Optimised calibration algorithm of a bounding surface model for coarse-grained soils

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ABSTRACT

Several constitutive models have been developed over the years to capture the salient features of the undrained cyclic stress-strain response of sandy soils, that is of crucial interest for assessing the behaviour of geotechnical systems under seismic loading. Among them, the bounding surface plasticity theory turned out to be a valuable framework for reproducing the hardening soil response under both drained and undrained conditions. However, such models usually require a non-straightforward calibration of many parameters, employing also trial-and-error procedures that inhibit the physical meaning of the parameters and their eventual correlation. In this view, the present study proposes an optimised procedure for calibrating the trial-and-error parameters of bounding surface constitutive models for coarse-grained soils. The proposed approach is applied to a modified version of the model developed by Papadimitriou and Bouckovalas (2002), which was recently implemented in OpenSees by the Authors to investigate liquefaction-related phenomena. Based on the obtained results, a preliminary correlation between the critical parameters and a significant response quantity to identify liquefaction triggering is proposed with reference to a well-characterised soil. Considerations on the ongoing developments and of the extension of the method to other classes of models are finally provided.

Keywords: Soil Constitutive Modelling, NTUASand02, Calibration, Liquefaction, Optimisation

1 INTRODUCTION

Reliable numerical modelling of the cyclic and dynamic response of saturated coarse-grained soils is a challenging goal in earthquake engineering. Over the years, advanced constitutive models based on the bounding surface theory turned out to be particularly effective in the description of the behaviour exhibited by sandy soils, even at large-strain levels and during liquefaction (Dafalias and Manzari, 2004; Boulanger and Ziotopoulou, 2017; Limnaiou and Papadimitriou, 2022).

On the other hand, these models need many parameters to be calibrated, where some of them can be identified by using trial-and-error procedures. This approach often inhibits the physical meaning of the constitutive parameters and their eventual correlation. Furthermore, the procedure can be non-trivial and time-consuming (Machaček et al., 2023).

For the reasons above, this paper presents a preliminary assessment of an optimisation algorithm aimed at calibrating the parameters requiring a trial-and-error procedure of bounding-surface constitutive models. In particular, the approach is applied to a modified version of the NTUASand02 model (named MNTUASand02), implemented by the Authors in OpenSees (Fierro, 2022; Fierro et al., 2024).

As a preliminary step, a parametric study is carried out to evaluate the effects on the soil response of the two model parameters requiring a trial-and-error procedure. To this aim, different element tests are performed in OpenSees (McKenna et al., 2010). Then, a preliminary assessment of the optimisation algorithm is discussed, providing a correlation law between the critical MNTUASand02 constitutive parameters and the number of cycles triggering liquefaction.

2 THE REFERENCE CONSTITUTIVE MODEL

2.1 Formulation

The NTUASand02 constitutive model was developed by Papadimitriou and Bouckovalas (2002) to describe the drained and undrained, monotonic and cyclic response of coarse-grained soils. The model relies on the bounding surface theory and represents an evolution of the formulation proposed by Manzari and Dafalias (1997). For the sake of brevity, only the relevant features of the model are recalled in the following.

State dependency of the soil response is included in the formulation through the state parameter $\psi=e-e_{cs}$

(Been and Jeffries, 1985), where *e* represents the current void ratio and e_{cs} is the void ratio at the Critical State. The latter varies logarithmically with the effective mean stress, *p'*.

The elastic-plastic hardening response of the model is controlled by the following four loci: yield, Critical State, dilatancy, and bounding surfaces. The hardening response triggers when the stress state lies on the yield surface, while the elastic-plastic response depends on the distance between the current stress state and the remaining three surfaces, according to a radial mapping rule.

In Fig.1a, the constitutive framework in the *p'-q* invariants plane is schematically depicted: each surface is represented through a cone with apex in the origin of the axes. In Fig. 1b, the intersection between the model and the π-plane is reported. In particular, $\mathbf{r}_i$ is the deviatoric stress ratio of the i[th] principal effective stress, $\mathbf{s}_i$, to the mean effective stress, *p'*. Here, only the yield surface is independent of the Lode angle θ and is consequently circular, while the remaining surfaces are conical and wedge-shaped. The yield surface evolves according to a kinematic hardening law, whereas its diameter in the π-plane is controlled by the parameter *m*. Its position with reference to the hydrostatic axis is defined through the back-stress ratio tensor $\boldsymbol{\alpha}$. The latter is the internal variable of the constitutive model, and a non-associated flow rule is included in the formulation.

