Transfers in porous media

JULY 2022

VERSION 3.0

Contents

- Characterization of porous media
- Fluid flow equation
- Mass transport

First Part: Porous Media Characterization

POROSITY

SPECIFIC SURFACE

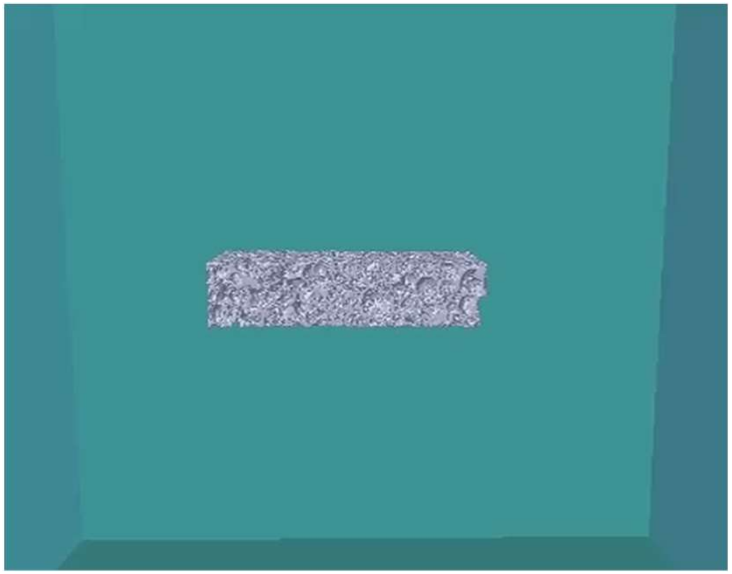
GRANULOMETRY

CAPILLARITY

Contents

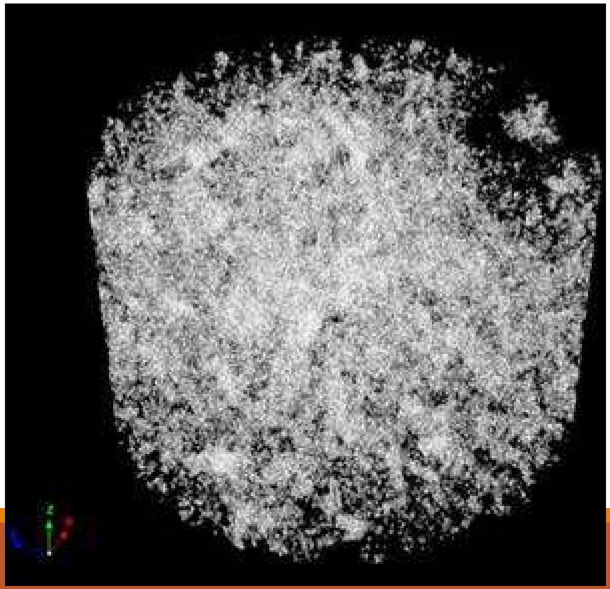
This first course will intend to introduce concepts, and main properties we will use

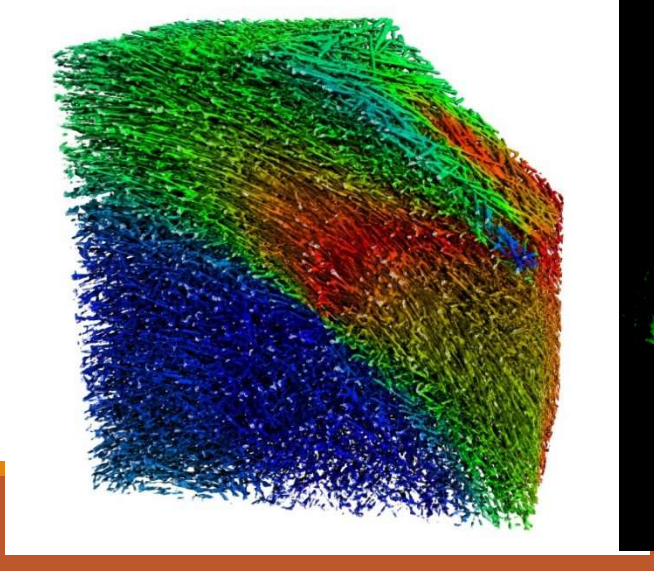
First of all, what is a porous medium ?

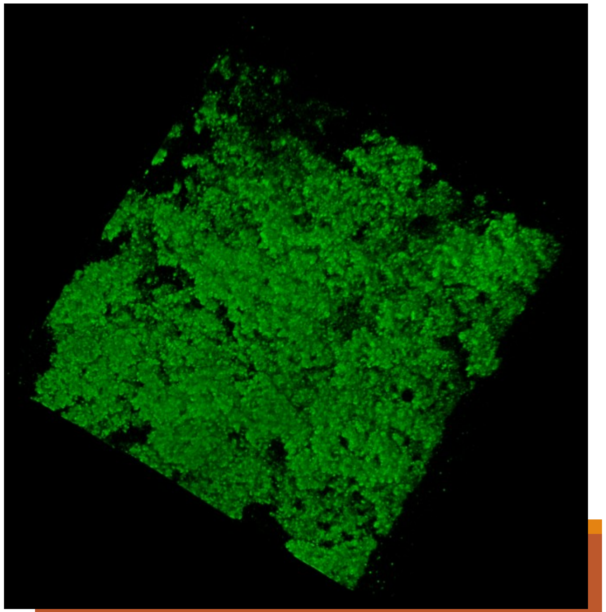


Definition

A porous medium is a medium composed of a solid structure and empty spaces called pores. These pores can be connected or not, and filled partially or completely with liquid or gas. The porous media can be consolidated, such as rock for example, or unbound, such as sand or a stack of logs.







Definition?

Porosity is the set of interstices (connected or not) of a rock or other material that may contain fluids (liquid or gas).

Porosity is also a numerical value that characterizes these interstices, the ratio of void volume of the material divided by the total volume. This value is usually noted Φ.

There are two categories of porosity: the porosity of cracks and the porosity of pores.

A crack is an empty space, two dimensions of which are much larger than the third. The crack porosity is related to mechanical or thermal stresses. In the oil and gas industry or in other contexts, hydraulic fracturing of the rock is intended to increase the macro porosity, and in some cases the micro-porosity.

Source: wikipedia

So what is the main problem

Just propose me some ideas and let's discuss

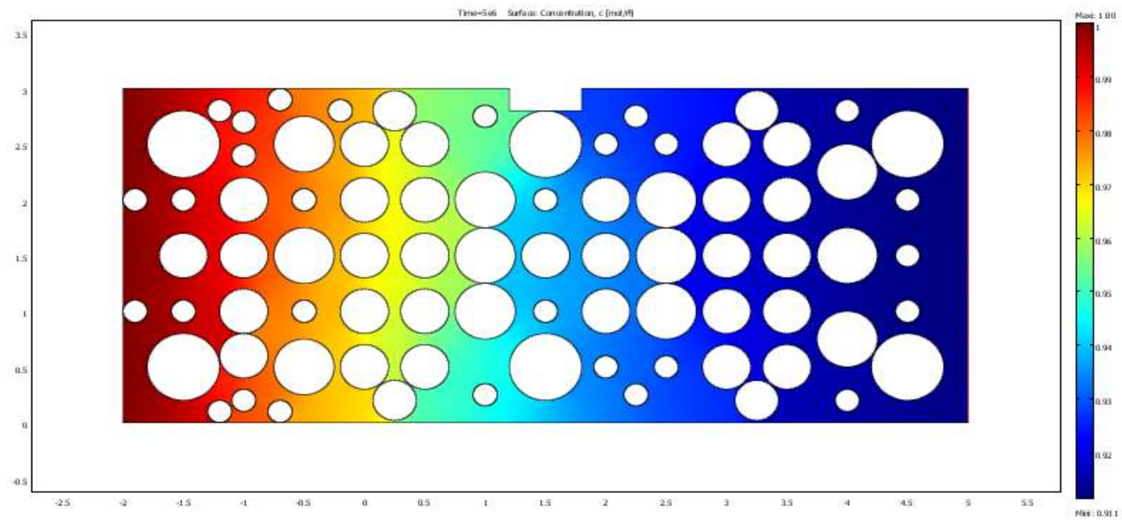
In conclusion, what are we going to do in this course?

