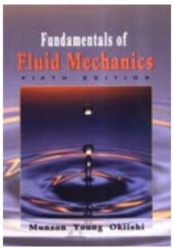
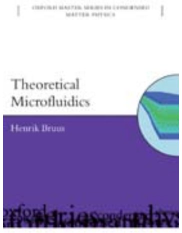
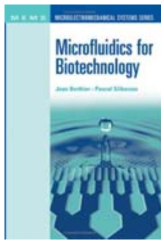
Fluid dynamics and Microfluidics







<u>Synopsys (tentative)</u>
Introduction. Basic properties of fluids
Statics of fluids
Fluid dynamics.
Navier-Stokes equations
Dynamic Similarity. Laminar and turbulent flow
Experimental flow characterisation
Numerical flow simulation
Electrofluidics
Flow with Diffusion. Two phase flow.
Basic microfabrication techniques
Microfluidic devices. Design examples: Valves, Pumps and Sensors.

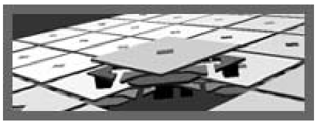
Lecture plan

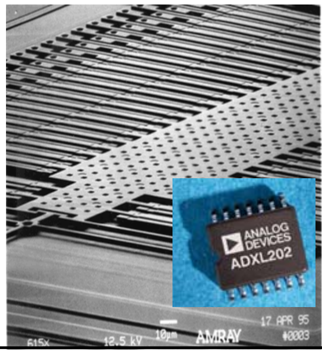
- Introduction: concept of microfluidics, applications and challenges
- Continuum hypothesis and fluid particles
- Properties of liquids:
  - Compressibility
  - Viscosity and No-Slip condition
  - Surface tension
- Wetting phenomena and digital microfluidics
- Problem session

Introduction

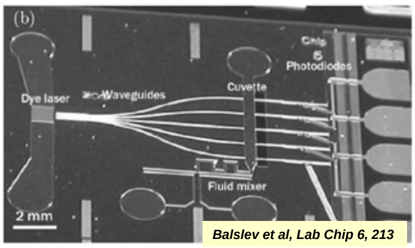
- **Miniaturization in microelectronics** – Moor's Law, doubling integration density every 18 monthy. According to Intel who currently uses 50nm features they will be able to follow Moor's Law for another 10 years at least (32nm and 15nm lithography is under development)

- **Miniaturization of non-electronics** devices started in late 70s as MEMS (MicroElectroMechanical Systems) but also extends to fluidics and optical components.

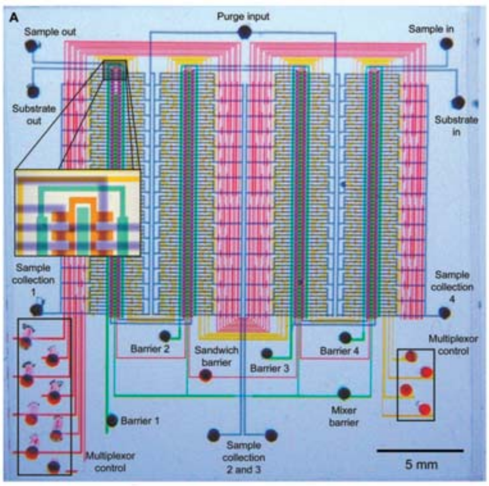




Microfluidics circuits



Balslev et al, Lab Chip 6, 213

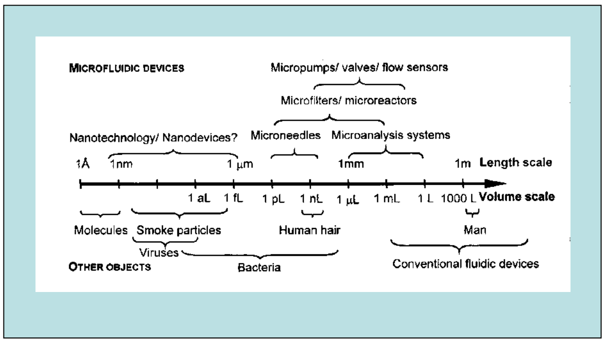


S. Quake et al, Science 298, 580

- Can include active and passive elements: pumps, mixers, reaction chamber
- Range of sensors
- Light sources
- Electronic circuitry

What size we are speaking about?

- Volume goes as L^3, so fairly small decrease in size leads to dramatic reduction of sample volume

