A micromechanical μ UNSAT effective stress expression for stress-strain behaviour of wet granular materials

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Abstract

The definition of an effective stress variable for idealized triphasic granular media as the contact stress arising from interparticle forces is examined through discrete element modelling computations in concert with appropriately derived analytical stress expressions based on homogenization. The latter take a more practical importance, in that they also circumvent the need for direct measurements of interparticle contact forces. Considering dry or pendular-regime conditions for slightly polydisperse dense and loose packings, the contact stress-strain behaviours in dry or wet conditions are compared along a variety of loading paths, depending on the level of plastic dissipation involved. The contact stress indeed emerges as an effective stress variable with a remarkable stress-strain character along contractant loading paths and for dense solid packings where the behaviour is close to be non-dissipative. Along more dilatant loading paths or for looser packings, plastic dissipation increases and the coincidence of the constitutive behaviour in both dry and triphasic conditions is restricted to the initial stages of the loading paths, limiting the applicability of the contact stress to the estimation of initial stiffnesses. The stark constitutive differences between the proposed effective stress and Bishop's stress are also highlighted.

Keywords: effective stress, Discrete Element Method (DEM), granular, pendular, μ UNSAT

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1. Introduction

Energy and Environmental Engineering operations require a precise mechanical description of multiphase porous media such as in oil and gas reservoirs, or partially water-saturated (unsaturated) soils. Obviously, the presence of various fluids within the pore space network of these multiphase materials greatly modifies their mechanical behaviour with respect to the dry (air-saturated) state which is well understood. For biphasic (or two-phase) porous media penetrated by a single pore fluid, a unified mechanical description by way of dry state constitutive models actually exists whatever the pore fluid and its pressure are following Terzaghi's and Biot's effective stress equations [1, 2]. Turning to triphasic (or three-phase) conditions with an immiscible fluid mixture, it would also be highly beneficial to extend this effective stress concept so that triphasic materials can be described by just inserting an adequate single effective stress into models designed for dry materials. In other words, the objective is to obtain a stress-strain-strength effective stress that would allow failure criterion and constitutive relations from dry conditions, all together, to be applied to triphasic conditions in order to easily predict limit stress states and strains. However, the exact determination of such a single effective stress has revealed to be highly challenging ever since the early Bishop's attempts [3].

When describing failure in triphasic media, it has been often possible to resort to an effective stress framework based on limit stress states according to dry shear strength criteria [4, 5, 6, 7, 8]. In these works, the effective stress is either phenomenologically deduced from Bishop's equation with appropriate expressions for χ coefficient [4, 7], or as the contact forces stress contribution which can be indirectly accessed by subtracting a so-called suction stress from the total stress [5, 6, 8]. The suction stress [5] encompasses all relevant stress contributions in triphasic materials, excluding the contact stress stemming from the contact forces between the solid grains of the skeleton, and can be identified for granular materials with the capillary stress since other physico-chemical forces are then negligible. As for the contact stress, the latter appears as a

31 logical stress-strength effective stress since pore water is reported to have little
32 or no influence onto the contact-scale local frictional threshold [9, 10], which
33 thus leads to unique limit states for the macroscopic contact stress and a unified
34 failure description irrespective of saturation.

35 Whereas in the biphasic case unique constitutive relations are related to
36 strains via Biot’s effective stress, no effective stress has yet been found that
37 would relate to strains in triphasic conditions through dry constitutive relations
38 [7]. As such, the application of an effective stress principle to triphasic materials
39 has often been challenged since Bishop himself [3], with alternate approaches
40 relying on total stress and another stress variable such as matric suction to de-
41 scribe unsaturated conditions using additional constitutive equations that are
42 specific to these triphasic conditions [11, 12]. A compromise may, nevertheless,
43 be found in that quasi-elastic behaviour, e.g. volume change along overconsoli-
44 dated oedometric loadings, may still be described in triphasic conditions using an
45 effective stress framework [4, 13, 14]. Recent micromechanical results by the au-
46 thors [8, 15] suggest that the same contact stress also enjoys such a quasi-elastic
47 strain-stress effective nature, in addition to its stress-strength character. This
48 seems to be indeed coherent because granular material strains derive from solid
49 particle relative displacements that relate to contact forces through a unique
50 contact law, irrespective of saturation.

51 The present work aims to provide new evidences that demonstrate the stress-
52 strain effective character of the contact stress in any regime showing small plastic
53 dissipation by considering a wide range of loading paths which were absent from
54 previous studies [8, 15].

55 It is further noted that direct measurements of contact forces and contact
56 stresses are still beyond reach in triphasic materials in spite of a current research
57 in the field [16]. To address this shortcoming, the present paper first recalls in
58 Section 2 the μ UNSAT expressions that enable one to indirectly access the con-
59 tact stress through capillary stresses and the fluid phase microstructures, whose
60 measurements appear to be more feasible thanks to e.g. computed tomography
61 [17, 18]. For the purpose of the paper, the choice is actually made to con-

62 sider a Discrete Element Method (DEM) model for wet granular materials [19],
 63 presented in Section 3, which allows both direct and indirect measurements of
 64 the contact stress from a comprehensive description of the microstructure of all
 65 solid and fluid phases, including interfaces. Numerical comparisons of dry-wet
 66 behaviours for slightly polydisperse materials along various loading paths are
 67 then presented in Section 4, validating the stress-strain effective nature of the
 68 contact stress in regimes with small dissipation, and hence the present μ UNSAT
 69 effective stress expression. Section 5 finally evidences the fundamental differ-
 70 ences in the pendular regime between the present μ UNSAT effective stress and
 71 Bishop's stress, whose inapplicability to wet conditions is once again demon-
 72 strated.

