CHEM420 Selected Topics in Analytical Chemistry

Analytical Applications of Microfluidics

Lecture 3: Flow in Idealized Devices

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Outline

Poiseuille Flow

Fluidic Circuits

Summary of Lecture 2

- **Continuity Equation** and **Navier-Stokes Equations** represent *conservation of mass* and *Newton's Second Law*, respectively for fluids.

$$\nabla \cdot \boldsymbol{v} = 0 \quad \text{Continuity Equation for Incompressible Fluid}$$

$$\underbrace{\rho(\partial_t \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v})}_{\text{inertial terms}} = \underbrace{-\nabla p + \eta \nabla^2 \boldsymbol{v}}_{\text{forcing terms}} \quad \text{N.S. Equation (no body forces)}$$

- Reynolds number $\mathrm{Re} = \frac{\rho V_0 L_0}{\eta}$ is ratio of **inertial** to **viscous** forces.
  - $\mathrm{Re} < 1$ - laminar (ordered) flow
  - $\mathrm{Re} \gg 1$ - turbulent (chaotic) flow. Roughly 2000 for microfluidics
  - intermediate Re - inertial effects present, but not turbulence.
- Small scale and low fluid velocity in microfluidics means low Reynolds number and therefore laminar flow

Motivation: Toward Real Devices

We have an idea of what forces matter in microfluidics, but how does fluid actually respond?

We would like solutions $\boldsymbol{v}(r, t)$ to the Navier-Stokes equations for idealized device geometries (i.e. domains).

Today, we'll introduce

- Poiseuille Flow - pressure driven, steady state flow
- Hagen-Poiseuille Law - Ohm's Law for microfluidics. Hydraulic *resistance* and *capacitance* (compliance)

(On Wednesday we'll talk about mixing and numerical methods for understanding real devices.)

Poiseuille Flow

Definition Pressure-driven, steady state flow

Physical origin Fluid driven through long, straight channel by imposing Δp across channel

For selected channel geometries, can analytically solve Navier-Stokes equation to calculate steady-state velocity profile across channel. (For everything else, there's COMSOL. More later.)

Poiseiulle Flow: Problem Setup

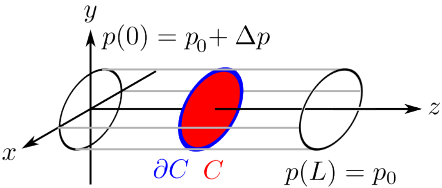
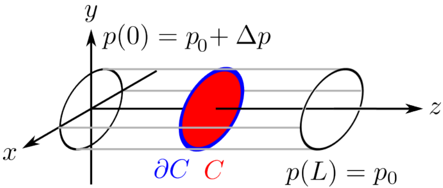


Figure: Circular channel of length L with pressure difference Δp across it. The cross-sectional area $\mathcal{C}$ is bounded by boundary $\partial\mathcal{C}$. (Adapted from Bruus.)

Assumptions:

- translation invariant along z-axis
- constant cross section
- **Pressure Boundary Conditions**: $p(0) = p_0 + \Delta p$ at inlet, $p(L) = p_0$ at outlet
- **Non-slip Boundary Conditions**: $\boldsymbol{v} = 0$ for $x, y \in \partial\mathcal{C}$

Poiseiulle Flow: Problem Setup



Simplifying Navier-Stokes equations...

- assume gravity $\boldsymbol{g}$ is balanced by hydrostatic pressure gradient in y-direction i.e. neglect $\rho \boldsymbol{g}$
- translational invariance in z and no net forces in xy plane suggest $\boldsymbol{v}$ is independent of z **and** only z-component is non-zero
  i.e. $\boldsymbol{v}(\boldsymbol{r}) = v_z(x, y)\boldsymbol{e}_z$
- This means convection term $(\boldsymbol{v} \cdot \nabla)\boldsymbol{v} = 0$ i.e. **laminar flow**! (We'll see later on that this is characterized by low Reynolds Number)

Wait, how is convection $(\boldsymbol{v} \cdot \nabla)\boldsymbol{v} = 0$?

Recall that $\boldsymbol{v}(\boldsymbol{r}) = v_z(x, y)\boldsymbol{e}_z$.

