Micromechanics of three-phase granular materials

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Plan

- 1. Wet granulars
- 2. DEM modeling
- 3. Macroscopic results and validation
- 4. Upscaling
- 5. Generalized effective stress
- 6. Discussion
Capillarity in Unsaturated Granular Materials

Air vapor
Solid Grain
Liquid (water)

hygroscopic  pendular  funicular  capillary

Sr
Capillarity in Unsaturated Granular Materials

At low water content levels, interfacial phenomena lead to intergranular water menisci.
Capillarity in Unsaturated Granular Materials

In granular soils (silts and sands), capillary effects are of primary significance in the unsaturated induced strength increase.

[Mitchell: Fundamentals of soil behavior, Wiley Inter Science, 1993]
Capillarity in Unsaturated Granular Materials

Capillary Theory (Laplace): \[ \Delta u = u_a - u_w = \sigma C \]

\[ C = f[y(x)] ; y(x) \text{ is the interface profile} \]

\[ F_{\text{capillary}} = 2\pi\sigma y_0 + \pi\Delta uy_0^2 \]

\[ V_{\text{meniscus}} = \pi \int y^2(x) \, dx \]
Capillarity in Unsaturated Granular Materials

Evolution of the capillary force at constant suction:

\[ U_n \]
Capillarity in Unsaturated Granular Materials

Evolution of the capillary force at constant suction:

$$\Delta u = u_a - u_c = \text{cst}$$
DEM simulations and results: suction variation

Water retention hysteresis:

Local hysteresis « ink bottle effect »
DEM simulations and results: suction variation

The range of simulated saturation degree

(a) 

(b)
DEM modelling

using YADE - open DEM  (http://yade-dem.org)
(based upon the pioneering work of Cundall and Strack, 1979)

Resultant forces and moments

Law of Motion
(Newton's 2nd Law)
applied to each particle

Force-Displacement Law
applied to each interaction

Positions and contacts update
(finite difference scheme)
DEM modelling

using YADE - open DEM  ([http://yade-dem.org](http://yade-dem.org))
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Resultant forces and moments

Law of Motion
(Newton's 2\textsuperscript{nd} Law)
applied to each particle

Capillary force

Position vs.
(contact)

Capillary force

\[ F_{\text{cap}} \]

Positions and contacts update
(finite difference scheme)
DEM simulations and results

DEM Sample:

- 10,000 spherical particles randomly positionned into a cubic box
- A unique value of succion in the sample (thermodynamic equilibrium)
- compacted through radius expansion to ensure the isotropy of the packing
- rigid frictionless boundary walls guarantee the homogeneity of the loading
Triaxial loading : dry sample

\begin{align*}
\Delta 5 \text{kPa} \\
\Diamond 10 \text{kPa} \\
\triangle 20 \text{kPa}
\end{align*}

<table>
<thead>
<tr>
<th>Nombre de grains</th>
<th>$E_{global}$ (Pa)</th>
<th>$k_n/k_t$</th>
<th>$\phi_c$ (deg.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10000</td>
<td>$5 \times 10^7$</td>
<td>0.5</td>
<td>30</td>
</tr>
</tbody>
</table>

$\Phi = 28^\circ$
Triaxial loading : wet sample

For several capillary pressure \( (u_a - u_w) \) in the pendular regime \( (0 < Sr < 12\%) \)

<table>
<thead>
<tr>
<th>( u_c ) (kPa)</th>
<th>5000</th>
<th>3000</th>
<th>50</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Sr_{init} ) (%)</td>
<td>0,001</td>
<td>0,01</td>
<td>2,5</td>
<td>10</td>
</tr>
<tr>
<td>( w_{init} ) (%)</td>
<td>0,0006</td>
<td>0,006</td>
<td>1,5</td>
<td>6,0</td>
</tr>
</tbody>
</table>

![Graph showing triaxial loading for wet samples](image-url)
Yield surfaces in the \((q,p)\) plane

No significant changes in the internal friction angle

Comparing well with experiments and simulations done in Montpellier (Richefeu and al.) for \(<D> = 0.045\) mm

\[ c^{DEM} = 5 \, kPa \]
Triaxial loading: wet sample

Quantitative validation:


\[
\frac{\sigma_I(D_{\text{DEM}})}{\sigma_I(D_{\text{Sand}})} = \frac{D_{\text{Sand}}}{D_{\text{DEM}}} = 0.45
\]

\[
\frac{0.45}{0.045}
\]
A DEM model, so what?

