

# **NUMERICAL MODELLING OF THE CYCLIC RESPONSE OF A CAPROCK MATERIAL WITH AN ELASTO-VISCOPLASTIC CONSTITUTIVE MODEL ACCOUNTING FOR DEBONDING**

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### **Abstract**

The energy transition is a paradigm shift that affects the entire economic, social and industrial trajectory of our country. In this context, large-scale underground storage of hydrogen is seen as an effective way of overcoming the drawback associated with the seasonal nature of renewable energy sources in meeting the needs of energy demand. However, the injection/production cycles will produce a seasonal cyclic pressure of the stored gas, which in turn will induce stress changes in both the host formation and the caprock material. Such geomechanical variations can seriously compromise the sealing capacity of the caprock, increasing the risk of leakage. It is then of paramount importance to appropriately model the fatigue behaviour of the caprock material. This work investigates the ability of an existing elasto-plastic framework developed for structured soils to model the experimental response of an Italian stiff clay, which represents a typical caprock material. The existing framework is enhanced by introducing a viscous strain component to reproduce the observed time-dependency of the caprock response, which is shown to be crucial in modelling the material behaviour under different cyclic loading conditions.

## **1. Introduction**

To address the rise in greenhouse gas emissions, policymakers have reached several climate change agreements (e.g., Paris Agreement, 2015). In order to meet these climate targets, there is an increasing focus on the implementation of carbon capture and storage operations and the use of renewable energy sources. Nevertheless, renewable energy systems such as solar, wind, hydropower, and biofuels are highly subjected to seasonal variations and need to be regulated efficiently.

In this context, underground storage systems, such as depleted hydrocarbon reservoirs and saline aquifers, are being considered to use hydrogen as an energy carrier. The latter is converted from surplus renewable energy to meet energy demand on a large scale, respecting the household purpose. However, the injection of non-native fluids into the porous and permeable reservoir formations raises concerns about the storage integrity of the overlying sealing caprock formation (Miocic et al., 2023). Storage of hydrogen in the porous formation implies replacement of the existing brine, which can lead to complex multiphase displacement patterns (Heinemann et al., 2021). The low density of hydrogen compared to brine can lead to the formation of a hydrogen cap directly below the caprock. In addition, the cyclic injection and production of hydrogen will result in cyclic changes in the effective stress state of the reservoir formation, which in turn will affect the state of the caprock. These cyclic stress variations can induce fatigue-related risks, creating leakage pathways within the caprock. Other potential undesirable effects are fault reactivation, surface heave and induced seismicity (Heinemann et al., 2021). To ensure safe storage it is therefore necessary to properly model the response of the caprock to the strain field imposed by the operations in the reservoir.

Most commonly, caprocks are sedimentary clayey rocks bonded to different extents. Bonding provides a larger strength and stiffness with respect to the same material in a remoulded state. Ciancimino et al. (2024) found a strong strain-softening response during monotonic shear of these structured materials, which is attributed to bond breakage. Also, Ciancimino et al. (under prep.) highlighted the nonnegligible influence of loading frequency on these structured clays. In this paper, the relevance of viscosity is firstly shown by comparing experimental trends obtained from cyclic tests conducted on an Italian stiff carbonatic clay with numerical predictions coming from a widely used constitutive model for the cyclic response of structured materials. Then, an existing elasto-plastic model including debonding (e.g., Seidalinov and Taiebat, 2019) is enhanced by introducing a viscous strain-component to model the time-dependent behaviour of the material. The proposed model is finally verified with the experimental results to show its effectiveness in assessing the fatigue life of the caprock material.

