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 ($\gamma$)

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

\[ E = \gamma.A \]

\[ F \cdot dh = dE = \gamma.L.dh \]

\[ F = \gamma.L \]

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

<table>
<thead>
<tr>
<th></th>
<th>Contact Angle (°)</th>
<th>Surface Tension (mN/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>72.8</td>
<td>10^{-3}</td>
</tr>
<tr>
<td>Benzene</td>
<td>28.8</td>
<td></td>
</tr>
<tr>
<td>Blood</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>Mercury</td>
<td>486</td>
<td></td>
</tr>
</tbody>
</table>
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 $\rightarrow$ Contact angle $\rightarrow$ molecular interactions

<table>
<thead>
<tr>
<th>Substance</th>
<th>Contact Angle (θ)</th>
<th>Surface Tension (γ)</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>72.8°</td>
<td>$10^{-3}$ N.m$^{-1}$</td>
<td>Highly polar with high hydrogen bonding</td>
</tr>
<tr>
<td>Benzene</td>
<td>28.8°</td>
<td></td>
<td>Non-polar, only dispersion</td>
</tr>
<tr>
<td>Blood</td>
<td>60</td>
<td></td>
<td>Polar (mostly made of water)</td>
</tr>
<tr>
<td>Mercury</td>
<td>486</td>
<td></td>
<td>Metallic bonds</td>
</tr>
</tbody>
</table>
Introduction to wetting

- Wettability $\Rightarrow$ Contact angle $\Rightarrow$ Intermolecular interactions

Owens and Wendt + Young:

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

Subscripts “$d$” and “$p$” refers to dispersive and polar contributions respectively.
Introduction to wetting

- Capillary action

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

\[ F_s = \gamma 2\pi r \cos \theta \]

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

Competition between depression under the meniscus and weight of the water column
Introduction to wetting

• Tears of wine (Larmes du vin)

Less alcohol

More alcohol
Introduction to wetting

- Capillary action

\[ F_c = 2\pi\gamma r \cos \theta \]

Introduction to wetting

- Agglomeration and coating

**Fluidized bed coater**

**Nozzle**

**Coating solution** (dispersed particles)

**Food particles**

**Hot Air**

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

- Primary particles
- Binder or coating solution
- Aggregate
- Coated particle

**Wetting**

**Drying**
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.

\[
W_l = 2\gamma_l \quad \text{Cohesion}
\]

\[
W_{ls} = \gamma_l + \gamma_s - \gamma_{ls} \quad \text{Adhesion}
\]

Wetting is the balance between cohesive and adhesive forces
Introduction to wetting

- Work of Adhesion/cohesion

Girifalco and Good

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

\[ \Phi_V = \frac{4(v_i v_s)^{1/3}}{(v_i^{1/3} + v_s^{1/3})^2} \]

\[ \Phi_I = \frac{\epsilon_{ls}}{(\epsilon_i \epsilon_s)^{0.5}} \]

Wu

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

\[ \phi_{ls} = 2 \left( \frac{x_i^d x_i^d}{g_i x_i^d + g_s x_s^d} + \frac{x_i^p x_s^p}{g_i x_i^p + g_s x_s^p} \right) \]

\[ x_i^p = \frac{\gamma_i^p}{\gamma_i} \quad x_i^d = \frac{\gamma_i^d}{\gamma_i} \quad i = l \text{ or } s \]

\[ g_s = \frac{\gamma_s}{\gamma_l} \quad g_i = \frac{\gamma_i}{\gamma_s} \]

\[ W_{\bullet\bullet} > W_{\bullet} > W_{\circ} \]

\[ W_{\bullet\bullet} > W_{\circ\circ} > W_{\bullet\circ} \]

\[ W_{\bullet\bullet} > W_{\bullet\circ} > W_{\circ\bullet} \]

- No affinity

- surrounds
Introduction to wetting

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

\[ S = W_{ls} - W_l \]

If \( S > 0 \)  Spontaneous spreading

Adhesion  \[ \uparrow \]  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**

**Heptanediol**

Without surfactants

With surfactants
Introduction to wetting

- Surfactants

Water: Higher surface tension

Ink: contains surfactants \( \Rightarrow \) 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.

