

Evaluating Discontinuity Behavior in CO₂ Storage Reservoirs: Experimental Data and Numerical Modelling

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ABSTRACT: Understanding the integrity of geological reservoirs for supercritical CO₂ (scCO₂) storage requires a detailed analysis of the hydromechanical behavior of natural discontinuities. This study investigates the influence of scCO₂ exposure on the shear strength and dilatant behavior of rock-rock interfaces in glauconitic sandstone, combining experimental and numerical approaches. A series of direct shear tests were performed on natural discontinuities before and after CO₂ exposure, revealing significant changes in shear strength and dilatancy. These experimental results provide a robust basis for calibrating a numerical model designed to evaluate the long-term hydromechanical behavior of discontinuities under CO₂ pressurization. The numerical model, implemented using the finite element method in COMSOL Multiphysics, simulates biphasic flow within a representative caprock-reservoir-caprock system intersected by mechanical discontinuities. The model incorporates experimentally derived parameters to capture the effects of scCO₂ on the mechanical and hydraulic properties of the discontinuities. A parametric study evaluates various distributions and orientations of discontinuities, investigating their role in fluid migration pathways, capillary pressure alterations, and potential reactivation mechanisms. Key findings demonstrate that scCO₂ exposure not only degrades the shear strength of natural discontinuities but also enhances their hydraulic conductivity, potentially facilitating fluid leakage. The parametric analysis reveals the critical influence of discontinuity geometry and pressurization rates on the stability of reservoir-caprock systems. The implications of these findings are discussed in the context of shadow reservoir mechanics, emphasizing the need for careful monitoring and management of discontinuity networks in scCO₂ storage projects. This study highlights the importance of integrating experimental data with advanced numerical modeling to predict the coupled hydromechanical response of reservoirs to scCO₂ injection. The findings contribute to the safe design and optimization of geological storage systems, offering valuable insights into the long-term stability of storage sites under pressurization conditions.

KEYWORDS: CO₂ storage, COMSOL Multiphysics, discontinuities, shear test, coupled numerical simulation.

1 INTRODUCTION

Researchers from all around the world have become increasingly interested in CO₂ underground storage (Jahanbakhsh et al. (2021), Hawkes et al. (2005), Casagrande et al. (2022), Stroisz et al. (2019)). This topic has become a well-known alternative to mitigating global warming while green energies are studied. In this context, different possible CO₂ injection sites are currently being studied (Rathnaweera et al. (2015), Jahanbakhsh et al. (2021), Marbler et al. (2012)).

Among the suitable formation types for CO₂ storage, depleted oil and gas reservoirs are commonly studied for two reasons. The first one relies on the fact that depleted oil and gas reservoirs present a series of characteristics that make them suitable for long-term CO₂ storage. For instance, these formations have high porosities and permeabilities which indicate great storage volumes and easy injection. The second one is related to the availability of underground information, due to previous geomechanical and hydraulic studies performed for the exploitation of oil and gas.

When considering the feasibility a certain oil and gas reservoir has as CO₂ storage, the long-term integrity of the underground must be studied. As it might be observed in Figure 1, in which a schematic drawing of CO₂ storage is presented, there are different aspects to be considered when studying long-term integrity. On the one hand, the changes produced in the rock matrix due to its exposure to CO₂ should be analyzed. On the other hand, the discontinuities present must be individually studied to analyze the consequences its failure would produce.

Several authors have tackled the study of discontinuities from different points of view. For example, in terms of wellbore cement-reservoir rock and wellbore cement-reservoir rock-caprock discontinuities, Cerasi et al. (2015) and Stroisz et al. (2019) focused their study on the debonding of the interface. Another point of view is the one proposed by Casagrande et al.

(2022), in which the mechanical behavior of the discontinuity is analyzed in terms of its surface roughness. Finally, more authors have addressed discontinuities studying the chemical interactions developed due to their exposure to CO₂ (Jobard (2013), Manzanal et al. (2013), Jahanbakhsh et al. (2021)). However, there seems to be a lack of information in the analysis of the changes produced in the mechanical behavior of discontinuities when exposed to CO₂.

