Introduction to Microfluidics Modeling: 
Part I - Fluid Mechanics

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Introduction

- **Continuum Mechanics**: conservation laws for variables continuously defined on a whole domain (e.g., pressure, temperature)

- **Molecular Dynamics**: multi-particle system with mutual interaction; Newton’s law

- **Statistical Physics**: from molecular level to continuum. E.g., Thermodynamics – Kinetic Gas Theory
Definition of Microfluidics

- **small scale effects**: micro in terms of (affected) volume rather than lengths
- **multi-scale problems**: e.g., CE: capillary length/diameter \( \approx 6000 \)
- **multi-physics problems**:

  - **Analyte Dynamics**
    - Advection–diffusion equation
    - in case of small concentration: algebraic slip model

  - **Microflow Simulation**
    - Navier–Stokes equation
    - electrophoretic body force
    - small Debye lengths: electroosmotic slip condition

  - **Electric Double Layer (EDL)**
    - Poisson–Boltzmann equation or Nernst–Planck equation
    - small Debye length: analytic solution

  - **Temperature Distribution**
    - heat equation
    - conduction
    - convection
    - external cooling
    - electric heating

  - **Electrostatic Potential**
    - Laplace equation
    - simple geometries: analytic solution
Typical Scales

spatial scales

- molecules
- viruses
- cells, bacteria
- blood vessel
- human body
- smoke particles
- microparticles
- macro particles
- normalized technology
- microneedles
- microchips
- microfilters/reactors
- classical fluidic devices
- microfluidic devices/sensors
Typical Scales

**spatial scales**

- Molecules: 1 Å - 1 nm
- Viruses: 1 nm - 1 μm
- Cells, bacteria: 1 μm - 1 mm
- Blood vessel: 1 mm - 1 m
- Hum. body

**temporal scales**

e.g., N₂ \( (p = 1 \text{ atm}, \ T = 20^\circ \text{ C}) \)

Analyte dynamics (CE)

\[ \nu_{\text{coll}}^{-1} = (\lambda_{\text{free}}/v_{\text{rms}})^{-1} \approx 10^{-10} \text{s} \]

\[ t = l/\nu_{\text{EP}} \approx (0.1 - 1 \text{ mm s}^{-1})/(10 \text{ cm}) \Rightarrow 10^2 - 10^3 \text{ s} \]
Typical Concentrations

- HIV in blood
- DNA fingerprinting
- cholesterol
- cancer detection
- biothreat agents detection
- estrogens
- uric acid

10^x copies/mL

larger sample volume → smaller sample volume
Typical Concentrations

Sample volume size:

\[ V_s = \frac{1}{(\eta \cdot N_A \cdot C)} \]

\[ 0 \leq \eta \leq 1, \quad N_A = 6.02 \cdot 10^{23} \]
Fluid Mechanics in a Nutshell

Fluid Mechanics is a Continuum Theory \( \Rightarrow \) sufficient large ensemble of molecules makes a fluid particle

\[ p, T, \rho, \tau \]

\[ v \]
What is a Fluid?

**fluid**: substance that shows continuing shear deformation in response to continuously applied shear forces
What is a Fluid?

**fluid** : substance that shows continuing shear deformation in response to continuously applied shear forces

**gas** : is a fluid that tends to evenly fill its containment

**liquid** : is a fluid that tends to take on the shape of its containment but conserves its volume; inter-molecular forces responsible for build up of free surfaces and/or droplets and bubbles (e.g., capillary effects)
**Nomenclature**

**compressibility**: dependency of density, $\rho$, upon dynamic (shear rate) and thermodynamic (pressure, temperature) variables; e.g., ideal gas law $\rho = \frac{p}{(R \cdot T)}$; under normal conditions liquids in contrary to gases can be treated as incompressible; criterion gases: Mach-number, $\text{Ma} = \frac{v}{c} < 0.3$
Nomenclature

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(shear) stress, $\tau$: surface force on a fluid particle

shear rate, $\dot{\gamma}$: temporal change of angle of deformation, $\gamma$ (in 2d plane configuration)
Nomenclature (cont.)

**Newtonian fluid**: shear stress linear proportional to shear rate (in 2d plane configuration), $\tau = \mu \cdot \dot{\gamma}$; most common liquids and gases; **viscosity**: $\mu$
Nomenclature (cont.)

Newtonian fluid: shear stress linear proportional to shear rate (in 2d plane configuration), \( \tau = \mu \cdot \dot{\gamma} \); most common liquids and gases; viscosity: \( \mu \)

Non-Newtonian fluid: Bingham or plastic fluid (dashed line) with yield stress \( \tau_0 \) (e.g., tooth-paste), pseudo-plastic (e.g., emulsions) and dilatant (fluids containing high levels of deflocculated solids)
Nomenclature (cont.)

