

Lawrence Berkeley National Laboratory

LBL Publications

Title

An Elastoplastic Constitutive Model for Anisotropic Hydro-Mechanical Response of Opalinus Clay

Permalink

<https://escholarship.org/uc/item/1dn4q0bx>

Journal

Minerals, 16(10)

ISSN

2075-163X

Authors

Nuus, Matthijs
Rinaldi, Antonio Pio
Guo, Guanlong
[et al.](#)

Publication Date

2026-09-24

DOI

10.3390/min16100981

Copyright Information

This work is made available under the terms of a Creative Commons Attribution License, available at <https://creativecommons.org/licenses/by/4.0/>

Peer reviewed

Article

An Elastoplastic Constitutive Model for Anisotropic Hydro-Mechanical Response of Opalinus Clay

Matthijs Nuus ^{1,*}, Antonio Pio Rinaldi ¹, Guanlong Guo ² and Jonny Rutqvist ²

¹ Swiss Seismological Service (SED)—ETH Zürich (Swiss Federal Institute of Technology Zürich), 8092 Zürich, Switzerland; antoniopio.rinaldi@sed.ethz.ch

² Lawrence Berkeley National Laboratory (LBNL), Berkeley, CA 94720, USA; gguo@lbl.gov (G.G.); jrutqvist@lbl.gov (J.R.)

* Correspondence: matthijs.nuus@sed.ethz.ch

Abstract

Opalinus Clay is currently proposed as the host rock for a deep geological repository (DGR) for radioactive waste in Switzerland. Gas is expected to be generated within the repository due to anoxic corrosion of metallic components and the degradation of organic material, and understanding gas migration is therefore critical, as pressure build-up may induce fracturing and potentially compromise the long-term integrity of the repository. One relevant gas transport mechanism is dilatancy-controlled flow, in which localized dilatant pathways can lead to transient increases in permeability, facilitating gas migration and potentially affecting the barrier performance of the host rock. To investigate and simulate such processes, a constitutive model is required that captures hydro-mechanical (HM) behavior, including the influence of bedding-induced anisotropy, yield behavior, and strain-dependent hardening and softening. In this study, consolidated undrained (CU) triaxial tests performed on Opalinus Clay specimens with varying bedding orientations (in increments of 15°) are used to calibrate and evaluate the columnar-basalt (COMBA) constitutive model implemented in FLAC3D. The model allows for the explicit representation of bedding through oriented joint sets, enabling orientation-dependent failure criteria, anisotropic stiffness, and strain-dependent evolution of strength parameters. The constitutive model is subsequently applied to a coupled hydro-mechanical simulation of a gas injection experiment conducted at the Mont Terri Rock Laboratory. Comparison with a previously applied ubiquitous-joint formulation shows that the COMBA constitutive model reproduces the observed hydraulic response and deformation localization, while providing a more accurate prediction of the timing of deformation measured by distributed fiber-optic sensing, although the accumulated deformation is overpredicted at later times. The improved representation of bedding anisotropy further provides a clearer insight into the gas migration mechanism, with the close correspondence between plastic shear strain and gas breakthrough supporting shear-slip dilation along the bedding planes as a likely mechanism for pathway formation.



Academic Editor: Andrey G. Kalinichev

Received: 7 August 2026

Revised: 20 September 2026

Accepted: 20 September 2026

Published: 24 September 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

Keywords: Opalinus Clay; constitutive model; anisotropy; hydro-mechanical; columnar-basalt (COMBA); FLAC3D; TOUGH-FLAC; dilatancy

1. Introduction

Opalinus Clay (OPA) is currently proposed as the host rock for a nuclear waste repository in Switzerland due to several favorable properties, including extremely low

intrinsic permeability, potential capacity for self-sealing [1] and high sorption capacity [2]. However, after repository closure, gas is expected to be generated primarily through the anoxic corrosion of metallic components and the degradation of organic materials [3]. As gas accumulates, pressure may build up within the low-permeability system, altering the hydro-mechanical conditions in the near field of the repository.

Gas migration in argillaceous rocks occurs through several mechanisms depending on pressure and stress conditions, including dissolved gas transport, two-phase flow, dilatancy-controlled flow, and fracturing, as conceptualized by Marschall et al. [4]. Of particular importance is the dilatancy-controlled regime, which occurs when gas pressure approaches the minimum principal stress, leading to localized damage and the formation of transient, high-permeability pathways. At the onset of this regime, the integrity of the host rock as a barrier may be compromised, making dilatancy-controlled flow a critical process for repository safety assessment.

The initiation of dilatant pathways is strongly controlled by the deformation and damage evolution of the host rock. In OPA, this behavior is highly anisotropic due to its pronounced bedding structure. Mechanical properties such as stiffness and strength are strongly dependent on the orientation of loading relative to bedding. Recent experimental and in situ studies (e.g., Cuss et al. [5]; Nuus et al. [6]) have further demonstrated that bedding orientation plays a key role in controlling the onset and propagation of dilatant flow paths. In particular, the numerical analysis in the GT experiment by Nuus et al. [6] indicated that permeability enhancement and gas breakthrough are predominantly associated with shear reactivation and dilation along the bedding planes. These observations highlight the need for constitutive models that can accurately represent anisotropic deformation and damage evolution under coupled hydro-mechanical conditions.

Numerous studies have investigated specific aspects of the deformation and strength behavior of OPA, such as its directional stiffness, orientation-dependent strength, and the development of strain localization [7–9]. Despite these advances, a consistent integration of anisotropic deformation into coupled hydro-mechanical models remains limited. Many approaches simplify material behavior or do not explicitly account for deformation-induced permeability changes, which are essential for simulating processes such as dilatancy-controlled flow and self-sealing [10]. As a result, the predictive capability of current models for gas migration in clay-rich rocks remains limited.

This study is carried out within the DECOVALEX-2027 HyMar task [11], which focuses on developing robust constitutive models to describe mechanical damage and failure, and to capture anisotropic behavior of clay rocks under coupled hydro-mechanical conditions. Laboratory consolidated undrained (CU) triaxial tests on OPA conducted by Winhausen et al. [12], performed at varying confining stresses and bedding orientations, provide detailed observations of pore pressure evolution, deformation, and failure behavior, and clearly demonstrate the strong anisotropic response of the material. These experiments form part of HyMar Task 1, aimed at developing and calibrating constitutive models based on laboratory and microscopic observations [11].

The columnar-basalt (COMBA) formulation [13], as implemented in FLAC3D [14], is used in this study, as it allows for the representation of multiple arbitrary orientations of weakness within an anisotropic elastoplastic matrix, while failure is still governed by a Mohr–Coulomb criterion, the formulation allows for anisotropic elastic behavior governed by bedding orientation and, in contrast to models with a single ubiquitous-joint orientation, the inclusion of multiple joint sets along which deformation and failure can occur. The CU triaxial test data are used to assess the capability of this formulation to reproduce the key features of anisotropic deformation and failure, with particular relevance for hydro-mechanical processes governing the onset of dilatant pathways.

The resulting framework provides the basis for subsequent simulations within Hy-Mar Task 3, which focuses on the simulation of an in situ gas injection experiment in OPA at the Mont Terri Rock Laboratory. The COMBA constitutive model is incorporated into an existing hydro-mechanical framework for dilatancy-controlled gas flow that was previously applied to the Gas Transport (GT) experiment using the bilinear strain-softening/hardening ubiquitous-joint (SUBI) model implemented in FLAC3D, hereafter referred to as the ubiquitous-joint model, thereby enabling a direct comparison between the two constitutive models. The objective is therefore not to recalibrate the GT model, but to evaluate how the explicit representation of bedding-controlled anisotropic elasticity in COMBA affects the simulated hydro-mechanical response compared with the ubiquitous-joint formulation.

2. Experimental Methods

2.1. Laboratory Experiments

CU triaxial compression tests were performed on cylindrical OPA specimens with dimensions of 30 mm in diameter and 60 mm in length. The specimens were prepared with different bedding orientations, including perpendicular (S), parallel (P), and inclined configurations (Z) at varying angles relative to the loading direction (Figure 1). All specimens were fully saturated prior to testing. The experiments considered in this study were conducted under an effective confining stress of 10 MPa, defined according to Terzaghi's effective stress principle as $\sigma'_c = \sigma_c - p_0$. During the consolidation stage, the total confining stress σ_c and pore pressure were increased until the desired effective confining stress σ'_c was reached. Axial loading was then applied under strain-controlled conditions at rates ranging between 5×10^{-8} and $5 \times 10^{-7} \text{ s}^{-1}$.

Specimens were prepared at orientations ranging from 0° to 90° relative to the bedding plane in increments of 15° . A detailed description of the experimental procedures is provided by Winhausen et al. [12,15].

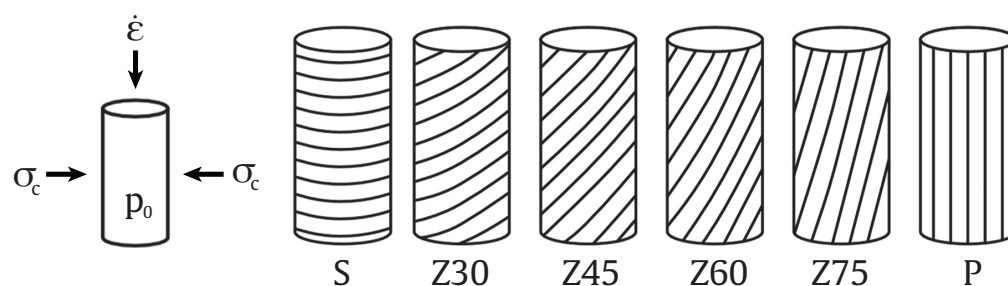


Figure 1. Schematic representation of specimen orientations used in CU triaxial tests (S, Z, and P configurations) relative to the axial strain rate $\dot{\epsilon}$ and applied confining stress σ_c . The initial pore pressure p_0 varies depending on the imposed effective confining stress. Modified from Winhausen et al. [12].

2.2. In Situ Gas Injection Experiment (GT Experiment)

The GT experiment was conducted in OPA at the Mont Terri Rock Laboratory, where helium was injected over a period exceeding one year to investigate gas migration under in situ conditions [5]. The experimental setup consists of a central injection borehole surrounded by eight observation boreholes arranged in a circular pattern with a radius of approximately 1 m. All boreholes are drilled perpendicular to bedding and, with the exception of BGT-2 and BGT-10, are instrumented with cemented fiber-optic cables to monitor deformation (Figure 2). A detailed description of the experimental setup is provided by Cuss et al. [5].

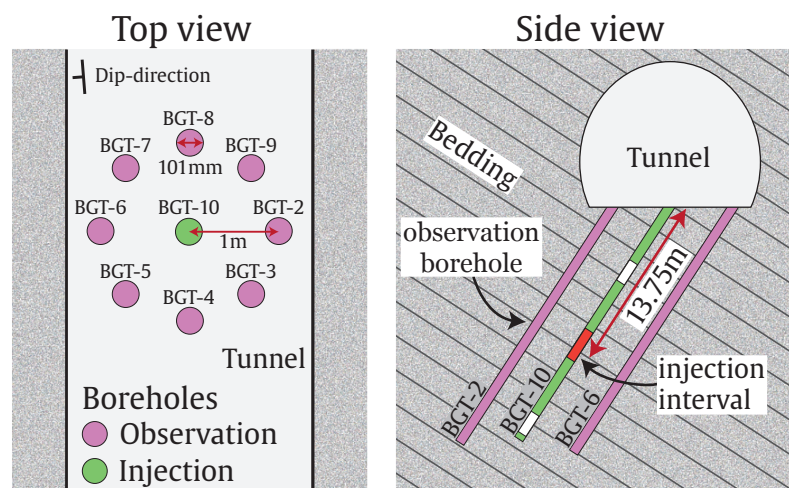


Figure 2. Arrangement of injection and observation boreholes in the GT experiment, showing the top view (left) and side view (right).