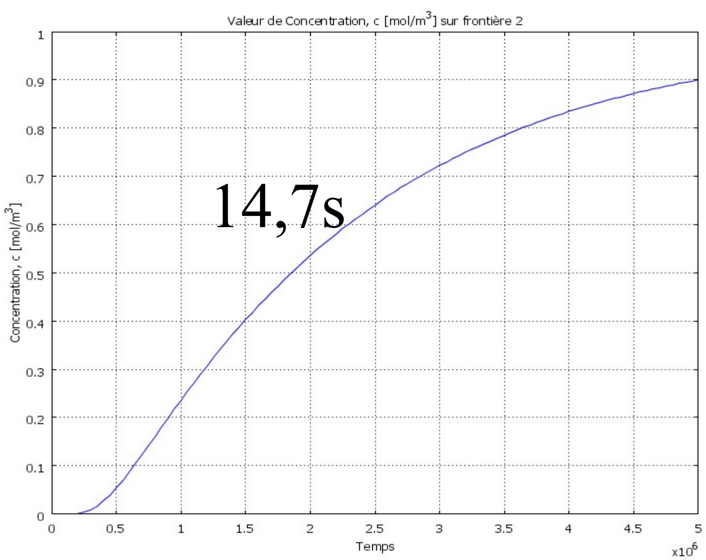
$$\underbrace{\rho \left(\frac{\partial \overrightarrow{u}}{\partial t} + \overrightarrow{u} \cdot \triangledown \overrightarrow{u}\right)}_{\text{Acceleration}} = \underbrace{-\triangledown p}_{\text{Pressure}} + \underbrace{\nu \triangle \overrightarrow{u}}_{\text{Viscosity}}$$

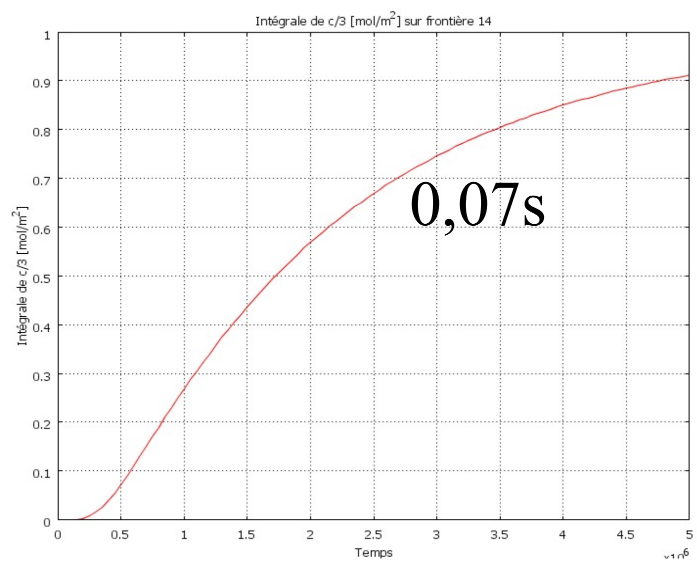
$$\underbrace{\triangledown \cdot \overrightarrow{u} = 0}_{\text{Continuity Equation}}$$

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\vec{v} c) + R$$

Upscaling in porous media….

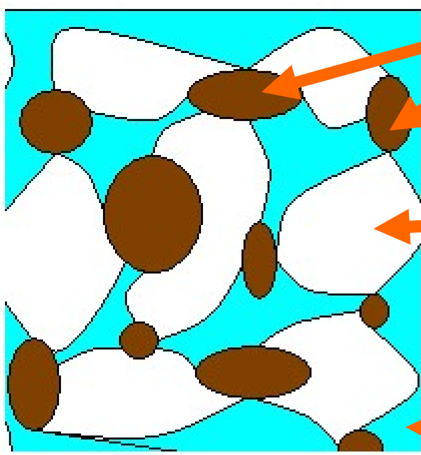






I-1 porosity

Granular porous medium of soil type



Solid phase: grains (silica, limestone, metallic oxides ...) + MO Volume Vs, Mass Ms

Gas phase

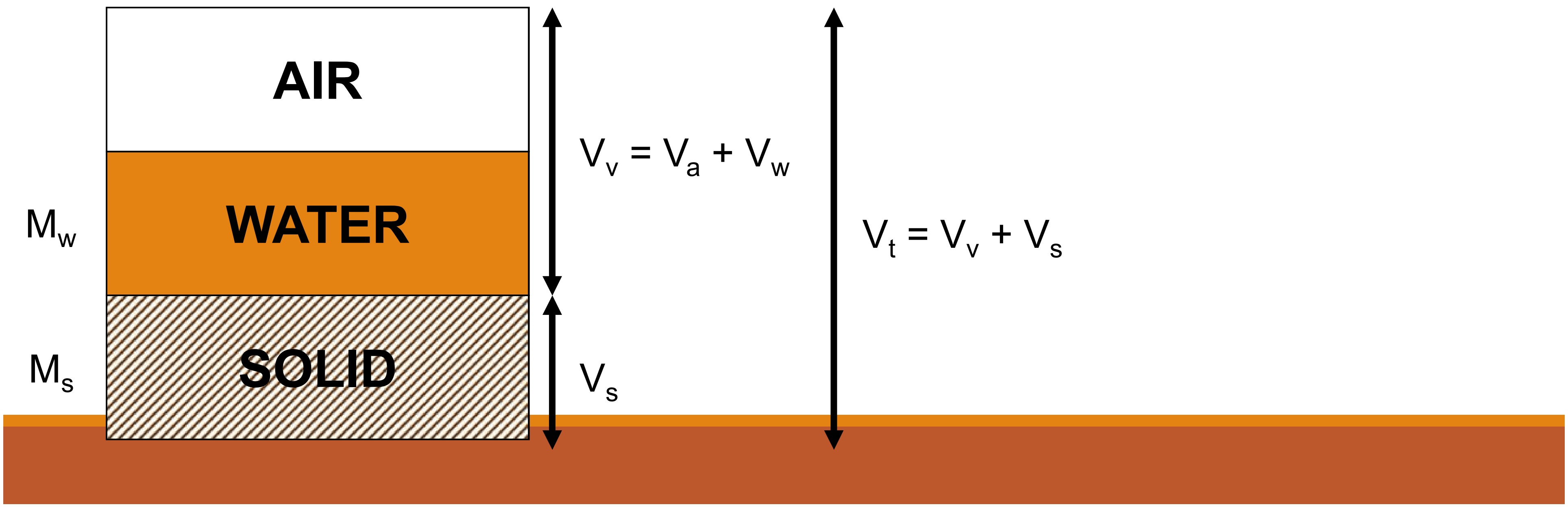
Liquid phase: leaching water (properties of H_2O: good solvent, considered incompressible, Volume **Vw**, Mass **Mw**

Void space volume: $\mathbf{V_v = V_w + V_a}$

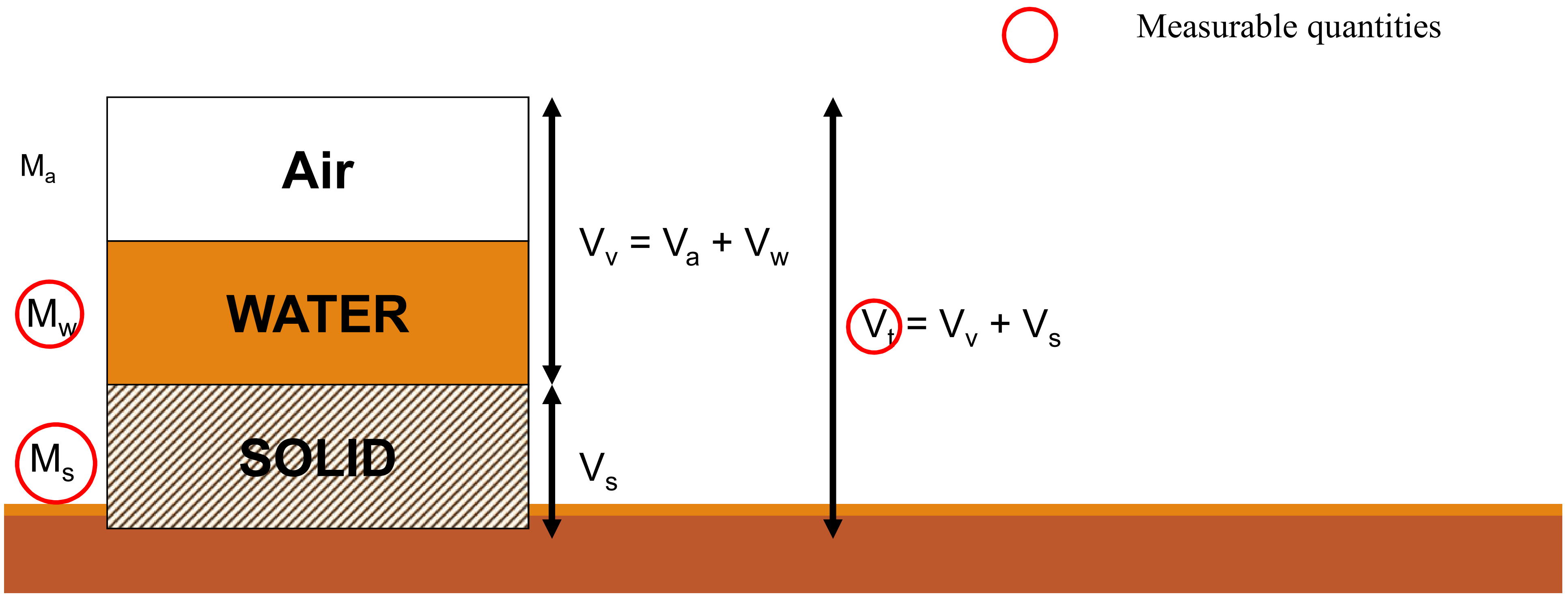
= blue + white area

I-1 porosity

For balance sheets, quantity and volume are represented as follows:



I-1 porosity

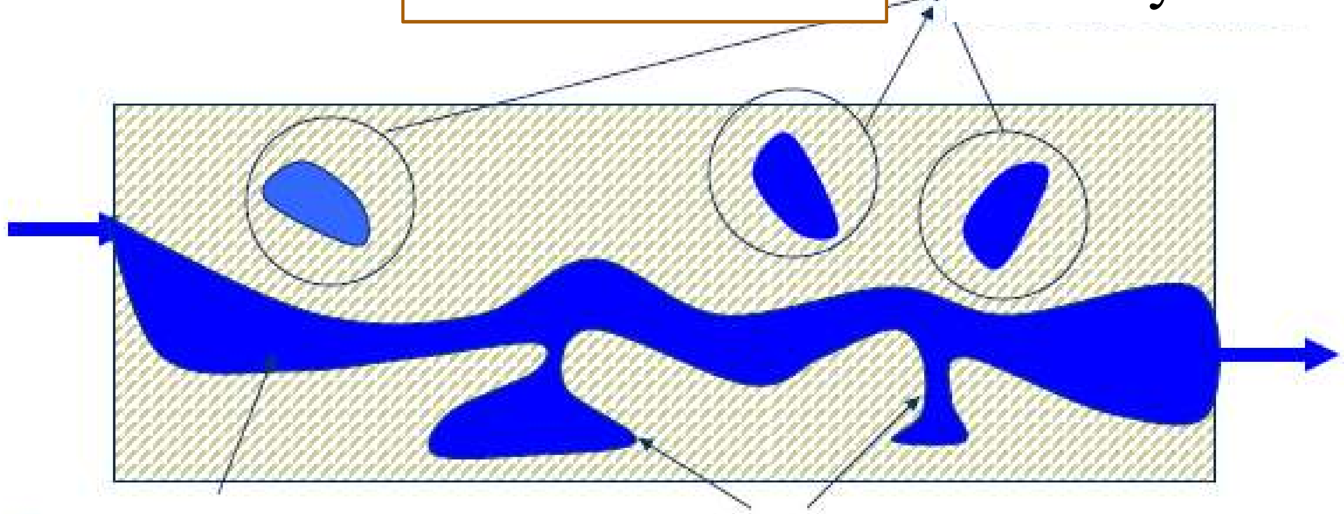

Measurable quantities
M_a
Air
M_w
WATER
M_s
SOLID
$V_v = V_a + V_w$
V_s
$V_t = V_v + V_s$

I-1 porosity

Characterisation

- porosity

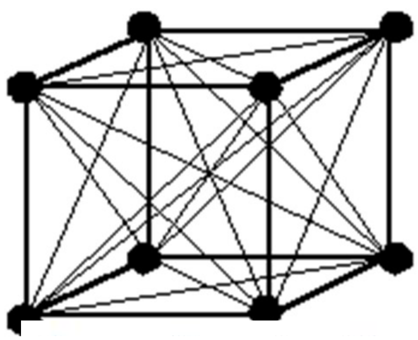
$$\varepsilon = \frac{V_{void}}{V_{total}} = 1 - \frac{V_s}{Vt}$$

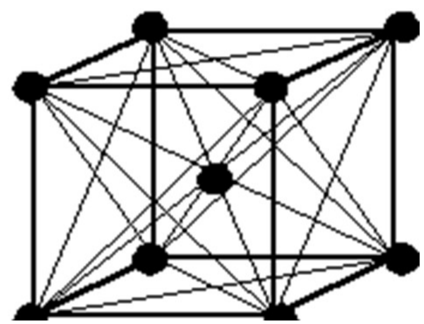


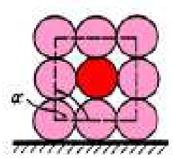
I-1 porosity

$$\varepsilon = \frac{V_{void}}{V_{total}} = 1 - \frac{V_s}{Vt}$$

Estimates

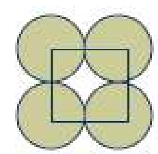


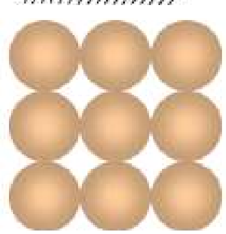


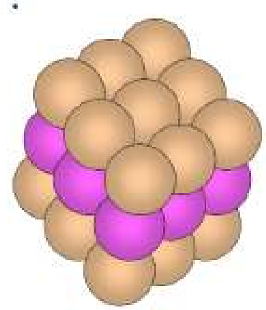


ε ?

ε ?







I-1 porosity

Characterization

Porosity $\varepsilon = \frac{V_{void}}{V_{total}} = 1 - \frac{V_s}{Vt}$

Apparent density of porous media $\rho_{app} = \frac{Ms}{V_{total}}$

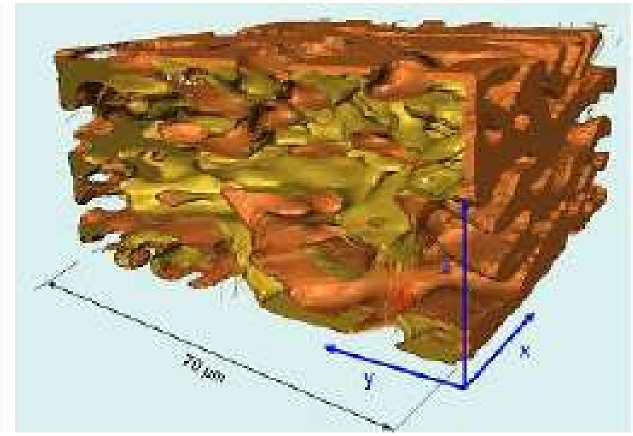
$$\varepsilon = 1 - \frac{\rho_{ap}}{\rho_s}$$

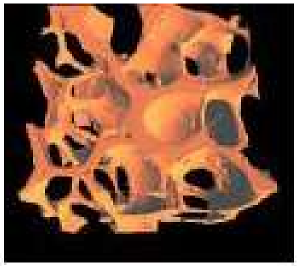
From 0.9 (fibers) to 0.01marble

I-1 porosity

Porosity estimates

$$\varepsilon = \frac{V_{vide}}{V_{total}} = 1 - \frac{V_{solide}}{V_{total}}$$





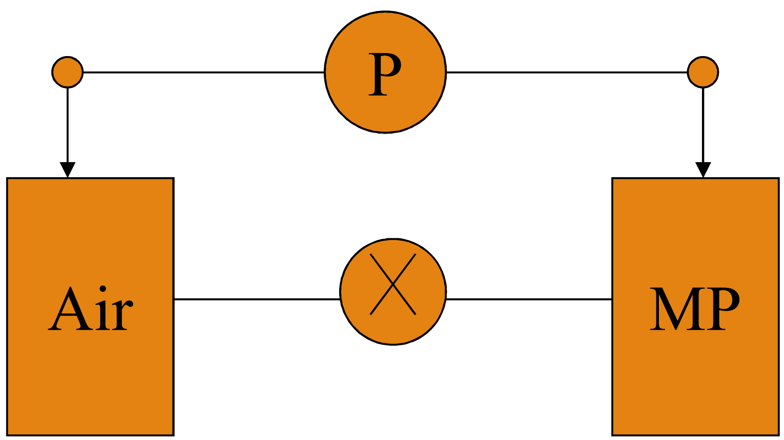
Estimates using water infiltration

Numerical estimates using microtomography

I-1 porosity

Air Pycnometer :

Easy to use and to develop. How does it work?