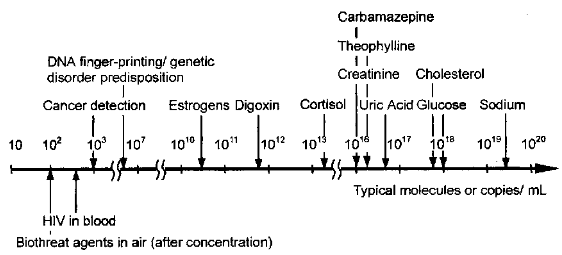


Unit Prefixes

zepto 10^{-21}

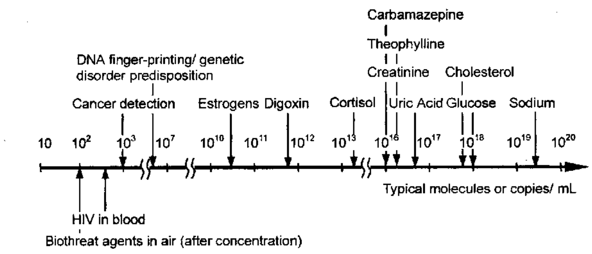
Atto	*Femto*	*Pico*	*Nano*	*Micro*	*Milli*	*Centi*	*Deka*	*Hecto*	*Kilo*	*Mega*	*Giga*
10^{-18}	10^{-15}	10^{-12}	10^{-9}	10^{-6}	10^{-3}	10^{-2}	10	10^{2}	10^{3}	10^{6}	10^{9}

What amount do we need



Digoxin – heart stimulating drug;
Cortisol – stress hormon synthesised by adrenal gland
Creatinine - protein produced by muscle and released into the blood. The creatinine level in the serum is a measure of kidney function
Theophylline – drug used in therapy to treat respiratory diseases e.g. Asthma
Uric acid – Uric acid is the end product of purine metabolism produced in the body is excreted by the kidneys. An overproduction of uric acid occurs when there is excessive breakdown of cells, which contain purines, or an inability of the kidneys to excrete uric acid

What amount do we need

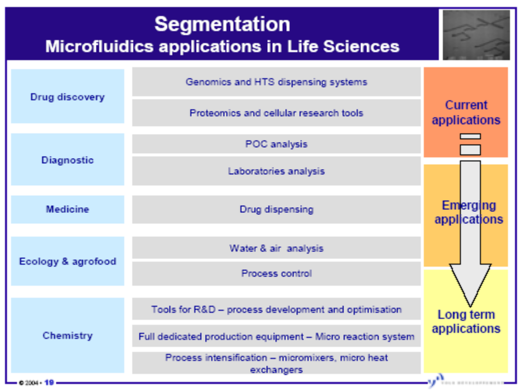


$$V = \frac{1}{\eta_s N_A A_i}$$

where η_s is the sensor efficiency $(0 \le \eta_s \le 1)$, $N_A = 6.02 \times 10^{23}$ is Avogadro number, and A_i is the concentration of analyte i.

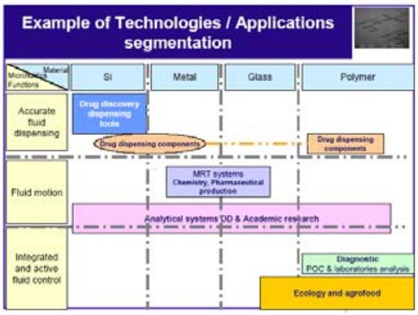
Samples volumes that are too small may contain not enough target molecules!

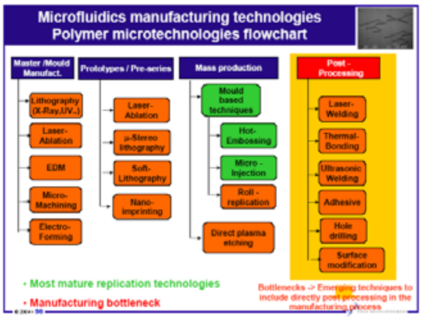
Major applications



Advantages:
Fast analysis due to small quantaties
Massively parallel automated analysis

Microfluidics technology





Due to large size of most microfluidics components relatively few devices can be placed on a wafer making silicon microfabrication technology too expensive. Plastic moulding is the technology of choice for most applications.

Microfluidics development

• Miniaturisation approach: shrinking down conventional devices (pumpes, valves etc.) using silicon micromachinig. Problem: as surface to volume ration increases viscosity role increases that requires excessive power for actuators

•Exporation of new effects: e.g. electrokinetic pumping, surface tension driven flow, electrowetting etc.

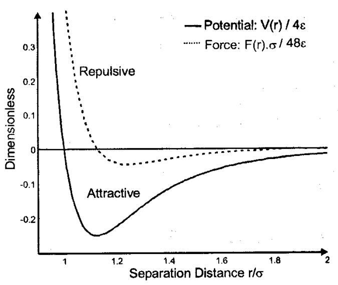
•Developing new applications: e.g. Distributed termal management, chemical production using distributed microreactors.

Droplet transport by electrowetting in a ring structure (Duke University, NC)

Basic Properties of Flowing Fluids

- Thermodynamic properties (e.g.pressure, temperature, density, surface tension)
- Transport properties (e.g.viscosity, thermal conductivity, diffusivity)
- Kinematic properties (e.g.linear and angular velocity, vorticity, acceleration, strain rate)

Intermolecular forces



$$V_{ij}(r) = 4\varepsilon\left[c_{ij}\left(\frac{r}{\sigma}\right)^{-12} - d_{ij}\left(\frac{r}{\sigma}\right)^{-6}\right]$$

$$F_{ij}(r) = -\frac{\partial V_{ij}(r)}{\partial r} = \frac{48\varepsilon}{\sigma}\left[c_{ij}\left(\frac{r}{\sigma}\right)^{-13} - \frac{d_{ij}}{2}\left(\frac{r}{\sigma}\right)^{-7}\right]$$

