CHEM420 Selected Topics in Analytical Chemistry Analytical Applications of Microfluidics

Lecture 2: Fundamentals of Transport in Microfluidics

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Outline

Transport Phenomena

The Continuum Hypothesis

The Continuity Equation

Navier-Stokes Equations

The Reynolds Number and Fluid Flow Regimes

Summary of Lecture 01: Introduction to Microfluidics

- Microfluidics is the science and technology of systems which manipulate very small fluid volumes (approximately nanoliters or less) in microscale channels. Or, study of how fluid flows behave and how they can be controlled at the micron scale
- Development of academic field driven by broad trends in miniaturization: of analytical instrumentation, defense sensing applications, high-throughput molecular biology, and electronics
- Microfluidic technologies are mostly hidden from view. Examples include inkjet printing, point of care blood glucose monitoring, lipid nanoparticle synthesis, and oilfield analytics
- Modern microfluidic research is in fundamental aspects of fluid flow (more today!), materials science, miniaturizing analytical methods, sample handling and preparation, and device integration

Motivation: Understanding Transport Phenomena



In Lecture 1, we were introduced to four successful microfluidic technologies. Each exploited an aspect of fluid flow to achieve an analytical or processing goal:

- ► Surface tension driven droplet breakup for precise inkjet printing
- ► Capillary filling of an electrochemical cell for quantitative blood glucose measurement
- ► Rapid, reproducible mixing of reagents for RNA/lipid nanoparticle synthesis
- ► Flow properties which mimic enhanced oil recovery conditions

Understanding transport phenomena is central to microfluidic design

What do we mean by Transport Phenomena?

The mathematical description of the movement of *momentum*, *mass*, and *energy* is unified by the study of **transport phenomena**.

In microfluidics, we are concerned with

- ► Fluid Mechanics/Dynamics How fluids flow under the action of applied forces
- Mass Transport How molecules move through fluids by diffusion, advection, and migration
- ► Energy Transfer Primarily heat transfer from integrated heaters, exo/endothermic reactions (Not so much in this short module.)

A Quick Orientation

We're going to get into some Intense Math, so here's a quick roadmap.

The governing equations for fluid mechanics are called the **Continuity Equation** and the **Navier-Stokes Equations**. They're basically statements of *conservation of mass* and *Newton's Second Law* but for fluids. To derive them, we will

- treat fluids as continuous media described by vector fields
- \blacktriangleright work in terms of *volumetric properties* like density ρ and force density f

Ultimately, we'll see that in most situation in microfluidics we can use the much simpler **Stokes Equation**.

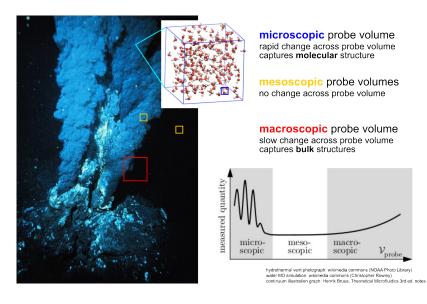
Fluid mechanics treat continuous media

A *fluid* is a chunk of matter with no fixed shape. Can be liquid (fixed volume) or gas (no fixed volume).

More technically, "a fluid deforms continuously under action of external forces, particularly small shear forces, which result in large changes in arrangements of fluid elements." (Bruus)

Do we need to worry about the molecular nature of fluids? (Spoiler: For us, no.)

The Continuum Hypothesis



How small is small enough?

Recap: Continuum hypothesis says there is some element size which is small enough that fluid properties are constant over element volume but big enough that we can ignore molecular nature of fluids.

This is an interesting break from ordinary mechanics where we often deal with point masses or charges. In Fluid Mechanics, basic constituent of fluid has finite size! So how small is it?

Physically, need fluid element to contain enough molecules that *statistical* fluctuations are small and well-defined average values are obtained. A **lower bound** is clearly dimensions of e.g. water molecule (about 0.3 nm).