The injection protocol involved a step-wise increase in gas pressure, with increments of approximately 0.5 MPa applied over periods of about two weeks, followed by phases of constant pressure. This sequence was continued until a pressure of approximately 4.2 MPa was reached, at which point a sudden pressure drop of about 0.9 MPa was observed (Figure 3). Such pressure responses are interpreted as indicative of the onset of dilatancy-controlled flow, where deformation-induced damage leads to the formation of transient, high-permeability pathways [5,6]. A second, larger pressure drop of approximately 2.5 MPa occurred later in the experiment following an increase in the injection rate. This was interpreted by Cuss et al. [5] as the formation of a partially open macro-feature associated with bedding-plane splitting (Figure 3 in Cuss et al. [5] and Figure 4 in Nuus et al. [6]). The present study focuses exclusively on the first pressure-drop event and the associated permeability enhancement, consistent with the modeling approach of Nuus et al. [6]. The GT experiment therefore provides a valuable field-scale dataset for evaluating the capability of numerical models to reproduce the coupled hydro-mechanical processes governing dilatant gas migration in OPA.

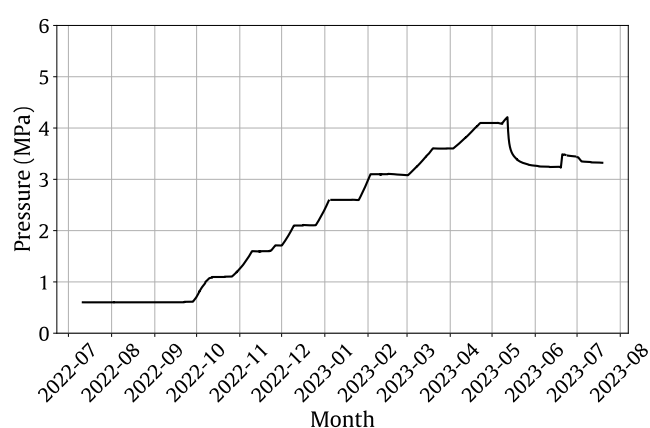


Figure 3. Pressure evolution measured in the injection interval of borehole BGT-10.

3. Constitutive Model

The coupled hydro-mechanical response of the system is simulated using FLAC3D v9.5 [14] for the fluid-saturated laboratory experiments and TOUGH3-FLAC3D [16] for the coupled

hydro-mechanical simulation in the in situ experiment. Regardless of the coupling approach, mechanical equilibrium is obtained in FLAC3D by solving the momentum equation:

$$\sigma_{ij,j} + \rho b_i = \rho \frac{dv_i}{dt} \quad (1)$$

where $\sigma_{ij,j}$ denotes the divergence of the Cauchy stress tensor, b_i is the body force per unit mass, ρ is the rock density, and $\frac{dv_i}{dt}$ is the material derivative of the velocity.

The coupling between fluid flow and deformation is described using Biot's theory of poroelasticity [17]. The total stress is related to the effective stress, denoted by a prime ('), and pore pressure according to

$$\sigma_{ij}^{\text{tot}} = \sigma'_{ij} - \alpha p \delta_{ij} \quad (2)$$

where σ'_{ij} is the effective stress, α is Biot's coefficient, p is the pore pressure, and δ_{ij} is the Kronecker delta. Positive stresses denote tension, and negative stresses denote compression.

Variations in pore pressure, saturation, and volumetric strain result in changes in fluid content, as described by the mass balance equation:

$$\frac{1}{M} \frac{\partial p}{\partial t} + \frac{\phi}{s} \frac{\partial s}{\partial t} = \frac{1}{s} \frac{\partial \zeta}{\partial t} - \alpha \frac{\partial \varepsilon}{\partial t} \quad (3)$$

where M is the Biot modulus, ϕ is porosity, s is saturation, ζ is the fluid content, and ε is the volumetric strain. Assuming isothermal conditions, the thermal term is neglected.

The relationship between stress and strain is governed by the constitutive model. In this study, the COMBA model [13] is adopted, in which the stress–strain response is obtained through the superposition of strain contributions from the rock matrix and embedded joints.

3.1. Elastic Behavior

The rock matrix is assumed to behave as an isotropic linear elastic material following Hooke's law, characterized by Young's modulus E and Poisson's ratio ν . In incremental form, the matrix contribution to the strain–stress relation can be written in Voigt notation as

$$\{\dot{\varepsilon}^e\} = \begin{bmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G} \end{bmatrix} \{\dot{\sigma}'\} \quad (4)$$

The local elastic strain increment contribution of joint set i is expressed as

$$\{\dot{\varepsilon}^e\}^i = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{k_i^n S_i} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{k_i^s S_i} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{k_i^s S_i} \end{bmatrix} \{\dot{\sigma}'\} \quad (5)$$

where S_i is the spacing of joint set i , and k_i^n and k_i^s are the normal and shear stiffnesses of the joint, respectively. A local coordinate system is defined for each joint set, in which axis 3

is oriented normal to the joint plane, axis 1 is aligned with the dip direction, and axis 2 is oriented along the strike direction. The compliance matrix of the joint is transformed to the global coordinate system, and the result is added to the global compliance matrix [13].

3.2. Yield Criterion and Plastic Behavior

The failure criterion on the joint, whose orientation represents the dip of the bedding, is described by a Mohr–Coulomb envelope with a tension cut-off. Shear failure on the joint is initiated when the following condition is satisfied:

$$f^s = \sqrt{\sigma'_{13}{}^2 + \sigma'_{23}{}^2} + \sigma'_{33} \tan \phi - c = 0 \quad (6)$$

where ϕ is the joint friction angle, and c is the joint cohesion.

Tensile failure occurs when

$$f^t = \sigma'_{33} - \sigma^t = 0 \quad (7)$$

where σ^t is the tensile strength of the joint.

Shear yielding on the weak plane follows a non-associated flow rule, with the plastic potential given by

$$g^s = \sqrt{\sigma'_{13}{}^2 + \sigma'_{23}{}^2} + \sigma'_{33} \tan \psi \quad (8)$$

where ψ is the dilation angle of the joint.

Tensile yielding is governed by an associated flow rule, with the corresponding potential function

$$g^t = \sigma'_{33}. \quad (9)$$

The yield conditions are evaluated on the weak planes, and if yielding is detected, a stress correction is applied to the elastic trial state in accordance with plasticity theory. A detailed description of the numerical implementation is provided by Meng et al. [13].

In the COMBA model, plastic yielding is restricted to the predefined joint sets, such that failure can only occur along these planes. This differs from, for example, the ubiquitous-joint model, in which both the matrix and the embedded joints may undergo plastic yielding. Upon yielding, the joint cohesion and friction angle are allowed to evolve through strain hardening and softening. These parameters are defined as a function of an evolution parameter that measures the accumulated plastic shear strain on the joint [13]. The increment of this evolution parameter is computed from the square root of the second invariant, $\sqrt{J_2}$, of the incremental plastic shear-strain deviator tensor:

$$\Delta\kappa_j^s = \sqrt{\frac{1}{3}(\dot{\epsilon}_{33}^p)^2 + \left(\frac{\dot{\epsilon}_{13}^p}{2}\right)^2 + \left(\frac{\dot{\epsilon}_{23}^p}{2}\right)^2} \quad (10)$$

where $\Delta\kappa_j^s$ is the plastic shear strain increment of joint set j . The local plastic strain-rate components $\dot{\epsilon}_{33}^p$, $\dot{\epsilon}_{13}^p$, and $\dot{\epsilon}_{23}^p$ correspond to the normal component and the two shear components associated with the joint plane, respectively. The accumulated plastic shear strain is obtained by summing $\Delta\kappa_j^s$ over the loading history.

4. Numerical Model

The COMBA constitutive model is applied at two different scales in this study. First, laboratory-scale models of the CU triaxial tests are used to calibrate and evaluate the constitutive response for different bedding orientations directly in FLAC3D v9.5. Subsequently, the calibrated constitutive model is applied to a TOUGH3–FLAC3D coupled

hydro-mechanical model of the in situ GT experiment at the Mont Terri Rock Laboratory. The numerical setups for both applications are described below.

4.1. Numerical Model of the CU Triaxial Tests

Given the saturated conditions of the CU tests, simulations of the experimental results are performed using the hydro-mechanical coupling implemented in FLAC3D. Porosity and permeability are assumed to remain constant throughout the laboratory simulations.

4.1.1. Model Geometry and Boundary Conditions

The numerical model consists of a cylindrical OPA specimen with a diameter of 30 mm and a height of 60 mm. To represent the loading platens, two additional cylinders are attached at the top and bottom, each with a thickness of 3 mm and the same diameter as the specimen (Figure 4). The mesh consists of 1782 elements.

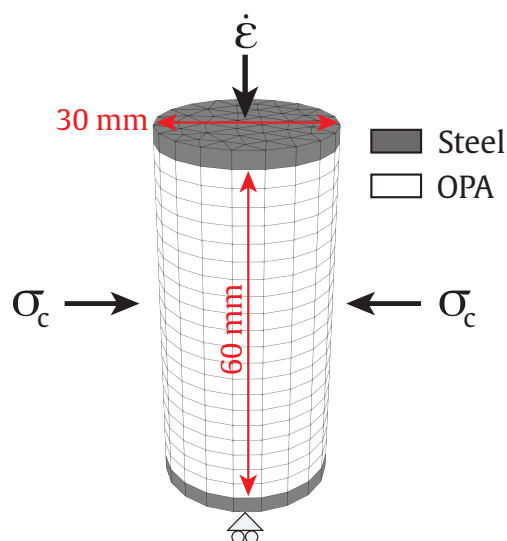


Figure 4. Numerical model geometry and boundary conditions.

The experimental conditions are replicated by applying a confining stress σ_c on the lateral surface of the cylinder. The magnitude of the applied total confining stress depends on the initial pore pressure p_0 and the target effective stress σ'_c . For example, for a specimen tested at an effective confining stress of 10 MPa with an initial pore pressure of $p_0 = 2.5$ MPa, a total confining stress of 12.5 MPa is applied.

A roller boundary condition is imposed at the bottom of the lower steel plate, while the top steel plate is constrained in the lateral directions. Axial loading is applied by prescribing a constant strain rate at the top of the specimen.

4.1.2. Elastic Material Parameters

The Young's modulus parallel to bedding was determined from the initial linear portion of the stress–strain response of the Z75 and P specimens. As non-linearity initiates at relatively low axial strains, only the range up to an approximately 0.1% axial strain was considered. This resulted in a value of $E = 5.45$ GPa.

In the present formulation, the Young's modulus E (Equation (4)) represents the stiffness parallel to bedding, i.e., $E = E_{11} = E_{22}$. The stiffness perpendicular to bedding is described by E_{33} , which is controlled through the normal joint stiffness k_n . In the COMBA

formulation, the Young's modulus normal to bedding (E_{33}) is obtained by superposition of the matrix and joint contributions, such that

$$\frac{1}{E_{33}} = \frac{1}{E} + \frac{1}{k_n S_i} \quad (11)$$

where S_i is the joint spacing, assumed to be 1 m in the present study. Note that the elastic contribution of the joint set is governed by the product of the stiffness and the spacing. The joint spacing of 1 m therefore represents a reference spacing and does not reflect the actual bedding spacing of Opalinus Clay. For example, the same response can be obtained by reducing the joint spacing to 0.01 m and increasing the corresponding joint stiffness by a factor of 100.

Based on the experimental results of Winhausen et al. [12], Young's moduli parallel and perpendicular to bedding were determined from triaxial tests at 50% of the peak deviatoric stress under an effective confining stress of 10 MPa, resulting in an anisotropy ratio of approximately 3.3. To reproduce this anisotropy ratio within the COMBA framework, the normal joint stiffness was set to $k_n = 2.4$ GPa/m.

The Poisson's ratio is assumed isotropic and is set to $\nu = 0.25$, as the COMBA model does not allow for directional variation in this parameter. The joint shear stiffness k_s is treated as a calibration parameter to account for shear compliance along the embedded joint sets.

4.1.3. Yield Criterion and Hardening–Softening Behavior

Peak and residual cohesion and friction angle were determined separately for two groups of specimens based on bedding orientation: (i) specimens with bedding dips between 30° and 75° , represented by *joint set 1*, and (ii) specimens with bedding orientations that are unfavorable for failure to occur along the bedding plane (S and P), represented by *joint set 2*.

For joint set 1, failure is assumed to occur along the bedding plane. At the time of peak failure, the effective maximum and minimum principal stresses were reconstructed from the peak deviatoric stress q_{peak} and the corresponding mean effective stress p'_{peak} using $\sigma'_1 = p' + 2q/3$ and $\sigma'_3 = p' - q/3$. The corresponding Mohr circles were then constructed from these principal effective stresses. Using the bedding orientation of each specimen, the effective normal and shear stresses acting on the bedding plane at peak failure were determined from the corresponding Mohr circle. A Mohr–Coulomb failure envelope was subsequently fitted through these stress points to determine the peak cohesion and friction angle.