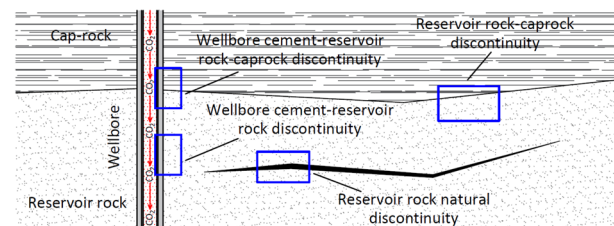


Figure 1. CO₂ underground storage schematic representation.

Once the different rock layers and discontinuities present in the underground storage of CO₂ have been characterized, reservoir-scale numerical studies are conducted. Researchers adopt this practice to analyze the long-term behavior of the reservoir, and verify its integrity is maintained in time (Mortezaei and Vahedifard (2015), Rinaldi et al. (2014), Mazzoldi et al. (2012)). Some of the aspects studied are the effects of fault reactivation such as seismic events and CO₂ leaks (Urpi et al. (2015), Mazzoldi et al. (2012)).

The presented research has as main aim the study of the Salamanca Formation long-term integrity as a CO₂ underground storage. To do this, an experimental study was conducted to assess the evolution of the behavior of natural rock discontinuities due to its exposure to CO₂. These results combined with previous characterization of the reservoir rock and caprock composing the Salamanca Formation, were used as

input parameters for the numerical simulations performed. Poroelastic and hydraulic phenomena were coupled for a better understanding of the geomechanical behavior of the underground, while a two-phase flow analysis considering the injection of CO₂ into the water-saturated underground was developed to study the CO₂ saturation plume.

2 MATERIALS AND METHODS

2.1 Experimental study

2.1.1 Specimen preparation

Prior to specimen preparation, it was necessary to obtain samples from Banco Verde. These were extracted from outcrop due to the high costs associated with obtaining reservoir depth specimens. Since the study focused on analyzing the mechanical properties of natural discontinuities, special attention was paid to extracting blocks that contained the discontinuity studied discontinuity. Afterwards, 5cm-side prisms were extracted, carefully ensuring that the horizontal faces were parallel to the discontinuity (Figure 2.a).

To study the evolution of the properties of natural discontinuities due to their exposure to CO₂, half of the samples were exposed to a CO₂-rich environment. Samples were paired according to their similar properties, considering that, if both were tested, they should present similar results. Half of the discontinuity test specimens were stored in their pristine state. The remaining samples were placed in the carbonation cell (Figure 2.b), where supercritical CO₂ conditions (temperature of 31.48°C and pressure of 7.38 MPa according to Ranjith et al. (2013)) were maintained for 30 days. Once this process was complete, the samples were stored in a temperature and humidity-controlled chamber until they were tested.



Figure 2. a. Discontinuity specimen. b. Carbonation cell.

2.1.2 Direct shear test

Direct shear tests were performed following the ASTM D 5607-16 (2016) guidelines. The natural discontinuity specimen was placed inside the shear box and set with a gypsum mixture. It was carefully verified that the discontinuity matched with the contact plane of the upper and lower parts of the shear box. Considering that both parts of the box had to be independent from each other, the specimen was also fixed independently. In this context, sawdust was placed in the transition between the two parts of the box.

Having properly secured the specimen to the shear box, the direct shear test began. First, the shear box was placed on the testing equipment. Once the axial stresses at which the tests would be performed had been selected, the axial load was applied to the testing device. It should be noted that the axial stresses chosen were 10MPa, 20MPa, and 30MPa, with the aim of covering the possible pressures reached at reservoir depth. Afterwards, the LVDTs were carefully installed. The test began by applying a controlled horizontal load to the top of the shear box, causing a relative displacement at a constant speed of 5 mm/s. The applied horizontal load and the horizontal and

vertical displacements were recorded until the shear stress became constant.

2.2 Numerical simulations

2.2.1 Calculation software and interest parameters

When developing the numerical simulation of CO₂ injection into the Banco Verde stratum of the Salamanca Formation, COMSOL Multiphysics 5.6 calculation software was chosen. This software was selected as it allows coupling phenomena, allowing a comprehensive analysis of the studied problem.

An underground formation composed of interbedded reservoirs and caprocks, crossed by a subvertical discontinuity, into which a flow of CO₂ is injected, was the case study. It was considered appropriate to perform two separate analysis. The first one, a two-phase flow study, carried out to analyze the evolution in saturation of CO₂ along the interbedded rock layers composing the designed underground. The second one, a hydromechanical study, performed with the aim of analyzing the fault reactivation and the tenso-deformational behavior of the reservoir.