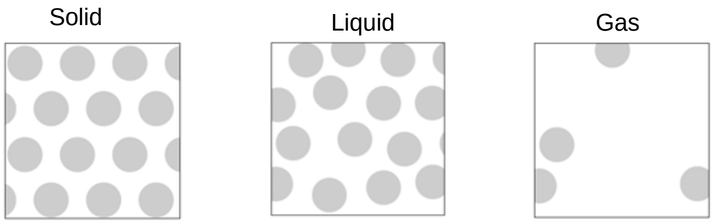
$$\tau = \sigma\sqrt{\frac{m}{\varepsilon}}$$

Fluid	*ε/K (K)*	*σ (nm)*
Air	97	0.362
N_2	91.5	0.368
CO_2	190	0.400
O_2	113	0.343
Ar	124	0.342

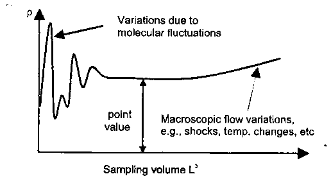
Phases	*Intermolecular Forces*	*Ratio of Thermal Vibration Amplitude Compared to σ*
Solid	Strong	« 1
Liquid	Moderate	~ 1
Gas	Weak	» 1

$K_B = 1.38 \cdot 10^{-23}\, J/K$

Validity of continuum approach



Thought experiment:
measuring density (or any other thermodynamic quantity)



Properties of a Typical Gas and Liquid at Standard Conditions (After [10])

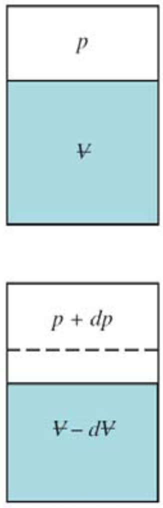
Property	*Gas (N_2)*	*Liquid (H_2O)*
Molecular diameter	0.3 nm	0.3 nm
Number density	3×10^{25} m^{-3}	2×10^{28} m^{-3}
Intermolecular spacing	3 nm	0.4 nm
Displacement distance	100 nm	0.001 nm
Molecular velocity	500 m/s	1,000 m/s

Microfluidics is still in the early stage of development.
Exciting field to join!!!

Compressibility of fluids

- Bulk module of elasticity

$$E_v = \frac{dp}{d\mathcal{V}/\mathcal{V}} = \frac{dp}{d\rho/\rho}$$



Water: E_v=2.15 *10^9 N/m^2
1% compression would require 2*10^7 N/m^2 =200 atm!!!.

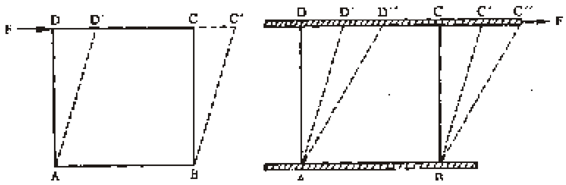
- Speed of sound

$$c = \sqrt{\frac{E_v}{\rho}}$$

Check the dimension!

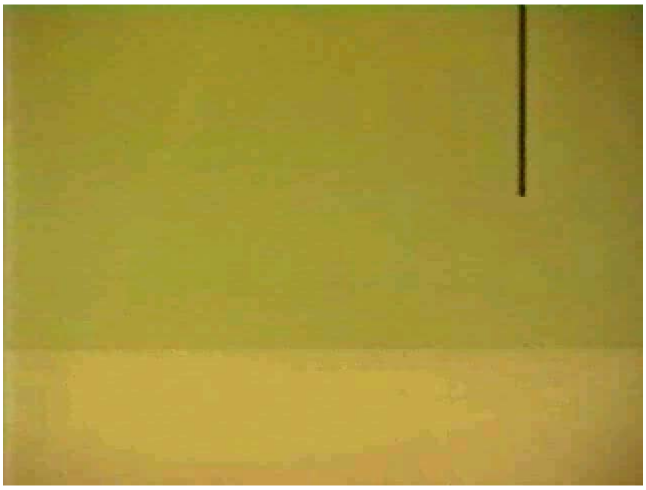
Definition of fluid

”a substance that deforms continuosly under the application of shear (tangential) stress, no matter how small the stress may be”



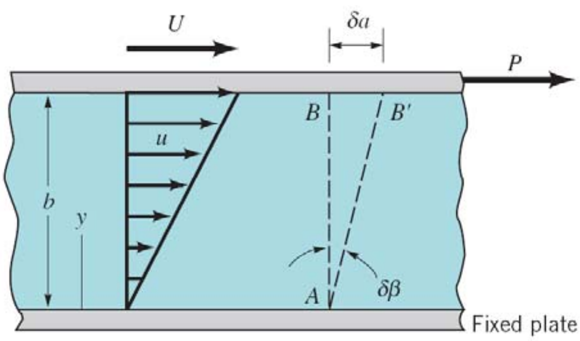
Solid Fluid

No-slip condition



- As a fluid flows near a solid surface, it "sticks" to the surface, i.e., the fluid matches the velocity of the surface. This so-called **"no-slip"** condition is a very important one that must be satisfied in any accurate analysis of fluid flow phenomena.

