Lawrence Berkeley National Laboratory

LBL Publications

Title

Modeling of fluid injection-induced fault reactivation using coupled fluid flow and mechanical interface model

Permalink

https://escholarship.org/uc/item/8h98921v

Authors

Park, Jung-Wook Guglielmi, Yves Graupner, Bastian <u>et al.</u>

Publication Date 2020-08-01

DOI

10.1016/j.ijrmms.2020.104373

Peer reviewed

1 2	
3	
4 5	Modeling of Fluid Injection-Induced Fault Reactivation Using Coupled
6	Fluid Flow and Mechanical Interface Model
7	
8	
10	
11	
13	Jung-Wook Park ^{1,*} , Yves Guglielmi ² , Bastian Graupner ³ , Jonny Rutqvist ² , Taehyun Kim ¹ , Eui-Seob
14	Park ¹ , Changsoo Lee ⁴
15	
10	¹ Korea Institute of Geoscience and Mineral Resources (KIGAM), 124 Gwahak-ro, Yuseong-gu,
17	Daejeon 34132, Republic of Korea
10	² Lawrence Berkeley National Laboratory (LBNL), Berkeley, CA 94720, USA
20	³ Swiss Federal Nuclear Safety Inspectorate (ENSI), 5200 Brugg, Switzerland
20	* Korea Atomic Energy Research Institute (KAERI), 111 Daedeok-daero, 989 beon-gil, Yuseong-gu,
21	Daejeon 3405/, Republic of Korea
22 23	
24	
25	
26	
27	* Corresponding author
28	Jung-Wook Park
29	E-mail: jwpark@kigam.re.kr
30	Telephone: +82-42-868-3246
31	Fax: +82-42-868-3416
32	
33	
34	
35	
36	
37	
38	
39	

40 Abstract

41 The present study is aimed at developing a numerical model to reproduce coupled hydro-mechanical 42 processes associated with fault reactivation by fluid injection in low permeability rock, as part of the 43 DECOVALEX-2019 project Task B. We proposed a modeling approach for simulating the processes 44 using the TOUGH-FLAC simulator, and modeled a fault reactivation experiment conducted at Mont 45 Terri Rock Laboratory in Switzerland. The first step of the study involved benchmark calculations 46 considering a simplified fault plane and geometry. Fluid flow along a fault was modeled using elements 47 of aperture-sized thickness on the basis of Darcy's law and the cubic law in TOUGH2, whereas the 48 mechanical behavior of a single fault was represented by zero-thickness interface elements in FLAC3D 49 upon which a slip and/or separation is allowed. A methodology to connect a TOUGH2 volume element 50 to a FLAC3D interface element was developed for handling the hydro-mechanical interactions on the 51 fault during fluid injection. Two different fault models for describing the evolutions of hydraulic 52 aperture by elastic fracture opening and failure-induced aperture increase were considered in the 53 benchmark calculations. In the coupling process, the changes in geometrical features and hydrological 54 properties induced by mechanical deformation were continuously updated. The transient responses of 55 the fault and host rock to stepwise pressurization were examined during the simulation. The hydro-56 mechanical behavior, including the injection flow rate, pressure distribution around the borehole, stress 57 conditions, and displacements in normal and shear directions were monitored in the surrounding rock 58 and along the fault. The results of benchmark calculations suggest that the developed model reasonably 59 represents the hydro-mechanical behavior of a fault and the surrounding rock. This modeling approach 60 was applied to the fault reactivation experiment of the Mont Terri Rock Laboratory. In this interpretive 61 modeling, a parametric study was conducted to examine the effects of input parameters regarding in 62 situ stress and fault properties on the hydro-mechanical responses of the fault to water injection. Then, 63 an optimal parameter set to reproduce the field experiment results was chosen by trial-and-error. The 64 injection flow rate and pressure response during fault reactivation closely matched those obtained at the 65 site, which indicates the capability of the model to appropriately capture the progressive pathway 66 evolution during fault reactivation tests at the site. The anchor displacements were overestimated by the 67 model, but a fair agreement was obtained in terms of the order of magnitude and the variation tendency. 68

- Keywords: Fault Reactivation, Water Injection, DECOVALEX-2019, Mont Terri Rock Laboratory,
 TOUGH-FLAC, Coupled Hydro-Mechanical Analysis
- 71 72
- 73
- 74

75 **1. Introduction**

76 The importance of an appropriate assessment on the fault reactivation by fluid injection into rock is 77 increasingly recognized, as promoted by rising demands for the technologies associated with geological 78 CO2 sequestration, shale gas development, enhanced geothermal systems, and enhanced oil/gas 79 recovery. Injected fluid changes the prevailing stress state in a reservoir and pre-existing faults and 80 fractures, and thus potentially triggers fault slip and seismicity. Fault activation may also be induced 81 associated with deep geological nuclear waste disposal, especially in low permeability rock, where 82 thermally driven fluid pressure increases (thermal pressurization) and pressure increases due to gas 83 generation could be significant. The fault reactivation process is a combination of hydrological and 84 mechanical interactions, such as hydraulic aperture evolution, hydrological properties change, effective 85 stress induction, and mechanical strength degradation. Development of technologies for understanding 86 and estimating the behavior is essential in ensuring safe and reliable operation of relevant energy 87 facilities and gaining public acceptance of potential hazards such as induced seismicity.