Write $\nabla \boldsymbol{v}$:

$$\nabla \boldsymbol{v} = \frac{\partial}{\partial x} v_z \boldsymbol{e}_x + \frac{\partial}{\partial y} v_z \boldsymbol{e}_y + \cancel{\frac{\partial}{\partial z} v_z}\, \boldsymbol{e}_z$$

Last term is zero due to translation invariance along z.

Write $\boldsymbol{v} \cdot \nabla \boldsymbol{v}$:

$$\boldsymbol{v} \cdot \nabla \boldsymbol{v} = v_x \frac{\partial}{\partial x} v_z \boldsymbol{e}_x + v_y \frac{\partial}{\partial y} v_z \boldsymbol{e}_y + v_z \cdot 0$$

But v_x and v_y are both 0! So

$$\boldsymbol{v} \cdot \nabla \boldsymbol{v} = 0$$

Simplifying the Navier-Stokes Equation

What cancels?

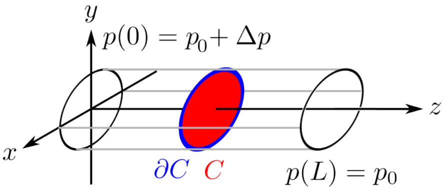
$$\rho(\cancel{\partial_t \boldsymbol{v}} + \cancel{(\boldsymbol{v} \cdot \nabla)\boldsymbol{v}}) = -\nabla p + \eta \nabla^2 \boldsymbol{v} + \cancel{\rho \boldsymbol{g}}$$

For Poiseiulle flow, can write steady-state Navier-Stokes equation:

$$0 = \eta \nabla^2 \boldsymbol{v} - \nabla p \qquad \text{(Stokes Equation)}$$

Need to figure out the pressure gradient...

Pressure Gradient Along z Only



We said earlier that v_x and v_y were zero because no force gradients in those directions. So pressure gradient only exists along z-axis i.e. $p(\boldsymbol{r}) = p(z)$.

Just need to write z-component of Stokes equation:

$$0 = \eta \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) v_z(x, y) - \frac{\partial p(z)}{\partial z}$$

Pressure Gradient is Linear

Rearranging last equation we have

$$\eta \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) v_z(x, y) = \frac{\partial p(z)}{\partial z}$$

Notice that LHS is $f(x, y)$ while RHS is $f(z)$! Only way for this to be true and non-zero is if both sides equal constant K.

This means that $p(z)$ is linear along z-axis! By integration, $p(z) = \frac{\Delta p}{L}(L - z) + p_0$ and $\partial p/\partial z = -\Delta p/L$

Equations To Be Solved - Finally!

To get analytical expression for $\boldsymbol{v}$ over cross-section $\mathcal{C}$ in Poiseiulle (pressure-driven) flow, need to solve second order PDE:

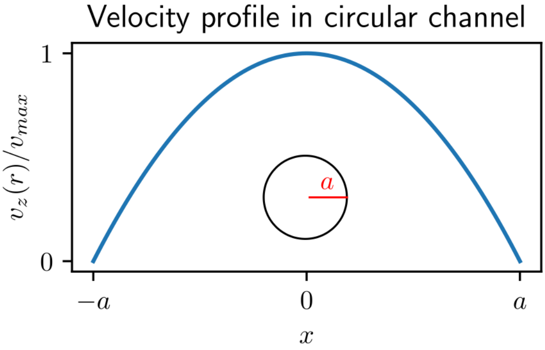
$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) v_z(x,y) = -\frac{\Delta p}{\eta L} \quad \text{for } (x,y) \in \mathcal{C} \qquad \text{(Stokes Equation)}$$

$$v_z(x,y) = 0 \quad \text{for } (x,y) \in \partial\mathcal{C} \qquad \text{(Non-Slip BC)}$$

Circular Channel

For channel of radius a and length L,

$$v_z(x, y) = -\frac{\Delta p}{4\eta L}(a^2 - x^2 - y^2)$$



Rectangular Channel

Surprisingly, no analytical solution exists! But we can write an approximate solution in terms of a Fourier Series

$$v_z(x, y) = \frac{4h^2 \Delta p}{\pi^3 \eta L} \sum_{n,\ \mathrm{odd}}^{\infty} \frac{1}{n^3} \left[1 - \frac{\cosh(n\pi \frac{x}{h})}{\cosh(n\pi \frac{w}{2h})} \right] \sin\left(n\pi \frac{y}{h} \right)$$

where L is length, h is height and w is width.