For joint set 2, the bedding orientation is unfavorable for shear failure, resulting in insufficient shear stress mobilization along the bedding plane. To account for this, a secondary joint set was introduced with a fixed orientation of 58° , representing a more favorably oriented failure plane. A dilation angle of 5° was used for joint set 2 to improve the agreement with the experimental response. The Mohr–Coulomb parameters for this joint set were determined in the same manner as for the first group, using the normal and shear stresses evaluated on a plane with a dip of 58° . It is important to note that, for the S and P specimens, joint set 2 is introduced in addition to joint set 1, such that both joint sets remain active. Joint set 1 remains aligned with the bedding and controls the bedding-related anisotropic elastic response. Joint set 2 primarily serves as the more favorably oriented failure plane. The same normal stiffness as for joint set 1 was assigned to joint set 2, while an arbitrarily large value of 1.0×10^5 GPa/m was used for the shear stiffness.

The resulting Mohr circles and corresponding failure envelopes for both groups are shown in Figure 5.

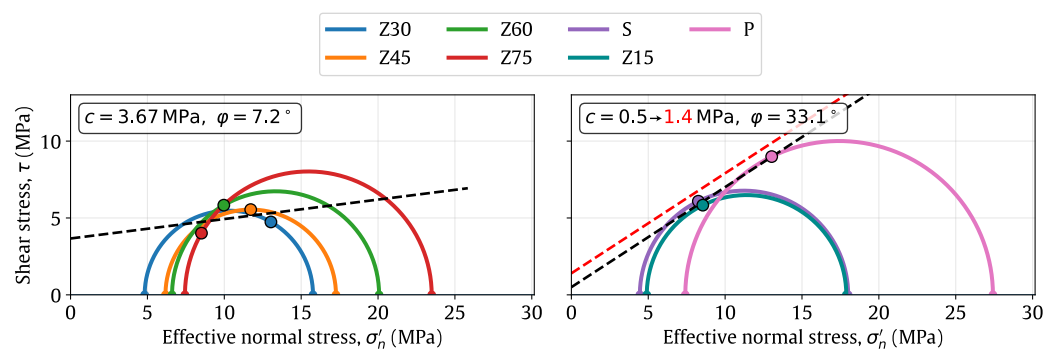


Figure 5. Mohr circles at peak deviatoric stress for *joint set 1*, assumed to fail along the bedding plane (**left**) and *joint set 2*, assumed to fail along a plane inclined at 58° (**right**), with fitted Mohr–Coulomb failure envelopes (black dashed lines) and the adjusted failure envelope for joint set 2 (red dashed line).

The same procedure was applied to determine the residual strength parameters, based on the residual deviatoric stress q_{res} and the corresponding mean effective stress p' at the residual state. For joint set 1, the friction angle was kept equal to the peak value, while for joint set 2, a constant cohesion was assumed. The resulting residual strength envelopes for both joint sets are shown in Figure 6.

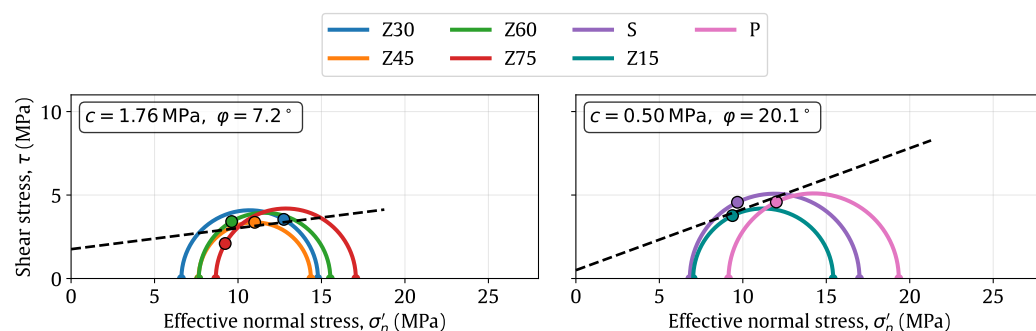


Figure 6. Mohr circles at residual deviatoric stress for the two joint groups, with fitted Mohr–Coulomb failure envelopes (black dashed lines).

The resulting hardening and softening curves for cohesion and friction angle are shown in Figure 7. The black markers indicate the discrete values defined in the FLAC3D tables, with linear interpolation applied between these points. The accumulated plastic strain at which softening initiates was manually adjusted to improve the fit to the experimental response and differs between the two joint sets, with values of 0.0075 for joint set 1 and 0.01 for joint set 2. For joint set 1, an initial cohesion of 0.60 MPa was adopted based on manual fitting to the experimental response. For joint set 2, the initial cohesion was set to 0.5 MPa following Figure 5. However, this resulted in premature failure associated with an overestimation of the simulated pore pressure. A hardening behavior was therefore introduced, with cohesion increasing to 1.4 MPa before softening back to its initial value of 0.5 MPa. For the joint set 2 specimens, the initial friction angle and peak cohesion were additionally adjusted to improve the agreement with the experimental response, with the corresponding peak failure envelope shown by the red dashed line in Figure 5. These adjustments are discussed further in Section 5.1. All remaining modeling parameters are summarized in Table 1.

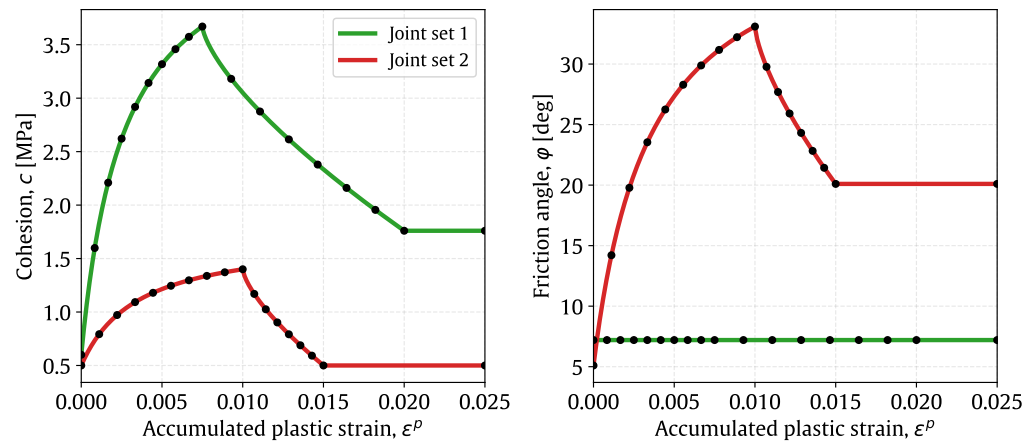


Figure 7. Hardening and softening evolution of friction angle and cohesion for joint sets 1 and 2.

Table 1. Model parameters used in the CU simulations.

Parameter	Symbol	Value	Unit
<i>Elastic parameters</i>			
Young's modulus	E	5.45	GPa
Poisson ratio	ν	0.25	—
Normal joint stiffness (1)	k_n^1	2.4	GPa/m
Shear joint stiffness (1)	k_s^1	1.0×10^3	GPa/m
Normal joint stiffness (2)	k_n^2	2.4	GPa/m
Shear joint stiffness (2)	k_s^2	1.0×10^5	GPa/m
Joint spacing	S	1	m
<i>Hydraulic parameters</i>			
Biot coefficient	α	1.0	—
Biot modulus	M	11.6	GPa
Permeability	k	5×10^{-20}	m ²
Porosity	ϕ	0.10	—
<i>Strength parameters</i>			
Friction angle (1)	φ^1	7.2	°
Initial friction angle (2)	φ_b^2	5.0	°
Peak friction angle (2)	φ_p^2	33.1	°
Residual friction angle (2)	φ_r^2	20.1	°
Dilation angle (1)	ψ^1	1.0	°
Dilation angle (2)	ψ^2	5.0	°
Initial cohesion (1)	c_i^1	0.60	MPa
Peak cohesion (1)	c_p^1	3.67	MPa
Residual cohesion (1)	c_r^1	1.76	MPa
Initial cohesion (2)	c_i^2	0.5	MPa
Peak cohesion (2)	c_p^2	1.4	MPa
Residual cohesion (2)	c_r^2	0.5	MPa

4.2. Numerical Model of the GT Experiment

4.2.1. Model Geometry and Boundary Conditions

The numerical model of the GT experiment closely follow the one proposed by Nuus et al. [6]. In brief, the computational domain consists of a tilted inner cube surrounded by an outer cube (Figure 8). The inner cube is oriented with the same bedding orientation as the Opalinus Clay, with a dip of 33° and a dip direction of N140°, and is discretized using prismatic layers aligned with the bedding. This allows the hydraulic properties to be assigned parallel and perpendicular to the bedding. At the center of the

inner cube, a cylindrical injection interval with a diameter of 0.101 m and a height of 0.5 m represents the helium injection interval used during the in situ experiment. During the simulations, helium is injected into this interval using the measured injection-rate history of the GT experiment.

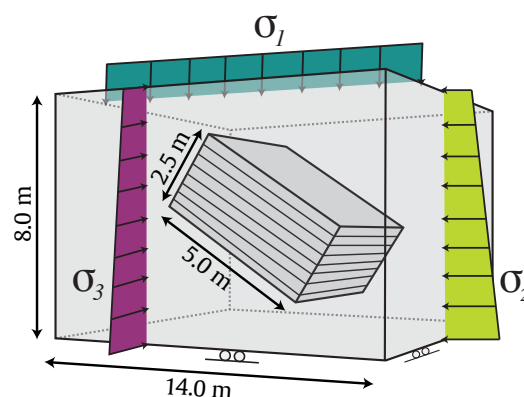


Figure 8. Model geometry of the GT experiment showing the tilted inner cube representing the bedded Opalinus Clay formation, the surrounding outer cube, and the applied stress boundary conditions.

The surrounding outer cube is oriented such that its faces are aligned with the principal stress directions, allowing the principal stresses to be applied directly normal to the model boundaries. Based on the local stress measurements [18], principal stresses of $\sigma_1 = 6.5$ MPa, $\sigma_2 = 4.5$ MPa, and $\sigma_3 = 2.9$ MPa are applied at the depth of the injection interval in the vertical, N320°, and N050° directions, respectively. The orientations of σ_2 and σ_3 are therefore parallel to the bedding dip direction and bedding strike. A lithostatic stress gradient of 0.025 MPa/m is assumed for the vertical principal stress. Assuming that the principal stress ratios remain constant with depth and that the orientation of the stress tensor does not change, the corresponding stress gradients are 0.017 MPa/m for σ_2 and 0.011 MPa/m for σ_3 . These stress gradients are imposed as linearly varying boundary conditions, ensuring that the in situ stress state evolves consistently with depth throughout the model domain.

Hydraulic pressure boundary conditions are imposed through thin layers located at the top and bottom of the model domain. A hydrostatic pressure gradient is initialized using the measured pore pressure at the injection interval (0.65 MPa) as a reference, resulting in fixed pressures of 0.61 MPa and 0.69 MPa at the top and bottom boundaries, respectively. These pressures are held constant throughout the simulation, while no-flow boundary conditions are applied to the remaining model boundaries.

4.2.2. Hydro-Mechanical Coupling and Permeability Evolution

The simulations are performed using the TOUGH3–FLAC3D framework, which couples the multiphase flow simulator TOUGH3 with the geomechanical solver FLAC3D [16]. In TOUGH3, two-phase flow is applied using a van Genuchten model for capillary pressure and relative permeability [19,20], while the mechanical response is simulated in FLAC3D. The effective stress entering the constitutive model is calculated according to Equation (2), in which the pore pressure is taken as the maximum of the gas and water pressures.

In contrast to the Mohr–Coulomb model with a ubiquitous-joint formulation used by Nuus et al. [6], the present study employs the COMBA constitutive model to represent the anisotropic mechanical response of the Opalinus Clay. For the GT model, only a single joint set, aligned with the bedding, is considered. Because the maximum principal stress is vertical and the bedding dip is 33°, the stress configuration is comparable to that of the Z30 specimen and therefore to the *joint set 1* specimens in the CU triaxial tests. Thus, the

main distinction from the ubiquitous-joint formulation is the representation of anisotropic mechanical behavior.