Rôle dans le développement de modèles micromécaniques d'homogénéisation

En particulier : modèle micro-directionnel de F. Nicot (Sholtès et al. 2009a), modèle micro-structurel de Chang et Hicher (Sholtès et al. 2009b)
Effective stress

Effective stress tensor in saturated granular materials (Terzaghi 1936):

« All measurable effects of a change of stress of the soil, that is, compression, distortion, and change of shearing resistance, are exclusively due to changes in the effective stress. »

\[
\sigma_{ij} = \sigma'_{ij} + u_w \delta_{ij}
\]

Generalization for porous elastic materials Biot (1955):

\[
\sigma'_{ij} = \sigma_{ij} - \left(1 - \frac{C_s}{C}\right) u_w \delta_{ij}
\]

Standard sand: \( E_y = 100 \) Mpa, \( \nu = 0.2 - 0.4 \)
Silice: \( E_y = 100 \) Gpa, \( \nu = 0.16 \)
Biot's alpha coefficient: 0.999 ~ 1
Effective stress tensor in saturated granular materials (Terzaghi 1936):

« All measurable effects of a change of stress of the soil, that is, compression, distorsion, and change of shearing resistance, are exclusively due to changes in the effective stress. »

\[
\sigma_{ij} = \sigma'_{ij} + u_w \cdot \delta_{ij}
\]
Generalized effective stress

Effective stress tensor in saturated granular materials (Terzaghi 1936):

« All measurable effects of a change of stress of the soil, that is, compression, distorsion, and change of shearing resistance, are exclusively due to changes in the effective stress. »

\[ \sigma_{ij} = \sigma'_{ij} + u \cdot \delta_{ij} \]

« Seating solely in the solid skeleton, the effective stress enter the constitutive equations of the soil matrix, linking a change in stress to strain-like quantity of the skeleton. […] A unique stress is necessary and sufficient to describe the mechanical behaviour. »

Generalised effective stress

Partial saturation:
Bishop and Blight, Géotechnique (1963)

\[ \sigma_{ij}' = \sigma_{ij} - (u_a + \chi (u_a - u_w)) \delta_{ij} \]

?
Generalised effective stress

A common assumption: \( \chi = S_r \)
Generalised effective stress

Yield surfaces in the (p',q') plane:

\[
\chi = \begin{cases} 
\left( \frac{s}{s_c} \right)^{-0.55} & \text{if } s > s_c \\
1 & \text{if } s \leq s_c
\end{cases}
\]

Khalili and Khabbaz, Géotechnique (1998)

A unique relationship for \( \chi \)...

The advantages of an effective stress is pointed out.

After Nuth and Laloui (2007)
Generalised effective stress

Yield surfaces in the \((p',q')\) plane for simulated low saturations:

\[ \chi = Sr \]

Khalili and Khabbaz (1998)

None of the common definitions will result in a unique yield surface...
Generalised effective stress

Interpretation of the suction term as an additional confinement:

\[ \sigma_{ij}' = \sigma_{ij} - (u_a + \chi (u_a - u_w)) \delta_{ij} \]

\[ \chi = Sr \]

\[ \chi = \begin{cases} \left( \frac{s}{s_e} \right)^{-0.55} & \text{if } s > s_e \\ 1 & \text{if } s \leq s_e \end{cases} \]