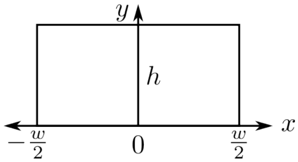
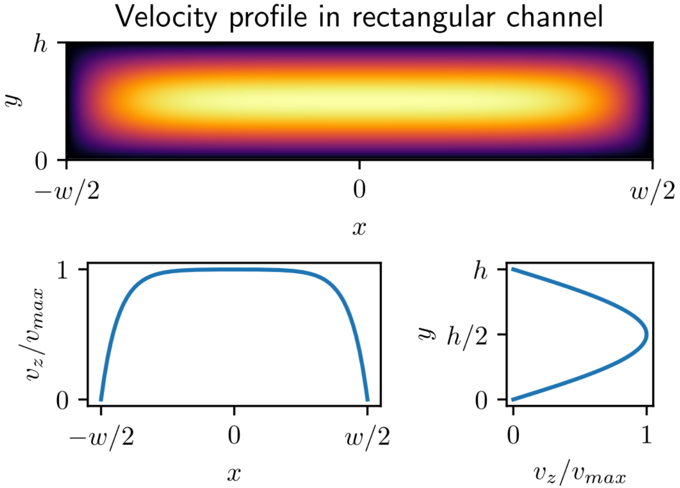


Figure: Rectangular channel geometry. Adapted from Bruus.

Rectangular Channel



Some Pitfalls

Distribution of fluid velocities in channel - dispersion in *residence time* for fluid elements

We can measure volumetric flow rate Q experimentally using a beaker and a timer. Dividing by cross sectional area gets us average linear flow velocity $\tilde{\boldsymbol{v}}$ **but** remember $\boldsymbol{v}(x, y) \neq \tilde{\boldsymbol{v}}$!

Volumetric Flow Rates

Found by integrating velocity profiles. Define Q as volumetric flow rate (units m^3/s)

$$
\begin{aligned}
Q_{circ} &= \frac{\pi}{8}\frac{a^4}{\eta L}\Delta p && \text{(Circular)} \\
Q_{rect} &= \frac{h^3 w \Delta p}{12\eta L}\left[1 - \sum_{n,\mathrm{odd}}^{\infty} \frac{1}{n^5}\frac{192}{\pi^5}\frac{h}{w}\tanh(n\pi\frac{w}{2/h})\right] && \text{(Rectangular)} \\
&\approx \frac{h^3 w \Delta p}{12\eta L}\left[1 - 0.630\frac{h}{w}\right] && \text{(for } h < w\text{)}
\end{aligned}
$$

Hagen-Poiseiulle Law

Notice from last slide we could write

$$\Delta p = \text{constant}(h, w, L, \eta) \cdot Q$$

Hagen-Poiseiulle Law wraps up the constant as the *hydraulic resistance*, R_{hyd}, in analogy to Ohm's Law for circuits:

$$\Delta p = R_{hyd} Q \qquad \text{(Hagen-Poseiulle Law)}$$

A constant pressure difference Δp results in constant volumetric flow Q *via* proportionality R_{hyd}. R_{hyd} depends on geometric factors (again, compare Ohm's Law)

What does this mean for us?

Can use Hagen-Poiseiulle Law to calculate Δp required for desired Q if we know R_{hyd}. Consequences for:

- sizing pressure controller / pump
- pressure source stability
- material choice (bond strength, stiffness)

Important to note that H.P. Law is only valid for $\mathrm{Re} \approx 0$.