For the hydromechanical analysis, the rock layers were considered linear elastic materials. Since the objective was to study the reactivation of the fault, the Mohr-Coulomb failure criterion was proposed. From the coupled study, the shear and effective normal stresses developed over time along the fault were obtained. The point of study was chosen considering fault's reactivation point is usually located along the fault in the surroundings of the interface between the lower caprock and the reservoir into which CO₂ is injected (Urpi et al. (2015)).

Once the fault's reactivation time was determined, it is possible to determine derived results such as the seismic event magnitude. To do this, it was first necessary to determine the associated seismic moment (M_0), defined as:

$$M_0 = \eta d A \quad (1)$$

where η represents the instant shear modulus of the fault, d is the average displacement suffered by the discontinuity, and A is the area of the fault-surface rupture (Hanks and Kanamori (1979)). On the other hand, according to Wells and Coppersmith (1994), the earthquake magnitude (M) is calculated as follows:

$$M = \frac{2}{3} [\log_{10}(M_0) - 9.1] \quad (2)$$

To determine both the seismic moment and the earthquake magnitude, the fault's failure time was used.

2.2.2 Problem design

According to Feruglio (1949), the Salamanca Formation is composed of five different strata. The lower layer, known as Lignitifero, is composed of gray clays with a thickness ranging from 15 to 20 m (TERMAP S.A. (2011)). Directly in contact with the aforementioned is the Glauconítico (10-30 m), a layer of glauconitic sandstones with low clay content. The Fragmentosa layer is characterized for being the thickest layer of the Salamanca Formation (134 m), representing the caprock of the Glauconítico, composed of gray claystone. The two upper strata, Banco Verde and Banco Negro, from bottom to top, represent the shallowest oil and gas deposit in the Golfo San Jorge Basin and its corresponding caprock. The special interest they present as a possible geological storage site for CO₂ lies in the fact that the Banco Verde reservoir rock is partially depleted. In addition, this layer is composed of greenish-gray sandstone with discontinuities (Foix (2009)). According to Rodríguez et al. 2014, Banco Verde is characterized by high porosity and permeability values, making it a suitable reservoir rock for CO₂ injection. The Banco Negro layer represents the

caprock of the Banco Verde reservoir, adding security to the potential underground storage of CO₂. This claystone is composed of dark gray clays, characterized by low permeability values, which make it a potentially effective rock for sealing possible gas leaks.

In terms of the geometric design of the underground, it was considered appropriate to simulate a 1km wide reservoir. Furthermore, considering that the Salamanca Formation is not the shallowest Formation in the Golfo San Jorge Basin, a rock layer representing the upper rocks was included in the design. Accordingly, an overburden pressure was not introduced, including instead the aforementioned layer representing the lithological pressure above the Salamanca Formation.

Regarding the particularities of the design, a series of additional mentions should be made. On the one hand, it was mentioned earlier that a discontinuity would be included in the model. In this case, it was decided to introduce a subvertical discontinuity, with an 80° inclination and a length of 100 m, intersecting most of the layers (Figure 3). On the other hand, it should be noted that CO₂ was injected through a point in the middle of the vertical boundary of the left side of the Banco Verde stratum, with a flow rate of 0.01 kg/m.s.

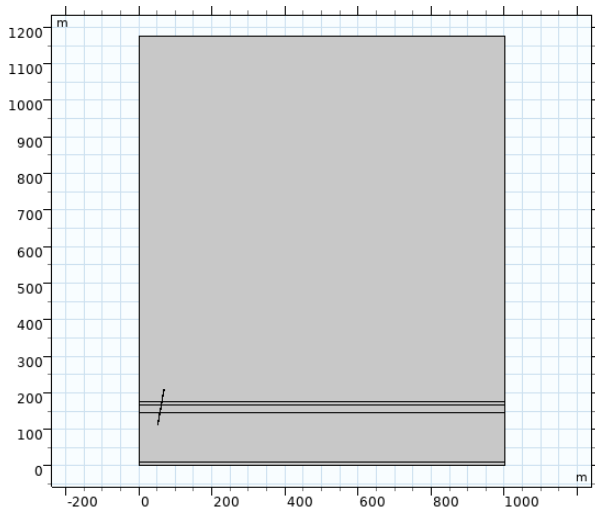


Figure 3. Geometrical design of the underground.