## **2. Elasto-plasticity theory with debonding**

Experimental results on natural and reconstituted clays highlighted the role of bonding on the compressibility and the shear strength of undisturbed structured materials (e.g., Ciancimino et al. 2024). The bonding degree of a natural clay depends on the physical and chemical conditions that occur during deposition, consolidation, ageing and unloading. In constitutive modelling, it is assumed that bonding is responsible for the different mechanical behavior of intact soil with respect to the reconstituted soil. Gens and Nova (1993) proposed to account for the mechanical consequences of bonding by increasing the size of the yield surface of reconstituted material via a new internal variable. The post-yielding disruption of the bonded material is then modelled as a progressive damage, assumed related to the reduction of the bonding degree variable occurring during plastic straining.

Following this framework, Seidalinov and Taiebat (2019) developed the Saniclay-B, a constitutive model to simulate the response of structured clays under cyclic loading. The Saniclay-B extends the formulation of the Saniclay model (Dafalias et al., 2006) incorporating the bounding surface plasticity concept. In this concept, the purely elastic response is restricted within an elastic nucleus, typically characterized by a very small size. The plastic modulus depends on the current state of stress along with the image state of stress on the bounding surface, allowing inelastic strains within the bounding surface. A shape hardening parameter is introduced to simulate the degradation of stiffness during cyclic loading. The model adopts an isotropic destructuration mechanism to capture the sudden post-yield increase of compressibility and strain softening response under shearing. According to the formulation of Saniclay-B, the cyclic response of bonded materials due to fatigue loading evolves due to both progressive debonding and cyclic degradation of the plastic modulus.

From the existing knowledge, loading scenario during underground gas storage can be idealized as a sinusoidal one-way deviatoric loading applied around a mean deviatoric stress  $q_{mean}$  with an amplitude *A* which gives a maximum deviatoric stress  $q_{max} = q_{mean} + A$ . Considering the storage operations,  $q_{max}$  is related to the maximum amount of fluid injected into the reservoir. To study the fatigue behaviour of a typical caprock formation, a series of undrained monotonic and cyclic triaxial tests were carried out at the Geotechnical Laboratory of Politecnico di Torino on an Italian stiff carbonatic clay. Fig 1a shows the dependency of number of cycles to failure  $N_f$  on  $A$  with the results obtained from three cyclic triaxial tests (Ciancimino et al., under prep.), where the specimens were anisotropically consolidated up to the expected in-situ stress state (mean effective stress  $p' = 8.1$  MPa, deviatoric stress  $q = 6.3$  MPa). A sinusoidal deviatoric loading with a time period  $T = 5$  min was applied with  $q_{max} =$ 12.5 MPa and with different values of *A* = 5.25 MPa, 4.25 MPa and 3.25 MPa. Under the scenario of keeping  $q_{max}$  constant and varying *A*, it is observed that smaller the value of *A*, the lower the number of cycles to failure  $N_f$ .

To evaluate the performance of the Saniclay-B in a similar scenario, undrained cyclic tests were simulated for two sensitive marine clays, the Cloverdale and the Ariake clay. The simulations refer to specimens isotropically consolidated up to  $p' = 200$  kPa and then subjected to sinusoidal one-way loadings with *qmax* of 100 kPa. The results are presented in Fig 1b. The Saniclay-B model parameters and the initial state parameters are taken from the validation performed by Seidalinov and Taiebat (2019) and Palmieri and Taiebat (2024) for the Cloverdale and the Ariake clay, respectively. The trends in Fig 1b are in contrast with the experimental results shown in Fig 1a. The degradation mechanisms, as predicted by Saniclay-B, are such that an increase in *A* corresponds to a larger plastic modulus degradation, and thus to progressive debonding. The opposite trend is observed in the laboratory results. This could be explained accounting for the highly time-dependent behaviour of clays. The experimental evidence for this caprock material when subjected to cyclic loading as the one considered in this paper suggests that the introduction of the viscous mechanism is critical to appropriately reproduce the measured fatigue response. In addition, it should be noted that, at the reservoir scale, the loading periods will be much larger than the ones used in the experiments; this may raise concerns that the viscous mechanism may be even more significant than observed. In this respect, a simple and effective elastoviscoplastic framework is proposed, as explained in Section 3.