Viscosity



Shearing stress, τ:

$\tau = F / A \;\; [N/m^2]$

Newtonian fluid:

$$\tau = \mu \frac{du}{dy}$$

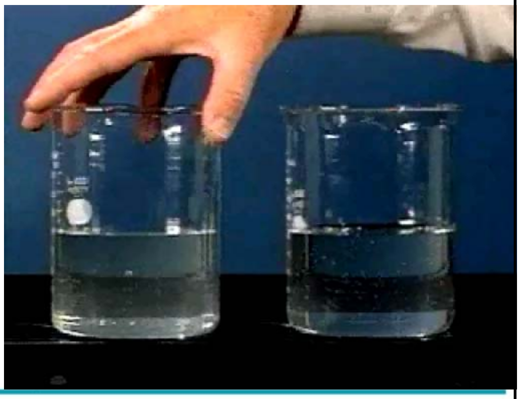
Rate of shearing strain (velocity gradient)

dynamic viscosity [N/m² / (m/s / m) = **N s/m²**]

kinematic viscosity $\upsilon = \tau / \rho$

Viscosity

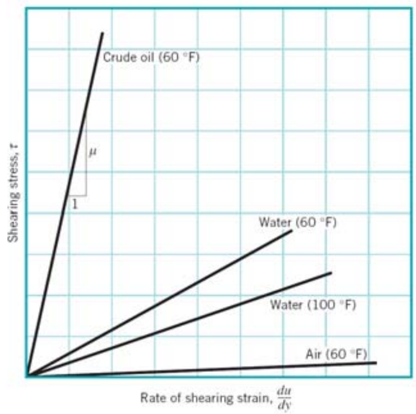
- Viscosity, one of the important properties, is responsible for the shear force produced in a moving fluid.

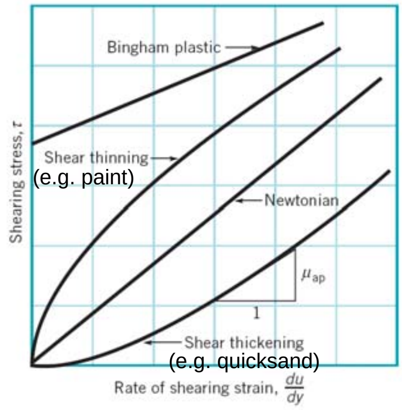


Although the two fluids shown look alike (both are clear liquids and have a specific gravity of 1), they behave very differently when set into motion. The very viscous silicone oil is approximately 10,000 times more viscous than the water

Liquid	Temperature (°C)	Density, ρ (kg/m^3)	Specific Weight, γ (kN/m^3)	Dynamic Viscosity, μ (N · s/m^2)	Kinematic Viscosity, ν (m^2/s)	Surface Tension,[a] σ (N/m)	Vapor Pressure, p_v [N/m^2 (abs)]	Bulk Modulus,[b] E_v (N/m^2)
Carbon tetrachloride	20	1,590	15.6	9.58 E − 4	6.03 E − 7	2.69 E − 2	1.3 E + 4	1.31 E + 9
Ethyl alcohol	20	789	7.74	1.19 E − 3	1.51 E − 6	2.28 E − 2	5.9 E + 3	1.06 E + 9
Gasoline[c]	15.6	680	6.67	3.1 E − 4	4.6 E − 7	2.2 E − 2	5.5 E + 4	1.3 E + 9
Glycerin	20	1,260	12.4	1.50 E + 0	1.19 E − 3	6.33 E − 2	1.4 E − 2	4.52 E + 9
Mercury	20	13,600	133	1.57 E − 3	1.15 E − 7	4.66 E − 1	1.6 E − 1	2.85 E + 10
SAE 30 oil[c]	15.6	912	8.95	3.8 E − 1	4.2 E − 4	3.6 E − 2	—	1.5 E + 9
Seawater	15.6	1,030	10.1	1.20 E − 3	1.17 E − 6	7.34 E − 2	1.77 E + 3	2.34 E + 9
Water	15.6	999	9.80	1.12 E − 3	1.12 E − 6	7.34 E − 2	1.77 E + 3	2.15 E + 9

Non-Newtonian fluids





Fluids for which shearing stress is not linearly related to the rate of shearing strain are designated as non-Newtonian fluids.

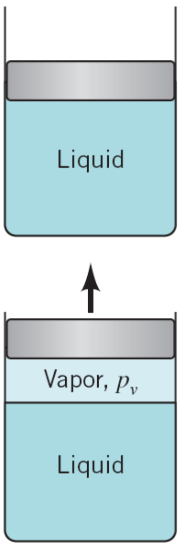
Non-Newtonian Fluids

A mixture of water and corn starch, when placed on a flat surface, flows as a thick, viscous fluid. However, when the mixture is rapidly disturbed, it appears to fracture and behave more like a solid. The mixture is a non-Newtonian shear thickening fluid which becomes more viscous as the shearing rate is suddenly increased through the rapid action of the spoon.

