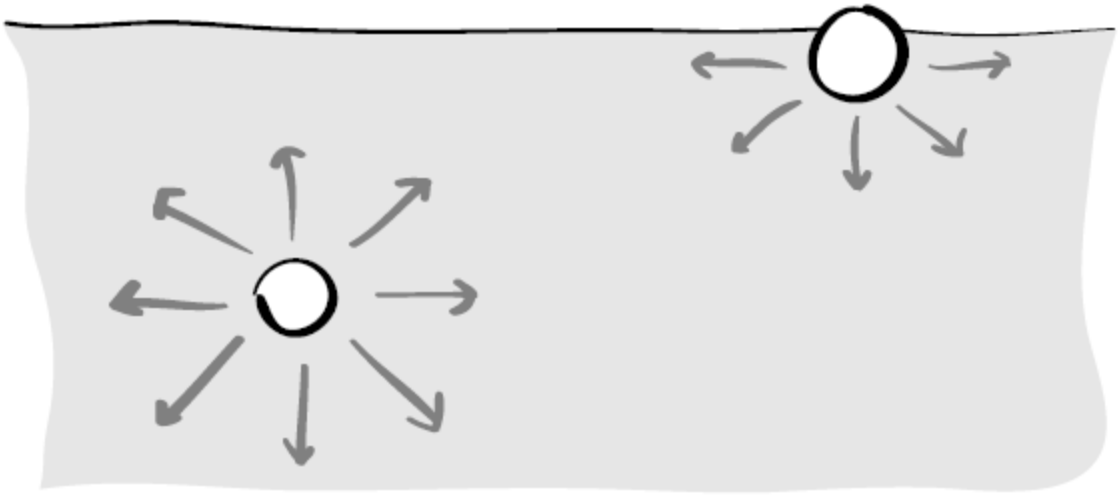
Multiscale wetting phenomena and grains

Jarray Ahmed

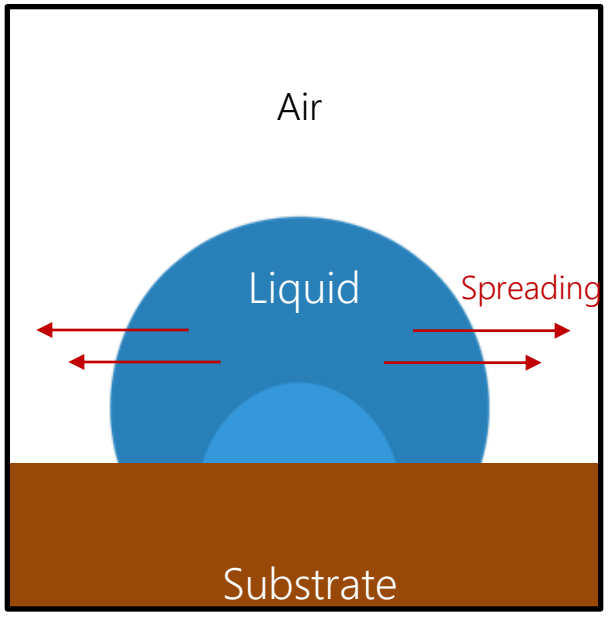


Introduction to wetting

- Wettability and Spreading?

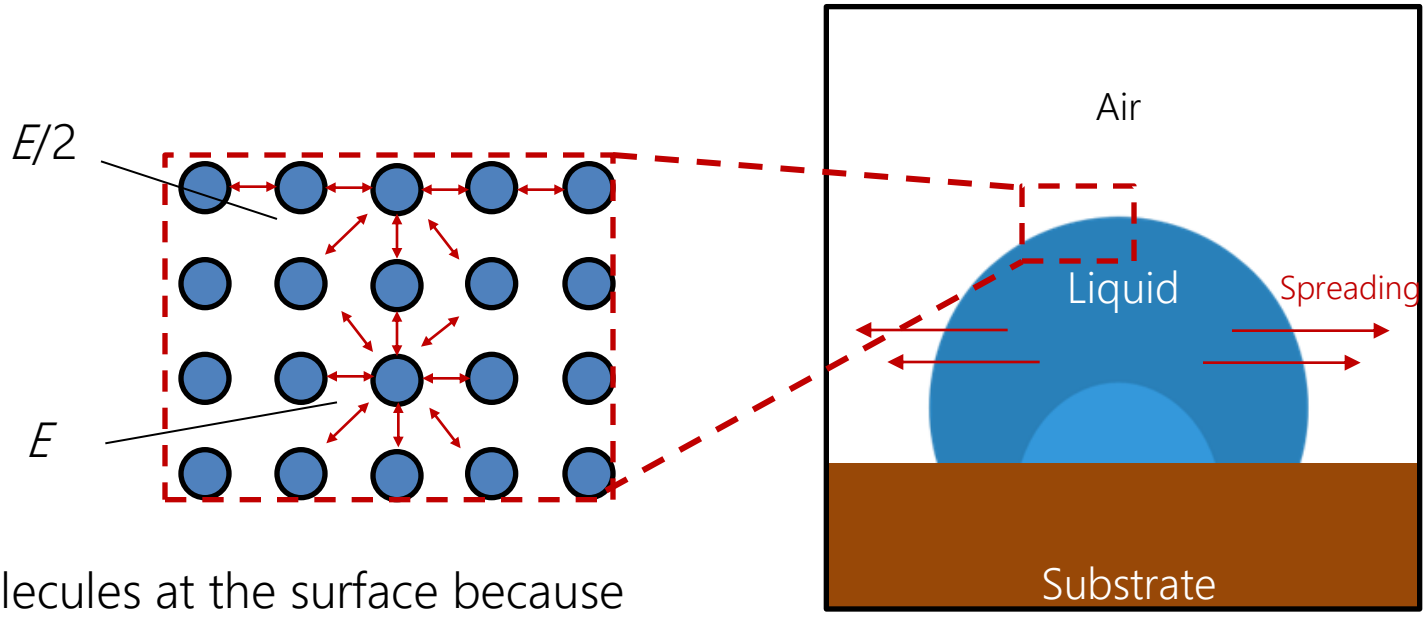
Wettability is the tendency of one fluid to spread on or adhere to a solid surface in the presence of other immiscible fluids.

Wettability refers to interaction between fluid and solid phases.



Introduction to wetting

- Wettability ➔ Surface tension (γ)



"Unhappy" molecules at the surface because they are missing half their attractive interactions

$$E = \gamma.A$$

$$F.dh = dE = \gamma.L.dh$$

$$F = \gamma.L$$

Water does not overflow

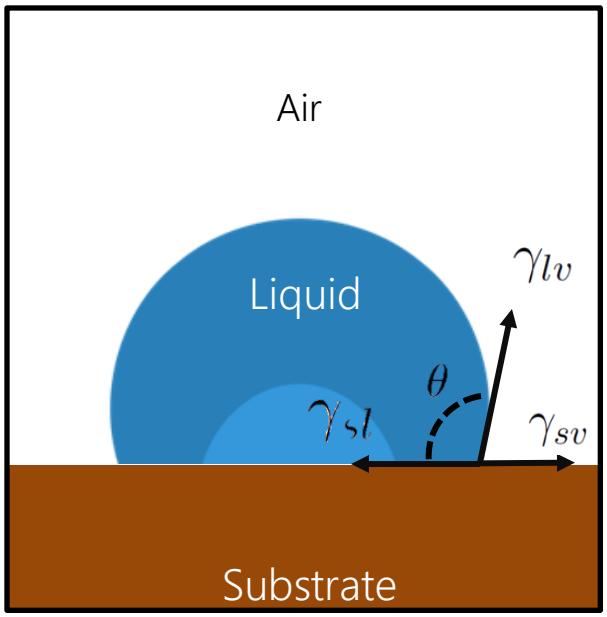
Introduction to wetting

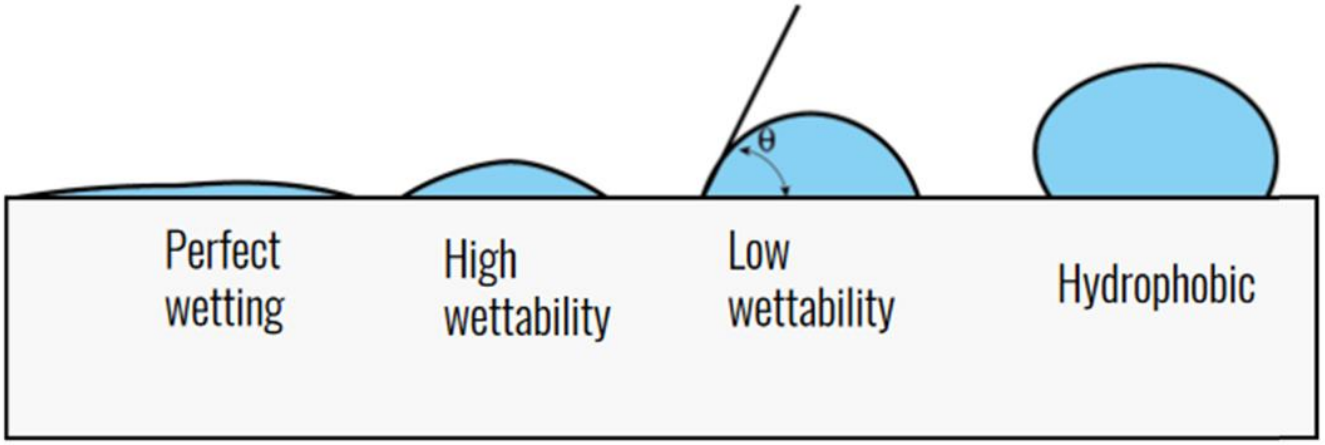
- Wettability ➔ Contact angle

Young equation: $\gamma_{sv} = \gamma_{sl} + \gamma_{lv} cos\theta$

Spreading coefficient: $S = \gamma_{sv} - (\gamma_{sl} + \gamma_{lv})$

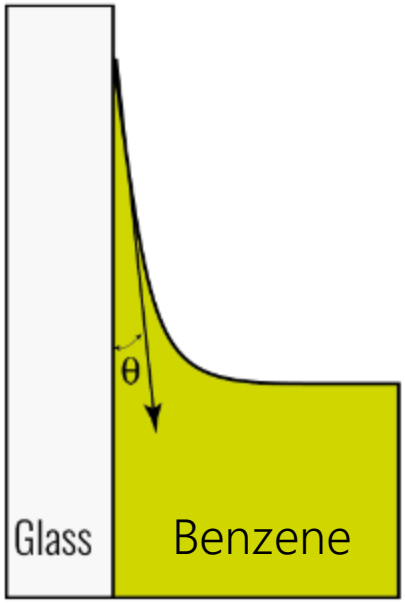
If $S > 0$ Spontaneous spreading

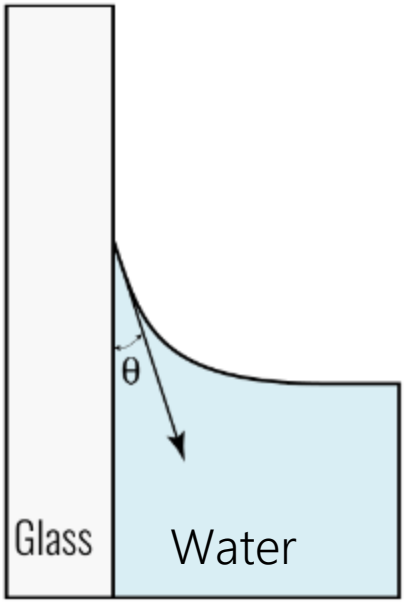


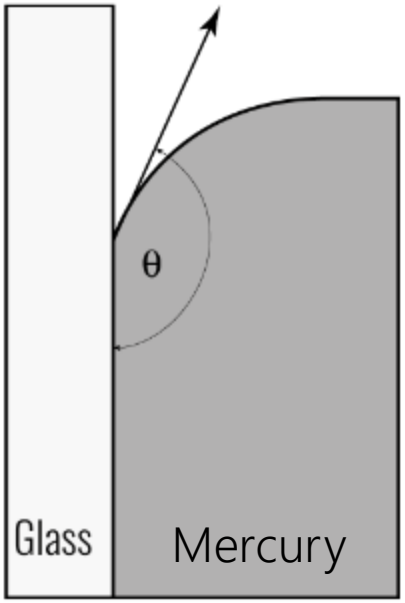


Introduction to wetting

- Wettability ➔ Contact angle







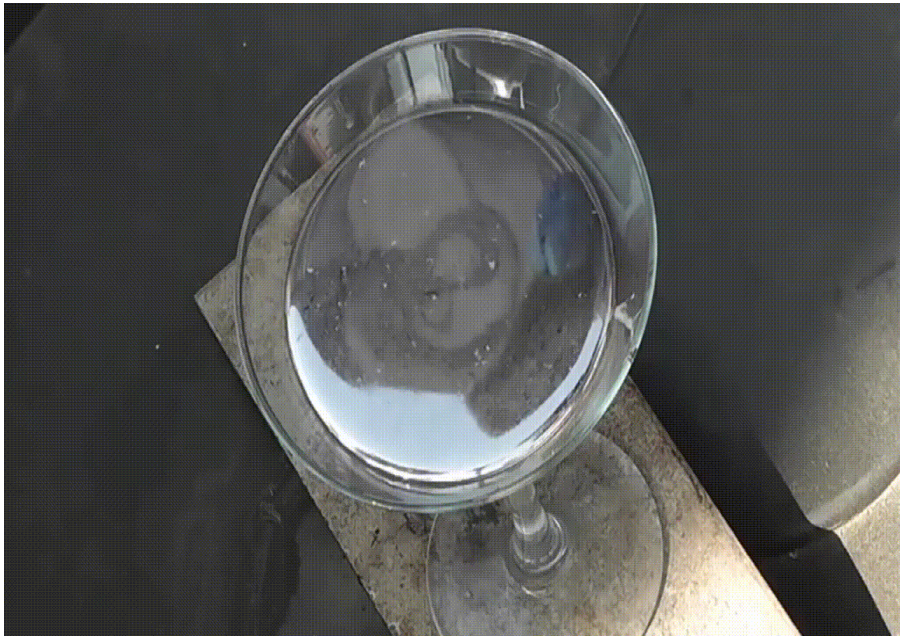
Water	72.8	10^{-3} N.m^{-1}
Benzene	28.8	
Blood	60	
Mercury	486	

Introduction to wetting

- Wettability ➔ Contact angle

Water (72.8 10^{-3} $N.m^{-1}$)

Mercury (486 10^{-3} $N.m^{-1}$)

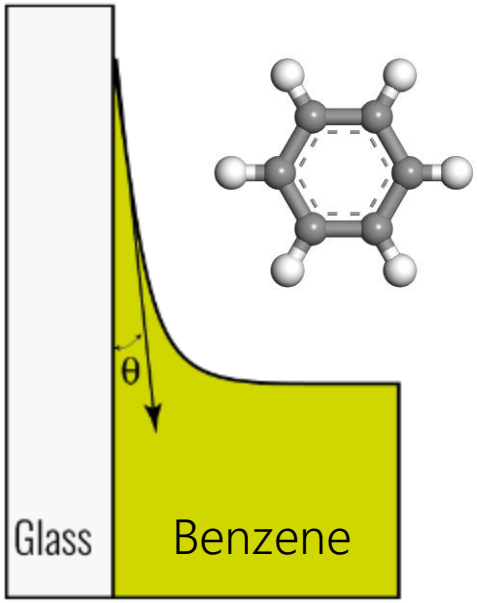


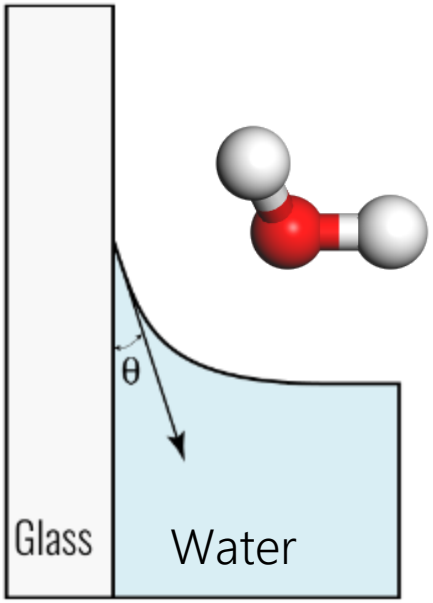
This also depends on the type of substrate (or sponge) used!

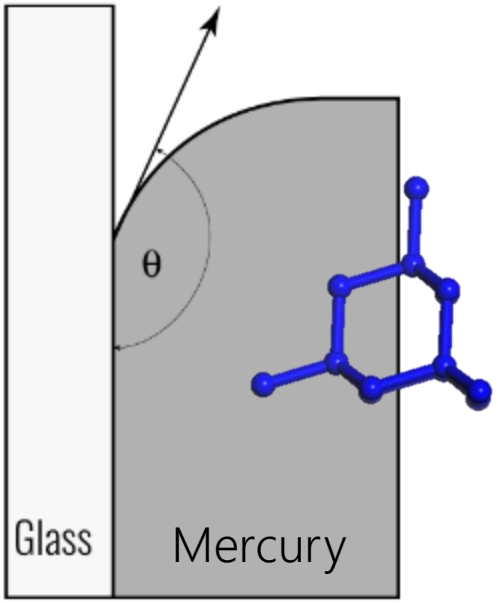
But why exactly?

Introduction to wetting

- Wettability ➔ Contact angle ➔ molecular interactions







Water	72.8	10^{-3} N.m^{-1}	Highly polar with high hydrogen bonding
Benzene	28.8		Non-polar, only dispersion
Blood	60		Polar (mostly made of water)
Mercury	486		Metalic bonds

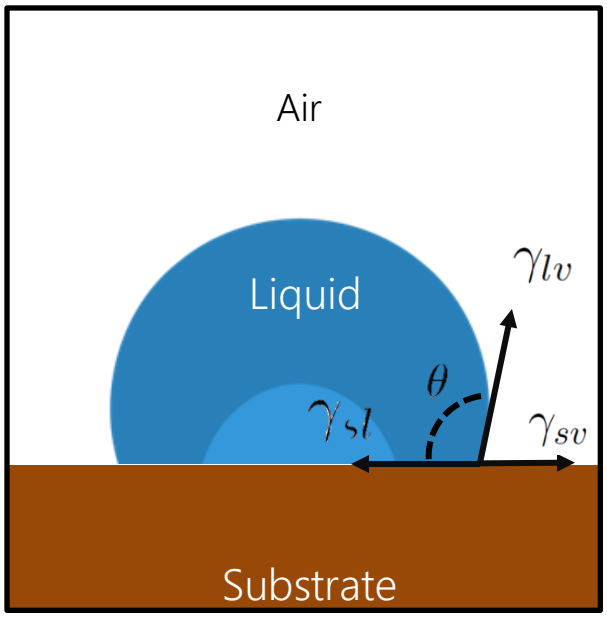
Introduction to wetting

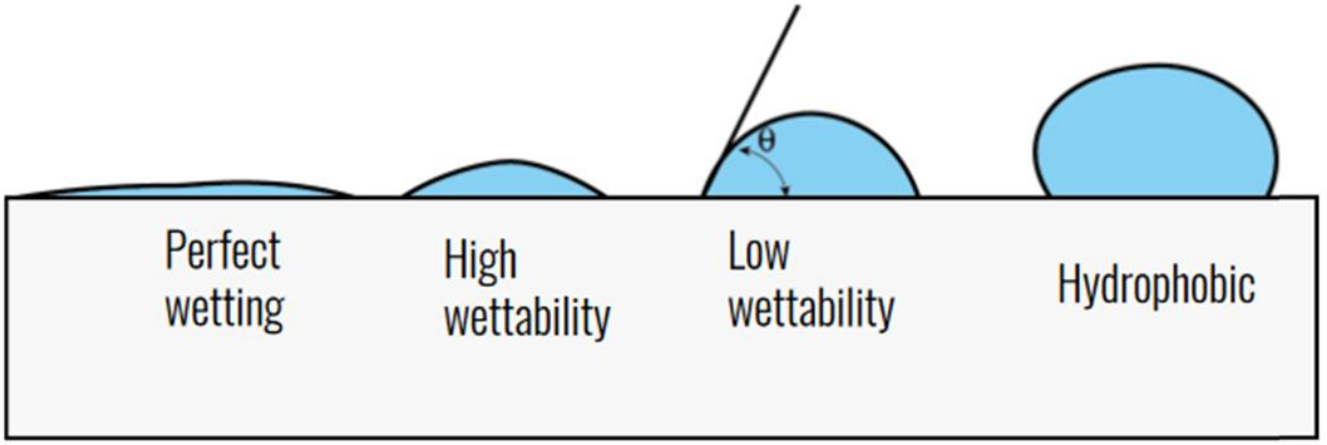
- Wettability ➔ Contact angle ➔ Intermolecular interactions

Owens and Wendt + Young:

$$cos\theta = -1 + 2\frac{\sqrt{\gamma_s^d \gamma_f^d}}{\gamma_f} + 2\frac{\sqrt{\gamma_s^p \gamma_f^p}}{\gamma_f}$$

Subscripts "*d*" and "*p*" refers to dispersive and polar contributions respectively.