The fault reactivation potential can be assessed using analytical and numerical methods. An analytical method estimates the possibility and extent of fault failure from theoretical calculations of fault plane stress states, which generally relies on the Coulomb failure criterion for shear strength.¹ The fault stability and fault slip critical pressure threshold can be determined depending on fault direction based on a simple approach.^{2, 3} Analytical methods, however, imply many assumptions and simplifications, and thus have interpretation limitations for the complicated hydro-mechanical process in faults and reservoirs, although they are useful tools in the preliminary design stage.

95 Numerical methods can offer a viable alternative for more comprehensive analysis on the fault 96 reactivation risk. For example, numerical modeling enables consideration of the initial and induced 97 stresses, progressive changes of hydrological and mechanical properties, and failure processes. 98 Mechanically, fault representation by numerical approaches can be classified into two categories: 99 continuum and discontinuum approaches, depending on whether the fault is modeled as a continuum 100 material or as a discontinuity. In the former approach, which is widely employed in geomechanics, the 101 fault is modeled as layer of finite thickness in a continuum model (finite element method or finite 102 difference method).⁴⁻⁷ The fault is assumed to have the same mechanical responses as an equivalent 103 continuum, and then relationships can be derived between fault properties and equivalent continuum 104 properties. The latter approach defines a fault as a zero-thickness discontinuity (interface in continuum 105 model or a series of contact formations in the discrete element method).⁸⁻¹⁵ This model is available to 106 represent fault surfaces as distinct planes upon which slip and/or separation are allowed based on shear 107 and tensile failure criteria. Cappa and Rutqvist¹⁰ showed that different fault modeling approaches using 108 finite-thickness elements and zero-thickness interfaces produced similar results, and therefore, the least 109 complex approach using finite thickness elements was appropriate for fault representation from a

110 comparative simulation on fault reactivation induced by CO2 injection. However, the study was based 111 on the one-way coupled hydro-mechanical analysis not considering hydraulic aperture change due to 112 mechanical deformation. It is still questioned whether the finite thickness element modeling with 113 equivalent properties can adequately reproduce the effect of continually changing hydraulic aperture in 114 a two-way coupled analysis.

115 Both modeling approaches have limitations and assumptions for conceptualization of fault behavior. 116 The choice is dependent upon the scale of interest, required properties of the associated model, and 117 conditions of rock mass and discontinuities.^{1, 16} In the continuum model, the failure state is characterized 118 by plastic strain and the displacement across a fault is a continuous approximation. Thus, the results can 119 be dependent on grid resolution and may be unrealistic when predicting large displacement. In field-120 scale problems where the fault thickness is negligible compared to the scale of interest, it may also be 121 challenging to generate a thin layer that approximates the fault. To explicitly represent fault behavior in 122 large-scale problems, a single discontinuity may be preferable, although the discontinuum approach 123 requires cautious selection of fault stiffness to avoid numerical instability.

124 The present study is aimed at developing a numerical method to reproduce the hydro-mechanical 125 behavior of a fault by fluid injection using the TOUGH-FLAC simulator as suggested by Rutqvist et 126 al.¹⁷ We propose a modeling approach through benchmark calculations with two different fault models, 127 and demonstrate its applicability by reproducing the field experiment results obtained at the Mont Terri 128 Rock Laboratory in Switzerland. This study has been conducted as part of the DECOVALEX 129 (Development of Coupled models and their VALidation against EXperiments) project, an international 130 research and model comparison collaboration for understanding and modeling of coupled thermo-131 hydro-mechanical-chemical processes in geological systems.¹⁸ The current phase is DECOVALEX-132 2019 running from 2016 through 2019, and this study falls under Task B entitled 'Modeling the induced 133 slip of a fault in argillaceous rock'. Seven modeling teams participate in analyzing fluid injection tests 134 using different modeling approaches.¹⁹ Task B consists of three steps related to modeling of fault 135 reactivation experiments performed at the Mont Terri Rock Laboratory. Step 1 is the model inception 136 based on the benchmark calculation of a single fault plane, and Step 2 and Step 3 are for the interpretive 137 modeling of fault reactivation experiments at the site.

In this study, we describe our Step 1 and Step 2 research results. Section 2 introduces the developed numerical model and Section 3 presents the results of Step 1, the benchmark calculations. Section 4 discusses the results of Step 2, the application of the developed model to a minor fault slip experiment at the Mont Terri Rock Laboratory, which is then followed by a few conclusions.

142 2. Development of numerical model using the TOUGH-FLAC simulator

143 **2.1 Description of benchmark simulations**

The objective of DECOVALEX-2019 Task B is to develop, compare, and validate numerical models for simulating fault reactivation induced by fluid injection.¹⁹ Step 1 of Task B is a model inception with well-defined models based on a simplified representation of the fault plane and geometry. The key concerns focus on the coupling between the fracture hydraulic properties and the slip-induced displacement during fault reactivation. Therefore, an appropriate estimation of progressive evolution of hydraulic aperture is the most critical factor determining the coupled hydro-mechanical process occurring along the fault.

The host rock is represented as a box-shaped region with a side length of 20 m containing a fault dipping 65° in its center. The estimated properties for Opalinus Clay with a minor fault and the injection scheme used in the field experiment on a minor fault are applied to the benchmark simulations. Fig. 1 shows the injection pressure scheme consisting of nine steps: the pressure is increased up to 6.302 MPa until the eighth step, and then decreased to 3.382 MPa for the last step.