The main innovative features of the constitutive model are the non-linear elastic formulation of shear and bulk moduli and the definition of a scalar parameter h_f. The former property allows for a more realistic modeling of the small-strain response if compared to the conventional elastic relationships. The latter directly scales the plastic modulus to define the evolution of the fabric tensor.

The original formulation of NTUASand02 was modified to improve the numerical stability in boundary value problems (Fierro et al., 2024), referred in the following to as MNTUASand02. The formulation of the evolution law for the deviatoric part of the fabric tensor, **f**, was originally defined as:

$$d\boldsymbol{f} = -H\langle -d\varepsilon_v^p\rangle[C\boldsymbol{n} + \boldsymbol{f}] \qquad (2)$$

where H is a coefficient that includes the effects of the state parameter ψ and the major principal effective stress at consolidation on the fabric tensor, while ε_v^p represents the plastic volumetric strain. The C coefficient, initially computed as $\mathrm{C} = \max\left|\mathrm{f_p}\right|^2$, in MNTUASand02 is instead assumed equal to 5 to avoid rapid variations of the fabric tensor **F**, which can generate anomalous hardening response and convergence issues. A different, constant value for C was also proposed by Miriano (2010) and Miriano et al. (2016) for the evaluation of the seismic performance of diaphragm walls. The reader can refer to Fierro et al. (2024) for a comprehensive assessment of the response of MNTUASand02.

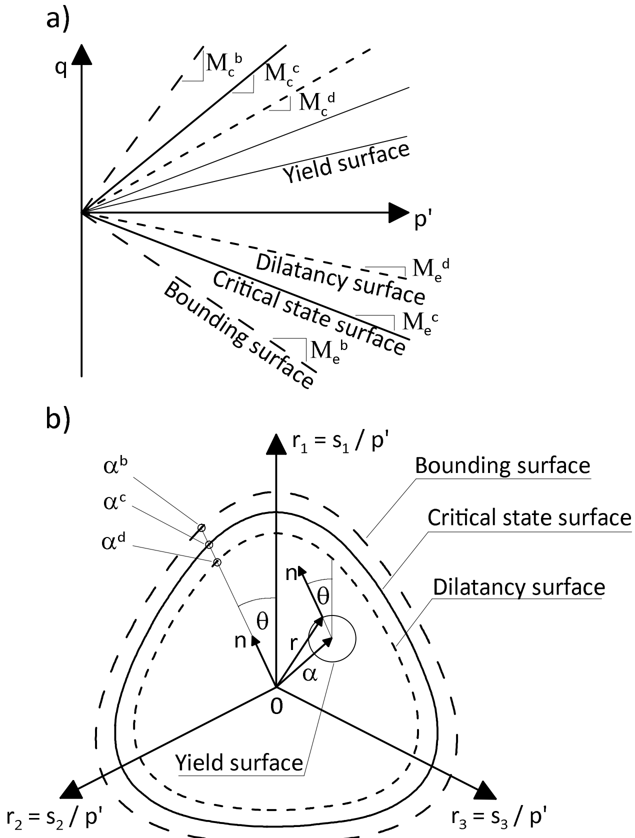

Fig. 1. (a) Representation of the model surfaces on the p'-q plane and (b) on the π-plane (reproduced from Papadimitriou and Bouckovalas, 2002).

2.2 Model parameters

The constitutive model requires the calibration of 15 material constants describing key features of the behavior of coarse-grained materials, such as the elastic response (m, B, ν, a_1, γ_1), Critical State ($e_{cs,a}$, λ, M_c^c, M_c^e), and the effect of the state parameter ψ on the peak strength (k_c^b) and the dilatancy surface (k_c^d). Additional input parameters are the dilatancy factor (A_o), the plastic modulus (h_0), and fabric-related constants (H_0, ζ).