Introduction to wetting

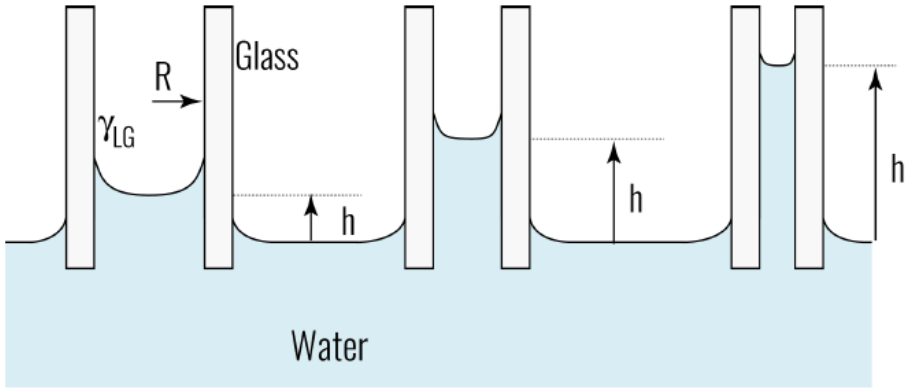
- Capillary action

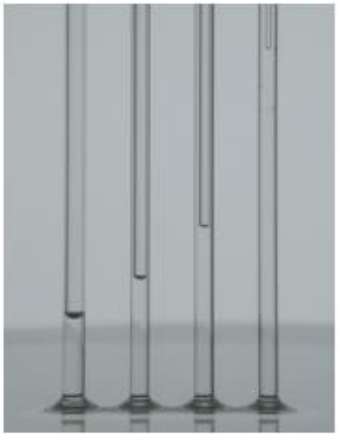
Competition between depression under the meniscus and weight of the water column

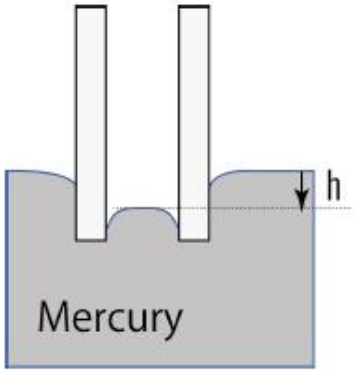
$$F_g = \rho h(\pi r^2)g$$

$$F_s = \gamma 2\pi r cos\theta$$

$$\gamma = \frac{1}{2cos\theta}\rho r g h$$

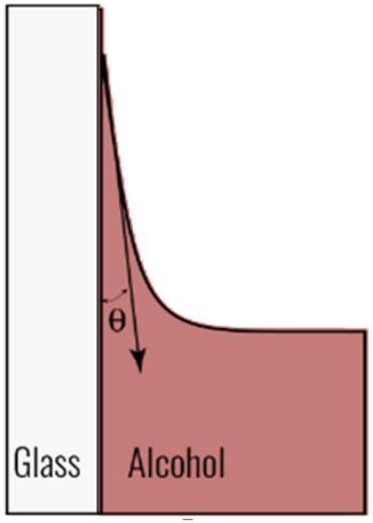


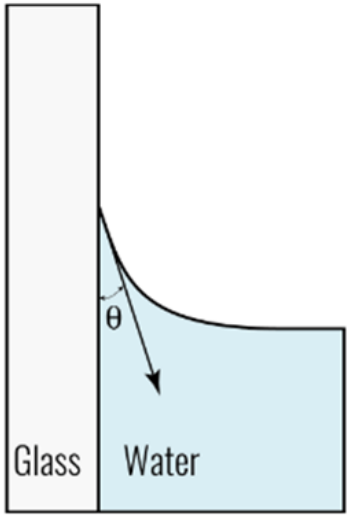




Introduction to wetting

- Tears of wine (Larmes du vin)

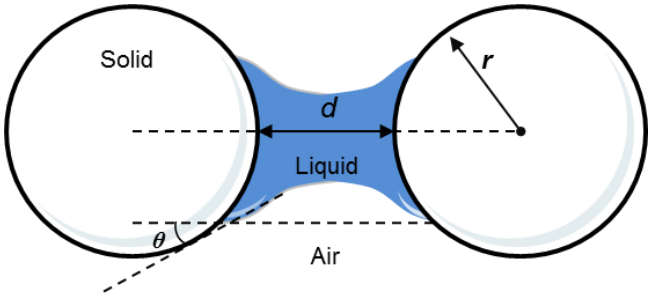


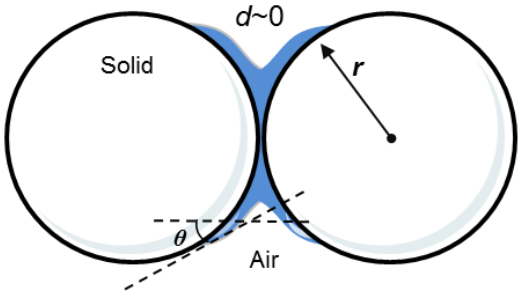


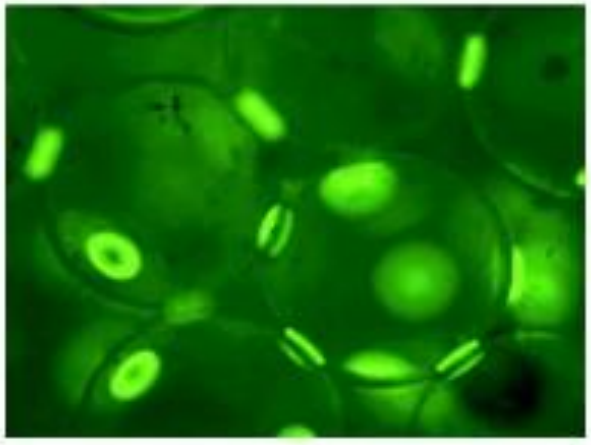
Introduction to wetting

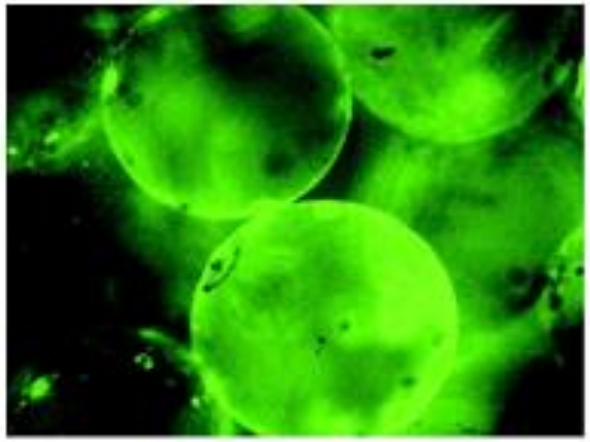
- Capillary action

$$F_c = 2\pi\gamma r\cos\theta$$





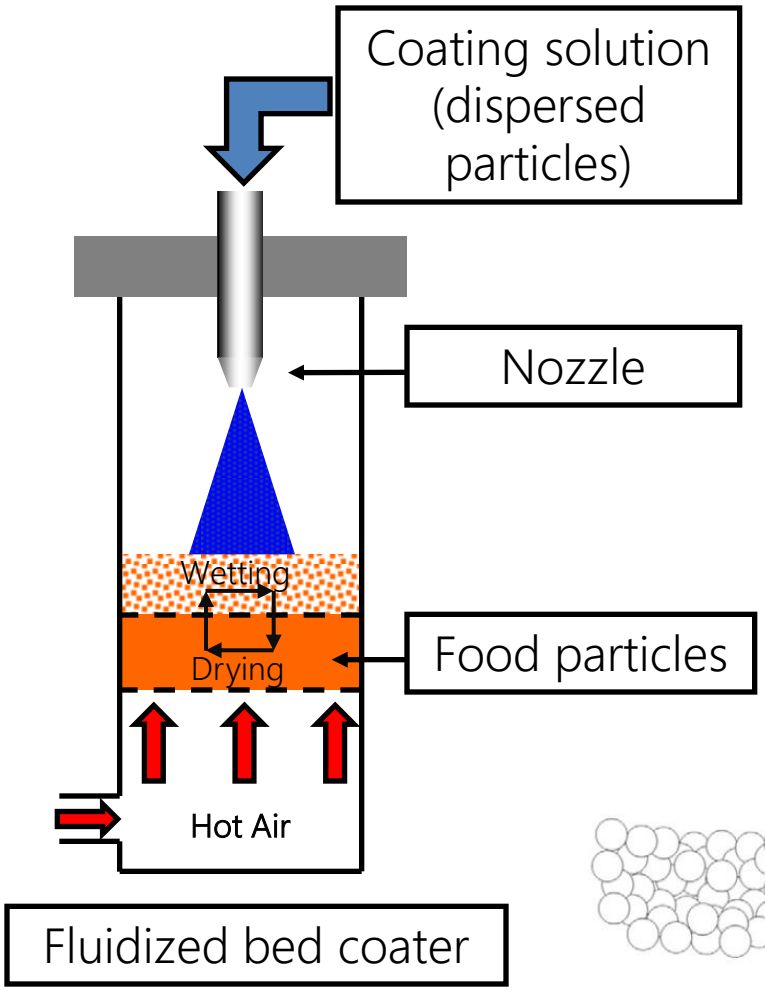


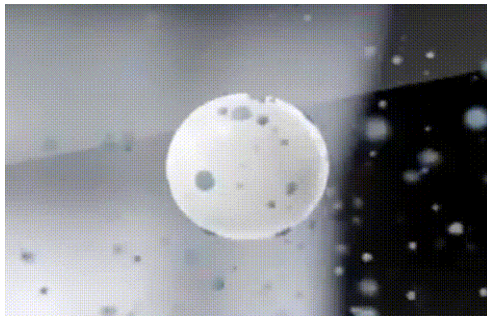


[1] Y.I. Rabinovich, M.S. Esayanur and B.M. Moudgil, Langmuir 21 (2005), 10992-7.

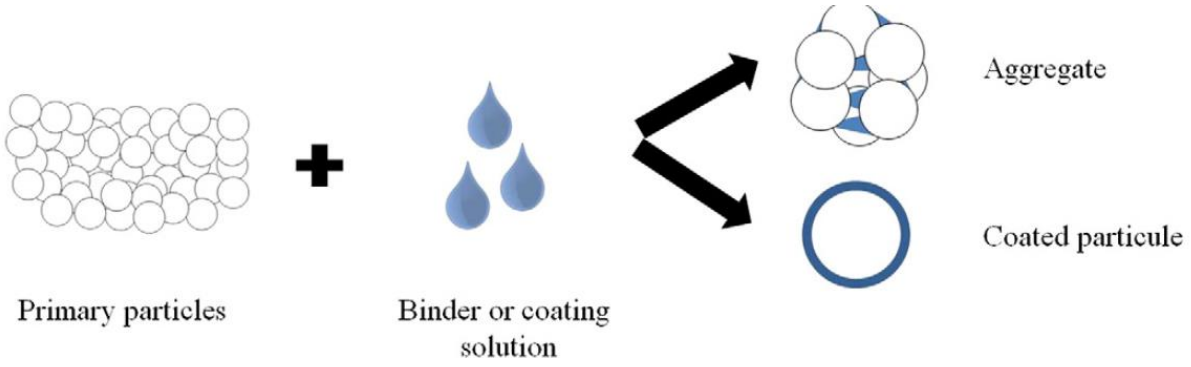
Introduction to wetting

- Agglomeration and coating



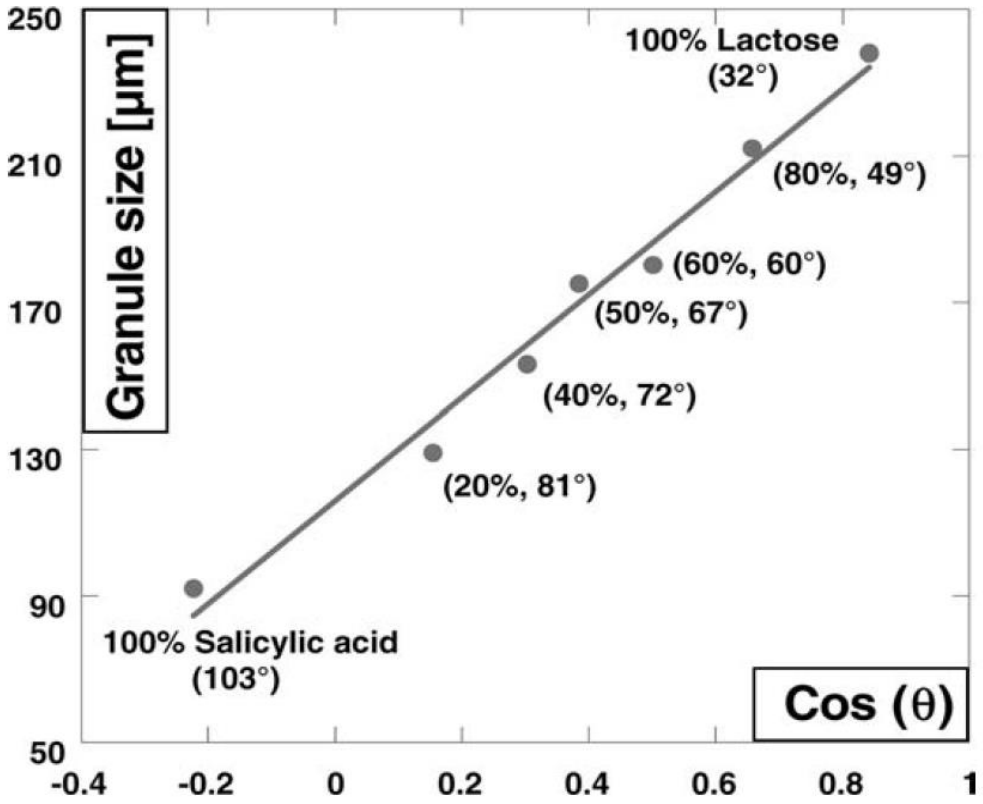


3D Example of Agglomeration due to capillary bridges in a fluidized bed.



Introduction to wetting

- Agglomeration



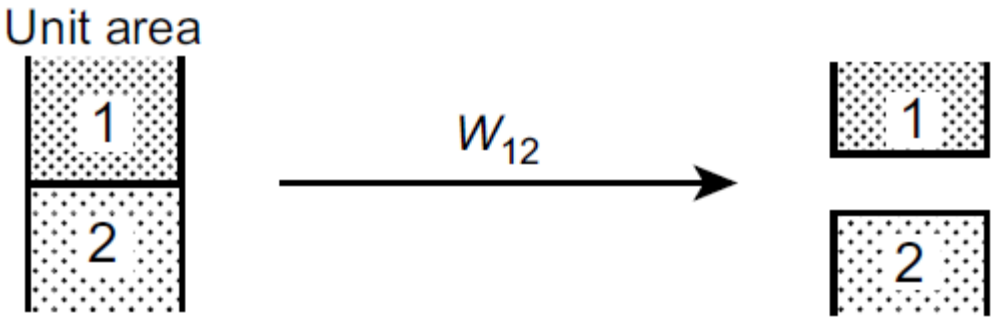
Introduction to wetting

- Work of Adhesion/cohesion

The *work of adhesion*, is the energy required to break the attraction between the unlike molecules.

$$W_l = 2\gamma_l$$ Cohesion

$$W_{ls} = \gamma_l + \gamma_s - \gamma_{ls}$$ Adhesion



Wetting is the balance between cohesive and adhesive forces

Introduction to wetting

- Work of Adhesion/cohesion

Girifalco and Good

$$W_{ls} = 2\Phi_I \Phi_V (\gamma_l \gamma_s)^{0.5}$$

$$\Phi_V = \frac{4(v_l v_s)^{1/3}}{(v_l^{1/3} + v_s^{1/3})^2}$$

$$\Phi_I = \frac{\varepsilon_{ls}}{(\varepsilon_l \varepsilon_s)^{0.5}}$$

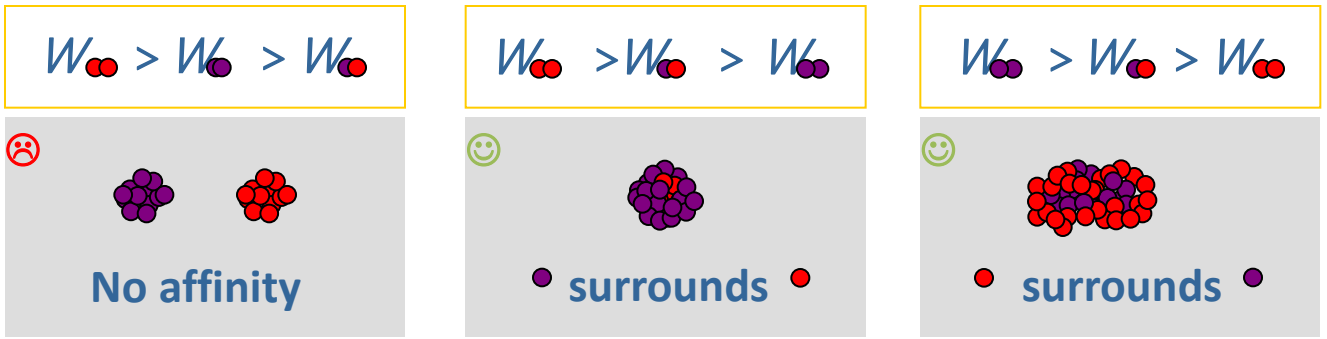
Wu

$$W_{ls} = 2\phi_{ls} (\gamma_l \gamma_s)^{0.5}$$

$$\phi_{ls} = 2\left(\frac{x_l^d x_s^d}{g_l x_l^d + g_s x_s^d} + \frac{x_l^p x_s^p}{g_l x_l^p + g_s x_s^p} \right)$$

$$x_i^p = \frac{\gamma_i^p}{\gamma_i} \qquad x_i^d = \frac{\gamma_i^d}{\gamma_i} \qquad i = l \text{ or } s$$

$$g_s = \frac{\gamma_s}{\gamma_l} \qquad g_l = \frac{\gamma_l}{\gamma_s}$$



Introduction to wetting

- Work of Adhesion/cohesion➔ Spreading coefficient (v.2)

$$S = W_{ls} - W_l$$

If $S > 0$ Spontaneous spreading

Adhesion Cohesion

Wetting is the balance between cohesive and adhesive forces

How to control/reduce the wettability?

Introduction to wetting

- Surfactants

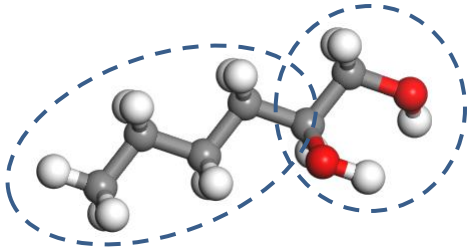
Hydrophilic

(polar head)

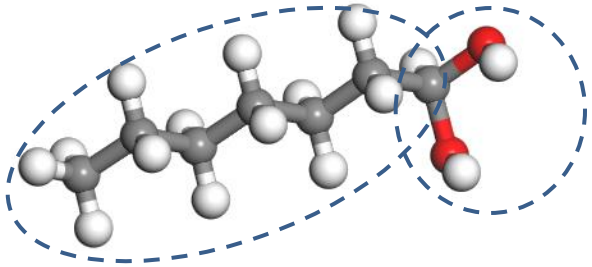
Hydrophobic

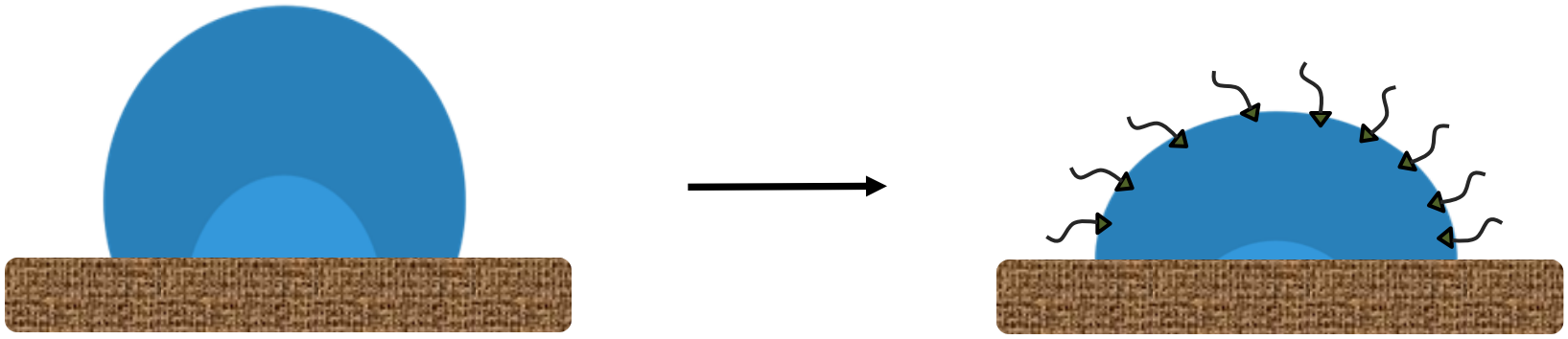
(non-polar tail - hydrocarbon)

Hexanediol



Heptandiol



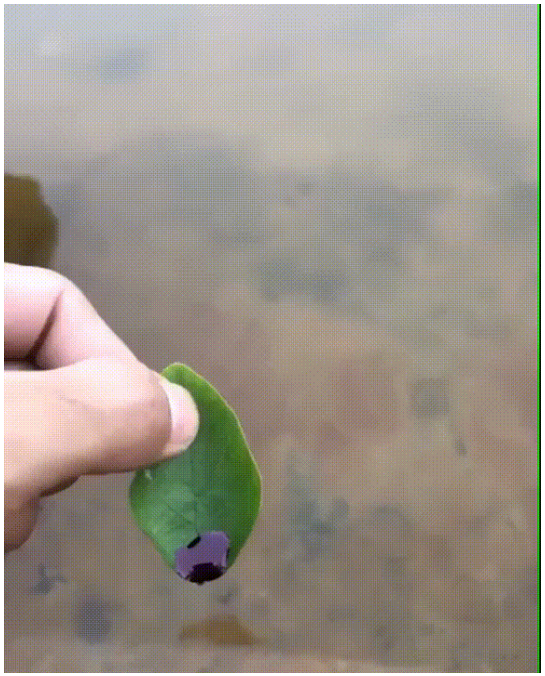


Without surfactants

With surfactants

Introduction to wetting

- Surfactants



Water: Higher surface tension

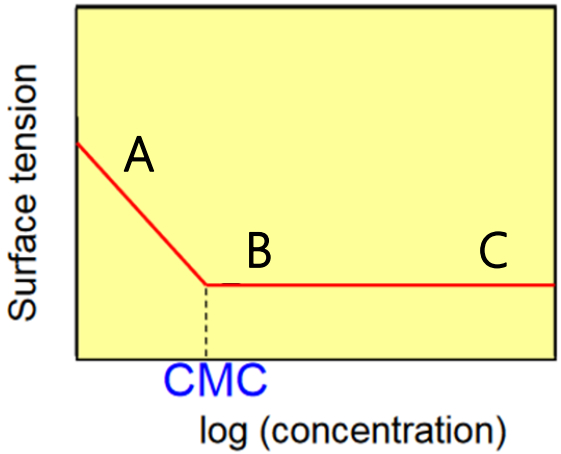
Ink: contains surfactants ➔ Lower surface tension

Surface tension gradient: Marangoni effect.

Introduction to wetting

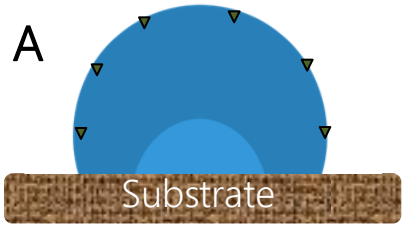
- Surfactants

  Wettability in the presence of surfactant depends on the critical micelle concentration (CMC) of the surfactant in the solvent.