156 In the benchmark simulation, it is assumed that the host rock is impermeable and that the injected 157 water flows only through the fault. Two different fault models, FM1 and FM2, are considered to handle 158 the hydraulic aperture evolution. The main difference between the models is that the fracture is closed 159 until failure occurs in the former, while it is initially open in the latter. The model FM1 is based on the 160 modeling experience with fault reactivation tests conducted at the Tournemire in Southern France.²⁰ In 161 their study, analysis of measured data indicated that the hydraulic aperture increase was higher than the 162 approximation by the dilation during slip. In FM1, it is assumed that the fluid flow only occurs through 163 the fractured (open) parts of the fault, which is initially closed before the stress state reaches the shear 164 or tensile failure criterion. After failure, an open part is created, and an irreversible aperture called 165 'creation aperture' is assigned as its current hydraulic aperture. The open part can thereafter experience 166 elastic normal displacement in response to effective normal stress. Note that the fault is assumed to be 167 initially open and permeable around the injection well to a distance of 0.5 m. This implies the existence 168 of an initially created fracture. The hydraulic aperture of FM1 can be formularized into Eq. 1:

$$b_{h} = \Delta b_{he} + b_{hc} \qquad r_{f} \le 0.5 \ m$$

$$b_{h} = 0 \qquad r_{f} > 0.5 \ m, \ before \ failure$$

$$b_{h} = \Delta b_{he} + b_{hc} \qquad r_{f} > 0.5 \ m, \ after \ failure$$
(1)

¹⁷⁰ where b_h is the hydraulic aperture of fault, Δb_{he} is elastic deformation in normal direction, b_{hc} is the ¹⁷¹ creation aperture induced by tensile or shear failure, and r_f is radius of the circular zone corresponding ¹⁷² to the initially created fracture.

173

The elastic deformation is determined by the effective normal stress increment and the normal

¹⁷⁴ stiffness of the fault.

175

184

$$\Delta b_{he} = \frac{\Delta \sigma'_n}{K_n} \tag{2}$$

¹⁷⁶ where $\Delta \sigma'_n$ is the effective normal stress increment and K_n is the normal stiffness of the fault.

Model FM2 is a more conventional approach in which hydraulic aperture is assumed to be consistent
 with mechanical aperture. FM2 consists of a non-zero initial aperture, elastic normal deformation, and
 slip-induced dilation. The hydraulic aperture is expressed as Eq. 3.

 $b_h = b_{hi} + \Delta b_{he} + \Delta b_{hs} \tag{3}$

¹⁸¹ where b_{hi} is the initial aperture and Δb_{hs} is the aperture induced by shear dilation along the fault zone.

¹⁸² The dilation occurring at slip is approximated as a linear equation using the dilation angle, ψ , and ¹⁸³ shear displacement increment, Δu_s .

$$\Delta b_{hs} = \Delta u_s \tan \psi \tag{4}$$

In FM1, initially b_{hi} is zero and b_{hc} is 28 μ m within a distance of 0.5 m from the injection. After shear or tensile failure occurs, the hydraulic aperture is determined by the elastic deformation and 28- μ m creation aperture. In FM2, b_{hi} is 10 μ m, and Δb_{hs} is determined by a dilation angle of 10° after shear rupture initiation. The host rock and fault are considered to be elastic and elastic-perfectly plastic, respectively. Table 1 lists the input parameters of the host rock, fluid, and fault zone.

190 2.2 Numerical model

191 In the present study, we adopted the TOUGH-FLAC simulator, which was initially developed by 192 Rutqvist et al.¹⁷ as pragmatic approach for modeling thermal-hydrological-mechanical (THM) processes 193 in porous and fractured geological media. The TOUGH-FLAC simulator is based on linking two well-194 established existing codes, TOUGH2²¹ and FLAC3D²². The respective merits of both codes have 195 allowed the TOUGH-FLAC simulator to be widely applied to many THM problems in geological media, 196 such as CO2 injection, natural gas production, geothermal reservoir engineering, nuclear waste disposal and energy storage systems in rock caverns.7, 23-30 In this approach, TOUGH2 and FLAC3D are 197 198 executed sequentially. The TOUGH2 calculates multi-phase pressures and temperatures and transfers 199 the results to the FLAC3D, and then the FLAC3D conducts a quasi-static mechanical analysis at the 200 TOUGH2 time step and updates the changes in input parameters for the next calculation in TOUGH2. 201 The procedures to link the two codes are provided in detail in Ref. 17. 202 Fig. 2 shows the benchmark model domain and mesh for the mechanical model built in FLAC3D.

²⁰³ P1 is the injection point, and P2 and P3 are the monitoring points for mechanical and hydrological

204 responses to water injection. The monitoring points are located 1.5 m from the injection point in the 205 strike and dip directions of the fault. The relative displacements between two anchors are monitored 206 during the simulation. The anchors are installed at the fault hanging wall and footwall, respectively, and 207 spaced at a vertical distance of 0.5 m. The host rock and fault are characterized by elastic and elastic-208 perfectly plastic models, respectively, in FLAC3D. A zero-thickness mechanical interface model upon 209 which slips and/or separation are allowed represents a single fault. The interface model is available to 210 simulate distinct interfaces between zone elements, thereby simulating the presence of faults, joints, or 211 fictional boundaries. If an interface element is defined and attached on a zone element face (host face), 212 interface nodes are automatically created at every interface element vertex. The fundamental contact 213 relation is defined between the interface node and its contacting zone element face (target face), and 214 characterized by normal and shear stiffnesses and sliding properties.²² The shear and tensile failure are 215 characterized by Coulomb shear strength and tensile strength. Based on an effective stress calculation, 216 a slip and/or tensile separation can occur along the interface elements.

