A thermodynamics-based constitutive model for clays accounting for double porosity

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Abstract Clays are natural materials characterised by a complex internal microstructure consisting of particles often arranged to form aggregates. Recent advances in experimental techniques, such as mercury intrusion porosimetry (MIP) combined with digital image correlation analysis from scanning electron microscopy (SEM), make it possible to identify at least two levels of porosity, one related to the intra-aggregate pores and another one related to the inter-aggregate voids, and to track their evolution upon loading. In continuum mechanics, constitutive modelling of clays can benefit from the aforementioned experimental evidence to identify measurable micro-inspired internal variables to back-predict the observed macroscopic response. In this perspective, in this study we propose a constitutive model for clays developed within the framework of thermodynamics with internal variables, in which we have selected two scalar internal variables, intra-aggregate and inter-aggregate porosities to track the clay response. The formulation takes advantage of a new strategy of initialisation of the inter-aggregate and intra-aggregate porosities based on the results of the MIP and the analysis of SEM images to reproduce the whole mechanical response of clays, from the early irreversible response to failure.

Keywords: clays, double porosity, thermodynamics with internal variables, continuum modelling

1 Introduction

Clays are multi-scale materials characterised by small particles often assembled in randomly oriented edge-to-face contacts or in iso-oriented domains of face-to-face contacts to form clusters of aggregates and stacks. Scanning electron microscope (SEM) images reveal that the single particle size is equal or lower than 2 μm, while the scale of the aggregates is typically of tens of μm (e.g. Delage and Lefebvre, 1984; Hattab *et al.*, 2013). This internal microstructure leads to a larger porosity due to the inter-aggregate voids, and a smaller one, called intra-aggregate porosity, within the aggregates, as detected by experimental tests performed by mercury intrusion porosimetry (MIP) (e.g. Chow *et al.*, 2019; Guglielmi *et al.*, 2022; Zheng *et al.*, 2023) and Nitrogen Gas

Adsorption test (N_2GA) (e.g. Bertagnolli *et al.*, 2011; Zheng and Baudet, 2024). These techniques allow to quantify the double porosity of clays and to track their evolution during loading through *post-mortem* measurements. Therefore, inter- and intra-aggregate porosities are suitable internal variables to describe the state of the material in constitutive models formulated within the continuum mechanics framework.
In this paper we propose an isotropic elasto-plastic constitutive model for clays developed within the framework of thermodynamics with internal variables (Maugin and Muschik, 1994), that requires the definition of two scalar potential functions, the free energy and the rate of dissipation, for the complete identification of the constitutive behaviour. The proposed formulation takes inspiration from the recent works by Amorosi *et al.* (2023) and Dadras-Ajirlou *et al.* (2024) and adopts the inter- and intra-aggregate void ratios as internal variables to reproduce the evolution of the double scale porosity of an illitic clay detected by Zheng and Baudet (2024) through MIP and N_2GA during different stages of one-dimensional compression. A new initialisation procedure of the internal variables is presented and the performance of the model to reproduce the macroscopic response of clays is illustrated through a series of ideal simulations of conventional laboratory tests.

2 Key features of the model

In the present formulation the void ratio is the summation of two terms e_o and e_i related to the volume of the inter- and intra-aggregate voids, respectively. Adopting the additive decomposition of elastic and plastic strains and assuming that the plastic volumetric strain rates are only related to a variation of the volume of the voids (i.e. the solids deform elastically according to Collins *et al.*, 2010), one has:

$$e = e_i + e_o \quad ; \quad \dot{\varepsilon}_v^p = -\frac{\dot{e}}{1+e} = -\frac{\dot{e}_i}{1+e} - \frac{\dot{e}_o}{1+e} = \dot{\varepsilon}_{vi}^p + \dot{\varepsilon}_{vo}^p \tag{1}$$

where the subscript v denotes the volumetric strain, i and o the intra- and inter-aggregate contributions of strains and void ratios, and the superscript p stands for plastic. The free energy function of the model is an extension of the Houlsby *et al.* (2005) expression to account for the dependency on the inter-aggregate void ratio e_o and the intra-aggregate plastic strains:

$$\varphi = \exp\left[\frac{r\left(N_{eo} - e_o\right)}{\lambda_o^*\left(1-n\right)}\right]\frac{p_r}{k\left(2-n\right)}\bar{r}_0^{\frac{2-n}{1-n}} + p_r \exp\left[A\left(\xi\varepsilon_{vi}^p + \left(1-\xi\right)\varepsilon_{si}^{py}\right)\right] \tag{2}$$

with

$$\bar{r}_0^2 = k^2\left(1-n\right)^2\left[\varepsilon_v^{e2} + \frac{3g}{k\left(1-n\right)}\varepsilon_s^{e2}\right] \tag{3}$$