  ![Diagram](attachment:image.png)

  - **Surfactants**
    - A: $\gamma_{\text{droplet}} > \gamma_{\text{surfactant}}$
      - $C_{\text{surfactant}} < \text{CMC}$
    - B: $\gamma_{\text{droplet}} \approx \gamma_{\text{surfactant}}$
      - $C_{\text{surfactant}} = \text{CMC}$
    - C: $\gamma_{\text{droplet}} \approx \gamma_{\text{surfactant}}$
      - $C_{\text{surfactant}} > \text{CMC}$
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)
- Wet granular flow is ubiquitous in nature and industry.

- Industrial applications of granular materials involve high number of particles.
Wetting and granular flow

- Different Regimes

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

- **Pendular**
  \[ 0.05 < S^* < 0.3 \]
  No capillary forces between the particles

- **Funicular**
  \[ 0.3 < S^* < 0.9 \]
  Capillary forces/cohesion active between the particles

- **Capillary**
  \[ S^* > 0.9 \]
  Liquid volume

- **Void volume**

Capillary forces/cohesion active between the particles
Wetting and granular flow

- Different Regimes
Wetting and granular flow

- Willet model

The bridge rupture distance is defined by:

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

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
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: \( V_{new} = \min\left( V_{old} + \frac{V_{rup}}{2N}, V_b^{\text{max}} \right) \)
- If \( V_{new} > V_b^{\text{max}} \) then \( V_{new} = V_b^{\text{max}} \)

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

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

\[ \eta = 3 + \frac{Z - 3}{n_A + (1 - n_A)c^2} \]

\[ n_A = 1 - n_B = \frac{N_A}{N_A + N_B} \]

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

Wetting and granular flow

- Liquid migration

Soulié (2005)

Wetting and granular flow

- Capillary number

\[ Ca = \frac{\mu \nu}{\gamma} \]

- Dynamic liquid bridge: \( Ca > 1 \)
- Static liquid bridge: \( Ca < 10^{-3} \)

\( \gamma \): Surface tension of liquid
\( \mu \): Dynamic viscosity of liquid
\( \nu \): Relative velocity between particles
Wetting and granular flow

- Capillary forces and flowability

- Rotating drum apparatus

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

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drum, R×L (mm)</td>
<td>60.5×22</td>
</tr>
<tr>
<td>Glass beads radii r (mm)</td>
<td>0.85, 1.25 and 2</td>
</tr>
<tr>
<td>Rotation speed (rpm)</td>
<td>3 to 57</td>
</tr>
<tr>
<td>Particle density $\rho_p$ (kg.m$^{-3}$)</td>
<td>2500</td>
</tr>
<tr>
<td>Filling level $\beta$</td>
<td>35% (125 g)</td>
</tr>
<tr>
<td>Volumetric liquid content $v_{liq}$(ml)</td>
<td>4</td>
</tr>
</tbody>
</table>
Wetting and granular flow

- Capillary forces and flowability

\[ F_r = \frac{\omega^2 R}{g} \]
Wetting and granular flow

- Effect of the rotation speed

We will focus on the continuous steady flow.
**Dry case:** Effect of the rotation speed and the particle size.

The dynamic angle of repose collapses into one linear profile.
Three regions can be distinguished: static, creeping and flowing region.

Velocity gradient and granular temperature

\[
\varphi = \sqrt{\left(\vec{v}_x - \vec{\Omega}_x \right)^2 + \left(\vec{v}_y - \vec{\Omega}_y \right)^2}.
\]

\[
T_g = \langle v^2 \rangle - \langle v \rangle^2.
\]

- Wall driven Velocity
- Gravity driven Velocity
- Flowing region
- Creeping region
- Static region

Flow Velocity \( \varphi \) (m/s)

Granular Temperature \( T \) (m^3/s^2)
- **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.

  \[ F_c = 2\pi r \cos \theta \]

- Capillary forces can be tuned.