Hydrodynamic Resistances for Common Geometries

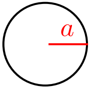
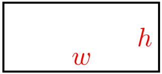
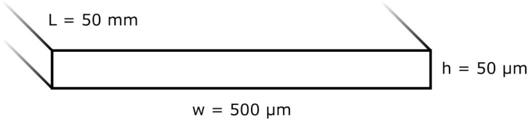
Shape	R_{hyd}	$R_{hyd}/\frac{Pa \cdot s}{m^3}$
	$\frac{8}{\pi}\eta L\frac{1}{a^4}$	254×10^9
	$\frac{12\eta L}{1-0.63(h/w)}\frac{1}{h^3 w}$	2049×10^9

Figure: Sample calculation shown for typical device dimensions. Assumes $a = 100$ µm, $w = 500$ µm, $h = 50$ µm, $l = 10$ mm, and $\eta = 1$ mPa (water at 25 °C).

Note that R_{hyd} is linear with L and η!

Example: Pressure required to drive flow



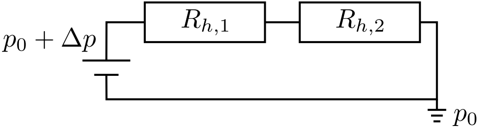
Example

Assume $w = 500$ µm, $h = 50$ µm, $L = 50$ mm. We want to flow at $Q = 1\ \mathrm{mL\,h^{-1}}$. What pressure is required? Assume $\eta_{H2O} = 1$ mPa s.

Answer: $R_{hyd} = 1.02 \times 10^{13}\ \mathrm{Pa\,s\,m^{-3}}$, $\Delta p = 2850$ Pa $= 28$ mbar

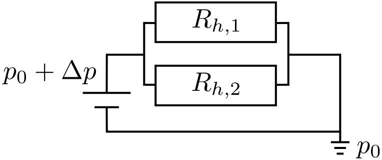
Adding Hydraulic Resistances

Assuming flow is laminar, can add R_{hyd} just like resistors. Let $R_{h,1}$ and $R_{h,2}$ be two hydraulic resistances.



Series

$$\Delta p = (R_{h,1} + R_{h,2})Q$$



Parallel

$$\Delta p = \left(\frac{1}{R_{h,1}} + \frac{1}{R_{h,2}}\right)^{-1} Q$$

Figure: Adding hydraulic resistances in series and parallel. (Adapted from Bruus.)

Bubbles are bad: Hydraulic Compliance

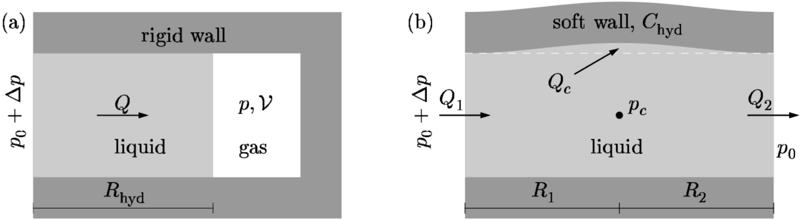


Figure: Compressible gas bubbles (left) or flexible walls (right) introduce hydraulic compliance. From Bruus.

Hydraulic compliance $C_{hyd} = -\partial\mathcal{V}/\partial p$ is analogous to capacitance in electrical circuits. Gas bubbles and deformable walls take time to "charge up" - compare RC charging time. Outcome is that microfluidic responds much slower to pressure changes!

Compressibility and compliance

Define *compressibility* K of gas bubble with volume $\mathcal{V}$ by

$$K_{bubble} = -\frac{1}{\mathcal{V}}\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}p}$$

where negative sign is chosen because bubble shrinks as pressure increases.

Define *dilatability* K for tube or device by

$$K_{tube} = \frac{1}{\mathcal{V}}\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}p}$$

where positive sign indicates tube or device volume expands as pressure increases.

Then hydraulic compliance can be calculated by $C_{hyd} = \mathcal{V}K$.

Example: Compressing a bubble

For a bubble with some initial volume $\mathcal{V}$ at atmospheric pressure p_0, and assuming small pressure deviations, $C_{hyd,bubble} \approx \mathcal{V}/p_0$

Example

Assume a bubble of equivalent diameter 500 μm is stuck in the channel from slide 21 (recall $R = 1.02 \times 10^{132}\ \mathrm{Pa\,s\,m^{-3}}$). What is the hydraulic compliance $C_{hyd,bubble}$ and RC charging time of the bubble?

