Mathematical Exploration of New Ideas Surrounding Capillarity Understanding in Science (M.E.N.I.S.C.U.S.)

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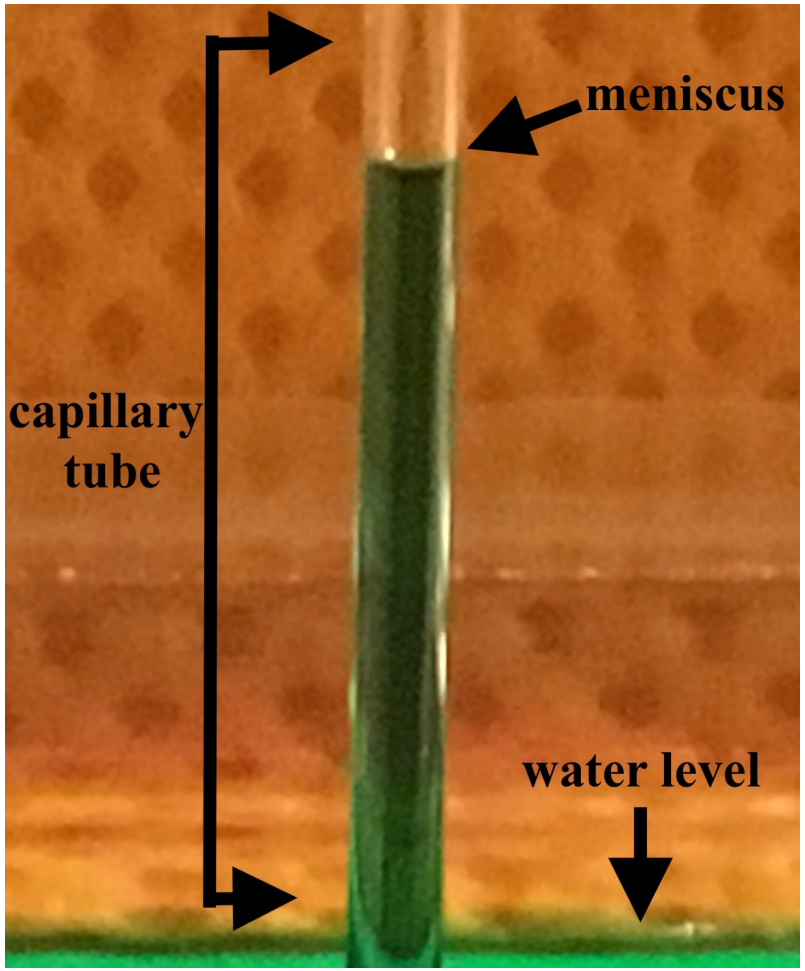
April 30, 2021

Overview

- Capillary Action: Dynamics of Fluid Rise and Porous Media
- Literature: Mixture Theory, Lago & Araujo, Brooks & Corey
- Quasi-Steady Model: Theory, Algorithm, and Results
- Unsteady Flow
- Ideas Moving Forward

What is Capillary Action?

- Fluid molecules stick to their container and to each other.
- This creates **surface tension**.
- Fluid rises through its container.
- Can happen in a **tube** or a **porous material**.



Capillary Dynamics

Navier-Stokes Equations (circa 1821)

$$\rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u}\right) = -\nabla P + \mu\nabla^2\vec{u} + \rho\vec{g}$$

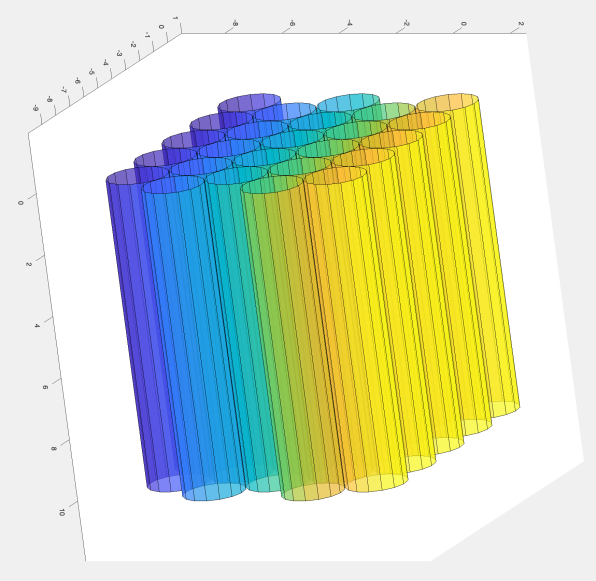
$$\nabla\cdot\vec{u} = 0$$

- We can add extra restrictions and boundary conditions to model capillary action in a tube.
- Let h be the **capillary height**.

