OPEN GEOMECHANICS

Review History for “Micromechanically inspired, finite deformation hyperplasticity for crushable, cemented granular materials ”

Kateryna Oliynyk, Claudio Tamagnini *2020*

Summary

This paper was sent to two reviewers: one anonymous reviewer (Reviewer 1) and Arghya Das, IIT Kanpur (Reviewer 2). The two reviewers remained anonymous during the entire review process. After the reviewing process was complete, Reviewer 2 agreed to disclose their identity. In Review Round 1, both reviewers provided a series of comments for the authors. Reviewer 1 recommended that revisions were required while Reviewer 2 recommended that the authors rework the manuscript and resubmit it for review. In Review Round 2, both Reviewers recommended the manuscript for publication with no reservations. At this stage the managing Editor decided to accept the manuscript for publication.

Review Round 1

Reviewer 1

In this paper a finite deformation model for soft rocks is proposed. The paper is clear, well-structured and well written. Perhaps section 3 could be moved into an appendix as the manuscript is quite long. Despite this suggestion, on top of extending Tengattini’s et al model to a finite strain formulation, there are several novel features arising from this work. In particular the feature of the model which does not prevent the possibility of modelling non–associative plastic flow in Kirchhoff or Cauchy stress spaces is, to the reviewer opinion, very interesting, as the model is non–associated within a thermodynamically consistent framework. There are some minor comments however that the authors must address before publication:

On the micromechanical features of the model and its calibration

The word “micromechanically” in the title and within the text is quite misleading. One would either expect detailed microscale experimental analyses and or DEM simulations in order to define a model micromechanical inspired. The “micro” aspect of the model is sort of immediately lost when statistical homogenization is performed. Please comment on this aspect as at it stands there is not so much micro inspiration here.

Also, the material parameters such as the elastic constants (K_g , K_b, G_g and G_b) in the end seem to be calibrated using macroscopic quantities directly. In fact it is stated that ‘The calibration of the elastic constants can be performed indirectly from the measurements of the pre–yield response of the material upon isotropic compression and during the deviatoric stage of a drained triaxial compression test” and that “the mineralogic composition of grains and intergranular bonds can provide a reasonable estimate of the ratios". However, in the paper a calcarenite rock is modelled. This is 98% $CaCO_3$. According to the reviewer, the bulk and shear moduli of calcium carbonate used here should be 3 to 4 orders of magnitude larger to give realistic values. Also, when calibrating E_{BC} and E_{DC}, the macroscopic trends are used and or their ratio is always diverted to "a reasonable estimate from the mineralogical composition".

On the numerical examples:

- *General comments.* Why no experimental data (oedometric tests) are reported? It would be interesting to see these here too. Also, is it possible to represent the unloading path? The unload here would highlight the damage effects on the stiffness degradation. It would be interesting to highlight the differences between the two formulations. Figure 7: the small strains and finite response diverges quite rapidly from the very beginning. I would have expected such changes to develop more gradually. Please comment on this as I would have expected the post yield tangent of the two curves to almost coincide.
- *On the Plane strain BVP analyses.* Das et. Al (2014) use a Perzyna–type rate–dependent viscoplastic approach to regularize the BVP used for the bifurcation analyses in the small strain regime. In this work no sort of regularization is performed and yet post peak (localization) issues are discussed here. According to the reviewer all the discussion is interesting but is it Objective? Fig. 18 shows the fine and coarse mesh results; is it possible to add the element test response of the same test? Also, in the bifurcation analysis one would expect a discussion on the acoustic tensor or equivalent in large deformations? Finally, for a material such as a calcarenite it is hard to believe that the failure mechanism of a pillar of rock would buckle and look like the one obtained with the large strain simulations. Perhaps contours of incremental deviatoric strains would have helped in the result interpretation. Said this please comment on the objectivity of the results presented and for each analysis please add the element test response.
- On the literature review. In the introduction, when discussing grain crushing from phenomenological view, please also refer to more recent formulations, e.g., Kikumoto et al. [2010].