73 **2. Micromechanical μ UNSAT effective stress expression**

74 *2.1. Total stress decomposition from micromechanics*

75 The μ UNSAT approach expresses the contact stress by isolating from the
 76 macroscopic total stresses Σ , all microscopic stress contributions due to the
 77 various phases and interfaces that encompass triphasic granular media. First,
 78 the solid s and fluid (n, w) bulk phases are considered with their corresponding
 79 volumes V_s , V_n and V_w . Here, n stands for the non-wetting fluid, e.g. air,
 80 whereas w refers to the wetting one, e.g. water. Additionally, all three interfaces
 81 $S_{\alpha\beta}$, $\alpha, \beta = n, s, w$ are as well included in the approach since the corresponding
 82 surface tensions $\gamma_{\alpha\beta}$ necessarily belong to the internal forces of the triphasic
 83 material. As such, the total stresses are given as follows:

$$\Sigma = \frac{1}{V} \left(\sum_{\alpha=n,s,w} \int_{V_\alpha} \sigma_\alpha dV + \sum_{\alpha,\beta=n,s,w} \int_{S_{\alpha\beta}} \pi_{\alpha\beta} dS \right) \quad (1)$$

84 In Eq. (1), the fluid stresses σ_α , $\alpha = n, w$, are directly given by the corre-
 85 sponding pressures $u_\alpha \delta$ with δ as the identity tensor, whereas the solid stress
 86 σ_s can be classically expressed in terms of the tractions acting along the solid
 87 particles surfaces S_p [20]. The surface stress tensors $\pi_{\alpha\beta} = \gamma_{\alpha\beta} (\vec{n} \otimes \vec{n} - \delta)$,
 88 with $\vec{n}$ as the normal to $S_{\alpha\beta}$, finally describe the surface tension fields acting as
 89 internal forces within any interface $S_{\alpha\beta}$ [21, 22, 23, 24].

Algebraic manipulations applied to Eq. (1) lead to the following μ UNSAT decomposition of Σ into the contact stress σ^{cont} and the capillary stress σ^{cap} , to which the solid fluid surface tensions $\gamma_{s\alpha}$ eventually do not contribute in the case of rigid solid particles [20, 22, 24]:

$$\Sigma - u_n \delta = \sigma^{cont} + \sigma^{cap} \quad (2)$$

$$\sigma^{cont} = \frac{1}{V} \sum_c \vec{f}^c \otimes \vec{l} \quad (3)$$

$$\begin{aligned} \sigma^{cap} &= -\frac{1}{V} \left[u_c \left(V_w \delta + \int_{S_{sw}} \vec{n} \otimes \vec{x} dS \right) \right. \\ &\quad \left. + \gamma_{nw} \left(\int_{S_{nw}} (\delta - \vec{n} \otimes \vec{n}) dS + \int_{\Gamma} \vec{\nu} \otimes \vec{x} dl \right) \right] \\ &= -\frac{1}{V} \left[u_c (\mu_{Vw} + \mu_{Ssw}) + \gamma_{nw} (\mu_{Snw} + \mu_{\Gamma}) \right] \end{aligned} \quad (4)$$

Eq. (3) refers to the standard definition of the contact stress tensor σ^{cont} from the contact forces $\vec{f}^c$ between solid particles, and the corresponding branch vector $\vec{l}$ connecting the centroids of contacting particles.

In Eq. (4), the capillary stress σ^{cap} encompasses the remainder of the internal forces that arise both from the fluid-fluid surface tension γ_{nw} and the capillary pressure $u_c = u_n - u_w$ that is equal to suction in granular materials. Four microstructure tensors μ_X reflect the tensorial nature of these internal forces, with μ_{Vw} the only one being always spherical since it corresponds to the isotropic action of suction within V_w . Other microstructure tensors have a general, non-spherical, tensorial expression with e.g. μ_{Ssw} depending on the orientation of the wetted surface S_{sw} since the latter sustains suction along its normal only. Also, μ_{Snw} , μ_{Γ} reflect the orientations of the interface S_{nw} and of the three-phase contact lines Γ that are subjected to fluid-fluid surface tension, where $\vec{\nu}$ in Eq. (4) is the tangent to S_{nw} being normal to Γ [20].

2.2. μ UNSAT contact stress expression

Isolating σ^{cont} in Eq. (2)-(4), the following μ UNSAT expression for the contact stress is eventually obtained:

$$\sigma^{cont} = \Sigma - u_n \delta + \frac{1}{V} \left[u_c (\mu_{Vw} + \mu_{Ssw}) + \gamma_{nw} (\mu_{Snw} + \mu_{\Gamma}) \right] \quad (5)$$

Such an expression is believed to provide an easier access to σ^{cont} during experiments than the direct definition of Eq. (3). Imaging techniques such as computed tomography indeed are very promising in allowing precise measurements of the fluid phase microstructures [17, 18]. Then, one would be able to compute the microstructure tensors μ_X in Eq. (5), as opposed to requiring more complex contact force measurements [16] that enter the direct contact stress expression, Eq. (3).

Leaving any experimental endeavour aside for now, Eq. (5) is herein used within the framework of DEM to investigate the very role of the contact stress in connection with strains, and whether it may serve as a strain-stress-strength effective stress expression.

3. DEM multiscale modelling of triphasic granular materials

Numerical DEM models indeed provide a convenient multiscale description of triphasic granular materials whereby the microstructure of all solid and fluid phases is easily measured. As such, the contact stress can be readily estimated using either Eq. (3) or (5) along various loading paths and for different packings.

