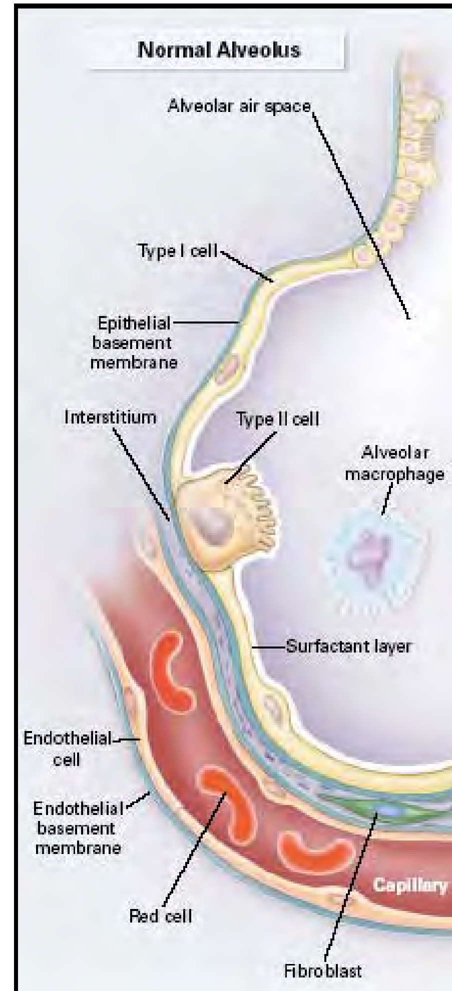
Pulmonary System





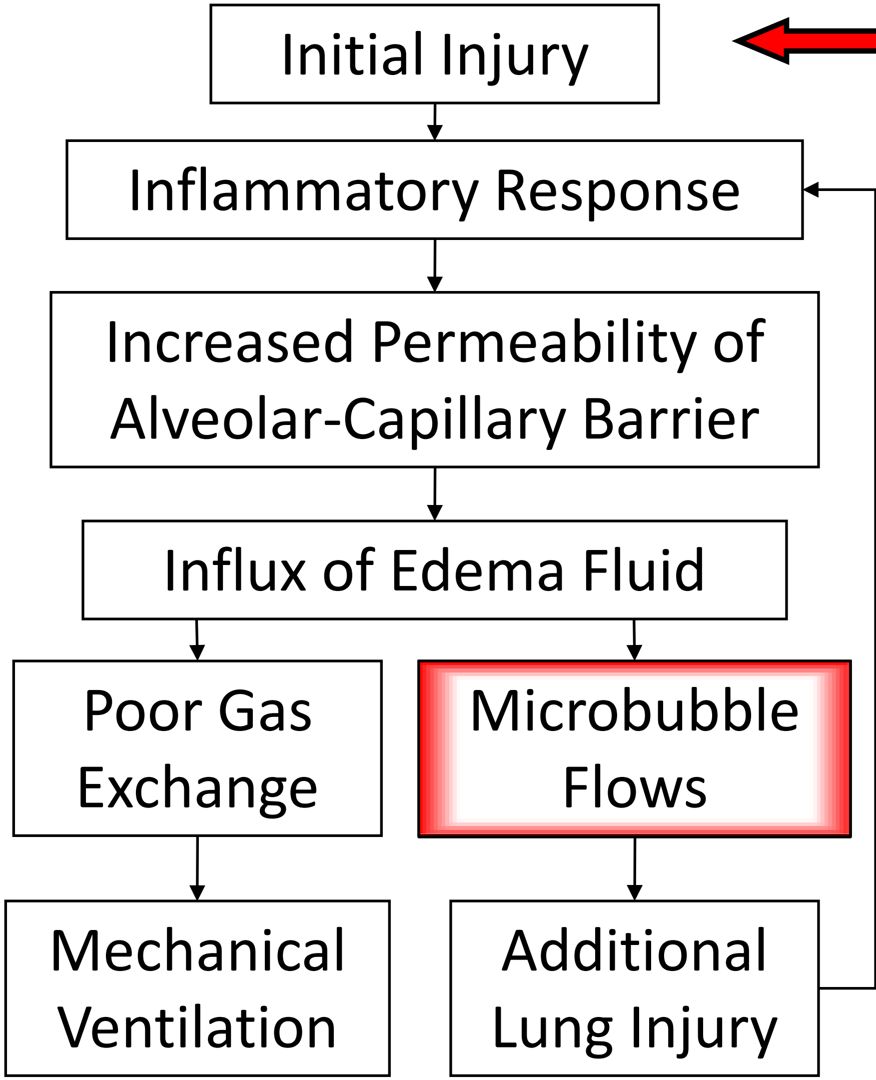


Ware LB & Matthay MA, *New Eng J Med* 342(18): 1334-1339 (2000)