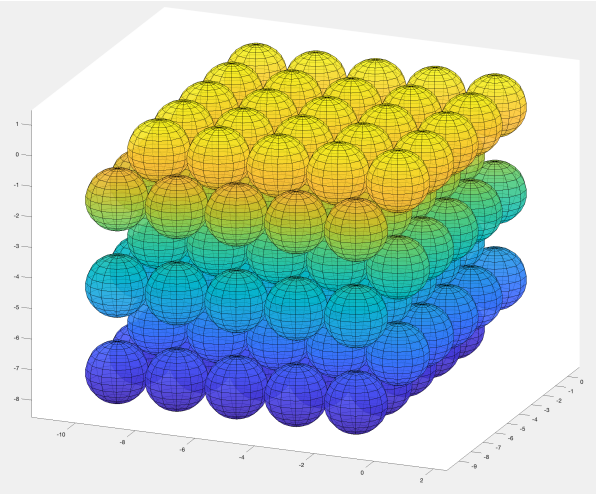
Washburn Equation (1921)

$$h(t) = \sqrt{Dt}, \text{ where } D := \frac{\gamma r\cos\theta}{2\mu}$$

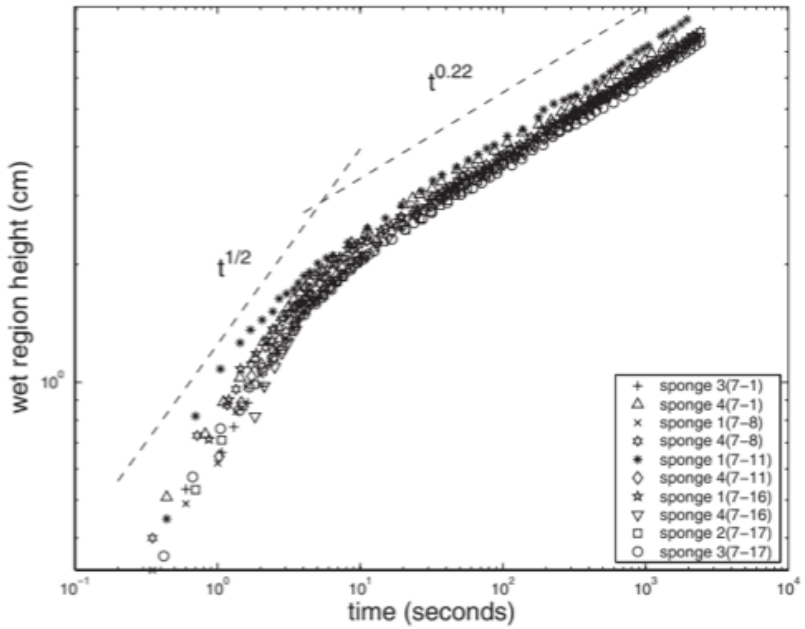
Porous Materials



Washburn[5]: **tube bundle** model



Lago and Araujo[3]: **regular sphere packing** model



Siddique, Anderson, and Bondarev[4]

- Washburn's $t^{1/2}$ model effective for small t
- Experimental results suggest different power law for longer t
- Lago and Araujo's sphere packing model more accurate for longer t

Mixture Theory

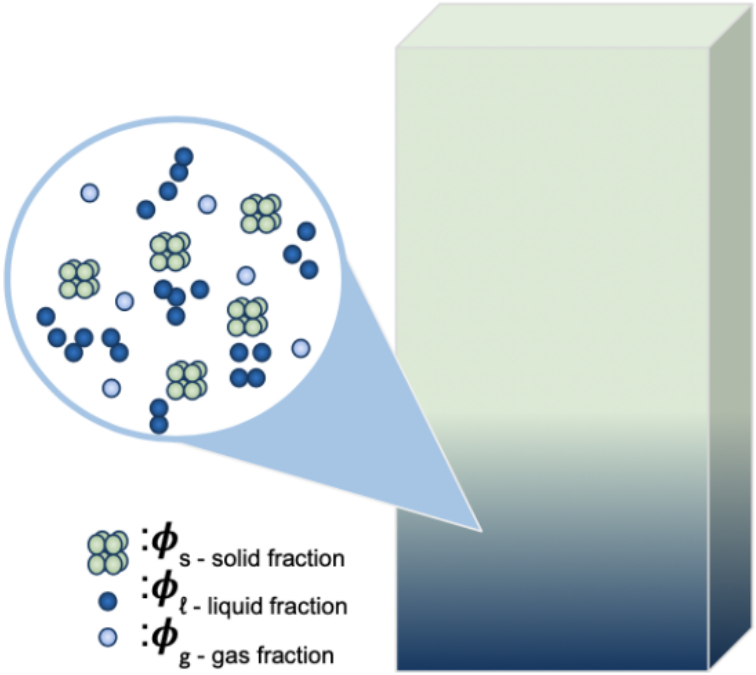


Figure: A partially saturated sponge.

