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

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Overview

- Introduction to Capillary Rise
- Capillary Statics
 - Jurin's Law for Tubes
 - Complex Geometries
- Capillary Dynamics
 - Navier-Stokes Equations
 - Washburn's Solution and Improvements
- Classical Results and Experiments
- Future Directions

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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**.
- Can express the force as **capillary pressure** instead.





Capillary Statics

Jurin's Law for Tubes (circa 1718)

$$h_{eq} = \frac{2\gamma\cos(\theta)}{
ho gr} = \frac{P_c}{
ho gr}$$

- *h_{eq}* : equilibrium height of the fluid
- γ : surface tension coefficient
- θ : contact angle
- ρ : fluid density
- g : gravitational constant
- r : radius of tube
- P_c : capillary pressure

Obtained by solving $\sum \vec{F} = \vec{0}$



Capillary Statics: Complex Geometries

Goal: Find expressions for the vertical force and capillary pressure in terms of saturation.



2D Example: Fluid Area Bounded by Circles

 $F_V(S) = \pi \sigma (2R_0 \sin(\pi S) - I_0) \sin(\pi S + \theta)$

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Capillary Statics: Complex Geometries (Cont.)

Going from 2D to 3D, we make the transformation $S \mapsto \frac{S}{f(I_0, R_0)}$



3D example: Volume of Fluid Bounded by Spheres

$$F_V(S) = \pi \sigma \left(2R_0 \sin \left(\frac{\pi S}{f(l_0, R_0)} \right) - l_0 \right) \sin \left(\frac{\pi S}{f(l_0, R_0)} + \theta \right)$$
$$f(l_0, R_0) \approx \frac{7.7789R_0 - 3.4231}{l_0 - 1.53R_0} - 0.35066R_0 + 1.2225$$

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- Washburn^[4]: **tube bundle** model
- Lago and Araujo^[2]: regular sphere packing model (more accurate)
- Use geometry to find capillary pressure and equilibrium height.
- [2] considers one packing, but there are several more.



Regular Sphere Packings



- Regular packings made of **unit cells**.
- First, calculate surface tension on a sphere.
- We can calculate P_c(φ) for a regular packing.

•
$$h_{eq} = \frac{P_c^{\min}}{\rho g}$$



Regular Sphere Packings (Cont.)

Packing Type	Unit Cell	APF ^[5]	P _c
Simple Cubic		52.36%	$\frac{\pi\sin\phi\sin(\phi+\theta)}{4-\pi\sin^2\phi}\cdot\frac{2\gamma}{R}$
BCC		68.02%	$\frac{\pi\sin\phi\sin(\phi+\theta)}{\frac{16}{3}-\pi\sin^2\phi}\cdot\frac{2\gamma}{R}$
FCC		74.05%	$\frac{\pi \sin \phi \sin(\phi + \theta)}{4 - \pi \sin^2 \phi} \cdot \frac{2\gamma}{R}$
HCP		74.05%	$rac{\pi\sin\phi\sin(\phi+ heta)}{2\sqrt{3}-\pi\sin^2\phi}\cdotrac{2\gamma}{R}$

Reminder:
$$P_c = \cos \theta \cdot \frac{2\gamma}{R}$$
 for a tube.

Capillary Tube: Fluid Dynamics

Navier-Stokes Equations (circa 1821)

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

(2)

(1)

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

- \vec{u} : fluid velocity P: fluid pressure t: time ρ : density
- μ : viscosity \vec{g} : gravity

- (1) is $m\vec{a} = \vec{F}$ applied to fluids.
- (2) means the fluid is incompressible.
- We can add extra restrictions and boundary conditions to model capillary action.

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Capillary Dynamics in Porous Materials

Washburn Equation (1921)

$$h(t)=\sqrt{Dt}, ext{ where } D:=rac{\gamma r\cos heta}{2\mu}$$

- Navier-Stokes solved for capillary tube
- Extends to bundles of tubes
- Square root function for *h*(*t*) also models flow between two parallel plates.

• Assumptions:

- One-dimensional flow
- Approximately steady flow
- Constant capillary pressure
- Gravity is negligible.
- No-slip condition and conservation of mass



h

- Remove the assumption that the velocity is constant over time.
- The pressure gradient does not depend on the position coordinates but can depend on time.

• Special case: Assume a constant pressure gradient $\frac{\partial P}{\partial z} = -G$.

• More complex case: Assume $\frac{\partial P}{\partial z} = -\frac{P_C}{h(t)}$.

Under a constant pressure gradient the solution is

$$w(r,t) = \frac{G - \rho g}{4\mu} (R^2 - r^2)$$

$$- \frac{2(G - \rho g)R^2}{\mu} \sum_{n=1}^{\infty} \frac{1}{\lambda_n^3 J_1(\lambda_n)} J_0\left(\lambda_n \frac{r}{R}\right) e^{-\lambda_n^2 \frac{\mu}{\rho R^2} t}$$

$$h(t) = \frac{(G - \rho g)R}{3\mu} t$$

$$+ \frac{2\pi\rho(G - \rho g)R^3}{\mu^2} \sum_{n=1}^{\infty} \frac{1}{\lambda_n^5} H_0(\lambda_n) \left(e^{-\lambda_n^2 \frac{\mu}{\rho R^2} t} - 1\right)$$

where w is the velocity distribution and h is the height of the fluid.

Integro-Differential Equations for Extended Washburn

Assume
$$\frac{\partial P}{\partial z} \equiv -\frac{P_C}{h(t)}$$
.

The system is given by

$$\frac{\partial w}{\partial t} - \frac{1}{\rho} \frac{P_C}{h(t)} - \frac{\mu}{\rho} \frac{\partial}{\partial r} \left(r \frac{\partial w}{\partial r} \right) + g = 0$$
$$\frac{dh}{dt} - \frac{2}{R^2} \int_0^R w(r, t) r dr = 0$$
$$w(R, t) = 0$$
$$w(r, 0) = 0$$
$$h(0) = 0$$

Numerical Simulation of Unsteady Flow

- We studied an analogous 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.



Numerical Simulation Details

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

• Assume that:





Experiments: Unsteady Flow



Unsteady Flow in a Magic Eraser

- 1% food coloring in DI water solution
- Fluid reservoirs at different heights joined by plastic tubing
- In general: $h \propto t^p$
- Power law least-squares approximation:

 $p \approx 0.2322$

Experiments: Classical Results



Lago and Araujo (2000) Oil, Glass Column, Sand Packing



Water, Sponge

Experiments: Different Porous Materials



















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Experiments: Different Porous Materials

Method used: tap water in stationary fluid reservoir



Experiments: Different Fluids

 $\begin{array}{ll} \mbox{Method used: 1\% food coloring in DI water, oil in stationary fluid reservoir} \\ H_{eq(oil)} \approx 7.5 mm & H_{eq(water)} \approx 24 mm & p_{water} \approx 0.1772 \end{array}$



Ideas Moving Forward

- Mixture Theory: How liquids and gases permeate a material
- **Deformable Materials:** How material expansion and deformation affect capillarity
- More Simulations: Numerically solve the problem of unsteady flow in a tube, like we did for parallel plates
- Random Sphere Packings: A better approximation for porous materials





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