217 Generally, the modeling approach using the TOUGH-FLAC simulator employs a compatible 218 numerical mesh for both codes. In the present study, however, it is assumed that the host rock is 219 impermeable and its poroelastic responses to water injection are negligible compared to the processes 220 in fault, and thus the flow analysis and hydro-mechanical coupling for the host rock are not taken into 221 account in the simulations. For this reason, only the flow along the fault was simulated in TOUGH2. 222 By taking advantage of flexibility of space discretization in TOUGH2, we directly generated a very thin 223 layer in which element thickness was identical to the real size of fault hydraulic aperture with a uniform 224 porosity value of 1.0. The mesh included some non-orthogonal connections between two adjacent 225 interface elements, which arose from the procedure to install triangular interface elements on 226 quadrilateral zone faces of the FLAC3D grid. These non-orthogonal connections could cause some 227 errors in pressure calculation, ^{31, 32} although the effect was not taken into consideration in the simulations.

228 Fig. 3 shows the mesh for the fluid flow analysis. The injection well has a radius of 0.07 m and 229 consists of 24 elements marked in blue. The mesh in the figure is only for the initial state calculation. 230 The mesh geometrical features (volume and connectivity) are continuously updated based on the 231 displacement calculated by FLAC3D through the hydro-mechanical coupling process. In FM1, the 232 central elements denoted by the red indicate the initial fracture zone, which has a hydraulic aperture of 233 $28 \ \mu m$ (creation aperture). The remaining elements represent the closed zone of negligible thickness 234 $(10^{-3} \mu m)$. The elements for the closed fracture are potential flow paths, but are treated as inactive 235 elements in the fluid flow calculation at the initial stage. Each TOUGH2 element corresponds to a 236 FLAC3D interface element. After shear or tensile failure of an interface element is detected in FLAC3D, 237 the corresponding element is switched to an active element for the subsequent flow calculation in 238 TOUGH2. In FM2, every element initially has a thickness of 10 μ m according to the initial hydraulic 239 aperture.

The benchmark calculation assumes that the fluid flow is governed by Darcy's law and the cubic relationship between flow rate and hydraulic aperture.³³ In the present study, the fluid flow within a fault is approximated by two-dimensional horizontal flow within parallel walls separated by a hydraulic aperture and characterized by transmissivity and storativity, which have been primarily used for the flow in well hydraulics in confined aquifers of a finite-thickness.³⁴ The fault transmissivity, T_f , is proportional to the cube of the hydraulic aperture:

$$T_f = \frac{\rho_f g}{12\mu} b_h^3 \tag{5}$$

where ρ_f is fluid density, g is the gravitational acceleration, μ is fluid dynamic viscosity, and b_h is hydraulic aperture.

Thus, the permeability,
$$k_f$$
, is written as a function of the hydraulic aperture:

$$k_f = \frac{b_h^2}{12} \tag{6}$$

Storativity describes the volume of water released from storage per unit decline in hydraulic head in the aquifer, per unit area of the aquifer. Assuming that a fault is an aquifer with the hydraulic aperture, b_h , and a porosity of 1.0, the fracture storativity can be expressed as follows: ³⁵

254 $S_f = \rho_f g b_h (\alpha_f + \beta) \tag{7}$

²⁵⁵ where α_f and β are fault and fluid compressibility, respectively.

The storativity is related to the compressibility of both the fault and the fluid. If we simplify the deformation of the fault as a one-dimensional problem in the normal direction, the fault compressibility can be determined using the fault normal stiffness as follows:

$$\alpha_f = \frac{\Delta b_h / b_h}{\Delta \sigma'_n} = \frac{1}{b_h K_n}$$
(8)

260 Fig. 4 illustrates the data transfer process between TOUGH2 and FLAC3D in the present study. The 261 execution of each program and the data transfer process are repeated at each time step of a TOUGH2 262 iteration. First, TOUGH2 calculates the pressure of each element and transfers the results to the 263 corresponding interface elements in FLAC3D. Then, the mechanical responses, including fault 264 deformation, are calculated based on an effective stress analysis in which the Biot effective stress 265 coefficient³⁶ is assumed to be equal to 1.0. The permeability and compressibility of each element are 266 modified according to Eqs. 6 and 8. The geometrical change induced by fault deformation and failure 267 is also updated by rebuilding the mesh for the next calculation in TOUGH2. In this procedure, for each 268 interface element of FLAC3D, a 6-noded prism-shaped element is generated using the updated 269 coordinates of host face and target face. Then, the volume and coordinates of the element, and its 270 connection information, including interface area, nodal distances for the interface, and orientation of 271 the nodal line, are reset for TOUGH2 analysis. Basically, the porosity is calculated by compressibility 272 in TOUGH2, but the value is reset to 1.0 at a beginning of a time step in our simulation because the 273 geometrical change is also updated. The hydraulic aperture is calculated as the distance between the 274 centroids of host face and target face. In FM1, the effect of creation aperture is considered by translating 275 the interface node and its corresponding vertex on the target face by one-half of creation aperture size 276 in opposite directions along the fault normal vector. In the benchmark simulation, the field principal 277 stresses are given by $\sigma_x = 3.3$ MPa, $\sigma_y = 6.0$ MPa, and $\sigma_z = 7.0$ MPa. However, it was observed from the 278 simulation of model FM1 that fracture propagation and fault slip were rarely induced under this stress 279 condition. A few modeling teams of TASK B reported similar findings in the benchmark simulations.¹⁹ 280 To identify the difference between FM1 and FM2 more effectively, we increased the initial shear stress 281 acting on the fault by reducing the intermediate principal stress, σ_{y} , so that the newly created fracture 282 could reach monitoring points P2 and P3 at 1.5 m from the injection point. Note that we present the 283 results of simulations with the initial stress condition of $\sigma_x = 3.3$ MPa, $\sigma_y = 5.3$ MPa, and $\sigma_z = 7.0$ MPa 284 in the present study. The fracture propagated up to the monitoring points under a lower σ_{v} of 5.3 MPa 285 in both models. Roller boundaries are set on all six sides of the model and the boundary planes are fixed 286 in the respective normal direction. The initial pressure is set to 0.5 MPa, as estimated from 287 measurements at the site, and the boundary pressure is kept constant during the simulation.