- treats a point in the porous media as a small volume containing some proportion of solid, liquid, and gas.
- define fluid velocity and pressure at each point

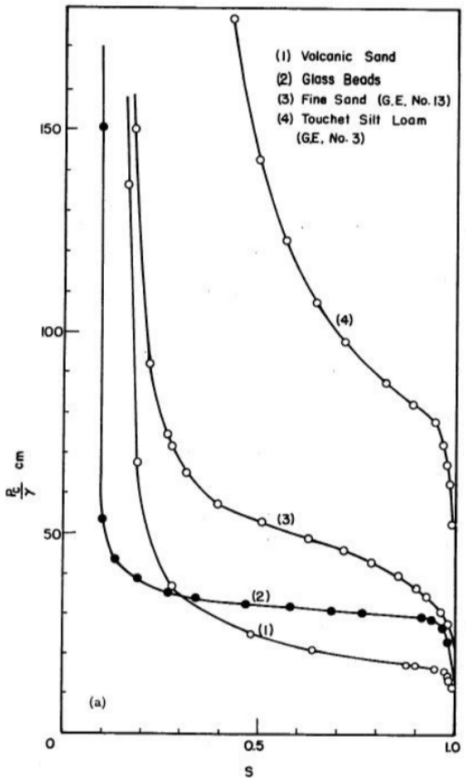
Saturation of Porous Media

$$\phi_\ell + \phi_s + \phi_g = 1$$

$$S := \frac{\phi_\ell}{1 - \phi_s}$$

Brooks & Corey (1964): Background

- investigation of drainage and irrigation models
- Earlier models neglected partial saturation and air/water pressure differential
- assumes flow of immiscible gas/liquid phases within continuous porous network



- Materials studied: Volcanic Sand, Fine Sand, Glass Beads, Silt Loam, Sandstone, and Clay/Sandstone/Sand mixture
- Figure: Capillary Pressure versus Saturation. Note asymptotic behavior as $S \to S_r$

Brooks & Corey (1964): Models

Capillary Pressure

$$p_c(S) = p_c^0 \left(\frac{1 - S_r}{S - S_r} \right)^{1/\lambda}$$

Relative Permeability (Burdine Equations)

$$k_{r\ell}(S) = \left(\frac{S - S_r}{1 - S_r} \right)^{3+2/\lambda}$$

- $S :=$ saturation
- $S_r :=$ residual saturation constant
- $\lambda :=$ pore size distribution index

Mixture Theory

- Assume only **vertical flow**
- **Mass Balance:**

$$\frac{\partial \phi_\ell}{\partial t} = -\frac{\partial}{\partial z}(w_\ell \phi_\ell)$$

- **Momentum Balance (Darcy's Law):**

$$\frac{\partial p_c}{\partial z} = \frac{K_{s\ell}}{\phi_\ell} w_\ell + \Delta\rho g$$

- Hence:

$$w_\ell = \frac{\phi_\ell}{K_{s\ell}} \left(\frac{\partial p_c}{\partial z} - \Delta\rho g \right)$$

$$\boxed{\frac{\partial \phi_\ell}{\partial t} = -\frac{\partial}{\partial z} \left[\frac{\phi_\ell^2}{K_{s\ell}} \left(\frac{\partial p_c}{\partial z} - \Delta\rho g \right) \right]}$$

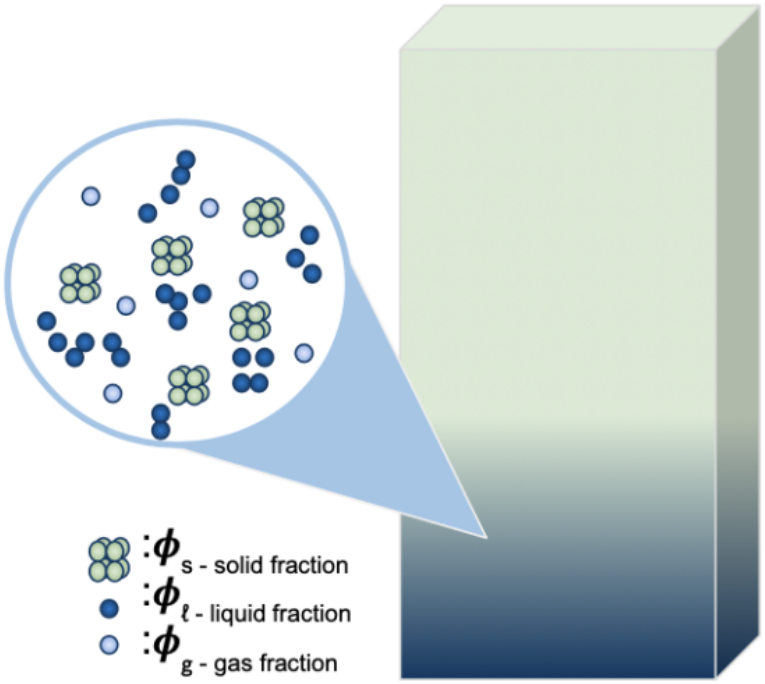


Figure: A partially saturated sponge.

- w_ℓ: liquid velocity
- $\Delta\rho = \rho_\ell - \rho_g$: density difference
- $p_c = p_\ell - p_g$: capillary pressure
- $K_{s\ell}$: friction coefficient ($\propto k_{r\ell}^{-1}$)

Mixture Theory (Cont.)