Recommendation: Revisions Required

Reviewer 2 (Arghya Das)

The paper presents a finite deformation hyperplastic model by enhancing the constitutive model proposed by Tengattini et al. (2004) for cemented granular materials. While the mathematical approach given in section 4 is interesting, the reviewer has a few concern over certain choices in the model:

1. Tengattini et al. (2014) used non–linear elasticity in the volumetric stress–strain relationship. The present manuscript uses linear elasticity in both volumetric and shear part (Eq. 59). The reviewer feels that such linear elasticity results in a $(1-D)^2$ term in the denominator of χ_D (Eq.) which is the stress conjugate of damage. Please note strain energy is added with respect to the volume fraction of cement and grain. Thus, strain must be the same in both phases. Therefore, Eq. 67 can be expressed in terms of stress on the cement phase alone along with a $(1-D)^2$ term in the denominator. The consequence is $(1-D)^2$ in the third term of Eq. 73 cancels. Therefore the model may not capture any cement damage effect other than cohesion.
2. Section 2 and 3 can be compressed since it is mostly same as Tengattini et al. 2014.
3. The authors aim to use the model for dissolution-prone granular materials. However, the model still lacks with volume dilation component. This issue needs to be addressed.

Recommendation: Resubmit for Review

Review Round 1: Author Response

Reviewer's comments are typed in grey, Author's replies in black.

Reply to Reviewer 1

1) In this paper a finite deformation model for soft rocks is proposed. The paper is clear, well-structured and well written. Perhaps section 3 could be moved into an appendix as the manuscript is quite long. Despite this suggestion, on top of extending Tengattini's et al model to a finite strain formulation, there are several novel features arising from this work. In particular the feature of the model which does not prevent the possibility of modelling non–associative plastic flow in Kirchhoff or Cauchy stress spaces is, to the reviewer opinion, very interesting, as the model is non–associated within a thermodynamically consistent framework.

The authors thank the anonymous reviewer for his constructive comments, which have helped us in improving the quality of the manuscript. To address the reviewer's comment, Sects. 2 and 3 have been merged into Sect. 2 and reduced in size.

2) The word "micromechanically" in the title and within the text is quite misleading. One would either expect detailed microscale experimental analyses and or DEM simulations in order to define a model micromechanical inspired. The "micro" aspect of the model is sort of immediately lost when statistical homogenization is performed. Please comment on this aspect as at it stands there is not so much micro inspiration here.

We agree with the reviewer about the "weak" link between the model formulation and the micromechanical concepts behind the definition of the internal variables B and D. The wording "micromechanically inspired", first used — to our knowledge — by Tengattini et al. (2016), has been used in this context to convey the fact that the part of the state variables of the (macroscopic) continuum hyperplasticity model are rooted in micromechanical concepts. This is why we supported the use of the verb "inspire" in place of stronger alternatives such as "derive" or "upscale". As the notion of "micromechanically inspired continuum models" has already been introduced in the literature, we decided to keep it, adding a short sentence in the introduction (p. 2) to stress that the adopted formulation is not a multiscale one. In addition, we changed the title, removing "micromechanically inspired" to avoid possible misunderstandings, and to make more clear that the paper is focused to the finite deformation extension of the infinitesimal hyperplasticity theory, and the main results of the paper are applicable to a whole class of models for granular materials with bonding and grain crushing.

3) Also, the material parameters such as the elastic constants (K_g , K_b, G_g and G_b) in the end seem to be calibrated using macroscopic quantities directly. In fact it is stated that 'The calibration of the elastic constants can be performed indirectly from the measurements of the pre–yield response of the material upon isotropic compression and during the deviatoric stage of a drained triaxial compression test" and that "the mineralogic composition of grains and intergranular bonds can provide a reasonable estimate of the ratios".