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laminar - turbulent: turbulence is the occurrence of flow patterns of random nature; \( \text{Re} = \rho \cdot v \cdot L / \mu > 2000 \)
Microfluidics in a Nutshell

Modeling of systems that include fluidic materials...

- of small volumetric amount
- that show small scale effects
- that contain objects of microscopic size

Microfluidics to a high degree is application oriented
Continuum Assumption

point values

$$\rho = m \cdot \left( \frac{N}{V} \right) = m \cdot n$$

error < 1% \(\Rightarrow\) 

$$N = 10^4 \text{ molecules;}$$

$$V = \frac{N}{n} = 10^4/n$$
Continuum Assumption

point values
\[ \rho = m \cdot \left( \frac{N}{V_{pt}} \right) = m \cdot n \]

error < 1% \( \Rightarrow \) \( N \approx 10^4 \) molecules;
\[ V_{pt} = \frac{N}{n} = \frac{10^4}{n} \]

gas
\[ n \approx 3 \cdot 10^{25} \]
\[ \Rightarrow V_{pt} = 3.3^{-22} \text{ m}^3 \]
\[ \Rightarrow L_{pt} \approx 7 \cdot 10^{-8} \text{ m} = 70 \text{ nm} \]

fluid
\[ n \approx 2 \cdot 10^{28} \]
\[ \Rightarrow V_{pt} = 5^{-25} \text{ m}^3 \]
\[ \Rightarrow L_{pt} \approx 8 \cdot 10^{-9} \text{ m} = 8 \text{ nm} \]
Gas Flow

**number density:** from ideal gas law: \( n = p/KT \),
(standard conditions: \( n = 2.7 \cdot 10^{25} \text{ m}^{-3} \))

**molecular diameter:** e.g. for N\(_2\): \( d = 0.3 \text{ nm} \)

**molecular spacing:** \( \delta = n^{-1/3} \), (standard conditions: \( \delta = 3.3 \text{ nm} \))

**mean free path:** \( \lambda_{\text{free}} = (\sqrt{2} \cdot \pi \cdot d^2 \cdot n)^{-1} \)
(standard conditions: \( \lambda_{\text{free}} \approx 100 \text{ nm} \))
characteristic scale for exchange properties:
\( L_{\text{ex}} = 10 \cdot \lambda_{\text{free}} \approx 10 \cdot 10^{-7} \text{ m} \)
\( \Rightarrow V_{\text{ex}} = L_{\text{ex}}^3 = 1 \cdot 10^{-18} \text{ m}^3 = 10^{-3} \text{ aL} \)
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specific gas constant: \( R = \frac{R_u}{M} \), \( R_u = 8.314 \text{ J/mol K} \)

mean thermal velocity: \( \bar{c} = \sqrt{\frac{2 \cdot E_{\text{kin}}}{M}} = \sqrt{3 \cdot R \cdot T} \)

kinematic viscosity: \( \nu = \frac{\mu}{\rho} = \lambda_{\text{free}} \cdot \bar{c}/2 \)

speed of sound: \( c = \sqrt{\kappa \cdot R \cdot T}, \ \kappa = c_p/c_v \)
Gas Flow

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(standard conditions: \( n = 2.7 \cdot 10^{25} \text{m}^{-3} \))
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speed of sound: \( c = \sqrt{\kappa \cdot R \cdot T} \), \( \kappa = c_p / c_v \)

**Mach number:** \( \text{Ma} = \frac{v}{c} = \frac{v}{\sqrt{\kappa \cdot R \cdot T}} < 0.3 \)

**Reynolds number:** \( \text{Re} = \frac{u \cdot L}{\nu} = \frac{2 \cdot u \cdot L}{\lambda_{\text{free}} \cdot \bar{c}} < 2000 \)
Gas Flow: The Knudsen Number

\[ Kn = \frac{\lambda_{\text{free}}}{L} \]

continuum approach:

\( Kn < 0.1 \)
Liquid Flow

molecules in permanent contact

⇒ no kinetic theory available

*rule of thumb*: interaction length $\lambda_{\text{int}} \approx$ molecular diameter

⇒ $L_{\text{ex}} = 10 \cdot \lambda_{\text{int}} \approx 10 \text{ nm}$
Fluid Flow: Max Shear-rate