Khalili and Khabbaz, Géotechnique (1998)
A unique relationship for $\chi$...

\[ \rightarrow 10 \text{ kPa} < s < 10^4 \text{ kPa} \]

Cohesion vs Saturation degree
Generalised effective stress : micromechanical definition

\[ \sigma_{ij} = \frac{1}{V} \sum_{c=1}^{N_{\text{contacts}}} F^\text{cont}_{ij} + \frac{1}{V} \sum_{m=1}^{N_{\text{menisci}}} F^\text{cap}_{ij} \]

\[ \Rightarrow \sigma = \sigma_{\text{contact}} + \sigma_{\text{capillary}} \]
Generalised effective stress: micromechanical definition

\[ \sigma_{ij} = \sigma^c_{ij} + \sigma^{cap}_{ij} \]
Possible definition of the effective stress: \[
\sigma_{ij}^{\text{contact}} = \frac{1}{V} \sum_{c=1}^{N_{\text{contacts}}} F_{i}^{\text{cont}} l_{j}
\]

Yield surfaces in the \((p^{\text{cont}}, q^{\text{cont}})\) plane:
Generalised effective stress : numerical results

\[ \sigma_{ij}^{cap} = \frac{1}{V} \sum_{m=1}^{N_{\text{menisci}}} F_{i}^{cap} l_{j} \]

Provides an explanation of the plateau in \( c \) vs. \( S_r \) curves. As suggested in e.g. Richefeu et al. (2006), the magnitude of capillary effects scales like:

\[ \sigma_t = \frac{3}{4\pi} \frac{s \kappa \Theta z_m}{D_{\text{grains}}} \]
Generalised effective stress: numerical results

\[ \sigma_{ij}^{\text{contact}} = \frac{1}{V} \sum_{c=1}^{N_{\text{contacts}}} F_{i}^{\text{cont}} l_{j} \]

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![Graph showing the relationship between stress and strain](image)
Generalised effective stress : numerical results

« Wetting » vs. « drying » initial states :

The shear strength is larger in the drying phase than in the wetting one.

No significant changes in the volumetric strain (nor in the internal friction angle).

Common residual stress state.
Generalised effective stress: numerical results

« Wetting » vs. « drying » initial states:

The difference in the shear strength is linked to the number of liquid bridges inside the sample.

The liquid bridges tend to the same distribution with the deformations.
Generalised effective stress: numerical results

The usual formalism fails to describe the anisotropy of the fluid contribution:

\[ \sigma_{ij}^{\text{contact}} = \sigma_{ij} - \sigma_{ij}^{\text{capillary}} \quad \Leftrightarrow \quad \sigma_{ij}' = \sigma_{ij} + \chi (u_a - u_w) \delta_{ij} \]

Contacts and Menisci orientation distributions
Generalised effective stress: numerical results

The usual formalism fail to describe the anisotropy of the fluid contribution:

\[ \sigma_{ij}^{contact} = \sigma_{ij} - \sigma_{ij}^{capillary} \quad \Leftrightarrow \quad \sigma_{ij}' = \sigma_{ij} + \chi (u_a - u_w) \delta_{ij} \]

\[ \Psi = 2 \frac{\sigma_{1}^{cap} - \sigma_{2}^{cap}}{\sigma_{1}^{cap} + \sigma_{2}^{cap}} \]

\[ \Psi = 0 \quad \text{if} \quad \sigma_{cap} = \chi (u_a - u_w) \]

The graph shows the peak load \( q_{peak} \) and the stress \( \Psi \) as a function of the strain \( \varepsilon_1 \) for different values of \( 0.001\% \), \( 0.01\% \), \( 2.5\% \), and \( 10\% \).
Generalised effective stress: numerical results

The usual formalism fail to describe the anisotropy of the fluid contribution:

\[ \sigma_{ij}^{contact} = \sigma_{ij} - \sigma_{ij}^{capillary} \quad \iff \quad \sigma_{ij}' = \sigma_{ij} + \chi \left( u_a - u_w \right) \delta_{ij} \]
Generalised effective stress : discussion