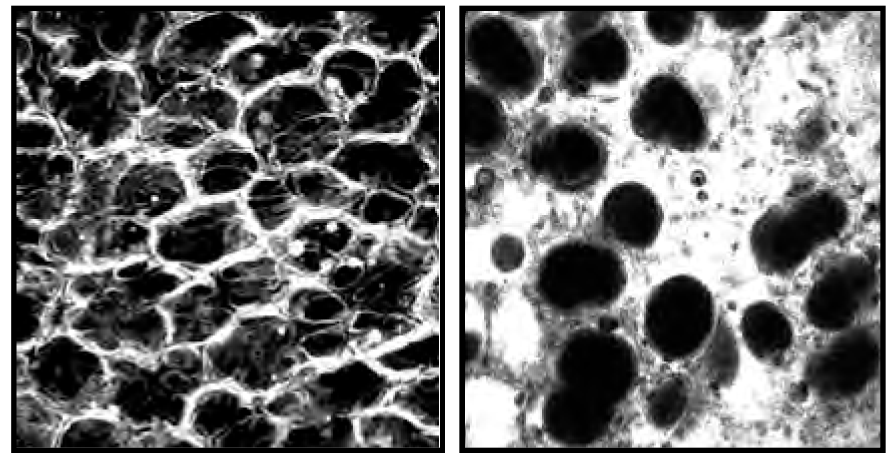
Bifurcating airway tree ends in air sacs called *alveoli*. Terminal airways are less than 500 μm in diameter.

A biological sandwich of endothelial cells (blood side) and epithelial cells (lung side) forms the *alveolar-capillary barrier*.

Motivation-- Acute respiratory distress syndrome (ARDS)



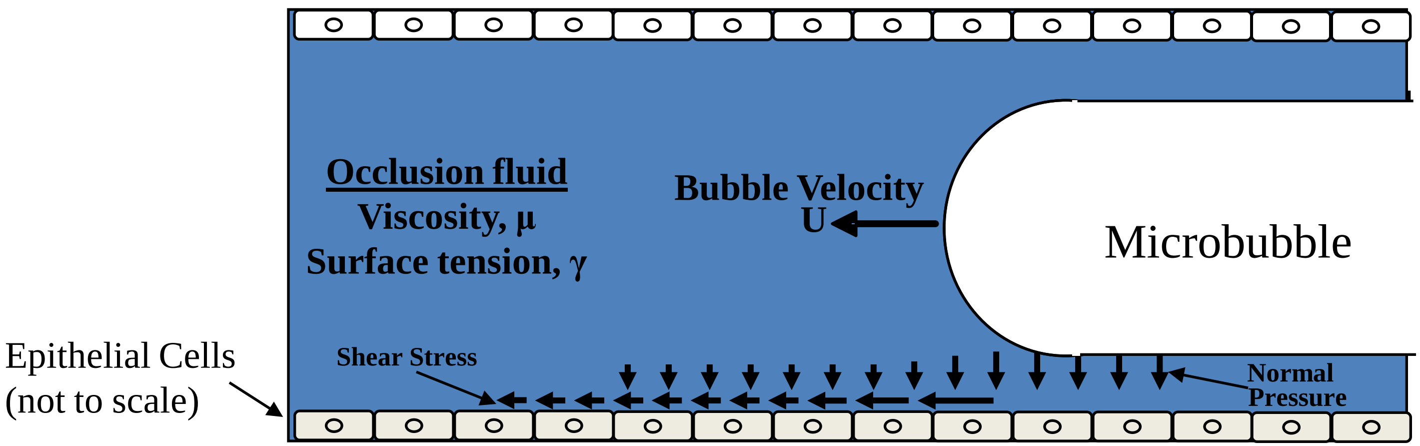
Common Causes:
Pneumonia, Sepsis, Trauma



Hubmayr RD, *Am J Respir Crit Care Med*, 165(12), pp. 1647-1653 (2002).

Comsol Mutiphysics Simulations

Mechanobiology of Airway Reopening



Airway Reopening Conditions

- Hydrodynamic stresses (Bilek, JAP 2004; Yalcin, JAP 2007).
- Cell Morphology (Yalcin, JAP 2007)
- Cytoskeletal Structure / Cell Mechanics

Mechanical Response

- Cell deformation
- Membrane rupture (necrosis)
- Cell detachment

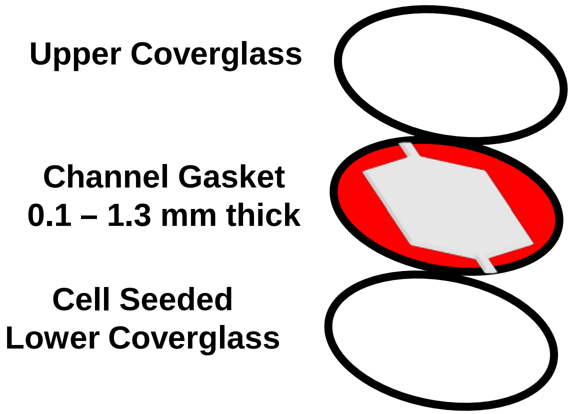
New treatment options (pharmaco-protective)