Breakdown of Newtonian behavior:

\[ \dot{\gamma} \leq \dot{\gamma}_c = \frac{2}{\tau} \]

\[ \tau = \sigma \sqrt{\frac{m}{\varepsilon}} \]
Fluid Flow: Max Shear-rate

Breakdown of Newtonian behavior:

\[
\dot{\gamma} \leq \dot{\gamma}_c = \frac{2}{\tau} \quad \tau = \sigma \sqrt{\frac{m}{\epsilon}}
\]

Lennard-Jones potential:

\[
V(r) = 4\epsilon \cdot \left[ c \cdot \left( \frac{r}{\sigma} \right)^{-12} - d \cdot \left( \frac{r}{\sigma} \right)^{-6} \right]
\]

\[
F(r) = -\frac{d V(r)}{dr} = \frac{48\epsilon}{\sigma} \cdot \left[ c \cdot \left( \frac{r}{\sigma} \right)^{-13} - \frac{d}{2} \cdot \left( \frac{r}{\sigma} \right)^{-7} \right],
\]

\[
r' = \frac{r}{\sigma}, \quad V'(r') = \frac{V(r/\sigma)}{4\epsilon}, \quad F'(r') = \frac{F(r/\sigma) \cdot \sigma}{48\epsilon}
\]
Wall Boundaries: Gas

\[ u - u_{\text{wall}} = \mathcal{L} \cdot \left. \frac{\partial u}{\partial y} \right|_{\text{wall}} \quad \text{← (wall slip)} \]

\[ + \quad C \cdot \left. \frac{\partial T}{\partial x} \right|_{\text{wall}} \quad \text{← (thermal creep)}, \]

\[ T - T_{\text{wall}} = \mathcal{F} \cdot \left. \frac{\partial T}{\partial y} \right|_{\text{wall}} \quad \text{← (temperature jump)} \]
Wall Boundaries: Gas

\[ u - u_{\text{wall}} = \mathcal{L} \cdot \frac{\partial u}{\partial y} \bigg|_{\text{wall}} \leftarrow \text{(wall slip)} \]
\[ + C \cdot \frac{\partial T}{\partial x} \bigg|_{\text{wall}} \leftarrow \text{(thermal creep)} \]
\[ T - T_{\text{wall}} = \mathcal{F} \cdot \frac{\partial T}{\partial y} \bigg|_{\text{wall}} \leftarrow \text{(temperature jump)} \]

\[
\mathcal{L}(Kn, f_u) = Kn \cdot \frac{2 - f_u}{f_u},
\]
\[
C(\text{Re}, \frac{\Delta T}{T_0}) = \frac{3}{4} \frac{\Delta T}{T_0} \frac{1}{\text{Re}},
\]
\[
\mathcal{F}(Kn, f_T, \kappa) = \frac{2 - f_T}{f_T} \cdot \frac{2\kappa}{\kappa + 1} \frac{Kn}{\text{Pr}}
\]
\[
\text{Pr} = \frac{cp\mu}{k}
\]

**accommodation coefficients**

<table>
<thead>
<tr>
<th>tangential momentum, ( f_u )</th>
<th>temperature, ( f_T )</th>
</tr>
</thead>
<tbody>
<tr>
<td>specular reflection: ( f_u = 0 )</td>
<td>insulation: ( f_T = 0 )</td>
</tr>
<tr>
<td>diffuse reflection: ( f_u = 1 )</td>
<td>perfect transfer: ( f_T = 1 )</td>
</tr>
</tbody>
</table>

**real world values**

| \( 0.87 - 0.97 \) | \( 0.87 - 0.97 \) |
Wall Boundaries: Liquid

Navier condition: \[ u - u_{\text{wall}} = \mathcal{L} \cdot \left. \frac{\partial u}{\partial y} \right|_{\text{wall}} \]

slip length: \( \mathcal{L} \)
Wall Boundaries: Liquid

Navier condition:

\[ u - u_{\text{wall}} = \mathcal{L} \cdot \left( \frac{\partial u}{\partial y} \right|_{\text{wall}} \]

slip length \( \mathcal{L} \)

low shear-rates:

\[ \left( \frac{\partial u}{\partial y} \right|_{\text{wall}} \approx 0 \]

\[ u|_{\text{wall}} = u_{\text{wall}} \text{ (no-slip)} \]

\[ T|_{\text{wall}} = T_{\text{wall}} \text{ (zero-jump)} \]
Wall Boundaries: Liquid

Navier condition: \[ u - u_{\text{wall}} = \mathcal{L} \cdot \left. \frac{\partial u}{\partial y} \right|_{\text{wall}} \]