▼ Surfactants

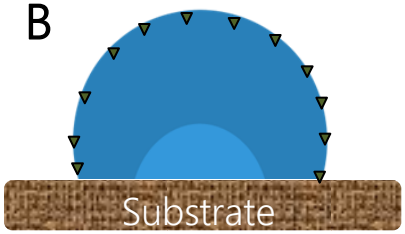
A



$C_{surfactant} < CMC$ ☹

$\gamma_{droplet} > \gamma_{surfactant}$

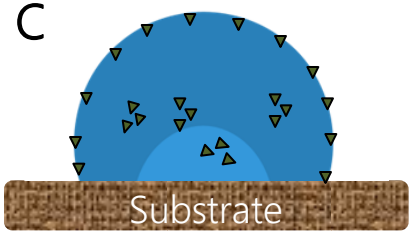
B



$C_{surfctant} = CMC$ ☺

$\gamma_{droplet} \approx \gamma_{surfactant}$

C



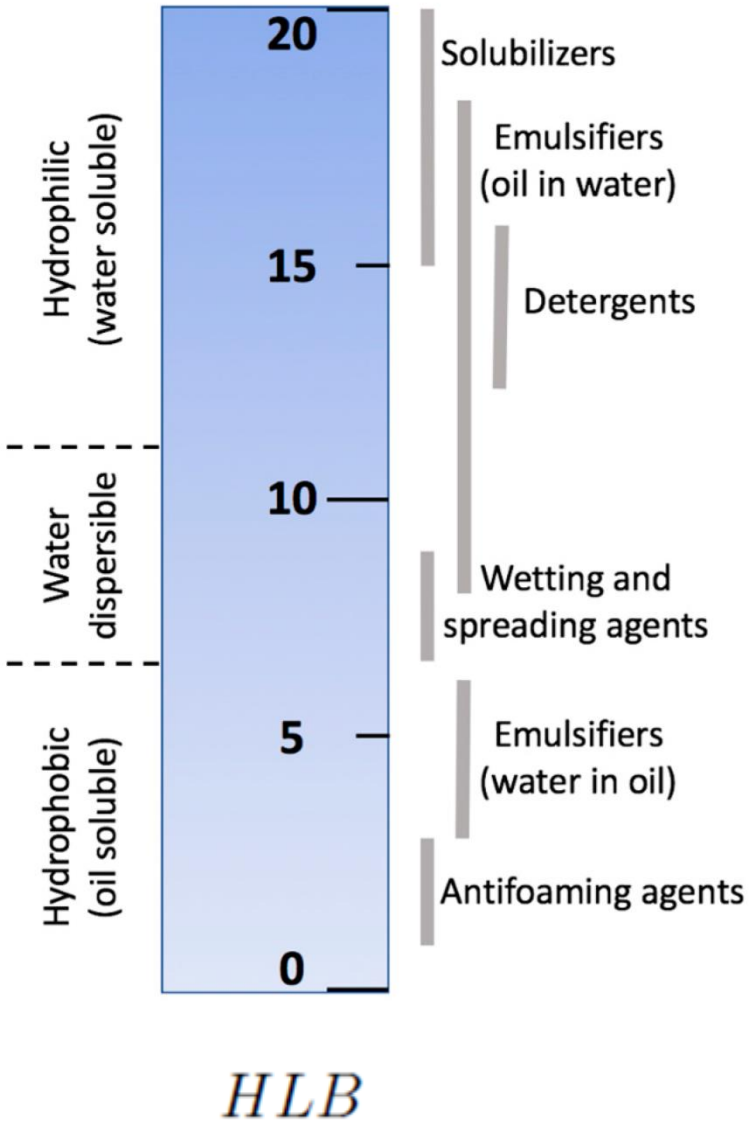
$C_{surfactant} > CMC$ 😐

$\gamma_{droplet} \approx \gamma_{surfactant}$

Introduction to wetting

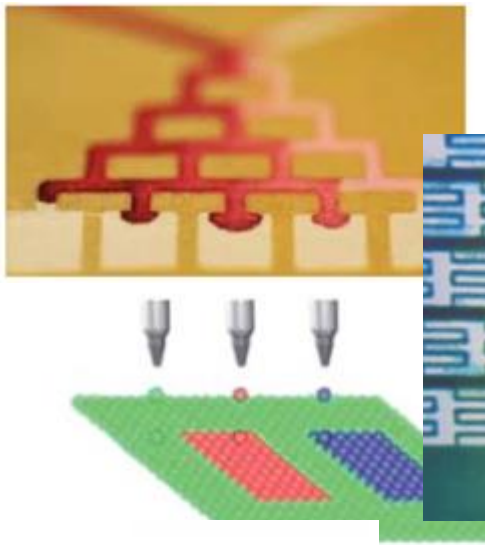
- Surfactants

$$HLB = 20M_h/M$$



Introduction to wetting

- Other wetting applications
  - Paper microfluidics
  - Nano and inkjet printing processes
  - Design oil-water separation material
  - Adhesives
  - Efficient deposition of pesticides on plant leaves.



Wetting and granular flow (Macroscopic)

Wetting and granular flow

- Wet granular flow is ubiquitous in nature and industry.
- Industrial applications of granular materials involve high number of particles.

Industry

Nature

Dry

Wet

Dry

Wet

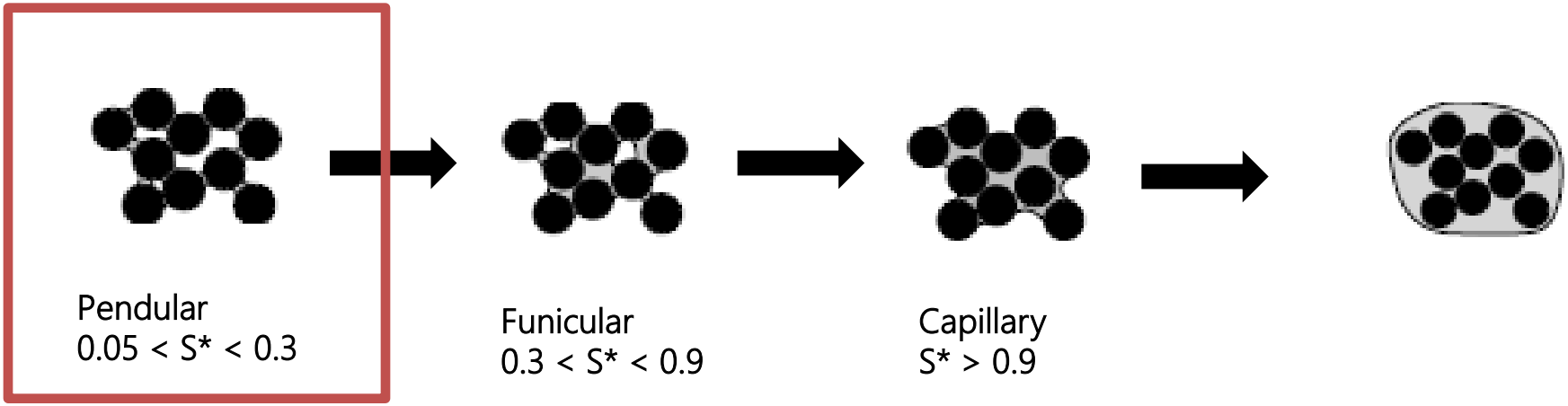
Wetting and granular flow

- Different Regimes

Bulk saturation: $S^* = \frac{V_l}{V_\phi}$

V_l: Liquid volume

V_ϕ: Void volume

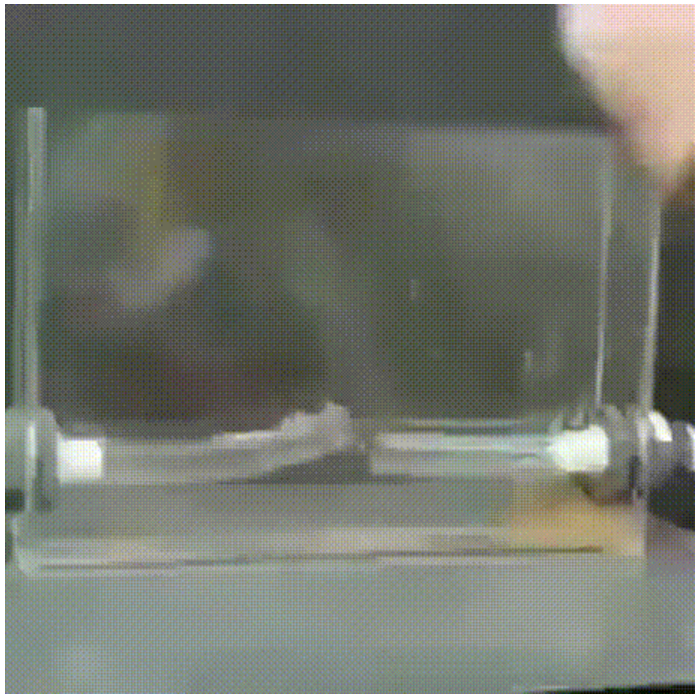


Capillary forces/cohesion active between the particles

No capillary forces between the particles

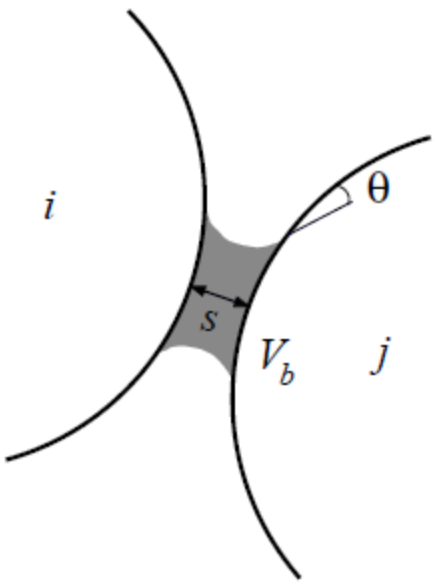
Wetting and granular flow

- Different Regimes



Wetting and granular flow

- Willet model



Capillary bridge force between equal-sized particles at finite distance :

$$F_{cij} = \frac{2\pi\gamma R\cos\theta}{1+1.05\bar{S}+2.5\bar{S}^2}$$

$$\bar{S} = S\sqrt{R/V_b}$$

$\theta \rightarrow$ Contact angle

$\gamma \rightarrow$ Surface tension

$R \rightarrow$ Mean radius

$V_b \rightarrow$ Liquid bridge volume

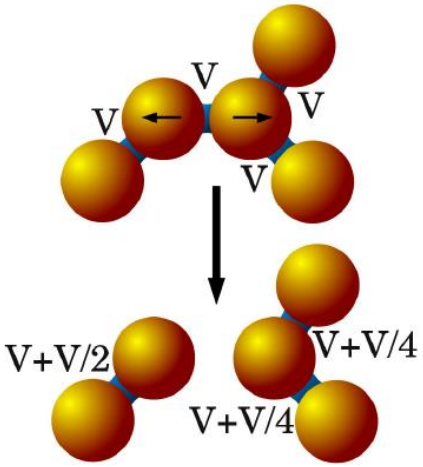
$S \rightarrow$ Separation distance

The bridge rupture distance is defined by:

$$S_c = \left(1+\frac{\theta}{2}\right)V_b^{1/3}$$

Wetting and granular flow

- Liquid migration
  - Distance between the interacting pair is greater than the critical rupture distance



- Ruptured bridge volume is split equally between the two interacting particles: $\frac{V_{rup}}{2}$
- Further distributed into '*N*' neighboring contacts: $\frac{V_{rup}}{2N}$
- New bridge volume : $V_{new} = \min\left(V_{old} + \frac{V_{rup}}{2N}, V_b^{\max}\right)$
- If $\left(V_{new} > V_b^{\max}\right)$ then $V_{new} = V_b^{\max}$

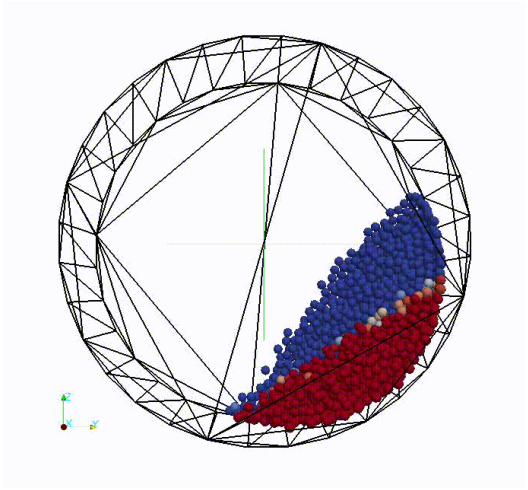
excess volume : $\left(V_{old} + \frac{V_{rup}}{2N} - V_b^{\max}\right)$

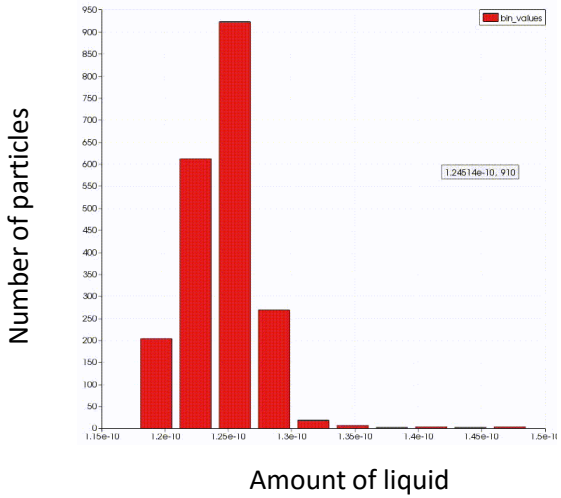
Mani R., Kadau D. and Herrmann H. , 2013. Liquid migration in sheared unsaturated granular media. Granular Matter. 15, 447-454

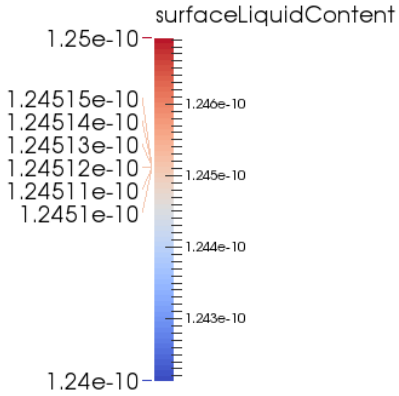
Wetting and granular flow

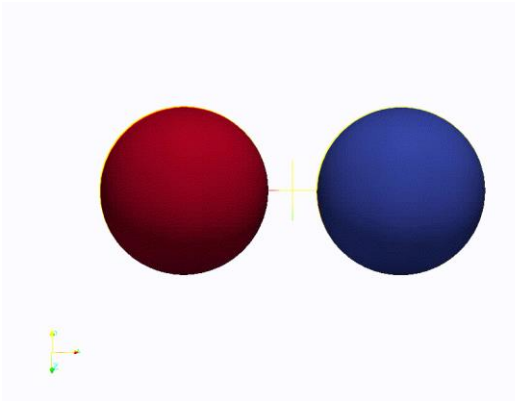
- Simulation of liquid migration

Percentage of water per particle volume: 0.5%



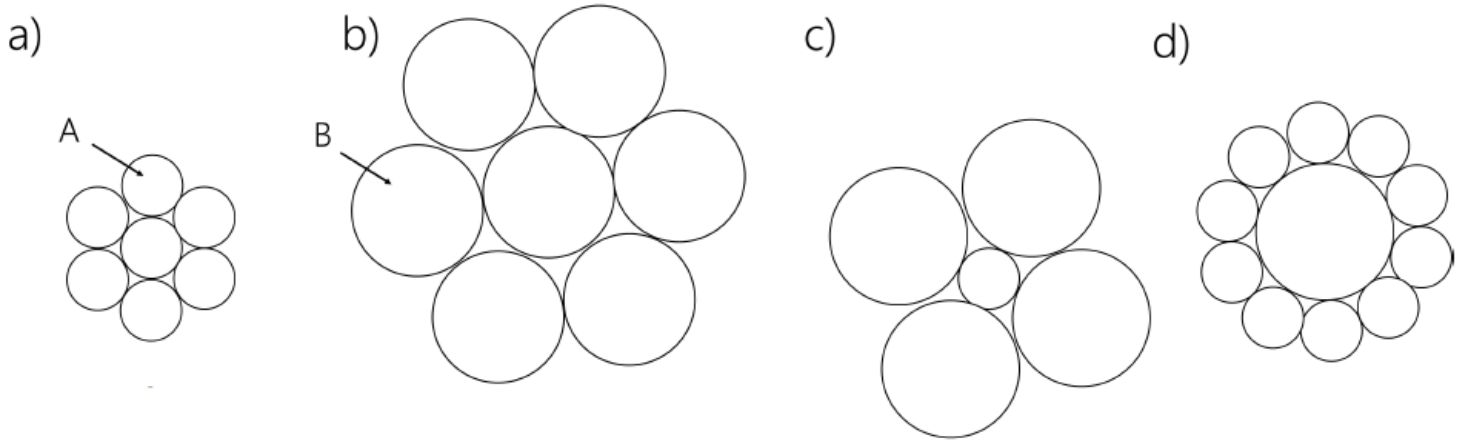






Wetting and granular flow

- Number of contacts



$$Z_{AA} = 3 + \eta - Z_{AB},$$

$$Z_{BB} = 3 + \eta c^2 - Z_{BA},$$

$$Z_{AB} = (9 + 3A + 3\eta c^2 + \eta^2 c^2)\frac{n_B}{Z},$$

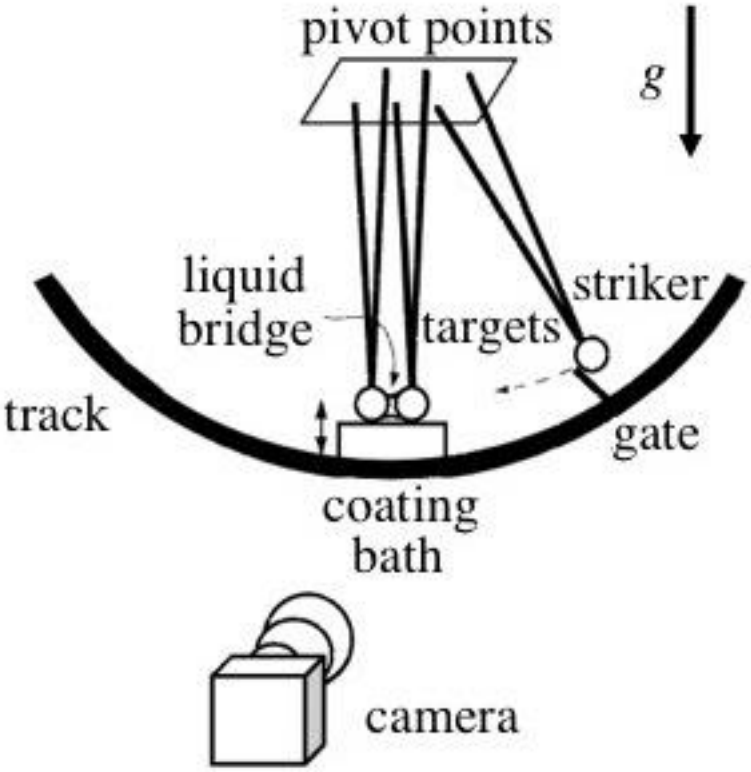
with

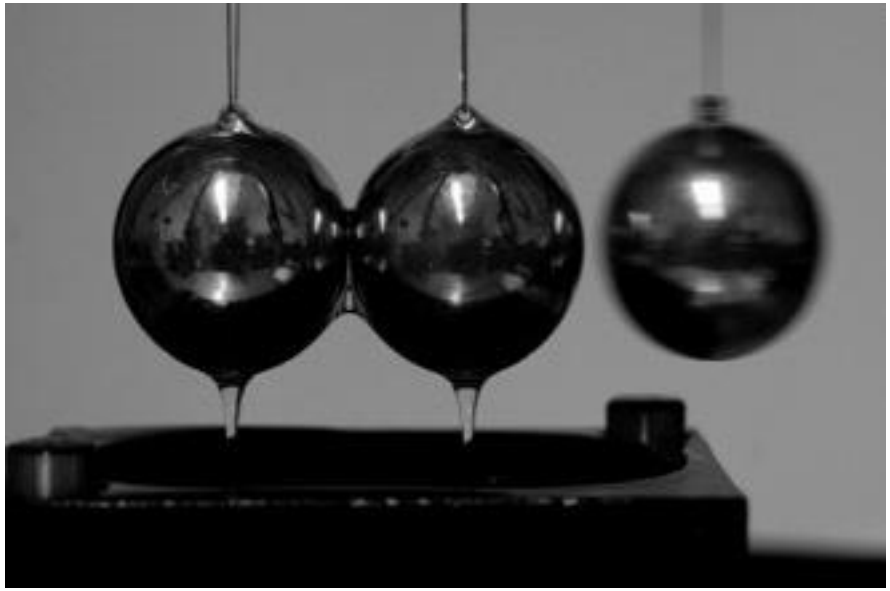
$$\eta = 3 + \frac{Z - 3}{n_A + (1 - n_A)c^2} \qquad n_A = 1 - n_B = \frac{N_A}{N_A + N_B}$$

Bouvard, D. & Lange, F. Relation between percolation and particle coordination in binary powder mixtures. Acta metallurgica et materialia 39, 3083–3090

Wetting and granular flow

- Liquid migration



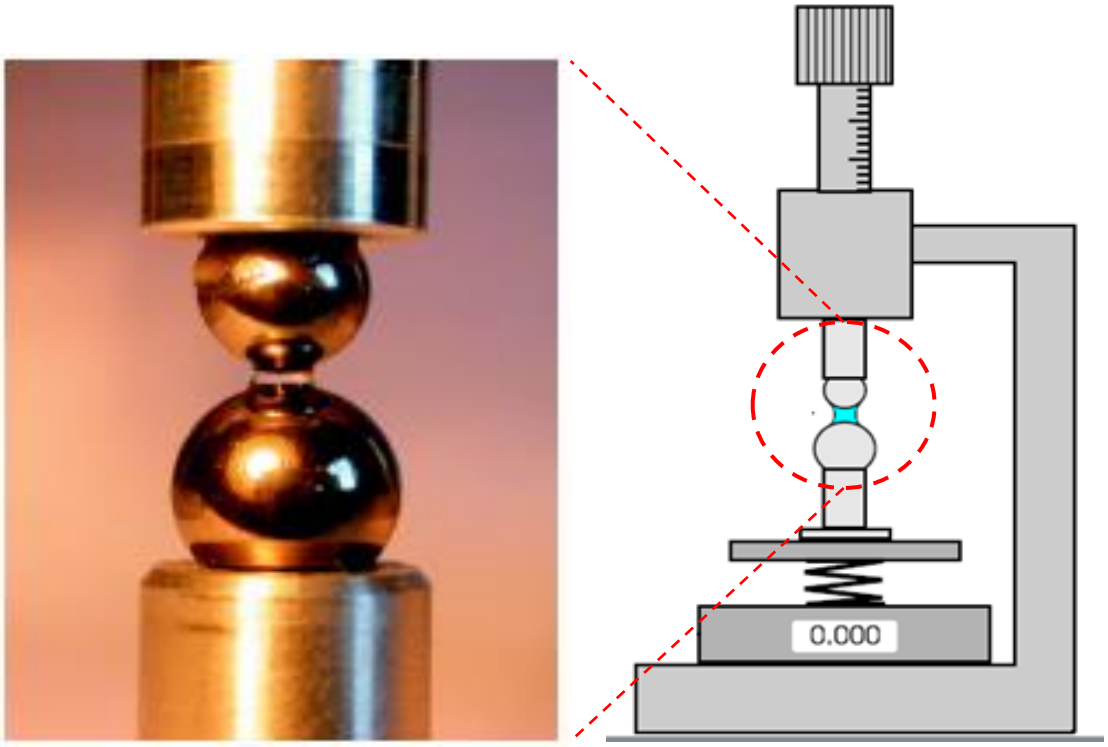


Wet Stokes's Cradle

Donahue, C. M. C. M. Hrenya, and R. H. Davis, *Stokes's cradle: Newton's cradle with liquid coating*, PRL 105 034501 (2010).

Wetting and granular flow

- Liquid migration



Soulié (2005)

F. Soulie, F. Cherblanc, M.S. El Youssoufi, and C. Saix, Influence of liquid bridges on the mechanical behaviour of polydisperse granular materials, International Journal for Numerical and Analytical Methods in Geomechanics, (2005), 30(3):213–228.