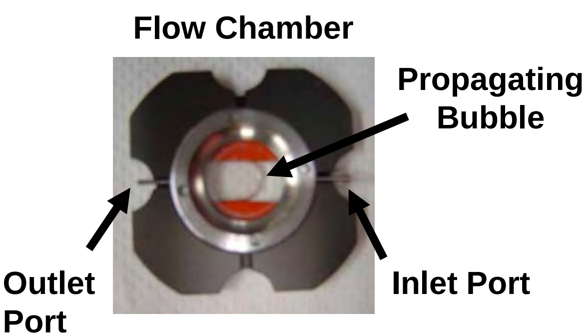
Biological Response

- Protein/Gene Expression
- Inflammatory pathways
- Surfactant secretion

Computational models → Mechanisms of Injury ← **In-vitro experiments**

Experimental Flow System and Boundary Element Method





Experiment Conditions:

Capillary number range: $Ca = \frac{\mu U}{\gamma}$ 3.7×10^{-6} to 3.7×10^{-4}

Reynolds number: Re from 0.1 to 10

Bubble Velocity range of 0.3 to 30mm/s

Channel height =0.5mm

H.C.Yalcin, S.F. Perry and S.N. Ghadiali, J Appl Physiol 103:1796-1807,2007.

BEM (Boundary Element Method)

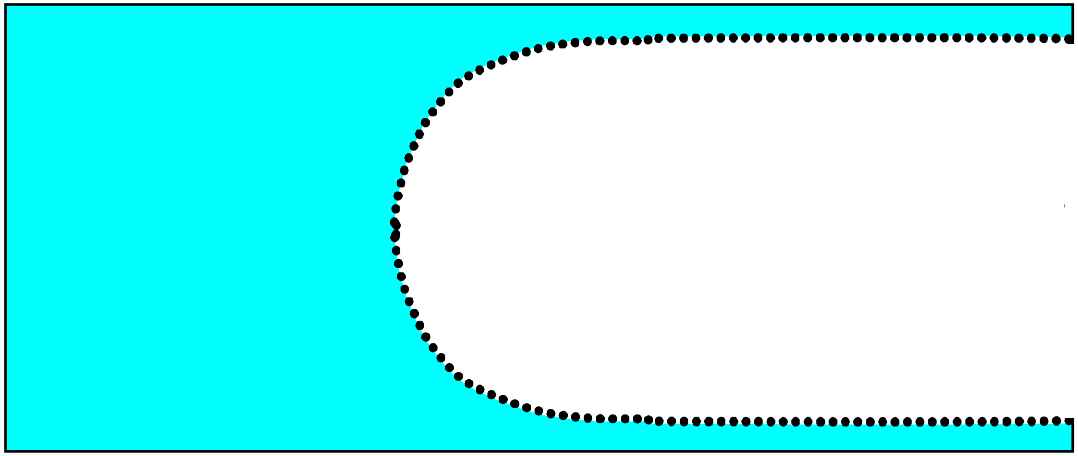
Limitations:

1) Only valid when $Ca > 10^{-3}$, far away from the experimental conditions

2) Only valid for zero Reynolds number flows such as Stokes flow while experimental Reynolds Numbers are O(1)

Ghadiali SN and Gaver DP 3rd, J. Fluid Mech. 478:165-196,2003

Goal



Current goal is to develop computational models that accurately characterize the microbubble flows that exist during experimental conditions and to develop a model that can be extended in the fluid structure interaction.

Overall goal is to develop novel treatment for ARDS that minimize the amount of cellular deformation and injury caused by microbubble flows

Governing Equations

Momentum Transport equations:

$$\mathrm{Re}\cdot\mathrm{Ca}\frac{\partial \mathrm{U}}{\partial \mathrm{t}} - \nabla\cdot[\mathrm{Ca}(\Delta\mathrm{U} + (\Delta\mathrm{U})^{\mathrm{T}})] + \mathrm{Re}(\mathrm{U}\cdot\nabla)\mathrm{U} + \nabla\mathrm{P} = \mathrm{F}$$

$$Re = \frac{\rho \mathrm{UD}}{\mu}, \mathrm{Ca} = \frac{\mu \mathrm{U}}{\gamma}, \mathrm{P} = \frac{\mathrm{p}}{\gamma/\mathrm{a}}$$ Dimensionless variables

Continuity Equation for Incompressible fluids:

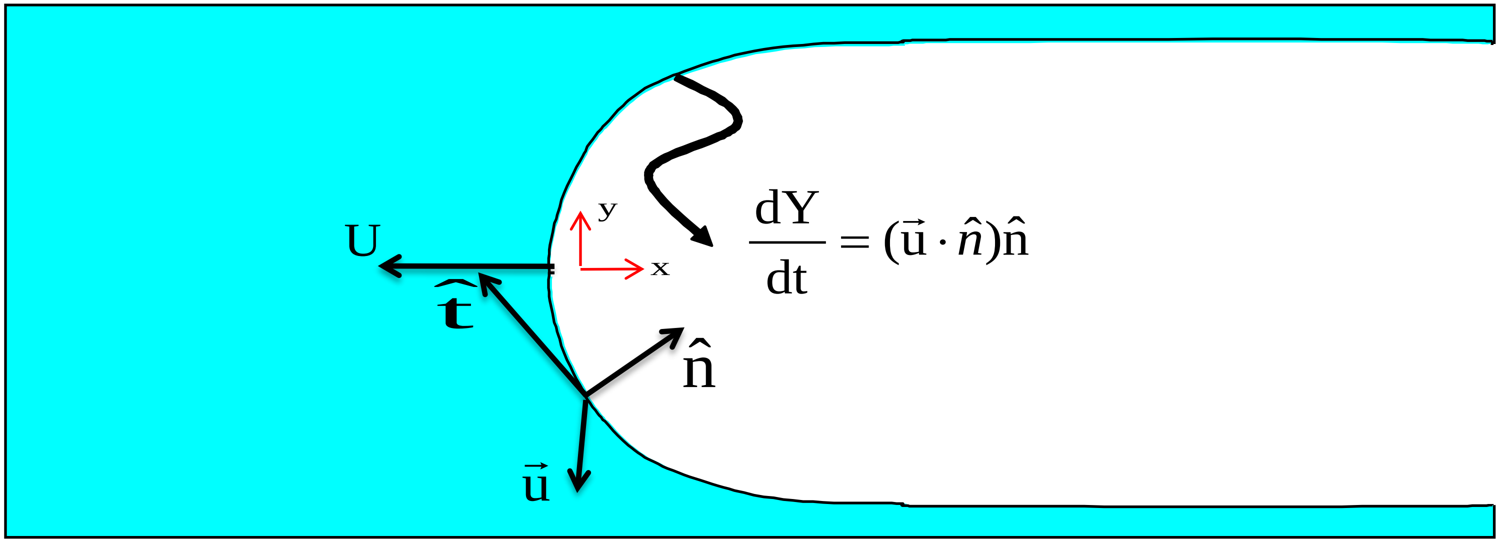
$$\nabla\cdot\mathrm{U} = 0$$

Laplace’s Law:

$$\nabla P = \mathrm{P_{in}} - \mathrm{P_{out}} = \kappa \quad \text{where } \kappa = \frac{\frac{dx}{ds}\cdot\frac{d^2y}{ds^2} - \frac{dy}{ds}\cdot\frac{d^2x}{ds^2}}{\left(\left(\frac{dy}{ds}\right)^2 + \left(\frac{dx}{ds}\right)^2\right)^{3/2}}$$

⇒ SPLINE Routine

Interface Motion Equation



$$\frac{dY}{dt} = (\vec{u}\cdot\hat{n})\hat{n}$$

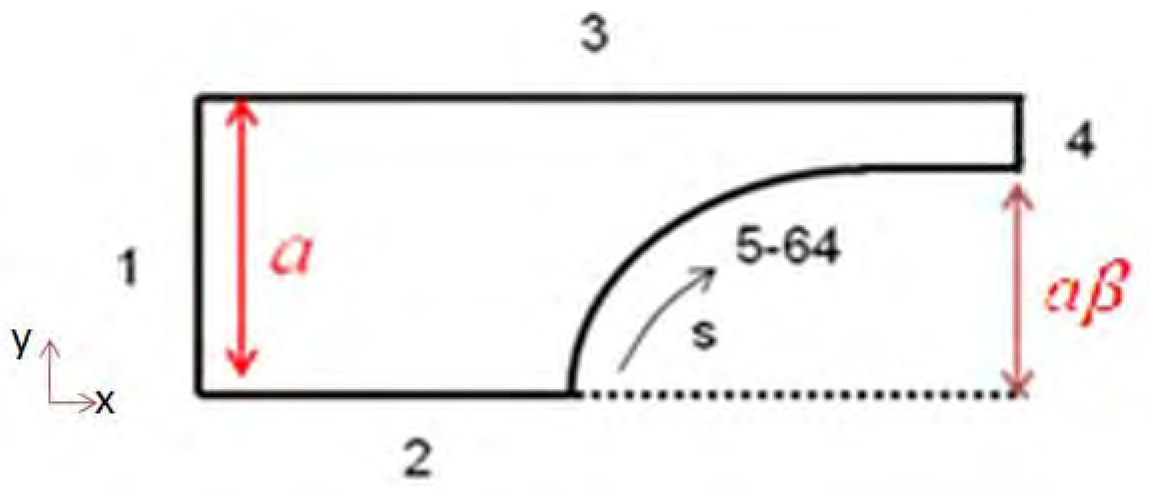
where $Y = x\hat{i} + y\hat{j}, \vec{u} = u_x\hat{i} + u_y\hat{j}, \hat{n} = n_x\hat{i} + n_y\hat{j}$

$$n_x = -\frac{\frac{dy}{ds}}{\left(\left(\frac{dy}{ds}\right)^2 + \left(\frac{dx}{ds}\right)^2\right)^{3/2}}$$

$$n_y = \frac{\frac{dx}{ds}}{\left(\left(\frac{dy}{ds}\right)^2 + \left(\frac{dx}{ds}\right)^2\right)^{3/2}}$$