288 **3. Results of benchmark simulations**

289 **3.1. Hydrological behavior**

This section describes the hydrological behavior of the different fault models, FM1 and FM2, in response to water injection. Figs. 5 and 6 show the profiles of hydraulic aperture and pressure along the fault strike direction (see Fig. 2a) for both fault models. In the figures, the results estimated at 100, 157, 420, 453, and 807 s of water injection are given, which correspond to the ends of injection steps at 1.919, 3.627, 5.484, 6.302, and 3.382 MPa, respectively (see Fig. 1).

295 The two fault models exhibited completely different evolutions of hydraulic aperture and pressure. 296 In FM1 with an initial 0.5 m radius fracture zone around the injection well, the fluid flowed only through 297 the zone until 420 s. In this phase, the hydraulic aperture increased as a result of elastic deformation 298 with increasing injection pressure and decreasing effective normal stress. Within the fracture zone, a 299 nearly uniform pressure corresponding to the injection pressure developed immediately due to the small 300 fracture volume. The stress conditions in close proximity to the well reached the shear failure criterion, 301 but newly created fracture was not observed until 420 s. Under a higher injection pressure of 6.302 MPa, 302 the shear failure initiated at 421.5 s along the edge of the initial fracture zone, and then propagated

rapidly until 453 s to a distance of 1.8 m. As the flow path expanded, the pressure gradient showed
 transient responses. Under a reduced injection pressure of 3.382 MPa between 453 s and 807 s, the
 hydraulic aperture decreased through elastic deformation recovery. Note that the creation aperture is
 irrecoverable in FM1.

307 In FM2, where the fault was assumed to be initially permeable with hydraulic aperture of 10 μ m, 308 the water flowed throughout the entire fault. The hydraulic aperture progressively increased with 309 injection pressure until 453 s by elastic deformation and/or slip-induced dilation, and then decreased by 310 elastic deformation between 453 s and 807 s. Generally, radial fluid flow by injection in a homogeneous, 311 isotropic, confined aquifer exhibits a pressure curve whose gradient decreases with distance from the 312 injection well.³⁴ The pressure distribution of FM2, however, showed a bell-shaped curve in the early 313 injection steps (157 s in Fig. 6). This might be ascribed to continually and progressively changing 314 fracture hydraulic aperture, permeability and compressibility during the injection. A preliminary study 315 to examine the hydro-mechanical coupling effect suggested that the uncoupled model with the same 316 properties produced the general shape of the pressure curve. In the present coupled model, an increase 317 in hydraulic aperture raised the permeability and reduced the compressibility, resulting in an increase 318 in hydraulic diffusivity. At the early steps, the hydraulic aperture around the well significantly increased 319 in response to water injection, and thus disproportionately high pressure quickly developed in the region. 320 As time proceeded, the injected water pressure transmitted to the boundaries of the model, as shown in 321 the profiles for 420 s and 453 s. It seemed that the chosen extent of the benchmark model domain was 322 not large enough to prevent boundary effects. It is expected that if the boundary condition of constant 323 pressure was not applied, the pressure at the boundaries would increase with time to become higher 324 than 0.5 MPa.

Fig. 7 shows the variations in pressures monitored at points P2 and P3, which are located 1.5 m from the injection point in the fault strike and fault dip directions, respectively (see Fig. 2a). In FM1, the pressures were unchanged at initial pressure of 0.5 MPa until approximately 445 s and then abruptly increased up to 4.2 MPa. Contrary to the nonconsecutive variation in FM1, the pressures in FM2 showed gradual change in response to the injection pressure, even though the pressure began changing at approximately 140 s.

331 The pressure development correlated closely to the injection flow rate. Fig. 8 shows the variations 332 in injection flow rate for both models. A comparison between the results showed that the FM1 model 333 produced a lower flow rate in the early steps. As mentioned above, the pressure within the initial fracture 334 zone quickly reached steady-state flow because of the small fracture volume. In each injection step, the 335 injection flow rate temporarily reached its peak initially, but decreased to a negligibly small value. With 336 the fracture propagation between 420 and 453 s, the pressure gradient showed transient behavior, and 337 the initial flow rate increased and plateaued during the injection. Newly opened fracture parts raised the 338 differential pressure head between the well and fault, resulting in abrupt changes in the injection flow

339 rate. In the last injection stage with the injection pressure of 3.382 MPa, a back-flow into the well 340 (negative flow rate) was observed in the simulation until the end of injection. The flow rate curve 341 changed slowly compared to those observed in other injection stages, which might be ascribed to the 342 increase in the storativity by irreversible creation aperture. This aspect can also be captured in Fig. 7; 343 after 453 s in FM1, the pressures at the monitoring points were greater than the injection pressure. In 344 FM2, the injection flow rate showed a more stepwise variation in response to injection pressure. FM2 345 produces higher injection flow rate than FM1 in the earlier steps, because higher differential pressure 346 head gradients developed within a wider range. Shear failure initiated at 215 s and progressively 347 propagated along the fault until 453 s, but the effect of shear failure on the flow rate was not evidently 348 observed contrary to the result of FM1.