- Let h_ℓ be the **height** of the liquid fraction:

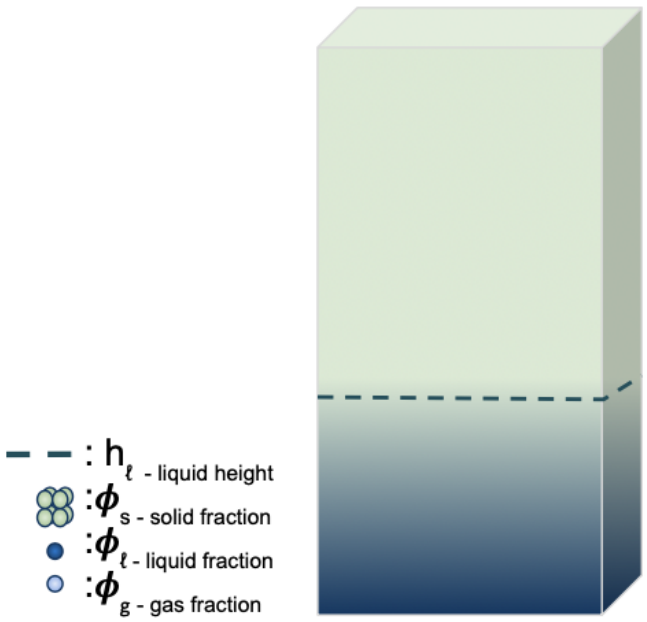
$$\frac{dh_\ell}{dt} = w_\ell(z = h_\ell)$$

$$\boxed{\frac{dh_\ell}{dt} = \frac{\phi_\ell}{K_{s\ell}} \left(\frac{\partial p_c}{\partial z} - \Delta\rho g \right) \Bigg|_{z=h_\ell}}$$

- Boundary Conditions:

$$\phi_\ell(z = 0) := \phi_\ell^0$$

$$\phi_\ell(z = h_\ell) := \phi_\ell^1$$



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Nondimensionalization

Let's **nondimensionalize** this:

$$z = \left(\frac{p_c(\phi_\ell^0)}{\Delta\rho g}\right)\bar{z}, \qquad t = \frac{\mu}{k_0 p_c(\phi_\ell^0)}\left(\frac{p_c(\phi_\ell^0)}{\Delta\rho g}\right)^2 \bar{t},$$

$$h_\ell(t) = \left(\frac{p_c(\phi_\ell^0)}{\Delta\rho g}\right)\bar{h}_\ell(t), \quad p_c(\phi_\ell) = \left(\frac{1}{p_c(\phi_\ell^0)}\right)\bar{p}_c(\phi_\ell)$$

Dimensional Forms $\Longrightarrow$ **Dimensionless Forms**

$$\frac{\partial \phi_\ell}{\partial t} = -\frac{\partial}{\partial z}\left[\frac{\phi_\ell^2}{K_{s\ell}}\left(\frac{\partial p_c}{\partial z} - \Delta\rho g\right)\right] \Longrightarrow \frac{\partial \phi_\ell}{\partial \bar{t}} = \frac{\partial}{\partial \bar{z}}\left[k_{r\ell}(\phi_\ell)\left(-\frac{\partial \bar{p}_c}{\partial \phi_\ell}\frac{\partial \phi_\ell}{\partial \bar{z}} + 1\right)\right]$$

$$\frac{dh_\ell}{dt} = \frac{\phi_\ell}{K_{s\ell}}\left(\frac{\partial p_c}{\partial z} - \Delta\rho g\right)\Bigg|_{z=h_\ell} \Longrightarrow \frac{d\bar{h}_\ell}{d\bar{t}} = -\frac{k_{r\ell}(\phi_\ell)}{\phi_\ell}\left(-\frac{\partial \bar{p}_c}{\partial \phi_\ell}\frac{\partial \phi_\ell}{\partial \bar{z}} + 1\right)\Bigg|_{\bar{z}=\bar{h}_\ell}$$

Quasi-steady Flow

- Goal: Solve for $\bar{h}_\ell(t)$

$$\frac{\partial \phi_\ell}{\partial \bar{t}} = \frac{\partial}{\partial \bar{z}}\left[k_{r\ell}(\phi_\ell)\left(-\frac{\partial \bar{p}_c}{\partial \phi_\ell}\frac{\partial \phi_\ell}{\partial \bar{z}} + 1\right)\right]$$

$$\frac{d\bar{h}_\ell}{d\bar{t}} = -\frac{k_{r\ell}(\phi_\ell)}{\phi_\ell}\left(-\frac{\partial \bar{p}_c}{\partial \phi_\ell}\frac{\partial \phi_\ell}{\partial \bar{z}} + 1\right)\Bigg|_{\bar{z}=\bar{h}_\ell}$$

- Assume flow is **quasi-steady**, i.e. $\dfrac{\partial \phi_\ell}{\partial \bar{t}} = 0$

$$0 = \frac{\partial}{\partial \bar{z}}\left[k_{r\ell}(\phi_\ell)\left(-\frac{\partial \bar{p}_c}{\partial \phi_\ell}\frac{\partial \phi_\ell}{\partial \bar{z}} + 1\right)\right]$$

$$\boxed{\begin{aligned} C(\bar{t}) &= k_{r\ell}(\phi_\ell)\left(-\frac{\partial \bar{p}_c}{\partial \phi_\ell}\frac{\partial \phi_\ell}{\partial \bar{z}} + 1\right) \\ \frac{d\bar{h}_\ell}{d\bar{t}} &= -\frac{C(\bar{t})}{\phi_\ell}\Bigg|_{\bar{z}=\bar{h}_\ell} = -\frac{C(\bar{t})}{\phi_\ell^1} \end{aligned}}$$