Wetting and granular flow

- Capillary number

$$Ca = \frac{\mu v}{\gamma}$$

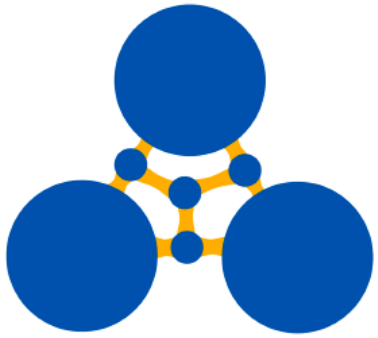
> 1 Dynamic liquid bridge

$< 10^{-3}$ Static liquid bridge

γ : Surface tension of liquid

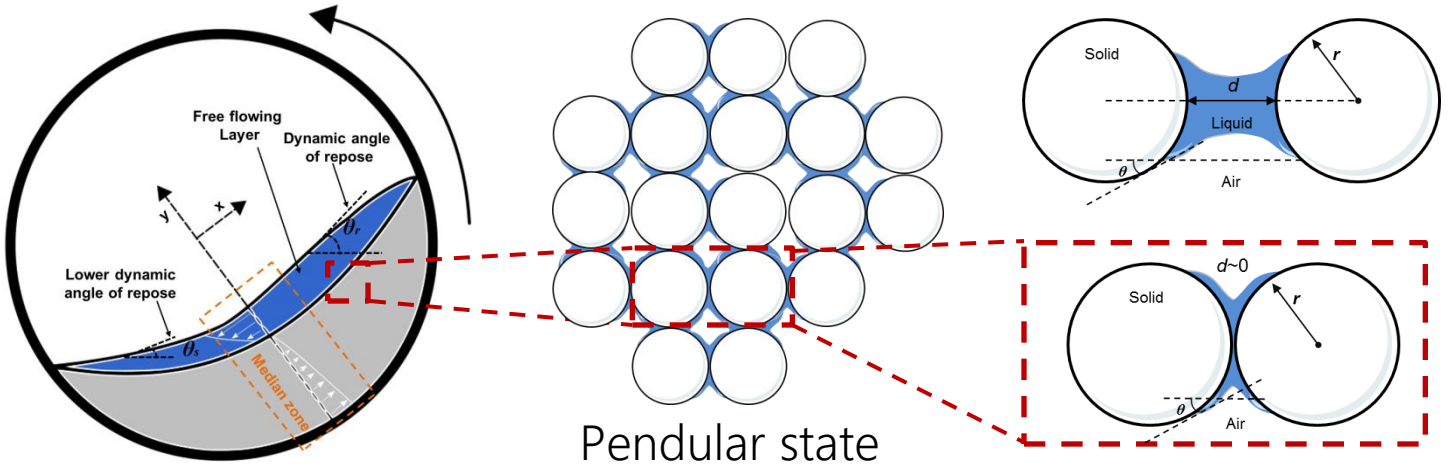
μ : Dynamic viscosity of liquid

v : Relative velocity between particles



Wetting and granular flow

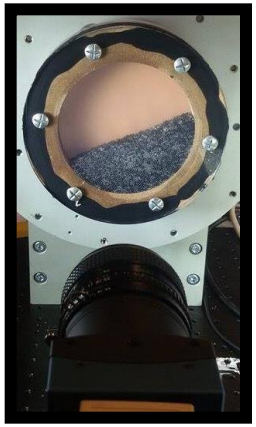
- Capillary forces and flowability

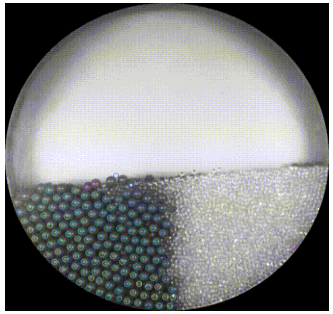


Pendular state

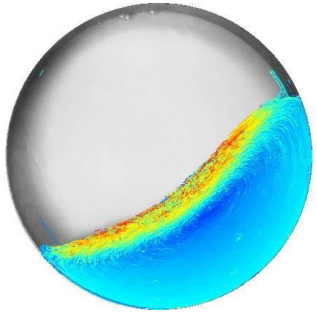
r is the particle radius
θ is the liquid contact ang
γ is the surface tension

- Rotating drum appartus





Particles tracking



Track linking/PIV and coarse-graining

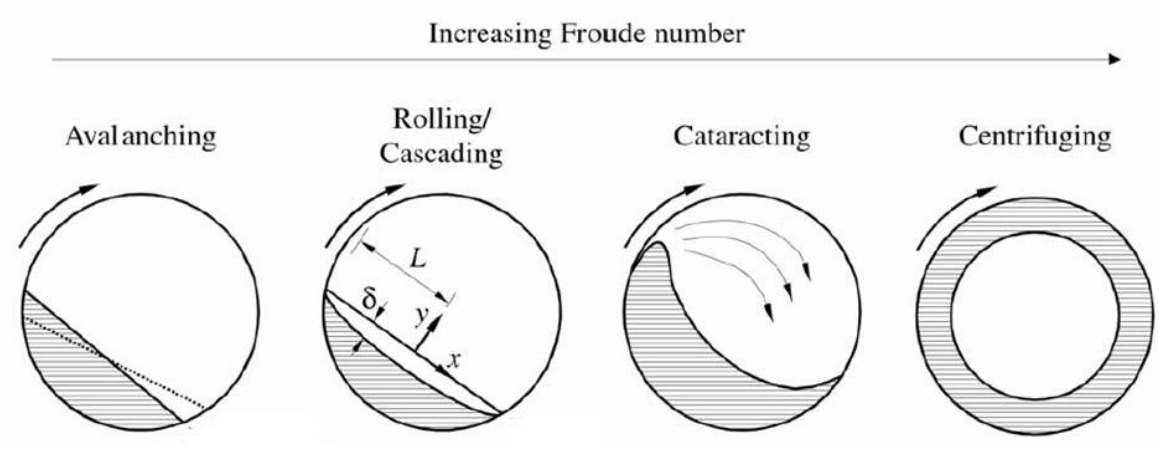
Table 1. Properties of the drum and the glass beads.

Properties	Value
Drum, R×L (mm)	60.5×22
Glass beads radii r (mm)	0.85, 1.25 and 2
Rotation speed (rpm)	3 to 57
Particle density ρ_p, (kg.m^{-3})	2500
Filling level β	35% (125 g)
Volumetric liquid content v_{liq} (ml)	4

Wetting and granular flow

- Capillary forces and flowability

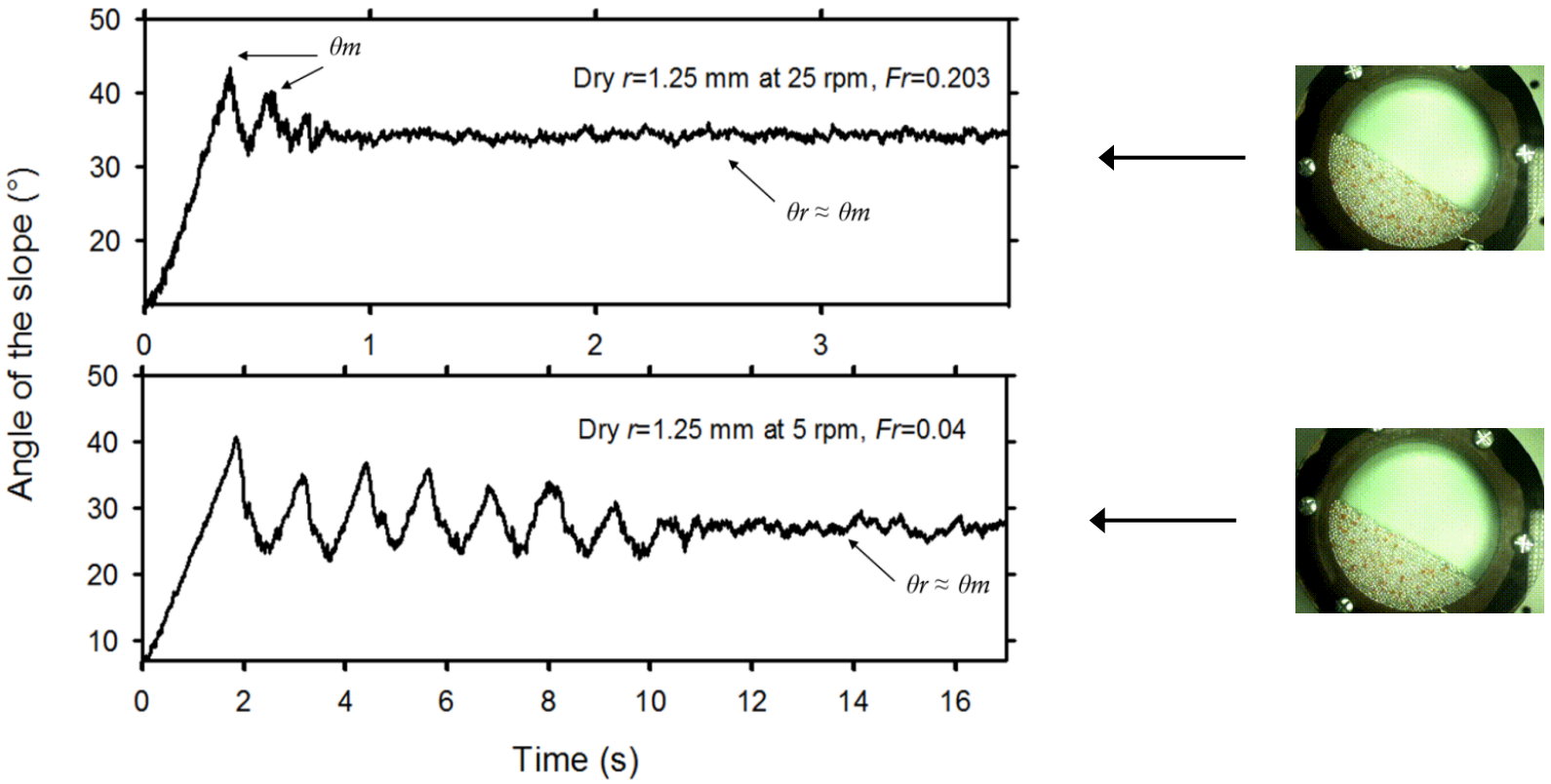
$$F_r = \frac{\omega^2 R}{g}$$



Fr<0.001 | 0.001<Fr<0.01 | 0.01<Fr<1 | 1<Fr

Wetting and granular flow

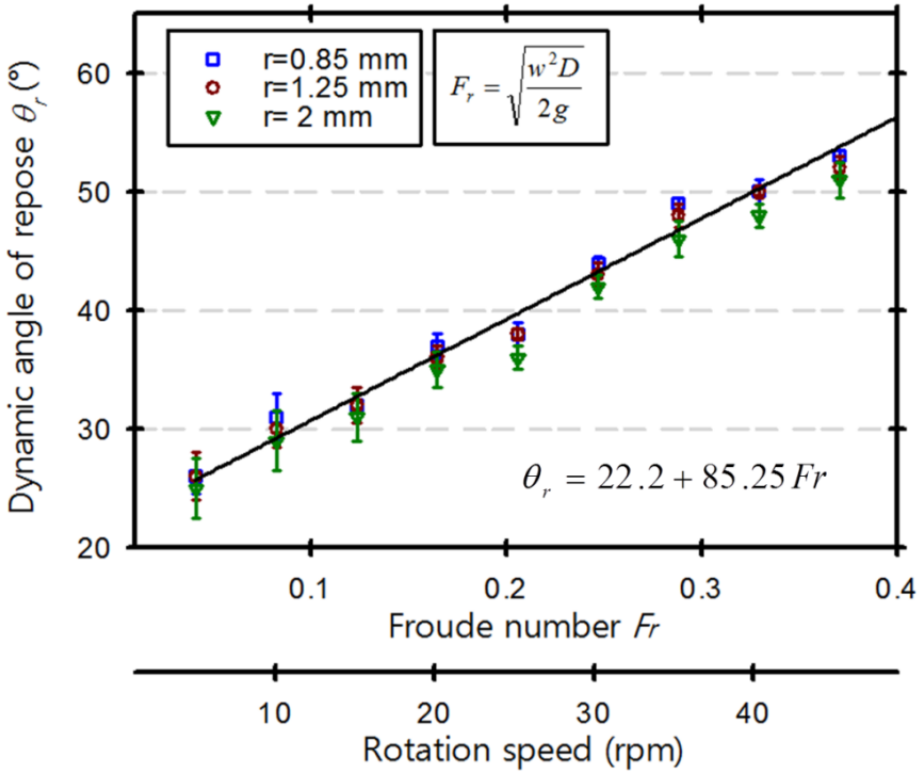
- Effect of the rotation speed

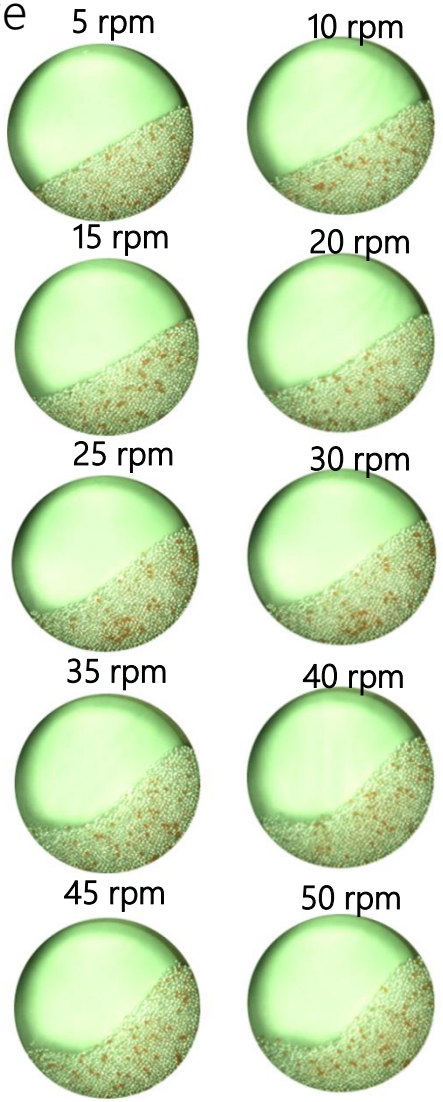


- We will focus on the continuous steady flow.

Wetting and granular flow

- **Dry case:** Effect of the rotation speed and the particle size





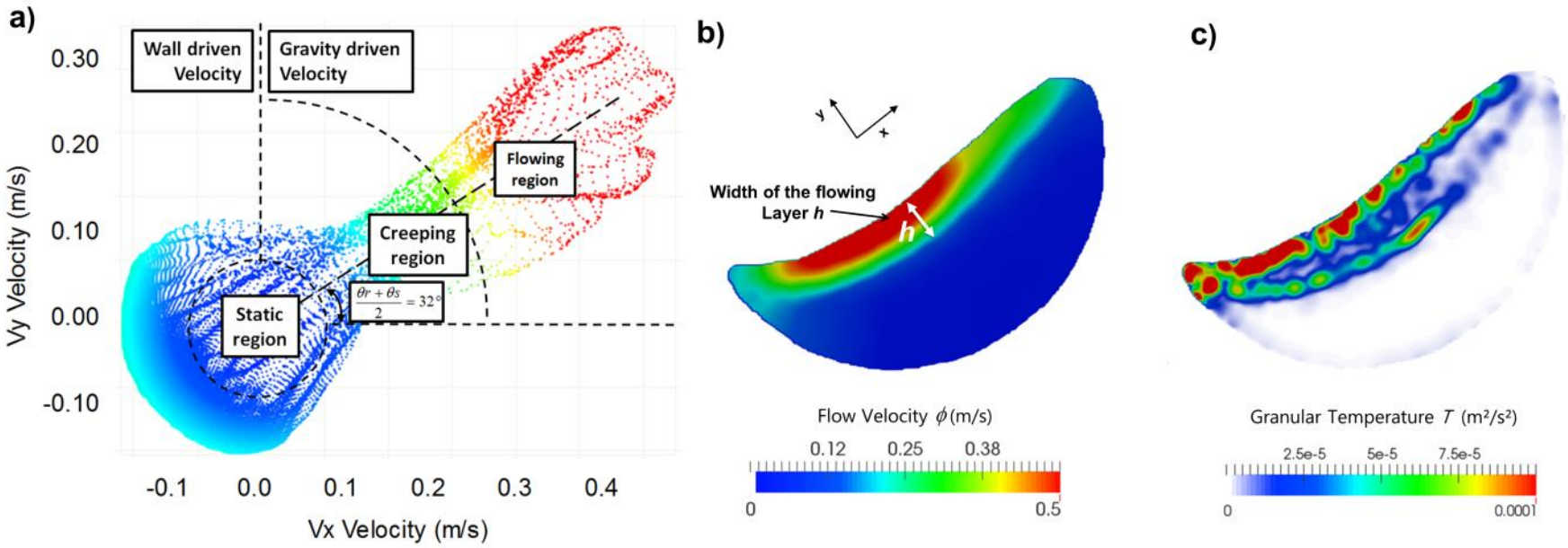
- The dynamic angle of repose collapses into one linear profile.

Wetting and granular flow

- Velocity gradient and granular temperature

$$\varphi = \sqrt{(\vec{v}_x - \vec{v}_{\Omega x})^2 + (\vec{v}_y - \vec{v}_{\Omega y})^2}\,.$$

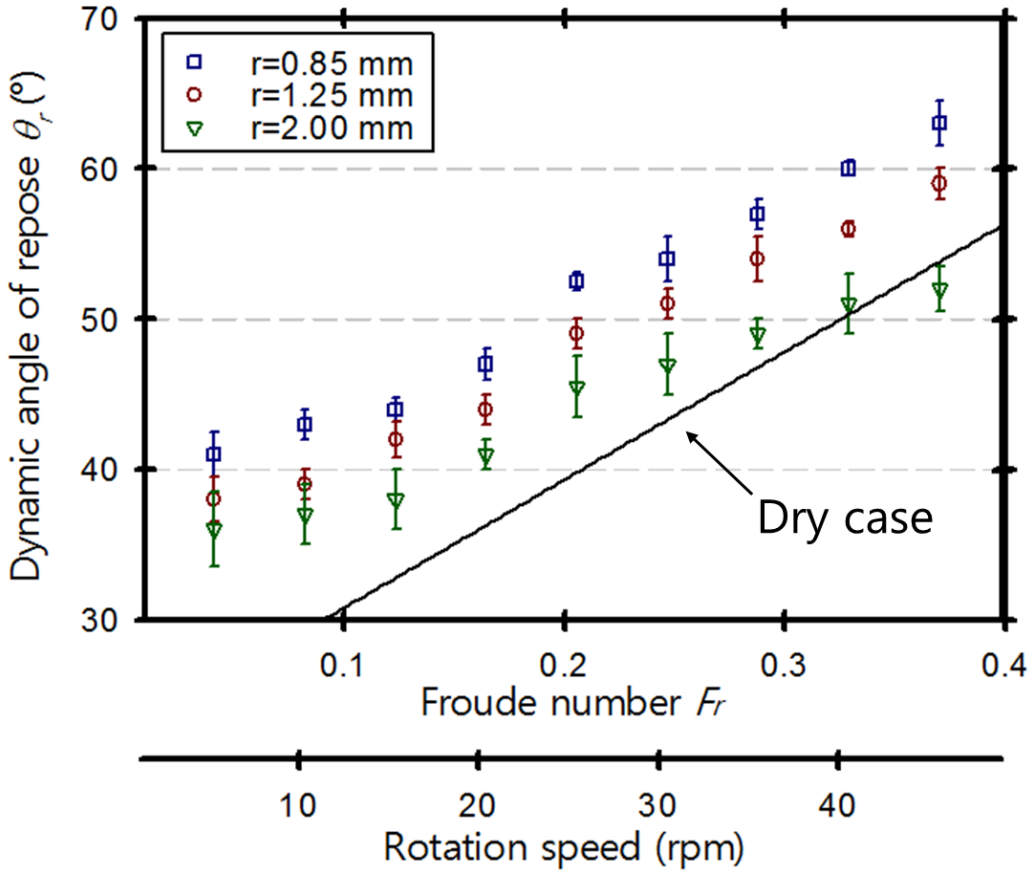
$$T_g = \langle v^2 \rangle - \langle v \rangle^2$$



- Three regions can be distinguished: static, creeping and flowing region.

Wetting and granular flow

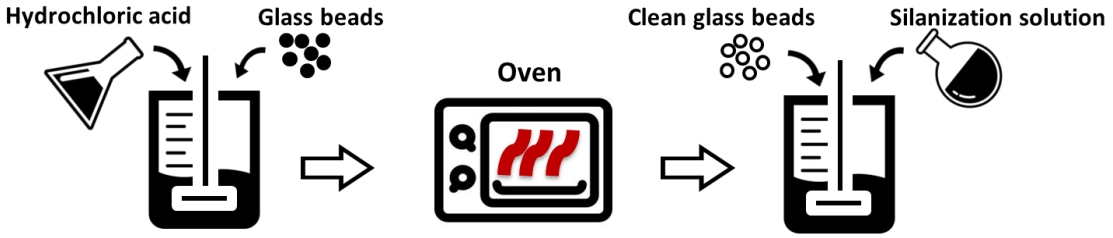
- **Wet case:** Effect of the drum rotation speed and particle size



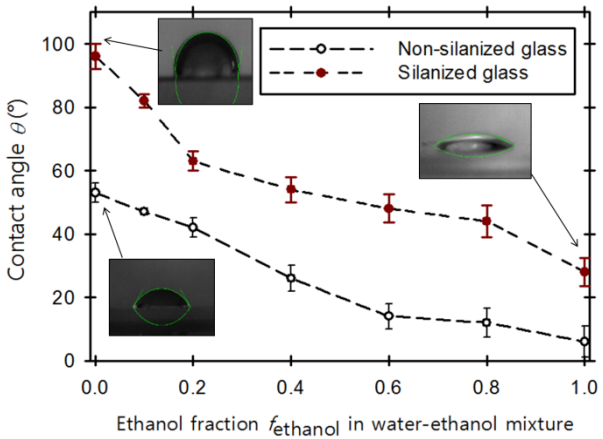
⚠ How to predict and control the flow in the wet case?

Wetting and granular flow

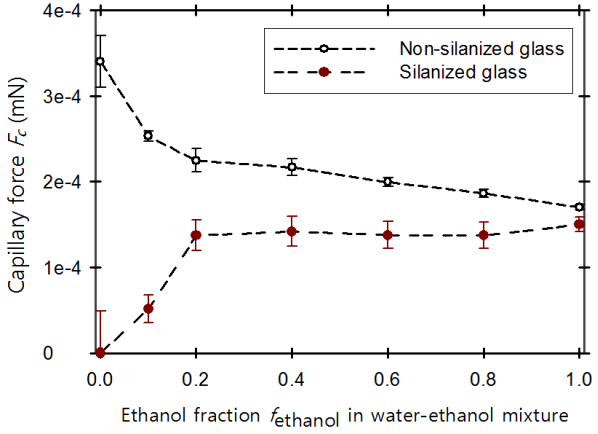
- **Wet case:** How to control the flow of the particles
  - Surface modification of glass beads using silanization.
    - Hydrophobic glass beads.



