

Double structure hydromechanical coupling formalism and a
model for unsaturated expansive clays

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Abstract

1

2 A formalism for double structure hydromechanical coupled modelling of aggregated unsatu-
3 rated soils has been developed. Independent coupled hydromechanical models are considered
4 for each structural level, including independent measures of macromechanical and microme-
5 chanical effective stresses. The models are linked using a coupling function to obtain the
6 global response. The individual components have been selected to represent the behaviour
7 of compacted expansive clays. The macrostructural mechanical model is based on the ex-
8 isting hypoplastic model for unsaturated soils. Hydromechanical coupling at each structural
9 level is efficiently achieved by linking the effective stress formulation with the water retention
10 model. An essential component of the model is representation of microstructural swelling.
11 It is demonstrated that its calibration on wetting induced expansion measured in oedomet-
12 ric (mechanical) tests leads to a correct global hydraulic response, providing a supporting
13 argument for the adopted coupling approach. An interesting consequence of the model for-
14 mulation is that it does not suffer from volumetric ratchetting, which is often regarded as one
15 of the main drawbacks of hypoplasticity. The proposed model has a small number of material
16 parameters. Its predictive capabilities have been confirmed by simulation of comprehensive
17 experimental data set on compacted Boom clay.

18 **Keywords:** expansive soils; double structure; unsaturated soils; hypoplasticity; hydrome-
19 chanical behaviour; water retention curve

20 1 Introduction

21 Advances in understanding of the behaviour of expansive compacted soils, gained over the
22 last 20 years, reveal a crucial role of microstructure in modelling of their behaviour. The
23 soil compacted dry of optimum has a structure with two distinct pore systems. Gens and
24 Alonso (1992) and Alonso et al. (1999) developed a pioneering mechanical model for expansive
25 clays, which combined an existing model for unsaturated soils with low plasticity with a simple
26 reversible model for microstructure, linked by a coupling function. The role of microstructure
27 in the soil hydraulic behaviour has been understood by Romero (1999) and Romero et al.
28 (1999), and recently combined into a complete water retention model by Romero et al. (2011).
29 The above two models considered separately two levels of structure and linked the responses
30 using a coupling function. The first model focused on the mechanical behaviour (Alonso et al.
31 1999), while the second on the hydraulic behaviour (Romero et al. 2011).

32 From different perspective, recent past advances in modelling of the hydromechanical be-
33 haviour of unsaturated soils reveal crucial role of hydromechanical coupling. Volumetric
34 deformation (mechanical response) of soil skeleton influences the degree of saturation and
35 the air entry value of suction (hydraulic response), which in turn influence soil effective stress
36 and thus affect its mechanical properties (see, e.g., models and discussion in D’Onza et al.
37 2011).

38 Following the above brief summary, expanded in Sec. 2, the behaviour of the two structural
39 levels will be in this work considered as separate, linked by a suitable coupling function to

1 obtained the global response. Such an approach is schematized in Fig. 1. The four partial
 2 constitutive models will be denoted as \mathbf{G}^M , \mathbf{G}^m , H^M and H^m (macrostructure and mi-
 3 crostructure mechanical and hydraulic models respectively). The hydromechanical coupling
 4 mechanisms for microstructure and macrostructure are denoted as $\mathbf{G}^M H^M$ and $\mathbf{G}^m H^m$ re-
 spectively.

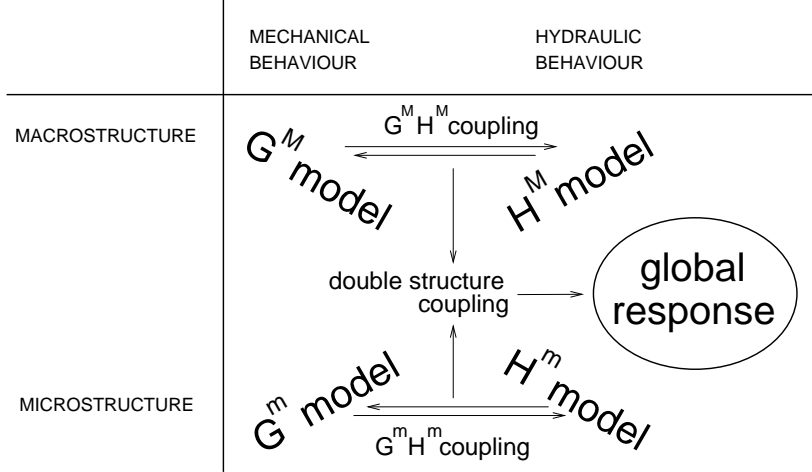


Figure 1: Schematic representation of the modelling approach adopted in this paper.

5

6 Existing constitutive models for double structure soils can be divided into two main groups.
 7 Models from the first group do not consider independent behaviour of macrostructure and
 8 microstructure, they are defined using global quantities. Sun and Sun (2011) developed such
 9 a model for expansive soils, considering full hydromechanical coupling. Cui et al. (2002)
 10 (realistically) assumed that the role of macroporosity in swelling of soils with dense structure
 11 may be neglected, and developed the global mechanical model based on the microstructural
 12 \mathbf{G}^m model. Similarly, Koliji et al. (2008) and Najser et al. (2012) described the behaviour
 13 of double porosity lumpy soils using a model based on the microstructural behaviour (\mathbf{G}^m),
 14 with phenomenological incorporation of the influence of macrostructure.

15 The primary idea of this paper is to use separate formulations for the behaviour of macrostruc-
 16 ture and microstructure. This approach is regarded as advantageous, as it is not necessary to
 17 search for a new and often intricate global constitutive model, and it is possible to use existing
 18 and well-evaluated models for each structural level. Success of the existing models considering
 19 double structure coupling supports this assumption. Soil mechanical behaviour has in this
 20 way been described by models by Gens and Alonso (1992), Alonso et al. (1999), Yang et al.
 21 (1998), Sánchez et al. (2005) and Thomas and Cleall (1999). Soil hydraulic behaviour by the
 22 model by Romero et al. (2011). Alonso et al. (2011) presented an advanced double structure
 23 based model considering all four \mathbf{G}^M , \mathbf{G}^m , H^M and H^m components. However, their model
 24 neglected the dependency of water retention behaviour on volumetric deformation ($\mathbf{G}^M H^M$
 25 and $\mathbf{G}^m H^m$ couplings are thus not fully accounted for). Similar advanced model is attributed
 26 to Gens et al. (2011). Della Vecchia et al. (2011) developed a fully coupled hydro-mechanical

1 model for double structure soils as an extension of the model by Romero et al. (2011). It
2 considered all the above mentioned coupling mechanisms, different in details when compared
3 to the present contribution.

4 One of the main means of hydromechanical coupling at each of the two structural levels
5 is the definition of the effective stress (often linked to hydraulic quantities). All the above
6 models use the effective stress defined in terms of global quantities. Thus, \mathbf{G}^M and \mathbf{G}^m
7 cannot be considered as fully independent. This drawback can be eliminated by adopting
8 an approach by Alonso et al. (2010), who suggested to attribute the main features (such as
9 shear strength) of the double structure soil behaviour to the behaviour of macrostructure,
10 and analyse it using effective stress measure independent of the microstructural quantities.
11 Such an approach will be used throughout this work, for each structural level. Different
12 approach has been suggested by Khalili et al. (2005) and Bagherieh et al. (2009). Based
13 on the microstructural interpretation, they developed a formulation for the *global* effective
14 stress within double porous medium. It may then be used within global constitutive equation,
15 where independent consideration of the two structural levels is no-more needed. The double
16 structure coupling mechanism has thus in their work been moved from the "external" double
17 structure coupling function into the effective stress equation.

18 The structure of this paper is as follows. After summary of the behaviour of compacted
19 expansive soils, a formal formulation of the double structure hydromechanical model based
20 on fully independent models for the two structural levels is developed. In the next part of
21 the paper, specific components of the proposed general model are selected so that they lead
22 to a concise fully coupled model for expansive clays. The model is then evaluated using
23 comprehensive experimental data on unsaturated compacted Boom clay by Romero (1999).

24 *Notation and conventions:* Compact tensorial notation is used throughout. Second-order
25 tensors are denoted with bold letters (e.g. $\boldsymbol{\sigma}$, \mathbf{N}) and fourth-order tensors with calligraphic
26 bold letters (e.g. $\boldsymbol{\mathcal{L}}$, $\boldsymbol{\mathcal{A}}$). Symbols "." and ":" between tensors of various orders denote
27 inner product with single and double contraction, respectively. The dyadic product of two
28 tensors is indicated by " \otimes ", and $\|\dot{\boldsymbol{\epsilon}}\|$ represents the Euclidean norm of $\dot{\boldsymbol{\epsilon}}$. The trace operator
29 is defined as $\text{tr } \dot{\boldsymbol{\epsilon}} = \mathbf{1} : \dot{\boldsymbol{\epsilon}}$; $\mathbf{1}$ and $\boldsymbol{\mathcal{I}}$ denote second-order and fourth-order unity tensors,
30 respectively. Following the sign convention of continuum mechanics, compression is taken
31 as negative. However, Roscoe's variables $p = -\text{tr } \boldsymbol{\sigma}/3$ and $\epsilon_v = -\text{tr } \boldsymbol{\epsilon}$, and pore fluid and
32 gas pressures u_w and u_a are defined to be positive in compression. The operator $\langle x \rangle$ denotes
33 the positive part of any scalar function x , thus $\langle x \rangle = (x + |x|)/2$. The effective stress is
34 denoted as $\boldsymbol{\sigma}$, net stress $\boldsymbol{\sigma}^{net} = \boldsymbol{\sigma}^{tot} + u_a$, where $\boldsymbol{\sigma}^{tot}$ is total stress. Matric suction is defined
35 as $s = u_a - u_w$. Macrostructural quantities are denoted by superscript M , microstructural
36 quantities by superscript m .

2 Double structure of expansive soils and its evolution with mechanical and hydraulic loading

It has now been well understood that the soil compacted dry of optimum has a structure with two distinct pore systems. The role of aggregated structure in constitutive modelling of the mechanical behaviour of unsaturated expansive soils has been recognised since the pioneering conceptual model by Gens and Alonso (1992), and later developed mathematical formalism by Alonso et al. (1999) (so-called BExM model). According to their approach, the behaviour of two structural levels may be considered separate, linked by coupling functions. Under the assumption of full saturation of the aggregates, they postulated that the deformation of the aggregates is purely volumetric and reversible, governed by the saturated effective mean stress $p = p^{net} + s$. The deformation of the macrostructure is governed by an existing model for unsaturated soils with low plasticity. Coupling between the two structural levels depends on the size of macropores (interaggregate pores). In soils with open macrostructure, aggregates during swelling invade the macropores, leading to the accumulated compression during cyclic changes of suction. Contrary, in soils with the initially closed macrostructure, macroporosity develops as a result of drying with less macropore invasion during wetting, leading to an accumulated expansion. In their development, Alonso et al. (1999) considered hydraulic and mechanical equilibrium between both levels of structure (both are subject to the same net stress and suction).

The different assumptions adopted in the above models have been subject of a detailed evaluation in a number subsequent studies. Microstructure evolution can be studied directly or indirectly. Among the direct methods, the most popular are mercury intrusion porosimetry (MIP) and environmental scanning electron microscopy (ESEM) (for complete review see Romero and Simms 2008). Indirect methods evaluate fabric evolution through measurement of the soil mechanical and water retention properties. A typical MIP result showing the development of microstructure with wetting is in Fig. 2a, with pore size density functions of a statically dry-of-optimum compacted London clay (Monroy et al. 2010). With decreasing suction, the microporosity increases, implying swelling of aggregates. The macroporosity, however, remains largely untouched, so the penetration of the aggregates into macropores is insignificant in this case. Only in the last step (wetting from suction 40 kPa to 0 kPa) the porosity becomes mono-modal, and the aggregated structure is not clear any more. Similar results were obtained by Lloret and Villar (2007), who reported also occlusion of macropores due to aggregate swelling. Romero et al. (2011) and Simms and Yanful (2001) observed that although the porosity is mono-modal upon saturation, the bi-modal porosity is recovered by subsequent drying. This process has been traced by Cuisinier and Laloui (2004) by testing compacted sandy loam along drying path (Fig. 2b). After re-establishment of the bi-modal pore size distribution, further drying caused reduction of macroporosity, with little influence on the microporosity (in fact, micropore volume slightly increased, as a result of closure of macrovoids which then added up to the microporosity). This has been confirmed by Romero et al. (2011), who dried the compacted Boom clay after saturation to very high suction (100 MPa). While the microporosity recovered to its original state, macroporosity was largely reduced.