Vapour pressure

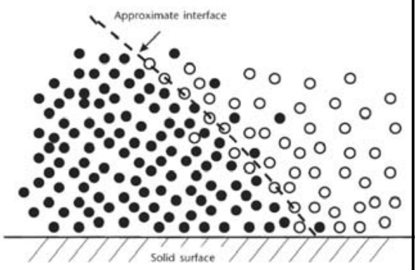
- Pressure of liquid vapour in equilibrium with liquid is called saturated vapour pressure (depends on T!)
- Boiling occurs when the total pressure is equal to the vapour pressure.

Water at 20C: p_v=1.77 10^3 N/m^2



Physics of wetting

- molecules on the interface interact to one half with the molecules of the same material and to the other half with the molecules of other liquid or gas.
- therefore surface possesses extra energy per unit of surface called **surface tension** (units N/m)



$$E = \gamma S$$

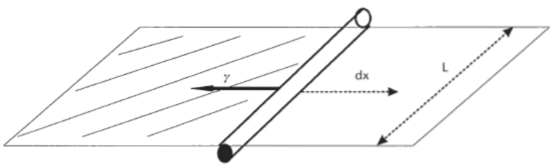
Table 2.1 Typical Values of Surface Tensions at Room Temperature

Type of Components	*Water/Air*	*Water/Oil*	*Glycerol/Air*	*Ethanol/Air*	*Cyclohexan/Air*	*Mercury/Air*
Surface tension [mN/m]	72	50	63	23	25	485

Physics of wetting

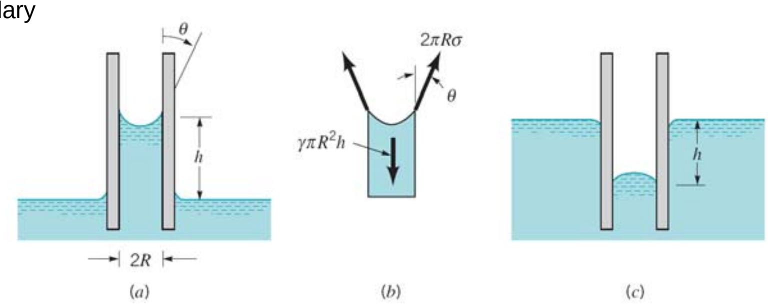
- Surface tension can be treated as force per unit length N/m
- Force on a free boundary:

$$\delta W = Fdx = 2\gamma Ldx$$



Capillary rise

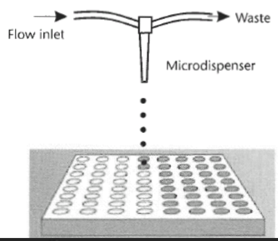
Surface tension causes liquid rise (or depression, depending on wetting) in a thin capillary



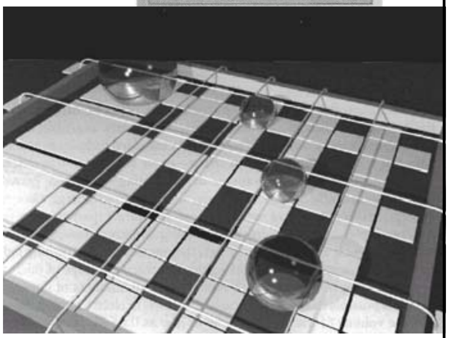
$$\rho g \pi R^2 h = 2\pi R\sigma \cos\theta \;\Rightarrow\; h = \frac{2\sigma\cos\theta}{\rho g R}$$

Microdrops in microfluidics

Why microdrops are important?



- Microdrops can be used directly to deliver sample to an array
- Microdrops can be used to transport and manipulate small samples in microfluidics systems:
  Advantages:
  - nonspecific adsorption to the walls is minimized
  - very small sample volumes (as low as 50 nl) can be used without diluting the sample
  - sample can be transported along the chosen trajectory



Physics of wetting

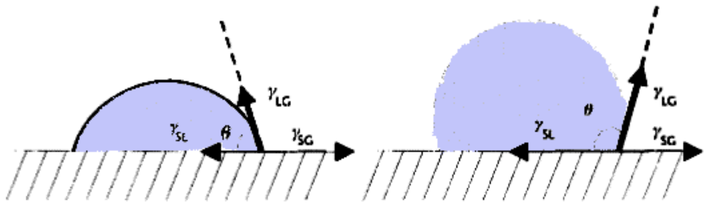
- Liquid droplet on solid surface:

partial wetting

total wetting $S=\gamma_{SG}-(\gamma_{SL}+\gamma_{LG})>0$

- In case of partial wetting a triple line is formed. Equilibrium along the triple line is described by **Young's law**

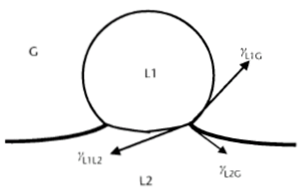
$$\gamma_{LG}\cos\theta=\gamma_{SG}-\gamma_{SL}$$