I-1 porosity

PYCNOMETER

t=0 $PaVa = n_1 RTa$

$P_{MP}\varepsilon V = n_2 RT_{MP}$

Opening the valves, we have

$Pa'Va = n_1' RTa'$

$P_{MP}'\varepsilon V = n_2' RT_{MP}'$

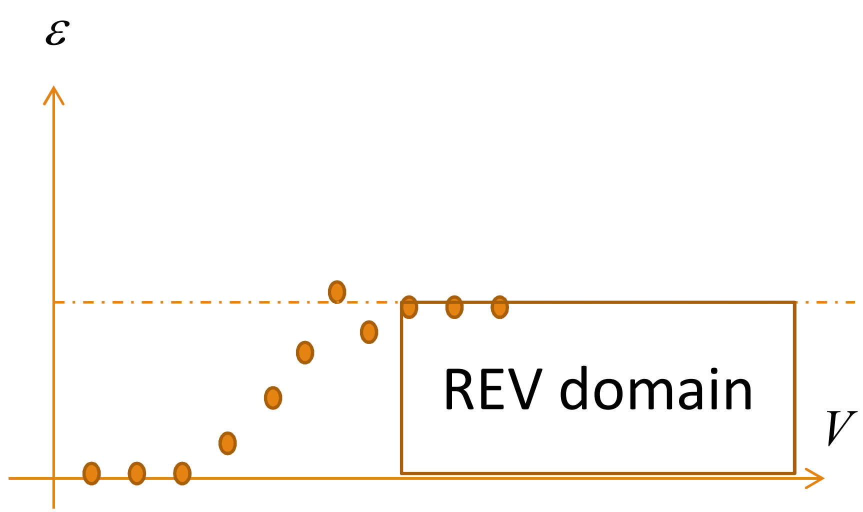
Number of moles is constant; hence we can write, assuming : $T_A = T_{MP}$

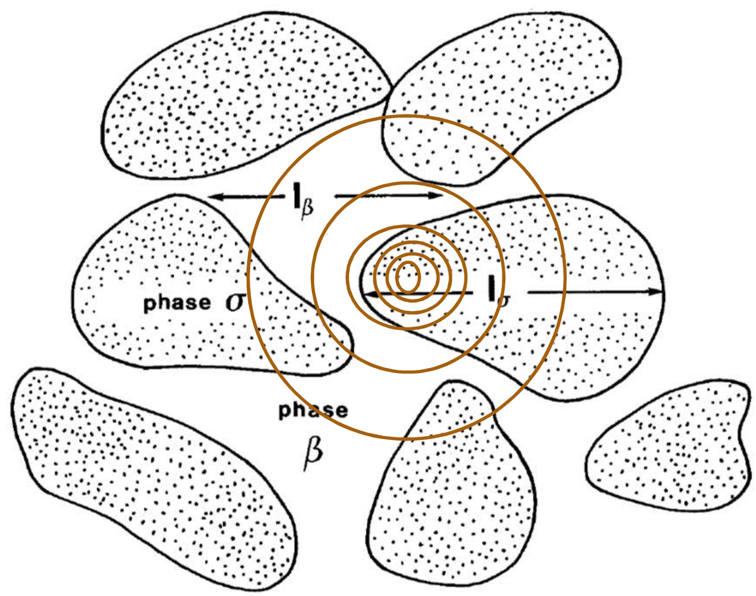
$$\epsilon = \frac{V_A}{V}\frac{T_{MP'}}{T_{A'}}\left[\frac{P_{A'} - P_A\frac{T_{A'}}{T_A}}{P_{MP}\frac{T_{MP'}}{T_A} - P_{A'}}\right]$$

I-1 porosity

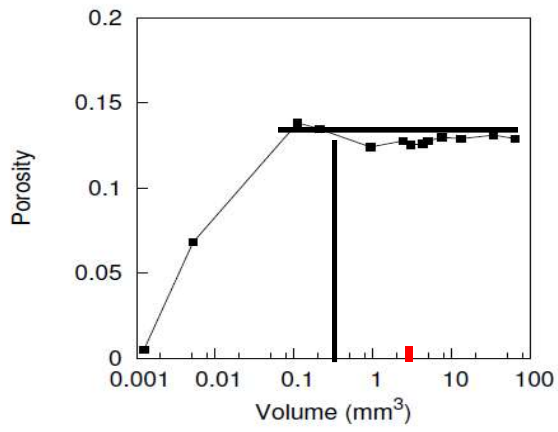
Let’s take this fictious domain…

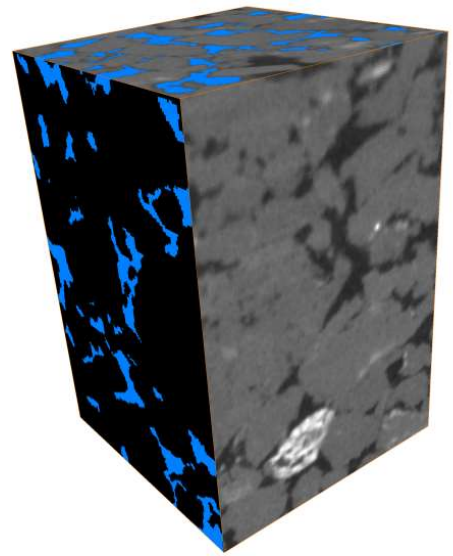
$$\varepsilon = \frac{V_\beta}{V_\beta + V_\sigma}$$

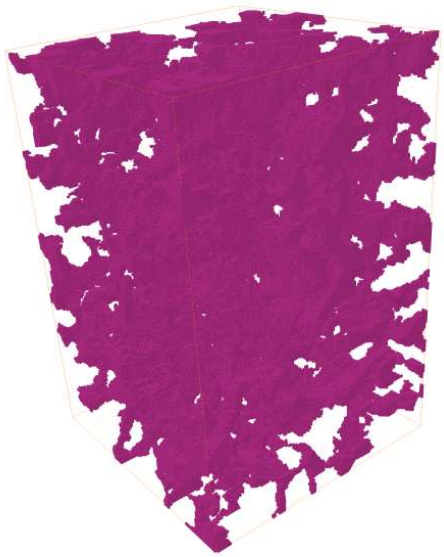




One important notion : REV







I- 2 Specific Surface

Sspec=Sip/Vs, Sip is the surface of the solid/fluid interface

<u>Ex</u> packing of n spheres radius R:

Sip= $n*4*\pi*R^2$

Vs=$n*4/3*\pi*R^3$

→ Sspec=?

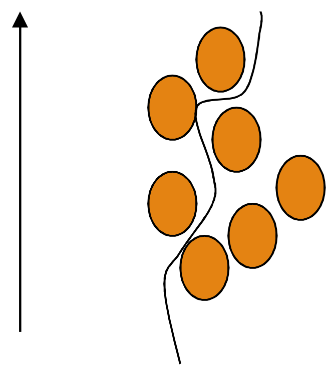
Vary from 1 to 10^n

Mass surface :

$$\Sigma m = Sip / Ms$$

I-3 tortuosity

ratio of the actual particle travel compared to that made in a straight line



It is noted τ and is from 1 to 10 for simple porous media.

How to measure it?

Ex of correlations Lanfrey et al (2010): $\tau = 1,23\frac{(1-\varepsilon)^{4/3}}{\varepsilon\phi^2}$

Φ is the sphericity index of the particles

I-4 Volumetric mass

Solid phase: $\rho s = Ms / Vs$ (~ 2000 kg / m3)

Apparent solid phase: $\rho o = Ms / Vt$ (1600 kg / m3)

The apparent density of a stacked granular material is lower than the actual density because it takes into account the porosity

I-5 Saturation

If we take it in weight or weight:

$\omega = Mw / Mt$.

In volume we have: $\theta = Vw / Vt$

We can also define the saturation:

$S = Vw / Vv$

What is θ if S is 1?

I-6 Granulometry

Dimension of a particle

Complex problem due to particle irregularity

Geometric diameter

2 Types:

- ❖Feret diameter (measured between two tangents)
- ❖Martin's diameter (average chord: length of … arent surface of the particle into two equal areas.)

- ❑Equivalent spherical diameter
- ❑Equivalent diameter of … $_s = 6/Sp$
- ❑Diamete…