After the thermodynamical approach of Gray and Schrefler (2006):

\[
\mathbf{t}^\text{Total} = \left(1 - \frac{K_T}{K_S}\right) (\mathbf{n}_s \cdot \mathbf{t}_s \cdot \mathbf{n}_s)^s + \varepsilon^s \tau^s
\]

with:

\[
-(\mathbf{n}_s \cdot \mathbf{t}_s \cdot \mathbf{n}_s)^s = x^{ws}_s p^{w}_{ws} + (1 - x^{ws}_s) p^n_{ns} - \frac{l^{wns}}{a_s} \gamma^{wn}_s \sin \psi^w
\]

- \(x^{ws}_s\): solid-liquid surface ratio (not volume fractions);
- last term reflects direct effects of surface tension
- still, the effect of the fluids are isotropic
Conclusions

- In the same way as frictional phenomena, water effects at low saturation degrees are adequately modelised at the grains scale.
- Capillary forces generate an apparent cohesion, which compares well with measured values.
- The mechanical behaviour of the sample is almost constant on the range of saturation degree [2%, 10%].
- The contribution of the liquid in the effective stress is anisotropic.
- Capillary forces homogeneized using Love-Weber stress provides a relevant quantity to describe the effect of capillary forces.
Generalised effective stress: micromechanical results

However...

\[ \sigma_{ij}^{\text{contact}} = \frac{1}{V} \sum_{c=1}^{N_{\text{contacts}}} F_{i}^{\text{cont}} l_{j} = \sigma_{ij} - \sigma_{ij}^{\text{cap}} \]

Elastic response to isotropic compression (\( \Delta \sigma \)) vs Wetting (\( \Delta \sigma^{\text{cap}} \))
Generalised effective stress: micromechanical results

$$\sigma_{ij}^{\text{contact}} = \frac{1}{V} \sum_{c=1}^{N_{\text{contacts}}} F_i^{\text{cont}} l_j = \sigma_{ij} - \sigma_{ij}^{\text{cap}}$$

Local kinematics are different:
P.D.Fs. of normal displacement at contacts

![Graph showing distribution of normal displacement at contacts with two curves: capillary loading (blue solid line) and external loading (red dashed line).]
Capillarity in Unsaturated Granular Materials

In the same as frictional phenomena, water effects at low saturation degrees are adequately modelised at the grains scale as a result of capillary menisci.

A multi-scale approach to analyse water induced phenomena then appears as a pertinent tool for critical examination of constitutive models.
Capillarity in Unsaturated Granular Materials

Challenges:

- range of water content: shape of the liquid bridges between 3, 4, N particles....

- kinetics: interfaces, transfers, variable wetting angle.

- constitutive macro-modeling

http://www.susqu.edu/facstaff/b/brakke/evolver/evolver.html
Suction Variation under isotropic loading: Wetting

\[ Sr = \frac{\sum_{m=1}^{N_{\text{meniscus}}} V_{\text{meniscus}}}{V_{\text{sample}}} \]

Hydric Domains:

Simulation Results: Water retention
Quantitative validation :

Tensile strength :

\[ \sigma_t = \frac{3}{4\pi} \frac{sk\Theta z_m}{D_{grains}} \]

*Shear strength properties of wet granular materials,*

Simulation Results :

Unsaturated triaxial paths

\[ \sigma_t = \frac{c}{\tan \varphi} \propto \frac{1}{D_{grains}} \]

\[ \frac{\sigma_t(DEM)}{\sigma_t(Sand)} = \frac{D(Sand)}{\overline{D}(DEM)} = \frac{0.45}{0.045} \]
Generalised effective stress

\[ \vec{F} = \vec{F}_{\text{cont}} + \vec{F}_{\text{cap}} \]
References