In Eq. (2), p_r is a reference pressure equal to 101 kPa, g and k are model constants related to the elastic stiffness, n controls the nonlinear dependence of the elastic stiffness with the current stress (or elastic strain), r modulates the effect of the current void ratio e_o on the elastic free energy, N_{eo} is the inter-aggregate void ratio at p_r, and λ_o^* is the slope of the isotropic compression line of e_o in the plane $e - \log p$. The second right-side term of Eq. (2) is the stored energy that introduces a non-linear kinematic hardening controlling the position of the centre of the yield surface in the Cauchy stress space as a function of the intra-aggregate plastic volumetric and deviatoric strains, in which the constants y, A and ξ modulate the intensity and the direction of the process.
The rate of dissipation function is:

$$\dot{d} = \frac{p_r}{2}\sqrt{\exp\left(2\frac{N_{eo}-e_o}{\lambda_o^*}\right)\left(\dot{\varepsilon}_{vo}^{p\,2} + M^2\dot{\varepsilon}_{so}^{p\,2}\right) + \exp\left(2\frac{N_{ei}-e_i}{\lambda_i^*}\right)\left(\dot{\varepsilon}_{vi}^{p2} + M^2\dot{\varepsilon}_{si}^{p2}\right)}$$
$$+\frac{p_r}{2}\left[\exp\left(\frac{N_{eo}-e_o}{\lambda_o^*}\right)\dot{\varepsilon}_{vo}^{p} + \exp\left(\frac{N_{ei}-e_i}{\lambda_i^*}\right)\dot{\varepsilon}_{vi}^{p}\right] + I_{\mathbb{K}}\left(\frac{\dot{e}_o}{1+e} + \dot{\varepsilon}_{vo}^{p}\right) + I_{\mathbb{L}}\left(\frac{\dot{e}_i}{1+e} + \dot{\varepsilon}_{vi}^{p}\right) \quad (4)$$

where M is the stress ratio at critical state, the quantities N_{ei} and λ_i^* are analogous parameters for the intra-aggregate void ratio, and $I_{\mathbb{K}}$ and $I_{\mathbb{L}}$ are the indicator functions (Rockafellar, 1970) that constraint the evolution of the void ratios of Eq. (1). Eq. (4) can be manipulated through convex analysis (Rockafellar, 1970; Han and Reddy, 1999) to obtain the yield function and the generalized flow rules. The shape of the yield surface is similar to the ellipse of the Modified Cam-Clay model, in which the void ratios e_o and e_i determine the size, and the dissipative processes related to the modification of the intra-aggregate pores control the position in the stress space.

3 Performance of the model

The predictive capability of the model is illustrated for the medium plasticity illitic clay (PI = 35.4) studied by Zheng *et al.* (2023) and Zheng and Baudet (2024). For this clay, pores smaller than 0.06 μm are identified as intra-aggregate pores, while the larger ones constitute the inter-aggregate porosity, consistently with *post-mortem* SEM observations carried out at different vertical stresses σ_v during 1D compression. The parameters of the model are summarised in Table 1.

Table 1 Model parameters

Parameter	Value	Parameter	Value	Parameter	Value
k	443	λ_o^*	0.153	M	1.07
g	332	λ_i^*	0.017	A	2200
n	0.57	N_{eo}	0.782	y	1.5
r	0.24	N_{ei}	0.235	ξ	0.05

The elastic constants *k, g, n* and *r* are calibrated to obtain the initial shear modulus provided by the empirical expression of Viggiani and Atkinson (1995), the critical state ratio *M* is given by Zheng et al. (2023), and the void ratios-related parameters are selected to reproduce the compressibility curves for 1D compression shown in Fig.1.

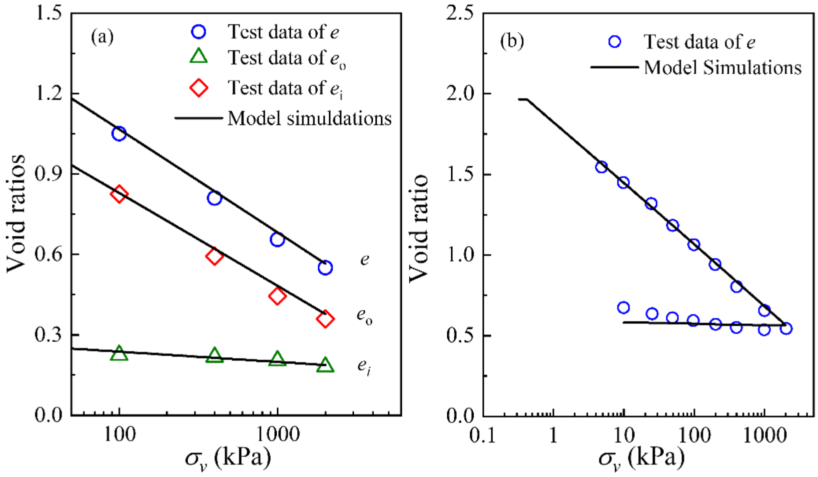

Fig. 1 Comparison between test data and simulated results of e, e_o and e_i during 1D compression

The model well reproduces the compressibility curve in terms of total void ratio during one-dimensional loading and unloading, and quantifies the evolution of the intra- and inter-aggregate void ratios upon loading, as detected through MIP and N_2GA measurements at different stages of the one-dimensional compression. The model response is also shown by means of ideal simulations of isotropically consolidated undrained triaxial compression tests for different over-consolidation ratios, OCR (Fig. 2).