The parameters describing the elastic response and those related to Critical State can be calibrated using resonant column and triaxial tests, respectively (Papadimitriou and Bouckovalas, 2002). With reference to A_o, it can be calculated using drained triaxial tests, while ζ can be assumed equal to 1 (Papadimitriou et al., 2001). The remaining parameters H_0 and h_0 require a trial-and-error procedure that can be sometimes difficultly performed and is time-consuming. For this reason, we performed a parametric study to analyse the effects of these parameters on the soil response at the element level. Hence, a cyclic direct simple shear test was simulated by varying H_0 and h_0, and a preliminary, optimised analytical relationship between these parameters and the number of cycles triggering liquefaction is developed in the following sections.

3 TEST SETUP AND PARAMETRIC STUDY

The parametric study refers to an undrained cyclic direct simple shear test carried out in the framework of VELACS project (Arulmoli et al., 1992). The test concerns a Nevada sand sample with relative density D_r=60%, corresponding to a void ratio e=0.66. In the consolidation stage an effective mean stress of 160 kPa and a shear stress of 5.9 kPa are applied to the sample. In the following deviatoric stage the sample is perturbed by 26 cycles of a harmonic shear stress with an amplitude of 13.7 kPa. In OpenSees, a quadrilateral finite element with four integration points providing a coupled hydro-mechanical response (named *quad-UP*) was employed to simulate the experimental data.

The calibration of the model proposed by Papadimitriou and Bouckovalas (2002) for Nevada sand is taken as a reference, except for the parameters H_0 and h_0, originally evaluated by trial-and-error, for which a systematic identification procedure is proposed herein. The fabric index H_0 includes the effect of the state parameter and of the major principal stress at consolidation in the fabric tensor evolution; h_0 is instead incorporated in the formulation through the quantity h_b, which accounts for the distance between the current stress state and its image stress point on the bounding surface. Using a trial-and-error procedure with reference to the experimental data of Nevada sand, Papadimitriou and Bouckovalas (2002) assumed H_0=68000 and h_0=5000. In addition, they suggested a range of variation for H_0, within 50000 and 100000, and h_0, between 1000-10000.

The proposed parametric study took the latter range as a reference for h_0, while a wider range was analysed for H_0, from 13600 to 122400. Five values were considered for each parameter, namely H_0=13600, 34000, 68000, 102000, 122400 and h_0=1000, 2500, 5000, 7500, 10000, resulting in 25 permutations H_0-h_0.

As an example, Fig. 2 illustrates the model response to the combination proposed by Papadimitriou and Bouckovalas (2002), that is H_0=68000 and h_0=5000, in terms of stress paths (Fig. 2a), hysteretic loops (Fig. 2b), excess pore water pressure ratio $r_u=\Delta u/\sigma'_{v0}$ (Fig. 2c), where Δu represents the excess pore water pressure and σ'_{v0} indicates the vertical effective stress at the end of consolidation. The numerical results are compared with the relative experimental data (Arulmoli et al., 1992).