Brooks & Corey Model

According to Brooks & Corey:

$$p_c(S(\phi_\ell)) = p_c^0 \left(\frac{1-\phi_s}{1-S_r}\phi_\ell + \frac{-S_r}{1-S_r} \right)^{-1/\lambda} =: \textbf{Capillary Pressure}$$

$$k_{r\ell}(S(\phi_\ell)) = \left(\frac{1-\phi_s}{1-S_r}\phi_\ell + \frac{-S_r}{1-S_r} \right)^{3+2/\lambda} =: \textbf{Relative Permeability}$$

$$-\frac{\partial \bar{p}_c}{\partial \phi_\ell} = \alpha\gamma(\alpha\phi_\ell + \beta)^{-1-\gamma}$$

$$k_{r\ell}(\phi_\ell) = (\alpha\phi_\ell + \beta)^{3+2\gamma}$$

Integration

- Plug these functions into our equation:

$$C(\bar{t}) = k_{r\ell}(\phi_\ell)\left(-\frac{\partial \bar{p}_c}{\partial \phi_\ell}\frac{\partial \phi_\ell}{\partial \bar{z}} + 1\right)$$

$$C(\bar{t}) = \alpha\gamma(\alpha\phi_\ell + \beta)^{2+\gamma}\frac{\partial \phi_\ell}{\partial \bar{z}} + (\alpha\phi_\ell + \beta)^{3+2\gamma}$$

- Separation of variables:

$$d\bar{z} = \frac{\alpha\gamma(\alpha\phi_\ell + \beta)^{2+\gamma}}{C(\bar{t}) - (\alpha\phi_\ell + \beta)^{3+2\gamma}}d\phi_\ell$$

$$h_\ell(\bar{t}) = \int_{\phi_\ell^0}^{\phi_\ell^1} \frac{\alpha\gamma(\alpha\phi_\ell + \beta)^{2+\gamma}}{C(\bar{t}) - (\alpha\phi_\ell + \beta)^{3+2\gamma}}d\phi_\ell$$

Numerical Simulation

$$\frac{d\bar{h}_\ell}{d\bar{t}} = -\frac{C(\bar{t})}{\phi_\ell^1} \tag{1}$$

$$h_\ell(\bar{t}) = \int_{\phi_\ell^0}^{\phi_\ell^1} \frac{\alpha\gamma(\alpha\phi_\ell + \beta)^{2+\gamma}}{C(\bar{t}) - (\alpha\phi_\ell + \beta)^{3+2\gamma}} d\phi_\ell \tag{2}$$

$$\phi_\ell(\bar{z} = 0) := \phi_\ell^0, \quad \phi_\ell(\bar{z} = \bar{h}_\ell) := \phi_\ell^1$$

- Let $F(\bar{h}_\ell) = C$ be the function given implicitly by (2)
- **Numerical approach:**

$\bar{t} \leftarrow \bar{t}_0; \quad \bar{h}_\ell(0) \leftarrow \bar{h}_\ell^0; \quad C(0) \leftarrow C_0$

```
While t̄ < t̄_max:
    h̄_ℓ ← h̄_ℓ − (C/φ_1)dt̄
    C ← F(h̄_ℓ)
    t̄ ← t̄ + dt̄
```

Zero Gravity

Suppose **gravity is negligible**, i.e. $g = 0$:

$$\textbf{Integrate:}\quad h_\ell(\bar{t}) = \int_{\phi_\ell^0}^{\phi_\ell^1} \frac{\alpha\gamma(\alpha\phi_\ell + \beta)^{2+\gamma}}{C(\bar{t}) - \cancelto{0}{(\alpha\phi_\ell + \beta)^{3+2\gamma}}}\, d\phi_\ell$$

$$\textbf{Substitute (1):}\quad C(\bar{t}) = \frac{\gamma(\alpha\phi_\ell^1 + \beta)^{3+\gamma} - \gamma(\alpha\phi_\ell^0 + \beta)^{3+\gamma}}{(3+\gamma)\bar{h}_\ell(\bar{t})}$$

$$\textbf{Solve ODE:}\quad \frac{d\bar{h}_\ell}{d\bar{t}} = -\frac{C(\bar{t})}{\phi_\ell^1} = \frac{\gamma(\alpha\phi_\ell^0 + \beta)^{3+\gamma} - \gamma(\alpha\phi_\ell^1 + \beta)^{3+\gamma}}{\phi_\ell^1(3+\gamma)\bar{h}_\ell(\bar{t})}$$

$$\boxed{\bar{h}_\ell(\bar{t}) = \sqrt{\bar{t}\left(\frac{\gamma(\alpha\phi_\ell^0 + \beta)^{3+\gamma} - \gamma(\alpha\phi_\ell^1 + \beta)^{3+\gamma}}{\phi_\ell^1(3+\gamma)}\right)}}$$