Wetting and granular flow

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

The dynamic angle of repose increases with the capillary force.
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

\[
We_g = \frac{e_p RV_p^2}{\gamma}
\]

Configurations inside the red circle have the same Weber number.
Wetting and granular flow

Wettability is important. How to predict it?
Wettability prediction
(Microscale)
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

1) Heating of Ice
   \[ q = mC_{\text{glace}}\Delta T \]

2) Ice melting
   \[ q = n\Delta H_{\text{fus}} \]

3) Heating of liquid water
   \[ q = mC_{\text{eau}}\Delta T \]

4) Vaporization of water
   \[ q = n\Delta H_{\text{vap}} \]

5) Heating water gaz
   \[ q = mC_{\text{vpeur}}\Delta T \]
Initialize

MD simulation and let the system reach equilibrium.

Measurement of physical properties.

• MD model

Atomistic model

Boundary conditions

Force field

Verlet algorithm

Thermodynamic ensemble

Statistical thermodynamics
Wettability prediction

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

### Bond Stretching

\[ \varphi_{\text{stretch}} = \sum_{\text{stretch}} k_b (r - r_0)^2 \]

![Bond Stretching Diagram](image)

### Angle Bend

\[ \varphi_{\text{angle}} = \sum_{\text{angle}} k_\theta (\theta - \theta_0)^2 \]

![Angle Bend Diagram](image)

### Dihedral Angle

\[ \varphi_{\text{dihedral}} = \sum_{\text{dihedral}} k_\chi \cos(n\chi - \Psi) \]

![Dihedral Angle Diagram](image)
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.
Popular potential: Lennard-Jones Potential

\[ \varphi_{ij} = \varepsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] \]

In reality, every atom interacts with every atom.

→ computationally demanding.

Lennard-Jones is often \textit{truncated} at \( r_{\text{cut}} = 2.5 \sigma \).
Popular potential: Lennard-Jones Potential

$\sigma_{ij}$

$\epsilon_{ij}$

$\phi_{ij}$

$r_{ij}$

$r > r_c$

$r < r_c$
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:

\[
\phi = \phi_{\text{intermolecular}} + \phi_{\text{intramolecular}}
\]
Wettability prediction

• Solubility parameter $\delta$ (i.e. cohesive energy density)
  
  • Measures the interactions of a molecule with its surroundings.

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

<table>
<thead>
<tr>
<th></th>
<th>$\delta_d$</th>
<th>$\delta_p$</th>
<th>$\delta_h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol</td>
<td>13.56</td>
<td>19.09</td>
<td>11.67</td>
</tr>
<tr>
<td>Pentane</td>
<td>15.20</td>
<td>0.01</td>
<td>0.01</td>
</tr>
</tbody>
</table>
Wettability prediction

• Overall procedure in MD for the calculation of $\delta$:

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 $\delta$ 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 $\delta$ (i.e. cohesive energy density)

<table>
<thead>
<tr>
<th>Components</th>
<th>$\delta_{Total}$</th>
<th>$\delta_d$</th>
<th>$\delta_P$</th>
<th>$\delta_h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solvents/liquids</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>45.9</td>
<td>0</td>
<td>38.78</td>
<td>24.52</td>
</tr>
<tr>
<td>Toluene</td>
<td>18.98</td>
<td>18.8</td>
<td>1.922</td>
<td>1.76</td>
</tr>
<tr>
<td>Glycerol</td>
<td>35.85</td>
<td>11.61</td>
<td>27.97</td>
<td>19.18</td>
</tr>
<tr>
<td>Acetone</td>
<td>20.16</td>
<td>16.19</td>
<td>11.99</td>
<td>0.78</td>
</tr>
<tr>
<td>Styrene</td>
<td>19.6</td>
<td>19.49</td>
<td>1.84</td>
<td>0.98</td>
</tr>
<tr>
<td>Ethylene Carbonate</td>
<td>28.39</td>
<td>23.68</td>
<td>15.64</td>
<td>0.88</td>
</tr>
<tr>
<td>Formamide</td>
<td>30.598</td>
<td>12.372</td>
<td>20.35</td>
<td>19.28</td>
</tr>
<tr>
<td>Heptane</td>
<td>16.14</td>
<td>16.1</td>
<td>1.088</td>
<td>0.31</td>
</tr>
</tbody>
</table>