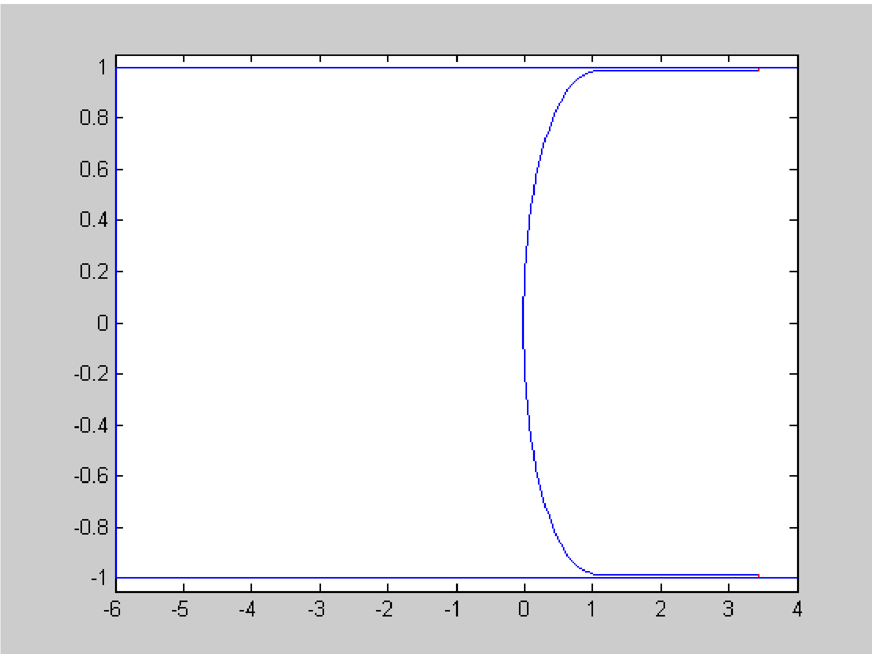
ODE Solver, Interface Tracking

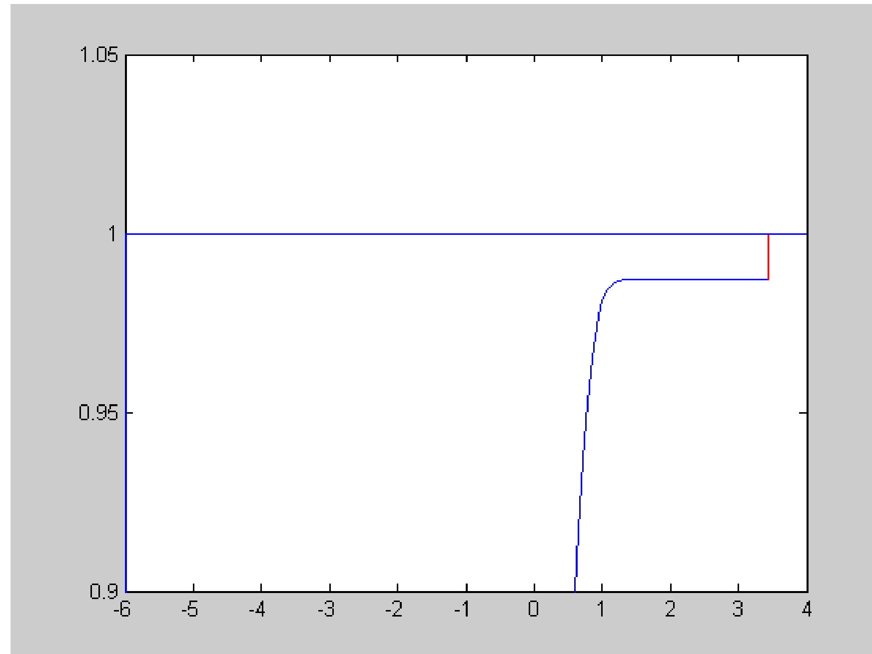
Model Domain in the Lab Frame



Boundaries	Boundary conditions
1	Parabolic flow $U = 3a\beta/2(y^2 - 1)$, $v = 0$
2	Symmetry
3	$u = 0$, $v = 0$
4	$u = 0$, $v = 0$
5-64	stress balance $\tau = \kappa n$