As the reviewer correctly observe, Sect. 4.5 addresses the issue of model constant calibration starting from macroscopic experimental evidence. We considered including this part since we believe that, in most practical applications, this kind of data is the only available from the geotechnical site characterization. However, the data reported in Tab. 1 for the model constants adopted in the numerical simulations of Sect. 7 have been taken directly from the paper of Das et al. (2014). The only exception is represented by the bulk moduli K^g and K^b, which have been taken equal to:

$$K^g = \frac{2(1+\nu^g)}{3(1-2\nu^g)} G^g \qquad\qquad K^b = \frac{2(1+\nu)^b}{3(1-2\nu^b)} G^b$$

with $\nu^g = \nu^b = 0.2$ (Poisson coefficients for grains and bonds, respectively). This has been necessary since, in this work, we have adopted a linear elastic relation between the mean stress and volumetric elastic strains, while in the paper of Das et al. (2014), a nonlinear model for $p(\epsilon_v^e)$ is used.

4) However, in the paper a calcarenite rock is modelled. This is 98% $CaCO_3$. According to the reviewer, the bulk and shear moduli of calcium carbonate used here should be 3 to 4 orders of magnitude larger to give realistic values.

The moduli of calcium carbonates, as for all the other constants, have been taken from Das et al. (2014). The reason why Das et al. (2014) report such low values of K^g — and consequently of K^b — are unknown to us. We can only speculate that, since the calcarenite grains are mostly made of empty calcareous shells, their stiffness could be much lower than the stiffness of crystalline $CaCO_3$.

5) Also, when calibrating E_{BC} and E_{DC}, the macroscopic trends are used and or their ratio is always diverted to "a reasonable estimate from the mineralogical composition".

Again, the values of E_{BC} and E_{DC} used in the simulations of Sect. 7 have been taken from Das et al. (2014), and no macro-