  - Using different mixture of ethanol-water.



$$F_c = 2\pi\gamma r\cos\theta$$

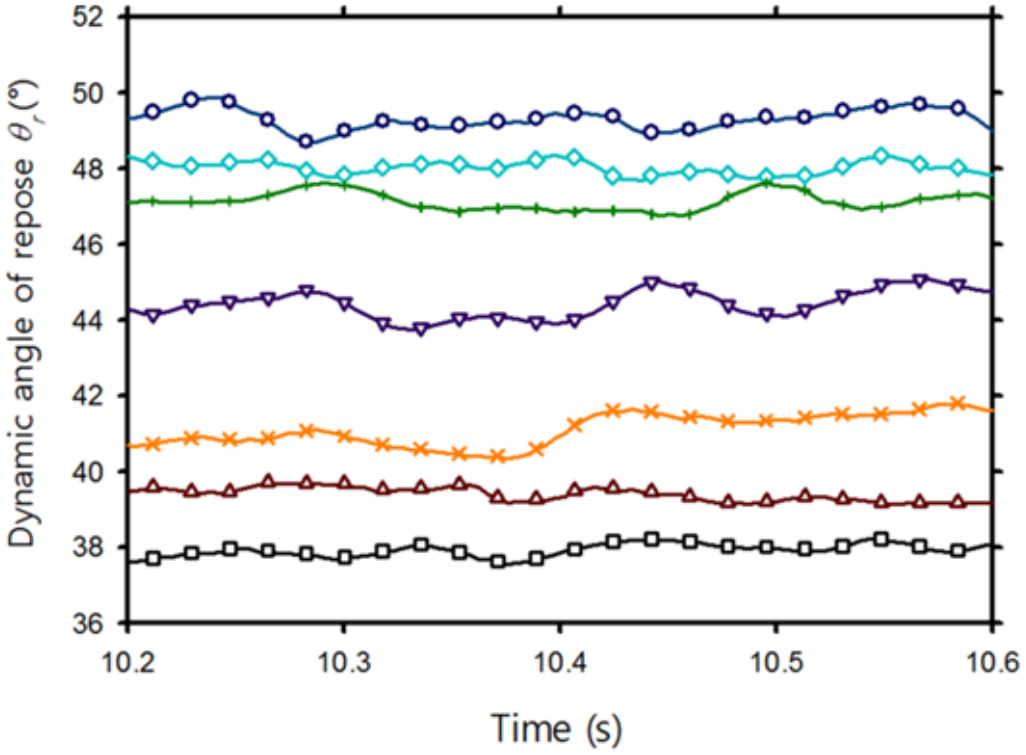


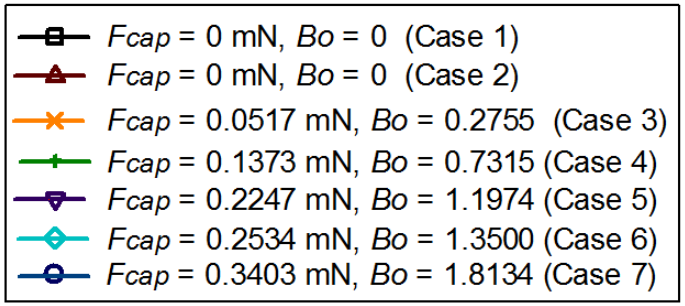
  - Capillary forces can be tuned.

[2] G. Vazquez, E. Alvarez, J. M. Navaza, J. Chem. Eng. Data , 40 (3), 611–614 (1995).

Wetting and granular flow

- **Wet case:** Effect of capillary force on the flow



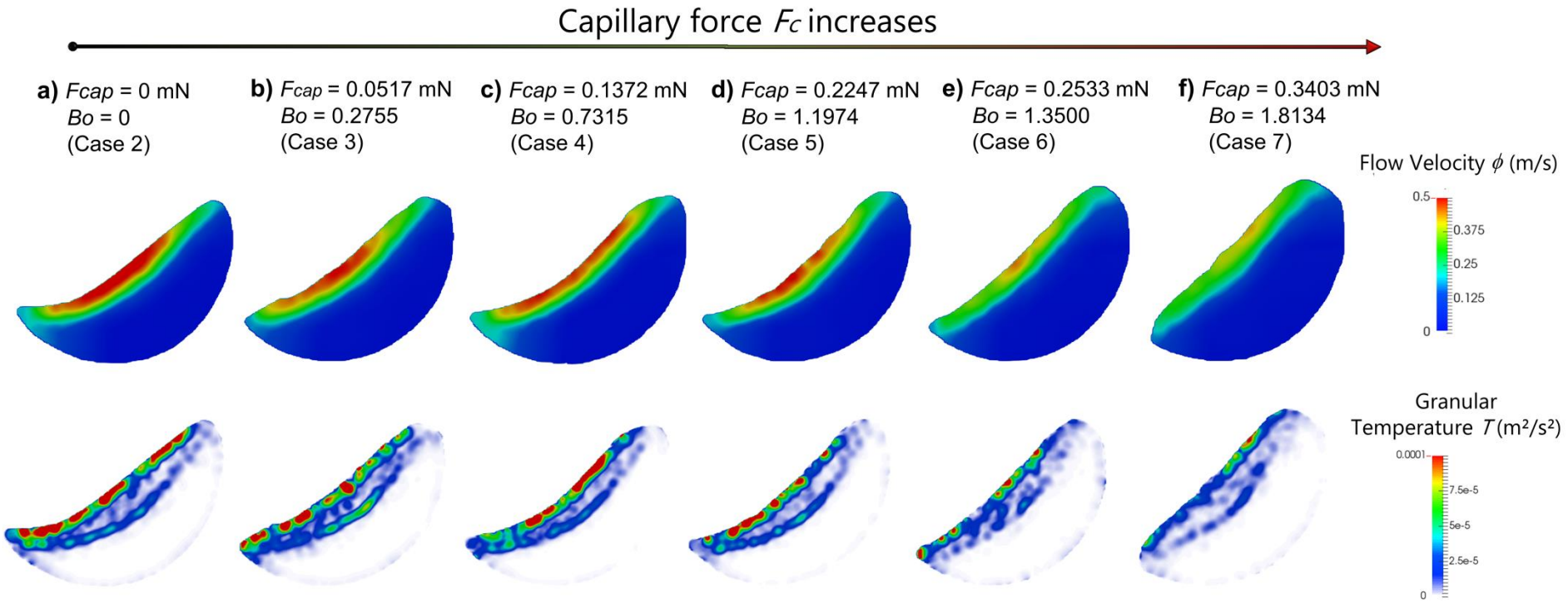


Case number	Silanized	Ethanol fraction
Case 1	no	Dry case here
Case 2	Yes	0
Case 3	yes	0.1
Case 4	yes	0.2
Case 5	no	0.2
Case 6	no	0.1
Case 7	no	0

▶ The dynamic angle of repose increases with the capillary force.

Wetting and granular flow

- **Wet case:** Effect of capillary force on the flow

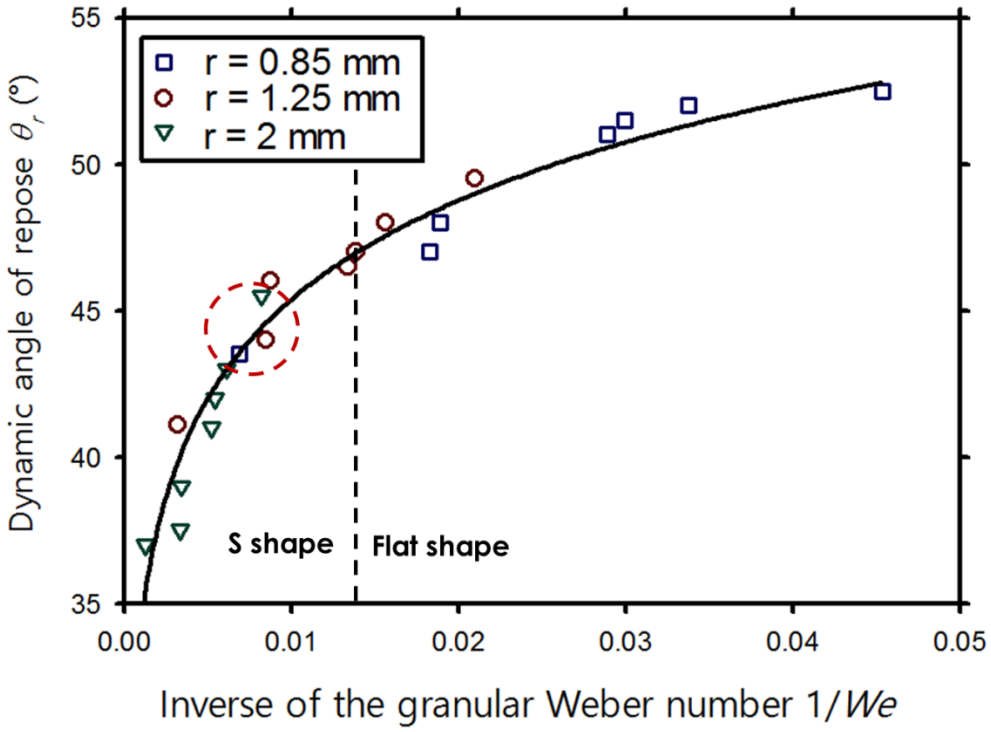


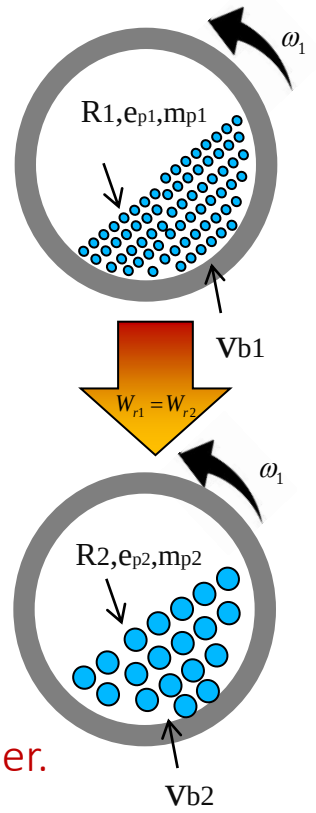
- The capillary force reduces the flow velocity but increases the width of the flow.
- The flow is controlled by an interplay between inertial forces and capillary forces.

Wetting and granular flow

- **Wet case:** Scaling

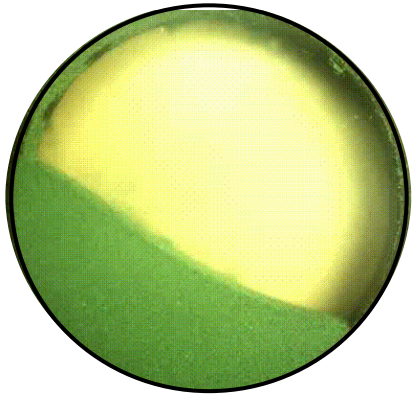
We scale with respect to the Weber number $We_g = \dfrac{e_p R V_p^{\,2}}{\gamma}$



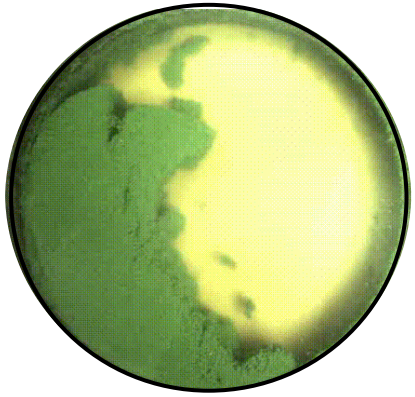


Configurations inside the red circle have the same Weber number.

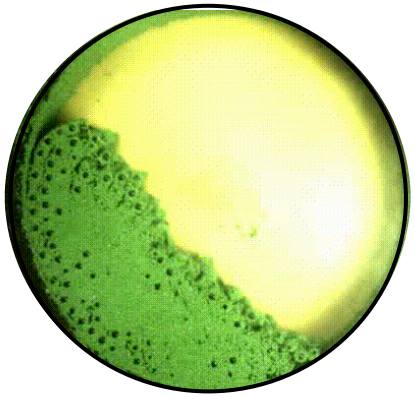
Wetting and granular flow



Dry



Wet



Wet + Larger particles

Wettability is important, How to predict it?

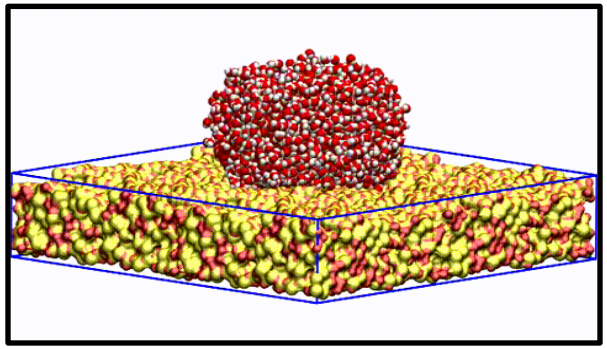
Wettability prediction
(Microscale)

Wettability prediction

- Basic concept

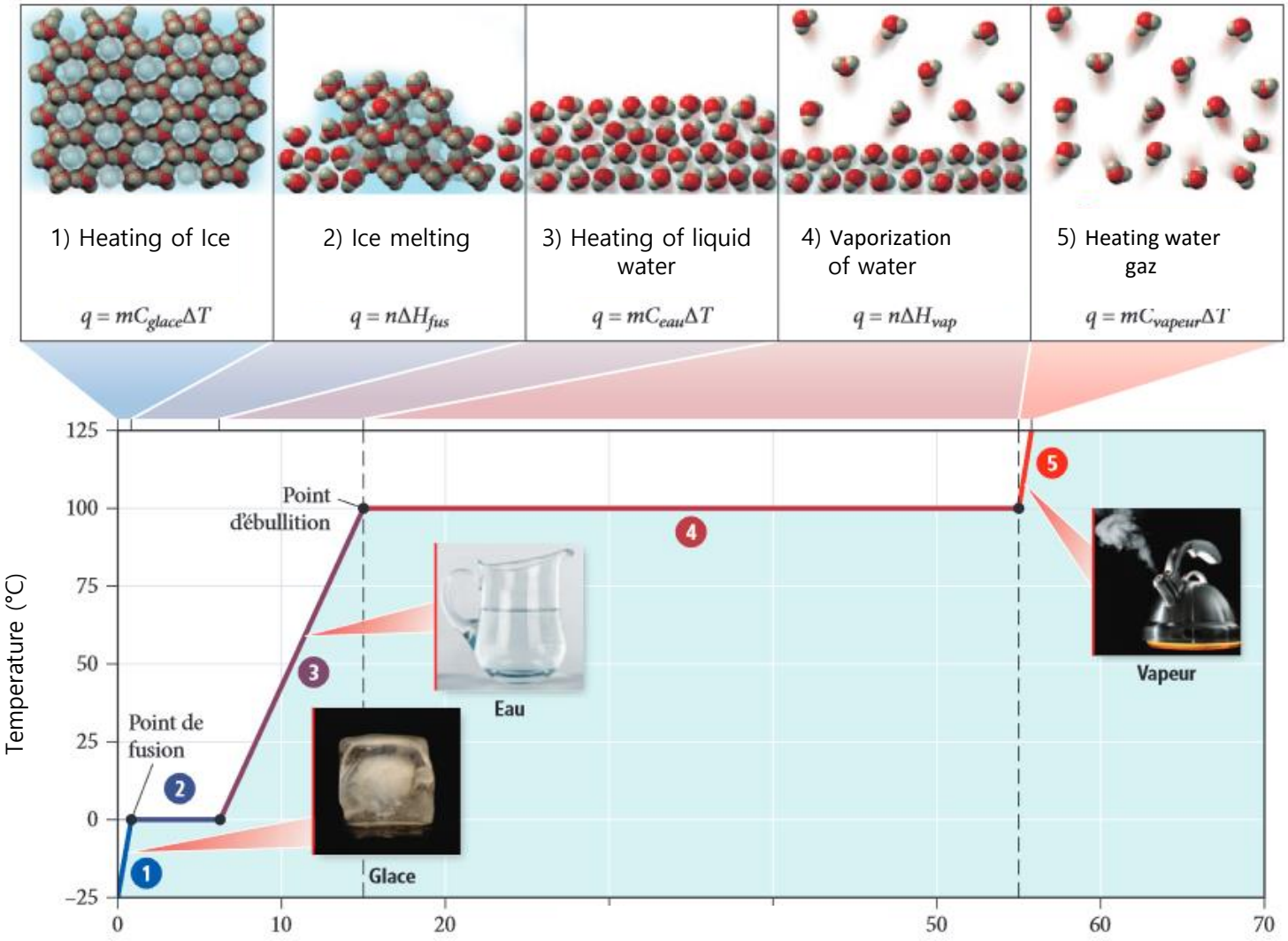
A water droplet is just a bunch of H2O molecules.

Atoms and molecules will 'move' in the computer, bumping into each other, vibrating about a mean position (if restrained), or wandering around (if the system is fluid), oscillating in waves in concert with their neighbours, perhaps evaporating away from the system if there is a free surface, and so on, in a way similar to what real atoms and molecules would do.



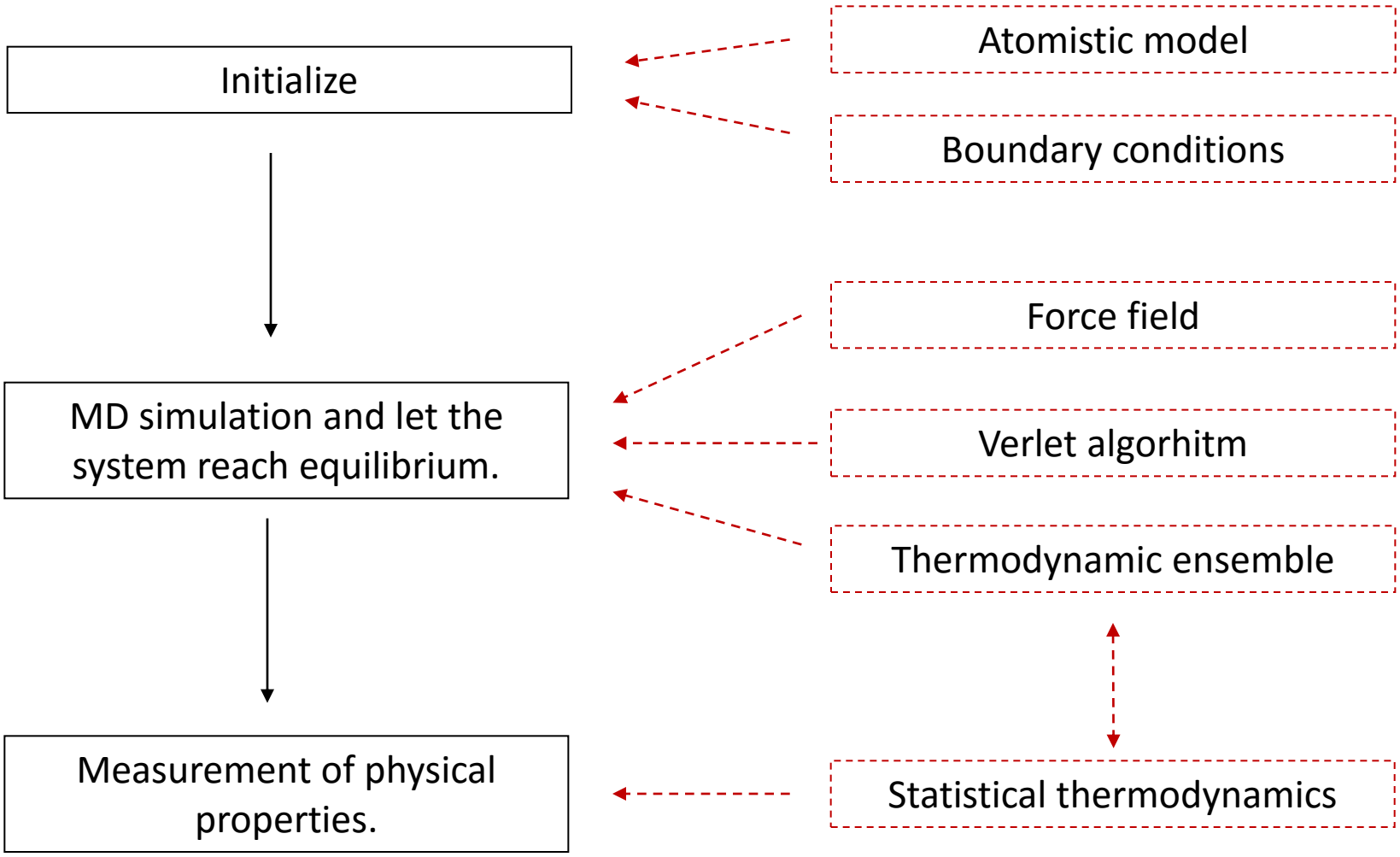
Wettability prediction

- Basic concept



Wettability prediction

- MD model

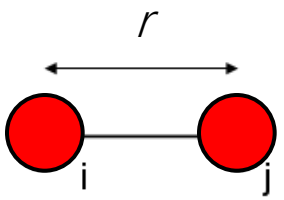


Wettability prediction

- Force field (set of potential interactions)
  - Bonded pair interactions (included in the intramolecular interactions)

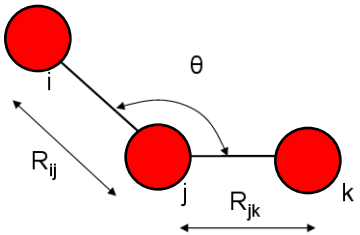
Bond Stretching

$$\varphi_{stretch} = \sum_{stretch} k_b (r - r_0)^2$$



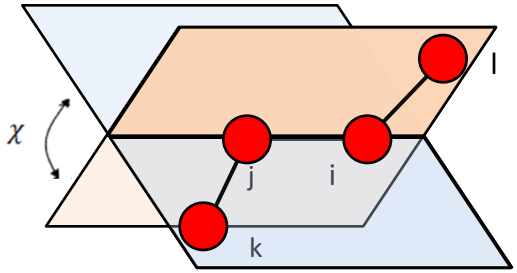
Angle bend

$$\varphi_{angle} = \sum_{angle} k_\theta (\theta - \theta_0)^2$$



Dihedral angle

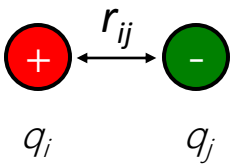
$$\varphi_{dihedral} = \sum_{dihedral} k_\chi \cos(n\chi - \Psi)$$



Wettability prediction

- Force field (set of potential interactions)
  - Non-bonded pair interactions:

Van der Waals potential $$\varphi_{\text{vdWaals}} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

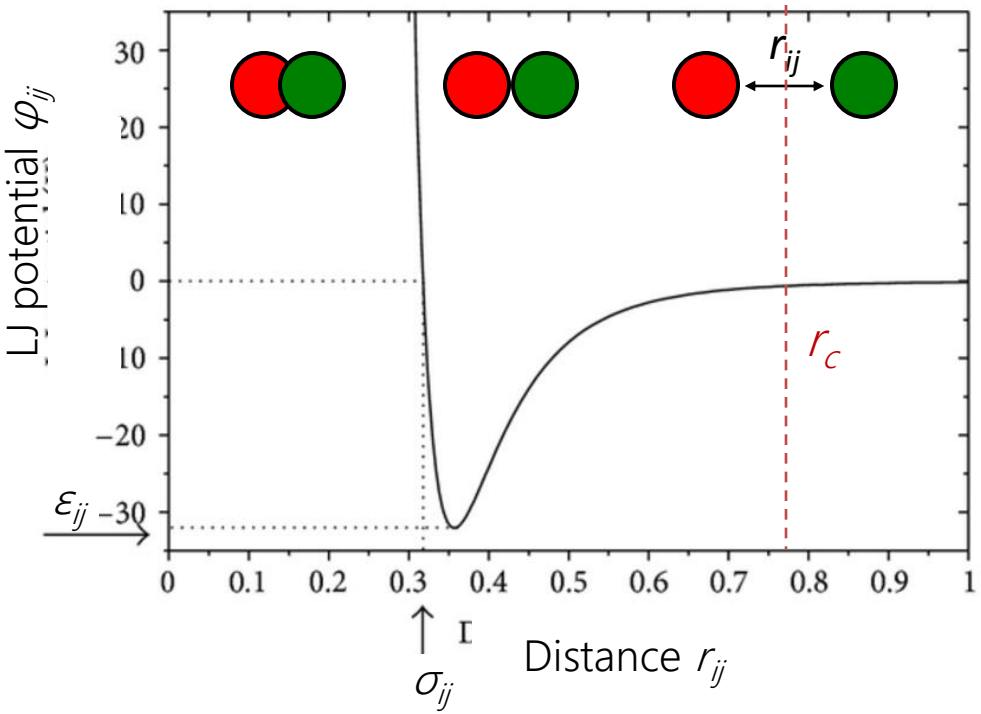


Electrostatic interaction (Coulomb) $$\varphi^{**}_{\text{Coulomb}} = \frac{1}{4\pi\varepsilon_0}\frac{q_i q_j}{r_{ij}}$$

Other function forms can also be found depending on the molecules and atoms placed in the cell.