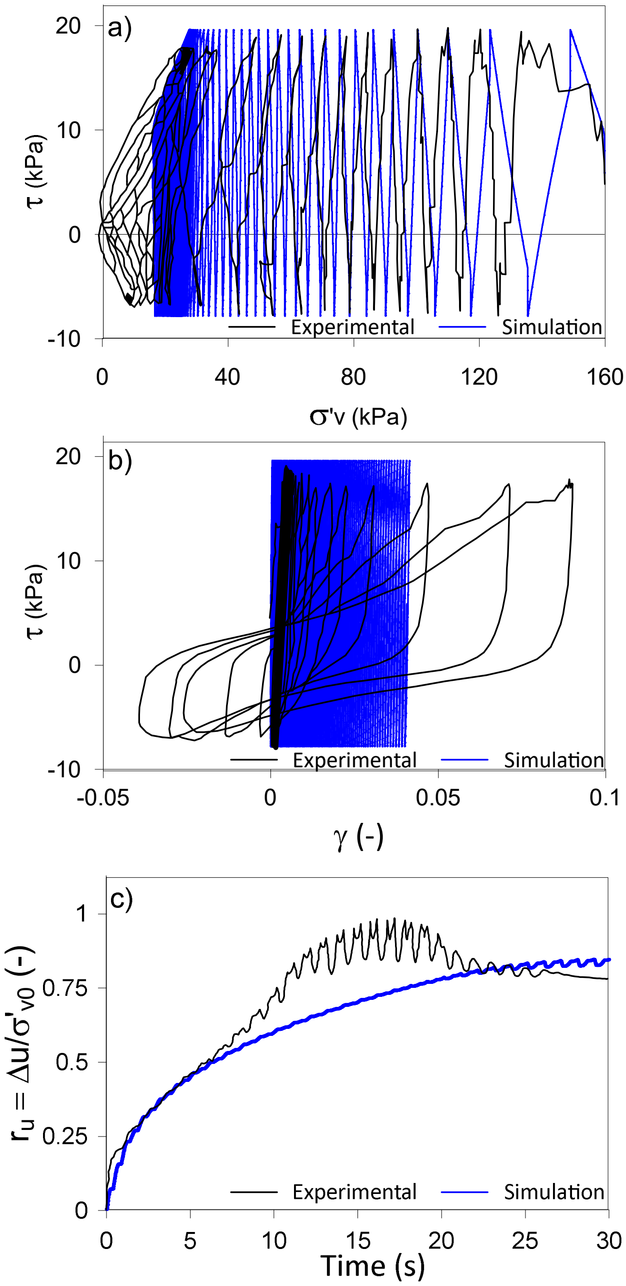

Fig. 2. Comparison between the model response for H_o=68000 and h_0=5000 (blue line) and the experimental data (black line): (a) stress paths in the τ-σ'$_v$ plane, (b) hysteretic loops, (c) excess pore water pressure ratio time-history.

In terms of stress path (Fig. 2a), the numerical result is in a good agreement with the experimental data during the first cycles, while discrepancies arise towards the attainment of liquefaction, with important underestimation of the irreversible shear strain (Fig. 2b). From the time evolution of the pore water pressure ratio obtained with MTUASand02 (Fig. 2c), it can be noticed that liquefaction triggers when r_u is equal to 0.8. The initial calibration of MNTUASand02 leads to a trend of the excess pore water pressure almost overlapped to the experimental data up to cycle No. 7; conversely, the model provides a progressively higher underestimation of r_u in the subsequent cycles, with consequent, significant delay in the attainment of liquefaction, occurring after 22 cycles instead of the 11 cycles associated with the experimental data.

The test above was then simulated for the considered couples of H_0-h_0. Tab.1 reports the computed number of cycles at liquefaction, N_{liq}, for all the analyses, referring to r_u = 0.8 as the value corresponding to the attainment of liquefaction.

Table 1. Number of cycles at liquefaction, N_{liq}, for all the parameters permutations examined.

		h_0 = 1000			
H_0	13600	34000	68000	102000	122400
N_{liq}	1	2	5	10	14
		h_0 = 2500			
H_0	13600	34000	68000	102000	122400
N_{liq}	2	4	12	24	33
		h_0 = 5000			
H_0	13600	34000	68000	102000	122400
N_{liq}	3	8	22	46	64
		h_0 = 7500			
H_0	13600	34000	68000	102000	122400
N_{liq}	5	11	33	68	95
		h_0 = 10000			
H_0	13600	34000	68000	102000	122400
N_{liq}	6	14	43	89	100

4 OPTIMISATION ALGORITHM

On the basis of the results discussed in Section 3, an optimisation algorithm was developed for the calibration of the critical parameters H_0 and h_0. The algorithm searches for the best-fitting of n samples using functions of various typology. It compares the candidate functions and, for each of them, returns the values of the respective coefficients. The goodness of fit is quantified by means of two common statistical parameters, that are the Coefficient of Determination, R^2, and the Root Mean Square Error, RMSE, whose description is left out for the sake of brevity. The objective of the optimization process consists of maximizing R^2 and minimizing RMSE (a perfect match corresponds to R^2=1 and RMSE=0).