Finally, the properties of each of the strata are detailed in Table 1. It should be noted that the characteristic values for the Banco Verde and Banco Negro layers were obtained through laboratory tests from previous studies (Laskowski et al. (2023a, b), (2024), (2025)). As for the properties of the Upper Formations, Fragmentosa, and Glauconítico layers, estimates were made based on the available literature (Foix (2009) and Rodríguez et al. (2014)). Finally, it should be noted that the mechanical and hydraulic properties of the discontinuity will be determined based on the results of the direct shear tests, which will be detailed later in this article.

Table 1. Stratum properties. UP: Upper Formations, BN: Banco Negro, BV: Banco Verde, F: Fragmentosa, y G: Glauconítico.

Properties	Strata				
	UF	BN	BV	F	G
Thickness [m]	1000	10	20	134	10
Porosity [%]	10	5	13	5	13
Permeability [m ²]	10 ⁻¹⁷	10 ⁻¹⁸	10 ⁻¹⁶	10 ⁻¹⁸	10 ⁻¹⁶
Capillary Pressure [MPa]	8	15	0,4	15	0,4
Young Modulus [GPa]	10	10	10	10	10
Poisson's Ratio	0,3	0,2	0,25	0,2	0,25
Density [kg/m ³]	2394	2530	2340	2530	2340
Biot-Willis Coefficient	1	1	1	1	1

3 RESULTS AND DISCUSSION

3.1 Natural discontinuity: evolution of the shear behavior

In Figure 4, the results obtained from the set of direct shear tests on both pristine and CO₂-aged natural discontinuities. As it can be observed, there is a reduction in the peak and residual shear strength for all test pressures chosen. This general behavior could be related to the interaction between CO₂, and the minerals present in the rock's discontinuity.

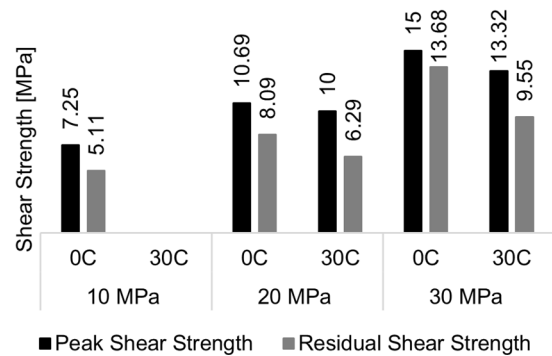


Figure 4. Peak and residual shear strength in terms of the CO₂ exposure time and the normal stress applied.

To analyze the evolution in the dilatant behavior of the specimens, Figure 5 shows an example of normal stress vs. shear displacement curves for natural discontinuities subjected to a normal pressure of 20 MPa. It might be noted that both pristine and 30-day carbonated specimens have contractive behavior. This analysis seems to indicate there are no changes in the dilatant behavior of the natural discontinuity due to its exposure to a CO₂-rich-environment.

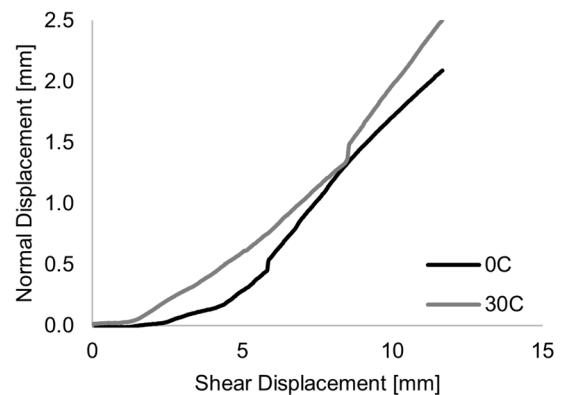


Figure 5. Normal displacement vs. Shear displacement.

From analyzing the results obtained in the direct shear tests performed on the natural discontinuities of the pristine rock (Figure 4), it seems that the discontinuity exhibits both a peak and a residual shear strength. Furthermore, with increasing normal stress, the peak becomes less evident. This behavior can also be detected by analyzing Figure 6. Additionally, it can be observed that while the Mohr envelope for peak shear strength values shows a cohesion around 0.57 MPa, the envelope corresponding to residual shear strength is cohesionless. According to several authors (Shapiro and Dinske (2021) and Nacht et al. (2010)), fault reactivation is related to residual shear strength and discontinuities without cohesion. Therefore, the behavior of the Banco Verde discontinuity will be that of the post-peak.