Example

Assume cube of sidelength L with an average of N molecules. Standard deviation of randomly counted sample is \sqrt{N} . Intermolecular distance of water is roughly $\lambda=0.3$ nm. What is sidelength L if relative uncertainty is $\alpha=\sqrt{N}/N=0.01$?

Consequences of the Continuum Hypothesis

Our approach will be to treat fluids as *continuous media* composed of small but finite *fluid elements*.

- 1. can use continuum mechanics math (common in engineering and physics) to treat fluids in terms of *vector fields* (see next slide)
- 2. microfluidics have dimensions $\mathcal{O}(1-100\mu\text{m})$ so continuum hypothesis works very well
- 3. for nanofluidics (dimensions $\leq \mathcal{O}(10nm)$) continuum hypothesis breaks down

Math review: Scalars, vectors, and fields

Solutions to transport equations take the form of scalar or vector fields. Scalars and vectors can be used to describe physical quantities.

- scalar a physical quantity with magnitude only
 - ▶ e.g. T, P, c, ρ , others.

vector a physical quantity with magnitude and direction

- e.g. **v**, **F**, **J**, others. *Note:* positions can be expressed as position vectors **r**.
- field a mathematical object which assigns physical quantities to all points \mathbf{r} in a domain Ω .
 - \triangleright can be scalar or vector valued e.g. $c(\mathbf{r},t)$ or $\mathbf{v}(\mathbf{r},t)$

Example

Temperature and velocity fields in this room. (Eulerian description)

Reference frames: Eulerian and Lagrangian description

On the last slide, I used an Eulerian description of fluid motion.

Eulerian description: describe time-dependence of velocity field for fluid elements at fixed positions r i.e. v(r, t)

Ex. flow profile in complex microchannel

Lagrangian description: follow individual fluid elements in motion as they move through system along streamlines i.e. $\mathbf{v}(\mathbf{r}(t),t)$ or simply $\mathbf{v}(t)$

Ex. streamlines of droplets flowing

Both useful in different contexts. We'll stick with Eulerian (fixed fluid elements). And note that Newton's Second Law is a Lagrangian description!

Conservation of Mass: the Continuity Equation

Intuition: in any fixed region of space Ω , net mass flowing through surface and mass accumulation in volume must be equal.

Derivation: Consider flux through surface $\mbox{d}\Omega$ and apply Gauss' theorem (see Bruus)

Continuity Equation for Compressible Fluid¹

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$

What does this say?

¹Bruus uses a funny notation for the time derivative: $\partial_t \equiv \frac{\partial}{\partial t}$

The Continuity Equation Explained

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$

This is the time derivative of the density field, $\partial_t \rho$, i.e. the accumulation (or loss) of mass over time plus the net rate of flow into or out of a point, $\nabla \cdot (\rho \mathbf{v})$.

It's equivalent to write

$$\partial_t \rho = -\nabla \cdot (\rho \mathbf{v})$$

which says that for a *compressible fluid* any change in density (accumulation of mass) can only come from flux into or out of that point.

Continuity Equation for Incompressible Fluids

For incompressible fluid, density does not change in space or time. So we have

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$

 $0 + \rho \nabla \cdot (\mathbf{v}) = 0$

and finally

Continuity Equation for Incompressible Fluids

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

which says divergence of velocity field is zero everywhere. Easy!

Consequences of Continuity Equation for Incompressible Fluids

Continuity Equation for Incompressible Fluids

$$abla \cdot \mathbf{v} = 0$$

- 1. This will greatly simplify math going forward!
- 2. Physically, $\nabla \cdot \mathbf{v} = 0$ says that for incompressible fluids *volume is conserved*. E.g. a flow through a converging pipe adjusts only by changing its velocity because water is incompressible

When can we assume fluids are incompressible?

Fluid mechanics can generally describes gases, plasmas, and liquids. Gases and plasmas are compressible, but we'll ignore them in microfluidics.