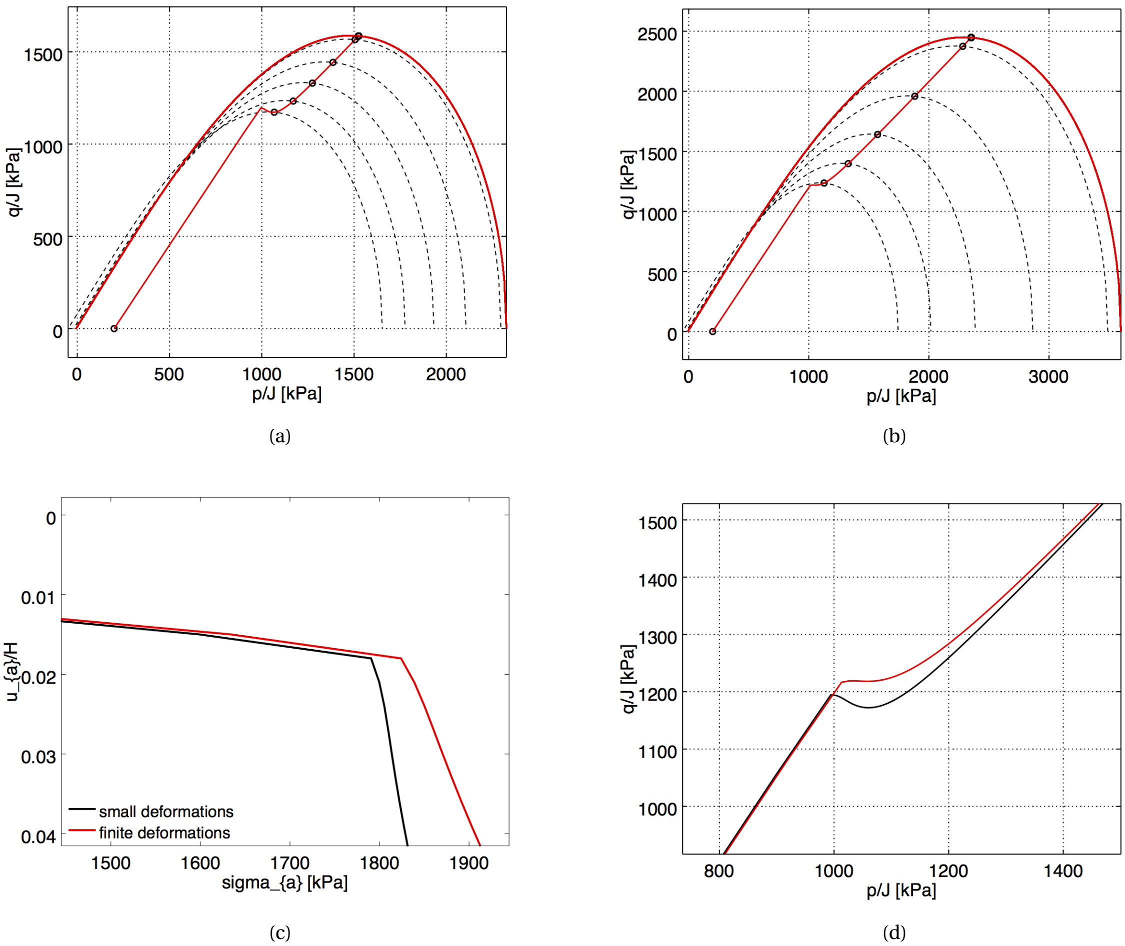

Figure 1: Oedometric test of Fig. 7. Stress paths and details of the compressibility curve close to the first yield point. Note: (p,q) = Kirchhoff stress invariants; $(p/J,q/J)$ = Cauchy stress invariants. The two quantities are coincident in the small strain case, for which $J=1$.

scopic data has been used for their calibration. The recipes for their calibration given in Sect. 4.5 have been included to provide a possible alternative to the (very difficult) direct measurement of these quantities at the microscopic scale.

6) Why no experimental data (oedometric tests) are reported? It would be interesting to see these here too. Also, is it possible to represent the unloading path? The unload here would highlight the damage effects on the stiffness degradation. It would be interesting to highlight the differences between the two formulations.

The reason why no experimental data have been reported in the paper is that we were mainly interested in showing the effects of non–linear kinematics in the model performance at both the element and at the BVP level, rather than demonstrating that the model is capable of reproducing the behavior of real geomaterials —- which has already been done at length by the developers of the original model (Tengattini et al. 2014; Das et al. 2014). We stress again that the model in Sect. 4 has only been adopted as a suitable example of application of the general concepts of finite deformation hyperplasticity, outlined in Sect. 3. Therefore, we believe that further explorations on the potentialities of the model is outside the scope of the present work.

7) Figure 7: the small strains and finite response diverges quite rapidly from the very beginning. I would have expected such changes to develop more gradually. Please comment on this as I would have expected the post yield tangent of the two curves to almost coincide.

We examined in detail the results of the oedometric tests in Fig. 7, by looking at the stress paths as well as to the compressibility curves. In figure 1, we report: a) the stress path of the SD simulation (fig. 1a); b) the stress path of the FD simulation (fig. 1b); c) an enlargement of the compressibility curves for SD and FD close to the first yield point; d) an enlargement of the stress paths for SD and FD close to the first yield point. As the oedometric test is performed under purely kinematic control, the stress path is a response of the material. This means that, as soon as the material yields the two formulations provide slightly different stress paths, due to the much larger volumetric stress rate as compared to the previous elastic behavior. This means that not only the tangent stiffness but also the positions of the yield points in the $u/H : \sigma_a$ plane are slightly different in the two solutions. This, in our opinion, explains the apparent inconsistency pointed out by the reviewer. We added a small sentence in the description of the test results – end of p. 19, beginning of p. 20 – to clarify this point.

8) Das et. al (2014) use a Perzyna–type rate–dependent viscoplastic approach to regularize the BVP used for the bifurcation analyses in the small strain regime. In this work no sort of regularization is performed and yet post peak (localization) issues are discussed here. According to the reviewer all the discussion is interesting but is it Objective?

When planning the simulations program for the plane strain tests, it was not our intention to analyze in detail the potentialities of the selected model in predicting the occurrence of bifurcation in shear band mode. This point has already been explored in detail in the paper of Das et. al. (2014). What we were interested in was to explore the effects of non–linear kinematics on the post–bifurcation solution. A significant result of our simulations is that FD kinematics may trigger a bifurcation mode (buckling) which cannot be obtained with the linearized kinematics.