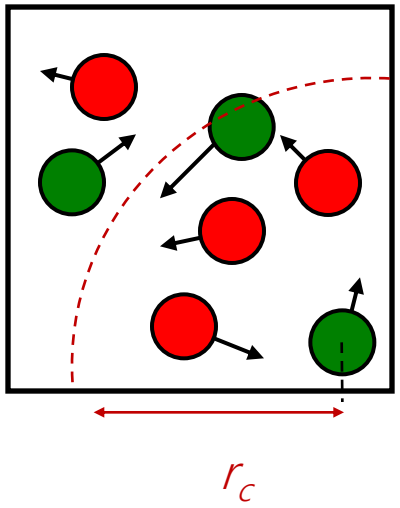
Wettability prediction

Popular potential: Lennard-Jones Potential



Shift to eliminate energy discontinuity

$$\varphi_{\mathrm{LJ,T}}(r_{ij}) = \begin{cases} \varphi_{\mathrm{LJ}}(r_{ij}) - \varphi_{\mathrm{LJ}}(r_c) & r \le r_c \\ 0 & r \le r_c \end{cases}$$



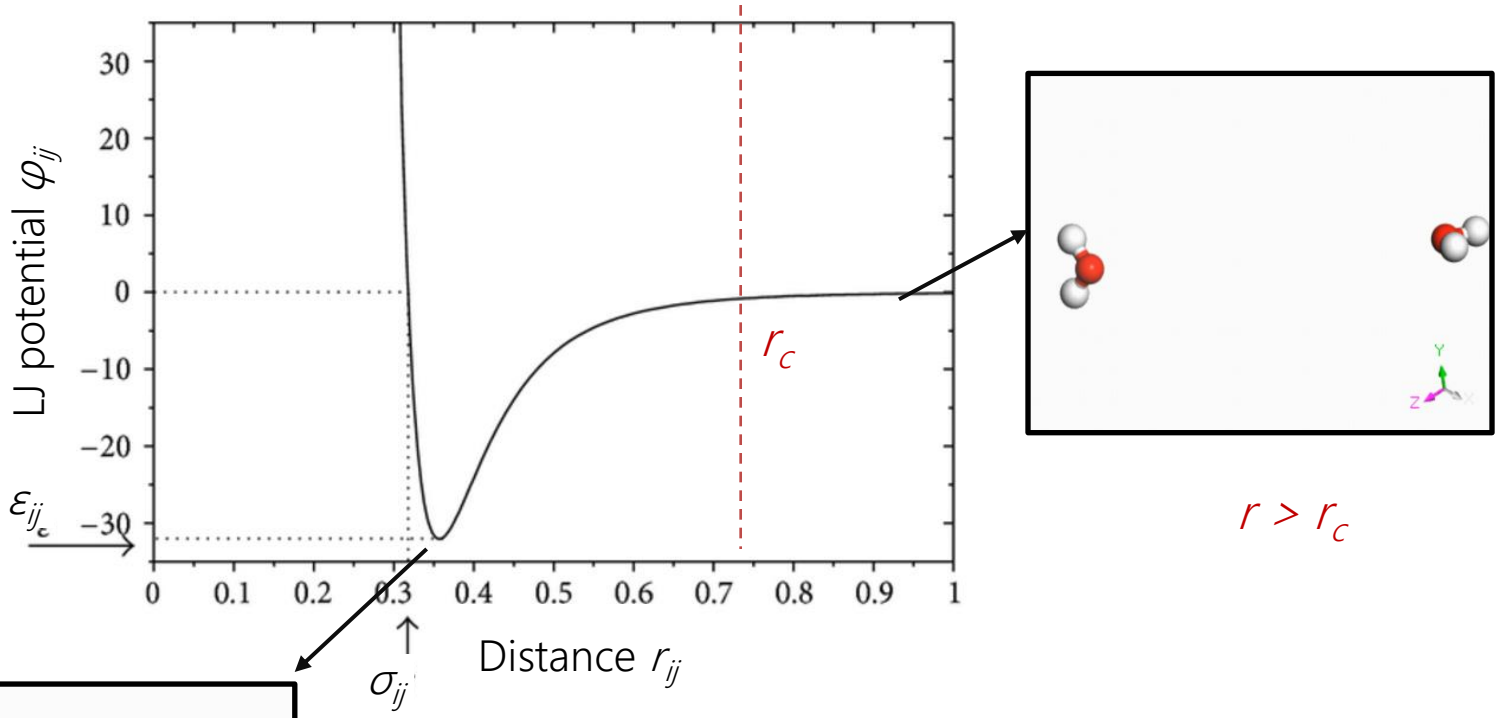
In reality, every atom interacts with every atom.

→ computationally demanding.

Lennard-Jones is often *truncated* at $r_{\mathrm{cut}} = 2.5\ \sigma$.

Wettability prediction

Popular potential: Lennard-Jones Potential



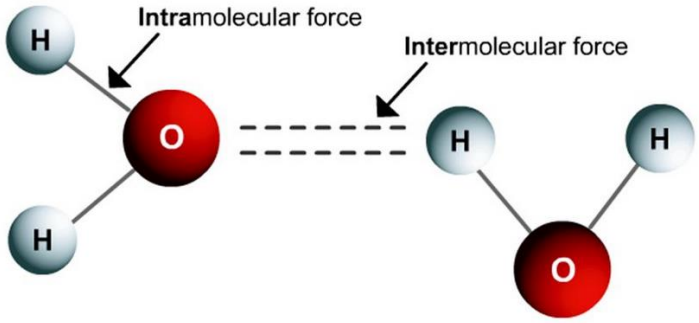
Wettability prediction

- Force field (set of potential interactions)

The heart of any molecular dynamics scheme is the force model used to analytically describe the atomistic interactions.

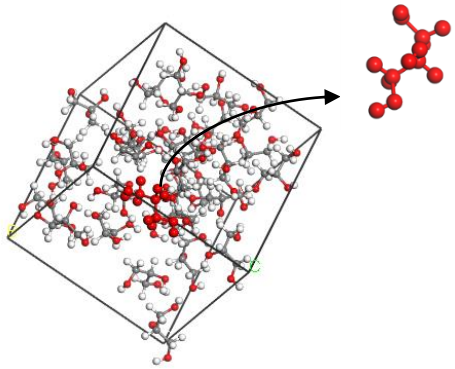
A force field can be divided into contributions from the intramolecular and intermolecular interactions:

$$\phi = \phi_{\text{int}ermolecular} + \phi_{\text{int}ramolecular}$$



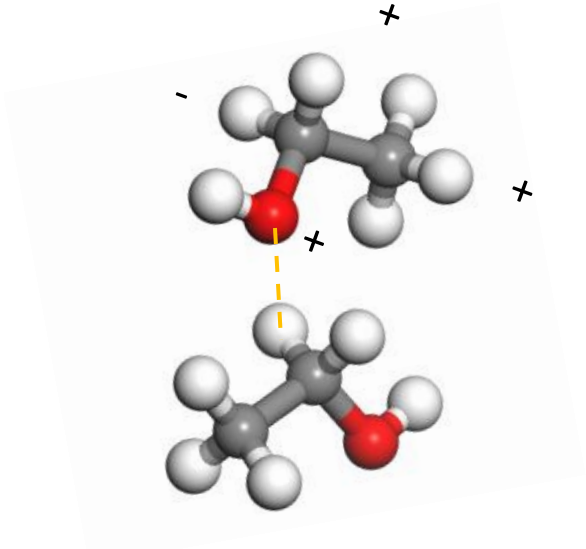
Wettability prediction

- Solubility parameter δ (i.e. cohesive energy density)
  - Measures the interactions of a molecule with its surroundings.



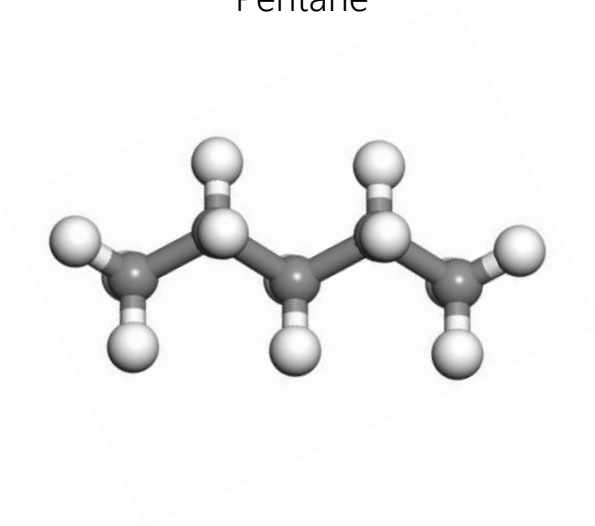
$$\delta = \sqrt{\delta_d^2 + \delta_p^2 + \delta_h^2} \qquad (J.cm^{-3})^{1/2}$$

Ethanol



δ_d = 13.56 δ_p = 19.09 δ_h = 11.67

Pentane



δ_d = 15.20 δ_p = 0.01 δ_h = 0.01

Wettability prediction

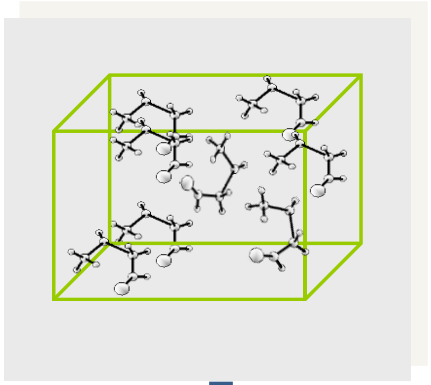
- Overall procedure in MD for the calculation of δ :

1) Cubic periodic unit cell with N molecules.

2) Dreiding forcefield.

3) Charge equilibration.

4) Geometry optimization.



5) First NPT then NVT with T = 298K (Nose-Hoover thermostat).

6) MD over 200 ps with a time step of 1 fs.

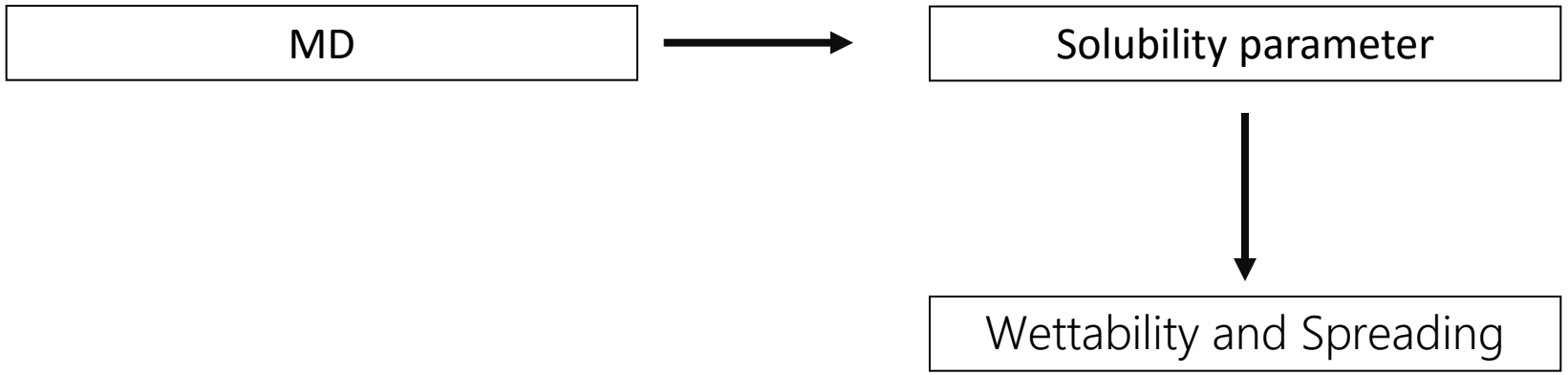
7) Average δ over the last 20 ps, where $\delta = \sqrt{CED} = \sqrt{\frac{< \sum_{i=1}^{n} E_i^k - E_c^k >}{N_{av} < V_{cell} >}}$

Wettability prediction

- Solubility parameter δ (i.e. cohesive energy density)

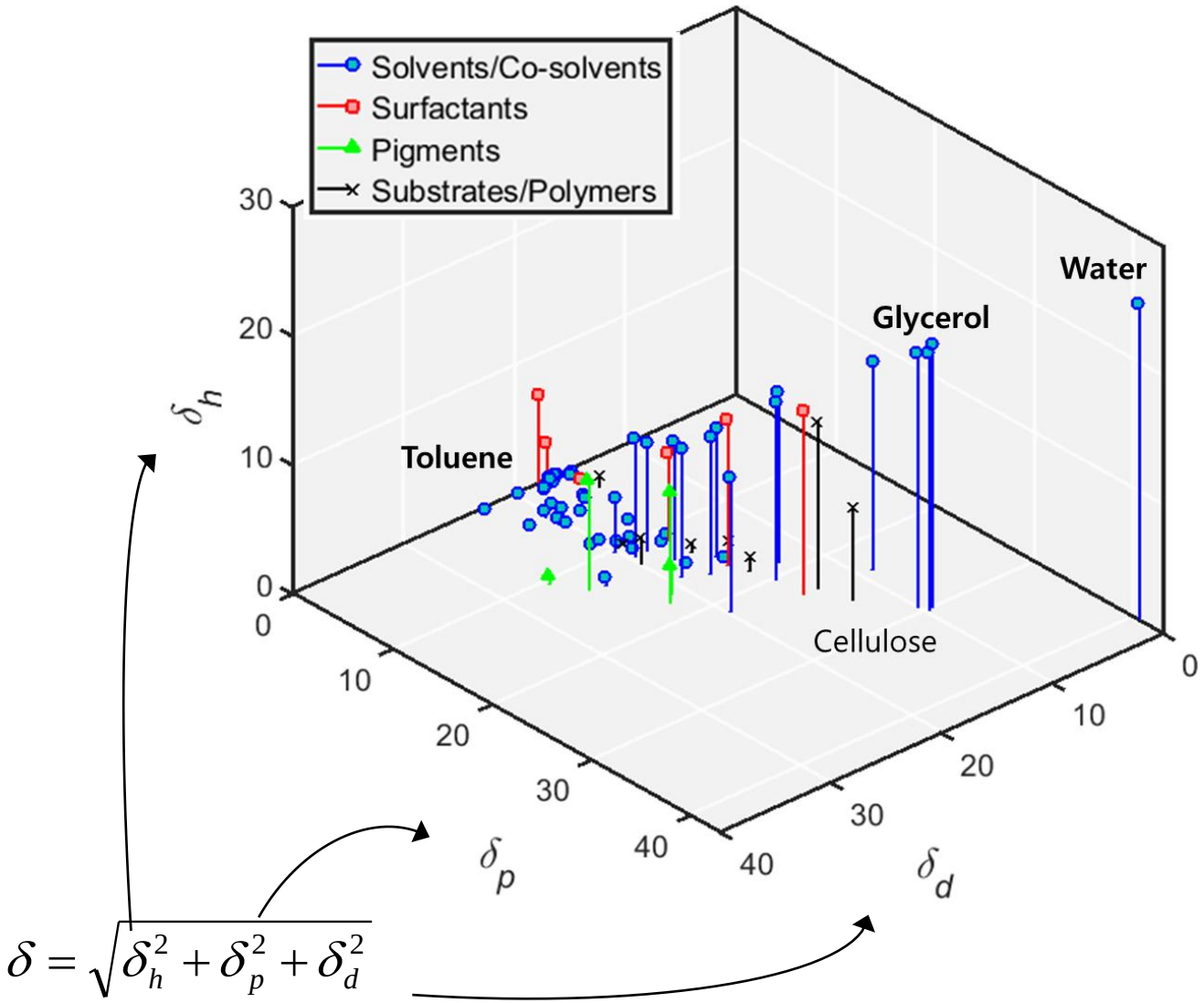
	Solubility parameters $(J.cm^{-3})^{0.5}$				
Components	*δTotal*	*δd*	*δP*	*δh*	
Solvents/liquids					
Water	45.9	0	38.78	24.52	Does not spread
Toluene	18.98	18.8	1.922	1.76	Spread
Glycerol	35.85	11.61	27.97	19.18	Does not spread
Acetone	20.16	16.19	11.99	0.78	Spread
Styrene	19.6	19.49	1.84	0.98	Spread
Ethylene Carbonate	28.39	23.68	15.64	0.88	-
Formamide	30.598	12.372	20.35	19.28	Does not spread
Heptane	16.14	16.1	1.088	0.31	Spread

Wettability prediction



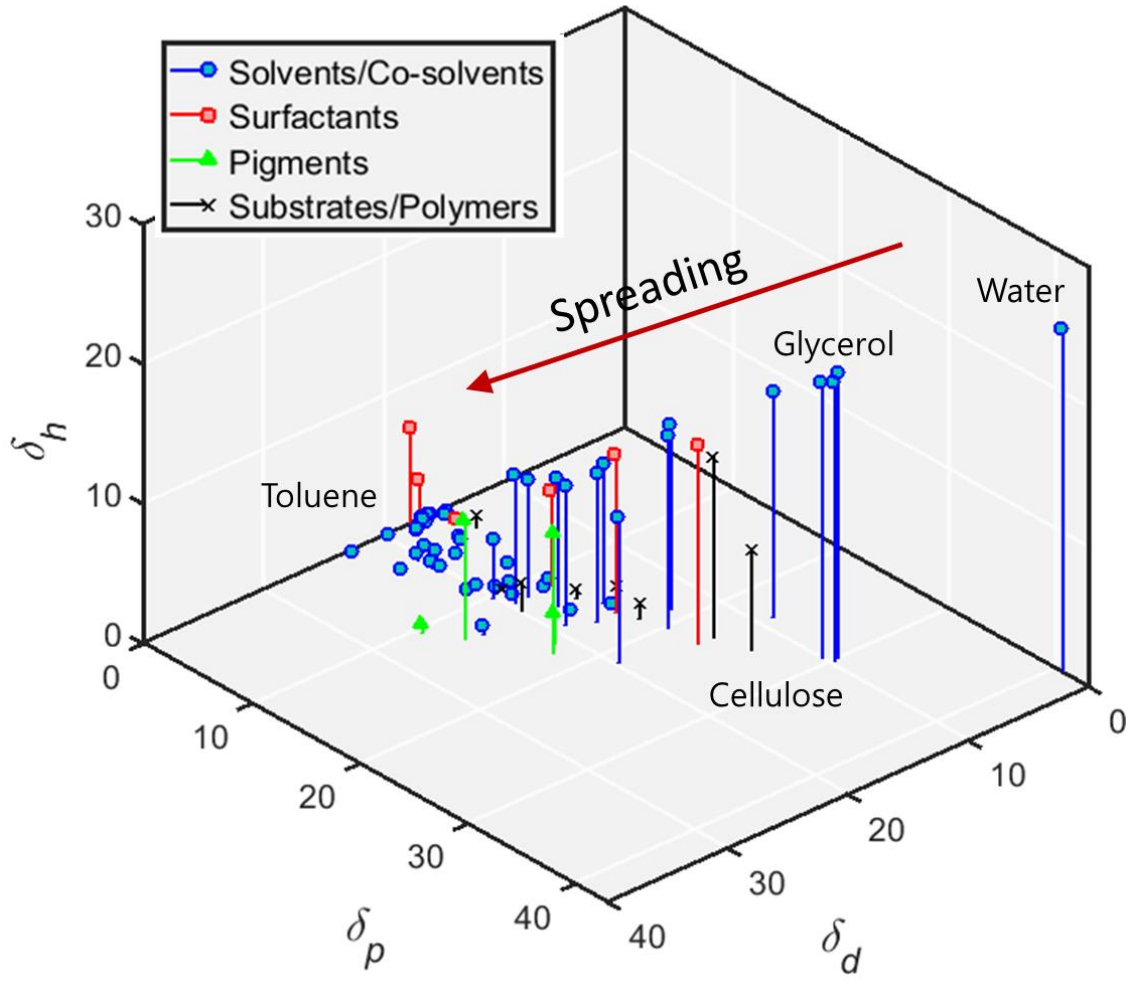
Wettability prediction

- Solubility parameters obtained from **MD** placed in the Hansen graph



Wettability prediction

- Spreading



Wettability prediction

- Wetting

$$\gamma = k\delta^2 V_m^{1/3}$$

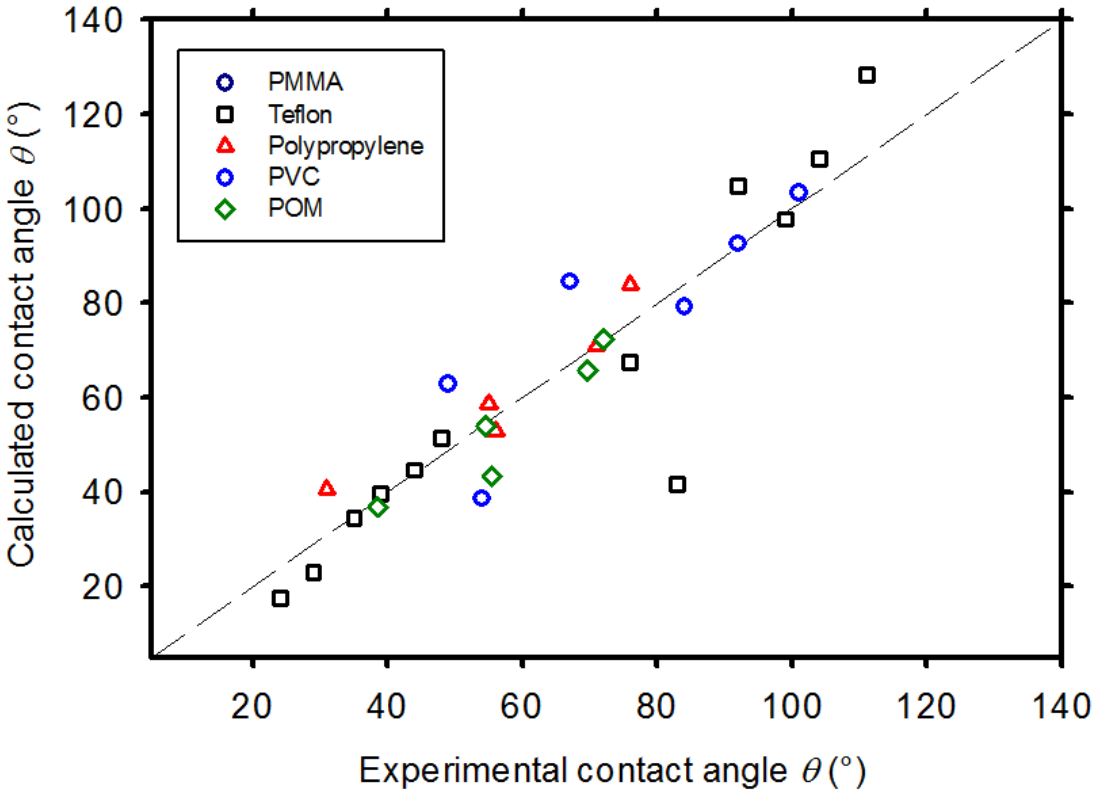
Owens and Wendt + Young:

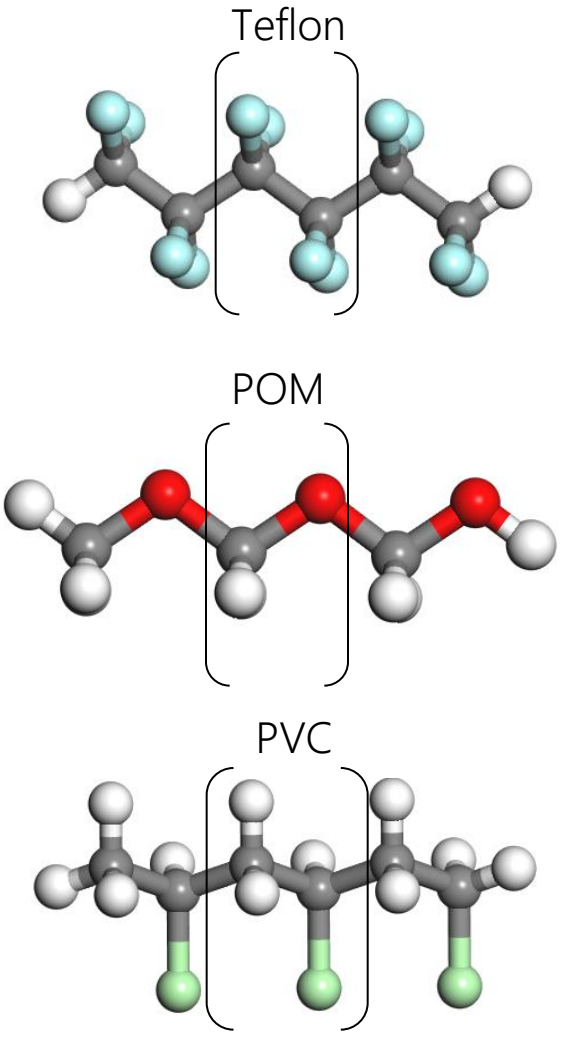
$$cos\theta = -1 + 2\frac{\sqrt{\gamma_s^d \gamma_f^d}}{\gamma_f} + 2\frac{\sqrt{\gamma_s^p \gamma_f^p}}{\gamma_f}$$

$$\longrightarrow \quad cos\theta = -1 + 2\frac{V_{ms}^{1/6}}{V_{mf}^{1/6}}\left(\frac{\delta_s^d \delta_f^d}{\delta_f^2} + \frac{\delta_s^p \delta_f^p}{\delta_f^2} + \frac{\delta_s^h \delta_f^h}{\delta_f^2}\right)$$

Wettability prediction

- Wetting





PVC: Polyvinyl chloride, Teflon: Polytetrafluoroethylene,
POM: Polyoxymethylene, PMMA: Poly(methyl methacrylate)

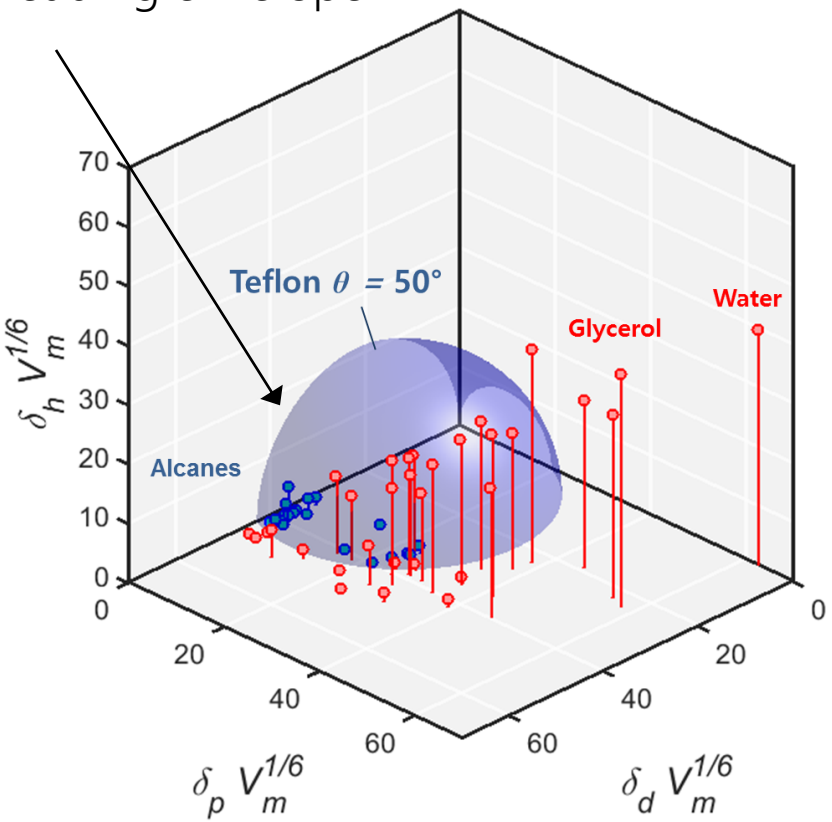
Ozkan, Orkun, and H. Yildirim Erbil. *Surface Topography: Metrology and Properties* 5.2 (2017): 024002.
Burdzik, Andrea, et al., International Journal of Adhesion and Adhesives 82 (2018): 1-7.

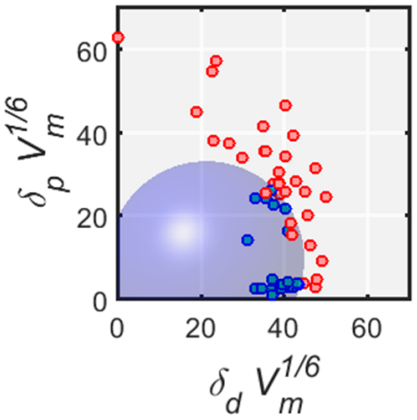
Wettability prediction

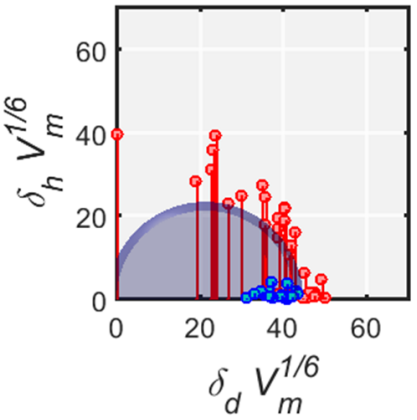
- Wetting

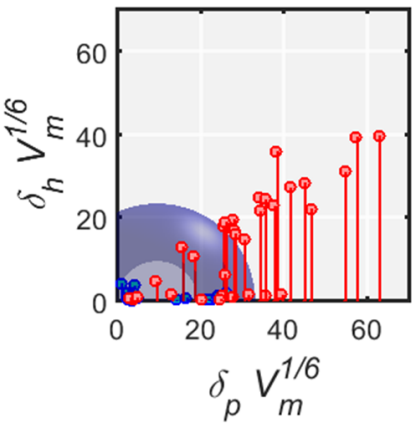
$$cos\theta = -1 + 2\frac{V_{ms}^{1/6}}{V_{mf}^{1/6}}\left(\frac{\delta_s^d\delta_f^d}{\delta_f^2} + \frac{\delta_s^p\delta_f^p}{\delta_f^2} + \frac{\delta_s^h\delta_f^h}{\delta_f^2}\right)$$

Spreading envelope



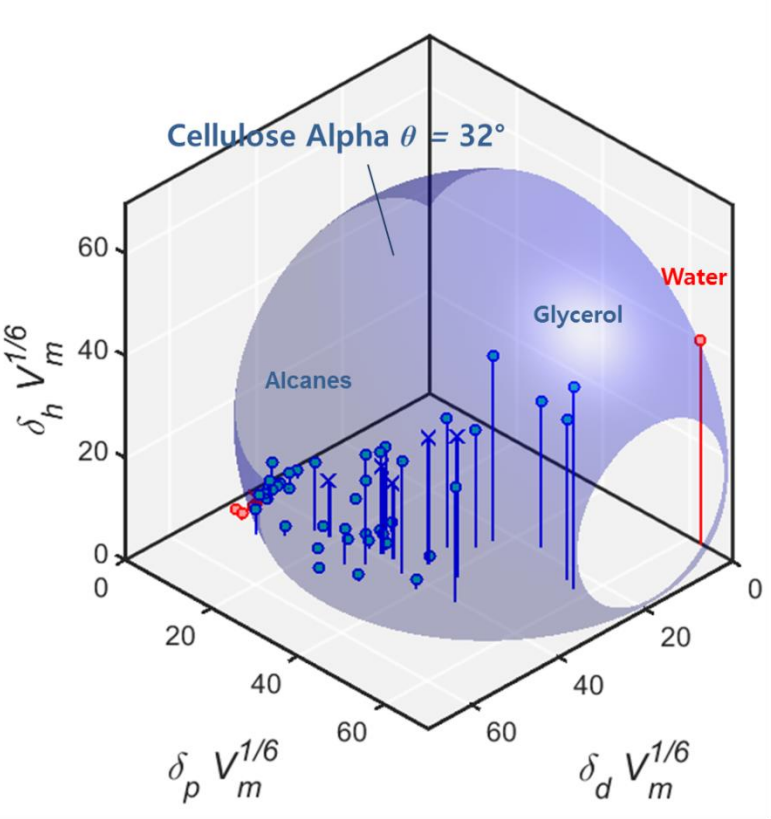


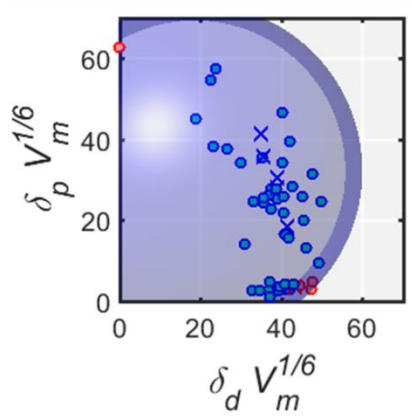


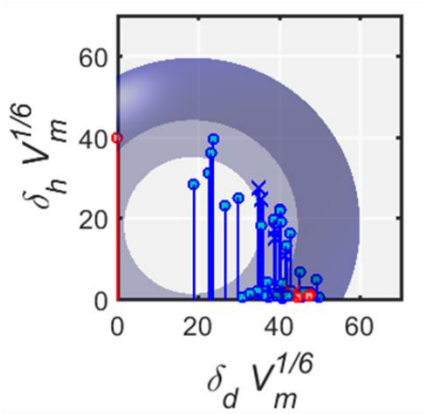


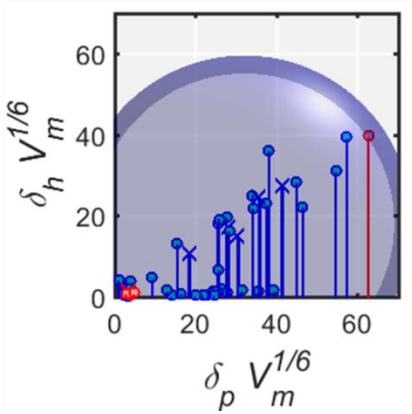
Wettability prediction

- Wetting





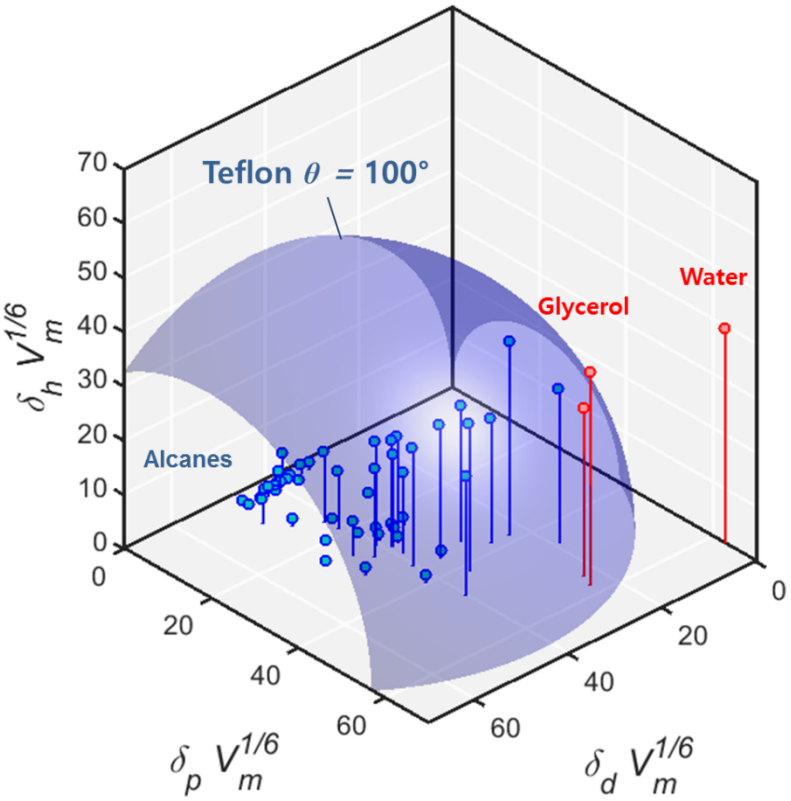


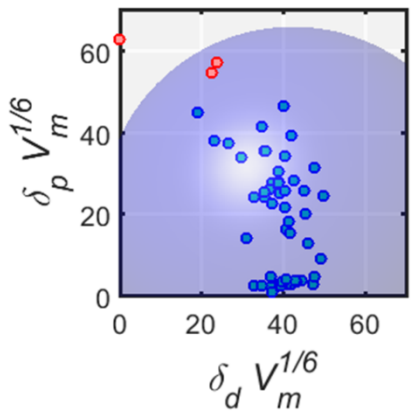


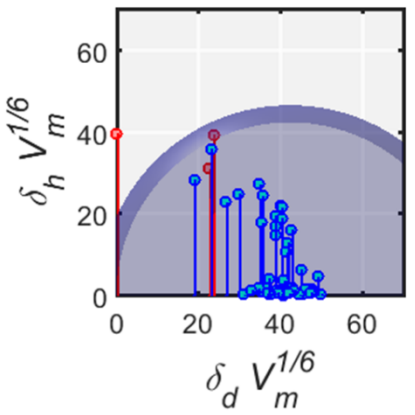
Wettability prediction

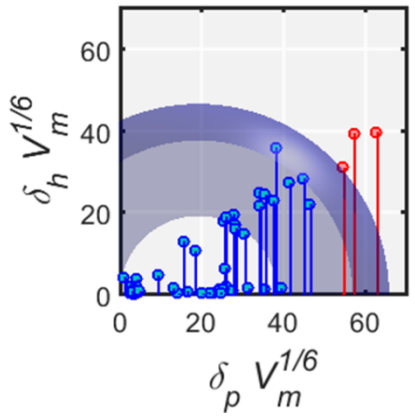
- Wetting

$$cos\theta = -1 + 2\frac{V_{ms}^{1/6}}{V_{mf}^{1/6}}\left(\frac{\delta_s^d\delta_f^d}{\delta_f^2} + \frac{\delta_s^p\delta_f^p}{\delta_f^2} + \frac{\delta_s^h\delta_f^h}{\delta_f^2}\right)$$









Wettability prediction

- Work of adhesion

$$W_{ls} = 2\phi_{ls}\left(\frac{\delta_l}{k}\right)^{1/2}\left(\frac{\delta_s}{k}\right)^{1/2}(v_l v_s)^{1/6}$$

$$\phi_{ls} = 2\left(\frac{x_l^d x_s^d}{g_l x_l^d + g_s x_s^d} + \frac{x_l^p x_s^p}{g_l x_l^p + g_s x_s^p}\right)$$

$$x_i^p = \frac{\gamma_i^p}{\gamma_i} \qquad x_i^d = \frac{\gamma_i^d}{\gamma_i} \qquad g_l = \frac{\gamma_l}{\gamma_s} \qquad g_s = \frac{\gamma_s}{\gamma_l}$$

$$S = W_{ls} - W_l$$


MD
Wettability and Spreading

Wettability prediction

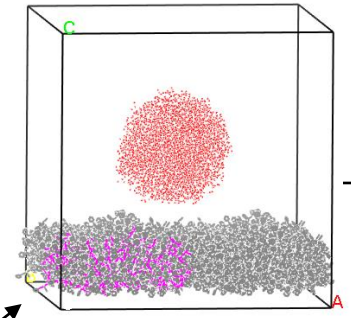
Polystyrene

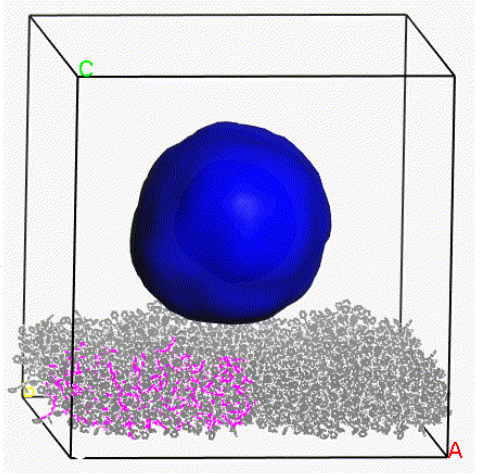
Cubic cell

Supercell

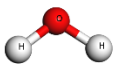
Put droplet above surface. And give it a little push (5A/s)

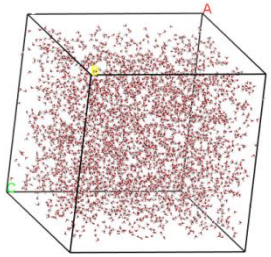
Isosurface





Water





Perform third MD simulation

Contact angle measurement

Construction

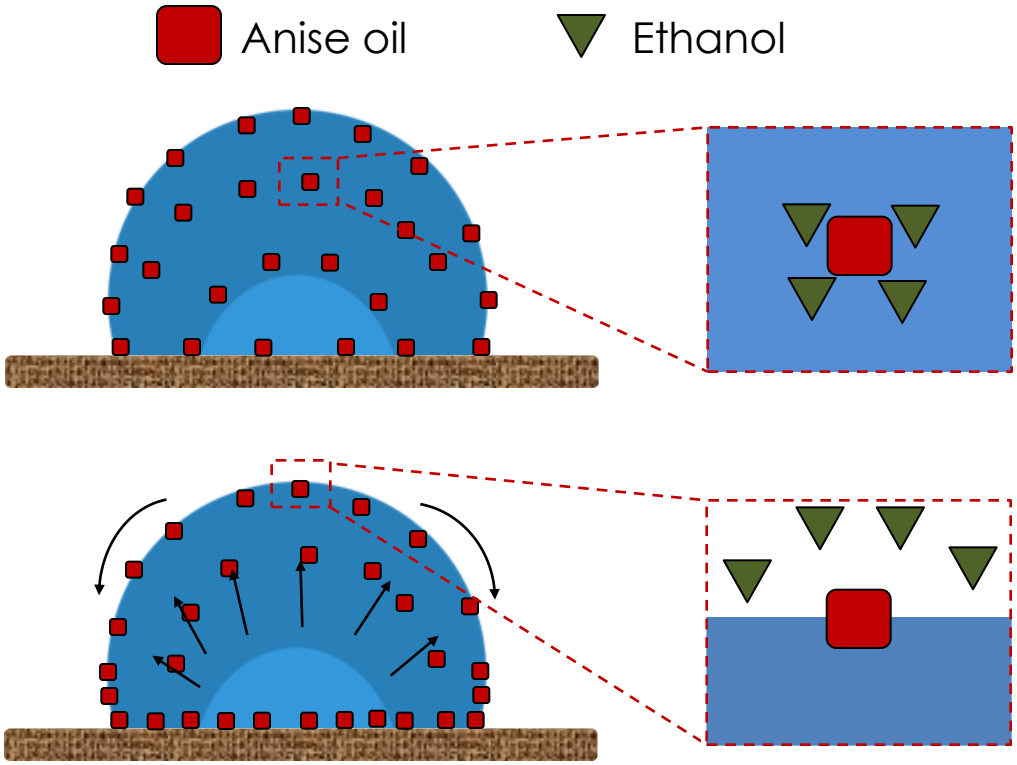
Optimization and MD simulation With the same procedure described previously.

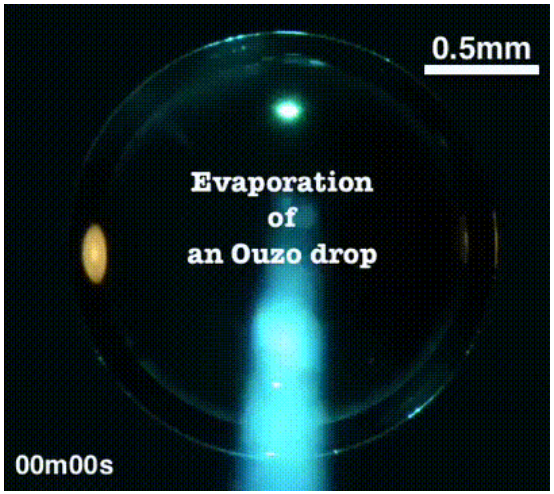
Second MD simulation until droplet formation

Research work on wettability

Research work on wettability

- Ouzo effect



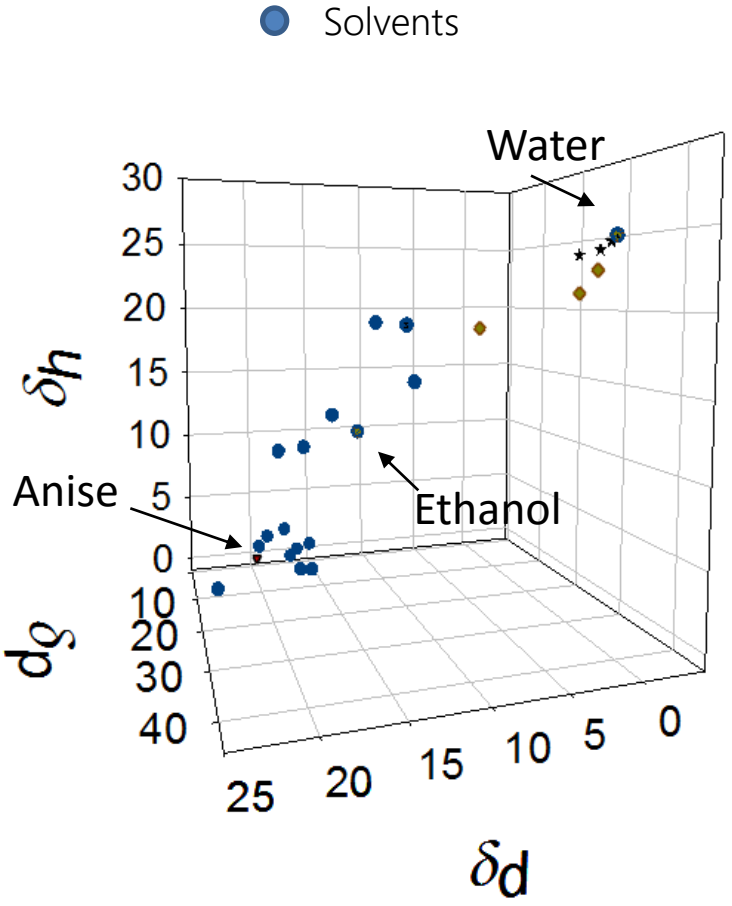


- Hypothesis: Ethanol have high affinity with Anise oil. Ethanol tend to surround Anise molecules (Ethanol interacts strongly with Anise oil). This explains the formation of oil droplets.
- Once on the surface, Ethanol evaporates and Anise oil microdroplets migrate to to the rim forming a ring.