3.1. Model formulation

Previously proposed in [19] and implemented in the Yade code [25], the considered DEM model addresses the case of spherical solid particles and a wetting fluid distribution in terms of distinct capillary bridges, i.e. menisci between particles pairs (Fig. 1), in accordance with the so-called pendular regime, also referred to as wet conditions. Such conditions correspond to a low wetting saturation, S_w , only, where S_w is defined as:

$$S_w = \frac{V_w}{V_w + V_n} \quad (6)$$

In line with another DEM approach [26], the model does not compute any biphasic pore flow, but instead assumes thermodynamic equilibrium and uniform capillary pressure conditions. As such, the menisci properties are computed

Figure 1: A capillary bridge

from the following Laplace-Young equation (7) which relates capillary pressure to surface tension and the interface curvature $\text{div}(\vec{n})$, with $\vec{n}$ being the normal to S_{nw} pointing from n to w :

$$u_c = \gamma_{nw} \text{div}(\vec{n}) \quad (7)$$

According to the thermodynamic equilibrium assumption, Eq. (7) is solved for uniform values of u_c throughout the sample, also considering a uniform and constant contact angle θ (Fig. 1) [19]. As discussed in greater depth in [19], Eq. (7) is actually solved depending on the particles radii and their distance, in addition to imposed u_c and θ . Based on the S_{nw} interface profile, the numerical solution procedure finally outputs the resultant capillary force $\vec{f}^{cap}$ and other relevant microstructural quantities such as $\mu_{S_{nw}} = \int_{S_{nw}} (\delta - \vec{n} \otimes \vec{n}) dS$ for instance, thus enabling one to apply the μ UNSAT Eq. (5) and measure contact stresses during DEM simulations [19].

The model actually inserts capillary bridges at each new contact between solid particles, with properties given by the Laplace-Young equation. In the instance the particles subsequently separate, the capillary bridge remains until some limit distance beyond which the Laplace-Young equation does not yield any solution. This hysteretic mechanism of bridge formation and rupture is consistent with experimental observations [27] and occurs in the model in a fully drained manner. The presence of a capillary bridge between two particles corresponds to a capillary interaction with the corresponding attractive capillary force $\vec{f}^{cap}$ due to the capillary pressure and surface tension loadings along the wetted surfaces S_{sw} and the contact lines Γ .

In addition, the interaction between touching particles is governed by classical elastic-plastic frictional (cohesionless) contact laws whereby normal and

162 tangential relative displacements between particles are restricted by normal and
163 tangential contact forces f_n^c and f_t^c [8, 19]. A simplified linear elastic behaviour
164 of the contact interaction is first defined by the normal and tangential local
165 stiffnesses, k_n and k_t , which are directly obtained from the average diameter $\bar{D}$
166 of any pair of contacting particles and the model parameters $k_n/\bar{D}$ and k_t/k_n :

$$k_n = \frac{k_n}{\bar{D}} \bar{D} \quad (8)$$

$$k_t = \frac{k_t}{k_n} k_n \quad (9)$$

167 with the consideration of an elastic shear stiffness being eventually restricted by
168 the following Coulombian friction threshold, with μ the friction coefficient:

$$|f_t^c| \leq \mu f_n^c \quad (10)$$

169 Table 1 lists all parameters of the DEM model. The retained values for the
170 contact interaction parameters, $k_n/\bar{D}$ and k_t/k_n , are similar to previous studies
171 [8, 24, 19, 20]. As for the capillary interaction, the latter is fully determined
172 by the fluid-fluid surface tension γ_{nw} , the contact angle θ and the particle size
173 distribution. Air-water surface tension at ambient temperature is considered for
174 γ_{nw} while a low though not zero θ -value corresponds to the wetting of glass beads
175 by water, having at the same time the convenience of enhancing the mechanical
176 effects of triphasic conditions [19]. Finally, silt-like particle diameters are chosen
177 with a narrow particle size distribution being uniform in number between D_{min}
178 and D_{max} .

Contact			Capillarity		Packing	
$k_n/\bar{D}$	k_t/k_n	μ	γ_{nw}	θ	D_{min}	D_{max}
(MPa)	(-)	(-)	(N/m)	(°)	(μm)	(μm)
10	0.5	0.5	0.073	10	21	25

Table 1: DEM model parameters

179 While the dynamic scheme of the DEM is classically carried out using some
180 numerical damping, in order to obtain more easily a quasi-static evolution of the
181 system, the damping coefficient [25] is taken as low as 0.05 to avoid numerical

artifacts. Quasi-staticity is systematically verified through low values of the particle unbalanced forces [25] which were below 1% during all loading cases. As such, particle inertia (mass) does not play any role in the computations, which allows the use of density scaling with an artificially high density value ($\rho = 20,000 \text{ kg/m}^3$ instead of $2,600 \text{ kg/m}^3$) for the particles. Without any consequence on the quasi-static rheology, density scaling reduces computational costs through larger time steps, even though loading rates have to be marginally reduced for quasi-staticity to still hold.

The DEM sample is a parallelepiped, initially a cube approximately 0.6 mm a side depending on packing density, with 6 rigid walls that enclose a total number of 20,000 spherical Discrete Elements (DE). Similar numbers (10,000 to 20,000) are classically used in material-scale DEM analyses [26, 19, 20, 28] in order to avoid numerical result dispersion from one numerical sample to another as well as field heterogeneity, in conformity with the Representative Elementary Volume (REV) concept. The DE sample is packed at various levels to produce different states in density as quantified by the porosity n and the average coordination number z_c :

$$n = \frac{V_n + V_w}{V_s + V_n + V_w} = \frac{V_v}{V} \quad (11)$$

$$z_c = \frac{2 N_c - N_1}{N_p - N_1 - N_0} \quad (12)$$

with N_c the total number of contacts, and $N_0 + N_1$ the number of excluded rattlers, i.e. particles with zero or only one contact, and N_p the total number of DE. All considered packings are initially isotropic and prepared such that dry vs wet comparisons can be conducted in an unbiased manner.