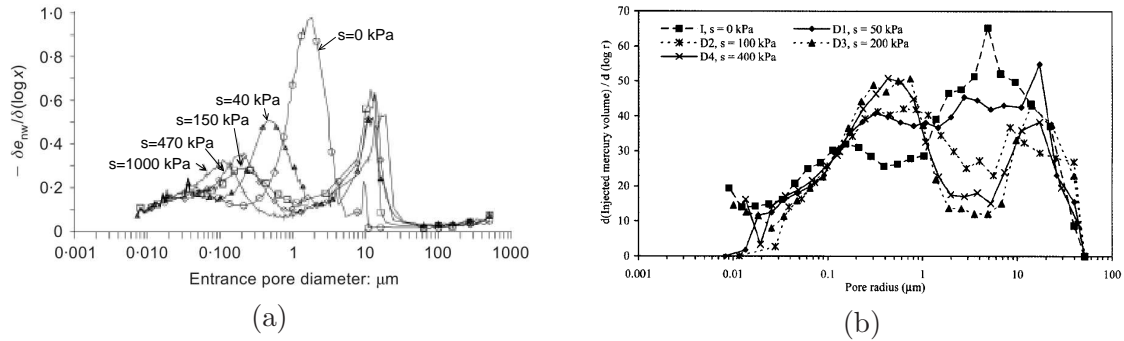


Figure 2: (a) Development of microstructure of compacted London clay with wetting (Monroy et al. 2010, modified). (b) Microstructural changes of a compacted sandy loam during drying (Cuisinier and Laloui 2004).

1 Loading under constant suction or constant water content was studied by Sivakumar et al.
 2 (2006), Miao et al. (2007), Thom et al. (2007), Lloret and Villar (2007), Simms and Yanful
 3 (2001), Alonso et al. (2011), Romero et al. (2011), Romero and Simms (2008) and Cuisinier
 4 and Laloui (2004). They all reported that loading (compaction) influenced predominantly the
 5 macrovoids, which closed up with increasing load. Microporosity remained either untouched
 6 (Fig. 3a), or it slightly increased with increasing compaction effort (Fig. 3b). A possible
 7 interpretation is that upon high stress compaction a proportion of macrovoids closed up and
 8 thus added up to microporosity. Note that this result does not imply the aggregates to be
 9 undeformable with load. Rather, it implies that the aggregate deformation is reversible, as
 10 the porosity of the samples compacted to different stresses is measured on samples removed
 11 from the testing apparatuses, and thus on unloaded samples. Reversibility (though hysteretic)
 12 of the aggregate deformation subject to suction variation this time has also been confirmed
 13 by Romero and Simms (2008), who extracted the microscale volume change from the overall
 14 volume change by digital image analysis of ESEM micrographs.

15 Microstructural changes reported above are manifested in the soil response to hydromechanical
 16 loading. The aggregates swell upon wetting, but the overall soil volumetric behaviour
 17 depends on the amount of occlusion of macropores by aggregates and on the stability of the
 18 macrostructure. It, in turn, depends on the level of relative opening of the soil macrostruc-
 19 ture (which increases with increasing void ratio and with increasing stress). Consequently,
 20 some authors report accumulated soil expansion with cyclic suction variation (for example,
 21 Gens and Alonso 1992, Romero and Simms 2008, Romero 1999) and some authors report
 22 accumulated compaction (e.g., Airò Farulla et al. 2010, Airò Farulla et al. 2007, Romero
 23 1999). The magnitude of swelling/compaction depends on the stress level and void ratio
 24 (Airò Farulla et al. 2007, Romero 1999, Alonso et al. 1995, Taibi et al. 2011, Villar 1999). It
 25 is also important to recognise that the magnitude of swelling depends, from the quantitative
 26 point of view, not only on the level of occlusion of macropores by aggregates, but also on
 27 the stress level dependency of swelling of individual aggregates. This issue requires consid-
 28 erable attention, as important portion of the overall aggregate volume change is related to
 29 the physico-chemical phenomena at the particle-scale level (osmotic swelling and crystalline

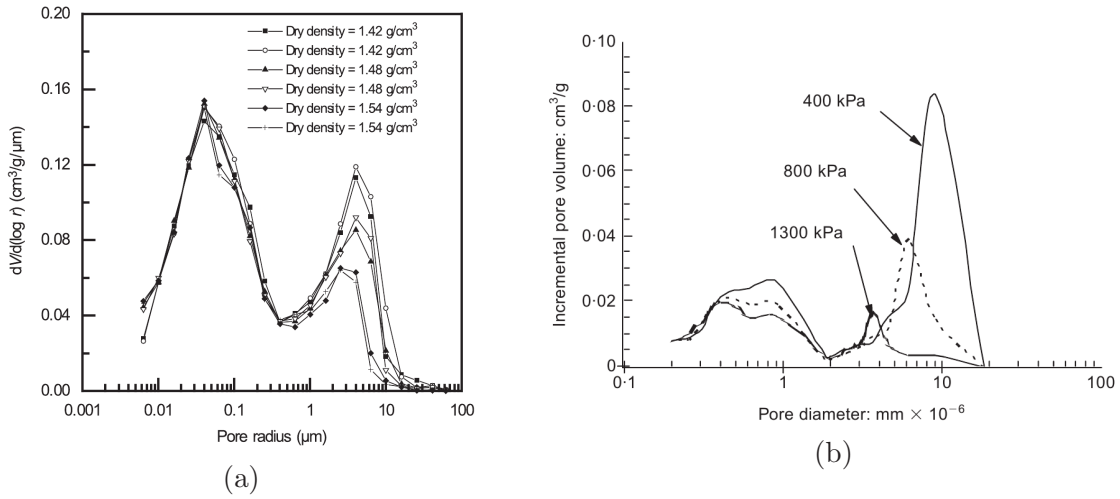


Figure 3: (a) Pore size density of compacted Guangxi expansive soil at various dry densities (Miao et al. 2007). (b) Microstructure of compacted kaolin after static compaction to different static pressures (Sivakumar et al., 2006).

1 swelling). This issue is discussed in more detail by (Mašín and Khalili 2012).

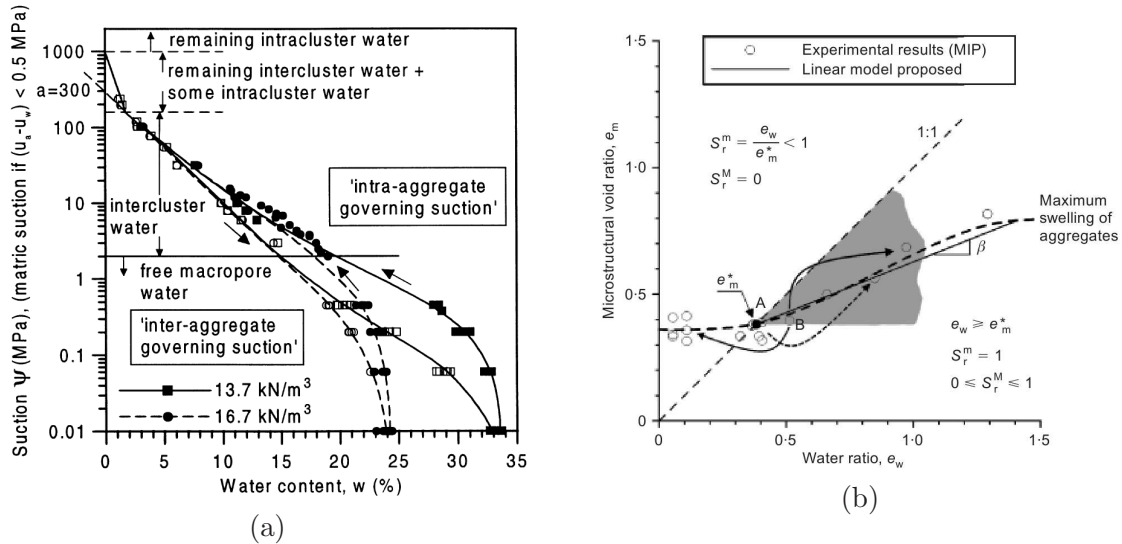


Figure 4: (a) Main wetting and drying water retention curves of Boom clay compacted to different densities (Romero et al. 1999). (b) Microstructural interpretation of the water retention behaviour of double structure soils by Romero et al. (2011).

2 Double structure of compacted soils is also evinced in their water retention behaviour, as put
 3 forward by Romero (1999) and Romero et al. (1999) and recently combined into a unified
 4 modelling framework by Romero et al. (2011). Fig. 4a shows water retention curves of a
 5 Boom clay compacted to two different initial densities. Clearly, water retention curves are

1 independent of density in the high suction range. In this case, the water is retained inside
2 the clay aggregates (macroporosity is dry). The results are thus consistent with the MIP
3 results presented above (recall that the size of micropores was found to be independent of
4 the compaction load). In the lower suction range, micropores are (thanks to smaller pore
5 size and thus higher air entry value of suction) saturated, and the water retention behaviour
6 is governed by the partially saturated macrostructure. As the water retention behaviour is,
7 in general, dependent on porosity (Sun et al. 2008, Sun et al. 2007, Gallipoli et al. 2003,
8 Nuth and Laloui 2008, Mašín 2010), so are the lower suction portions of water retention
9 curves of double structure soils. Similar experimental results were obtained by Airò Farulla
10 et al. (2011), who tested compacted scaly clay from Sicily. Conceptual interpretation of
11 this behavior by Romero et al. (2011) is in Fig. 4b in terms of microstructural void ratio
12 e^m (micropores volume over solid volume) vs. water ratio e_w (volume of water over solid
13 volume). For e_w higher than a threshold value e_m^* (at the suction s_m^*) representing fully
14 saturated micropores and dry macropores, the e^m changes with e_w along a line with slope
15 β . $\beta = 0$ implies no aggregate swelling, whereas $\beta = 1$ implies maximum swelling in which
16 aggregates fully occlude the macroporosity. β is for the given pore-fluid composition in the
17 model considered as a soil-specific parameter.

18 3 Formalism for double structure coupling

19 3.1 Coupling of micro and macrostructural strain measures

20 In the case of no occlusion of macropores by the swelling aggregates, the following additive
21 equation for the total strain rate $\dot{\epsilon}$ holds true:

$$\dot{\epsilon} = \dot{\epsilon}^M + \dot{\epsilon}^m \quad (1)$$

22 Here $\dot{\epsilon}^m$ describes the deformation of the aggregates and $\dot{\epsilon}^M$ measures the deformation of
23 the macroskeleton. The three strain rates are coupled with rates of corresponding porosity
24 measures, namely with the rates of total void ratio (\dot{e}), microvoid ratio (\dot{e}^m) and macrovoid
25 ratio (\dot{e}^M) through

$$\frac{\dot{e}}{1+e} = \text{tr } \dot{\epsilon} \quad (\text{a}) \quad \frac{\dot{e}^M}{1+e^M} = \text{tr } \dot{\epsilon}^M \quad (\text{b}) \quad \frac{\dot{e}^m}{1+e^m} = \text{tr } \dot{\epsilon}^m \quad (\text{c}) \quad (2)$$

26 Khalili et al. (2010) demonstrated that the volume change of individual grains in soil skeleton
27 imply no change of the skeletal void ratio (pore volume over solid volume), provided the
28 skeleton configuration remains unchanged. It follows that, due to the grain swelling, the pore
29 volume increases in the same fraction as solid volume to keep the void ratio constant. To
30 be consistent with this observation, microvoid ratio e^m is defined as the ratio of micropore
31 volume (V_p^m) over total solid volume (V_s), macrovoid ratio e^M is defined as the ratio of
32 macropore volume (V_p^M) over the total volume of aggregates (V_A) and the total void ratio is
33 $e = (V_p^m + V_p^M)/V_s$, as normal. Note that the usually adopted definition of $e^M = V_p^M/V_s$
34 (Gens et al. 2011, Sánchez et al. 2005), implying $e = e^M + e^m$, is not consistent with the

1 above comment, as it leads to a nil change of V_p^M with the change of V_p^m . The definition of
 2 the porosity measures adopted in this work imply

$$e = e^M + e^m + e^M e^m \quad (3)$$

3 Water volume fractions of the two pore systems will be, consistently with the definition of void
 4 ratios, described by the total degree of saturation S_r (water volume V_w over V_p), microscopic
 5 degree of saturation S_r^m (water volume in micropores V_w^m over V_p^m) and macroscopic degree
 6 of saturation S_r^M (water volume in macropores V_w^M over V_p^M). The following relation then
 7 holds true

$$S_r = S_r^M + \frac{e^m}{e}(S_r^m - S_r^M) \quad (4)$$

8 Note that the adopted definition of S_r^M is equal to the "effective degree of saturation" S_r^e by
 9 Alonso et al. (2010).