Figure 6. Peak and residual shear strength in terms of normal stress, results obtained from the direct shear tests performed.

As it was previously mentioned, the results obtained from direct shear tests performed on pristine natural discontinuity specimens will be used as input parameters for the numerical simulation. Table 2 details the characteristic properties of the fault which will be introduced in the simulation of the CO₂ injection into the Salamanca Formation.

Table 2. Discontinuity's properties.

Properties	Values
Length [m]	100
Porosity [%]	20
Permeability [m ²]	10 ⁻¹⁷
Capillary Pressure [MPa]	12
Young's Modulus [GPa]	0,64
Poisson's Coefficient	0,27
Cohesion [MPa]	0
Friction Angle [°]	23,9

3.2 CO₂ underground storage: reservoir-scale numerical analysis

3.2.1 Two-phase flow analysis

CO₂ saturation distribution is presented in Figure 7. As it might be noted, CO₂ flows through different interfaces, developing the saturation distribution shown. On the one hand, the CO₂ injected initially flows through Banco Verde reservoir, saturating to a greater extent the zone under the Banco Negro caprock, reaching saturation levels of 0.8. This is due to the difference presented by Banco Verde and Banco Negro in terms of capillary pressures. On the other hand, once the CO₂ flow reaches the discontinuity, given the fact that the fault's capillary pressure is lower than the caprock's, the fluid migrates through it. Furthermore, as CO₂ moves forward in the fault, it spreads to different areas. Horizontally, CO₂ re-enters Banco Verde layer, while vertically it takes longer for CO₂ to enter Upper Formations layer due to the high capillary pressure values characterizing them. In this context, higher saturation values develop in the fault, reaching values around 0.9.

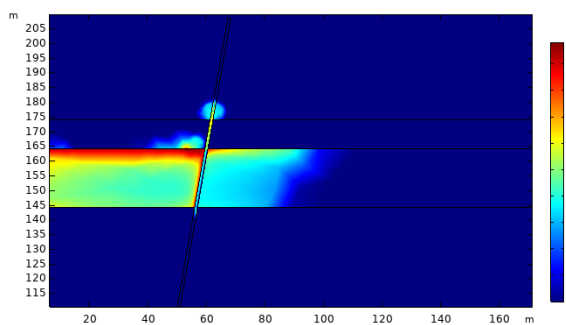


Figure 7. Zoom in to CO₂ saturation distribution in the Salamanca Formation.

3.2.2 Hydromechanical analysis

According to the literature (Urpi et al. (2015)), fault reactivation occurs at the interface between the rock used as a reservoir where the fluid is injected and the underlying caprock. In this context, to determine the fault reactivation time, the point of analysis chosen was located at the discontinuity between the Fragmentosa and Banco Verde layers. Figure 8 shows the behavior of shear stress vs. effective normal stress at the selected point of analysis. As it can be seen, the reactivation shear stress is around 0.2 MPa, taking 9 days to develop. With this information, and by determining the average displacement suffered by the discontinuity (Equation 1 and Equation 2), it is possible to determine the magnitude of the earthquake produced. Specifically, the magnitude of the earthquake related to the reactivation of the Salamanca Formation discontinuity is 0.3, which represents an event that cannot even be classified as minor.

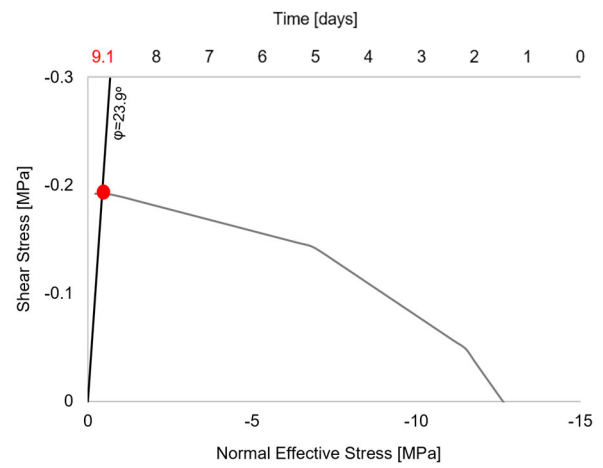


Figure 8. Fault's reactivation time determination.