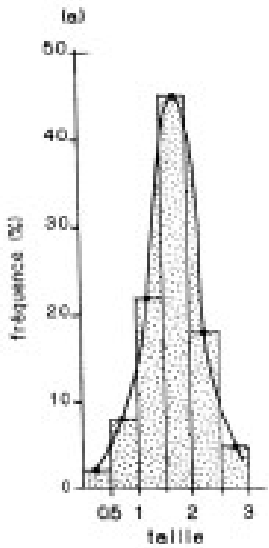
$$d_a = \sqrt{S_p/\pi}$$

$$d_{st} = \sqrt{\frac{18\mu u}{(\rho_s - \rho_l)g}}$$

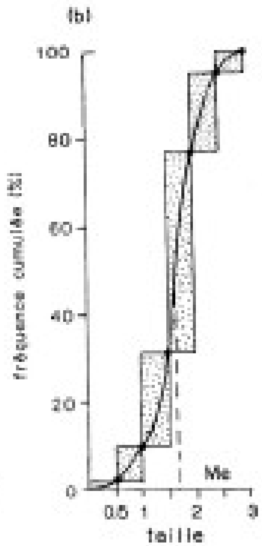
USEFUL TO SIMPLIFY CLASSIC RELATIONS
WHAT WE WILL SEE

I-6 Granulometry

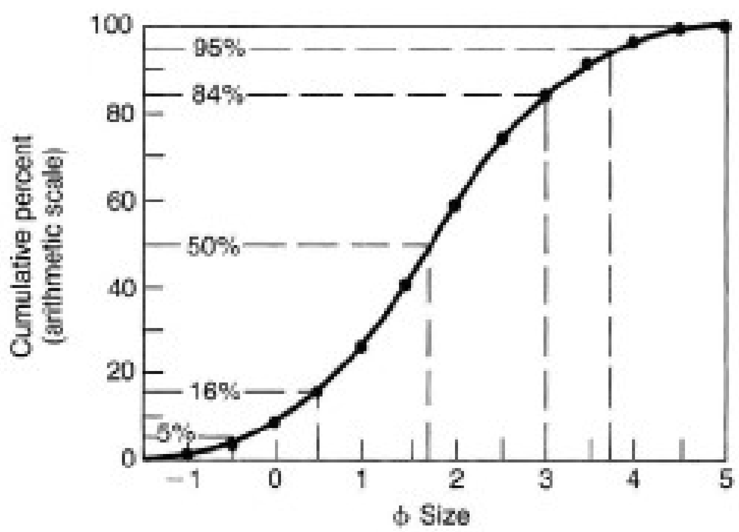
Sediments often consist of particles of very different sizes and an easy way to appreciate their particle size is to sift the sediment according to the classes defined below, then weigh the respective weight of each class. From these data, we can draw up a histogram of the distribution by class or a cumulative frequency curve



Histogram and smoothed curve



Cumulative curve



Cumulative curve

I-6 Granulometry

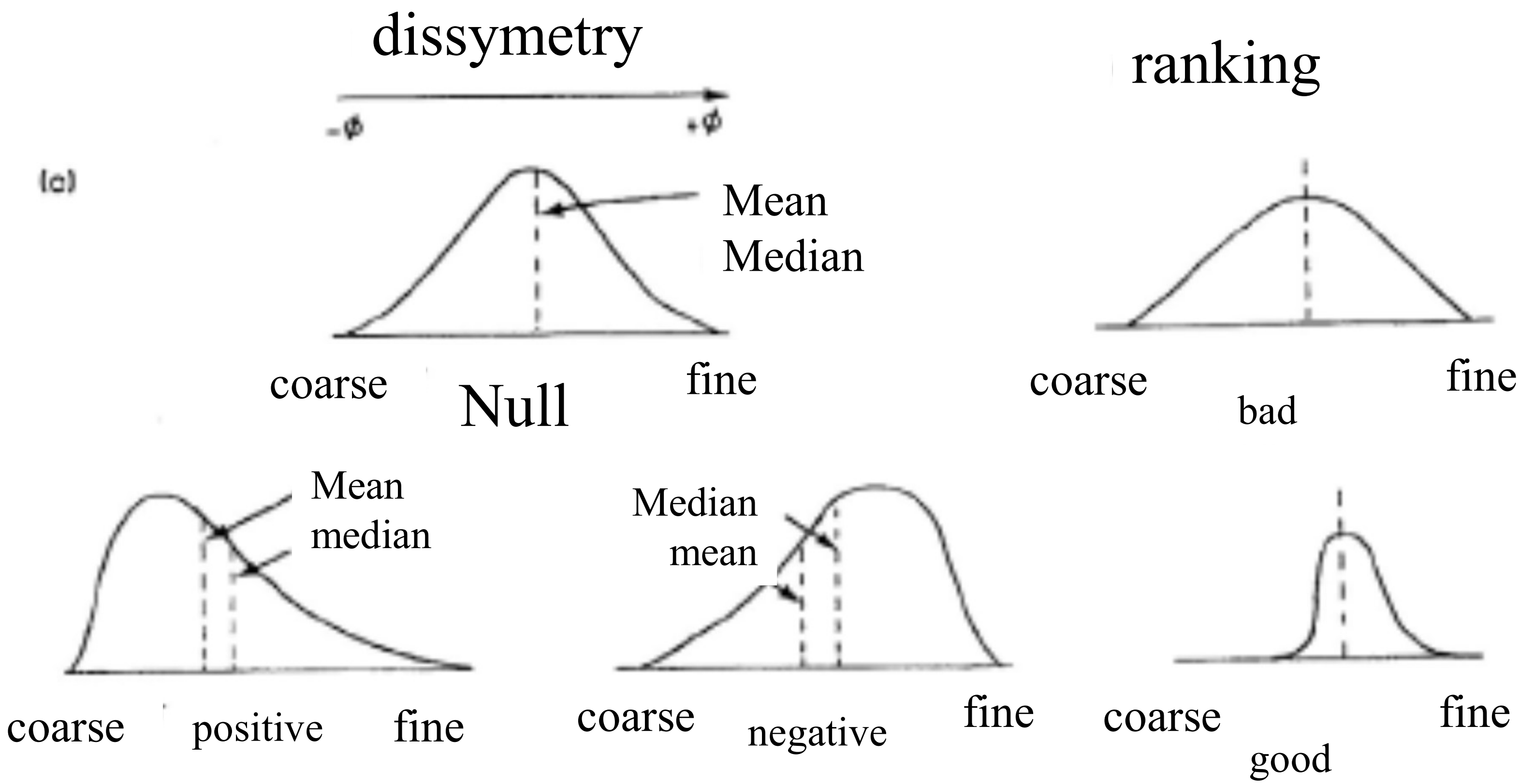
- The **mean** (M - mean), of formula (Φ16 + Φ50 + Φ84) / 3 and the median (Me - median), size corresponding to 50% of the grains on the cumulative curve. Mean and median reflect the average kinetic energy and the particle size distribution of the sediment.

- The **ranking index** (So - sorting) indicates the quality of the ranking (the index decreases with the ranking): (Φ84- Φ16) / 4+ (Φ95- Φ5) / 6. The ranking is linked to hydrodynamism and depends on sediment deposition mode.

- The **dissymmetry coefficient** (Sk - skewness). This parameter is often presented as an indicator of the sediment deposition environment:

  (Φ84 + Φ16-2 Φ50) / 2 (Φ84- Φ16) + (Φ95 + Φ5-2 Φ50) / 2 (Φ95- Φ5)

- The **acuity coefficient** (K - kurtosis), measures the shape of the peak of the curve: (Φ95- Φ5) / 2.44 (Φ75- Φ25)



Ranking		materials
<0.35ϕ	Very Well ranked	powders
0.35ϕ-0.5Φ	Well ranked	beaches
0.5-0.7Φ	Average to well ranked	beaches
0.7-1Φ	Average	rivers
1-2Φ	poor	Rivers, gravels
2-4Φ	bad	gravels

I-6 Granulometry

I-7 Particle form

Characterisation

- Sphericity Index(Wadell)

$$\phi = \frac{S_{sphère}}{S_{réelle}} \qquad \tau = 1,23\frac{(1-\varepsilon)^{4/3}}{\varepsilon\phi^2}$$

- Form Factor (Heywood)

$$\Psi_v = V_p / d_p^3$$

- Ratio d_{min}/d_{max}

Measurement

- Microscopy (optical ou FIB-SEM) + image analysis

II- Water (Fluid) behaviour in porous media

II- Various states of water in a porous medium:

a) Free water:

This is the water that flows freely, in macropores, cracks wide a few centimeters or smaller, the size of a few millimeters or less, but allow a flow under the effect of gravity.

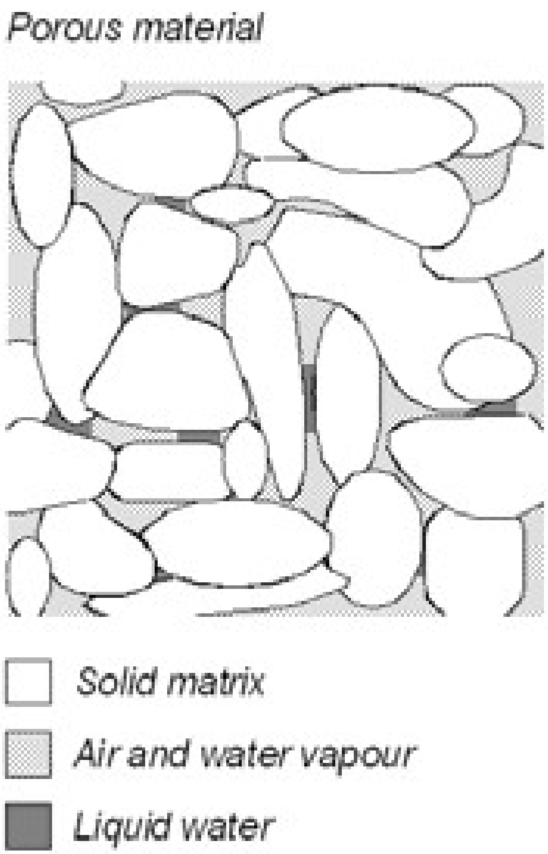
b) capillary water:

It fills capillary pores, so small that they have the size of a hair: displacements depend on laws no more of the gravity but of the capillarity. This is visible when placing a block of dry rock or even a dry sponge on a flat plate filled with water: the block or sponge "suck" the water from the bottom up, defying the laws of the severity

c) hygroscopic water and water of hydration:

Hygroscopic water is water that is trapped on the surface of pores. The water of hydration is the one, even more microscopic, which is included inside the minerals ... These two waters can not be moved by physical processes (gravity, atmospheric pressure, evaporation with the free air neither nor osmotic pressure related to the absorbent hairs of plant roots). They do not intervene at all in the balance sheets and transfers of water that are considered at the scale of a watershed and that could potentially feed more or less directly a watercourse.