Equilibrium height

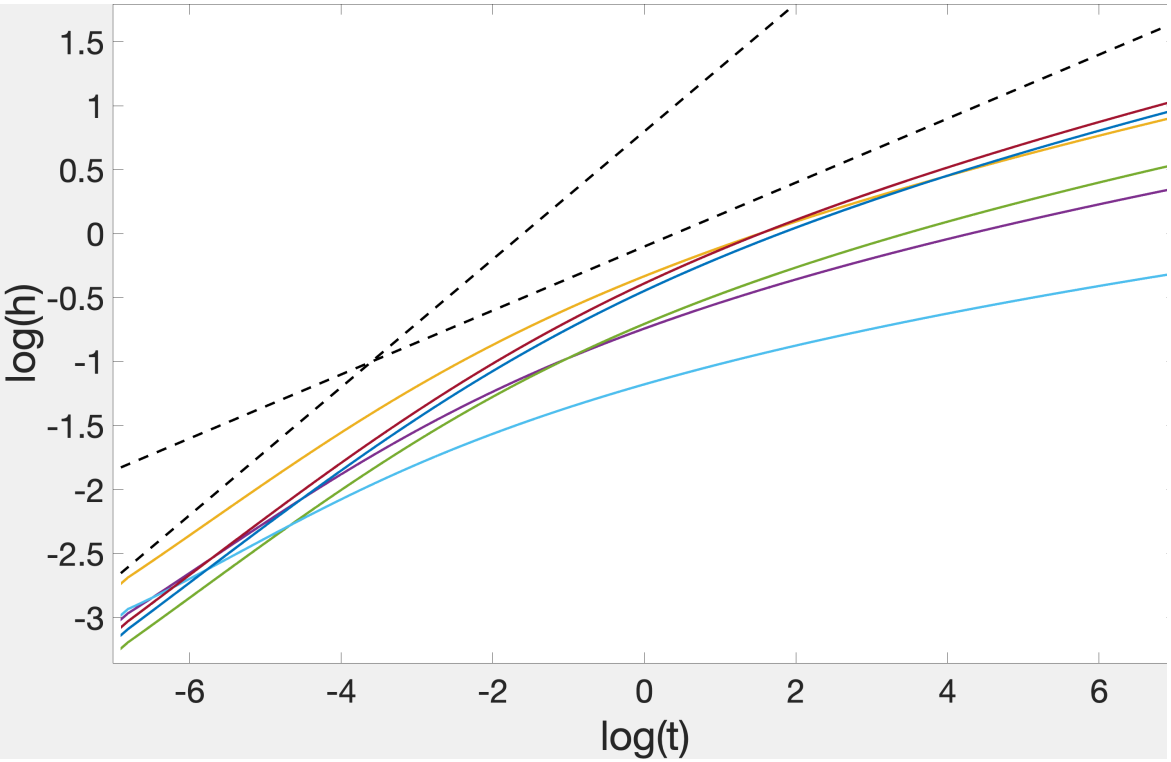
$$\frac{d\bar{h}_\ell}{d\bar{t}} = -\frac{C(\bar{t})}{\phi_\ell^1} = 0$$

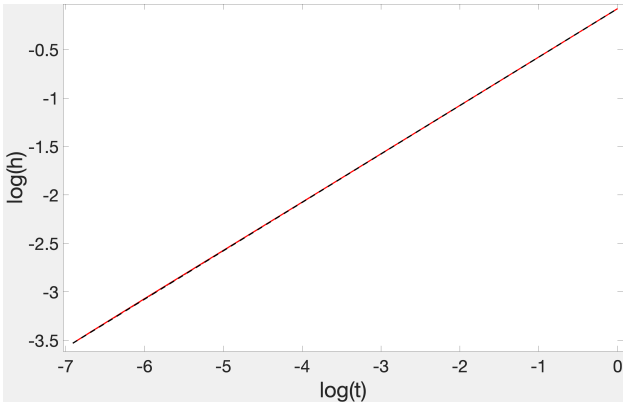
$$C(\bar{t}) = 0$$

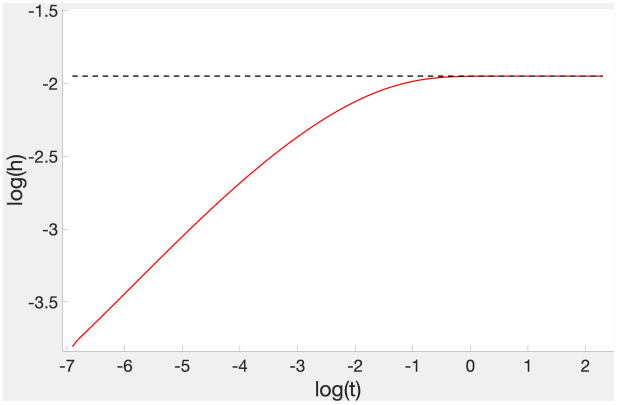
$$h_\ell^{eq} = \int_{\phi_\ell^0}^{\phi_\ell^1} \frac{\alpha\gamma(\alpha\phi_\ell + \beta)^{2+\gamma}}{\cancelto{0}{C(\bar{t})} - (\alpha\phi_\ell + \beta)^{3+2\gamma}} d\phi_\ell$$

$$\boxed{\bar{h}_\ell^{eq} = \frac{1}{(\alpha\phi_\ell^1 + \beta)^\gamma} - \frac{1}{(\alpha\phi_\ell^0 + \beta)^\gamma}}$$