As a preliminary step of this study, the focus is on the identification of the optimal number of cycles triggering liquefaction, N_{liq}, as a simple means for controlling the rate of the pore water pressure under cyclic loading. This is indeed a key point to be accounted for during the calibration of bounding surface models (Gorini, 2019; Gallese, 2022), typically set up with reference to the observed monotonic behaviour: the proposed, simple criterion aims instead at avoiding an exaggerate generation of the excess pore water pressure under cyclic conditions.

In the case at hand, the proposed algorithm was used to find the best-fitting function N_{liq}=*func*(H_0,h_0) of the numerical results in Table 1. Three constraints were introduced into the optimization problem, namely: R^2>0.98, RMSE<10.0, minimization of the coefficients number of the fitting.

The resulting, optimum function is illustrated in Fig. 3: it represents a paraboloid described by 5 coefficients p_i, automatically identified to meet the target. The relationship N_{liq}=*func*(H_0,h_0) reads:

$$N_{\text{liq}} = p_0 + p_1 \cdot h_0 + p_2 \cdot H_0 + p_3 \cdot h_0 \cdot H_0 + p_4 \cdot {H_0}^2 \quad (3)$$

For the considered initial conditions of the soil (σ'_{v0}=160 kPa, τ=5.9 kPa, e=0.66), the optimal values of the coefficients are: p_0=7.518, p_1=-1.4×10^{-3}, p_2=-3.5×10^{-4}, p_3=9.4×10^{-7}, p_4=3.0×10^{-9}. These correspond to R^2=0.98 and RMSE=4.3. This optimization procedure can be straightforwardly applied to find the parameters correlation for different initial states of the soil.

For the case at hand, the paraboloid shows a clear, regular correlation between N_{liq} and the pairs (H_0, h_0). The optimum function represents a preliminary tool for the calibration of the critical parameters of MNTUASand02.

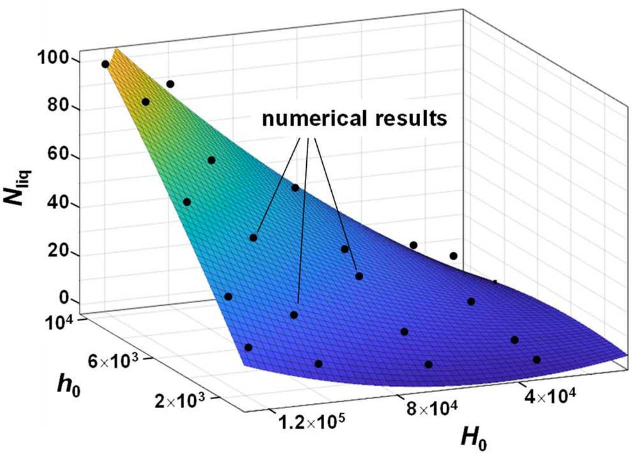

Fig. 3. Best-fitting of the numerical results: paraboloid surface describing the number of cycles triggering liquefaction, N_{liq}, as a function of the couples H_0 and h_0.

6 VALIDATION PROCEDURE

The proposed criterion for calibrating H_0 and h_0 is concisely validated with reference to the test in Section 3. To this end, the optimised equation for N_{liq} was used to reproduce the desired number of cycles triggering liquefaction, equal to 11 in the case at hand: the resulting values for h_0 and H_0 are 4341 and 47903, respectively. The corresponding response is depicted in Fig. 4.