349 **3.2. Mechanical behavior**

350 This section describes the mechanical behavior of the FM1 and FM2 models. To assess the mechanical 351 fault behavior, the histories of stress states along the fault were recorded during the simulations, and the 352 shear strength was calculated based on the Coulomb failure criterion using a friction angle of 22° and 353 effective normal stress. Note that if the stress state at the interface node satisfies the Coulomb failure 354 criterion in FLAC3D, sliding is assumed to occur. Then, the magnitude of shear stress is set to the 355 current shear strength with the direction preserved. If the stress state reaches tensile criterion, the fault 356 is assumed to be separated in the normal direction. Actually, a discontinuity in a rock is defined as any 357 significant mechanical break or fracture of negligible tensile strength that already reached failure state.³⁷ 358 Thus, 'tensile failure' in this study more exactly denotes 'tensile opening' induced by negative effective 359 normal stress.

360 Generally, in many of the transient subsurface flow problems with respect to fluid injection, it is 361 assumed that total normal stress is constant and the pressure of the injected fluid causes a change in 362 effective normal stress. Assuming that the Biot effective stress coefficient is equal to 1.0, the critical 363 injection pressures above which shear and tensile failure occur, P_{cs} and P_{ct} , can be theoretically derived 364 from the criteria and given conditions for in-situ stress, fault direction, and fault friction angle. The 365 theoretical predictions of P_{cs} and P_{ct} of the benchmark model are found to be 3.99 MPa and 5.60 MPa, 366 respectively. This indicates that shear failure and sliding, prior to tensile opening, is expected to take 367 place at P1.

Fig. 9 shows the variations in injection pressure, total normal stress, effective normal stress, shear stress, and shear strength monitored at injection point P1. The effective normal stress and shear strength showed a degradation or increase in response to change in injection pressure in the simulations. The stress state at P1 reached the shear failure condition when imposing an injection pressure much higher than the expectation; shear failure at P1 occurred at 5.484 MPa in FM1, and 4.511 MPa in FM2. Tensile fracture opening due to negative normal stress was not observed in either model. Contrary to the 374 theoretical assumption, total normal stress acting on the fault did not remain constant but increased in 375 the simulations, and therefore the effective normal stress and shear strength of the model were higher 376 than the calculation. This aspect might be ascribed to the physical constraint of normal displacement 377 and is more evident in FM1 than in FM2. In FM1, where the initial rupture zone was only allowed to 378 deform in the normal direction, compressive stress was concentrated along the edge, which raised the 379 total normal stress. After the additional fracture was created, total normal stress was reduced. The 380 increase in total normal stress until approximately 150 s observed in FM2 can be explained in the same 381 way.

Fig. 10 shows the fault shear displacement and failure zone, which were estimated at 453 s. In the displacement contour, the red denotes the maximum value and the blue denotes zero. Fig. 11 shows the variations in normal and shear displacements monitored at P1 and P2. In both models, the fault shear displacement occurred in the dip direction after shear failure and displacement in the strike direction was negligible. As mentioned, an increase in total normal stress shifted the point of the onset of shear failure to higher injection pressure, which caused FM2 to have a greater shear displacement and larger failure zone.

389 Fig. 12 shows the displacement contours of the surrounding host rock estimated at 420, 453, and 390 807 seconds of injection. Fig. 13 shows the relative displacement of the upper anchor to lower anchor. 391 The rock deformation was limited to small regions adjacent to the newly fractured zone in FM1, whereas 392 a large deformation was predicted along the entire fault in FM2. It is found from the anchor 393 displacement in Fig. 13 and the displacements at injection point P1 in Fig. 11a that the anchor 394 displacement is primarily correlated with the fault displacement. The anchor displacement was oriented 395 in the fault normal direction before shear failure, and then inclined towards the dip direction after shear 396 failure. The decreases in dy and dz between 420 and 453 s indicate that the upper surface of the hanging 397 wall moved downward relative to the lower surface of footwall due to fault slip. This is also evident 398 from the observations of rock and fault displacements in Fig. 12.

399 4. Application of developed model to fault slip experiment at Mont Terri Rock

400 Laboratory

401 **4.1 Descriptions of minor fault reactivation experiment**

The Mont Terri Rock Laboratory is an underground research facility located at a depth of 280 m below the surface in Saint Ursanne in the canton of Jura. The research facility can be accessed through the security gallery of the Mont Terri tunnel (Fig. 14). In the facility, various experiments have been conducted to investigate and analyze the hydrogeological, geochemical, and rock mechanical characteristics of argillaceous formations, specifically the Opalinus Clay layer, which has been considered as the preferred host rock for high-level waste disposal in Switzerland.³⁸

- ⁴⁰⁸ The Mont Terri rock laboratory is intersected by a major fault called the 'Main Fault'. The fault core
- ⁴⁰⁹ is 0.8 3.0 m thick and is bounded by two major fault planes oriented $156^{\circ}/45^{\circ}$ (dip direction/dip angle)

410 and $165^{\circ}/40^{\circ}$, respectively. Several fault planes were observed and they were almost parallel to bedding

⁴¹¹ planes oriented $145 - 155^{\circ}/50 - 55^{\circ}$. The dip directions and dip angles of the fault planes ranged from

412 120° to 150° and from 50° to 70°, respectively.