Research work on wettability

- Ouzo effect

Components	Density (g/cm³)	Solubility parameter $(J.cm^{-3})^{1/2}$				
		Exp. δt	MD Simulation			
			δt	δd	δp	δh
Ethanol	0.789	26.18	26.17	13.56	19.09	11.67
Anis oil	0.986	-	20.8	20.002	5.66	0.78
Water	0.997	47.9	45.9	0	38.78	24.56

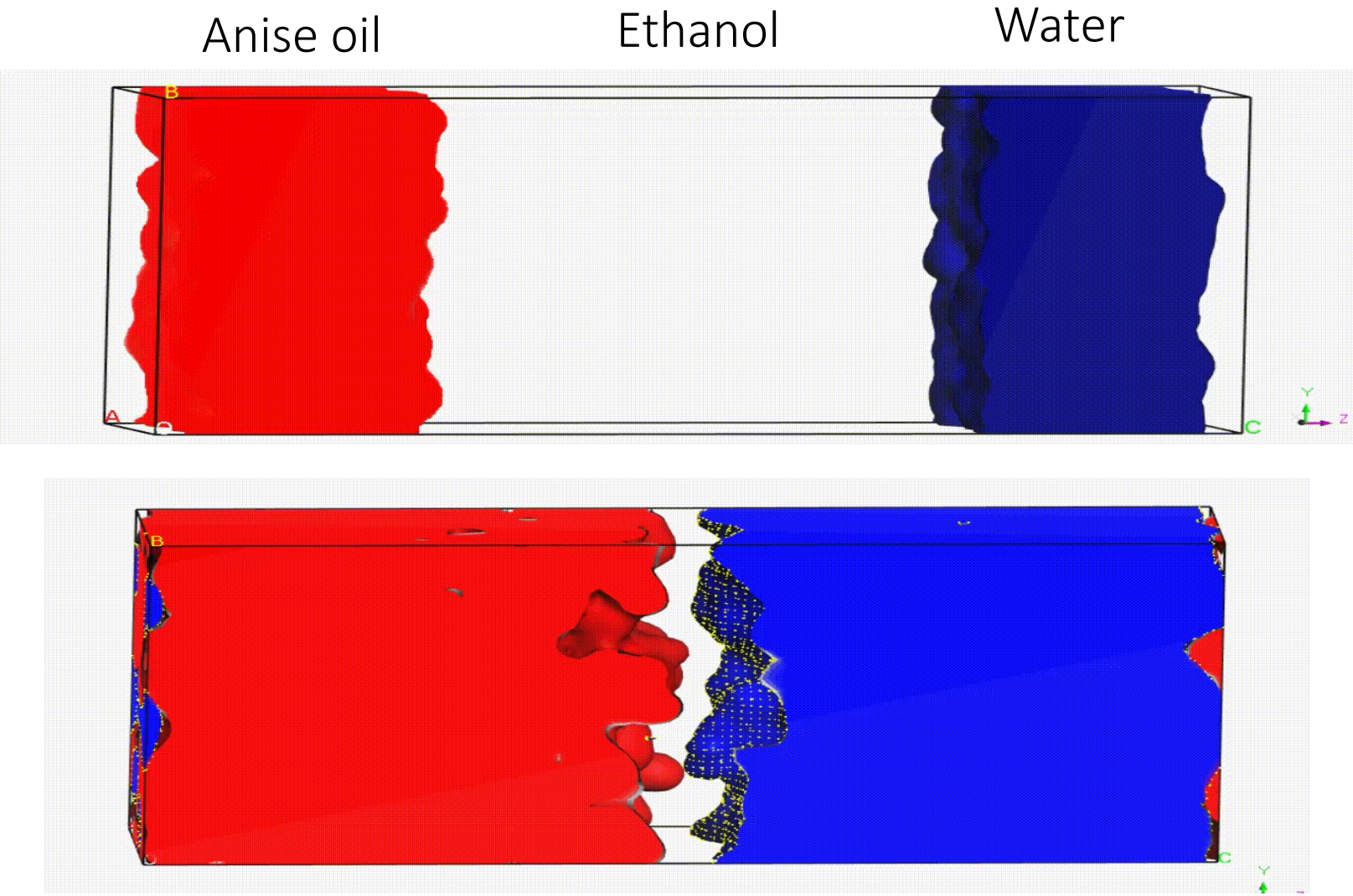


$$\Delta\delta_{Anise-Ethanol} = 20.64 \quad < \quad \Delta\delta_{Water-Ethanol} = 35.90$$

- Hansen graph: Ethanol has good affinity with both Water and Anis oil, but results suggest that this affinity is higher with Anise oil.

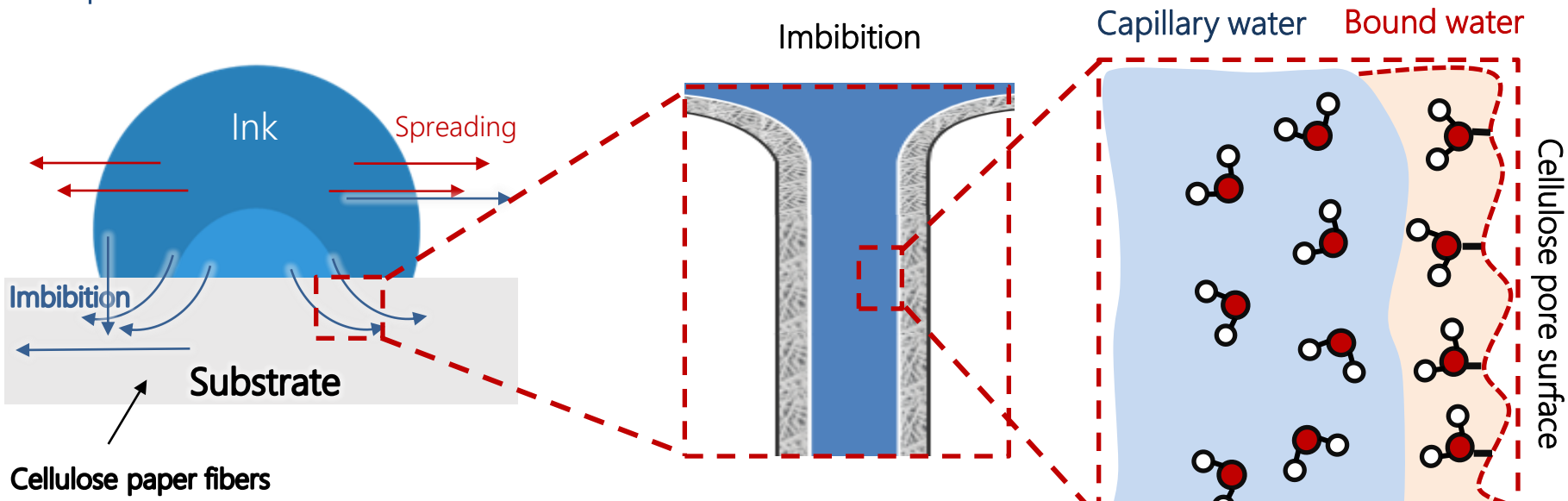
Research work on wettability

- Ouzo effect

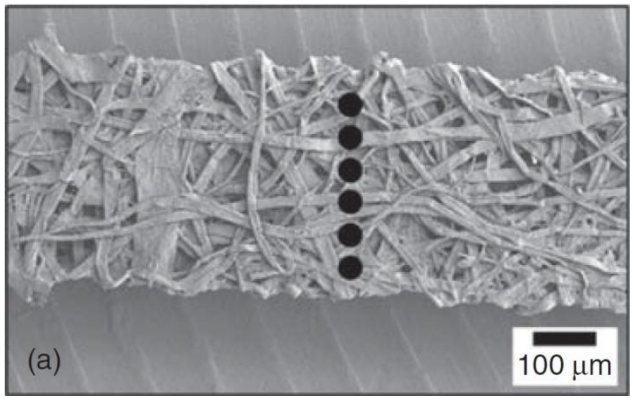


Research work on wettability

- Liquid imbibition



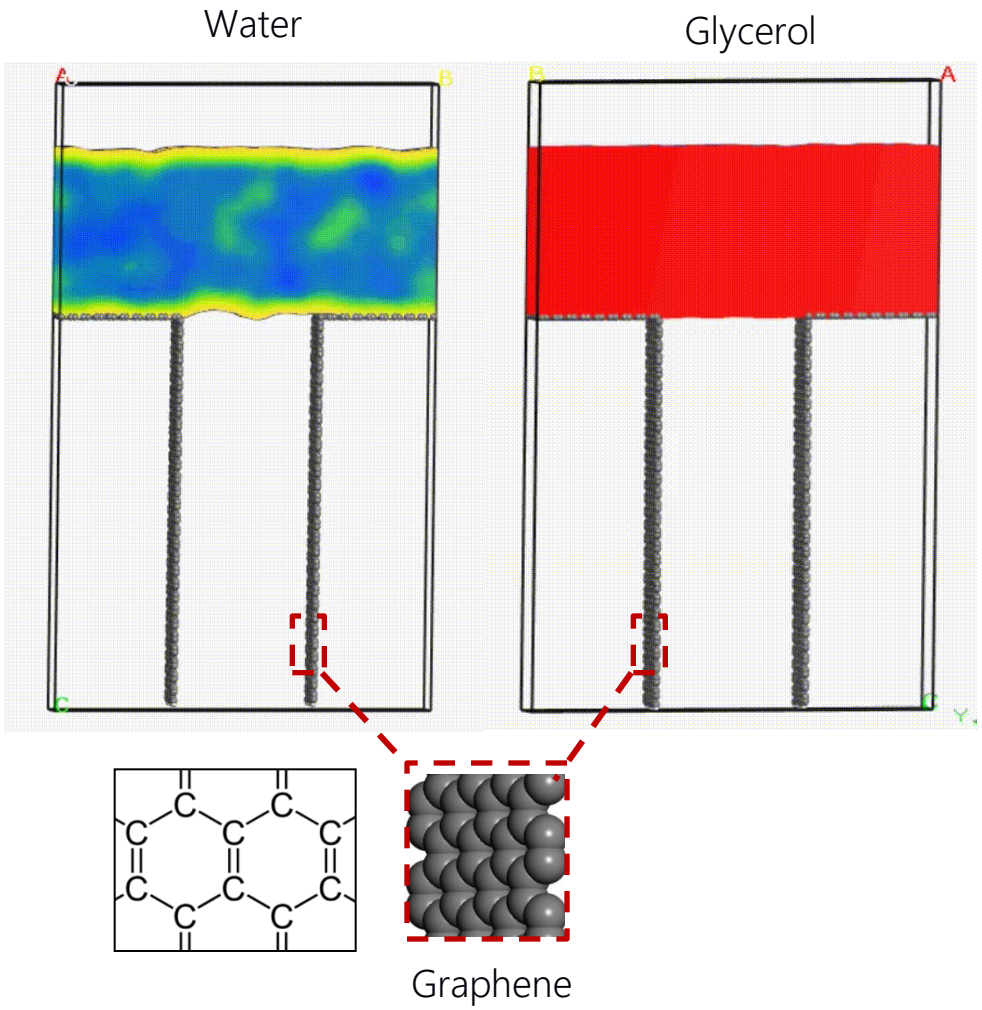
- Effect of the physico-chemical properties of the pore on the imbibition dynamics?
- Imbibition of multicomponents liquids?

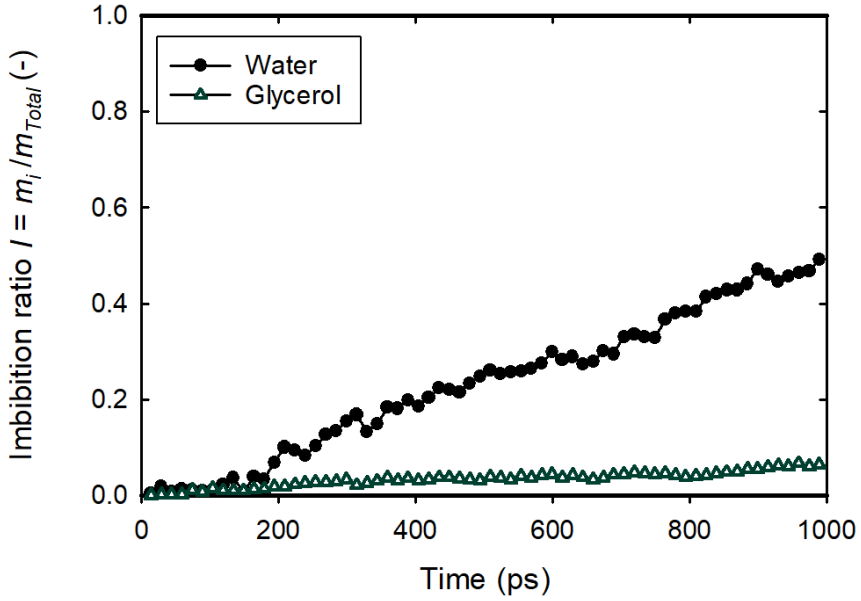


SEM of paper with black circles drawn to illustrate approximate scale of standard inkjet drops

Research work on wettability

- Liquid imbibition

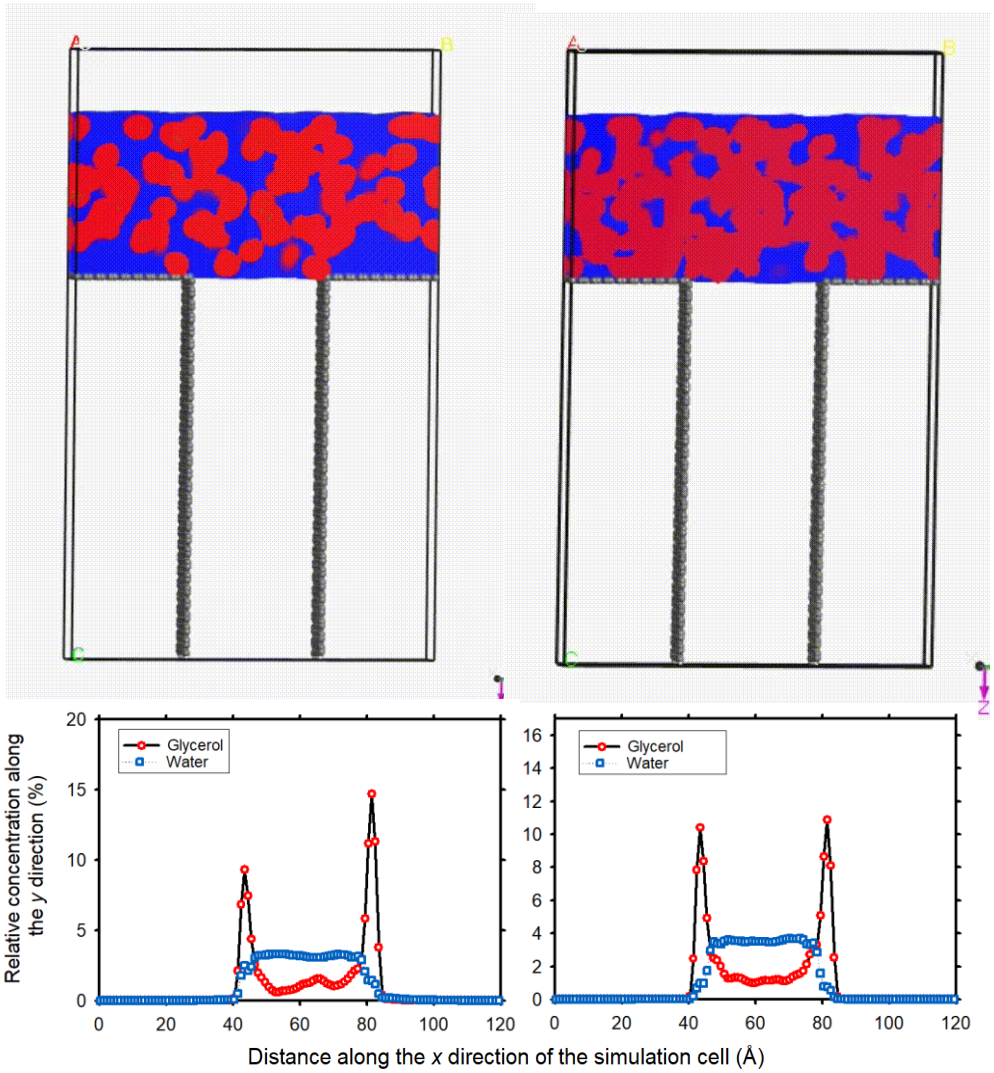


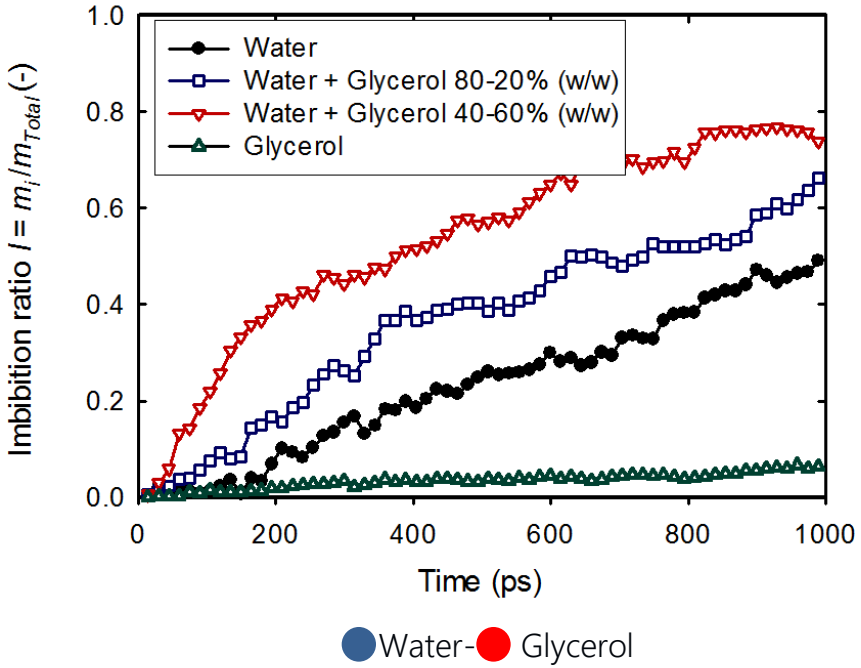


Research work on wettability

- Liquid imbibition

Water- Glycerol 80-20% (w/w) Water - Glycerol 60-40% (w/w)

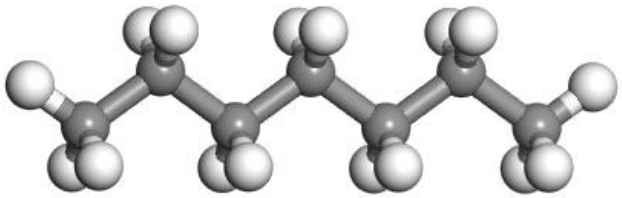




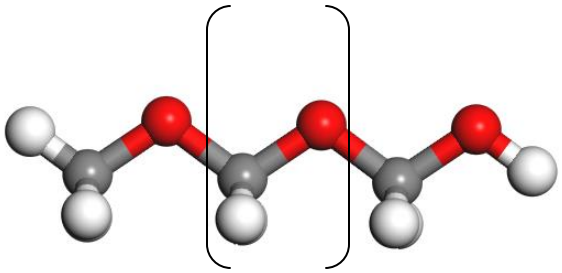
Exercices

1) An unknown component « A » does not wet very well POM substrate. By looking at the molecular structures of the liquids and POM, which one of the following liquids is most likely to be « A » and why:

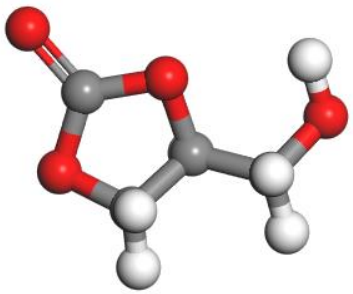
a) Heptane, b) Glycerol Carbonate, c) Cyclobutanone, d) Ethylene carbonate



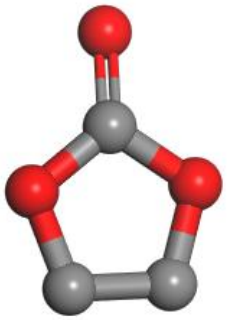
Heptane



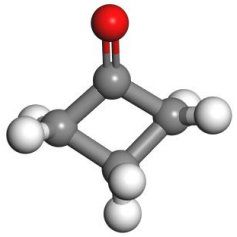
POM



Glycerol Carbonate



Ethylene carbonate



Cyclobutanone

Using the properties of the components in Table 1:

1) Calculate the contact angle of water, Toluene, Glycerol and Acetone on Teflon.

2) Which solvent have the highest affinity to water?

3) Acetophenone and Benzylamine have the same surface tension; do they have the same wettability on Teflon? Comment.

	Solubility parameters $(J.cm^{-3})^{0.5}$				
Components	δTotal	δd	δP	δh	Molar volume $(cm^3.mol^{-1})$
Solvents/liquids					
Water	45.9	0	38.78	24.52	18.03
Toluene	18.98	18.8	1.922	1.76	105.2
Glycerol	35.85	11.61	27.97	19.18	75
Acetone	20.16	16.19	11.99	0.78	72.4
Acetic acid	26.4	15.23	17.4	12.37	117.7
Acetophenone	22.53	20.614	9.09	0.19	109.8
Benzylamine	21.25	19.1	7.11	6.04	18.03
Substrate					
Teflon	21.38	16.38	13.72	0.74	76.2
Polyoxymethylene (POM)	29.5	12.55	25.71	7.189	41.1

Thank you!