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large shear-rates:
\[ \mathcal{L} = \mathcal{L}_0 \cdot \left( 1 - \frac{\dot{\gamma}}{\dot{\gamma}_c} \right)^{-1/2} \]
\[ \dot{\gamma}_c = \frac{2}{\tau} \]
Wall Boundaries: Liquid

Navier condition: 
$$u - u_{\text{wall}} = {\mathcal{L}} \cdot \left. \frac{\partial u}{\partial y} \right|_{\text{wall}}$$

slip length $\mathcal{L}$

low shear-rates:

$$\left. \frac{\partial u}{\partial y} \right|_{\text{wall}} \approx 0$$

$$u|_{\text{wall}} = u_{\text{wall}} \text{ (no-slip)}$$

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large shear-rates:

$$\mathcal{L} = \mathcal{L}_0 \cdot \left(1 - \frac{\dot{\gamma}}{\dot{\gamma}_c}\right)^{-1/2}$$

$$\dot{\gamma}_c = \frac{2}{\tau}$$

In most cases the no-slip and zero jump condition are justified!
Surface Forces

liquid-gas interface: attractive force \( \propto r^{-7} \)

\[ \Rightarrow \text{molecule sees more liquid molecules} \]

\[ \Rightarrow \text{attraction towards surface} \]

\[ \Delta p = \frac{\sigma_{lg}}{R} \]
Surface Forces

liquid-gas interface: attractive force $\propto r^{-7}$

$\Rightarrow$ molecule sees more liquid molecules

$\Rightarrow$ attraction towards surface

$$\Delta p = \frac{\sigma_{lg}}{R}$$

contact angle: $\Theta < 90^\circ \Rightarrow$ wetting liquid

$\Theta > 90^\circ \Rightarrow$ non-wetting liquid

contact line: horizontal force balance

$$\sigma_{ls} + \sigma_{lg} \cdot \cos \Theta = \sigma_{sg}$$
Capillarity

capillary pressure difference compensated by
hydrostatic pressure

\[ \rho \cdot g \cdot \Delta h = \Delta p = \frac{4 \cdot \sigma_{lg} \cdot \cos \Theta}{d} \]
Capillarity

capillary pressure difference compensated by
hydrostatic pressure

hydrophilic or wetting materials

hydrophobic or non-wetting materials

\[ \rho \cdot g \cdot \Delta h = \Delta p = \frac{4 \cdot \sigma_{lg} \cdot \cos \Theta}{d} \]

liquid is sucked in, \( \Delta h > 0 \)

liquid is pushed out, \( \Delta h < 0 \)
Pressure Driven Flows

linear pressure drop

\[
\frac{dp}{dx} = \text{const} = \frac{\Delta p}{\Delta L}
\]

low Reynolds number

(pressure drop) = (gradient of radial shear stress)
Pressure Driven Flows

linear pressure drop

low Reynolds number

Newtonian fluid with viscosity $\mu$

in circular channel of radius $R$

\[
\frac{d p}{d x} = \text{const} = \frac{\Delta p}{\Delta L}
\]

(pressure drop) = (gradient of radial shear stress)

\[
u = -\frac{\Delta p}{\Delta L} \cdot \frac{1}{4\mu} \cdot (R^2 - r^2)
\]
Electrokinetics

- four basic types of electrokinetic phenomenas:
  - **Electro-osmosis**: liquid moves relative to charged wall due to applied field
  - Electrophoresis: ions or charged particles move relative to fluid due to applied field
  - Streaming potential: induced field caused by charged particles moved by fluid
  - Sedimenting potential: induced field caused by charged particles moving in resting fluid
Electrokinetics

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- surface charges $\Rightarrow$ surface forces $\Rightarrow$ effects only on micro-scales
Electrokinetics

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  - Streaming potential: induced field caused by charged particles moved by fluid
  - Sedimenting potential: induced field caused by charged particles moving in resting fluid
- surface charges $\Rightarrow$ surface forces $\Rightarrow$ effects only on micro-scales
- easy to integrate in microsystems
Electrokinetics: Electrostatics

Poisson equation

\[
\frac{d}{dy} \left( \frac{d \Phi}{dy} \right) = \frac{d^2 \Phi}{dy^2} = -\frac{\rho_e}{\epsilon}
\]
Electrokinetics: Electrostatics

Poisson equation

\[
\frac{d}{dy} \left( \frac{d \Phi}{dy} \right) = \frac{d^2 \Phi}{dy^2} = -\frac{\rho_e}{\epsilon}
\]

Boundary conditions

fixed potential: \( \Phi|_{\text{wall}} = \Phi_{\text{wall}} \)

surface charge: \( \frac{d \Phi}{dy}|_{\text{wall}} = \sigma_e \)
Electrokinetics: Zeta-potential $\zeta$