10 So far, the deformation of macroskeleton and the deformation of aggregates were both fully
 11 contributing to the overall deformation. To include the possibility for the aggregates to
 12 occlude into the macropores, Eq. (1) is modified to

$$\dot{\epsilon} = \dot{\epsilon}^M + f_m \dot{\epsilon}^m \quad (5)$$

13 where the factor $0 \leq f_m \leq 1$ quantifies the level of occlusion of macroporosity by aggregates.
 14 When $f_m = 1$, pure swelling or shrinking of aggregates implies the same global swelling or
 15 shrinking of the soil sample ($\dot{\epsilon} = \dot{\epsilon}^m$), with no change of macrovoid ratio and no skeletal rear-
 16 rangement ($\dot{\epsilon}^M = \mathbf{0}$). Contrary, $f_m = 0$ means that the aggregates freely penetrate or recede
 17 from the macropores while implying no global sample deformation ($\dot{\epsilon} = \dot{\epsilon}^M$ independently of
 18 $\dot{\epsilon}^m$). With Eq. (5), Eqs. (2a) and (2c) are still valid, but not the Eq. (2b). Microstructure
 19 (aggregate) can penetrate macropores, and thus influence e^M . An updated form of Eq. (2b)
 20 reads

$$\frac{\dot{\epsilon}^M}{1 + e^M} = \text{tr} [\dot{\epsilon}^M + (f_m - 1)\dot{\epsilon}^m] \quad (6)$$

21 It is the macroskeletal strain rate $\dot{\epsilon}^M = \dot{\epsilon} - f_m \dot{\epsilon}^m$ which is to be controlled by the constitutive
 22 model for macrostructure, $\dot{\epsilon}^m$ by the model for microstructure, and the factor f_m which
 23 quantifies the double-structural coupling.

24 3.2 Effective stress measures and constitutive relationships

25 As indicated in Sec. 1, the behaviour of the two structural levels will in this paper be
 26 considered separate (including the effective stress measures), and linked through relations
 27 from Sec. 3.1. The mechanical constitutive equations for the two structural levels then read,
 28 under full generality,

$$\dot{\sigma}^M = \mathbf{G}^M(\sigma^M, \mathbf{q}^M, \dot{\epsilon}^M) \quad (7)$$

$$\dot{\sigma}^m = \mathbf{G}^m(\sigma^m, \mathbf{q}^m, \dot{\epsilon}^m) \quad (8)$$

1 \mathbf{G}^M stands for a constitutive model for macroskeleton, \mathbf{G}^m for a constitutive model for
2 microstructure and $\boldsymbol{\sigma}^M$ and $\boldsymbol{\sigma}^m$ are two corresponding effective stress measures. \mathbf{q}^M and \mathbf{q}^m
3 are vectors of state variables, which typically include suction. The general expression for the
4 effective stress for unsaturated *single porosity* media is due to Bishop (1959):

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{net} - \mathbf{1}s\chi \quad (9)$$

5 with χ being the effective stress parameter. As the two structural levels are considered
6 separately, each of them may be considered as ordinary unsaturated single porosity medium.
7 For each of the structural levels we may thus write

$$\boldsymbol{\sigma}^M = \boldsymbol{\sigma}^{netM} - \mathbf{1}s^M\chi^M \quad (10)$$

$$\boldsymbol{\sigma}^m = \boldsymbol{\sigma}^{netm} - \mathbf{1}s^m\chi^m \quad (11)$$

8 A complete hydromechanical model for unsaturated soils requires also specification of a con-
9 stitutive relationship for soil hydraulic behaviour (water retention model). In this case, the
10 stress measure is represented by the value of suction. The corresponding strain-like quantities
11 are the macrostructural and microstructural degrees of saturation respectively (S_r^M and S_r^m).
12 The hydraulic constitutive relationships may be written as

$$\dot{S}_r^M = H^M(\dot{s}^M, s^M, \dot{\boldsymbol{\epsilon}}^M) \quad (12)$$

$$\dot{S}_r^m = H^m(\dot{s}^m, s^m, \dot{\boldsymbol{\epsilon}}^m) \quad (13)$$

13 with H^M and H^m being the water retention models for macrostructure and microstructure
14 respectively. Note the coupling between the hydraulic and mechanical parts. The hydraulic
15 models H^M and H^m depend on the mechanical strain measures $\dot{\boldsymbol{\epsilon}}^M$ and $\dot{\boldsymbol{\epsilon}}^m$. The mechanical
16 models \mathbf{G}^M and \mathbf{G}^m may depend on the hydraulic strain measures S_r^M and S_r^m through the
17 definition of the effective stress parameters χ^M and χ^m .

18 4 Model for expansive clays

19 Using formal model definition from Sec. 3, a complete hydromechanical model for double
20 structure medium requires specification of the effective stress measures $\boldsymbol{\sigma}^M$ and $\boldsymbol{\sigma}^m$, consti-
21 tutive relationships \mathbf{G}^M , \mathbf{G}^m , H^M and H^m , and the coupling function f_m . These will in
22 this section be developed for the specific case of compacted expansive soils. The equations
23 are limited to the ones needed for explanation of the proposed approach. A complete model
24 formulation is described in Appendix.

25 4.1 Macrostructural effective stress $\boldsymbol{\sigma}^M$ and the water retention model for 26 macrostructure H^M

27 The soils of the interest in this work, described in Sec. 2, have maximum aggregate sizes of
28 the order of tens of micrometers (see Figs. 2 and 3). For such a material, it is reasonable to

1 assume local hydraulic equilibrium between macro- and microstructure (Alonso et al. 1999),
 2 i.e. $s^m = s^M$. In addition, it is assumed that $\sigma^{netM} = \sigma^{netm}$. This equality is strictly valid
 3 only if the cross-sectional area of the aggregates is comparable to the cross-sectional area of
 4 the whole sample. Then,

$$\sigma^M = \sigma^{net} - \mathbf{1}s\chi^M \quad (14)$$

$$\sigma^m = \sigma^{net} - \mathbf{1}s\chi^m \quad (15)$$

5 It is recognised that this assumption is not valid for materials with bigger aggregate size,
 6 such as pellet material studied by Gens et al. (2011) and Alonso et al. (2011) or fissured
 7 material considered by Khalili et al. (2005).

8 For single porosity granular materials (sand, silt) and for aggregated materials with low to
 9 medium plasticity, the aggregates (respectively particles for single porosity media) are not
 10 substantially deformable when subject to stress and suction variation. The overall deforma-
 11 tion of the soil skeleton is then governed by the deformation of macrostructure, i.e. $\dot{\epsilon} = \dot{\epsilon}^M$,
 12 $\dot{\sigma} = \dot{\sigma}^M$ and

$$\chi = \chi^M \quad (16)$$

13 Shear strength and compressibility of such soils has been studied by Khalili and Khabbaz
 14 (1998) and Khalili et al. (2004). They searched for such a formulation of χ which permitted
 15 to represent the rebound volumetric behaviour and shear strength in a unique effective stress
 16 space. They reached the following expression for the χ parameter:

$$\chi = \begin{cases} 1 & \text{for } s < s_e \\ \left(\frac{s_e}{s}\right)^\gamma & \text{for } s \geq s_e \end{cases} \quad (17)$$

17 in which s_e is a suction at air-entry or air-expulsion, depending whether drying or wetting
 18 process is considered respectively. γ is a soil parameter, which was found to be for a broad
 19 range of soils close to a unique value of $\gamma = 0.55$. In light of the above explanation, Eq. (17)
 20 may well be considered to represent the value of χ^M .

21 A similar approach as Khalili and Khabbaz (1998) and Khalili et al. (2004) has been adopted
 22 by Alonso et al. (2010). They suggested that the parameter χ is related only to the free water
 23 partially filling the macropores, and that immobile pore fluid within aggregates does not affect
 24 the macrostructural effective stress. Following thermodynamically consistent definition of the
 25 parameter $\chi = S_r$ derived using different approaches for single porosity medium (Coussy 2007,
 26 Houlsby 1997, Laloui et al. 2003, Lewis and Schrefler 1987, Hutter et al. 1999), Alonso et al.
 27 (2010) suggested equality¹

$$\chi = S_r^M \quad (18)$$

28 They then demonstrated by studying critical shear strength and compressibility of different
 29 soils with aggregated structure that Eq. (18) successfully normalised the experimental data
 30 with respect to suction contribution.

¹Note that the definition of S_r^M in this work equals to the "effective degree of saturation" S_r^e by Alonso et al. (2010)

1 Combination of Eqs. (16), (17) and (18) yields a Brooks and Corey (1964) type water
 2 retention model for macrostructure

$$S_r^M = \chi^M = \begin{cases} 1 & \text{for } s < s_e \\ \left(\frac{s_e}{s}\right)^\gamma & \text{for } s \geq s_e \end{cases} \quad (19)$$

3 In light of this interpretation, the Khalili and Khabbaz (1998) parameter γ represents a slope
 4 of the macrostructural water retention curve (WRC) in the $\ln S_r^M$ vs. $\ln s$ plane. In granular
 5 soils, WRC depends primarily on the soil grain size distribution (Fredlund et al. 2002).
 6 Then, somewhat peculiar uniqueness of the parameter γ may be implied by the fact that the
 7 shape of the aggregate-size-distribution of different compacted soils is actually similar. As a
 8 reference, see Figs. 2 and 3. They show pore-size distribution of double structure soil, which
 9 gives an indirect indication of the aggregate size distribution.

10 To account for the effects of hydraulic hysteresis, the macrostructural water retention model
 11 from Eq. (19) is enhanced as shown in Fig. 5. s_{en} is the air entry value during drying process
 12 and a_e is a model parameter representing ratio of the wetting branch air-expulsion value of
 13 suction s_{exp} and drying branch air-entry value of suction s_{en} . γ is the slope of WRC. It is here
 14 considered as a material-independent constant $\gamma = 0.55$ to simplify the model calibration
 15 procedure, but for the sake of generality it may be considered as a material parameter if
 16 needed. The slope of the macrostructure hydraulic scanning curve was deliberately selected
 17 as $\gamma/10$. Note that the interpretation of χ^M using Fig. 5 will be less accurate for hydraulic
 reversal paths, as evidenced experimentally by Khalili and Zargarbashi (2010).

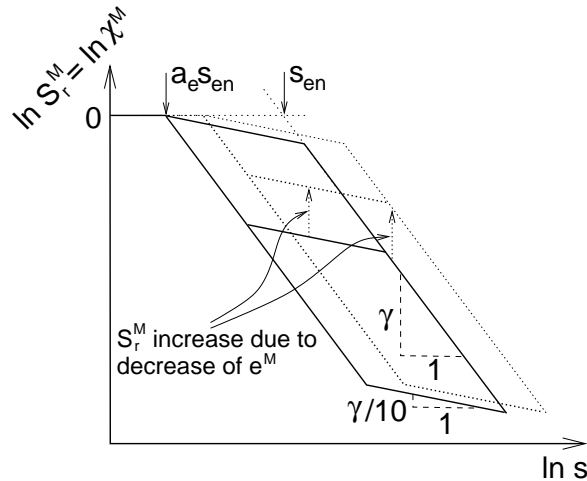


Figure 5: Water retention model for macrostructure.

18

19 Indeed, water retention curves are void ratio dependent (due to hydro-mechanical coupling),
 20 and this dependency must be considered in constitutive models to ensure accuracy of predic-
 21 tions (Sun et al. 2008, Sun et al. 2007, Gallipoli et al. 2003, Nuth and Laloui 2008, Mařín
 22 2010, Wheeler et al. 2003). Mařín (2010) derived a water retention model, in which the void
 23 ratio dependency of WRC is implied by the adopted form of the effective stress tensor. The

1 starting equation has originally been derived by Loret and Khalili (2000) from the assumption
 2 of existence of generalized elastic and plastic potentials. As detailed in Khalili et al. (2008),
 3 the existence of elastic potential $\Psi(\boldsymbol{\sigma}, u_a, u_w)$, quadratic in $\boldsymbol{\sigma}$, but a priori not in suction, the
 4 elastic strain components are related to the stress components so that they enjoy the major
 5 symmetry. Considering also the irreversible components of pore water and pore air volume
 6 changes (\dot{V}_w and \dot{V}_a), Khalili et al. (2008) finally derived

$$-\frac{\dot{V}_w}{V} = \psi \dot{\epsilon}_v - a_{11} \dot{u}_w - a_{12} \dot{u}_a \quad (20)$$

$$-\frac{\dot{V}_a}{V} = (1 - \psi) \dot{\epsilon}_v - a_{21} \dot{u}_w - a_{22} \dot{u}_a \quad (21)$$

7 with constitutive constants a_{ij} . Rearrangement of the above equations, considering definitions
 8 of S_r and e , yields (Khalili et al. 2008)

$$\frac{\partial S_r}{\partial e} = \frac{\psi - S_r}{e} \quad (22)$$

9 where ψ is the effective stress rate parameter given by $\psi = \partial(\chi s)/\partial s$. Mašín (2010) adopted
 10 the χ expression from Eq. (17) in his developments, and the water retention curve was
 11 characterised by a slope λ_p in the $\ln S_r$ vs. $\ln s$ plane. The derivations yielded a relatively
 12 complex semi-analytical expression relating the air entry (expulsion) value of suction s_e and
 13 the WRC slope λ_p to void ratio. The only special case, in which the expression simplified,
 14 was when $\lambda_p = \gamma$. Then, the slope λ_p was independent of void ratio and the air entry value
 15 could be calculated explicitly as $s_e = s_{e0} e_0 / e$, where s_{e0} represented the known value of
 16 the air entry suction at the reference void ratio e_0 . Unfortunately, as λ_p was always found
 17 substantially lower than γ (which meant $\chi \neq S_r$), the special case could not be used to
 18 simplify the calculations. λ_p in the above represented the slope of the WRC expressed in
 19 global terms (total degree of saturation S_r).