Hydrophilic contact, $\theta < 90°$ Hydrophobic contact, $\theta > 90°$

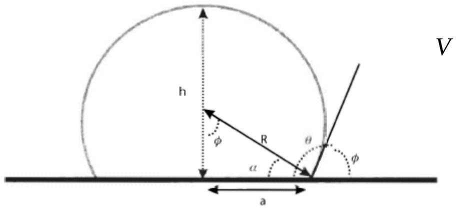
Physics of wetting

- in case of liquid drop on solid vertical force is balanced by the reaction of solid. In case of liquid drop on liquid balance in X and Y direction should be obtained



Equilibrium shape of a droplet

- assuming a spherical droplet (no gravity):



$$V = \pi R^3 \left(\frac{2}{3} - \frac{3\cos\theta}{4} - \frac{\cos 3\theta}{12} \right)$$

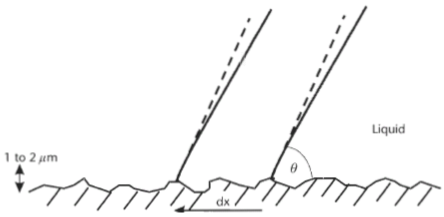
- the shape can be determined by minimizing energy with constant volume

$$E = (\gamma_{LS} - \gamma_{GS}) S_{LS} + \gamma_{LG} S_{LG} =$$
$$= \pi R^2 \left[(\gamma_{LS} - \gamma_{GS}) \sin^2\theta + 2\gamma_{LG}(1 - \cos\theta) \right]$$
$$dE = \frac{\partial E}{\partial R}(R,\theta) dR + \frac{\partial E}{\partial \theta}(R,\theta) d\theta = 0$$

- minimization will lead to Young's law

Droplet on rough surface: Wenzel's law

- assumption: roughness on a microscopic scale



- work along the contact line:

$$dE = dW = \sum F_x dx = (\gamma_{SL} - \gamma_{SG}) r dx + \gamma_{LG} \cos\theta dx$$
$$\gamma_{LG} \cos\theta = (\gamma_{SL} - \gamma_{SG}) r$$
$$\cos\theta = \frac{(\gamma_{SL} - \gamma_{SG}) r}{\gamma_{LG}} = r \cos\theta^*$$

on smooth surface

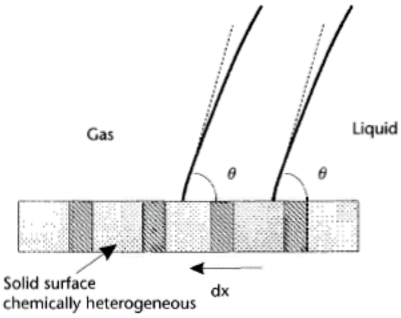
Wenzel's law

$\theta > \theta^*$ for hydrophobic surface ($\theta^* > 90^0$)

$\theta < \theta^*$ for hydrophilic surface ($\theta^* < 90^0$)

Cassie-Baxter law

- droplet on an inhomogeneous surface:

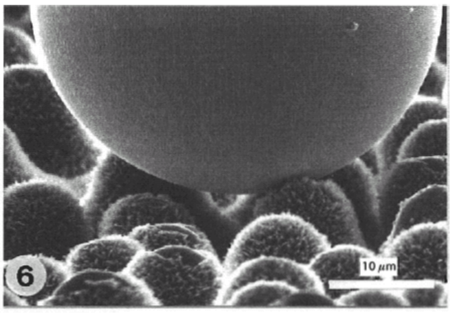


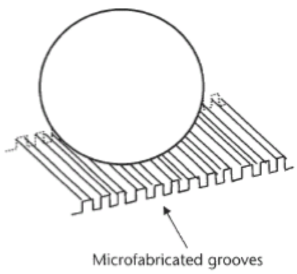
$$dE = dW = \sum F_x dx = (\gamma_{SL1} - \gamma_{SG1}) f_1 dx + (\gamma_{SL2} - \gamma_{SG2}) f_2 dx + \gamma_{LG} \cos\theta dx$$

$$\cos\theta = f_1 \cos\theta_1 + f_2 \cos\theta_2$$

Superhydrophobicity and Superhydrophilicity

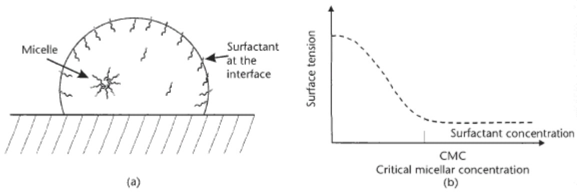
- Wenzel's law: hydrophobocity or hydrophilicity is enhanced by an increase in surface roughness
- In addition inclusion of air pores contributes to the superhydrophobicity $\cos\theta = f_1 \cos\theta_1 - f_2$ as $\theta_{AIR} = 180^0$





The effect of surfactants

- in the presence of surfactants the surface tension will be reduced (e.g. for water from 72 mN/m down to 30 mN/m)