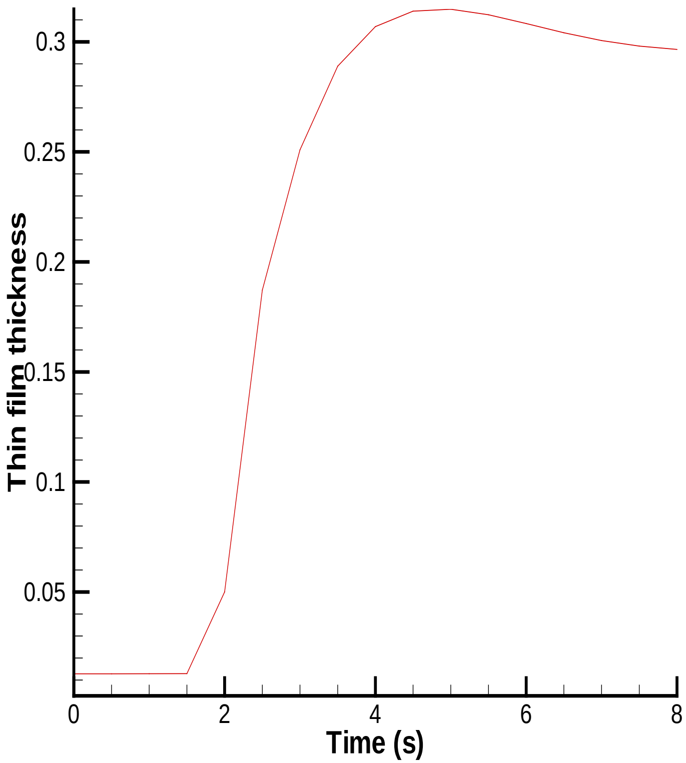
Simulation Results





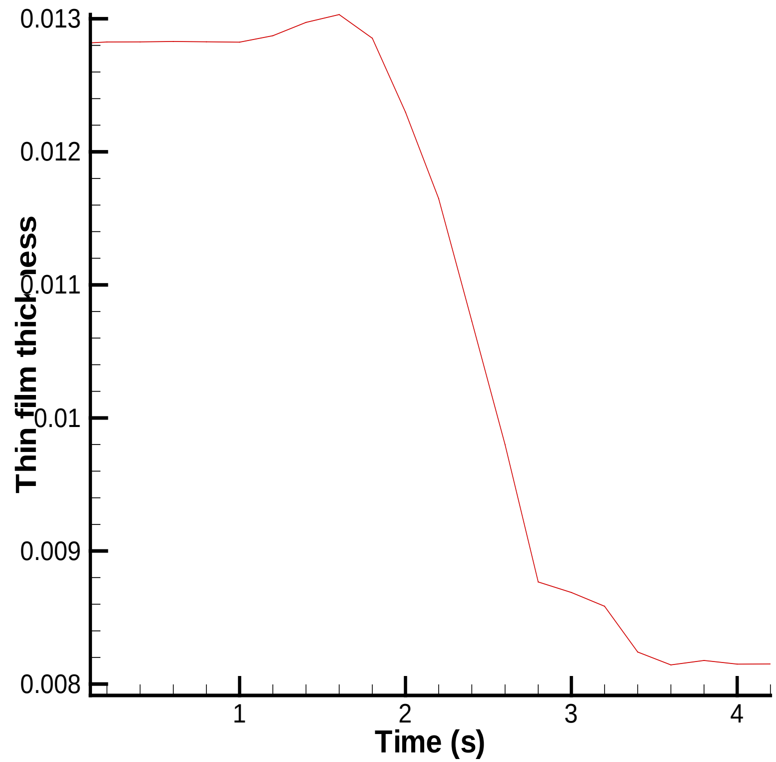
Bubble moving due to the change of capillary numbers from $\mathrm{Ca} = 0.001$ to 0.01 in the lab frame.

Thin Film Thickness Change



$Ca = 0.001 \rightarrow Ca = 0.5$

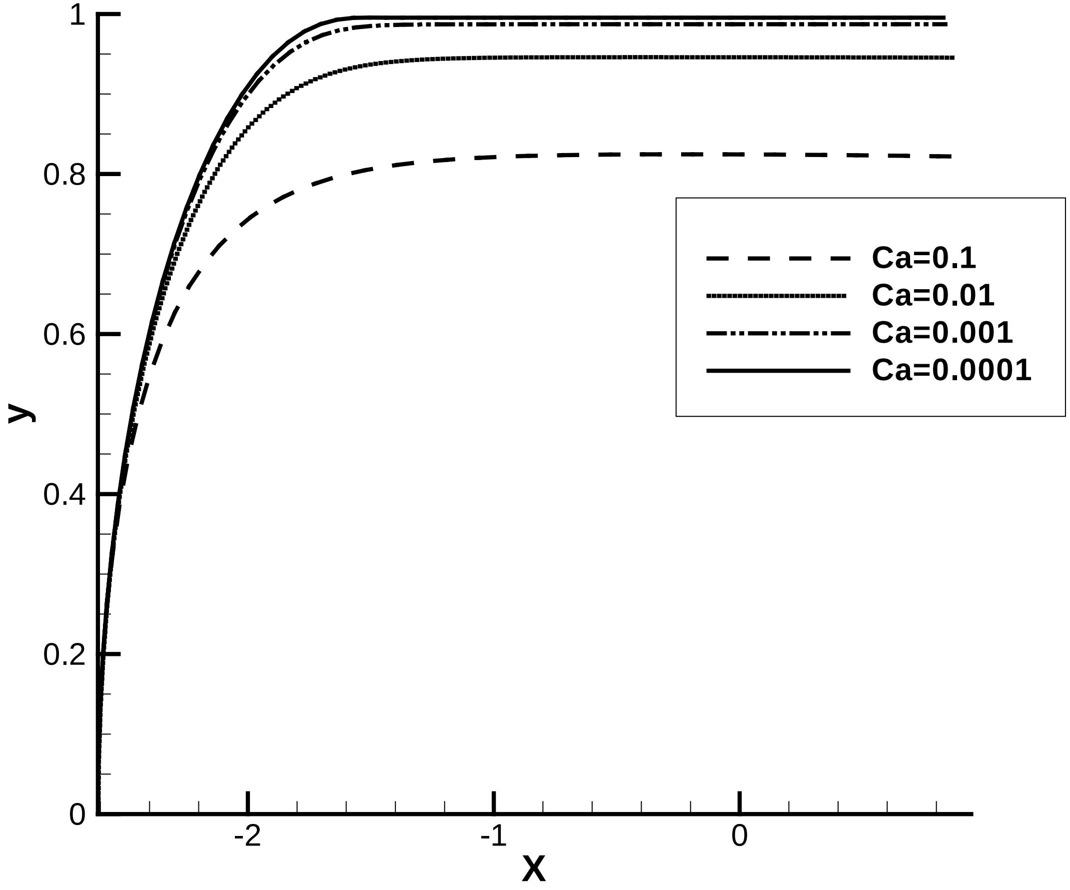
(a)