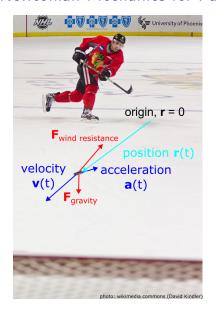
Liquids can be treated as incompressible in the absence of acoustic effects i.e. device flow velocities are below the speed of sound.

This will be true for all of the devices treated in this module.

Toward the Navier-Stokes Equations

- 1. Start from Newton's Second Law describes dynamics of *particle* under *applied forces F*
- 2. Express Newton's Second Law in volumetric properties like density ρ instead of mass m.
- 3. Introduce Material-Time Derivative
- 4. Describe typical force densites f in microfluidics

Newtonian Mechanics for Particles



Newton's Second Law:

$$\sum_{j} F_{j} = m\mathbf{a}(t) = m\frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}t}$$

with appropriate initial conditions can solve this ODE for $\mathbf{v}(t)$ or position $\mathbf{r}(t)$.

Key point: The solution r(t) is a complete description of the particle's trajectory through space for all times t! How do we get that for fluids???

Basic Navier-Stokes Equation

$$\sum_{j} \mathbf{F_{j}} = m \frac{\mathrm{d} \mathbf{v}}{\mathrm{d} t} \qquad \text{(Newton's Second Law)}$$

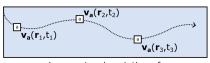
This is for discrete particles, but we need continuous fluids. Divide by volume \ensuremath{V} to get

$$\sum_{j} \mathbf{f_{j}} = \rho D_{t} \mathbf{v_{a}} \qquad \text{(Basic Navier-Stokes Equation)}$$

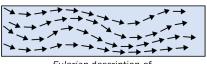
where

- f_j are force densities
- ρ is fluid density
- ν_a is the velocity of an arbitrary fluid element flowing through the system (a Lagrangian quantity!)
- $ightharpoonup D_t v_a \equiv \frac{Dv_a}{Dt}$ is called the *material time derivative* (next slides)

The Material-Time Derivative



Lagrangian description of fluid element velocity $\mathbf{v_a}(\mathbf{r}(t),t)$



Eulerian description of velocity field **v**(**r**,t)

The Material-Time Derivative

$$D_t \mathbf{v_a}(t) = \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v}$$

- D_t v_a(t) is the total rate of velocity change by a fluid element at a given location
- $\rightarrow \partial \mathbf{v}/\partial t$ (unsteady term) local rate of change of \mathbf{v} in time
- $(\mathbf{v} \cdot \nabla)\mathbf{v}$ (convective term) local rate of change of \mathbf{v} in space

Note that all terms have dimensions of acceleration.

Key Point: We've described a Lagrangian quantity, $v_a(t)$, in terms of Eulerian velocity fields, v.

Navier-Stokes Equation So Far

Knowing explicit expression for material-time derivative (acceleration term), can write

$$ho(\partial_t \mathbf{v} + (\mathbf{v} \cdot
abla) \mathbf{v}) = \sum_j \mathbf{f_j}$$

where $\mathbf{v} = \mathbf{v}(\mathbf{r}, t)$ is an Eulerian quantity.

This says LHS is density ρ times sum of time-varying and convective terms. Just need expressions for force densities f_j .

Typical Forces in Microfluidics

We'll consider four typical forces:

- Body Forces
- 1. electrical force \mathbf{f}_{el} on charged particles in external field
- 2. gravitational force \boldsymbol{f}_{grav}
- Surface Forces (Stresses)
- 3. pressure gradient force f_{pres}
- 4. viscous force f_{visc} arising from viscous stress

Body Forces $m{f}_{el}$ and $m{f}_{grav}$

A *body force* acts throughout the entire body of the fluid (force per unit volume). Compare a *surface force* (stress) which only acts on a surface element (force per unit area).

Two important body forces:

$$\mathbf{f}_{grav} = \rho \mathbf{g}$$
 (Gravity force)

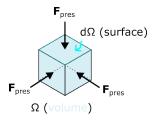
Gravity, a vector field, acts on a mass density ρ

$$\mathbf{f}_{el} = \rho_{el} \mathbf{E}$$
 (Electric force)

Electric field, a vector field, acts on charge density ρ_{el} ..