Shape of drops on solid surface

- large drops are not spherical as the gravity flattens the drop. Equilibrium shape can be found by minimization of energy

$$E = (\gamma_{LS} - \gamma_{GS})\pi R^2 \sin^2\theta + 2\pi R^2 \gamma_{LG}(1-\cos\theta) + R^4 \rho g \frac{2\pi}{3}(3+\cos\theta)\sin^6\left(\frac{\theta}{2}\right)$$

$$\frac{\partial E}{\partial R}(R,\theta)dR + \frac{\partial E}{\partial \theta}(R,\theta)d\theta = 0$$

$$\cos\theta - \frac{\gamma_{LS} - \gamma_{GS}}{\gamma_{LG}} + \frac{\rho g R^2}{\gamma_{LG}}\left[\frac{\cos\theta}{3} - \frac{\cos 2\theta}{12} - \frac{1}{4}\right] = 0$$

- Bond number represents the ration of gravitational forces and surface tension

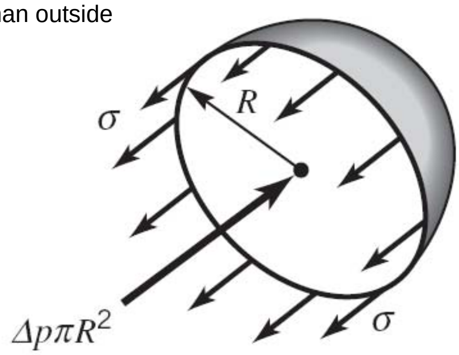
$$Bo = \frac{\rho g R^2}{\gamma_{LG}}$$

Typically: ρ=1000 kg/m^3, γ=72 mN/m, R=1mm, so Bo=0.15

Pressure inside the droplet

Pressure inside the drop is higher than outside

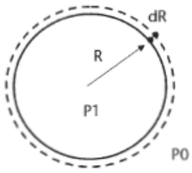
$$2\pi R\sigma = \Delta p \pi R^2 \quad \Rightarrow \quad \Delta p = \frac{\sigma}{R}$$



Laplace equation

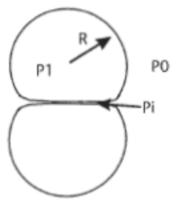
- Let's consider an infinitesimal change in droplet size:

$$dE = -P_1 dV_1 - P_0 dV_0 + \gamma dA =$$
$$= -4\pi(P_1 - P_0)R^2 dR + 8\pi\gamma R dR$$
$$P_1 - P_0 = 2\frac{\gamma}{R}$$



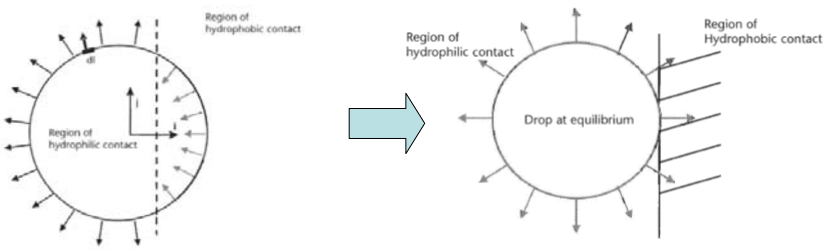
Generally:

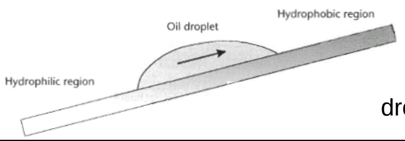
$$P_1 - P_0 = \gamma\left(\frac{1}{R} + \frac{1}{R'}\right)$$



Motion of drops under action of hydrophilic/Hydrophobic forces

- droplet deposited on a border between hydrophilic/hydrophobic region will move towards hydrophilic region





droplet running uphill

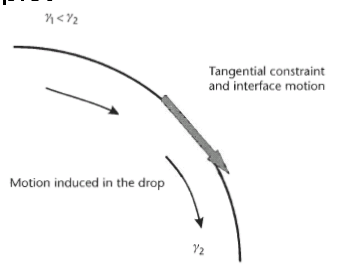
Marangoni effect

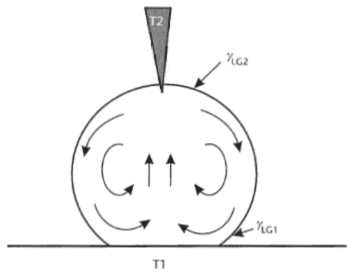
- surface tension depends on temperature as

$$\gamma = \gamma_0 (1 - \beta (T - T_0))$$

for water/air interface: γ_0=72mN/m and β=0.1 mN/(m K)

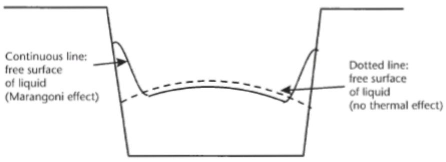
- surface tension distribution induces tangential force distribution on the interface and convective motion inside the droplet



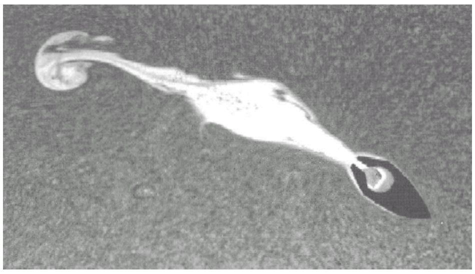


Marangoni effect

- Marangoni effect due to temperature in a microwell

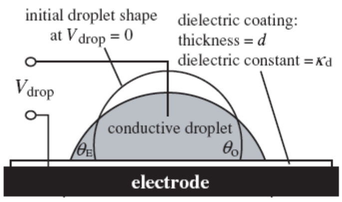


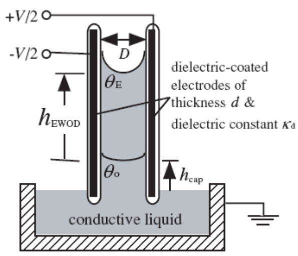
- Marangoni effect due to surfactant concentration



Electrowetting

Electrowetting on Dielectric film is a phenomenon where the surface property of a dielectric film can be modified between hydrophobic and hydrophilic states using an electric field. This process can cause a droplet of liquid to bead or spread out on the surface depending upon its surface state.