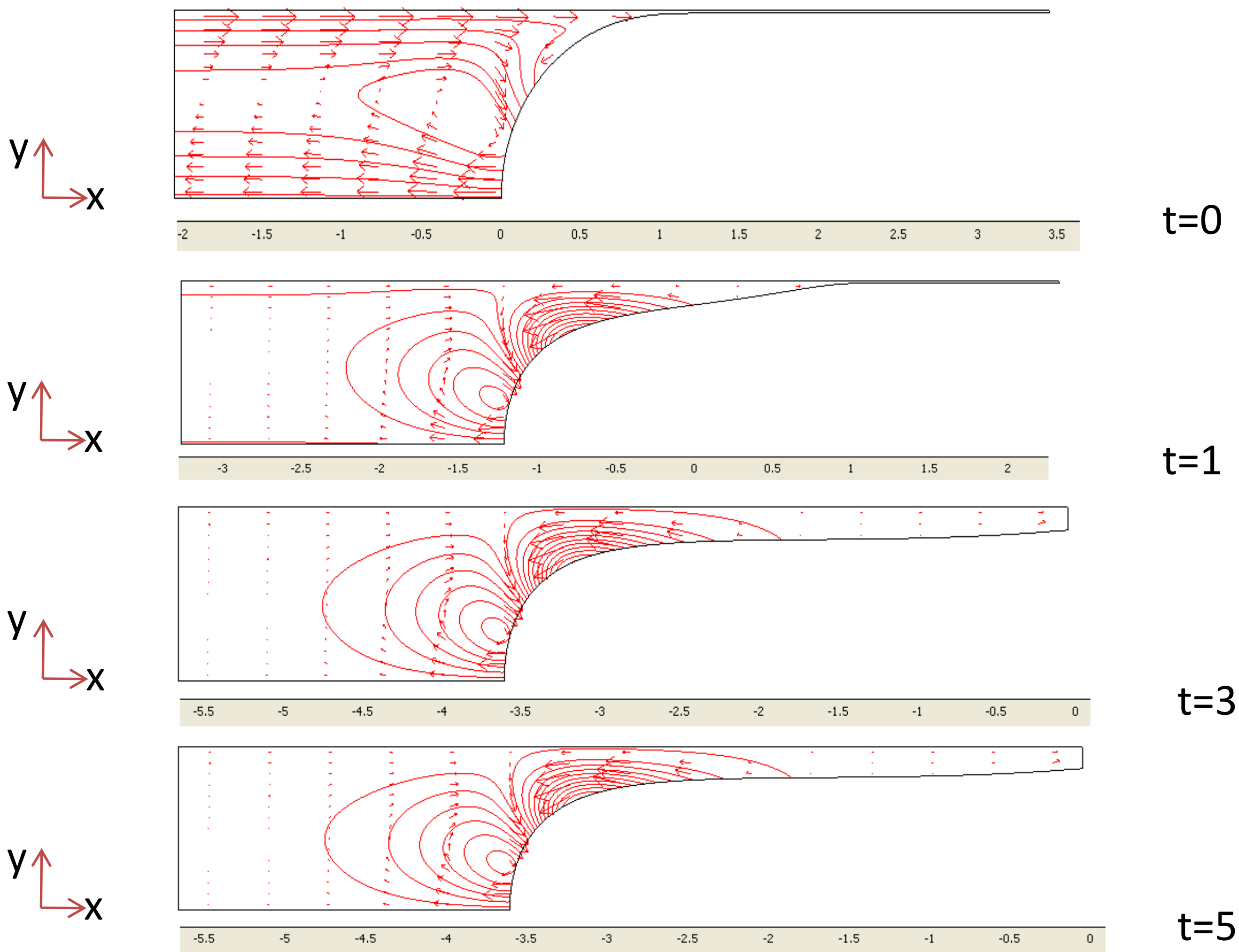
$Ca = 0.001 \rightarrow Ca = 0.0005$

(b)