Care is indeed taken in considering dry or wet solid packings to be comparable in terms of n and z_c as these parameters obviously affect the dry constitutive relation which should also be described in wet conditions by an effective stress. As such, an appropriate particle packing generation procedure is followed which first involves a classical isotropic compression until a desired confining pressure is reached to obtain dense or loose dry packings [26], without the consideration of any capillary interaction that is only introduced in a second stage for the

210 wet samples. In this manner, wet packings show initial states which are barely
 211 affected by the presence of capillary forces, and thus compare well with dry
 212 packings.

213 3.2. Dry and wet strain proportional loading paths

214 In order to investigate the stress-strain effective nature of the contact stress,
 215 the DEM model is used to explore the existence of a unique constitutive relation
 216 $\mathcal{F}$ between $\boldsymbol{\sigma}^{cont}$ and the strains $\boldsymbol{\varepsilon}$ in both dry (biphasic) and wet (triphasic)
 217 conditions. In the case of such an existence, $\mathcal{F}$ by definition would relate the
 218 current contact stress $\boldsymbol{\sigma}^{cont}(t)$ to the strain loading path $[\boldsymbol{\varepsilon}(\tau); -\infty < \tau \leq t]$
 219 such that:

$$\boldsymbol{\sigma}^{cont}(t) = \mathcal{F}([\boldsymbol{\varepsilon}(\tau); -\infty < \tau \leq t]) \quad (13)$$

220 Extending our previous work [8, 15] where classical triaxial paths were exam-
 221 ined, the validity of the same Eq. (13) in dry and wet conditions with a unique
 222 $\mathcal{F}$ is herein probed considering axisymmetric strain proportional loading paths,
 223 with ‘1’ as the axis of symmetry and ‘2,3’ the two other spatial directions:

$$d\varepsilon_1 = cst \geq 0 ; d\varepsilon_2 = d\varepsilon_3 ; d\varepsilon_1 + 2R d\varepsilon_3 = 0 \quad (14)$$

224 The loading parameter $R \geq 0$ is constant along a given path, $R = 1$ corresponds
 225 to an isochoric loading path, whereas dilatancy (resp. contractancy) is imposed
 226 for $0 < R < 1$ (resp. $R > 1$). The limiting case $R = 0$ is defined as another
 227 contractant path ($d\varepsilon_1 = 0 ; d\varepsilon_2 = d\varepsilon_3 = cst \geq 0$).

228 Let’s denote the volumetric strain as ε_V :

$$\varepsilon_V = \varepsilon_1 + 2\varepsilon_3 \quad (15)$$

229 and choose $\|\boldsymbol{\varepsilon}\|$ (the Euclidean norm of $\boldsymbol{\varepsilon}$) as a monotonously increasing loading
 230 parameter, i.e.

$$\|\boldsymbol{\varepsilon}\| = \sqrt{\varepsilon_1^2 + 2\varepsilon_3^2} \quad (16)$$

231 Accordingly, Fig. 2 illustrates the corresponding dilatancy rates of four loading
 232 paths with $R \in \{0; 0.2; 1; 5\}$ that will be considered in the following analysis. In
 233 all cases, imposed strain rates are low enough to ensure quasi-static simulations

Figure 2: Dilatancy rates of imposed loading paths for $R \in \{0; 0.2; 1; 5\}$

as verified from the corresponding low values of the particle unbalanced forces [25] which were below 1%.

The main objective of imposing such strain loading paths on both dry and wet packings is to verify the hypothesis, $\boldsymbol{\sigma}' = \boldsymbol{\sigma}^{cont}$, upon which is founded the μ UNSAT framework. If Eq. (13) holds, then the resulting contact stress paths should coincide in both dry and wet conditions. Recognizing the axial symmetry of the problem, it is convenient to associate the tensor $\boldsymbol{\sigma}^{cont}$ with the two classical scalars (invariants) p^{cont} and q^{cont} , i.e.

$$p^{cont} = \frac{\sigma_1^{cont} + 2\sigma_3^{cont}}{3} \quad (17)$$

$$q^{cont} = \sigma_1^{cont} - \sigma_3^{cont} \quad (18)$$

while similarly, p and q variables pertain to the total stress tensor $\boldsymbol{\Sigma}$:

$$p = \frac{\Sigma_1 + 2\Sigma_3}{3} \quad (19)$$

$$q = \Sigma_1 - \Sigma_3 \quad (20)$$

243 4. Validity of the μ UNSAT effective stress

244 4.1. Dense packings

245 Proportional strain loading paths are first imposed to dense solid packings.
 246 In essence, the same strain loading path is imposed to similarly dense packings
 247 in both dry and wet conditions with the resulting contact stress paths recorded.
 248 The contact stress obviously coincides with the total stress in dry conditions,
 249 whereas Eq. (3) or (5) can be indistinctly used to access the contact stress under
 250 wet conditions [28].

251 Four strain loading paths are considered with $R \in \{0; 0.2; 1; 5\}$, under two
 252 different confining pressures referred to as “A” and “B”. For each confining
 253 pressure A or B, and each R value, one dry and one wet test are considered,
 254 leading to 16 tests on dense packings in total. Table 2 gives details of the initial
 255 conditions for the dry-wet test pairs A, B pertaining to dense packings. These
 256 initial conditions are such that dry and wet tests of a given pair A or B show
 257 initial states (σ^{cont}, n, z_c) being as close as possible.

	Tests A		Tests B	
	Dry	Wet	Dry	Wet
Initial p (kPa)	11.1	2	20.6	10
Imposed u_c (kPa)	—	25	—	125
Initial S_w (%)	—	7.18	—	0.85
Initial n (-)	0.375	0.380	0.370	0.373
Initial z_c (-)	6.41	6.21	6.62	6.52

Table 2: Tests data for the dry and wet loading paths imposed on dense packings

258 Comparing the contact stress responses in dry and wet conditions (Fig. 3
 259 and 4), it is indeed verified that virtually unique behaviours are observed along
 260 the contractant or isochoric loading paths $R \in \{0; 1; 5\}$. As such, this establishes
 261 the validity of using the dry constitutive relation $\mathcal{F}$ together with σ^{cont} as an
 262 effective stress along these loading paths.