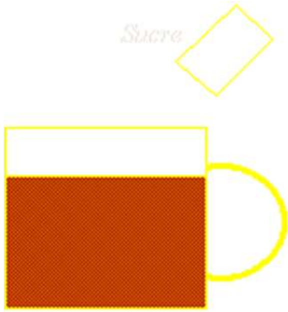
A balance?



Grunewald, J., Häupl, P., & Bomberg, M. (2003). Towards an engineering model of material characteristics for input to ham transport simulations-Part 1: an approach. *Journal of Thermal Envelope and Building Science*, *26*(4), 343-366.

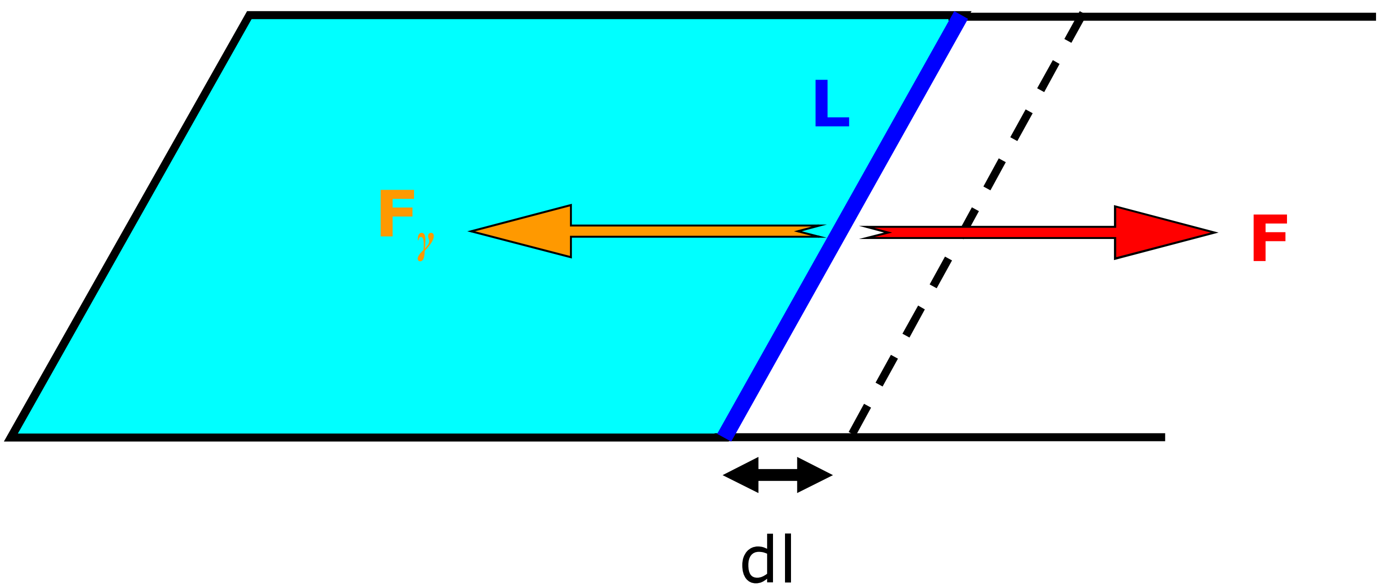
A weird thing ... interfacial effects

Highlighs



<u>Def:</u> Surface tension, or interface energy, or surface energy, is the tension that exists at the separation surface of two media. In fact, the surface tension, or surface tension, is that which exists between a solid or a liquid and a gas. The tension between two solids, two liquids, or a liquid and a solid is rather called interfacial tension.

Surface Tension Definition



Surface Tension γ en **$N.m^{-1}$**

Force to displace the layer by dl ?

$$F=2\gamma L$$

Energy consumed

$$dW=2\gamma L\,dl = \gamma\,dS$$

The factor 2 takes into account the fact that the film has a certain thickness along z and thus two faces, so that the length of the layer is twice the width of the film.

Surface tension definition

Values :

Liquide	γ (N.m^{-1})
Glycol	0,046
Glycerin	0.063
Water	0,07
Blood	0,073
Mercury	0,436

with $$\gamma = \left(\frac{\partial F}{\partial S}\right)_{T,V,n}$$

F=U-TSe

Liquid	0°C	20°C	40°C	60°C	80°C	100°C
water	75,64	72,75	69,56	66,18	62,61	58,85
Benzene	31,60	28,90	26,30	23,70	21,30	
Toluène	30,74	28,43	26,13	23,81	21,53	19,39
Carbon tetrachloride		26,80	24,30	21,90		
Methanol	24,50	22,65	20,90			15,70
Ethanol	24,05	22,27	20,60	19,01		
Acetone	26,21	23,70	21,16	18,60	16,20	

Effects of temperature on surface tension

Experimental results show a decrease in surface tension as temperature increases

Minimization of free energy

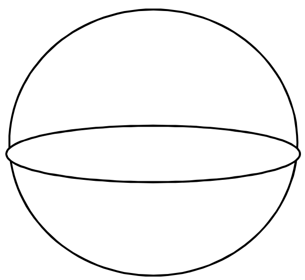
Surface minimization

$$E = \gamma S$$

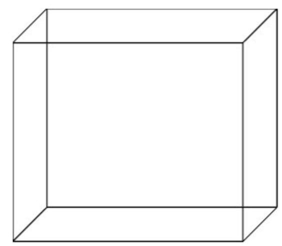
avec

$$\gamma = \left(\frac{\partial F}{\partial S}\right)_{T,V,n}$$

F=U-TS



V=1m^3



S=4.83 m^2

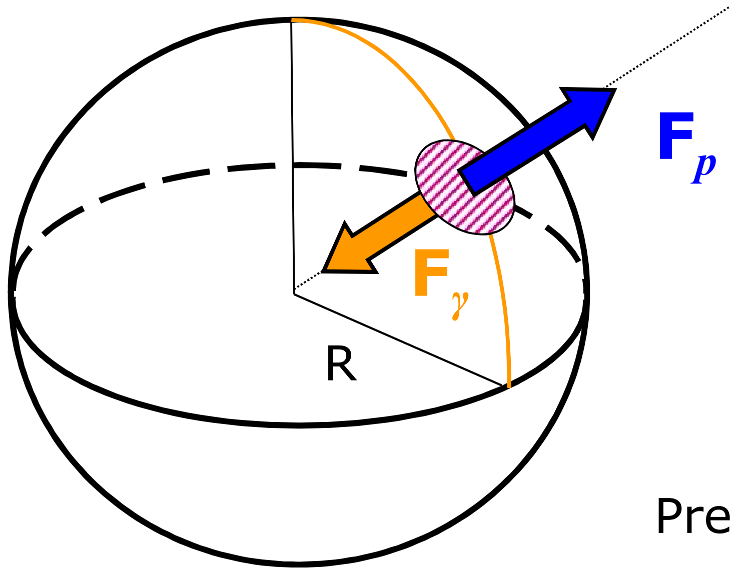
S=6 m^2

There is no cubic raindrop.

The interfacial tension tends to pull the surface inward in a state where the free energy will be minimal!