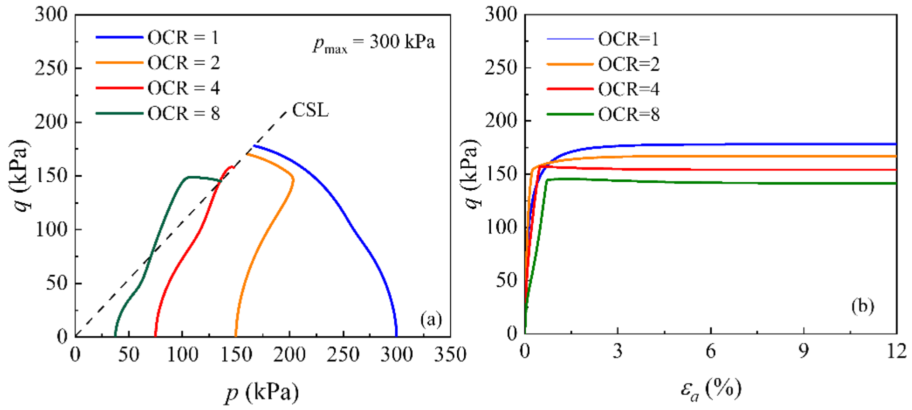

Fig. 2 Ideal simulations of undrained triaxial compression tests: (a) stress paths; (b) stress-strain curves

Another relevant feature of the model is the ability to reproduce the nonlinear early irreversible response of clayey soils in terms of secant shear modulus (G) reduction curves through a proper choice of the kinematic hardening parameters. Fig. 3 shows the comparison between the model predictions during undrained triaxial compression for OCR = 1, 2 and the corresponding curves as obtained by the empirical expression proposed by Darendeli (2001).

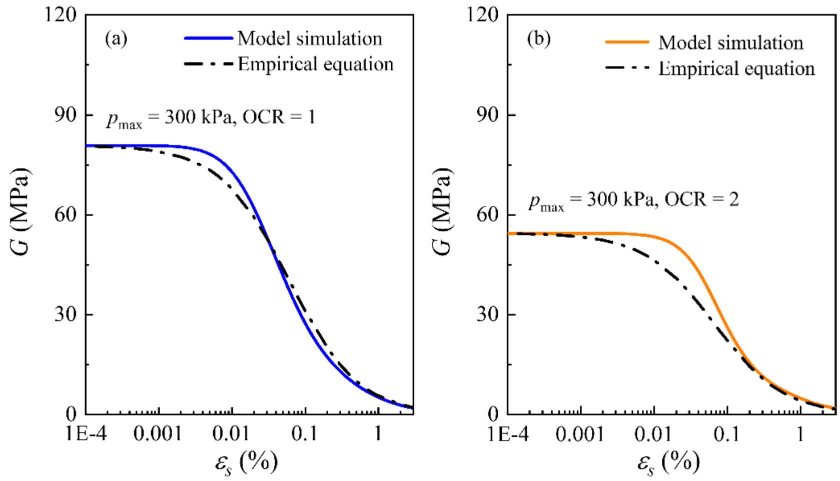

Fig. 3 Secant shear modulus reduction curves for different OCRs: comparison between model response and the empirical expression by Darendeli (2001).

4 Conclusions

In this paper we presented a constitutive model for clays developed within the framework of thermodynamics with internal variables, in which the intra- and inter-aggregate void ratios are evolving internal variables initialised through micro-scale measurements. The model accounts for many relevant aspects of the mechanical behaviour of clays, such as the early non-linear and dissipative response observed for small strain perturbations, the either dilatant or contractant behaviour expected along deviatoric stress paths, the evolution of the size and position of the yield surface in relation to the loading direction, and the attainment of critical state condition. Future investigations will be necessary to explore the predictive capability of the model under cyclic loading.

Acknowledgements Yang Yu is grateful to the China Grants Council (CSC no. 202306320333) for the award of a full scholarship support. Angelo Amorosi and Fabio Rollo acknowledge the financial support of the RETURN Extended Partnership and received funding from the European Union Next-GenerationEU (National Recovery and

Resilience Plan – NRRP, Mission 4, Component 2, Investment 1.3 – D.D. 1243 2/8/2022, PE0000005). Angelo Amorosi also acknowledges the Project DAMAGE, Prin 2022 - CUP B53D23005430006 - Grant Assignment Decree No. 961 adopted on 30/06/2023 by the Italian Ministry of Ministry of University and Research (MUR).

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