413 A series of fault reactivation experiments were conducted in the major and minor planes of the Main 414 Fault, which were aimed at quantifying hydraulic and mechanical characteristics of those major and 415 minor fault planes in response to water injection. Fig. 15 shows the locations and apparatus of the fault 416 reactivation experiments.^{39, 40} The fault reactivation experiments were conducted at four borehole 417 interval sections (at depths of 47.2 m of borehole BFS1 and 44.65, 40.6, and 37.2 m of BFS2). In each 418 test, a fault plane was stimulated by pressure-controlled water injection and the flow rate, pressure, 419 displacement variations, and induced seismicity were monitored in the injection and monitoring 420 boreholes. More detailed descriptions of the experiments are given by Gulglielmi et al.³⁹

The experiment for the numerical simulation of Step 2 of Task B corresponds to the injection test conducted at 37.2 m of BFS2. This section is the farthest from the fault core and the host rock is nearly intact rock affected by a few polished and striated secondary faults. The injection test was conducted for approximately 9,500 s. The initial period of 807 s was taken for the numerical simulation.

Fig. 16 shows the field experimental results. Fig. 16a shows the injection chamber pressure and injection flow rate measured at 37.2 m of borehole BFS2 and the pressure monitored at a packed-off interval in borehole BFS4. The monitoring point is located at a distance of approximately 1.5 m in the fault strike direction. Fig. 16b shows the vertical, northern, and western components of the relative displacement of upper anchor to lower anchor, which are initially spaced at a vertical distance of 0.5 m and installed in the hanging wall and footwall.

The pressure response at the monitoring point can be characterized by its abrupt increase occurring after 420 s of injection, which indicates the onset of fracture opening at the monitoring point. The consistent injection flow rate between 420 and 453 s reveals the increase in hydraulic conducting aperture followed by fracture propagation along the fault plane. The relative displacement of upper anchor to lower anchor initially corresponds to a normal closure of the fault, and then changes with injection pressure.

437 **4.2 Simulation of the experimental results**

The simulation of Step 2 is aimed at interpretively simulating the field experimental results by selecting appropriate boundary and initial conditions, constitutive models, and properties for the rock and fault. The modeling approach described in Section 2, including assumptions and constitutive laws, was taken for the simulation. We adopted the model FM1 to consider the hydraulic aperture evolution. The comparisons between field data in Fig. 16 and the results of benchmark simulations in Figs. 7, 8, and 443 13 reveal that FM1 can more reasonably capture the characteristics of the pressure build-up at the 444 monitoring point and the variation in injection flow rate observed in the site than FM2. In FM2, the 445 fault is assumed to be an open and permeable flow path regardless of fracture failure. Consequently, the 446 immediate effect of fracture opening on the change in the injection flow rate cannot be properly 447 simulated, even though the pressure build-up at monitoring points would be controlled by assigning a 448 smaller initial aperture.

449 According to Martin and Lanyon⁴¹ and Yong et al.⁴², the Mont Terri rock laboratory is subjected to 450 an in-situ stress state where the maximum principal stress, $\sigma_1 = 6 - 7$ MPa, the intermediate principal 451 stress, $\sigma_2 = 4 - 5$ MPa, and the minimum principal stress, $\sigma_3 = 0.6 - 3$ MPa. The average orientations 452 (trend/plunge) are analyzed to be 210°/70°, 320°/10°, and 50°/20°, respectively. Based on the studies, we 453 assume that σ_l corresponds to the vertical principal stress σ_v , and σ_s and σ_s to the two horizontal principal 454 stresses, σ_H and σ_h , which are oriented at 320° and 50° in the model. For simplicity of assigning the 455 boundary and initial stress conditions to the model, we made the axes of coordinate, x, y, and z, parallel 456 to directions of σ_h , σ_H , and σ_v , respectively, by rotating the geometric information of fault and in-situ 457 stresses.

Fig. 17 shows an example of a FLAC3D model rotated with respect to the *z* axis by 40°. As in the benchmark calculation, the boundaries were assigned a constant pressure in fluid flow analysis, and the grid points were fixed in the out-of-plane direction in mechanical analysis. The initial fluid pressure was set to 0.5 MPa, as estimated from measurements at the site.

A series of simulations were performed under various conditions to examine the effects of influencing factors and to reproduce the field data shown in Fig. 16. Table 2 lists the ranges of the input parameters for fault and in-situ stress. The values chosen in the simulations showing the best match (Case 1) and second-best match (Case 2) are also given in the table. The friction angle, dilation angle, and tensile strength of the fault were fixed in the calibration. The input parameters of the host rock and fluid are the same as those used for benchmark simulations (see Table 1).

With the priority given to the following characteristics observed from the field data, we calibrated the numerical model by improving the parameter set in a trial-and-error manner until the responses of the numerical model matched the field data.