The resulting strains are coupled to permeability evolution through a strain-dependent permeability formulation following Xu et al. [21]. The permeability update function is given by

$$\mathbf{k} = 10^{\mathbf{b}_1 \cdot \varepsilon_{\text{vol}}} \cdot \exp^{\mathbf{b}_2 \cdot \varepsilon^p} \cdot \mathbf{k}_{\text{ini}} \quad (12)$$

$$k_{\text{ini},\parallel} = \begin{cases} k_{\text{ini}} & \text{if } \varepsilon^p = 0 \\ k_f & \text{if } \varepsilon^p > 0 \end{cases} \quad (13)$$

$$k_{\text{ini},\perp} = \begin{cases} k_{\text{ini}} & \text{if } \varepsilon^p = 0 \\ 0.2 \times k_f & \text{if } \varepsilon^p > 0 \end{cases}$$

In these equations, ε_{vol} represents the volumetric strain, ε^p represents the plastic shear strain, and $\mathbf{b}_1$ and $\mathbf{b}_2$ represent empirical constants controlling the sensitivity of permeability to volumetric and plastic deformation, respectively. Within this formulation, the development of dilatant flow pathways is represented through the accumulation of plastic shear strain, with $\mathbf{b}_2$ controlling the magnitude of permeability enhancement associated with a given amount of accumulated plastic shear strain.

Once plastic strain develops within an element ($\varepsilon^p > 0$), the initial permeability k_{ini} in Equation (12) is replaced by a prescribed failure permeability k_f according to Equation (13). To represent the anisotropic nature of the dilatant pathways, the permeability perpendicular to the pathway is set to 20% of the permeability parallel to the pathway.

The porosity is updated following the porosity increment formulation of Kim et al. [22], as implemented in the TOUGH3–FLAC3D coupling by Rinaldi et al. [16]:

$$d\phi = A(\alpha, \phi, K) dp + \Delta\phi, \quad (14)$$

where $A(\alpha, \phi, K)$ describes the poro-elastic response as a function of the Biot coefficient α , porosity ϕ , and drained bulk modulus K , dp is the pore-pressure increment, and $\Delta\phi$ is a correction term accounting for mechanically induced porosity changes.

Because permeability enhancement is triggered by accumulated plastic shear strain, the onset of dilatant pathway formation is represented as a shear-failure process. Consequently, an appropriate failure criterion is required to determine when permeability enhancement is initiated.

4.2.3. Failure Criterion for Permeability Enhancement

The failure criterion for permeability enhancement is based on the simulated evolution of the effective normal and shear stresses acting on the bedding planes surrounding the injection interval. To enable a direct comparison with the reference ubiquitous-joint model, the same modeling parameters are adopted unless stated otherwise. The only additional mechanical parameters introduced in the present model are the normal and shear joint stiffnesses, k_n and k_s , as the ubiquitous-joint formulation, despite allowing for failure along the bedding planes, assumes isotropic elasticity and therefore does not include separate stiffness parameters for the bedding. The values of k_n and k_s are taken from the calibration of the CU triaxial tests (Table 1). To reproduce the timing of the observed pressure drop, the friction angle of the Mohr–Coulomb failure criterion was reduced from 17.3° to 16.6° , while the cohesion was retained at 0 MPa. Note that this failure criterion represents the onset of dilatant pathway formation and the associated permeability enhancement, modeled through shear failure along the bedding planes as described by Nuus et al. [6], rather than the full shear failure represented by the failure criterion calibrated against the CU triaxial tests. After failure, strain softening is applied by reducing the friction angle to 80% of

its peak value, following the same reduction adopted by Nuus et al. [6]. This results in a residual friction angle of 13.3°.

All material parameters used in the numerical model are summarized in Table 2. Finally, the empirical constant $\mathbf{b}_2$ in Equation (12), which controls the sensitivity of permeability to accumulated plastic strain, is reduced relative to the value used by Nuus et al. [6] to obtain a better match between the modeled and measured injection pressure response.

Table 2. Material parameters used in the numerical model of the GT experiment.

Parameter	Symbol	Value	Unit
<i>Elastic parameters</i>			
Young's modulus	E	7.0	GPa
Poisson ratio	ν	0.27	–
Normal joint stiffness	k_n	2.4	GPa/m
Shear joint stiffness	k_s	1.0×10^3	GPa/m
Joint spacing	S	1	m
<i>Strength parameters</i>			
Peak friction angle	φ	16.6	°
Residual friction angle	φ_r	13.3	°
Cohesion	c	0	MPa
<i>Hydraulic parameters</i>			
Biot coefficient	α	1.0	–
Biot modulus	M	18.3	GPa
Permeability (parallel)	$k_{\parallel}$	5×10^{-20}	m ²
Permeability (perpendicular)	$k_{\perp}$	1×10^{-20}	m ²
Porosity	ϕ	0.12	–
van Genuchten parameter	n	1.67	–
Apparent gas entry pressure	$1/\alpha$	60	MPa
Liquid saturation	S_{ls}	1.0	–
Residual liquid saturation	S_{lr}	0.01	–
Residual gas saturation	S_{gr}	0.0	–
<i>Permeability evolution parameters</i>			
Failure permeability	k_f	5×10^{-19}	m ²
Volumetric strain constant	$\mathbf{b}_1$	$\begin{bmatrix} 50 \\ 50 \\ 10 \end{bmatrix}$	–
Plastic strain constant	$\mathbf{b}_2$	$\begin{bmatrix} 21,000 \\ 21,000 \\ 4200 \end{bmatrix}$	–

5. Results

5.1. CU Triaxial Test Model

The measured and simulated response of the six CU triaxial tests is shown in Figures 9–11. Figure 9 presents the evolution of deviatoric stress q with axial strain, Figure 10 compares the stress paths in p' – q space, and Figure 11 shows the development of excess pore pressure with axial strain.

Figure 9 shows that the relationship between deviatoric stress and axial strain depends strongly on bedding orientation. Samples with lower bedding angles undergo larger axial strains at a given deviatoric stress than specimens with higher bedding angles. Using the selected values of k_n and k_s in the COMBA model and varying only the bedding orientation, the model reproduces this trend well.

The measured peak deviatoric stress generally increases with bedding angle and is captured by the simulations. An exception is the S specimen, which reaches a higher peak deviatoric stress than the Z30 and Z45 specimens. For all six orientations, the difference between the simulated and measured peak deviatoric stress remains within 20%. The

simulated peak deviatoric stress is slightly underestimated for the Z45 and Z60 specimens and overestimated for the Z75 and P specimens. Nevertheless, the overall deviatoric stress–axial strain response is reproduced well by the model.

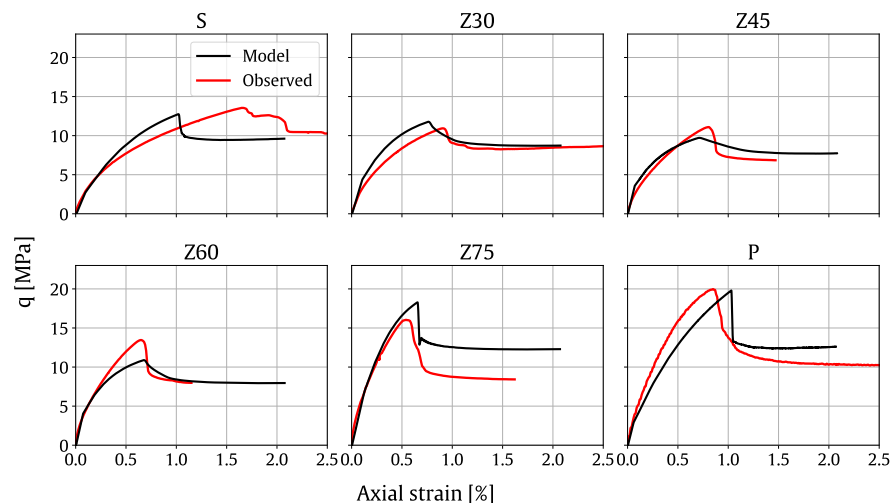


Figure 9. Modeled (black) and measured (red) axial strain ε [%] versus deviatoric stress q [MPa] of specimens with different bedding angles.

A similar anisotropic trend is observed in the stress paths shown in Figure 10. For low bedding angles, the mean effective stress p' decreases during loading as excess pore pressure accumulates, whereas for high bedding angles p' increases with increasing q . This behavior is consistent with the excess pore-pressure evolution shown in Figure 11, where specimens with lower bedding angles develop considerably larger excess pore pressures than specimens with higher bedding angles. The model reproduces both trends well, including the progressive reduction in excess pore-pressure generation and the transition from decreasing to increasing mean effective stress with increasing bedding angle. One notable discrepancy is observed for the S specimen. In the experiment, the stress path curves back toward higher values of p' after reaching its minimum effective stress, whereas this recovery is less pronounced in the model. This behavior is consistent with the excess pore-pressure evolution, where the measured S specimen exhibits a more gradual reduction in excess pore pressure following peak values than is reproduced by the simulation.

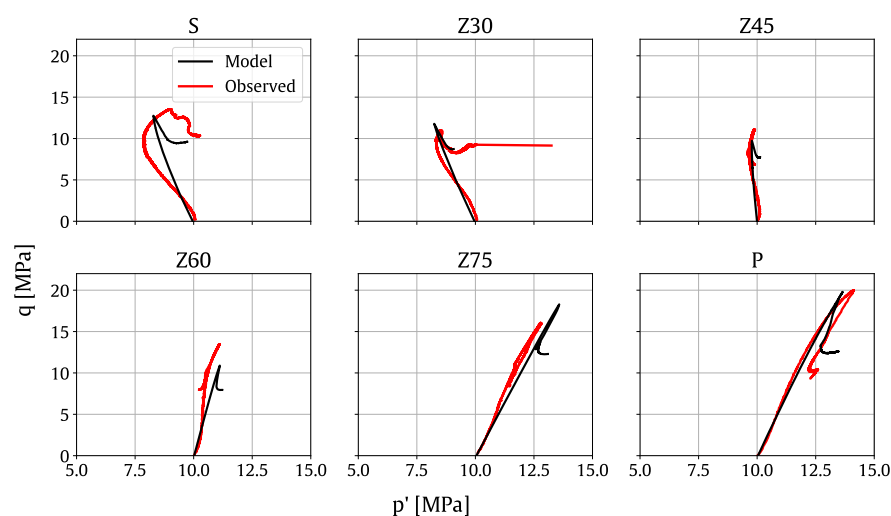


Figure 10. Modeled (black) and measured (red) mean effective stress p' [MPa] versus deviatoric stress q [MPa] of specimens with different bedding angles.

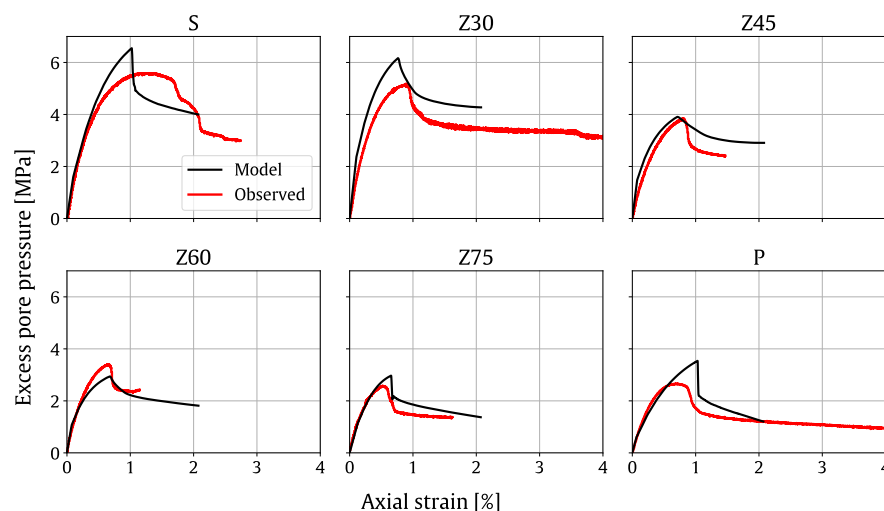


Figure 11. Modeled (black) and measured (red) axial strain ϵ [%] versus excess pore pressure p [MPa] of specimens with different bedding angles.