#### **3. Proposed elasto-viscoplastic constitutive framework**

The proposed model follows the hardening elasto-plasticity framework introduced by Gens and Nova (1993) for bonded soils, incorporating the Vermeer and Neher (1999) visco-plasticity theory formulated within the framework of Extended Overstress theory (see Kutter and Sathialingam, 1992).



*Fig 1. Influence of A on keeping as constant: a) experimental results of undrained cyclic triaxial tests carried out on intact caprock specimens imposing a sinusoidal deviatoric loading with T =5min,*  $q_{max} = 12.5MPa$ *and different amplitudes A; b) virtual cyclic tests performed on Cloverdale clay and Ariake Clay imposing a sinusoidal loading with*  $q_{max} = 100$  kPa *and varying* A.

The strain-rate tensor  $\dot{\boldsymbol{\epsilon}}$  is decomposed into an elastic  $\dot{\boldsymbol{\epsilon}}^e$  and a viscoplastic  $\dot{\boldsymbol{\epsilon}}^{vp}$  component:

$$
\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^{vp}
$$

The formulation of the model is presented in terms of the stress invariants  $p'$  and  $q$ , their conjugate strain variables being the volumetric strain  $\varepsilon_{vol}$  and the deviatoric  $\varepsilon_{dev}$  strain. Usually, natural sedimentary caprocks are characterized by elastic cross-anisotropic behaviour. For this the elastic behaviour accounted is according to the proposal of Graham and Houlsby (1983). The yield surface *f* is expressed according to Panteghini and Lagioia (2018):

$$
f = \frac{q^2}{M^2} \frac{\left[ (p' + p_t)(1 - 2\alpha_y) + \alpha_y (p_{cb} + p_t) \right]^2}{4(p_{cb} + p_t)^2 (1 - \alpha_y) \alpha_y^3} - (p' + p_t)(p_{cb} - p')
$$

where:  $\alpha_y$  and M are material parameters influencing the shape of the yield surface (in particular M is the critical state stress ratio);  $p_{cb}$  is the preconsolidation pressure of the material in the presence of bonding; and  $p_t$  is the tensile strength. The  $p_{cb}$  and  $p_t$  values are both linked to a scalar measure *b* of the degree of bonding, as in Gens and Nova (1993):

$$
\frac{p_{cb}}{p_c} = 1 + b \; ; \; \frac{p_t}{p_c} = \alpha_t b
$$

The model employs a non-associative flow rule, i.e.,  $f \neq g$  (being g the plastic potential), and  $p_c$  evolves as a function of both volumetric and deviatoric visco-plastic strain increments. The degree of bonding *b* is related to a damage variable *h*, which evolves with the visco-plastic strain increment:

$$
g = \beta_y \frac{q^2}{M^2} \frac{\left[ (p' + p_t)(1 - 2\alpha_y) + (p_{cb} + p_t) \right]^2}{4(p_{cb} + p_t)^2 (1 - \alpha_y)\alpha_y^3} - (p' + p_t)(p_{cb} - p')
$$
  

$$
b = b_0 e^{-(h - h_0)} \; ; \; \dot{h} = h_{dev} |\dot{\varepsilon}_{dev}^{vp}| + h_{vol} |\dot{\varepsilon}_{vol}^{vp}|
$$

where  $\beta_{y}$  is the material parameter influencing the shape of plastic potential.  $h_{dev}$  and  $h_{vol}$  are constitutive parameters weighing the influence of deviatoric and volumetric viscoplastic strain rate. In compliance with the Vermeer and Neher model, the viscoplastic strain rate  $\dot{\varepsilon}^{vp}$  is given as follows:

$$
\dot{\varepsilon}^{vp} = \frac{1}{\alpha_{VN}} \frac{\mu^*}{\tau} \left( \frac{p_{cb}^d + p_t^d}{p_{cb}^r + p_t^r} \right)^{\frac{\lambda^* - \kappa^*}{\mu^*}} \frac{\partial g}{\partial \sigma'}
$$