Laplace Law

Overpressure in drops of water and bubbles



Surface tension tends to decrease the surface

F_γ must therefore be compensated by the pressure forces F_p

Pressure: it is necessary to have $P_i > P_e$

$W_F = \gamma S = 4\pi R^2 \gamma$ if R varies dR ➡ $dW_F = \gamma dS = 8\pi R \gamma dR$

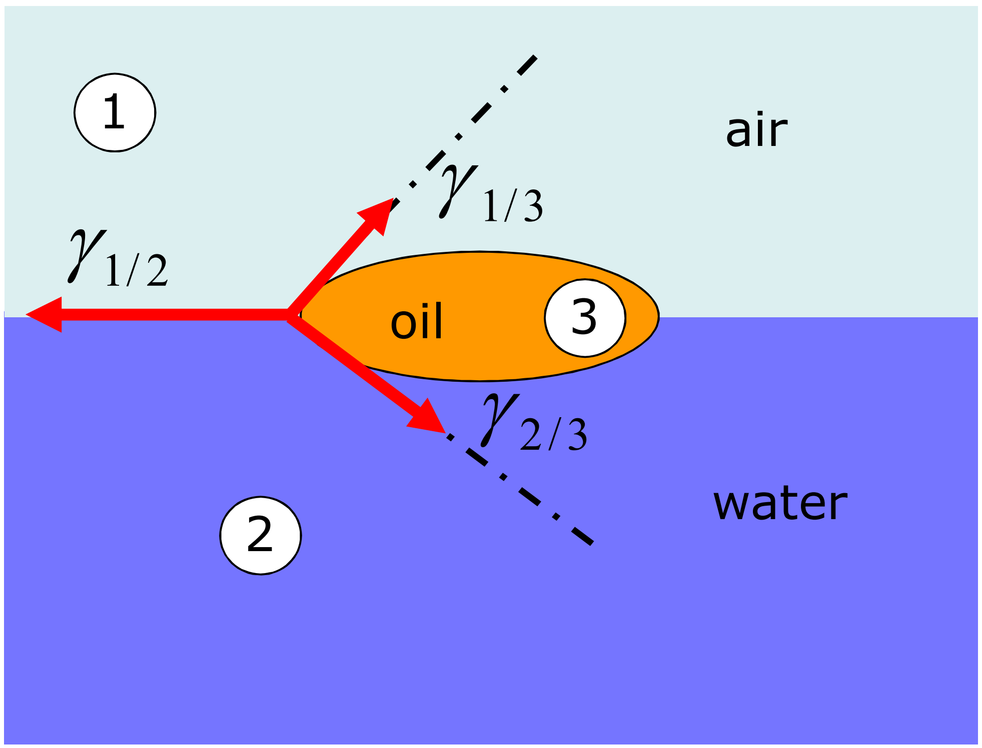
Let E be the total energy of the system (area and volume), if we contract the drop, this must be compensated by an increase in the pressure Δp $dF = -\Delta p dV + dW_F$

equilibrium, $dF = 0 = -\Delta p dV + \gamma dS = -\Delta p 4\pi R^2 dR + 8\pi R \gamma dR$

⇨ $$\Delta p = \frac{2\gamma}{R}$$

Wetting: Young's conditions

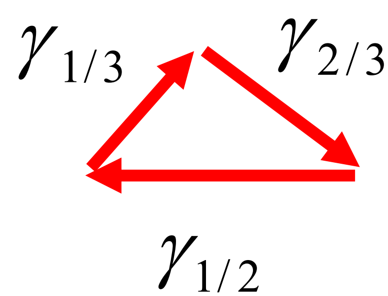
Liquid / solid balance



Balance at the contact point

$$\vec{F}_{1/2} + \vec{F}_{1/3} + \vec{F}_{2/3} = \vec{0}$$

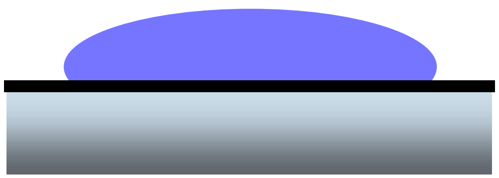
Contact Triangle:



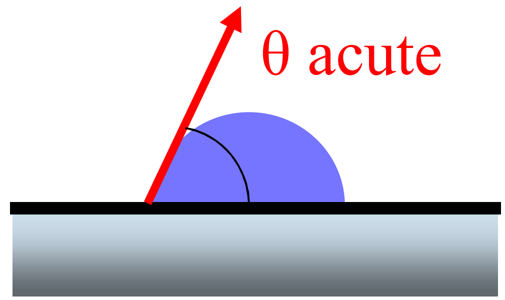
Wetting: Young's conditions

Contact Liquid/ gas/ solid

$\theta \sim 0$

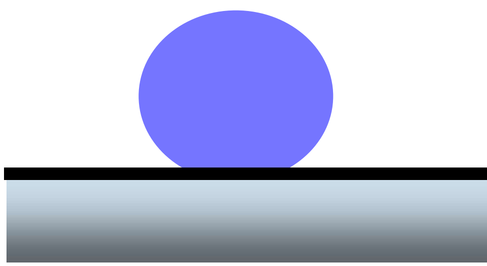


θ acute

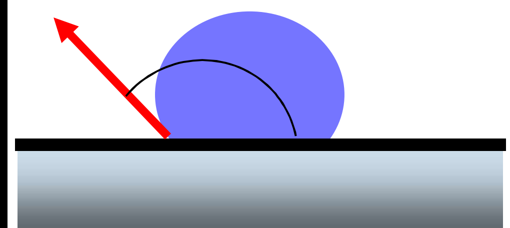


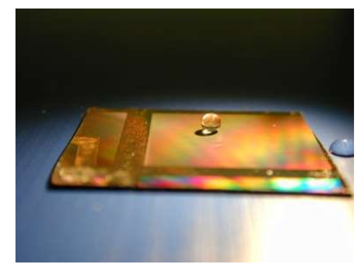
Strong wetting

$\theta = 180°$



θ obtuse



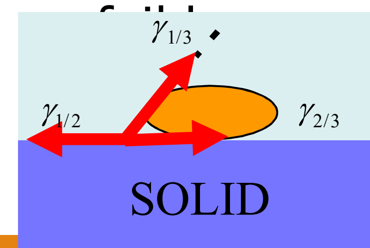


Weak wetting

Young expression

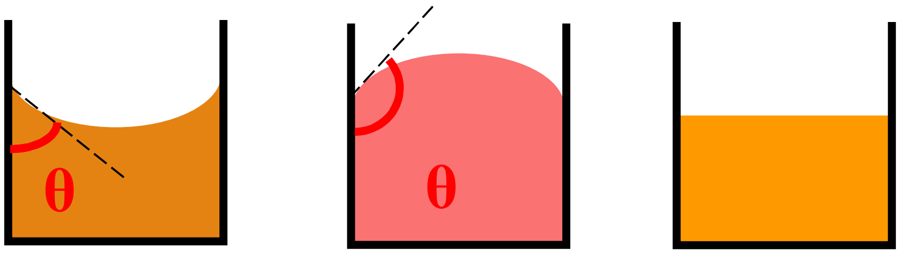
$$\gamma_{1/2} = \gamma_{1/3}\cos\theta + \gamma_{2/3}$$

$$\Rightarrow \cos\theta = \frac{\gamma_{1/2} - \gamma_{2/3}}{\gamma_{1/3}}$$

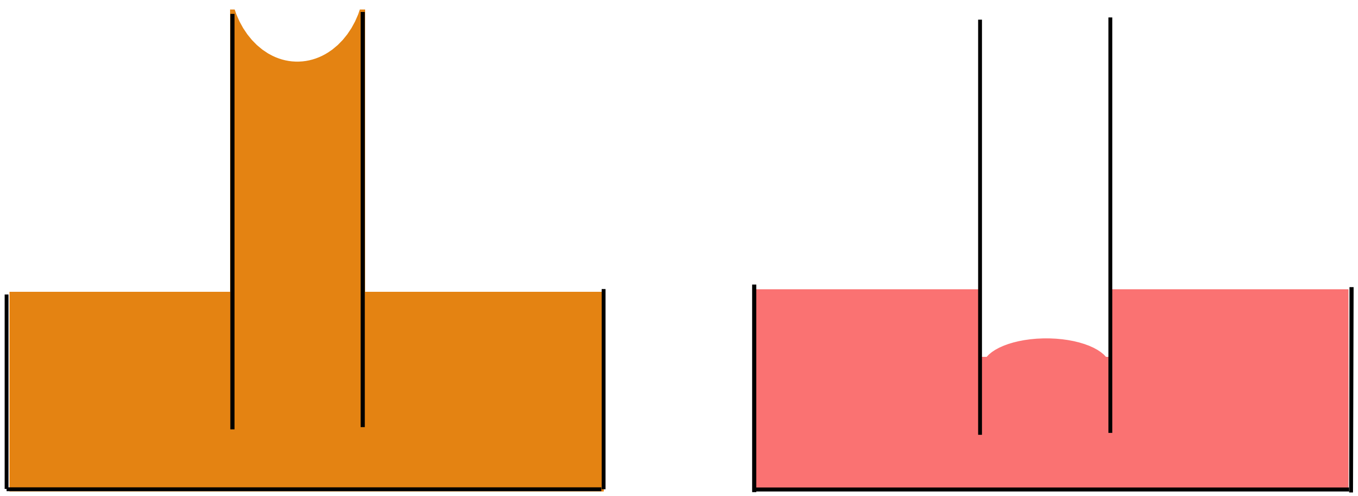


Capillarity

How is it possible to see this phenomenon?