263 As for the dilatant loading path $R = 0.2$, a unique behaviour is observed in
 264 the early stage of the test. Subsequently, the imposed dilatancy rate requires the
 265 stresses to eventually vanish in the dry case, whereas when wet the same packing

Figure 3: Contact stress response of a dense packing (Table 2) along contractant ($R = 0$) and isochoric ($R = 1$) strain loading paths (color version online)

Figure 4: Contact stress response of a dense packing (Table 2) along contractant ($R = 5$) and dilatant ($R = 0.2$) strain loading paths (color version online)

gains a propensity to dilate originating from liquid bridges, thus avoiding a loss in bearing capacity. Hence, for such a dilatant loading path, the role of the contact stress as an effective stress is limited to the initial part of the loading path, and could still be used to predict initial stiffnesses in triphasic conditions.

It is noted that all contact stress responses obtained in both dry and triphasic conditions are found to be bounded by the same cohesionless Mohr-Coulomb failure criterion (with $c = 0$ Pa ; $\varphi = 31^\circ$) that was previously measured in dry conditions for such packings [15]. The universal property of this limit stress line, irrespective of the phase condition, is another illustration of the previously mentioned stress-strength effective nature of the contact stress.

4.2. Loose packing

The same analysis procedure is now applied to loose packings (Table 3). The numerical results displayed in Figs. 5 and 6 reveal less of an agreement between dry and wet behaviours in comparison to the previous dense case study.

	Tests A		Tests B	
	Dry	Wet	Dry	Wet
Initial p (kPa)	8.1	2	17.3	10
Imposed u_c (kPa)	—	25	—	125
Initial S_w (%)	—	4.17	—	0.50
Initial n (-)	0.442	0.441	0.436	0.438
Initial z_c (-)	4.96	4.84	5.17	5.12

Table 3: Tests data for the dry and wet loading paths imposed on loose packings

In particular, the existence of a unique constitutive relation $\mathcal{F}$ between σ^{cont} and ε is identified for the most contractant loading path $R = 0$ only, and is somewhat approximated along the less contractant path $R = 5$.

As for the isochoric path $R = 1$, and at variance with the dense packing (Fig. 3), a dry-wet agreement is only obtained for the very initial phase during which p^{cont} remains constant, consistent with a possible relationship between σ^{cont} and ε through Hooke's elastic law. Then, the dry packing presents a 'liquefaction' behaviour with vanishing stresses, consistent with the constant volume condition and the underlying material contractant flow rule. In contrast,

Figure 5: Contact stress response of a loose packing (Table 3) along contractant ($R = 0$) and isochoric ($R = 1$) strain loading paths (color version online)

Figure 6: Contact stress response of a loose packing (Table 3) along contractant ($R = 5$) and dilatant ($R = 0.2$) strain loading paths (color version online)

similar packings under triphasic conditions gain a propensity to dilate due to liquid bridges, thus leading the mean contact stress to increase.

Some influence of the mean contact stress on the dry-wet comparison is finally observed along the dilatant loading path $R = 0.2$. Along such a path, dry conditions induce the stresses in this loose material to vanish as expected, while triphasic conditions enhance again the material dilatant nature, leading to non zero stress states. The exact behaviour of the wet material nevertheless depends on the confining pressure.

For a low confining pressure, the wet loose packing behaves similarly to the dense one because capillary stress plays an important part of the total stresses: $|p^{cap}|/p \approx 3.0$ and $|p^{cap}|/p^{cont} \approx 0.75$ at the initial stage of this test. The behaviour then changes into one with a greater propensity to dilate as a result of triphasic conditions.

On the other hand, upon increasing the confining pressure, the contact stress also increases while the capillary stress remains fairly constant, leading to $|p^{cap}|/p^{cont} \approx 0.42$ and $|p^{cap}|/p \approx 0.72$, initially. The changes in the relative contributions from contact and capillary stresses diminish the liquid bridge induced dilatancy in the loose packing.

Finally, and as previously noted for the dense packing, the plastic limit criterion ($c = 0$ Pa ; $\varphi = 21^\circ$) corresponding to this loose material under dry conditions [15] also applies to the contact stress under triphasic conditions, once again confirming the stress-strength effective nature of σ^{cont} .

4.3. Discussion: effective stress vs dissipation and elasticity

The influences of the loading path and the solid packing on the ability of σ^{cont} to act as a stress-strain effective stress are now interpreted in relation to the variable dissipation associated with the observed behaviours. From f_n^c and f_t^c the normal and tangential components of the contact forces $\vec{f}^c$, the specific elastic energy e^{el} of the material is:

$$e^{el} = \frac{1}{2V} \sum_{N_c} \left(\frac{(f_n^c)^2}{k_n} + \frac{(f_t^c)^2}{k_t} \right) \quad (21)$$

317 which is easily measured from the DEM model, together with its increment
 318 δe^{el} between successive states. Comparing this increment with the incremental
 319 external work $\Sigma : d\epsilon$, the following quantity λ quantifies the deviation of the
 320 mechanical behaviour of any dry test from a non-dissipative behaviour:

$$\lambda = \left| \frac{\Sigma : d\epsilon - \delta e^{el}}{\Sigma : d\epsilon} \right| \quad (22)$$

321 The quasi-static nature of the loading paths ensures that both the kinetic energy
 322 and the energy term associated to numerical damping are negligible, and thus
 323 do not contribute to the energy balance quantified by the quantity λ . As such,
 324 during a non-dissipative, e.g. elastic, dry loading path, λ is equal to 0 throughout
 325 since all external work is completely stored as elastic energy. On the other hand,
 326 increasing values of λ reveal an increasing dissipation. It is noted that λ may
 327 be greater than 1 in the instance of elastic energy loss ($\delta e^{el} < 0$).