20 In the present case, however, the above discussed assumption $\chi^M = S_r^M$ implies that the
 21 WRC slope λ^{pM} in *macro-structural terms* (S_r^M) coincides with γ . When the derivations by
 22 Mašín (2010) are repeated in terms of macrostructural quantities, the following expression
 23 for the air entry value of suction is obtained

$$s_{en} = s_{e0} \frac{e_0^M}{e^M} \quad (23)$$

24 with $\lambda^{pM} = \gamma$ independent of void ratio and of the applied suction. In Eq. (23) e_0^M is
 25 arbitrary reference macrovoid ratio and s_{e0} is the corresponding air-entry value of suction².
 26 Apart from the parameter a_e (refer to Fig. 5), the adopted formulation for the macrostructure
 27 water retention curve does not require any other parameter. As sketched in Fig. 5, it
 28 is assumed (without direct experimental evidence) that the change of e^M for states at the
 29 hydraulic scanning curve imposes the same change of S_r^M as if the state was on the main
 30 wetting or drying branch of WRC. In other words, "mechanical" wetting (or drying), in the
 31 sense defined by Tarantino (2009), does not change the relative position of a hydraulic state
 32 with respect to the main wetting and drying branches of WRCs.

²Note that in the present developments the microstructure has been considered as saturated, thus the superscript M has been omitted above s_{en} and s_{e0}

1 4.2 Macrostructural mechanical constitutive model \mathbf{G}^M

2 The mechanical behaviour of macroskeleton is described using a hypoplastic model for un-
 3 saturated soils by Mašín and Khalili (2008). The model has also been adopted as a reference
 4 model by Mašín and Khalili (2011), who enhanced it by the effects of temperature. In combi-
 5 nation with the water retention model by Mašín (2010), the model was evaluated by D’Onza
 6 et al. (2011) in their benchmarking exercise on the performance of different hydromechanical
 7 models for unsaturated soils.

8 As other hypoplastic models, the model is based on a single incrementally non-linear (see
 9 Mašín et al. 2006) relationship relating the effective stress rate to rates of total strain rate
 10 and of suction. The model is based on the critical state soil mechanics (Gudehus and Mašín
 11 2009), and implicitly predicts state boundary surface (Mašín and Herle 2005), similarly to
 12 other common elasto-plastic constitutive models based on the Cam-clay framework (Roscoe
 13 and Burland 1968). Unlike these models, however, the model predicts irreversible behaviour
 14 inside the state boundary surface, which gives it an important advantage in terms of its
 15 predictive capabilities (see D’Onza et al. 2011, Mašín 2012).

16 In terms of macrostructural quantities, the rate formulation of the model reads

$$\dot{\boldsymbol{\sigma}}^M = f_s (\mathcal{L} : \dot{\boldsymbol{\epsilon}}^M + f_d \mathbf{N} \|\dot{\boldsymbol{\epsilon}}^M\|) + f_u \mathbf{H} \quad (24)$$

17 f_s , f_d and f_u are three scalar factors, \mathcal{L} is the fourth-order constitutive tensor and \mathbf{N} and
 18 \mathbf{H} are two second order constitutive tensors, all calculated in terms of $\boldsymbol{\sigma}^M$ in place of $\boldsymbol{\sigma}$
 19 when compared to the original formulations. For their definition, see Appendix and the cited
 20 publications. The objective effective stress rate $\dot{\boldsymbol{\sigma}}^M$ is calculated from (14) as

$$\dot{\boldsymbol{\sigma}}^M = \dot{\boldsymbol{\sigma}}^{net} - \mathbf{1} \left[\frac{\partial(\chi^M s)}{\partial s} \dot{s} + \frac{\partial(\chi^M s)}{\partial e^M} \dot{e}^M \right] \quad (25)$$

21 which can be for the present case expressed as

$$\dot{\boldsymbol{\sigma}}^M = \dot{\boldsymbol{\sigma}}^{net} + \mathbf{1} \chi^M \left[(\gamma_a - 1) \dot{s} + \gamma s \frac{\dot{e}^M}{e^M} \right] \quad (26)$$

22 where $\gamma_a = \gamma$ for the states on the main drying and wetting branches of macrostructural
 23 WRC, $\gamma_a = \gamma/10$ for the states at the macrostructural hydraulic scanning curve and $\gamma_a = 0$
 24 otherwise (for $s \leq s_{exp}$). \dot{e}^M is calculated by Eq. (6).

25 Apart from the parameters of the macrostructural water retention curve (Sec. 4.1), the
 26 mechanical model requires altogether eight parameters. Five of them are parameters of the
 27 underlying model for saturated soils (Mašín 2005) (namely, N , λ^* , κ^* , φ_c and r), and they
 28 correspond to the parameters of the Modified Cam clay model. They are summarised in Sec.
 29 4.6. Important parameters, which control the size of the state boundary surface, are N and
 30 λ^* . They represent position and slope of the isotropic normal compression line in the $\ln p^M$
 31 vs. $\ln(1 + e)$ plane, given by the expression due to Butterfield (1979). For a saturated soil,

$$\ln(1 + e) = N - \lambda^* \ln(p^M/p_r) \quad (27)$$

1 with reference stress $p_r = 1$ kPa. In the model for unsaturated soils, $N(s)$ and $\lambda^*(s)$ depend
 2 on the current value of suction through the parameters n and l :

$$N(s) = N + n \ln \left(\frac{s}{s_e} \right) \quad \lambda^*(s) = \lambda^* + l \ln \left(\frac{s}{s_e} \right) \quad (28)$$

3 where s_e is the value of the air entry/expulsion value of suction. This expression is adopted
 4 also in the proposed model. In order to keep consistency of the predictions with the hysteretic
 5 hydraulic model, however, the value of s_e is calculated from Eq. (19), leading to $s_e =$
 6 $s(S_r^M)^{(1/\gamma)}$. Note that the normal compression lines are still defined in terms of the global
 7 void ratio, as considering e^M in place of it would complicate the parameter calibration.
 8 For many soils, it is reasonable to assume, as a first approximation, the slopes of normal
 9 compression lines independent of suction, i.e. $l = 0$ (see Mašín and Khalili 2008 and Mašín
 10 and Khalili 2011).

11 The last parameter of the model m controls the influence of overconsolidation ratio (OCR) on
 12 magnitude of wetting-induced collapse. It is incorporated in the following way. In Eq. (24),
 13 the wetting-induced collapse is introduced by the tensor \mathbf{H} . It is multiplied by the factor f_u ,
 14 which reads

$$f_u = \left(\frac{f_d}{f_d^{SBS}} \right)^{m/\alpha} \quad (29)$$

15 where α is a function of material parameters (see Appendix, Eq. (54)), f_d is the current
 16 value of the pyknropy factor and f_d^{SBS} is its value at the state boundary surface. The
 17 factor f_d is in the model decreasing with increasing OCR, f_d^{SBS} thus represents maximum
 18 value of f_d for the current stress state. Eq. (29) therefore implies that f_u , and thus also
 19 the magnitude of wetting-induced collapse, decreases with increasing OCR. The rate of this
 20 decrease is controlled by m , in such a way that for $m = 0$ the collapse is always fully present
 21 independently of OCR, whereas for $m \rightarrow \infty$ the collapse occurs at the state boundary surface
 22 only.

23 4.3 Microstructural effective stress σ^m , mechanical constitutive model \mathbf{G}^m 24 and water retention model H^m

25 To preserve certain simplicity of the model formulation, the microstructure is, thanks to its
 26 high air-entry value of suction, considered to be fully saturated. The microstructural water
 27 retention model thus reads simply

$$S_r^m = 1 \quad (30)$$

28 and the proposed model is considered not to be accurate for suctions higher than the mi-
 29 crostructure air entry value of suction. The second assumption is that validity of the effective
 30 stress in the Terzaghi sense (see Sec. 2) is assumed. The microstructural effective stress is
 31 then governed through

$$\chi^m = S_r^m = 1 \quad (31)$$

32 this implies $\sigma^m = \sigma^{net} - \mathbf{1}s = \sigma^{tot} + \mathbf{1}u_w$, i.e. the Terzaghi saturated effective stress. The
 33 above two assumptions have recently been supported by Mašín and Khalili (2012).

1 As demonstrated in Sec. 2, and as supported by Mašín and Khalili (2012), it is reasonable
 2 to assume the microstructure behaviour to be reversible. In this work, a simple volumetric
 3 model has been adopted:

$$\dot{\boldsymbol{\sigma}}^m = \mathbf{1} \frac{p^m}{\kappa_m} \text{tr} \dot{\boldsymbol{\epsilon}}^m \quad (32)$$

4 This model yields linear response when represented in the $\ln p^m$ vs. $\ln(1 + e^m)$ plane, i.e.

$$\ln(1 + e^m) = C - \kappa_m \ln p^m \quad (33)$$

5 with a constant C . At the zero net mean stress, $p^m = s$ holds true. Reference microstructural
 6 void ratio e_r^m corresponding to an arbitrary reference value of suction s_r at zero net mean
 7 stress may be considered as material parameters, yielding explicit formulation for e^m :

$$e^m = \exp \left[\kappa_m \ln \frac{s_r}{p^m} + \ln(1 + e_r^m) \right] - 1 \quad (34)$$

8 With an advantage, e^m and s_r may be considered equal to the microstructural void ratio
 9 (e_m^*) and suction (s_m^*) corresponding to the fully saturated micropores and dry macropores
 10 by Romero et al. (2011), but any other reference value of suction and corresponding e^m may
 11 be used.

12 4.4 Coupling function f_m

13 The last component in the proposed modelling framework is the coupling function f_m linking
 14 the responses of macrostructure and microstructure. Recall that this factor quantifies the
 15 level of occlusion of macroporosity by aggregates. When $f_m = 1$, pure swelling or shrinking
 16 of aggregates implies the same global swelling or shrinking of the soil. Contrary, $f_m = 0$
 17 means that the aggregates freely penetrate or recede from the macropores while inducing no
 18 global sample deformation. As indicated in Sec. 2, the actual deformation mode depends on
 19 the level of compaction of macrostructure, which is measured by void ratio e . Minimum void
 20 ratio e_d corresponds to $e^M = 0$, i.e. $e_d = e^m$ (note that e^m varies with stress level, so also
 21 e_d is a variable). Maximum void ratio e_i corresponds to the state at the isotropic normal
 22 compression line. For the proposed model,

$$e_i = \exp [N(s) - \lambda^*(s) \ln p^M] - 1 \quad (35)$$

23 It is then convenient to define relative void ratio r_{em} as

$$r_{em} = \frac{e - e_d}{e_i - e_d} \quad (36)$$

24 For the densest possible state $r_{em} = 0$ and for the loosest possible state $r_{em} = 1$. Similar
 25 measure of the relative void ratio has been adopted by Gudehus (1996) and von Wolfersdorff
 26 (1996) in their hypoplastic models.

1 For aggregate swelling (wetting or unloading process) $f_m \rightarrow 1$ corresponds to a dense
 2 macrostructure (no macropore occlusion), whereas $f_m \rightarrow 0$ corresponds to a loose macrostruc-
 3 ture (full occlusion of macropores by swelling aggregates). The following relationship satis-
 4 fying these limiting properties has been adopted for $\dot{p}^m < 0$:

$$f_m = 1 - (r_{em})^{m_c} \quad (37)$$

5 where m_c is a model parameter controlling the influence of r_{em} on f_m for intermediate values
 6 of r_{em} . For particle shrinkage ($\dot{p}^m > 0$), $f_m = 0$ has always been assumed. In combination
 7 with the adopted macrostructural model (which predicts softer response in loading), higher
 8 values were found to lead to excessive global shrinkage.

9 The parameter m_c controls the influence of macrostructure compaction on the structural
 10 coupling. Similar influence, now on the structural collapse, has parameter m of the model for
 11 macrostructural behaviour. As the physical interpretation of the two parameters is similar,
 12 they are in the following assumed to take the same values ($m_c = m$). If needed, additional
 13 calibration freedom can be gained by their separate calibration.