5.2. GT Experiment Model

Using the material parameters listed in Table 2, together with the permeability evolution described by Equations (12) and (13), a good agreement is obtained between the modeled and measured pressure evolution in the injection interval (Figure 12). The pressure response predicted using the COMBA constitutive model closely matches the response previously obtained using a ubiquitous-joint formulation [6], shown by the dashed colored lines in Figure 12. In both approaches, a good agreement with the measured injection pressure is achieved using the same hydraulic and (poro-)elastic parameters. The only notable difference is that the ubiquitous-joint model required slightly larger values of the empirical permeability constant b_2 to reproduce the observed pressure evolution.

The remaining modeled pressure and gas saturation curves correspond to evaluation points located at increasing down-dip distances from the injection interval. Up to the beginning of May 2023, gas migration remains confined within approximately 0.25 m of the injection interval, after which both gas saturation and pore pressure rapidly increase at the 0.25 m evaluation point. Following the pressure drop, gas migration accelerates, as indicated by the subsequent increase in gas saturation and pore pressure at the remaining evaluation points. For comparison, the pressure evolution predicted by the ideal gas law is also shown. The deviation between the ideal gas pressure and the measured injection pressure becomes apparent at approximately 2 MPa, indicating the onset of gas entry into the clay.

The stress evolution of a clay element located near the bottom of the injection interval is shown in Figure 13. The upper panel shows the evolution of the effective normal and shear stresses acting on the bedding plane, together with the corresponding Mohr circles and the peak and residual Mohr–Coulomb failure envelopes. The middle and lower panels show the pore pressure and accumulated plastic shear strain in the same element, respectively. As pore pressure increases, the stress state progressively approaches the peak failure envelope, although the stresses resolved on the bedding plane do not fully reach it. The highlighted blue Mohr circle (day 293) shows the stress state immediately before the onset of plastic deformation, whereas the red Mohr circle (day 295) shows the stress state immediately after plastic deformation has initiated. Between these two states, the stresses resolved on the bedding plane move to the residual Mohr–Coulomb failure envelope. Plastic shear strain first develops at approximately day 295 and increases to approximately 31 $\mu\epsilon$. At the onset of plastic deformation, the stresses resolved on the bedding plane shift toward the residual Mohr–Coulomb failure envelope. This is followed by a rapid decrease in pore pressure in

the selected element from 3.35 to 2.56 MPa. At approximately day 304, coinciding with the measured and modeled pressure drop in the injection interval, the accumulated plastic shear strain increases rapidly to approximately $158 \mu\epsilon$. This is accompanied by a rapid increase in pore pressure to approximately 3.6 MPa, followed by a gradual decrease to approximately 2.6 MPa.

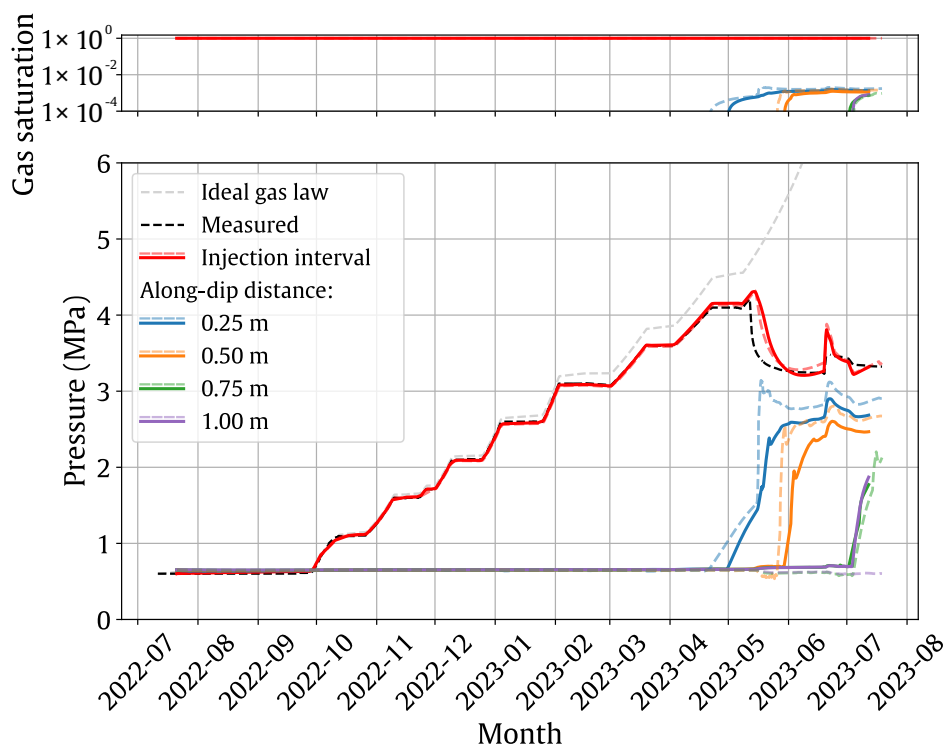


Figure 12. Modeled gas saturation (**top**) and pore pressure evolution (**bottom**) during the GT experiment. Colored curves represent the injection interval and observation locations at increasing down-dip distances (0.25, 0.50, 0.75, and 1.00 m) from the injection interval. Solid colored lines show the COMBA model results, while dashed colored lines show the corresponding ubiquitous-joint model results from Nuus et al. [6]. The black dashed line shows the measured injection pressure, and the gray dashed line shows the pressure predicted by the ideal gas law.

Figure 14 compares the modeled permeability parallel to the bedding plane one week after the initiation of the injection pressure drop using the COMBA model (left) and the ubiquitous-joint model of Nuus et al. [6] (right). In the COMBA model, the largest permeability enhancement develops at the lower end of the injection interval in the down-dip direction and at the upper end in the up-dip direction. Most activated elements exceed $1 \times 10^{-17} \text{ m}^2$, with peak permeabilities approaching $1 \times 10^{-15} \text{ m}^2$. The permeability-enhanced zone extends approximately 0.77 m in the down-dip direction and 0.96 m in the up-dip direction from the injection interval. In comparison, the ubiquitous-joint model shows a shorter down-dip extent of approximately 0.5 m, with the strongest permeability enhancement concentrated in the uppermost and lowermost mesh layers, reaching approximately $1.9 \times 10^{-16} \text{ m}^2$. The COMBA model results in activation of more elements immediately adjacent to the injection interval on the down-dip side, whereas the ubiquitous-joint model shows more extensive activation on the up-dip side and, overall, a larger number of activated elements directly surrounding the injection interval. However, the permeability of these surrounding elements is generally higher in the ubiquitous-joint model, reaching approximately $3 \times 10^{-17} \text{ m}^2$, compared with values around $1 \times 10^{-17} \text{ m}^2$ in the COMBA model.

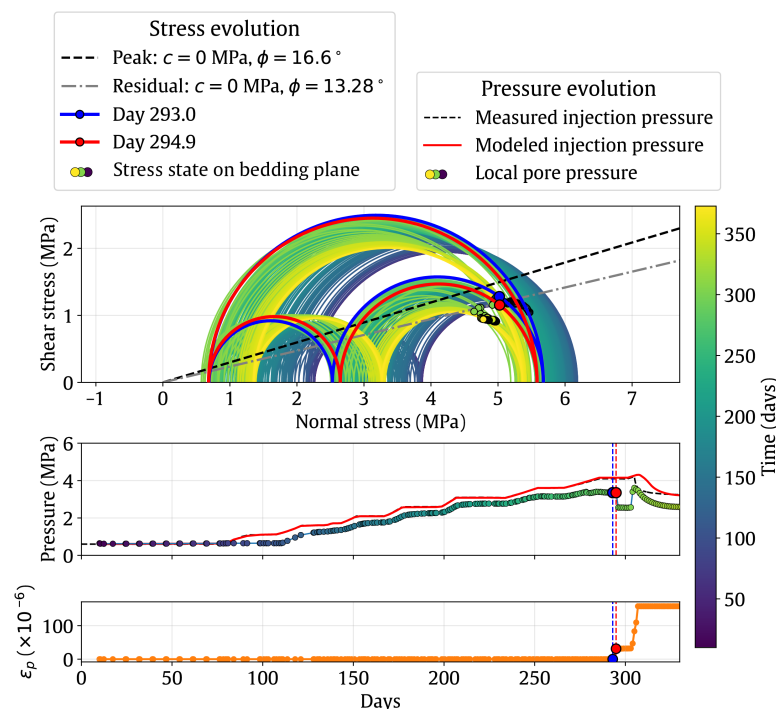


Figure 13. Stress evolution of a clay element near the bottom of the injection interval. Upper panel: Mohr circles and effective normal and shear stresses acting on the bedding plane, with peak and residual Mohr–Coulomb failure envelopes. Blue and red Mohr circles indicate the stress states immediately before (day 293) and after (day 295) the onset of plastic deformation. Middle panel: pore pressure evolution of the clay element and injection interval. Lower panel: accumulated plastic shear strain evolution of the clay element.

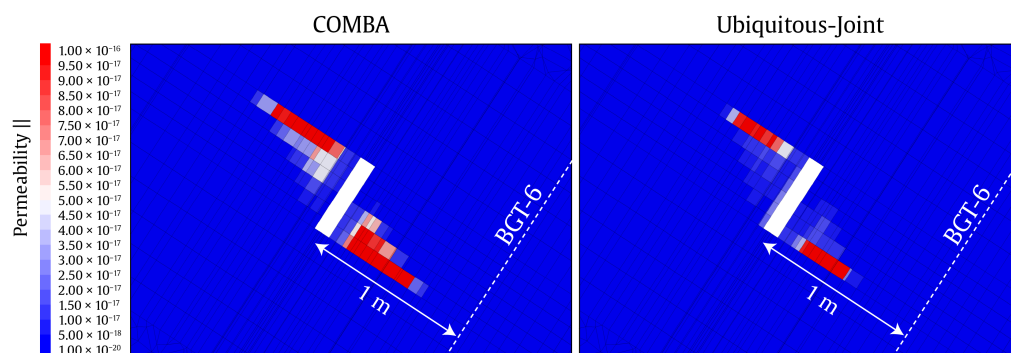


Figure 14. Cross-sections of the modeled permeability parallel to the bedding plane one week after the initiation of the injection pressure drop using the COMBA model (left) and the ubiquitous-joint model of Nuus et al. [6] (right).

The evolution of the measured and modeled strain along the fiber-optic cable in borehole BGT-6 is shown in Figure 15. The strain profiles represent the difference between one day before the initiation of the injection pressure drop and 5, 10, 15, and 25 days thereafter. Borehole BGT-6 is located down-dip from the injection interval (Figure 2) and exhibits the strongest deformation signal of the evaluated fiber-optic boreholes. Results for the additional boreholes BGT-4 and BGT-8, located along strike of the bedding relative to the injection interval, are presented in Appendix A.

The measured strain profiles are compared with the numerical results obtained using both the COMBA constitutive model used in this study and the ubiquitous-joint formulation of Nuus et al. [6]. In the measurements, the extension signal develops slightly below the equivalent depth of the injection interval projected onto the fiber-optic cable. This

localization is reproduced by both constitutive models, with the strongest modeled extension developing near the lower end of the equivalent injection interval in the down-dip direction, although the maximum is predicted at a slightly shallower depth than observed.

The two constitutive models differ substantially in the predicted magnitude and temporal evolution of the accumulated extension. Using the COMBA constitutive model, a localized extension of approximately $38 \mu\epsilon$ is predicted after 5 days, compared with a measured maximum extension of approximately $82 \mu\epsilon$. The maximum modeled extension subsequently increases to approximately 81, 166, and $314 \mu\epsilon$ after 10, 15, and 25 days, respectively. In contrast, the ubiquitous-joint model predicts only limited deformation during the first 15 days, with the maximum extension increasing from approximately 2 to $20 \mu\epsilon$, and reaching only about $78 \mu\epsilon$ after 25 days. A similar trend is observed for the boreholes located approximately along-strike of the bedding (Appendix A), where the COMBA constitutive model predicts an earlier onset of extension than the ubiquitous-joint formulation, followed by continued accumulation of deformation.