In the simulations of Fig. 18 and Fig. 22, the mesh sensitivity of the computed solutions has been evaluated by direct comparison of the coarse and fine mesh results. Objectivity – that is, the independence of the solution on the element size – has been verified in all our simulations, both in small and finite deformations. As explicitly stated in the text, the element size independence of the solution in the SD simulations (bifurcation into shear bands) is a consequence of the large width of the localized zone, larger than the adopted element sizes. As for the FD simulation, mesh independence is a consequence of the specific bifurcation mode (buckling) which is not characterized by strain localization.

9) Fig. 18 shows the fine and coarse mesh results; is it possible to add the element test response of the same test?

As for the "element behavior", we did not include it in the presentation of the results because our aim was to analyze the outcome of a typical laboratory test result as a boundary value problem in which inhomogeneities could develop (due to the random initialization of B and D) as soon as a bifurcation from the homogeneous equilibrium solution occurs, and to see if, in this case, the FD kinematics might have an effect on the overall response of the specimen. We believe that the results shown are sufficient to provide a clear answer to our original question.

10) Also, in the bifurcation analysis one would expect a discussion on the acoustic tensor or equivalent in large deformations?

We did not add a discussion on the localization condition for the adopted model because this has already been done by Das et al. (2014). Their results refer to the infinitesimal version of the model but, since shear banding occurs at relatively small strains, we do not expect that the extension to finite deformation kinematics introduces significant changes to their results. In addition, what is significant is that, in the FD case, bifurcation into shear bands is preceded by buckling, for which the instability condition is different.

11) Finally, for a material such as a calcarenite it is hard to believe that the failure mechanism of a pillar of rock would buckle and look like the one obtained with the large strain simulations. Perhaps contours of incremental deviatoric strains would have helped in the result interpretation. Said this please comment on the objectivity of the results presented and for each analysis please add the element test response.

The issue raised here by the reviewer is about the capabilities of the model of predicting the actual observed behavior of the material for which it is used. As we already pointed out, providing an assessment of the model capabilities was outside the scope of this work, since the focus of the paper is on extending the theory of hyperplasticity with micromechanically–based internal variables to finite deformations, and Tengattini et al. (2014) model has been chosen as an example from this class of models from those available in the literature. We agree with the reviewer that the buckling response predicted in the plane strain test simulations is rather unusual. However, this may be due to the fact that in common laboratory test equipments the horizontal displacements of the top platen are restrained, thus preventing buckling to occur. In our numerical tests, we reproduced a condition of free horizontal displacement of the top platen, as in the experimental apparatus of Finno et al. (1997). As for the addition of the element test response, please see our reply to remark no. (9).

12) In the introduction, when discussing grain crushing from phenomenological view, please also refer to more recent formulations, e.g., Kikumoto et al. [2010].

We thank the reviewer for pointing out this very interesting paper. The work of Kikumoto et al. (2010) has been added to the bibliography and a sentence summarizing the main points of this work has been included in the introduction (p. 2).

Reply to Reviewer 2

1) The paper presents a finite deformation hyperplastic model by enhancing the constitutive model proposed by Tengattini et al. (2004) for cemented granular materials. While the mathematical approach given in section 4 is interesting, the reviewer has a few concern over certain choices in the model.

The authors thank the anonymous reviewer for his constructive comments, which have helped us in improving the quality of the manuscript. In our replies to each specific remark made (listed below) we will try to address the reviewer's concerns about the specific model adopted in Sect. 4 (former Sect. 5 of the original manuscript). Before doing that, we would like to point out that the main goal of the paper was to extend the infinitesimal hyperplasticity theory with micromechanically–inspired internal variables to finite deformations, and we never claimed to present a new, original model for bonded granular materials with grain crushing. Instead, we choose the model of Tengattini et al. (2014) as a good prototype for a whole class of models, to which we could apply the general approach of Sect. 3, and the numerical integration algorithm of Sect. 5 (which is again of general applicability, and not necessarily related to the specific model adopted). We have been perfectly aware of the merits and the limitations of the model chosen, deciding from the start that the limitations could still be accepted, in view of the known merits of the formulation. The only case in which we made a significant modification to the original formulation is in the volumetric part of the free energy function, which has been changed from a cubic law to a quadratic law in elastic volumetric strain. The reasons behind this choice are detailed in the reply to remark (3).