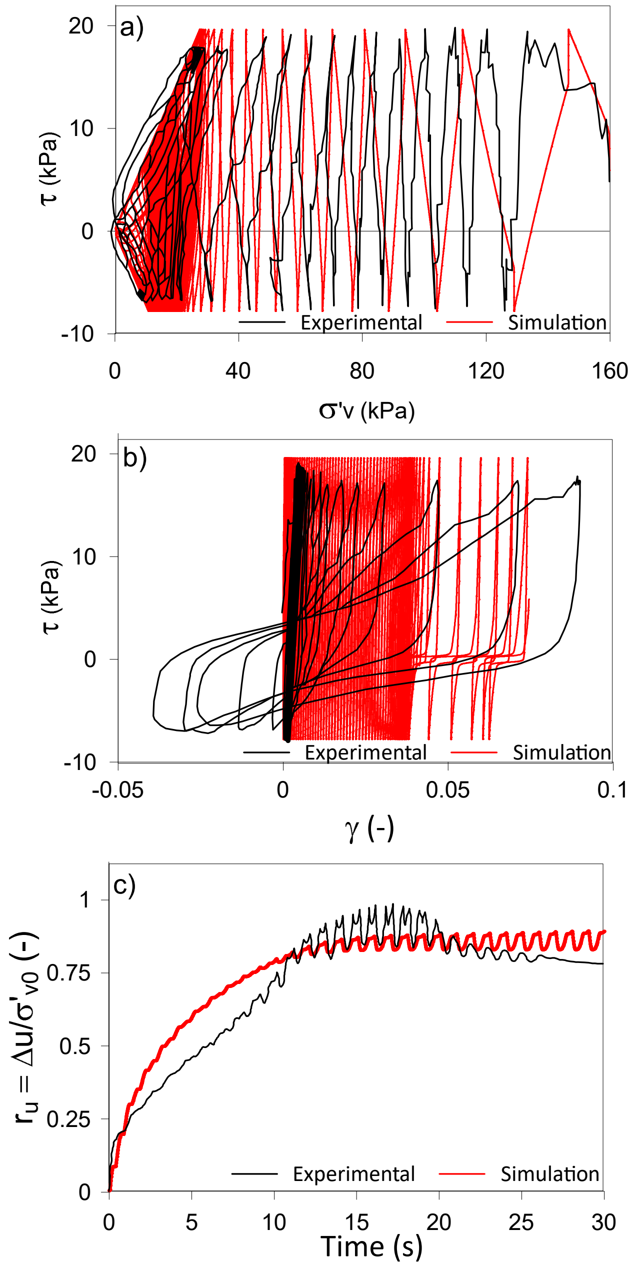

Fig. 4. Comparison between the optimised model response (red line) and the experimental data (black line): (a) stress paths in the τ-σ'$_v$ plane, (b) hysteretic loops, (c) excess pore water pressure ratio time-history.

It can be noted that the optimised calibration of the parameters h_0 and H_0 improves significantly the model response. Compared to the initial calibration by Papadimitriou and Bouckovalas (2002), the optimised response simulates more accurately the evolution of the stress state from small to large strain levels, with also a more realistic reproduction of the butterfly-shaped trend occurring at low stress levels.

The stress-strain relationship (Fig. 4b) obtained with the optimised calibration of MNTUASand02 still underestimates energy dissipation and the ratcheting effect, that is the progressive accumulation of a permanent shear strain as the cycles increase. Nonetheless, if compared with the initial calibration of the model, the proposed one leads to a first improvement of the response also in the τ-γ space.

The observation of Fig. 4c evidences that, in the first ten cycles, the optimised calibration overestimates of at most 30% the excess pore water pressure, but captures very well the attainment of the maximum value of r_u, as prescribed by the proposed liquefaction criterion, and its development until the end of the test, overcoming part of the limitations associated with the initial trial-and-error procedure (cf. Figs. 2c and 4c).

6 CONCLUSIONS

The current paper presented a numerical procedure for the optimised calibration of the advanced bounding surface constitutive model MNTUASand02. The critical parameters were related to the number of cycles triggering liquefaction, as a simple means for reproducing a realistic evolution of the pore water pressure under cyclic loading.

The preliminary results discussed in the paper highlighted the strong sensitivity of the soil response to the plastic modulus parameter h_o and the fabric tensor constant H_o. Through the implementation of a straightforward optimization algorithm, a close correlation was found between the number of cycles for liquefaction triggering and the parameters above. An analytical relationship between them was devised. The algorithm was preliminary validated with reference to the experimental data relating to a cyclic direct simple shear tests carried out on Nevada sand. In light of the promising results obtained so far, the proposed numerical procedure is currently being used i) to identify an optimized calibration of general validity for MNTUASand02, considering different initial conditions for the soil, and ii) to devise parameters correlations for a wider panorama of bounding surface models.

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