14 4.5 Calculation of the model response in terms of global quantities $\dot{\epsilon}$ and 15 S_r

16 The constitutive models for the micro- and macrostructural levels enable to quantify the
 17 behaviour of each of the levels using properly selected existing constitutive models. However,
 18 the primary goal is to obtain the response in terms of global, directly measurable quantities.
 19 As for the mechanical models, the global strain rate is calculated from the macrostructural
 20 and microstructural strain rates using the set of equations (5), (7) and (8). To obtain the
 21 global water retention response, S_r is calculated from the known S_r^m and S_r^M and void ratios
 22 e^m and e using Eq. (4).

23 The solution of the system is for the proposed model straightforward for the known $\dot{\sigma}^{net}$ and
 24 \dot{s} (provided the solution is unique and exists). For the prescribed global strain rate $\dot{\epsilon}$ and
 25 suction rate \dot{s} the equations become implicit in $\dot{\sigma}^{net}$, however. Eq. (24) can be with the aid
 26 of (1) written as

$$\dot{\sigma}^M = f_s [\mathcal{L} : (\dot{\epsilon} - \dot{\epsilon}^m) + f_d \mathbf{N} \|\dot{\epsilon} - \dot{\epsilon}^m\|] + f_u \mathbf{H} \quad (38)$$

27 where (from (32))

$$\dot{\epsilon}^m = \mathbf{1} \kappa_m \frac{\dot{p}^m}{p^m} \quad (39)$$

28 and thus

$$\dot{\sigma}^M = f_s \left[\mathcal{L} : \left(\dot{\epsilon} - \mathbf{1} \kappa_m \frac{\dot{p}^m}{p^m} \right) + f_d \mathbf{N} \left\| \dot{\epsilon} - \mathbf{1} \kappa_m \frac{\dot{p}^m}{p^m} \right\| \right] + f_u \mathbf{H} \quad (40)$$

29 $\dot{\sigma}^{net}$ appears in both the expressions for $\dot{\sigma}^M$ and \dot{p}^m . Development of a robust and efficient
 30 numerical scheme to solve (40) is outside the scope of the present paper. For the sake of
 31 the present evaluation, the system was solved using a trial-and-error numerical procedure,
 32 in which the solution was approached by variation of the unknown \dot{p}^m . Such an approach is
 33 feasible as long as the microstructural behaviour is governed by a simple elastic volumetric
 34 model.

1 4.6 Summary of model parameters

2 In its simple form, the complete model for the expansive clays requires specification of 10
3 parameters:

- 4 • φ_c : Critical state friction angle.
- 5 • λ^* : Slope of normal compression lines (isotropic/oedometric/critical state line) of a
6 saturated soil in the $\ln p^M/p_r$ vs $\ln(1 + e)$ plane.
- 7 • N : Position of the isotropic normal compression line, i.e. the value of $\ln(1 + e)$ for
8 $p^M = p_r = 1$ kPa.
- 9 • κ^* : Slope of the *macrostructural* isotropic unloading line.
- 10 • r : Parameter controlling stiffness in shear.
- 11 • n : Parameter controlling the dependency of the position of the isotropic normal com-
12 pression line on suction.
- 13 • m : Controls the dependency of wetting-induced collapse on the overconsolidation ratio
14 and the macropore occlusion by microporosity on relative void ratio.
- 15 • κ_m : Specifies the dependency of microstructural swelling/shrinkage on the microstruc-
16 tural effective stress (i.e. saturated effective stress).
- 17 • s_{e0} : The air entry value of suction for the (arbitrary) reference macrostructural void
18 ratio e_0^M .
- 19 • a_e : The ratio between the air expulsion and entry values of suction (controls the differ-
20 ence between the wetting and drying branches of water retention curves).

21 In addition, it is necessary to specify the initial values of the following state variables:

- 22 • e : global void ratio.
- 23 • e^m : microstructural void ratio. It may be advantageous to specify the initial value of
24 e^m by means of Eq. (34), thus specify the value of e_r^m for the (arbitrary) reference value
25 of suction s_r . A possible approach to initiation of e^m follows Romero et al. (2011).
26 e_r^m is then equal to the water ratio e_w (and s_r is the corresponding suction) at which
27 the macrostructure becomes dry in the drying test. At this value of suction, water
28 retention curves for different global void ratios merge into a single curve (see Fig. 4
29 and the associated discussion). In the absence of relevant data, e^m should be calibrated
30 using a trial-and-error procedure.
- 31 • S_r^M : The value of S_r^M is implied by the adopted water retention model for microstruc-
32 ture, but it is necessary to specify whether the current state belongs to the main drying
33 branch of macrostructural WRC, main wetting branch or to the macrostructural scan-
34 ning curve.

1 It is interesting to point out that, regardless the low number of material parameters, the model
 2 has advanced capabilities in predicting non-linear soil behaviour in compression and in shear,
 3 incorporates hysteretic water retention model coupled with the mechanical response, and
 4 predicts the inter-related behaviour of two structural levels. For comparison, the equivalent
 5 macrostructural model formed by a combination of the mechanical model by Mašín and
 6 Khalili (2008) and the water retention model by Mašín (2010) requires only one parameter
 7 less, but does not consider hysteretic water retention behaviour and double structure coupling.
 8 The pioneering and still popular model for expansive soils BExM by Alonso et al. (1999)
 9 requires 11 parameters and focuses on the mechanical response only.

10 5 Evaluation of the model

11 The model is evaluated using comprehensive experimental data set on unsaturated compacted
 12 Boom clay by Romero (1999), presented also in Romero et al. (1999) and Romero et al.
 13 (2011). The laboratory tests were performed on artificially prepared (dry side statically
 14 compacted) powder obtained from natural Boom clay. The soil is moderately swelling clay,
 15 containing 20-30% of kaolinite, 20-30% of illite and 10-20% of smectite. The liquid limit
 16 $w_L = 56\%$, plastic limit $w_P = 29\%$ and the amount of particles $< 2\mu\text{m}$ is 50%. The testing
 17 program included two main soil packings of clay aggregates fabricated at a moulding water
 18 content of 15%: high porosity structure with collapsible tendency and low-porosity structure
 19 with swelling tendency (Romero et al. 1999).

20 To demonstrate the capabilities of the proposed approach, the predictions are compared with
 21 predictions by the existing (denoted as "original") model, which is formed by a combination
 22 of the mechanical model by Mašín and Khalili (2008) and the water retention model by
 23 Mašín (2010). Both the models were calibrated using the experimental data used also for
 24 the evaluation of the models, and all the predictions were obtained using a single parameter
 25 set with no further parameter manipulation. The data by Romero (1999) did not include
 26 the tests needed for calibration of parameters φ_c and r . They were calibrated using different
 27 data set on saturated Boom clay by Coop et al. (1995). The parameters are in Tabs. 1 and
 2.

Table 1: *Parameters of the proposed hypoplastic model for expansive soils for Boom clay. Default values $\gamma = 0.55$ and $l = 0$ adopted. e_m initialised using $e_r^m = 0.38$ for $s_r = 2400$ kPa (from Romero et al. 2011).*

φ_c	λ^*	κ^*	N	r	n	m	κ_m	$s_{e0} (e_0^M)$	a_e
27°	0.08	0.008	1.05	0.4	0.025	2	0.04	200 kPa (0.18)	0.25

28

Table 2: Parameters of the original hypoplastic model for Boom clay. Default values $\gamma = 0.55$ and $l = 0$ adopted.

φ_c	λ^*	κ^*	N	r	n	m	λ_p	$s_{e0} (e_0)$
27°	0.08	0.008	1.05	0.4	0.025	2	0.17	70 kPa (0.75)

1 5.1 Unconfined wetting-drying tests

2 First, cyclic isotropic wetting-drying free swell test for three initial relative void ratios (loose,
3 medium dense and dense soil) is simulated to demonstrate qualitative response of the model
4 to cyclic loading. The model predictions for different values of the parameter m and constant
5 value of $\kappa_m = 0.04$ are shown Fig. 6 in terms of the relative void ratio r_{em} . In all cases,
6 the initially dense soil would accumulate swelling deformation during cyclic loading, and the
7 initially loose soil would accumulate cyclic compaction. The model predicts the asymptotic
8 cyclic state independent of further cycles. For given κ_m , the asymptotic state does not depend
9 on the initial state, but on the value of the parameter m only.

10 The influence of the parameters m and κ_m on the asymptotic cyclic state is shown in Figs.
11 7a,b in terms of global void ratio. Although both the parameters influence the asymptotic
12 state, the principle of their influence is fundamentally different – m controls wetting-induced
13 collapsibility of macrostructure and macroporosity occlusion by aggregate swelling, whereas
14 κ_m influence wetting-induced swelling of microstructure. This is clearly seen in Figs. 7c,d,
15 where the results are plotted in terms of e^m and e^M .

16 It is interesting to point out that the asymptotic state in cyclic loading is predicted not only
17 for suction cycles, but also for stress cycles in constant suction tests, even (but not only) in a
18 saturated state. Fig. 8 shows the results of a saturated cyclic isotropic test on initially loose
19 soil for two different values of the parameter m . The proposed model predicts asymptotic
20 cyclic state, which depends on m . This strongly contrasts with predictions by the original
21 model (in fact, for the saturated case the basic hypoplastic model for clays by Mašín 2005),
22 which predicts continuous cyclic accumulation of compression. The proposed model thus does
23 not suffer from volumetric ratcheting, which is often regarded as one of the main drawbacks
24 of hypoplasticity³.

25 5.2 Constant volume wetting-drying tests

26 Fig. 9 demonstrates the difference between the water retention curves plotted in terms of
27 global quantity S_r and macrostructural quantity S_r^M . The figure shows results of confined
28 wetting-drying test with constant global void ratio e and variable net stress σ^{net} (for the
29 evolution of σ^{net} in these tests, see Fig. 12 presented later). One test has been performed
30 on a high porosity packing sample (denoted here as "loose sample" with $e = 0.932$), and

³Note that the model does not limit ratcheting in shear, due to the purely volumetric model for microstructure.

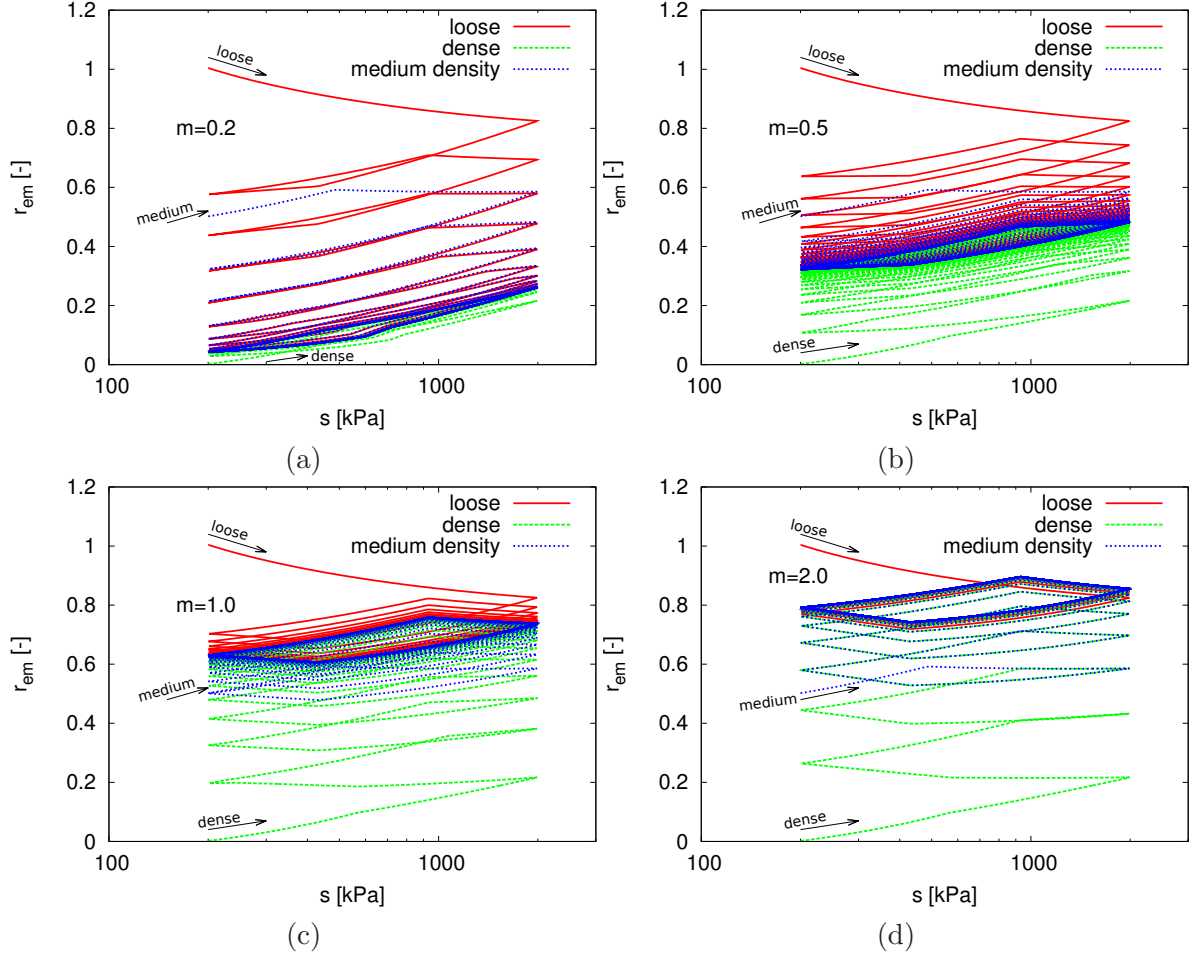


Figure 6: Response of the model to cyclic wetting-drying isotropic free swell test in terms of the relative void ratio r_{em} for different values of the parameter m .