Poisson-Boltzmann equation (symmetric electrolyte):

$$\frac{d^2 \Phi}{dy^2} = \frac{2 e_0 z n_{\text{bulk}}}{\epsilon} \cdot \sinh \left( \frac{z \epsilon_0 \Phi}{k_B T} \right) = -\frac{\rho_e}{\epsilon}$$

Debye Length:

$$\lambda_D = \frac{1}{2} \sqrt{\frac{\epsilon k_B T e_0^2}{z n_{\text{bulk}}}}$$

$$\lambda_D \ll h$$
Electrokinetics: Zeta-potential $\zeta$

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Electrokinetics: Zeta-potential $\zeta$

Poisson-Boltzmann equation (symmetric electrolyte):

$$\frac{d^2 \Phi}{d y^2} = \frac{2 e_0 z n_{\text{bulk}}}{\epsilon} \cdot \sinh \left( \frac{z \epsilon_0 \Phi}{k_B T} \right) = -\frac{\rho_e}{\epsilon}$$

Debye Length:

$$\lambda_D = \frac{1}{2} \cdot \sqrt{\frac{\epsilon k_B T}{e^2_0 z^2 n_{\text{bulk}}}}$$

$$\lambda_D \ll h:$$

$$\frac{d^2 \Psi}{d y^2} = \frac{\Phi}{\lambda_D^2}$$

$$\Rightarrow \Phi = \Phi_{\text{wall}} \cdot e^{-y/\lambda_D}$$
Electrokinetics: Electro-osmosis

Helmholtz-Smoluchowski velocity:

shear force = electrokinetic force

\[
\frac{d \tau}{d y} = -\rho_e E_x
\]
Electrokinetics: Electro-osmosis

Helmholtz-Smoluchowski velocity:

Shear force = electrokinetic force

\[ \frac{d \tau}{d y} = -\rho_e E_x \]

\[ \mu \cdot \frac{d^2 u}{d y^2} = \epsilon \cdot \frac{d^2 \Phi}{d y^2} E_x \]
Electrokinetics: Electro-osmosis

Helmholtz-Smoluchowski velocity:

shear force $= \text{electrokinetic force}$

$$\frac{d \tau}{d y} = - \rho_e E_x$$

$$\mu \cdot \frac{d^2 u}{d y^2} = \epsilon \cdot \frac{d^2 \Phi}{d y^2} E_x$$

$$u_{\text{wall}} = \frac{u_{\text{eof}}}{\mu} = \frac{\epsilon \zeta E_x}{\mu}$$
**Electrokinetics: Electro-osmosis**

**Helmholtz-Smoluchowski velocity:**

shear force = electrokinetic force

\[
\frac{d\tau}{dy} = -\rho_e E_x
\]

\[
\mu \cdot \frac{d^2 u}{dy^2} = \epsilon \cdot \frac{d^2 \Phi}{dy^2} E_x
\]

**EO mobility:**

\[
\mathbf{u}_{\text{eof}} = \frac{\epsilon \zeta E_x}{\mu}
\]

\[
\mathbf{u}_{\text{wall}} = \mathbf{u}_{\text{eof}} = \mu_{\text{eof}} \cdot E_{||}
\]
Electrokinetics: Electrophoresis

electrokin. force \_{\text{surface}} = \text{viscous drag \_{\text{surface}}}

\sigma_e \cdot \vec{E} = 6 \pi \mu a \vec{u}_{ep}
**Electrokinetics: Electrophoresis**

The equation for the electrokinetic force is given by

\[
\sigma_e \cdot \vec{E} = 6 \pi \mu a \vec{u}_{ep}
\]

\[\Rightarrow \vec{u}_{ep} = \frac{\sigma_e \cdot \vec{E}}{6 \pi \mu a}\]
Electrokinetics: Electrophoresis

\[ \frac{\text{electrokin. force}}{\text{surface}} = \frac{\text{viscous drag}}{\text{surface}} \]

\[ \sigma_e \cdot \vec{E} = 6\pi \mu a \vec{u}_{ep} \]

\[ \Rightarrow \vec{u}_{ep} = \frac{\sigma_e \cdot \vec{E}}{6\pi \mu a} \]

EP mobility: \( \vec{u}_{ep} = \mu_{ep} \cdot \vec{E} \)
Heat Transfer

convection + diffusion = production

e.g. Joule heating $\propto \sigma_\tau \cdot \vec{E}^2$
Heat Transfer: Thermal effects in HV-CE

induced convection dependent material properties
Heat Transfer: Simulation HV-CE