Numerical Results



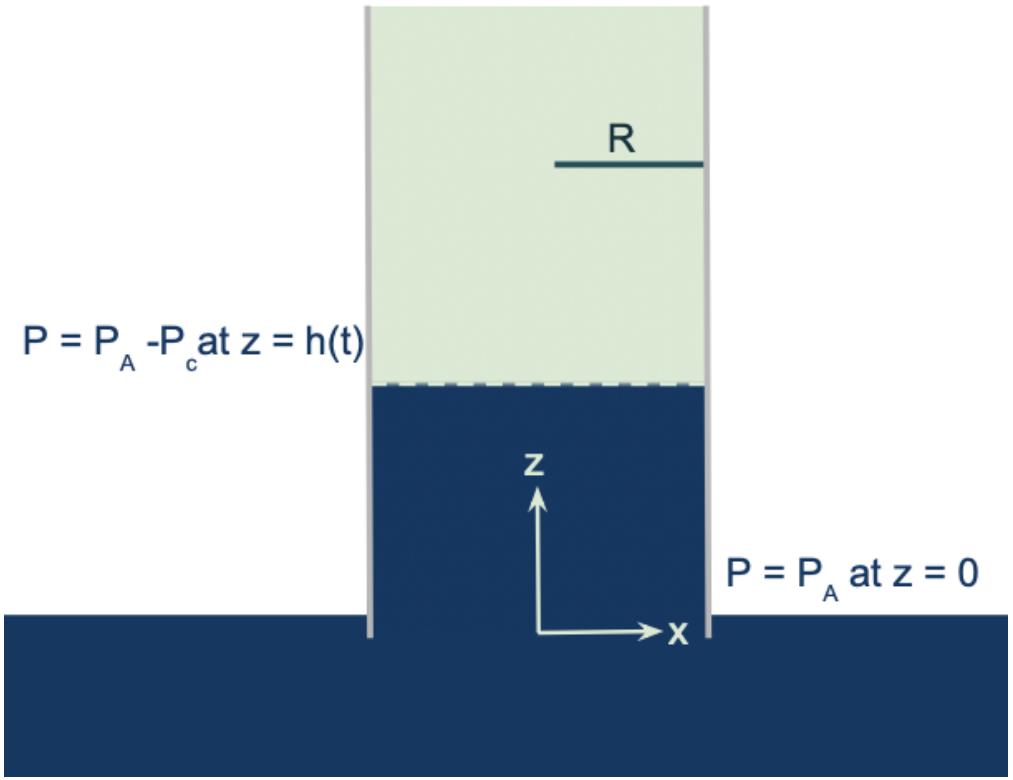




- Simulation behavior consistent with model in zero-gravity case
- Simulation equilibrium height consistent with model
- Similar shape as seen in experiments, but **no clear** $t^{1/2}$ **or** $t^{1/4}$ regimes

Numerical Simulation of Unsteady Flow

- We studied a problem involving the flow of a liquid confined between parallel walls.
- It is essentially a 2-dimensional problem, different from the 3-D problems of flow in tubes.
- Discretizing into a many distinct x-values allows us to convert the PDE into a system of many ODEs.
- zero gravity, but unsteady flow