N.B. We will usually ignore gravity and electric fields.

Pressure Gradient Force f_{pres}



Pressure force is a normal surface stress acting on surface $d\Omega$ of fluid volume Ω

Derivation: Find total external surface force \boldsymbol{F}_{pres} acting on surface $d\Omega$ due to pressure p by surface integral. Apply Gauss' theorem to convert surface to volume integral. Integrand of volume integral is force density due to pressure:

$$\mathbf{f}_{pres} = -\nabla p$$
 (Pressure Gradient Force)

Viscous Force f_{visc}

Physical origin is friction between adjacent fluid elements. The derivation is horrible. It involves **Tensor Math** so I am not going to do it.

$${m f}_{\it visc} = \eta
abla^2 {m v}$$
 (Viscous force for Incompressible Fluids)

where

- $\triangleright \eta$ fluid viscosity (scalar constant)
- $ightharpoonup
 abla^2 \equiv
 abla \cdot
 abla$ Laplace operator

This form is often seen in diffusion equations. The physical interpretation is that viscosity operates as *diffusion of fluid momentum*!

Viscous Stresses Result in Momentum Diffusion

Imagine several layers of fluid at rest (t=0). Then, impart velocity \mathbf{v} to one layer. As time progresses, interfacial stresses act to "pull" adjacent layers along.

Conservation of momentum applies, so momentum diffuses outward!

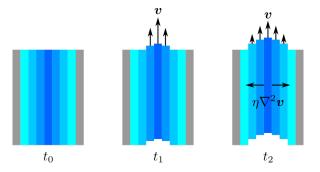


Figure: Illustration of viscous stresses as diffusion of fluid momentum

The Navier-Stokes Equations for Incompressible Fluids

$$\nabla \cdot \mathbf{v} = 0$$
 Continuity Equation

$$\rho(\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v}) = -\nabla p + \eta \nabla^2 \mathbf{v} + \rho \mathbf{g} + \rho_{el} \mathbf{E} \qquad \text{(Navier-Stokes Equation)}$$

where

- ightharpoonup
 ho fluid density (scalar constant)
- v velocity field (vector field)
- p pressure (scalar field)
- \triangleright η fluid viscosity (scalar constant)
- **g** gravity force (vector field)
- $ightharpoonup
 ho_{el}$ charge density (scalar field)
- **E** electric field (vector field)

Physical Interpretation of Navier-Stokes Equation

$$\rho(\underbrace{\begin{array}{ccc} \partial_t \textbf{\textit{v}} & + & \underbrace{(\textbf{\textit{v}} \cdot \nabla) \textbf{\textit{v}})}_{\text{convective term}} = \\ & \underbrace{\begin{array}{ccc} \nabla \rho & + & \underline{\eta} \nabla^2 \textbf{\textit{v}} + & \underline{\rho} \textbf{\textit{g}} + \rho_{el} \textbf{\textit{E}} \\ \\ \text{pressure gradient} & \text{friction} & \text{gravity and electric forces} \end{array}}$$

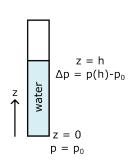
Key point: Just Newton's Second Law for a *continuous fluid*; compare $m \frac{d\mathbf{v}}{dt} = \sum_{i} \mathbf{F}$.

LHS: **Inertial terms** - represent changes in fluid inertia due to forcing terms. Changes in fluid flow manifest as temporal or spatial changes of velocity field.

RHS: Forcing terms: forces which drive these changes include applied pressure gradient across fluid, intrafluid viscous drag, and external fields (gravity and electric)

A quick example: Hydrostatic Pressure

Assume gravity acts along z-axis, $\mathbf{g}=-g\mathbf{e}_z$, where \mathbf{e}_z is unit vector along z. Assume **mechanical equilibrium** i.e. $\mathbf{v}=0$ and $\partial_t\mathbf{v}$ everywhere.