- 1 one on a high density packing sample (denoted here as "dense sample" with $e = 0.65$).
- 2 Both water retention curves have in terms of S_r^M similar slopes (controlled by $\gamma = 0.55$ and
- 3 variation of e^M) and different air entry/expulsion values of suction (calculated by Eq. (23)).
- 4 In terms of global quantity S_r , both water retention curves have different slopes, implied by
- 5 the initial value of e_m and its variation with microstructural mean effective stress. The global
- 6 water retention curves, which are controlled by the double structure coupling features of the
- 7 model, agree well with the experimental data by Romero (1999), shown also in Fig. 9. Note
- 8 that the modelled drying branches of WRCs in Fig. 9 represent results of a single constant
- 9 volume wetting-drying experiments with the wetting branch terminated at $s=450$ kPa. This
- 10 value of suction was sufficiently low to ensure compressive net stresses and constant volume
- 11 conditions. The experimental data plotted in Fig. 9, on the other hand, are extrapolated
- 12 from different test series for the given dry density, they could thus be plotted also in the
- 13 higher suction range. For details of the extrapolation procedure, see Romero (1999).

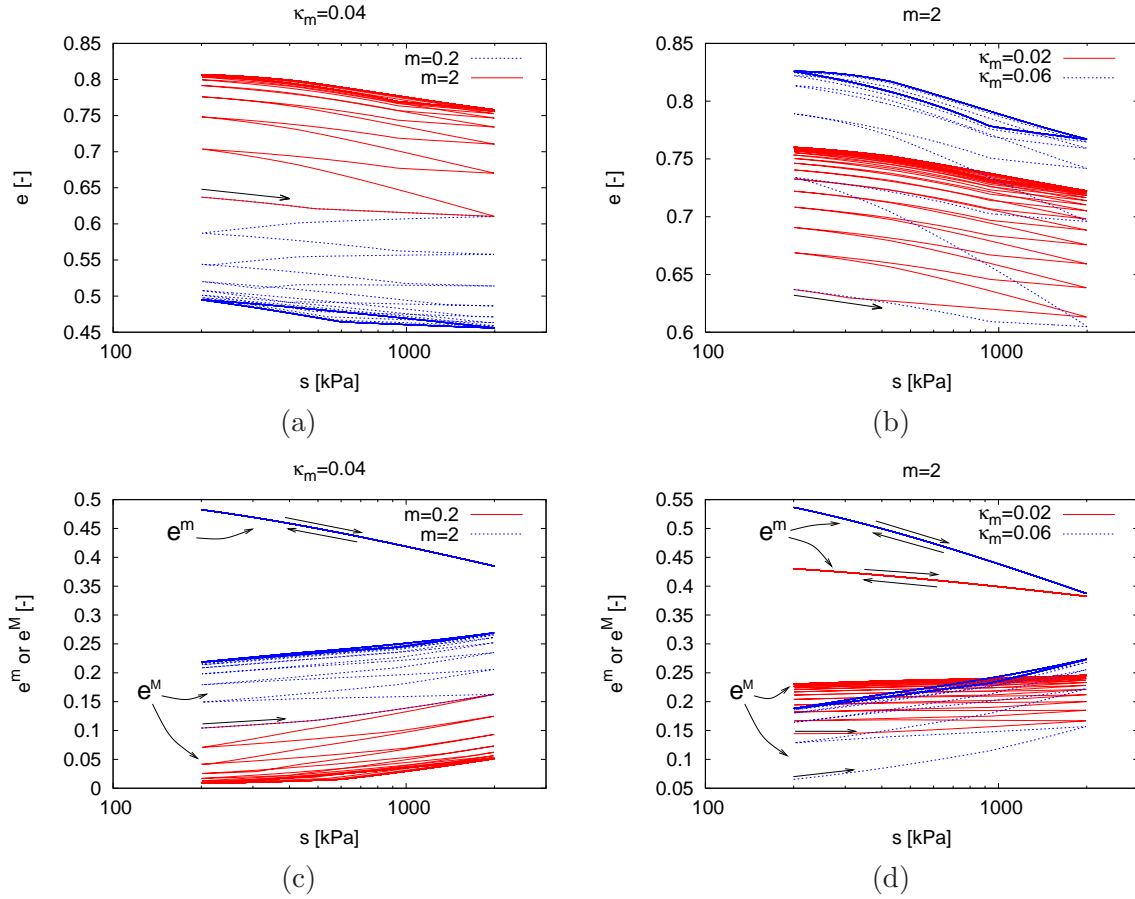


Figure 7: Response of the model to cyclic wetting-drying isotropic free swell test for medium dense soil and different values of parameter m (a,c) and κ_m (b,d). Results plotted in terms of global void ratio e (a,b) and e^m and e^M (c,d).

1 At this point, it is interesting to compare prediction of the proposed model with predictions
2 by the original water retention model (Mašín 2010). In the original model, the slope of
3 the global water retention curve is calibrated directly using parameter λ^p . The model then
4 predicts the change of the slope of water retention curve and variability of the air expulsion
5 value with void ratio using Eq. (22). Fig. 10 compares drying branches of water retention
6 curves predicted by the original and proposed models for different global void ratios. Clearly,
7 predictions by both models agree very closely. This once more supports the proposed coupling
8 mechanisms.

9 It is also interesting to investigate the development of microstructural void ratio e^m during the
10 tests. Fig. 11a shows that the model predicts reasonably correctly the water retention curves
11 in terms of water ratio e_w (as in the case of Fig. 9, predictions of a single constant volume
12 wetting-drying test are shown only). Fig. 11b shows development of e^m with e_w for different
13 values of the parameter κ^m (loose sample). Experimental data by Romero et al. (2011) are

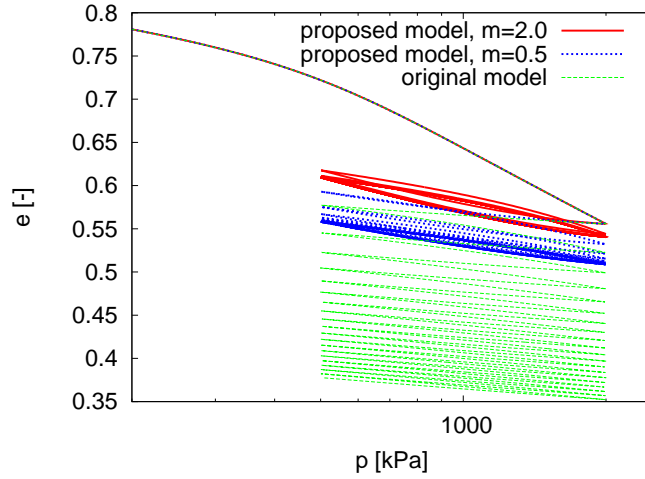


Figure 8: Response of the proposed and original models to cyclic isotropic test in a saturated state.

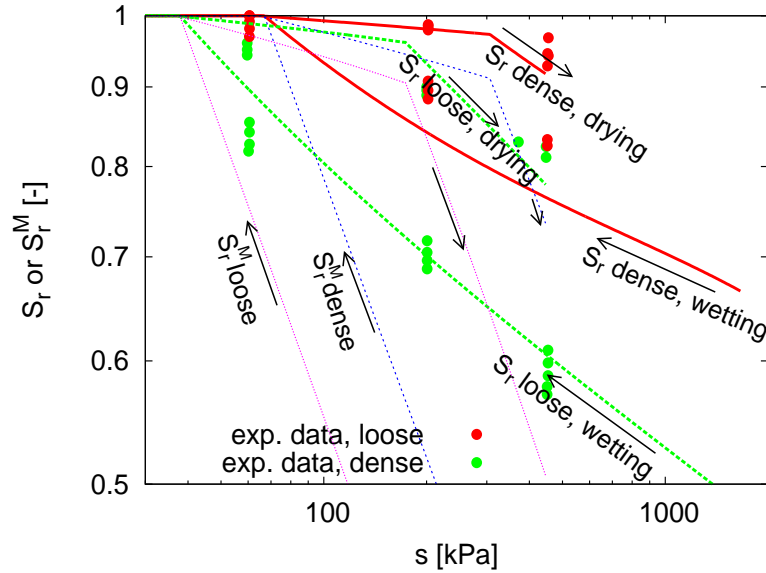


Figure 9: Constant global void ratio wetting-drying tests on Boom clay in terms of macrostructural degree of saturation S_r^M and a global quantity S_r . Experimental data by Romero (1999).

1 also included (taken from Fig. 4b). The parameter κ^m controls the development of e^m with
 2 e_w . It has thus the same effect as the parameter β of the model by Romero et al. (2011)
 3 (Fig. 4b). In the proposed model, this parameter has also a direct physical interpretation
 4 in terms of mechanical properties of microstructure. The parameter $\kappa^m = 0.04$, which was
 5 calibrated using results of oedometric swelling tests (Sec. 5.3), represents the data well,

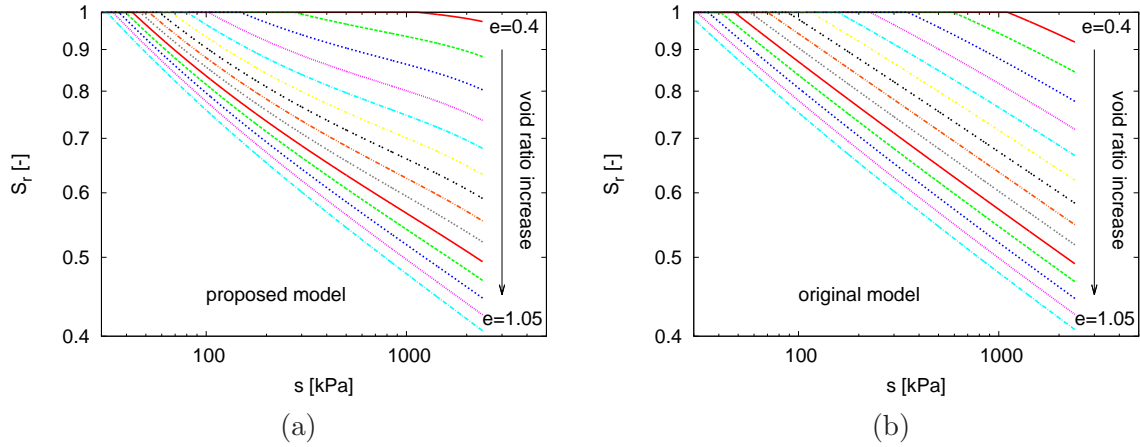


Figure 10: The dependency of the drying branch of constant volume water retention curve on void ratio predicted by the proposed microstructural model (a) and original model (Mašín 2010) (b).

- 1 giving another argument towards validity of the proposed double structure hydromechanical coupling approach.

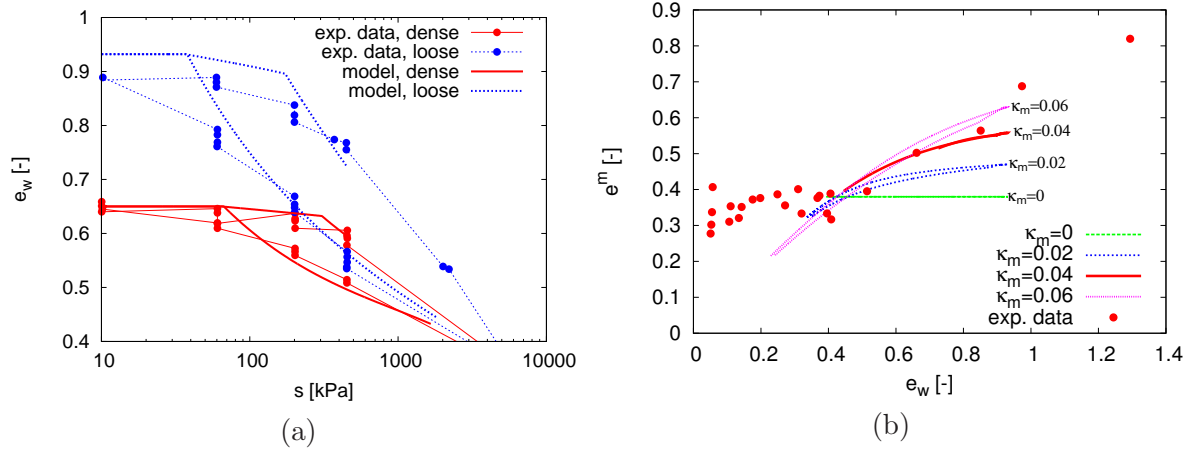


Figure 11: Constant volume water retention curves (a) and demonstration of microstructural swelling in terms of e_w vs. e^m graph (b). Experimental data by Romero et al. (2011).