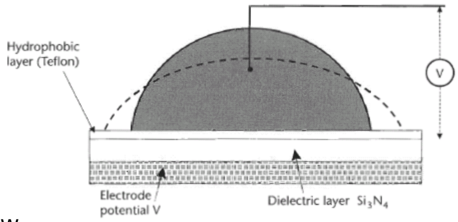


Applications

- liquid dispensers
- voltage-controlled fluidic switches
- laboratory-on-a-chip
- focused liquid lenses
- Optoelectronics couplers
- electronic paper displays

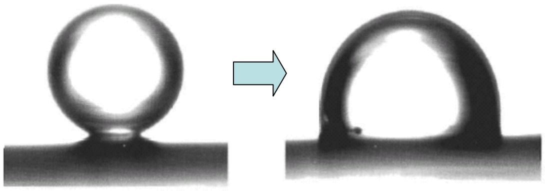
Electrowetting

- redistribution of charges under applied electric field causes change in wetting properties

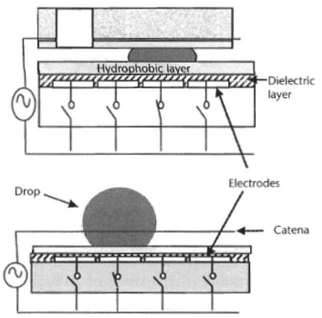


$$\gamma_{SL} = \gamma_{SL,0} + \frac{1}{2} CV^2$$ Lippmann's law

$$\cos\theta = \cos\theta_0 + \frac{1}{2}\frac{C}{\gamma_{LC}} V^2$$



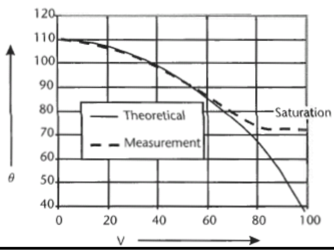
Electrowetting



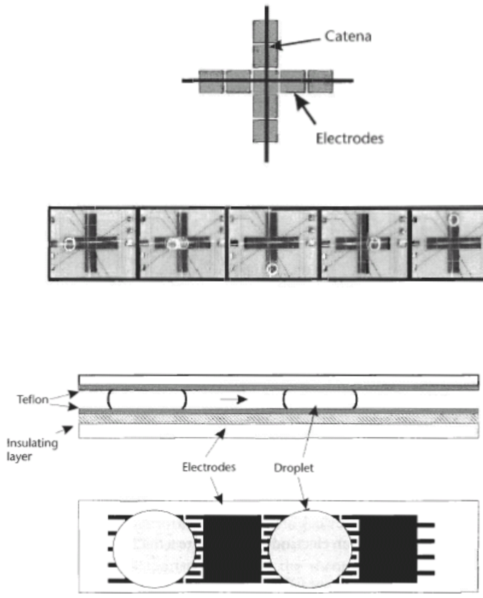
covered EWOD (Electro-Wetting On Dielectric) system

open EWOD system

- Experimentally observed a saturation of contact angle vs. applied potential

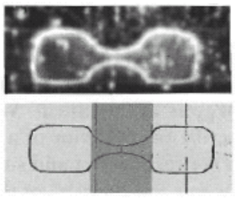


Electrowetting devices

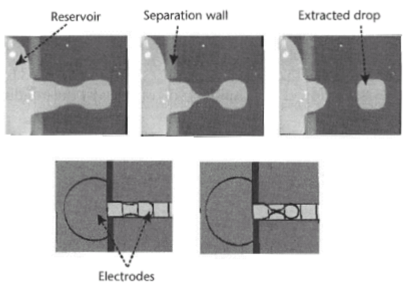


Electrowetting devices

- drop division



- drop formation by electrowetting



Problems

- Estimate the minimum size of air and water volume where the fluctuation of thermodynamics be less than 0.5%. Assume that air is an ideal gas at atmospheric pressure and fluctuations go as $\sqrt{N}/N$
- Munson1.92 Find the minimum length of the interface necessary to support a water strider. Assume the bug weighs 10^{-4} N and surface tension acts vertically upward.
  Surface tension of water σ=7.3 10^{-2} N/m.
- Munson1.41 The kinematic viscosity can measured in a capillary-tube viscometer as v=KR4t, where K is constant. Glycerin (calibration liquid) passed the tube in 1430s. A liquid with density 970 kg/m^3 did it for 900s. Find the dynamic viscosity of the liquid.