Interface Change



Flow Field for Ca=0.001



Verification

- For small $Ca < 2\times10^{-3}$ Bretherton showed that

$$\delta \to 1.337 \cdot Ca^{2/3} \text{ as } Ca \to 0$$

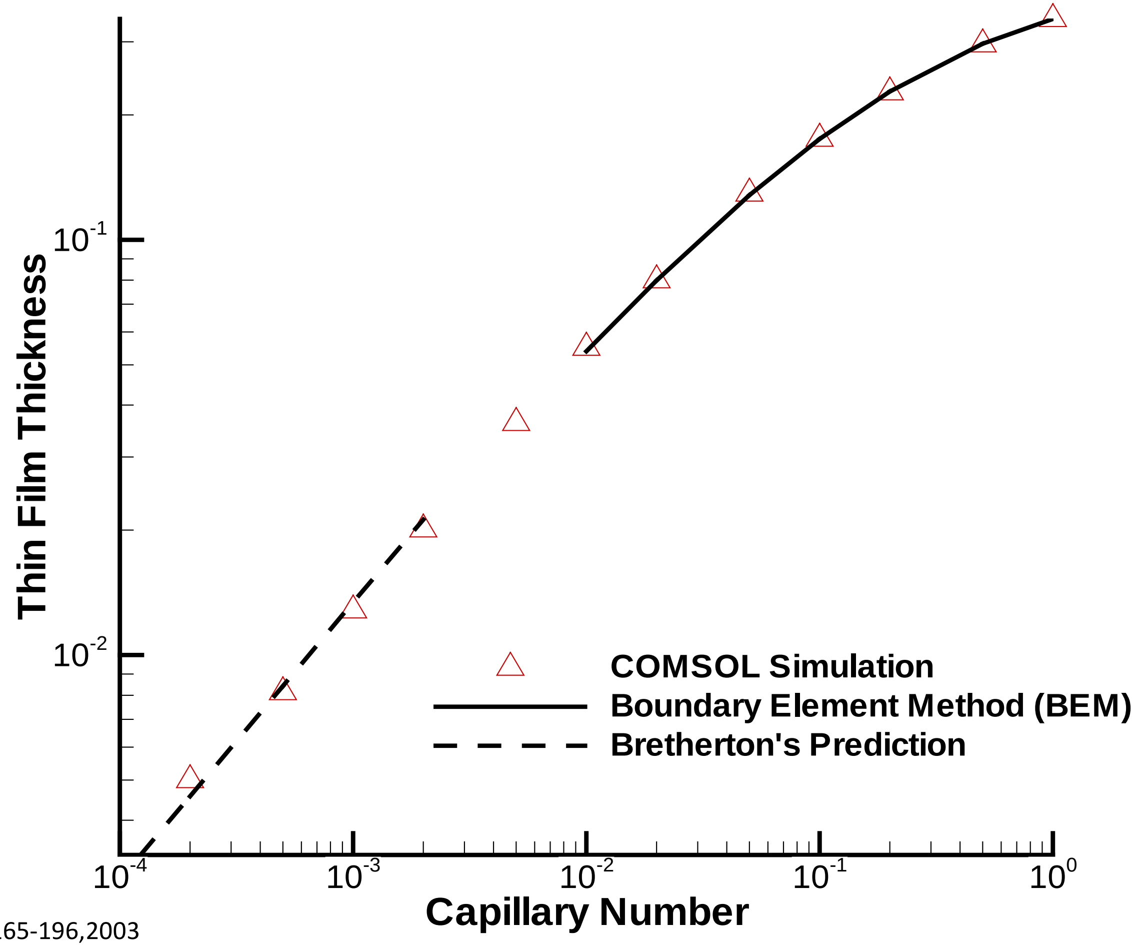
F.P.Bretherton. J. Fluid Mech. 10,166(1961)

Relative Error within 0.12%

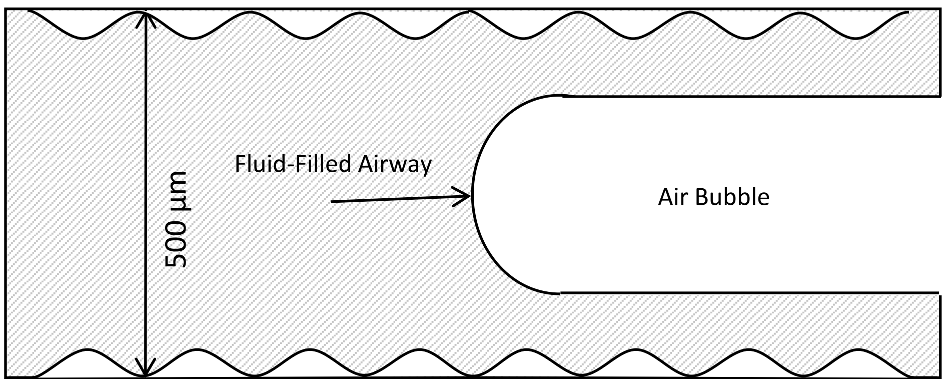
- For large $Ca > 10^{-2}$, we compare to BEM results

Relative Error within 0.15%

Ghadiali SN and Gaver DP 3rd, J. Fluid Mech. 478:165-196,2003



Application and Ongoing Work



Add cells and develop a fully coupled fluid and structure interaction model to assess how distortion of the air liquid interface.

Quantify cellular stress and strain under airway reopening conditions through the use of the models.

Acknowledgement

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