Answer: $C_{hyd,bubble} = 6.48 \times 10^{-16}\ \mathrm{m^3\,Pa^{-1}}$, $5\tau = 33$ ms.

Dilatability of common materials

What happens if the channel material is compressible? Roughly, the dilatability of channel or tubing materials is related to Young's modulus E by

$$K \approx \frac{1}{E}$$

A table of common materials is below.

Material	**E (GPa)**	**K (1/Pa)**	**K (1/bar)**
steel	200	5×10^{-12}	5×10^{-7}
Si	150	6.7×10^{-12}	6.7×10^{-7}
glass	64	1.6×10^{-11}	1.6×10^{-6}
PMMA	3	3×10^{-10}	3×10^{-5}
PTFE	0.6	1.7×10^{-9}	1.7×10^{-3}
Tygon	0.007	1.4×10^{-7}	0.14
PDMS	0.002	5×10^{-7}	0.05

Example: Pressurizing a microfluidic channel

Example

Recall the device from slide 21 ($R = 1.02 \times 10^{13}$ Pa s m^{-3}). What is the compliance, C, and RC charging time if the device is made from

1. PDMS (soft silicone elastomer)
2. PMMA (hard thermoplastic)
3. glass

Answers:
$C_{PDMS} = 6.3 \times 10^{-16}$ m^3 Pa^{-1}, $5\tau = 32$ ms
$C_{PMMA} = 3.8 \times 10^{-19}$ m^3 Pa^{-1}, $5\tau = 19$ μs
$C_{glass} = 2.0 \times 10^{-20}$ m^3 Pa^{-1}, $5\tau = 1$ μs

Plumbing considerations

In the last slide we showed that the choice of material for our microfluidic affects time required for pressure to equilibrate in the device.

Must also consider the time constant of the inlet and outlet tubing.

Example

Tygon and PTFE are typical tubing materials in microfluidics. Assuming an inner diameter of $\phi = 1$ mm and total length $l = 50$ cm, for both materials calculate the tubing compliance and the system's RC charging time. *Hint: Pay attention to the total resistance of the system.*

Answers:
Tubing internal volume $\mathcal{V} = 3.9 \times 10^{-7}$ m^3, $R_{tube} = 2.0 \times 10^{10}$ Pa s m^{-3}
Tygon: $C_{tube,tygon} = 5.5 \times 10^{-14}$ m^3 Pa^{-1}, $5\tau = 2.8$ s
PTFE: $C_{tube,PTFE} = 6.7 \times 10^{-16}$ m^3 Pa^{-1}, $5\tau = 30$ ms

Consequences for analytical measurements

Why does any of this matter? Imagine we have a coupled analytical measurement which takes some measurement time Δt. We could measure...

- GC-MS at device outlet - $\Delta t \approx 10$ min
- FTIR FPA image - $\Delta t \approx 5$ min
- FTIR absorbance spectrum - $\Delta t \approx 1$ s - 1 min
- a CMOS image sensor - $\Delta t \approx 30$ ms

Depending on time it takes device to reach steady state, we may only be measuring useful data for fraction of experimental time!

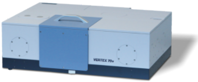



image credits: Agilent, Bruker, Zeiss

Design considerations for microfluidics

For fast device response times, it's good practice to

- avoid flexible tubing
- purge bubbles
- prefer solid construction materials

When designing for an analytical application, the engineering approach is to

- estimate measurement time and desired duty cycle
- draw equivalent circuit with key features
- estimate system τ from circuit
- choose appropriate materials

Lecture 3 Summary

- **Poiseuille Flow** - pressure driven, steady state flow
  - valid for $\mathrm{Re} \to 0$
  - **pressure boundary condition** imposes Δp across channel inlet and outlet
  - **non-slip boundary condition** means $\boldsymbol{v} = 0$ at all points on channel boundary
  - velocity varies across channel section! Distribution in residence times
- **Hagen-Poiseuille Law** is Ohm's law for fluidics

$$\Delta p = R_{hyd} Q$$

- **hydraulic resistance** related to channel cross section and length
- **hydraulic compliance** related to volume change of channel, tube, or bubble
- consider response time τ of system for given measurement technique