water mercury Alcool



rise descent

AN: teflon

$\gamma_{1/2} = \gamma_{s/g} = 19 mJ / m^2$

$\gamma_{2/3} = \gamma_{l/s} = 50 mJ / m^2$

$\gamma_{1/3} = \gamma_{l/g} = 73 mJ / m^2$

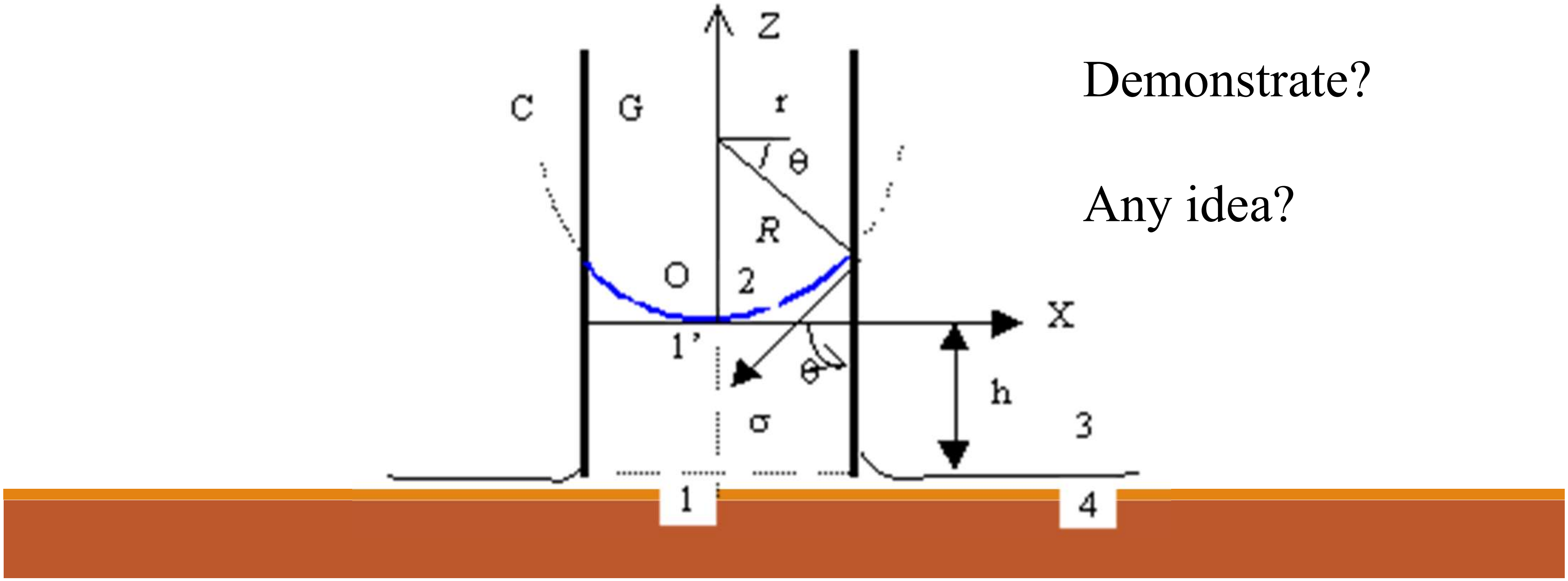
$\Rightarrow \cos\theta = -0,42$

$\theta \approx 120°$

Jurin's law

Capillary rise – Jurin's law

the phenomenon of capillary ascension can be understood by using the Laplace equation. When a small diameter cylindrical tube is immersed in a liquid, a difference in level is observed between the column of the liquid and the external reservoir. Let's calculate this level difference called **capillary rise height**

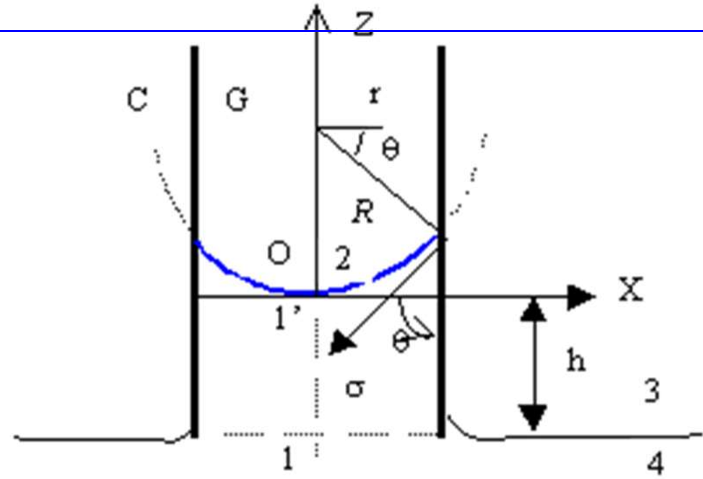


Your mission?

Demonstrate?

Any idea?

Jurin's law



Capillary Ascension

meniscus formed in a tube of radius r of spherical shape of radius R. Between 1 'and 2, Laplace's law is applied:

Then : (1) $p_2 - p_{1'} = \frac{2\gamma}{R} = \frac{2\gamma\cos\theta}{r}$ $\cos\theta = r/R$

On the other hand, the hydrostatic pressure difference between points 1 (or 4) and 1 'is (2): $p_{1'} - p_4 = -\rho_L g h$

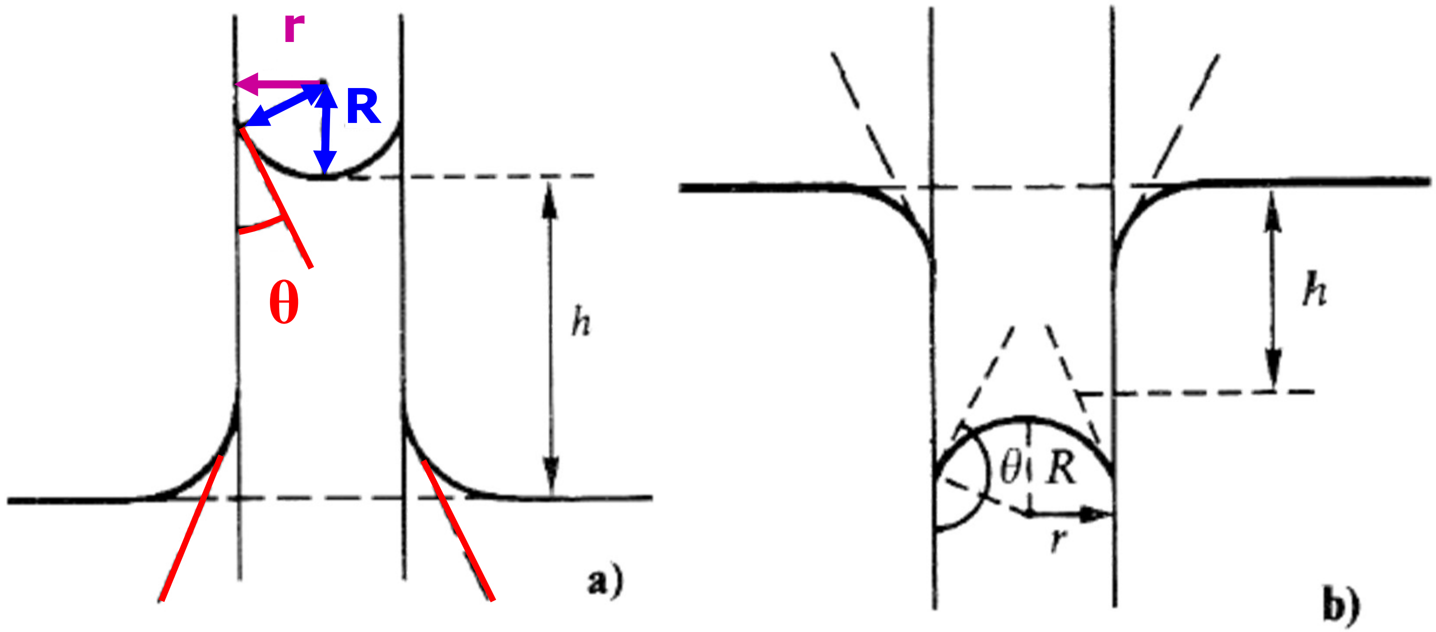
The difference in pressure that exists in the gas column between points 2 and 3 is (3): $p_3 - p_2 = \rho_G g h$

By performing the sum of these three equations, we find (4): $p_3 - p_4 = \frac{2\gamma\cos\theta}{r} + (\rho_G - \rho_L) g h$

Jurin's law.

$$h = \frac{2\gamma\cos\theta}{r(\rho_L - \rho_G) g}$$

Jurin's law



cos $\theta = r / R$

Laplace : $\Delta p = \dfrac{2\gamma}{R} = \dfrac{2\gamma\cos\theta}{r}$

Hydrostatics: $\Delta p = \rho g h$

$$h = \frac{2\gamma\cos\theta}{\rho g r}$$