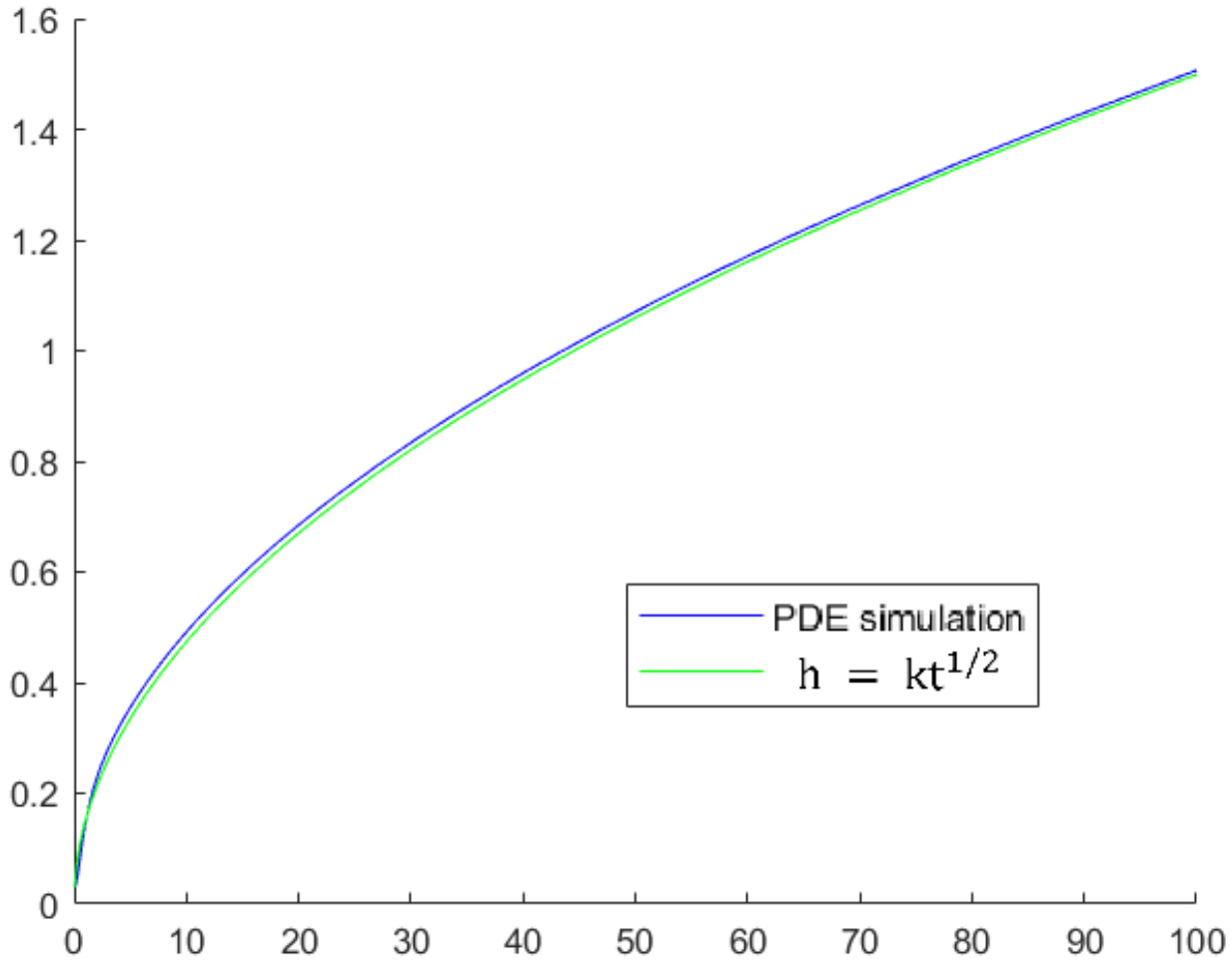


Assume that the meniscus is approximately flat, and that capillary pressure is constant

Numerical Simulation Details

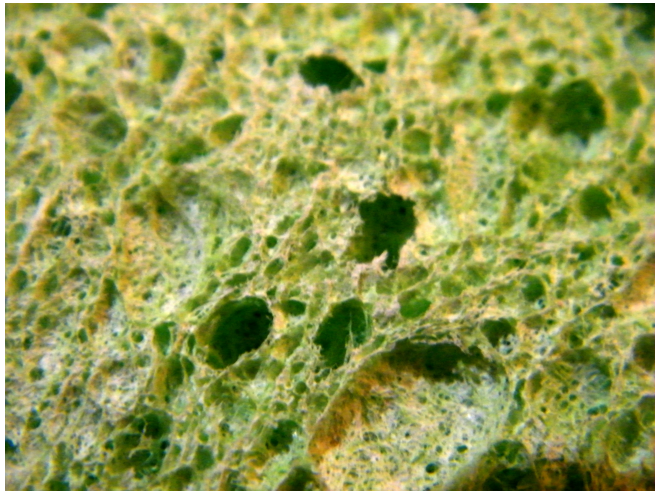
- Keep assumptions related to the Washburn-type model for parallel plates, but allow velocity to change over time.
- Assume that:

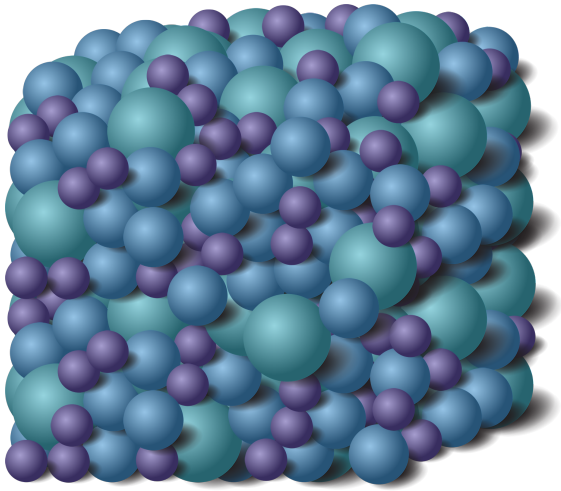
$$\frac{\partial P}{\partial z} = -\frac{P_C}{h(t)}$$



Future Work

- Further exploration using **numerical simulation**
- Use **asymptotic & perturbation methods** to find an analytic solution
- Attempt to solve without relying upon **quasi-steady assumption**
- Incorporate **material deformation**





Acknowledgements

We would like to thank our project mentor, Dr. Anderson. We would also like to thank Dr. Siddique, who joins us from Penn State; Matthew South, our Graduate Research Assistant; and MEGL for supporting our research.

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