As shown in Figure 9, the point at which fault reactivation begins is located between the Fragmentosa and Banco Verde layers. This graph corroborates the findings of Urpi et al. (2015) and validates our selection of the study point. Going deeper into the distribution of shear stress along the fault, it should be noted that the maximum shear stress produced at the reactivation point is 0.2 MPa, which corresponds to the value previously determined using the Mohr-Coulomb failure criterion as the fault shear stress.

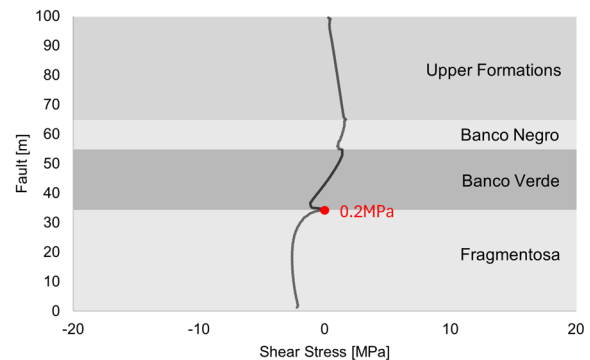


Figure 9. Shear stress distribution along the fault.

When analyzing the fluid pressure distribution, it should be mentioned that, as expected, the zone with the greatest increase is Banco Verde layer (Figure 10). Due to the great capillary pressure that characterizes both Banco Negro and Fragmentosa

layers, fluid pressure redistribution doesn't occur before the fault's reactivation.

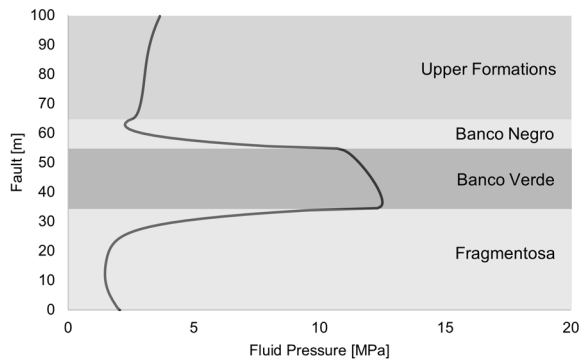


Figure 10. Induced fluid pressure throughout the fault.

4 CONCLUSION

The study presented had two main objectives. The first was to analyze the variation produced in the mechanical behavior of the discontinuities present in the reservoir rock proposed as a possible CO₂ storage site due to its exposure to a CO₂-rich environment. The second was to use the experimental results previously obtained to carry out a reservoir-scale numerical study of the Salamanca Formation when injecting CO₂. The aim was to study the long-term behavior of the underground, analyzing the effects produced by the fluid's injection.

In terms of the experimental study, it was observed that the changes produced in the natural discontinuity of Banco Verde after exposure to CO₂ were notable. Changes were detected in terms of the mechanical strength of the discontinuity, a weakening of the interface was observed. The changes were more notable in terms of peak shear strength, not so pronounced in the case of residual shear strength. However, no significant changes were observed in the dilation behavior of the sample. The changes aforementioned are attributed to chemical reactions between CO₂ and the reservoir rock, which weaken the rock (Laskowski et al. (2023a, b), (2024), (2025)).

Regarding the numerical simulations carried out, a series of interesting results were obtained. To begin with, it was observed that the seismic magnitude produced by the reactivation of the fault was 0.3, which does not even reach the level of a minor event (between 2 and 4). In addition, it was confirmed that the reactivation of the fault occurred between the reservoir layer into which the CO₂ was being injected and the underlying caprock, particularly in this case, between Banco Verde and Fragmentosa. This was observed from the results in terms of the distribution of shear stress along the fault. Finally, it was also noted that the induced fluid pressure was mainly concentrated in the reservoir rock, where the CO₂ was injected.

Considering the important findings achieved through the study presented, it would be interesting to develop similar analysis for other types of discontinuities. In particular, the wellbore cement-reservoir rock discontinuity could be studied, which would lay the foundations not only for studying the integrity of CO₂ storage sites but also of hydrogen and oil fields in full operation. In this way, the ultimate goal would be to simulate an underground reservoir that is as realistic as possible, composed not only of different materials but also of discontinuities.

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