- 2
- 3 Confined swelling tests lead to a development of swelling pressures. The overall volumetric
- 4 swelling is suppressed, and swelling of the aggregates occurs only to the extent allowed by
- 5 the amount of occlusion of macropores. Fig. 12 shows development of horizontal and vertical
- 6 net stresses with suction. Both the models predict correctly that higher swelling pressures
- 7 reach the denser soil. However, the original model, which predicts swelling of macrostructure
- 8 controlled by the macrostructural effective stress only, underpredicts the swelling pressure
- 9 magnitude. The proposed model predicts the swelling pressures in a reasonable agreement

with experiment, thanks to the additional contribution of the microstructural swelling.

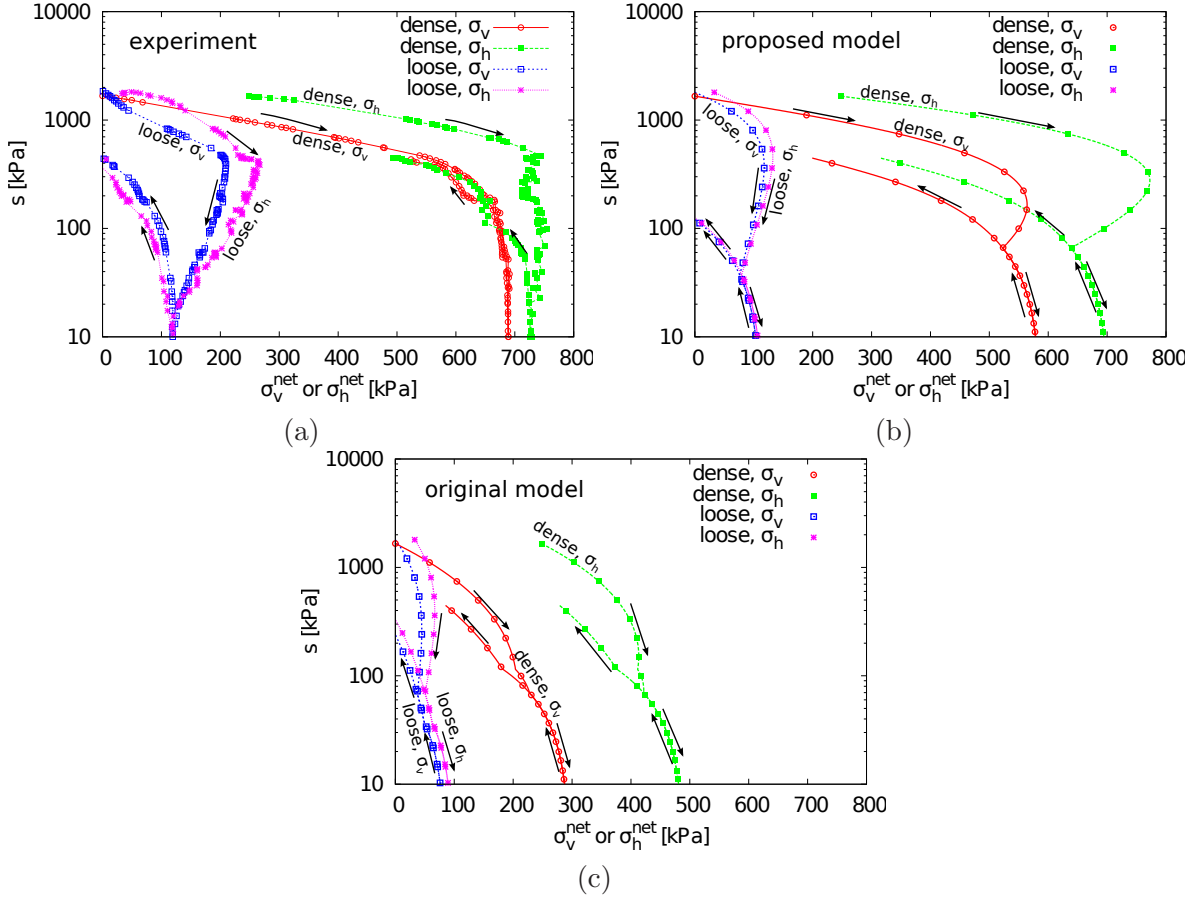


Figure 12: Development of swelling pressure with suction for denser and looser soil. Experimental data by Romero (1999) (a), compared with predictions by the proposed (b) and original (c) models.

1

2 5.3 Oedometric wetting-drying tests

3 Romero (1999) reported results of constant vertical net stress cyclic wetting-drying oedomet-
 4 ric tests on samples with high porosity and high density fabric. The experimental results
 5 are in terms of suction vs. void ratio shown in Figs. 13a,c. As expected, and as described
 6 in Sec. 2, soil with the dense macrostructure is prone to accumulated swelling, whereas
 7 the soil with initially loose structure is prone to accumulated compaction. The amount of
 8 swelling/compaction also depends on the stress level. Predictions by the proposed model
 9 are shown in Figs. 13b,d. The model, in general, represents the experimental data very closely.
 10 The only more important qualitative discrepancy is that in the second wetting-drying cycles
 11 of the tests on dense soil at low vertical stresses (Figs. 13c,d), the model does not represent

1 the hysteretic behaviour and thus slightly overpredicts the swelling strains. For comparison,
2 Figs. 13e,f show predictions by the original model. Predictions of the tests on loose soil do not
3 differ substantially from predictions by the proposed model. This is because the compaction
4 behaviour (collapse of structure due to wetting) is primarily controlled by the stability of
5 macrostructure, predicted the same by the original and proposed models. However, the re-
6 sults differ significantly in predictions of high density fabric tests. The original model predicts
7 only minor swelling strains, implied by the adopted effective stress formulation. Contrary, the
8 proposed model predicts the swelling behaviour relatively accurately, thanks to the predicted
9 swelling of the aggregated microstructure. For completeness, Fig. 14 shows predictions of
10 two tests in terms of degree of saturation. Clearly, also the hydraulic response is predicted
11 reasonably well.

12 **6 Summary and conclusions**

13 A formalism for double structure hydromechanical coupling has been developed. An essen-
14 tial component of the model is independent modelling of the behaviour of microstructure and
15 macrostructure (including separate effective stress measures), and considering hydromechan-
16 ical coupling at both structural levels. Individual components of the general model have been
17 selected to represent the behaviour of compacted expansive clays. Based on the recent findings
18 by Alonso et al. (2010), a link between different effective stress measures from the litera-
19 ture has been suggested. Namely, the effective stress representation by Khalili and Khabbaz
20 (1998) is considered to represent the macrostructural water retention model, following the ap-
21 proach by Alonso et al. (2010). It has been shown that using this assumption, formula from
22 Mašín (2010) yields explicit and simple expression for the dependency of macrostructural
23 water retention model on volumetric deformation of macroskeleton, simplifying substantially
24 the model formulation.

25 Thanks to the insight into the physical phenomena controlling the global response of double
26 structure soils, the proposed model has a small number of material parameters and state
27 variables. Still the model has advanced capabilities in predicting the non-linear soil behaviour
28 in compression and in shear, it incorporates hysteretic water retention model coupled with
29 the mechanical response, and predicts the inter-related behaviour of two structural levels.
30 Predictive capabilities of the model have been confirmed by simulation of comprehensive
31 experimental data set on compacted Boom clay by Romero (1999) using a single set of
32 material parameters.

33 An essential new component of the proposed model is representation of the microstructural
34 mechanical behaviour controlled by the parameter κ_m . It has been shown that calibration
35 of the parameter κ_m using volume change measured in swelling experiments leads to a cor-
36 rect global response in terms of degree of saturation, providing a support for the proposed
37 coupling approach. Additional confidence is gained by equality of the predictions with the
38 water retention model from Mašín (2010). Interestingly, the proposed approach have another
39 substantial consequence on the global response of the model. It limits volumetric ratchet-
40 ting, which is often regarded as one of the main drawbacks of hypoplasticity, the underlying

1 mechanical model for macrostructure.

2 In summary, the proposed model is considered as an advance with respect to the exist-
3 ing hypoplastic model for unsaturated soils by Mašín and Khalili (2008) and Mašín (2010).
4 Unlike the original model, the proposed model allows for predictions of soils with high plastic-
5 ity. When the microstructural behaviour is switched-off (by considering zero microstructural
6 volume change), the model reduces to the original model, while preserving its predictive
7 capabilities and including hysteretic hydraulic response.

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30 Appendix

31 The mathematical formulation of the proposed model for expansive soils is summarised in the following. The
32 behaviour of two structural levels is linked through

$$\dot{\epsilon} = \dot{\epsilon}^M + f_m \dot{\epsilon}^m \quad (41)$$

33 Different state variables are defined as $e = (V_p^m + V_p^M)/V_s$, $e^m = V_p^m/V_s$, $e^M = V_p^M/V_s$, $S_r = V_w/V_p$,
34 $S_r^m = V_w^m/V_p^m$ and $S_r^M = V_w^M/V_p^M$. For definition of volume measures V_x^y see Sec. 3.1. The quantities are
35 linked through

$$\frac{\dot{e}}{1+e} = \text{tr } \dot{\epsilon} \quad \frac{\dot{e}^M}{1+e^M} = \text{tr} \left[\dot{\epsilon}^M + (f_m - 1)\dot{\epsilon}^m \right] \quad \frac{\dot{e}^m}{1+e^m} = \text{tr } \dot{\epsilon}^m \quad (42)$$

1
$$e = e^M + e^m + e^M e^m \quad (43)$$

2
$$S_r = S_r^M + \frac{e^m}{e} (S_r^m - S_r^M) \quad (44)$$

3 The behaviour of macrostructure is governed by

$$\dot{\boldsymbol{\sigma}}^M = f_s \left(\boldsymbol{\mathcal{L}} : \dot{\boldsymbol{\epsilon}}^M + f_d \mathbf{N} \|\dot{\boldsymbol{\epsilon}}^M\| \right) + f_u \mathbf{H} \quad (45)$$

4 $\boldsymbol{\sigma}^M$ is the macrostructural effective stress defined by

$$\boldsymbol{\sigma}^M = \boldsymbol{\sigma}^{net} - \chi^M s \mathbf{1} \quad (46)$$

5 The macrostructural effective stress parameter χ^M coincides with the macrostructural degree of saturation
6 S_r^M , i.e.

$$S_r^M = \chi^M = \begin{cases} 1 & \text{for } s < s_e \\ \left(\frac{s_e}{s}\right)^\gamma & \text{for } s \geq s_e \end{cases} \quad (47)$$

7 where the drying branch of macrostructural WRC is described by $s_e = s_{en}$ and wetting branch by $s_e = s_{exp}$.
8 These two quantities are linked by

$$s_{exp} = a_e s_{en} \quad (48)$$

9 where a_e is a model parameter and

$$s_{en} = s_{e0} \frac{e_0^M}{e^M} \quad (49)$$

10 with parameters s_{e0} and e_0^M and $\gamma = 0.55$. Within the hysteretic model, the rate of S_r^M is given by

$$\dot{S}_r^M = -\gamma_a \frac{S_r^M}{s} \dot{s} - \gamma \frac{S_r^M}{e^M} \dot{e}^M \quad (50)$$

11 where $\gamma_a = \gamma$ for the main wetting and drying branches of WRC, $\gamma_a = \gamma/10$ at the hydraulic scanning curve
12 and $\gamma_a = 0$ for $s < s_{exp}$. Maximum value of S_r^M is limited to 1. The macrostructural effective stress rate
13 from Eq. (45) is given by

$$\dot{\boldsymbol{\sigma}}^M = \dot{\boldsymbol{\sigma}}^{net} + \mathbf{1} \chi^M \left[(\gamma_a - 1) \dot{s} + \gamma s \frac{\dot{e}^M}{e^M} \right] \quad (51)$$