What cancels?

$$\rho(\partial_{\mathbf{r}}\mathbf{v}) + (\mathbf{v} \cdot \nabla)\mathbf{v}) = -\nabla p + \eta \nabla^{2}\mathbf{v} + \rho \mathbf{g}$$

Continuity and Navier-Stokes reduce to...

$$\mathbf{v}(\mathbf{r}) = 0$$
 (continuity)
 $0 = -\nabla p - \rho g \mathbf{e}_z$ (Navier-Stokes)

A quick example: Hydrostatic Pressure

Need to solve $\nabla p = -\rho g \, \boldsymbol{e}_z$. Assume incompressible fluid (ρ constant) and integrate to find

$$p(z) = p_0 - \rho gz$$

where p_0 is p at arbitrarily defined z=0. Put another way,

$$\Delta p = p(z) - p_0 = \rho g h$$

So pressure difference is proportional to height h of fluid column, which is what we expect from first year physics.

Non-Dimensionalizing the Navier-Stokes Equation

Recall the Navier-Stokes equation (ignoring body forces):

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

We can non-dimensionalize NS to study general behaviour.

For any quantity x, we'll express it as the product of a dimensionless quantity, \tilde{x} and a critical scale, X_0 .

Reduced Quantities

Scale length by L_0 and velocity by V_0 :

$$r = L_0 \tilde{r}$$
 $v = V_0 \tilde{r}$

Scale time by $T_0=L_0/V_0$ and pressure by $P_0=\eta V_0/L_0$:

$$t = \frac{L_0}{V_0}\tilde{t} = T_0\tilde{t}$$
 $p = \frac{\eta V_0}{L_0}\tilde{p} = P_0\tilde{p}$

Write temporal and spatial derivatives:

$$\partial_t = \frac{1}{T_0} \tilde{\partial}_t \qquad \nabla = \frac{1}{L_0} \tilde{\nabla}$$

Reduced Navier-Stokes Equation

$$\rho\left[\frac{V_0}{T_0}\tilde{\partial}_t\tilde{\mathbf{v}}+\frac{V_0^2}{L_0}(\tilde{\mathbf{v}}\cdot\tilde{\nabla})\tilde{\mathbf{v}}\right]=-\frac{P_0}{L_0}\tilde{\nabla}\tilde{\rho}+\frac{\eta V_0}{L_0^2}\tilde{\nabla}^2\tilde{\mathbf{v}}$$

This is ugly, right? But define **Reynolds Number**, $\mathrm{Re}=\frac{\rho V_0 L_0}{\eta}$ and do some algebra to reveal

$$\operatorname{Re}\left[\tilde{\partial}_t\tilde{\boldsymbol{v}}+(\tilde{\boldsymbol{v}}\cdot\tilde{\nabla})\tilde{\boldsymbol{v}}\right]=-\tilde{\nabla}\tilde{\boldsymbol{\rho}}+\tilde{\nabla}^2\tilde{\boldsymbol{v}}$$

Physical Interpretation of the Reynolds Number

$$\operatorname{Re}\left[\tilde{\partial}_{t}\tilde{\mathbf{v}}+(\tilde{\mathbf{v}}\cdot\tilde{\nabla})\tilde{\mathbf{v}}\right]=-\tilde{\nabla}\tilde{p}+\tilde{\nabla}^{2}\tilde{\mathbf{v}}$$

Reynolds number $\operatorname{Re} = \frac{\rho V_0 L_0}{\eta}$ is ratio of **inertial** to **viscous** forces.

Two limiting cases:

- 1. ${
 m Re}\gg 1$ (**Turbulent Flow**) inertial forces (turbulence) dominate in fluid. Typically ${
 m Re}>2000$ is onset of turbulence in microfluidics.
- 2. ${
 m Re} \ll 1$ (Laminar Flow) inertial forces are negligible. System is dominated by viscous stresses!