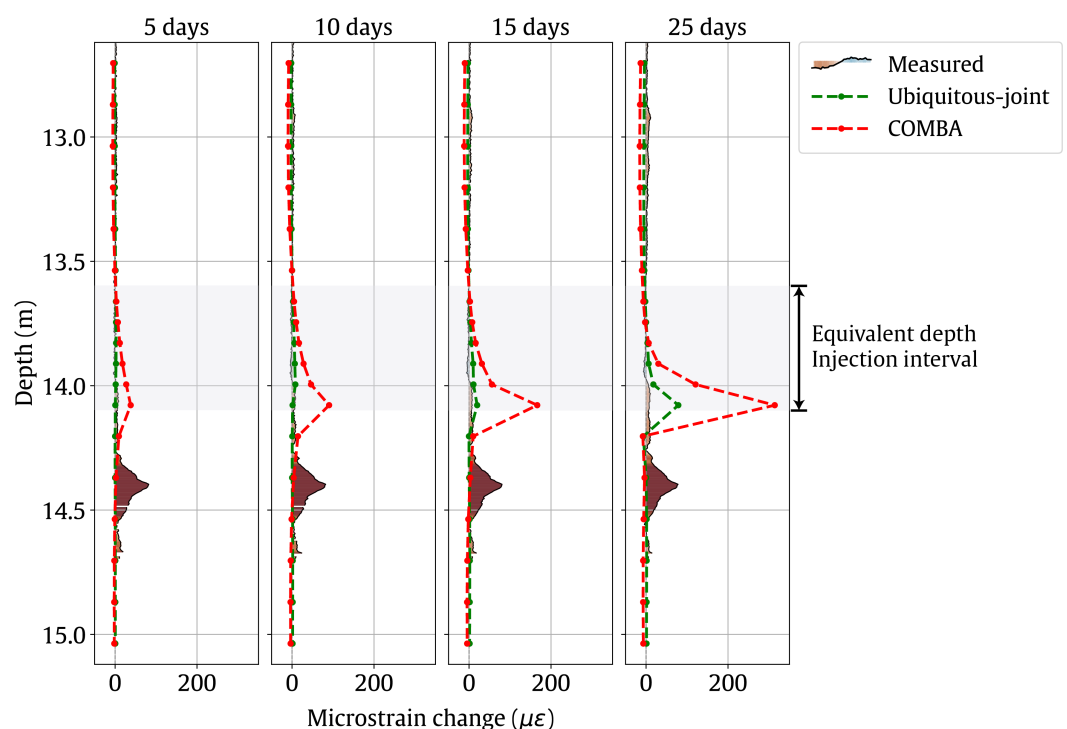


Figure 15. Modeled and measured strain changes along the fiber-optic cable in borehole BGT-6 (down-dip) between one day before and 5, 10, 15, and 25 days after the onset of the injection pressure drop. The COMBA model (red) is compared with the ubiquitous-joint model (green). The light gray shaded region indicates the equivalent depth of the injection interval.

6. Discussion

6.1. Evaluation Using the CU Triaxial Tests

The objective of the laboratory simulations was to evaluate the capability of the COMBA constitutive model to reproduce the anisotropic hydro-mechanical behavior of OPA observed under controlled laboratory conditions. Successful reproduction of the laboratory response increases confidence in applying the constitutive model to the in situ GT experiment.

For the *joint set 1* specimens, the adopted calibration procedure based on the Mohr circles (Figures 5 and 6) resulted in peak and residual strength parameters that reasonably reproduce the measured peak and residual deviatoric stresses for the different bedding orientations (Figure 9). In this calibration, failure was assumed to occur predominantly

along the bedding planes for specimens with bedding orientations between 30° and 75°, although some contribution of matrix shearing to the observed failure cannot be excluded. For example, if the Z30 and Z45 specimens had instead been included in the calibration of *joint set 2*, the calibrated strength parameters for both joint sets would likely differ, while a similar reproduction of the measured peak and residual strengths would still be targeted. However, because the introduction of a second joint set substantially increases the complexity of the calibration, and the response of the specimens between 30° and 75° is already reproduced reasonably well using the bedding-oriented joint set, these specimens were retained within the *joint set 1* calibration.

In addition to reproducing the strength, the simulations capture the anisotropic mechanical response reflected by the different slopes of the deviatoric stress–axial strain curves. This behavior is achieved through the explicit representation of the bedding orientation and the assignment of orientation-dependent joint stiffness values. The modeled effective stress paths (Figure 10) further demonstrate that the constitutive model reproduces the anisotropic hydro-mechanical response of the *joint set 1* specimens reasonably well, while the corresponding excess pore-pressure evolution is also captured satisfactorily.

The calibration focused primarily on reproducing the peak and post-peak behavior rather than the detailed hardening response. Consequently, no extensive calibration of the hardening law was performed, and the initial friction angle was assumed equal to the residual friction angle. Despite this simplification, the model provides a good overall representation of the observed mechanical behavior for the *joint set 1* specimens.

Application of the COMBA constitutive model to the *joint set 2* specimens proved more challenging. Since these specimens are not expected to fail predominantly along the bedding planes, an additional joint set was introduced to represent the observed failure orientation. Reproducing the pronounced hardening behavior of the S specimen required a substantially lower initial friction angle than the residual friction angle (Figure 7). Furthermore, simulations of the S specimen overpredicted the excess pore-pressure response, resulting in an earlier onset of failure than observed experimentally. To delay the onset of failure while maintaining the same hydraulic parameters used for the *joint set 1* specimens, the cohesion was changed from a constant value of 0.5 MPa to a strain-hardening law that increases from 0.5 MPa to 1.4 MPa, which improved the agreement with the experimental response of the S specimen. In addition to the strength parameters, the stiffness of *joint set 2* was adjusted to improve the combined agreement with the S and P specimens, with a normal stiffness of 2.4 GPa/m adopted in the final calibration. An additional sensitivity simulation in which the normal stiffness of joint set 2 was increased from the adopted value of 2.4 GPa/m to an arbitrarily large value of 1.0×10^5 GPa/m showed relatively little effect on the S specimen, but resulted in a poorer representation of the peak and residual deviatoric stress and excess pore-pressure evolution of the P specimen (Appendix A Figure A3). Altogether, the adopted approach reproduces the principal anisotropic trends observed in both the S and P specimens, but requires a considerably more elaborate calibration than for the *joint set 1* specimens. The sensitivity to the parameters of *joint set 2* also introduces uncertainty in the predictive capability of the model for configurations in which this additional joint set controls the response.

The laboratory simulations therefore demonstrate that the COMBA constitutive model is capable of reproducing the dominant anisotropic mechanical and hydro-mechanical behavior of OPA. Although the implementation becomes considerably more complex when deformation is not governed primarily by slip along the bedding planes, the overall agreement with the laboratory observations provides confidence that the constitutive model is suitable for application to the GT experiment, corresponding also to HyMar Task 3. Compared with the constitutive models developed by the other DECOVALEX teams [11],

the COMBA model shows somewhat larger discrepancies for the S and P specimens. More advanced anisotropic formulations, such as the model of Radeisen et al. [10], which combines anisotropic elasticity with a microstructure-tensor-based anisotropic yield criterion and hardening–softening behavior, provide a closer representation of the experimental response for these orientations. In contrast, for the Z45 specimen, where deformation is predominantly controlled by the bedding plane, the COMBA model performs comparably to, or better than, the other approaches. A comprehensive comparison of the different constitutive models and their results is provided by Nguyen et al. [11]. The main advantage of COMBA is its straightforward implementation of bedding-controlled anisotropic elasticity combined with strain hardening and softening within FLAC3D, and its direct applicability within the existing TOUGH3–FLAC3D framework. This makes the model particularly suitable for bedding-controlled deformation, as in the *joint set 1* specimens and the GT experiment, while its advantages diminish when additional failure orientations are required, as for the S and P specimens.

6.2. Application to the GT Experiment

6.2.1. Injection Pressure Response

Following the laboratory calibration and evaluation, the COMBA constitutive model was applied to the coupled hydro-mechanical model of the GT experiment. Compared with the ubiquitous-joint formulation of Nuus et al. [6], the principal modification is the explicit representation of the mechanical stiffness of the bedding planes through the COMBA constitutive model, while the hydraulic formulation and the remaining elastic and poro-elastic parameters were kept unchanged. This allows differences in the simulated hydro-mechanical response to be directly related to the explicit representation of bedding-controlled anisotropic deformation.

Using the material parameters presented in Table 2, a good agreement was obtained between the modeled and measured pressure evolution in the injection interval. Similar to the ubiquitous-joint approach, the observed pressure response could be reproduced using the strain-dependent permeability formulation. However, a reduction in the empirical permeability constant b_2 from 27,000 to 21,000 for permeability parallel to the bedding was required to obtain a comparable pressure response. Within the adopted permeability formulation, the permeability enhancement associated with the development of dilatant flow pathways is related to accumulated plastic shear strain through the empirical constant b_2 . The lower value of b_2 used for the COMBA model reflects the greater accumulation of plastic shear strain predicted by this model, such that a lower permeability enhancement per unit of accumulated plastic shear strain is required to obtain a comparable pressure response. Despite the lower value of b_2 , the resulting permeability enhancement is of a similar order of magnitude in both models, although its spatial distribution and peak values differ (Figure 14). The COMBA model shows a greater down-dip extent of permeability enhancement, which is consistent with the earlier development of the modeled extension signal along BGT-6. In contrast, the ubiquitous-joint model shows a smaller down-dip extent, but permeability enhancement occurs in a larger number of elements directly surrounding the injection interval. This more concentrated enhancement around the injection interval may explain why a similar injection pressure drop is obtained with both constitutive models, regardless of the differences in the spatial extent of the enhanced zone.

6.2.2. Comparison with Distributed Fiber-Optic Strain Measurements

This difference becomes evident in the comparison with the distributed fiber-optic strain measurements in borehole BGT-6 (Figure 15), while both constitutive models reproduce the location of the extension signal below the equivalent depth of the injection

interval reasonably well, they differ substantially in the predicted temporal evolution of the deformation. The ubiquitous-joint model captures the localization of the extension but predicts only limited deformation during the first two weeks following the pressure drop, with a pronounced extension signal developing only after approximately 25 days. In contrast, the COMBA constitutive model predicts localized extension immediately following the pressure drop, resulting in a considerably better agreement with the measured timing of deformation. The modeled extension reaches approximately half of the measured magnitude after 5 days and approaches the measured values after approximately 10 days.

A similar direction-dependent deformation pattern is predicted by both constitutive models, with the largest and more localized extension occurring in the down-dip direction, whereas a smaller and more uniform extension is predicted along-strike (Appendix A Figures A1 and A2). Along BGT-4, the measured response is predominantly compressive and is not reproduced by either model. A more detailed discussion of the measured distributed fiber-optic strain responses is provided by Cuss et al. [5], while the differences between the modeled and measured deformation patterns are discussed by Nuus et al. [6]. Focusing on the temporal evolution of the extension, the rapid extension observed along BGT-6 and BGT-8 is reproduced considerably earlier by the COMBA model than by the ubiquitous-joint model.

Despite the improved timing of the extension response, the continued accumulation of plastic shear strain in the COMBA model results in a significant overestimation of the measured extension at later times. A similar tendency is also observed for the ubiquitous-joint formulation, although the slower accumulation of plastic shear strain results in better agreement with the measured strain approximately 25 days after the pressure drop. This behavior suggests that the coupling between plastic shear strain and permeability enhancement in the current permeability evolution model may contribute to the continued accumulation of plastic shear strain, rather than this behavior being solely related to the constitutive formulation itself. As permeability increases, the permeability-enhanced pathway continues to propagate, promoting further plastic deformation and consequently additional permeability enhancement. One possible improvement would be to introduce a criterion that limits or halts permeability evolution once the pressure reduction associated with pathway formation occurs, thereby reducing the continued accumulation of plastic shear strain and the associated overestimation of deformation. A more detailed investigation of this coupling and the development of alternative permeability evolution formulations are, however, beyond the scope of the present study, which aims to compare the COMBA and ubiquitous-joint constitutive models when applied to the GT experiment.

6.2.3. Failure Process During Pathway Formation

Additional insight into the modeled failure process is provided by the stress evolution of a representative clay element located near the bottom of the injection interval (Figure 13) and the spatial distribution of accumulated plastic shear strain and permeability before and after the modeled pressure drop (Figure 16).