328 However, it is to stress out that a non-dissipative behaviour with negligi-
 329 ble values of λ does not necessarily correspond to a stress-strain path being
 330 reversible, even though the opposite is true. These intricacies are specific to
 331 granular materials whose elastic energy is contained in a contact network whose
 332 properties (for instance, N_c in Eq. (21)) fundamentally depend on irreversible
 333 strains. Also, granular materials are prone to irreversible yet non-dissipative
 334 local mechanisms such as contact losses. These very specific features can be
 335 interpreted in terms of a locked elastic energy concept [29] and have also been
 336 widely commented, e.g. in [30, 31], motivating here the distinction between the
 337 “non-dissipative” and “elastic” terminologies.

338 From the evolutions of λ shown in Figs. 7, and comparing with previous
 339 Figs. 3, it clearly appears that it is along the less dissipative loading paths that
 340 the stress-strain effective nature of σ^{cont} is the most marked, e.g. $R = 0$. Such
 341 a result includes and extends the finding previously reported in [4, 13] that an
 342 effective stress approach is possible in the elastic regime.

343 Another illustration of the role of dissipation in the effective stress discus-
 344 sion is proposed in Fig. 8 which considers an extreme case of the DEM model,
 345 referred to as $\mu = \infty$. In this extreme case of the DEM model, an ideal contact

Figure 7: Dissipative nature of the behaviour during various dry loading paths imposed on the dense packing (Tests A). Raw data have been smoothed without altering the average trends and λ -values for $R=0.2$ may be disregarded beyond $\|\epsilon\| \approx 1\%$ since stresses vanish at this point

description is adopted in which no frictional threshold (10) limit is imposed on the shear contact force: f_t^c just evolves linearly with the tangential relative displacement according to the shear stiffness k_t as long as a contact exists. The dry-wet comparisons shown in Fig. 8 then reveal an enhanced stress-strain effective character of σ^{cont} with this model, as opposed to the already discussed dry-wet comparisons with the classical friction coefficient $\mu = 0.5$ for the loose packing along the $R = 5$ loading path.

The present discussion finally sheds some light on the generality of thermomechanical approaches to effective stress, as proposed e.g. in [23, 32, 33]. Because the effective stress discussion herein appears to be widely different depending on the elastic or dissipative nature of the behaviour, and since such thermomechanical approaches usually rely on the assumption of an elastic behaviour for the solid phase with an appropriate potential, it is probably impossible to generalize the conclusions obtained through thermomechanics outside the assumed framework.

Figure 8: Influence of local friction μ on the contact stress' effective nature for a loose packing along a contractant loading path ($R = 5$)

5. Comparison with Bishop's stress

5.1. Qualitative discussion

The present μ UNSAT approach to effective stress is now compared with the commonly used effective stress expression as Bishop's stress σ^{Bish} :

$$\sigma' \stackrel{?}{=} \sigma^{Bish} = \Sigma - u_n \delta + u_c \chi \delta \quad (23)$$

Formally, significant differences appear between Bishop's equation (23) and the proposed μ UNSAT equation (5). It is herein recalled that the μ UNSAT equation includes a surface tension dependency in addition to that of capillary pressure, as well as the possibility of a non-spherical, microstructure-dependent, capillary stress contribution. Such features that characterize the microstructural details in triphasic materials go beyond the scope of Bishop's stress that relies on an average fluid pressure, being proportionnal to u_c and necessarily spherical. Since triphasic conditions by nature involve fluid-fluid interfaces and corresponding surface tension, the lack of γ^{nw} in Bishop's approach is questionable, as is the hypothesis of an averaged (isotropic) fluid pressure, while the wetted solid surfaces for instance experience capillary pressure along their normals only. Actually, the deviatoric nature of the capillary stresses has been repeatedly demonstrated in the pendular regime from modelling approaches [6, 26, 8, 24, 20], with possible variations in q^{cont} or q^{cap} independently of q

379 during microstructural changes of the fluid phases, contrary to Bishop’s general
380 equality between q and q^{Bish} .

381 5.2. Quantitative discussion

382 In order to illustrate the inadequacy of Bishop’s stress to serve as an effective
383 stress in the pendular regime, other dry-wet comparisons are presented for the
384 dense packing along the two loading paths $R \in \{1; 5\}$, from initial states pre-
385 sented in Table 4. The present discussion actually narrows down to the classical
386 choice $\chi = S_w$ for Bishop’s parameter, which can be continuously measured
387 during DEM simulations thanks to the complete description of the microstruc-
388 ture. As such, the stress response observed in dry conditions is now compared
389 to the Bishop’s stress response measured during triphasic conditions along the
390 same strain paths.

	Dry	Wet
Initial p (kPa)	11.5	10
Imposed u_c (kPa)	—	125
Initial S_w (%)	—	0.85
Initial n (-)	0.375	0.373
Initial z_c (-)	6.41	6.52

Table 4: Tests data for the dry-wet comparison in terms of Bishop’s stress

391 Such loading paths $R \in \{1; 5\}$ revealed a very good agreement of the $\sigma^{cont-\epsilon}$
392 behaviours in both dry and wet conditions (Figs. 3 and 4). However, the wet
393 behaviour in terms of Bishop’s stress here significantly deviates from the dry be-
394 haviour (Fig. 9), clearly showing that Bishop’s stress is a much less appropriate
395 effective stress measure along these loading paths than the contact stress. In
396 addition to this degraded stress-strain effective character of Bishop’s stress, it
397 is also clear from the present comparison that Bishop’s stress is also inadequate
398 to describe the strength of wet materials from the dry plastic limit criterion,
399 which σ^{Bish} violates. The consideration of Bishop’s stress in an effective stress
400 approach with some dry shear strength criterion in practice would thus lead
401 to an overestimation of the risk of material failure in the pendular regime, in

Figure 9: Bishop's or total stress responses along isochoric ($R = 1$) and contractant ($R = 5$) loading paths imposed on a dense packing

connection with an underestimation of capillary stresses already discussed in [20, 24].