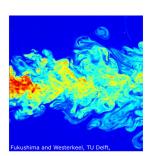
Note: As $\mathrm{Re} \to 0$ this becomes the Stokes Equation

$$0 = - \tilde{
abla} ilde{p} + \tilde{
abla}^2 ilde{oldsymbol{v}}$$

No inertial terms at all!

Fluid Flow Regimes

Two extremes for flow of liquids: turbulent and laminar flow.



LIF image of turbulent flow

false colour is fluorescence magnitude

Turbulent systems are dominated by **inertial effects**. Turbulent flow is characterized by

- ▶ high Re
- chaotic fluctuations in fluid velocity
- wide range of spatial and temporal scales
- presence of vortices and eddies (energy dissipation)
- high degree of mixing
- sensitive dependence on initial conditions

Intuition: fluid inertia so high that it overwhelms "restoring force" of viscosity

Fluid Flow Regimes



laminar flow of honey

Laminar systems are dominated by **viscous effects**. Laminar flow is characterized by

- ► low Re
- highly ordered flow with parallel layers ("lamellae") of co-flowing fluid
- stable flow without velocity or pressure fluctations
- minimal to no mixing
- deterministic and "easily" predicted

Intuition: fluid viscosity dominates inertia, causing flow to "creep"

Typical Values of Re in Microfluidics

Example

Calculate the Reynolds number for two limiting cases of typical microfluidic designs:

- 1. $V_0 = 1 \ \mu \text{m s}^{-1} \ \text{and} \ L_0 = 10 \ \mu \text{m}$
- 2. $V_0=1~{\rm cm}\,{\rm s}^{-1}$ and $L_0=500~{\rm \mu m}$

Recall that ${
m Re}=rac{
ho V_0 L_0}{\eta}.$ The density of water is $ho=1000~{
m kg/m^3}$ and the dynamic viscosity is $\eta_{H2O}=1~{
m mPa\,s}.$

Reynolds Number in Rectangular Channels

Last slide is true for circular channel of radius L_0 . Generally, for L_0 we use **hydraulic diameter**, $D_H = 4A/P$ where A is channel cross-sectional area and P is perimeter.

For rectangular channel,

$$D_H = \frac{2wh}{w+h}$$

Example

Calculate ${\rm Re}$ for a device with width $w=500~\mu m$ and height $h=50~\mu m$. Assume $V_0=1~{\rm cm\,s^{-1}}$ (average velocity for $Q=1~{\rm mL/s}$)

$$D_H = 9.09 \times 10^{-5} \text{ m, so } \mathrm{Re} = 0.9$$

Intermediate Values of Re

At intermediate ${\rm Re}$ (typically $\mathcal{O}(10$ - 100)), secondary flows may appear due to limited inertial effects. One example is called *Dean flow*, where fluids flow around a curved channel at intermediate ${\rm Re}$.

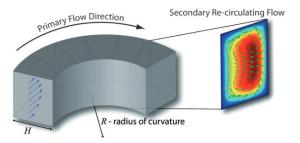


Figure: Secondary (Dean) flow in a curved rectangular channel. Adapted from "Inertial Microfluidics," Di Carlo, *Lab. Chip.*, 2009, **9**, 3038-3046.

In general, so-called "inertial microfluidics" exhibit flow which is not turbulent but may become chaotic. Note also these flows are *non-linear!* (More on this in a future lecture.)

When do we need to worry about Dean flow?

Define Dean number $\mathrm{De} = \sqrt{D_H/2R}\mathrm{Re}$ and calculate using last example's dimensions i.e. $D_H = 9.09 \times 10^{-5}$ m, choosing radius of curvature R = 1 mm, and recall $\mathrm{Re} = 0.9$. Then,

$$De = 0.19$$

which is less than the critical value of 1 so Dean flow is neglible. Can minimize Dean flow by using large radius of curvature in devices.

Summary of Lecture 2

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

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

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

- ► Reynolds number $Re = \frac{\rho V_0 L_0}{\eta}$ is ratio of **inertial** to **viscous** forces.
 - ▶ Re < 1 laminar (ordered) flow
 - $ightharpoonup {
 m Re} \gg 1$ 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