Plastic shear strain in the representative tracked element develops before the modeled pressure drop (Day 298) in the injection interval, indicating that shear failure initiates locally before a continuous permeable pathway is established. As shown in the top-left panel of Figure 16, the tracked element is already part of a locally developed region of accumulated plastic shear strain prior to the pressure drop. However, this region remains separated from the injection interval by one intact element. Since permeability enhancement is directly related to accumulated plastic shear strain in the model, the absence of plastic strain in this intervening element means that its permeability remains at the initial value of $5 \times 10^{-20} \text{ m}^2$. Consequently, a continuous permeability-enhanced connection between the locally failed

region and the injection interval has not yet been established, as shown in the bottom-left panel of Figure 16. The initial pressure drop observed in the tracked element is therefore attributed to pressure redistribution within this locally connected region. Following failure of the intervening element (right panels in Figure 16), the enhanced-permeability region becomes hydraulically connected to the injection interval, allowing gas to rapidly enter the previously disconnected region. This explains the temporary pore-pressure increase observed in the tracked element immediately after the injection-interval pressure drop, before pressure gradually dissipates throughout the enhanced pathway (Figure 13). At the same time, additional permeability-enhanced connections develop along the upper part of the injection interval, increasing the hydraulic connectivity of the pathway and contributing to the modeled pressure drop in the injection interval.

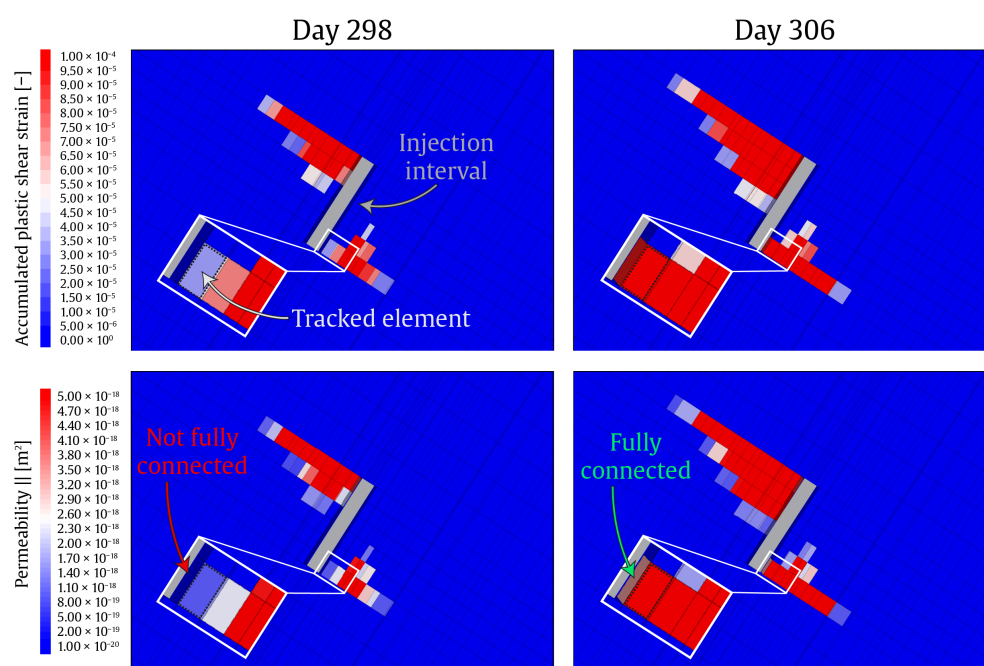


Figure 16. Distribution of accumulated plastic shear strain (**top**) and permeability (**bottom**) before (day 298) and after (day 306) the modeled pressure drop in the injection interval.

The stress evolution in Figure 13 provides further insight into the mechanical mechanism governing pathway formation. Despite the increase in pore pressure, the bedding plane remains under substantial effective normal compression when shear failure and gas breakthrough occur. Although tensile or bedding-plane opening mechanisms are not explicitly represented in the adopted permeability formulation, the modeled stress state does not reach tensile conditions during the simulated gas injection. The modeled stress evolution therefore suggests that shear-slip dilation along the bedding planes is a more likely mechanism for gas breakthrough than tensile opening [5,6].

It should be noted that the resolved stresses on the bedding plane shown in Figure 13 never fully reach the peak Mohr–Coulomb failure envelope. The closest stored stress state prior to yielding lies approximately 0.22 MPa below the peak failure envelope. This is most likely a consequence of the constitutive return-mapping algorithm in FLAC3D, whereby stresses are corrected back to the admissible yield surface once yielding occurs before they are stored for output.

6.3. Limitations and Future Work

The present study demonstrates that the COMBA constitutive model is capable of reproducing the principal hydro-mechanical behavior observed in both laboratory and

field-scale experiments. Nevertheless, several limitations remain. First, the current implementation assumes deformation to occur along predefined joint sets, while this is well suited for the *joint set 1* specimens and the GT experiment, additional failure planes were required to reproduce the behavior of the *joint set 2* specimens, increasing the complexity of the calibration. In particular, the orientation of *joint set 2* was prescribed at 58° , representing an assumed favorably oriented failure plane rather than a uniquely determined failure orientation. A different prescribed orientation would change the resolved stresses and consequently the calibrated cohesion and friction angle, resulting in a non-unique calibration. Second, the current permeability evolution formulation results in continued accumulation of plastic shear strain following pathway formation, leading to an overestimation of long-term deformation. Future work should therefore focus on introducing a mechanism that limits permeability evolution after pathway stabilization, while retaining the improved prediction of the onset of deformation demonstrated in this study.

A parameter optimization and sensitivity analysis would be valuable for further evaluating the field-scale application of COMBA. This could include the joint stiffness parameters, the empirical parameter b_2 controlling the relationship between plastic shear strain and permeability enhancement, and hardening–softening behavior. In particular, the hardening behavior observed in the CU tests was not implemented in the GT model in order to maintain a more direct comparison with the previous ubiquitous-joint model, which did not account for hardening. Although the rapid development of the extension signals observed in the distributed fiber-optic strain measurements suggests that permeability enhancement and subsequent strain softening may dominate the response following pathway formation, the influence of hardening prior to and during pathway initiation remains uncertain and would be valuable to investigate in future work.

The implications of the predicted permeability-enhancement patterns for the long-term sealing capacity of the host rock were not investigated in the present study. The simulated extents of permeability enhancement are specific to the duration and injection conditions of the GT experiment and should therefore not be interpreted as predictions of the long-term extent of the affected zone. Over longer timescales, continued pressure evolution and stress redistribution may alter both the extent and spatial distribution of the permeability-enhanced region. Future work could therefore assess the long-term evolution of these pathways and their implications for sealing capacity using different constitutive models.

7. Conclusions

This study evaluated the capability of the COMBA constitutive model to reproduce the anisotropic hydro-mechanical behavior of OPA at both laboratory and in situ scale. The constitutive model was first calibrated and evaluated using CU triaxial tests covering multiple bedding orientations before being applied to the coupled hydro-mechanical simulation of the GT gas injection experiment at the Mont Terri Rock Laboratory.

The laboratory simulations demonstrate that the COMBA constitutive model is capable of reproducing the principal anisotropic mechanical and hydro-mechanical behavior observed in the CU triaxial tests. In particular, the model captures the strength anisotropy associated with bedding orientation, the corresponding stress paths, and the excess pore-pressure response for specimens failing predominantly along bedding. Although reproducing the behavior of specimens failing away from the bedding required the introduction of an additional failure joint, the overall agreement with the experimental observations provides confidence in applying the constitutive model to field-scale simulations.

Application of the COMBA constitutive model to the GT experiment resulted in a pressure evolution that closely reproduces the measured injection pressure and is comparable to that previously obtained using a ubiquitous-joint formulation. However, the COMBA

constitutive model provides an improved representation of the timing of the extension response, particularly in the down-dip direction along BGT-6, predicting the onset of localized extension shortly after the pressure drop rather than several weeks later. The agreement is direction-dependent and the measured predominantly compressive response along BGT-4 is not reproduced by either model. This suggests that the explicit representation of bedding stiffness improves the simulated timing of the extension associated with dilatant pathway development, particularly in the down-dip direction, while maintaining a comparable hydraulic response. The stress evolution during pathway formation further indicates that the bedding remains under substantial effective normal compression at the onset of gas breakthrough, supporting shear–slip dilation along the bedding planes as a more likely mechanism for gas breakthrough than tensile opening within the conditions investigated.

The simulations also indicate that both the COMBA and ubiquitous-joint approaches continue to accumulate plastic shear strain following pathway formation, resulting in an overestimation of the deformation at later times. This behavior may partly result from the coupling between plastic shear strain and permeability enhancement in the adopted permeability evolution formulation. Future work should therefore focus on improving the permeability evolution formulation to better represent pathway stabilization while retaining the improved prediction of the timing of the extension response demonstrated in this study.

Author Contributions: Conceptualization, M.N. and A.P.R.; methodology, M.N., A.P.R. and G.G.; software, M.N., A.P.R. and G.G.; validation, M.N., G.G. and J.R.; formal analysis, M.N.; investigation, M.N.; data curation, M.N. and A.P.R.; writing—original draft preparation, M.N.; writing—review and editing, M.N., A.P.R., G.G. and J.R.; visualization, M.N.; supervision, A.P.R. and J.R.; project administration, A.P.R.; funding acquisition, A.P.R. All authors have read and agreed to the published version of the manuscript.

Funding: This study was supported by a research agreement between the SED and the Swiss Federal Nuclear Safety Inspectorate (ENSI) to conduct research for the DECOVALEX-2027 project. The authors appreciate and thank the DECOVALEX-2027 Funding Organizations Andra, BASE, BGE, BGR, CAS, CNSC, COVRA, DynaFrax (KORAD), US DOE, ENRESA, ENSI, KAERI, KIGAM, NWMO, RWM, SSM, SÚRAO, and Taipower for the financial and technical support of the work described in this paper.

Data Availability Statement: The experimental data used for the laboratory-scale simulations are openly available in the OSF repository of Winhausen et al. [12] at <https://osf.io/5s2cb/overview> (accessed on 30 September 2025). The experimental and modeled data of the GT experiment of Nuus et al. [6] are openly available in the ETH Zürich Research Collection at <https://www.research-collection.ethz.ch/entities/researchdata/0df75c5e-1488-47d3-a3da-af4cc9816c65> (accessed on 30 September 2025). Additional modeled data as part of the present study are available from the corresponding author upon request.

Acknowledgments: DECOVALEX is an international research project comprising participants from industry, government, and academia, focusing on the development of understanding, models, and codes related to complex coupled problems in sub-surface geological and engineering applications, including the geologic disposal of radioactive waste; DECOVALEX-2027 is the current phase of the project. The statements made in the paper are solely those of the authors and do not necessarily reflect those of the funding organizations. The GT experiment was made possible through the support of the Mont Terri Consortium project partners, including ENSI (CH), Swisstopo (CH), ETH Zürich (CH), FANC (BE), BASE (DE), BGR (DE), and SCK CEN (BE). We thank Manuel Sentis and Bastian Graupner (ENSI) for useful comments on a preliminary version of the manuscript.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

COMBA	Columnar-basalt
OPA	Opalinus Clay
CU	Consolidated undrained

Appendix A. Additional Fiber-Optic Strain Comparisons

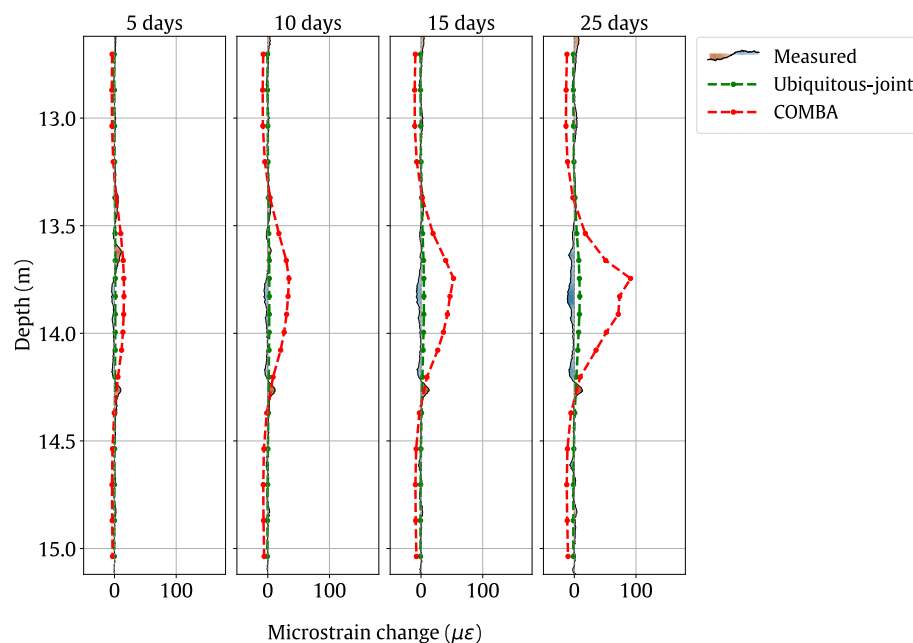


Figure A1. Modeled and measured strain changes along the fiber-optic cable in borehole BGT-4 (along strike) between one day before and 5, 10, 15, and 25 days after the onset of the injection pressure drop. The COMBA model (red) is compared with the ubiquitous-joint model (green).