6. Conclusion

Micromechanical modelling approaches showed evidence of a single effective stress variable that can be used together with dry constitutive relations to describe the strains of idealized slightly polydisperse granular media in the pendular regime. The appropriate variable is the contact stress whose direct evaluation requires the prior knowledge of the contact force network. Using the proposed μUNSAT expression, contact stresses can be alternatively calculated through measurements or estimations of the fluid phase microstructure (interconnects), which are easier to determine than forces.

Unique contact stress-strain relationships have indeed been numerically demonstrated along a variety of loading paths for both dry and wet (pendular regime) conditions. This lends strong support to applying the effective stress designation to contact stress. However, the considered loading paths have to induce small dissipation for the stress-strain effective stress approach to hold. Namely, contractant loading paths and dense packings are well suited for the application of the present μUNSAT approach to hold.

Previous experimental and phenomenological works by [4, 13] had restricted the existence of a single stress-strain effective stress in triphasic media to the

422 elastic regime. This work based on microstructural analysis suggests a less
423 restrictive condition by extending it to even the irreversible regime but with
424 small dissipation.

425 There remain open questions as to whether new definitions of strain quan-
426 tities could cast the presented results into an even more general framework.
427 The present approach actually relies on observable strains or particle relative
428 displacements that are due to both contact and capillary forces, through the
429 classical DEM workflow (second Newton’s law). Alternatively, it could be at-
430 tempted to define distinct, non-observable, strain components: first, a contact
431 strain uniquely caused by contact forces, and second, a capillary strain uniquely
432 due to capillary forces, with the combination of the two leading to the ob-
433 servable strains herein considered. Such an alternative framework may lead to
434 strictly unique constitutive relations between the contact stress and such a con-
435 tact strain, and shed some light on the dissipation role through the yet to be
436 defined link between contact strain and observable strain.

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- 440 [1] K. Terzaghi, The shearing resistance of saturated soils and the angle be-
441 tween the planes of shear, in: Proceedings of the 1st International con-
442 ference on soil mechanics and foundation engineering, Vol. 1, Cambridge,
443 1936, pp. 54–56.
- 444 [2] M. A. Biot, General theory of three-dimensional consolidation, Journal of
445 Applied Physics 12 (2) (1941) 155–164. doi:10.1063/1.1712886.
- 446 [3] A. W. Bishop, G. E. Blight, Some aspects of effective stress in saturated
447 and partly saturated soils, Géotechnique 13 (1963) 177–197.
- 448 [4] N. Khalili, F. Geiser, G. Blight, Effective stress in unsaturated soils: Review

- 449 with new evidence, *International Journal of Geomechanics* 4 (2) (2004) 115–
450 126. [doi:10.1061/\(ASCE\)1532-3641\(2004\)4:2\(115\)](https://doi.org/10.1061/(ASCE)1532-3641(2004)4:2(115)).
- 451 [5] N. Lu, W. Likos, Suction stress characteristic curve for unsaturated soil,
452 *Journal of Geotechnical and Geoenvironmental Engineering* 132 (2) (2006)
453 131–142. [doi:10.1061/\(ASCE\)1090-0241\(2006\)132:2\(131\)](https://doi.org/10.1061/(ASCE)1090-0241(2006)132:2(131)).
- 454 [6] P.-Y. Hicher, C. Chang, A microstructural elastoplastic model for unsat-
455 urated granular materials, *International Journal of Solids and Structures*
456 44 (7-8) (2007) 2304 – 2323. [doi:10.1016/j.ijsolstr.2006.07.007](https://doi.org/10.1016/j.ijsolstr.2006.07.007).
- 457 [7] M. Nuth, L. Laloui, Effective stress concept in unsaturated soils: Clar-
458 ification and validation of a unified framework, *International Journal for*
459 *Numerical and Analytical Methods in Geomechanics* 32 (7) (2008) 771–801.
460 [doi:10.1002/nag.645](https://doi.org/10.1002/nag.645).
- 461 [8] R. Wan, J. Duriez, F. Darve, A tensorial description of stresses in tripha-
462 sic granular materials with interfaces, *Geomechanics for Energy and the*
463 *Environment* 4 (2015) 73–87. [doi:10.1016/j.gete.2015.11.004](https://doi.org/10.1016/j.gete.2015.11.004).
- 464 [9] I. Cavarretta, I. Rocchi, M. Coop, A new interparticle friction apparatus
465 for granular materials, *Canadian Geotechnical Journal* 48 (12) (2011) 1829–
466 1840. [doi:10.1139/t11-077](https://doi.org/10.1139/t11-077).
- 467 [10] K. Senetakis, M. R. Coop, M. C. Todisco, The inter-particle coefficient of
468 friction at the contacts of leighton buzzard sand quartz minerals, *Soils and*
469 *Foundations* 53 (5) (2013) 746–755. [doi:10.1016/j.sandf.2013.08.012](https://doi.org/10.1016/j.sandf.2013.08.012).
- 470 [11] D. G. Fredlund, N. R. Morgenstern, R. A. Widger, The shear strength of
471 unsaturated soils, *Canadian Geotechnical Journal* 15 (3) (1978) 313–321.
472 [doi:10.1139/t78-029](https://doi.org/10.1139/t78-029).
- 473 [12] E. E. Alonso, A. Gens, A. Josa, A constitutive model for partially saturated
474 soils, *Géotechnique* 40 (3) (1990) 405–430.