Does not spread
Spread
Does not spread
Spread
- Does not spread
Spread
Wettability prediction

MD → Solubility parameter → Wettability and Spreading
Wettability prediction

- Solubility parameters obtained from MD placed in the Hansen graph

\[ \delta = \sqrt{\delta_h^2 + \delta_p^2 + \delta_d^2} \]
Wettability prediction

- Spreading

![Graph showing wettability predictions with various substances like Toluene, Glycerol, and Cellulose highlighted on the 3D plot.](image)
Wettability prediction

- Wetting

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

Owens and Wendt + Young:

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

\[ \rightarrow \quad \cos \theta = -1 + 2 \frac{V_{ms}^{1/6}}{V_{mf}^{1/6}} \left( \frac{\delta_s^d \delta_f^d}{\delta_f^2} + \frac{\delta_s^p \delta_f^p}{\delta_f^2} + \frac{\delta_s^h \delta_f^h}{\delta_f^2} \right) \]
Wettability prediction

- Wetting

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

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

\[ W_{ls} = 2 \phi_{ls} \left( \frac{\delta_l}{k} \right)^{1/2} \left( \frac{\delta_s}{k} \right)^{1/2} (\gamma_l \gamma_s)^{1/6} \]

\[ \phi_{ls} = 2 \left( \frac{x_i^d x_s^d}{g_l x_i^d + g_s x_s^d} + \frac{x_i^p x_s^p}{g_l x_i^p + g_s x_s^p} \right) \]

\[ x_i^p = \frac{\gamma_i^p}{\gamma_i} \quad x_i^d = \frac{\gamma_i^d}{\gamma_i} \quad g_l = \frac{\gamma_l}{\gamma_s} \quad g_s = \frac{\gamma_s}{\gamma_l} \]

\[ S = W_{ls} - W_l \]
MD \rightarrow \text{Wettability and Spreading}
Wettability prediction

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

Perform third MD simulation.

Contact angle measurement.

Optimization and MD simulation with the same procedure described previously.

Second MD simulation until droplet formation.
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 the rim forming a ring.
Research work on wettability

• Ouzo effect

<table>
<thead>
<tr>
<th>Components</th>
<th>Density (g/cm³)</th>
<th>Solubility parameter (J.cm⁻³)¹/²</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Exp. δt</td>
<td>MD Simulation</td>
</tr>
<tr>
<td>Ethanol</td>
<td>0.789</td>
<td>26.18</td>
</tr>
<tr>
<td>Anis oil</td>
<td>0.986</td>
<td>-</td>
</tr>
<tr>
<td>Water</td>
<td>0.997</td>
<td>47.9</td>
</tr>
</tbody>
</table>

\[ \Delta \delta_{\text{Anise-Ethanol}} = 20.64 < \Delta \delta_{\text{Water-Ethanol}} = 35.90 \]

- 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

Anise oil  Ethanol  Water
Research work on wettability

- Liquid imbibition

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

- Imbibition of multicomponents liquids?

Ink Spreading

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

100 µm
Research work on wettability

- Liquid imbibition

Water

Glycerol

Graphene

\[
\text{Imbibition ratio } I = \frac{m_i}{m_{\text{total}}}
\]

Graphene
Research work on wettability

- Liquid imbibition

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

Graph showing imbibition ratio vs. time for different mixtures of water and glycerol.
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
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 Benzyalmine have the same surface tension; do they have the same wettability on Teflon? Comment.

<table>
<thead>
<tr>
<th>Components</th>
<th>δTotal</th>
<th>δd</th>
<th>δP</th>
<th>δh</th>
<th>Molar volume (cm³.mol⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solvents/liquids</strong></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Water</td>
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<td>38.78</td>
<td>24.52</td>
<td>18.03</td>
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<td>Toluene</td>
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<td>Glycerol</td>
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<td>11.61</td>
<td>27.97</td>
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<td>19.1</td>
<td>7.11</td>
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<td><strong>Substrate</strong></td>
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<tr>
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<tr>
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<td>12.55</td>
<td>25.71</td>
<td>7.189</td>
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Thank you!