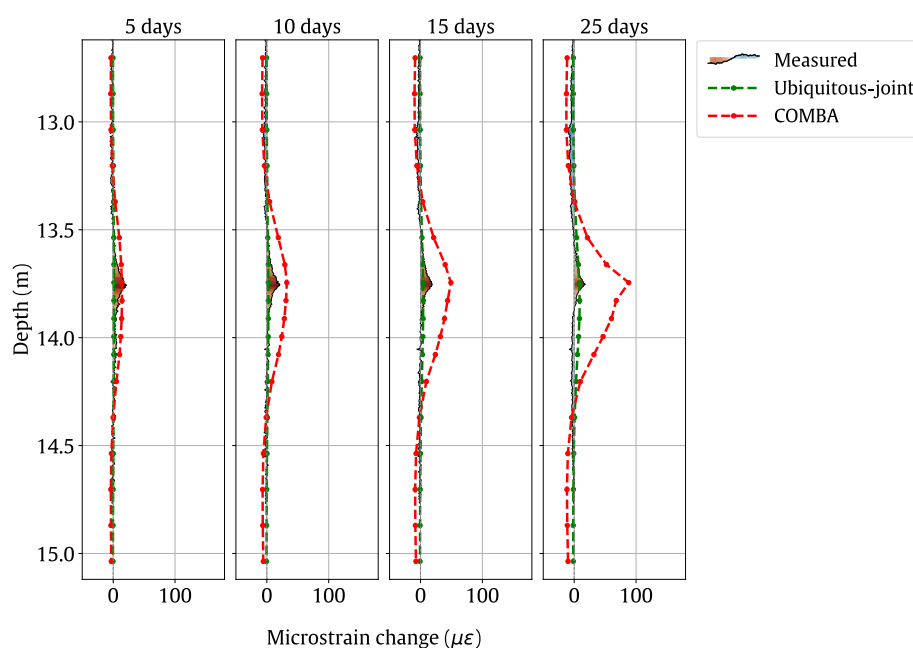


Figure A2. Modeled and measured strain changes along the fiber-optic cable in borehole BGT-8 (along strike) between one day before and 5, 10, 15, and 25 days after the onset of the injection pressure drop. The COMBA model (red) is compared with the ubiquitous-joint model (green).

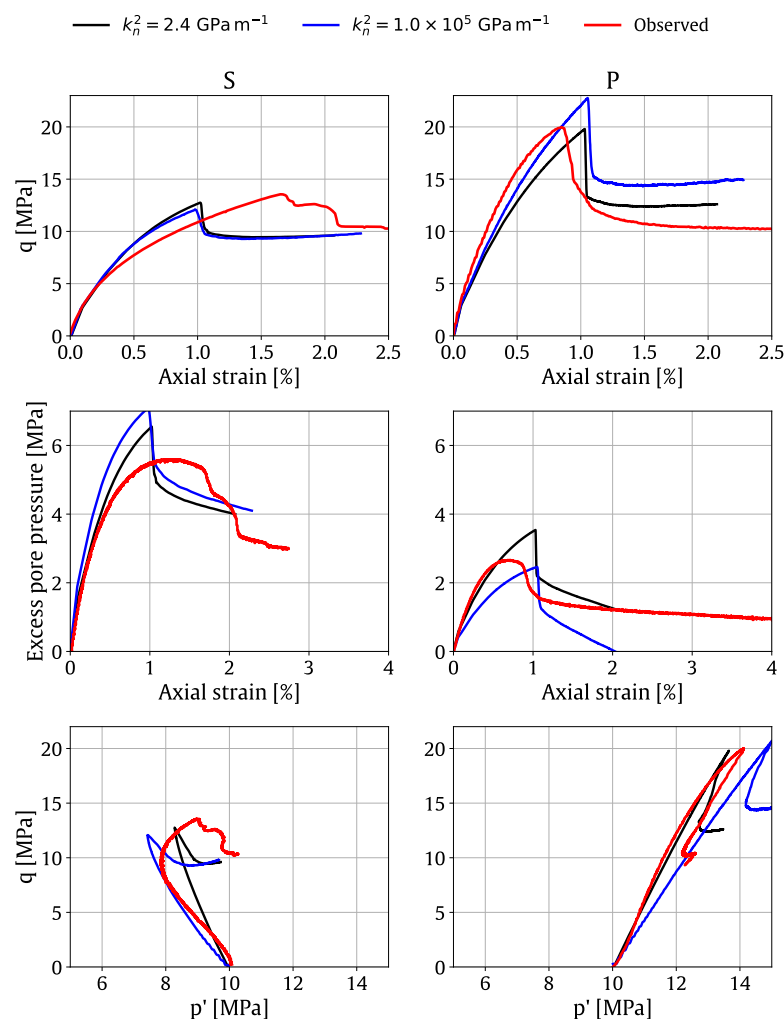


Figure A3. Comparison of the modeled response of the S and P specimens using $k_n^2 = 2.4 \text{ GPa/m}$ (black) and $k_n^2 = 1.0 \times 10^5 \text{ GPa/m}$ (blue) with the experimental observations (red). The top row shows axial strain versus deviatoric stress q , the middle row axial strain versus excess pore pressure, and the bottom row mean effective stress p' versus deviatoric stress q .

References

1. Corkum, A.; Martin, C. The mechanical behaviour of weak mudstone (Opalinus Clay) at low stresses. *Int. J. Rock Mech. Min. Sci.* **2007**, *44*, 196–209. [\[CrossRef\]](#)
2. Kulenkampff, J.; Zakhnini, A.; Gründig, M.; Lippmann-Pipke, J. Quantitative experimental monitoring of molecular diffusion in clay with positron emission tomography. *Solid Earth* **2016**, *7*, 1207–1215. [\[CrossRef\]](#)
3. NAGRA. *Effects of Post-Disposal Gas Generation in a Repository for Low- and Intermediate-Level Waste Sited in the Opalinus Clay of Northern Switzerland*; Technical Report 08-07; Nagra: Wettingen, Switzerland, 2008.
4. Marschall, P.; Horseman, S.; Gimmi, T. Characterisation of gas transport properties of the Opalinus Clay, a potential host rock formation for radioactive waste disposal. *Oil Gas Sci. Technol.* **2005**, *60*, 121–139. [\[CrossRef\]](#)
5. Cuss, R.J.; Gisiger, J.; Rinaldi, A.P.; Bird, E.J.M.; Jaeggi, D.; Nuus, M.H.; Sentis, M.L.; Graupner, B.J.; Bernier, F.; Magri, F.; et al. The role of gas injection rate on the advective movement of gas in Opalinus Clay at the field scale. *Saf. Nucl. Waste Dispos. Discuss.* **2026**, *in review*. [\[CrossRef\]](#)
6. Nuus, M.; Rinaldi, A.P.; Cuss, R.; Sentis, M.; Graupner, B.; Magri, F.; Bernier, F. Modeling in situ gas flow and coupled hydro-mechanical processes in the Opalinus Clay. *Int. J. Rock Mech. Min. Sci.* **2026**, *206*, 106643. [\[CrossRef\]](#)
7. Pietruszczak, S.; Mroz, Z. Formulation of anisotropic failure criteria incorporating a microstructure tensor. *Comput. Geotech.* **2000**, *26*, 105–112. [\[CrossRef\]](#)
8. Salager, S.; François, B.; Nuth, M.; Laloui, L. Constitutive analysis of the mechanical anisotropy of Opalinus Clay. *Acta Geotech.* **2013**, *8*, 137–154. [\[CrossRef\]](#)

9. Xu, W.; Shao, H.; Marschall, P.; Hesser, J.; Kolditz, O. Analysis of flow path around the sealing section HG-A experiment in the Mont Terri Rock Laboratory. *Environ. Earth Sci.* **2013**, *70*, 3363–3380. [[CrossRef](#)]
10. Radeisen, E.; Shao, H.; Hesser, J.; Wang, W. Hydro-Mechanical Modelling of Anisotropic Deformation and Failure Behaviour of Opalinus Clay Under Saturated and Unsaturated Conditions. *Minerals* **2026**, *16*, 279. [[CrossRef](#)]
11. Nguyen, T.S.; Chittenden, N.; Cuss, R.; Graupner, B.; Guo, G.; Nicholas, J.; Nuus, M.; Damians, I.P.; Olivella, S.; Radeisen, E.; et al. Constitutive model development to assess dilatant gas flow in bedded argillaceous rocks. *Res. Sq.* **2026**, preprint. [[CrossRef](#)] [[PubMed](#)]
12. Winhausen, L.; Khaledi, K.; Jalali, M.; Bretthauer, M.; Amann, F. The anisotropic behavior of a clay shale: Strength, hydro-mechanical couplings and failure processes. *J. Geophys. Res. Solid Earth* **2023**, *128*, e2023JB027382. [[CrossRef](#)]
13. Meng, G.; Detournay, C.; Cundall, P. Formulation and application of a constitutive model for multijointed material to rock mass engineering. *Int. J. Geomech.* **2020**, *20*, 04020044. [[CrossRef](#)]
14. Itasca Consulting Group, Inc. *FLAC3D—Fast Lagrangian Analysis of Continua in Three Dimensions, Version 9.0*; Itasca Consulting Group, Inc.: Minneapolis, MN, USA, 2023.
15. Winhausen, L.; Khaledi, K.; Jalali, M.; Urai, J.L.; Amann, F. Failure mode transition in Opalinus Clay: A hydro-mechanical and microstructural perspective. *Solid Earth* **2022**, *13*, 901–915. [[CrossRef](#)]
16. Rinaldi, A.P.; Rutqvist, J.; Luu, K.; Blanco-Martín, L.; Hu, M.; Sentís, M.L.; Eberle, L.; Kaestli, P. TOUGH3-FLAC3D: A modeling approach for parallel computing of fluid flow and geomechanics. *Comput. Geosci.* **2022**, *26*, 1563–1580. [[CrossRef](#)]
17. Biot, M. General three-dimensional theory of poroelasticity. *J. Appl. Phys.* **1941**, *12*, 155–164. [[CrossRef](#)]
18. Guglielmi, Y.; Nussbaum, C.; Rutqvist, J.; Cappa, F.; Jeanne, P.; Birkholzer, J. Estimating perturbed stress from 3 to D borehole displacements induced by fluid injection in fractured or faulted shales. *Geophys. J. Int.* **2020**, *221*, 1684–1695. [[CrossRef](#)]
19. Luckner, L.; Van Genuchten, M.T.; Nielsen, D. A consistent set of parametric models for the two-phase flow of immiscible fluids in the subsurface. *Water Resour. Res.* **1989**, *25*, 2187–2193. [[CrossRef](#)]
20. Jung, Y.; Pau, G.S.H.; Finsterle, S.; Doughty, C.A. *TOUGH3 User's Guide, Version 1.0*; Technical Report LBNL-2001093; Lawrence Berkeley National Laboratory: Berkeley, CA, USA, 2018.
21. Xu, W.; Shao, H.; Hesser, J.; Wang, W.; Schuster, K.; Kolditz, O. Coupled multiphase flow and elasto-plastic modelling of in situ gas injection experiments in saturated claystone (Mont Terri Rock Laboratory). *Eng. Geol.* **2013**, *157*, 55–68. [[CrossRef](#)]
22. Kim, J.; Sonnenthal, E.L.; Rutqvist, J. Formulation and sequential numerical algorithms of coupled fluid/heat flow and geomechanics for multiple porosity materials. *Int. J. Numer. Methods Eng.* **2012**, *92*, 425–456. [[CrossRef](#)]

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.