14 with \dot{e}^M calculated using Eq. (42)b. The fourth-order tensor $\boldsymbol{\mathcal{L}}$ is a hypoelastic tensor given by

$$\boldsymbol{\mathcal{L}} = 3 \left(c_1 \boldsymbol{\mathcal{I}} + c_2 a^2 \hat{\boldsymbol{\sigma}}^M \otimes \hat{\boldsymbol{\sigma}}^M \right) \quad (52)$$

15 with $\hat{\boldsymbol{\sigma}}^M = \boldsymbol{\sigma}^M / \text{tr} \boldsymbol{\sigma}^M$. The two scalar factors c_1 and c_2 are defined as:

$$c_1 = \frac{2(3 + a^2 - 2^\alpha a \sqrt{3})}{9r} \quad c_2 = 1 + (1 - c_1) \frac{3}{a^2} \quad (53)$$

16 where r is a model parameter and the scalars a and α are functions of the material parameters φ_c , λ^* and κ^*

$$a = \frac{\sqrt{3}(3 - \sin \varphi_c)}{2\sqrt{2} \sin \varphi_c} \quad \alpha = \frac{1}{\ln 2} \ln \left[\frac{\lambda^* - \kappa^*}{\lambda^* + \kappa^*} \left(\frac{3 + a^2}{a\sqrt{3}} \right) \right] \quad (54)$$

17 The second-order tensor \mathbf{N} is given by

$$\mathbf{N} = \boldsymbol{\mathcal{L}} : \left(Y \frac{\mathbf{m}}{\|\mathbf{m}\|} \right) \quad (55)$$

18 with the quantity Y

$$Y = \left(\frac{\sqrt{3}a}{3 + a^2} - 1 \right) \frac{(I_1 I_2 + 9I_3)(1 - \sin^2 \varphi_c)}{8I_3 \sin^2 \varphi_c} + \frac{\sqrt{3}a}{3 + a^2} \quad (56)$$

1 where the stress invariants are defined as

$$I_1 = \text{tr}(\boldsymbol{\sigma}^M) \quad I_2 = \frac{1}{2} \left[\boldsymbol{\sigma}^M : \boldsymbol{\sigma}^M - (I_1)^2 \right] \quad I_3 = \det(\boldsymbol{\sigma}^M)$$

2 $\det(\boldsymbol{\sigma}^M)$ is the determinant of $\boldsymbol{\sigma}^M$. The second-order tensor \mathbf{m} is calculated by

$$\mathbf{m} = -\frac{a}{F} \left[\hat{\boldsymbol{\sigma}}^M + \text{dev} \hat{\boldsymbol{\sigma}}^M - \frac{\hat{\boldsymbol{\sigma}}^M}{3} \left(\frac{6\hat{\boldsymbol{\sigma}}^M : \hat{\boldsymbol{\sigma}}^M - 1}{(F/a)^2 + \hat{\boldsymbol{\sigma}}^M : \hat{\boldsymbol{\sigma}}^M} \right) \right] \quad (57)$$

3 with the factor F

$$F = \sqrt{\frac{1}{8} \tan^2 \psi_h + \frac{2 - \tan^2 \psi_h}{2 + \sqrt{2} \tan \psi_h \cos 3\theta} - \frac{1}{2\sqrt{2}} \tan \psi_h} \quad (58)$$

4 where

$$\tan \psi_h = \sqrt{3} \left\| \text{dev} \hat{\boldsymbol{\sigma}}^M \right\| \quad \cos 3\theta = -\sqrt{6} \frac{\text{tr}(\text{dev} \hat{\boldsymbol{\sigma}}^M \cdot \text{dev} \hat{\boldsymbol{\sigma}}^M \cdot \text{dev} \hat{\boldsymbol{\sigma}}^M)}{[\text{dev} \hat{\boldsymbol{\sigma}}^M : \text{dev} \hat{\boldsymbol{\sigma}}^M]^{3/2}} \quad (59)$$

5 The *barotropy* factor f_s introduces the influence of the mean stress level

$$f_s = \frac{3p^M}{\lambda^*(s)} \left(3 + a^2 - 2^\alpha a\sqrt{3} \right)^{-1} \quad (60)$$

6 and the *pyknотropy* factor f_d incorporates the influence of the overconsolidation ratio.

$$f_d = \left(\frac{2p^M}{p_e} \right)^\alpha \quad p_e = p_r \exp \left[\frac{N(s) - \ln(1+e)}{\lambda^*(s)} \right] \quad (61)$$

7 where $p_r = 1$ kPa is the reference stress. Values of $N(s)$ and $\lambda^*(s)$ are represented by

$$N(s) = N + n \left\langle \ln \frac{s}{s_e} \right\rangle \quad \lambda^*(s) = \lambda^* + l \left\langle \ln \frac{s}{s_e} \right\rangle \quad (62)$$

8 N , λ^* , n and l are model parameters and

$$s_e = s(S_r^M)^{(1/\gamma)} \quad (63)$$

9 The tensorial term \mathbf{H} from Eq. (45) reads

$$\mathbf{H} = -c_i \frac{\boldsymbol{\sigma}^M}{s\lambda^*(s)} \left[n - l \ln \frac{p_e}{p_r} \right] \langle -\dot{s} \rangle \quad (64)$$

10 for $s > s_{exp}$ and $S_r < 1$, and $\mathbf{H} = \mathbf{0}$ otherwise. The factor c_i reads

$$c_i = \frac{3 + a^2 - f_d a \sqrt{3}}{3 + a^2 - f_d^{SBS} a \sqrt{3}} \quad (65)$$

11 f_d^{SBS} is the value of the pyknотropy factor f_d for states at the SBS, defined as

$$f_d^{SBS} = \|f_s \mathcal{A}^{-1} : \mathbf{N}\|^{-1} \quad (66)$$

12 where the fourth-order tensor \mathcal{A} is expressed by

$$\mathcal{A} = f_s \mathcal{L} + \frac{1}{\lambda^*(s)} \boldsymbol{\sigma}^M \otimes \mathbf{1} \quad (67)$$

13 The factor controlling the collapsible behaviour f_u reads

$$f_u = \left(\frac{f_d}{f_d^{SBS}} \right)^{m/\alpha} \quad (68)$$

14 with m being a model parameter.

1 The behaviour of microstructure is governed by

$$\dot{\boldsymbol{\sigma}}^m = \mathbf{1} \frac{\dot{p}^m}{\kappa_m} \text{tr} \dot{\boldsymbol{\epsilon}}^m \quad (69)$$

2 where κ_m is a model parameter and $\boldsymbol{\sigma}^m$ is the microstructural effective stress given by

$$\boldsymbol{\sigma}^m = \boldsymbol{\sigma}^{net} - s = \boldsymbol{\sigma}^{tot} + u_w \quad (70)$$

3 The value of e^m may be initialised through

$$e^m = \exp \left[\kappa_m \ln \frac{s_r}{p^m} + \ln(1 + e_r^m) \right] - 1 \quad (71)$$

4 with parameters e_r^m and s_r .

5 Finally, the coupling function f_m reads

$$f_m = 1 - (r_{em})^m \quad (72)$$

6 for $\dot{p}^m < 0$ and $f_m = 0$ otherwise. r_{em} is relative void ratio

$$r_{em} = \frac{e - e_d}{e_i - e_d} \quad (73)$$

7 with

$$e_i = \exp \left[N(s) - \lambda^*(s) \ln p^M \right] - 1 \quad (74)$$

8 and

$$e_d = e_m \quad (75)$$

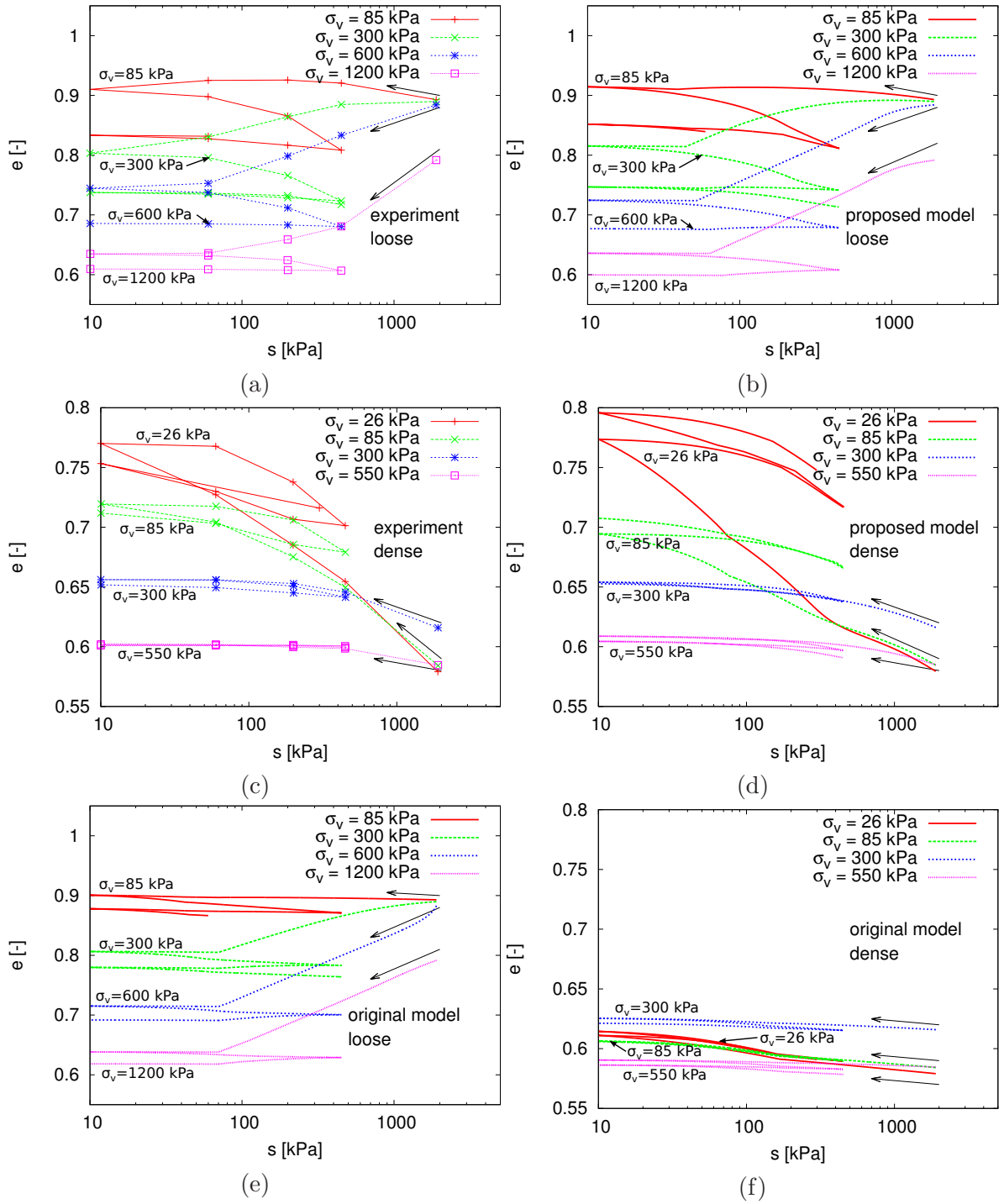


Figure 13: Constant σ_v^{net} wetting-drying oedometric experiments on Boom clay with loose and dense structures. Experimental data by Romero (1999) (a,c) compared with predictions by the proposed (b,d) and original (e,f) models.

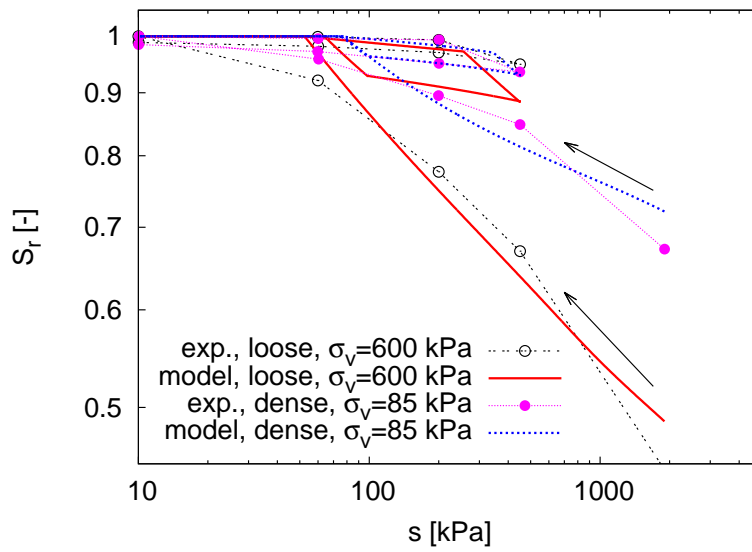


Figure 14: Constant σ_v^{net} wetting-drying oedometric experiments on Boom clay with loose and dense structures in terms of s vs. S_r . Experimental data by Romero (1999).