$$
\alpha_{VN} = abs\left( \frac{\partial g}{\partial p'} \right); \ \lambda^* = \frac{\lambda}{1 + e}; \ \kappa^* = \frac{\kappa}{1 + e}
$$

where  $\sigma'$  is the effective stress tensor,  $\mu^*$  is the viscous parameter obtained by the slope of the volumetric strain-time curve in natural logarithmic scale.  $\lambda$  and  $\kappa$  are the slope of compression and unloadingreloading line in void ratio  $e - \ln(p')$  plane. The superscript *r* and *d* denote respectively the reference and dynamic yield surfaces, as defined by the Extended Over Stress Theory (see Kutter and Sathialingam, 1992). The capabilities of the proposed model are validated against the experimental data obtained from cyclic triaxial tests performed on intact specimens of an Italian stiff carbonatic clay introduced in Section 2. The model parameters are reported below. For a detailed explanation of the calibration procedure see Ciancimino et al. (submitted).

		$\kappa$ $G$ $\alpha$ $\lambda$ $\mu^*$ $M$ $\alpha_y$ $\beta_y$ $p_{c0}^r$ $b_0$ $h_0$ $\alpha_t$ $h_{dev}$ $h_{vol}$					
		(-) (MPa) (-) (-) (-) (-) (-) (-) (MPa) (-) (-) (-) (-) (-)					
		0.033 300 0.83 0.102 0.0034 1 0.62 1.1 13.5 0.47 0 0 20 250					

*Table 1. Model parameters and initial values of the internal variables for proposed model to simulate undrained cyclic triaxial tests.* 

Fig 2 shows the comparison between the model simulations and the experimental results in terms of stress-strain response and effective stress paths. The cyclic test was performed with  $q_{max}$  =13.5 MPa,  $q_{mean}$  =7.55 MPa. The model captures well the accumulation of inelastic strain and the progressive debonding. As the framework is developed within Extended Overstress Theory, the concept of cyclic failure under stress control is associated with very large strains rather than with the attainment of certain failure stress. In Fig 3a the same test conditions  $(q_{max} = 13 \text{ MPa}, q_{mean} = 7.75 \text{ MPa})$  were simulated assuming different periods ( $T = 5$  min or 250 min). The behavior observed for intact specimens is reproduced by the model in terms of decrease of the number of cycles to failure as the loading period increases. From Fig 3b, it can be observed that the trends shown in Fig 1a are captured correctly, albeit the influence of *A* is more pronounced in the laboratory tests. This can be improved by formulating the model within the bounding surface plasticity concept but at the price of increasing its complexity and, possibly, limiting its applicability to simulate underground storage scenarios.



*Fig 2. Comparison between numerical simulations and experimental results of an undrained cyclic triaxial test: a) deviatoric stress vs axial strain; and b) effective stress path*



*Fig 3. Comparison between numerical simulations and experimental data of undrained cyclic triaxial tests in terms* of number of cycles to failure  $N_f$  as a function of: a) loading period; and b) amplitude.

### **4. Conclusions**

At the reservoir scale, the stress changes associated with injection and production cycles must be studied to ensure the sealing capacity of the caprock. However, the stress paths in the caprock during these pressure changes can be very complex and different from those studied in the laboratory. As a result, accurate numerical modelling of the caprock response becomes paramount. In this work, an existing framework for constitutive modelling of bonded materials was extended to reproduce the observed experimental response of caprocks under cyclic loading. The proposed framework introduced viscosity to the existing elasto-plastic theory, allowing a satisfactory reproduction of the experimental trends in terms of fatigue life as a function of both loading period and amplitude. The ability of the proposed simple approach to represent the caprock material behaviour makes it accessible to extend the simulations from an element scale to a boundary value problem to investigate the stress dynamics in the caprock.

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