2) Section 2 and 3 can be compressed since it is mostly same as Tengattini et al. 2014.

We agree with the reviewer. We have merged the original Sects. 2 and 3 into a new Sect. 2 and eliminated all the non–necessary parts. We decided to leave unaltered the parts in which we provide the references to previous works as well as the general outline of hyperplasticity theory with internal variables of Sect. 2.2, which could be of help in understanding the developments of the finite deformation theory in Sect. 3.

3) Tengattini et al. (2014) used non–linear elasticity in the volumetric stress–strain relationship. The present manuscript uses linear elasticity in both volumetric and shear part (Eq. 59). The reviewer feels that such linear elasticity results in a $(1-D)^2$ term in the denominator of χ_D (Eq.) which is the stress conjugate of damage. Please note strain energy is added with respect to the volume fraction of cement and grain. Thus, strain must be the same in both phases. Therefore, Eq. 67 can be expressed in terms of stress on the cement phase alone along with a $(1-D)^2$ term in the denominator. The consequence is $(1-D)^2$ in the third term of Eq. 73 cancels. Therefore the model may not capture any cement damage effect other than cohesion.

As we already pointed out before, our original intention was to use the model of Tengattini et al. (2014) as it is, without any modifications. However, after implementing and testing the original model, we realized that we needed to change the volumetric part of the free energy functions ψ_r^g and ψ_r^b to circumvent an important drawback in the volumetric part of the elastic constitutive equation. In the original model, the volumetric elastic stress–strain law (eq. 40a) reads:

$$p = n^g p_r (A^g)^2 (1-\theta^g B) + n^b p_r (A^b)^2 (1-D) \tag{1}$$

with:

$$A^g = \frac{1}{2}\overline{K}^g \epsilon_v^e + 1 \qquad\qquad A^b = \frac{1}{2}\overline{K}^b \epsilon_v^e + 1$$

Now, it is immediately apparent from eq. (1) that this elastic law cannot provide negative (tensile) mean stress values, as all the terms on the RHS are positive or zero. In addition, considering the case in which $\overline{K}^b = \overline{K}^g$, the elastic constitutive law is not invertible for $\epsilon_v^e < -2/\overline{K}^g (\simeq -5.8e-4)$, see Fig. 2a. These features of the original volumetric hyperelastic law make it unsuitable for cemented granular materials displaying cohesion values of the order of hundreds of kPa, and for which the admissible stress space extends significantly into the tensile region.

In addition, the original non–linear elastic model presents another (less serious) drawback at relatively low, positive values of p, which is typical of hyperelastic models with stress–dependent bulk stiffness and constant shear stiffness. At low mean stress levels, the tangent bulk modulus $K = dp/d\epsilon_v^e$ tends to be very low as compared to the shear modulus G, and therefore the apparent Poisson ratio, defined as:

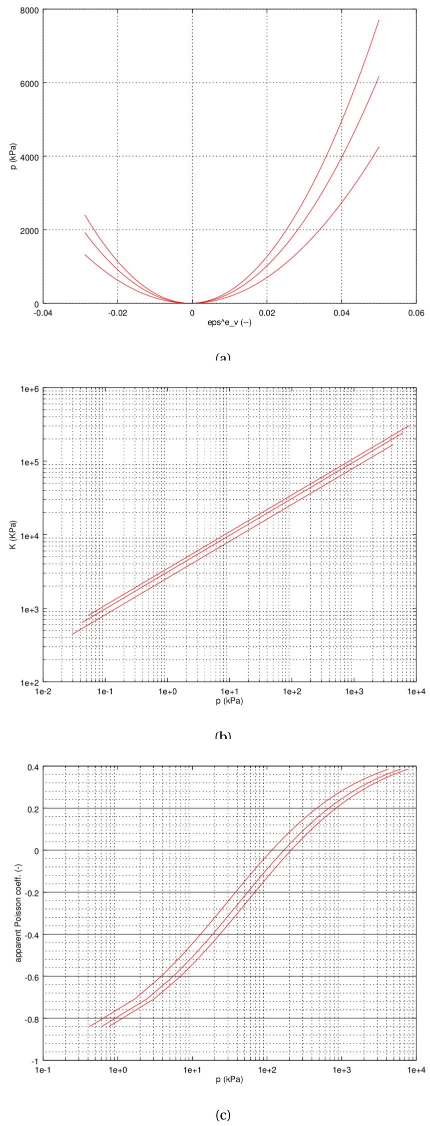

Figure 2: Volumetric elastic constitutive equation adopted in Tengattini et al. (2014) model. a) Mean stress vs. elastic volumetric strain curves for different B values and $D = 0$; b) Tangent elastic bulk modulus $K = dp/d\epsilon_v^e$ vs. mean stress p, for different B values and $D = 0$; c) Apparent Poisson ration $\nu_{app} := (3K/G - 2)/(2 + 6K/G)$ vs. mean stress p, for different B values and $D = 0$.

$$\nu_{app} := \frac{3K/G - 2}{2 + 6K/G}$$

becomes negative, approaching -1 as $K \to 0$. With the set of material constants reported by Das et al. (2014) for the calcarenite, the evolution of K and of ν_{app} with p is provided by Figs. 2b and 2c. The figures show that the tangent bulk modulus for $p < 100$ kPa predicted by the non–linear elastic law is unrealistically low, i.e., not larger than $1.0e4$ kPa, and that, in this range, the apparent Poisson ratio is negative. This aspect is of importance in all practical applications where the soil/rock mass has a free surface (e.g., slope stability problems, underground excavations, natural underground cavities), close to which the mean stress p is necessarily relatively low. All that considered, we choose to replace the original volumetric free energy functions with the simplest possible alternative, i.e., the standard quadratic free energy functions. This choice is not only more consistent with the observed behavior of calcarenites at low stress levels, but also more convenient in terms of calibration, as it only requires to assign realistic values to the Poisson's ratios of grains and bonds to determine the corresponding bulk moduli K^g and K^b. In the paper, we adopted $\nu^g = \nu^b = 0.2$.

4) The authors aim to use the model for dissolution–prone granular materials. However, the model still lacks with volume

dilation component. This issue needs to be addressed.

The scope of the paper is limited to the purely mechanical theory. We are aware of the fact that the model cannot capture dilatancy in the compressive stress range and we have discussed this feature in detail at the end of Sect. 4.4, providing indications on how to overcome this problem. This issue will be taken in due consideration in the future extension of the present work to the chemo–mechanical framework.

References

Kikumoto, M., Wood, D. M., and Russell, A. (2010). Particle crushing and deformation behaviour. *Soils and foundations*, 50(4):547–563.

Review Round 2

Reviewer 1

The authors addressed all my previous concerns and questions. I have no further comments to the revised manuscript. Perhaps I would suggest the authors to increase the font size of axis labels of figures 2-16 and 18-26. I also find the colorbar labels and the load displacement curves of figures19-26 quite small. Other than these editorial suggestions I recommend accepting the revised manuscript for publication.

Reviewer 2 (Arghya Das)

The authors have responded to the queries of the reviewers satisfactorily. Hence the manuscript can be accepted for publication.

Review Round 2: Author Response

We made our best to address the issues raised by Reviewer 1, by increasing the size of the text labels (by about 20%) in the revised manuscript no. 2. We hope that the graphical format of the figures is now acceptable.

Editorial Decision

At the end of Review Round 2, the managing Editor accepted the revised version of the manuscript for publication.