- [13] E. Alonso, J.-M. Pereira, J. Vaunat, S. Olivella, A microstructurally based effective stress for unsaturated soils, *Géotechnique* 60 (2010) 913–925(12).
[doi:10.1680/geot.8.P.002](https://doi.org/10.1680/geot.8.P.002).
- [14] W. Baille, S. Tripathy, T. Schanz, Effective stress in clays of various mineralogy, *Vadose Zone Journal* 13 (5). [doi:10.2136/vzj2013.06.0112](https://doi.org/10.2136/vzj2013.06.0112).
- [15] J. Duriez, R. Wan, M. Pouragha, Partially saturated granular materials: Insights from micro-mechanical modelling, in: *Proceedings of the 6th Biot Conference on Poromechanics*, 2017, pp. 441–448.
[doi:10.1061/9780784480779.054](https://doi.org/10.1061/9780784480779.054).
- [16] R. Hurley, E. Marteau, G. Ravichandran, J. E. Andrade, Extracting inter-particle forces in opaque granular materials: Beyond photoelasticity, *Journal of the Mechanics and Physics of Solids* 63 (2014) 154 – 166.
[doi:10.1016/j.jmps.2013.09.013](https://doi.org/10.1016/j.jmps.2013.09.013).
- [17] K. A. Culligan, D. Wildenschild, B. S. B. Christensen, W. G. Gray, M. L. Rivers, A. F. B. Tompson, Interfacial area measurements for unsaturated flow through a porous medium, *Water Resources Research* 40 (12).
[doi:10.1029/2004WR003278](https://doi.org/10.1029/2004WR003278).
- [18] J.-F. Bruchon, J.-M. Pereira, M. Vandamme, N. Lenoir, P. Delage, X-ray microtomography characterisation of the changes in statistical homogeneity of an unsaturated sand during imbibition, *Géotechnique Letters* 3 (2) (2013) 84–88. [doi:10.1680/geolett.13.00013](https://doi.org/10.1680/geolett.13.00013).
- [19] J. Duriez, R. Wan, Contact angle mechanical influence for wet granular soils, *Acta Geotechnica* 12 (1) (2017) 67–83.
[doi:10.1007/s11440-016-0500-6](https://doi.org/10.1007/s11440-016-0500-6).
- [20] J. Duriez, M. Eghbalian, R. Wan, F. Darve, The micromechanical nature of stresses in triphasic granular media with interfaces, *Journal of the Mechanics and Physics of Solids* 99 (2017) 495–511.
[doi:10.1016/j.jmps.2016.10.011](https://doi.org/10.1016/j.jmps.2016.10.011).

- [21] M. E. Gurtin, A. I. Murdoch, A continuum theory of elastic material surfaces, *Archive for Rational Mechanics and Analysis* 57 (4) (1975) 291–323. doi:10.1007/BF00261375.
- [22] X. Chateau, L. Dormieux, Homogenization of a non-saturated porous medium: Hill’s lemma and applications, *C. R. Acad. Sci. Paris, Série II* 320 (1995) 627–634.
- [23] W. G. Gray, B. A. Schrefler, Analysis of the solid phase stress tensor in multiphase porous media, *International Journal for Numerical and Analytical Methods in Geomechanics* 31 (4) (2007) 541–581. doi:10.1002/nag.541.
- [24] J. Duriez, R. Wan, Stress in wet granular media with interfaces via homogenization and discrete element approaches, *Journal of Engineering Mechanics* 142 (12). doi:10.1061/(ASCE)EM.1943-7889.0001163.
- [25] V. Šmilauer, et al., *Yade Documentation 2nd ed*, The Yade Project, 2015. doi:10.5281/zenodo.34073.
URL <http://yade-dem.org/doc/>
- [26] L. Scholtès, P.-Y. Hicher, F. Nicot, B. Chareyre, F. Darve, On the capillary stress tensor in wet granular materials, *International Journal for Numerical and Analytical Methods in Geomechanics* 33 (10) (2009) 1289–1313. doi:10.1002/nag.767.
- [27] S. Herminghaus, Dynamics of wet granular matter, *Advances in Physics* 54 (3) (2005) 221–261. doi:10.1080/00018730500167855.
- [28] J. Duriez, R. Wan, Subtleties in discrete-element modelling of wet granular soils, *Géotechnique* 67 (4) (2017) 365–370. doi:10.1680/jgeot.15.P.113.
- [29] I. F. Collins, The concept of stored plastic work or frozen elastic energy in soil mechanics, *Géotechnique* 55 (5) (2005) 373–382. doi:10.1680/geot.2005.55.5.373.

- 529 [30] R. Puebla, A. Relaño, Irreversible processes without energy dissipation in
530 an isolated Lipkin-Meshkov-Glick model, Phys. Rev. E 92 (2015) 012101.
531 [doi:10.1103/PhysRevE.92.012101](https://doi.org/10.1103/PhysRevE.92.012101).
- 532 [31] M. Pouragha, R. Wan, Non-dissipative structural evolutions
533 in granular materials within the small strain range, Interna-
534 tional Journal of Solids and Structures 110111 (2017) 94 – 105.
535 [doi:10.1016/j.ijsolstr.2017.01.039](https://doi.org/10.1016/j.ijsolstr.2017.01.039).
- 536 [32] A. Madeo, F. dell’Isola, F. Darve, A continuum model for deformable,
537 second gradient porous media partially saturated with compressible fluids,
538 Journal of the Mechanics and Physics of Solids 61 (11) (2013) 2196 – 2211.
539 [doi:10.1016/j.jmps.2013.06.009](https://doi.org/10.1016/j.jmps.2013.06.009).
- 540 [33] E. Nikoee, G. Habibagahi, S. Hassanizadeh, A. Ghahramani, Effective
541 stress in unsaturated soils: A thermodynamic approach based on the in-
542 terfacial energy and hydromechanical coupling, Transport in Porous Media
543 96 (2) (2013) 369–396. [doi:10.1007/s11242-012-0093-y](https://doi.org/10.1007/s11242-012-0093-y).