471

473

- 1) Flow rate and volume of injected water between 420 and 453 s
 - 2) Abrupt change in pressure at monitoring point after 420 s
- 474 3) Magnitude and direction of anchor displacement vector
- 475

The numerical and experimental results of injection flow rate and pressure at the monitoring point are compared in Figs. 18 and 19. The numerical results were obtained from the simulation case showing the best match. Note that little attempt was made for reproducing the variation in injection flow rate within the first 420 s during which the fracture failure was not expected to occur. The erratic variation observed in the field data in the duration is beyond the scope of the present study. In terms of the injection flow rate and injected water volume between 420 and 453 s, the numerical model showed good agreement with the experimental results. In the model, the injection flow rate showed an instantaneous rise to a peak followed by a quick drop to zero in each injection step before 430 s. Then, it increased up to 21 liter/min that was consistently maintained until 453 s.

- 485 Fig. 20 shows the pressure contours estimated at 425, 430, and 453 seconds. In the figure, r is the 486 radius of the created fracture zone at each moment. As seen in the figure, small regions around the initial 487 fracture zone only functioned as flow paths in the early stage, and therefore high pressure quickly 488 developed within the zone. As new fracture areas were created through rupture propagation, the pressure 489 developed in a transient manner, which resulted in continuous increases in the injection flow rate. The 490 stress state at the monitoring point reached the failure criteria at approximately 430 s, and then the 491 pressure started to increase. Even though the pressure curve obtained from numerical model exhibited 492 a higher peak and slower responses than field observations, it reasonably reproduced the overall 493 tendency, including timing of the increase. The volume of injected water between 420 and 453 s was 494 calculated to be 8.0×10^{-3} m³ in the numerical model, which corresponds well to 7.7×10^{-3} m³ that is 495 calculated from the curve of the field data. After 453 s, when a lower injection pressure of 3.382 MPa 496 was imposed, negative flow rate values were estimated, which indicated flow-back into the well due to 497 injection pressure being lower than the fault pressure. In the field, some flow-back was observed at the 498 very end of the test even though it was not measured.
- 499 The numerical and experimental results for variations in relative displacement between two anchors 500 are compared in Fig. 21. They are within reasonable agreement, even though the numerical model 501 estimated 3 - 4 times larger vertical components than the field data. In the numerical model, the upper 502 anchor moved upward and in a southeastern direction horizontally, while the lower one was displaced 503 in the exact opposite direction. If we decompose the relative displacement vector into two components 504 in fault shear and normal directions, it is evidently observed that the anchor displacements are reflective 505 of the fault movement. In Fig. 22, the components of the relative displacement vector in fault normal 506 and shear directions, d_n and d_s , are presented and compared to normal and shear displacements, u_n and 507 u_s , of injection point P1. The anchor movement was primarily affected by the elastic normal expansion 508 of the fault before 420 s, and then dominated by fault slip after 420 s. The upper anchor slid along the 509 fault, which resulted in a decrease in the vertical component between 420 and 453 s. With increasing 510 fault shear displacement, the magnitudes of the horizontal components increased as shown in Fig. 21. 511 After 453 s, the displacement in every direction was recovered due to elastic recovery in the fault normal 512 direction.
 - 15 -

513 **4.3 Discussion**

In the calibration procedure, it was found that the hydro-mechanical responses of the fault to injection were not only interrelated but also affected by input parameters in conflicting ways. The complicated effects of several input parameters made it difficult to find a parameter set that satisfactorily reproduced all the experimental data in Fig. 16. We placed more emphasis on producing a reliable representation of the characteristics regarding the fracture opening and propagation, and thus focused on the variations in injection flow rate and pressure response. As a result, the anchor displacement curve even in the best matching case was in relatively poor agreement with field data.

The injection flow rate and the pressure at the monitoring point were mainly dependent on the fracture opening and propagation process. In other words, the onset and extent of the failure can be controlled by adjusting the in-situ stress direction and magnitude, fault direction, and strength parameters. According to the theory of stresses in three dimensions⁴³, we can calculate the normal stress, σ_n , and shear stress, τ , on a fault plane whose normal vector in the principal coordinate system is n = (n_1, n_2, n_3) , as Eqs. 9 and 10.

$$\sigma_n = \sigma_1 n_1^2 + \sigma_2 n_2^2 + \sigma_3 n_3^2 \tag{9}$$

$$\tau^{2} = (\sigma_{1} - \sigma_{2})^{2} n_{1}^{2} n_{2}^{2} + (\sigma_{2} - \sigma_{3})^{2} n_{2}^{2} n_{3}^{2} + (\sigma_{3} - \sigma_{1})^{2} n_{3}^{2} n_{1}^{2}$$
(10)

⁵²⁹ Using the stresses and fault strength properties, theoretical estimates of the critical pressures above ⁵³⁰ which shear and tensile failures of fault occur, P_{cs} and P_{ct} , can be calculated based on the failure criteria. ⁵³¹ In the calibration process, we repeatedly adjusted the influencing input parameters in a trial-and-error ⁵³² manner so that the shear or tensile failure along the fault could be induced between 420 and 453 s. The ⁵³³ initial condition of stresses on the fault plane and cohesion were the dominant parameters determining ⁵³⁴ the onset and extent of the failure. Small normal stress and/or large shear stress and/or small cohesion ⁵³⁵ promoted the fault failures, and vice versa.

536 In the best matching case, the cohesion of interface elements was set to zero, and thus shear failure 537 was theoretically expected to occur prior to tensile failure: the calculated values of P_{cs} and P_{ct} were 4.93 538 MPa and 5.01 MPa. However, in the simulation, both shear and tensile failures initiated at 422 s within 539 the regions around the injection well. The fault effective normal stress dropped to a negative value 540 instantaneously due to the imposed injection pressure, and the stress condition simultaneously satisfied 541 the shear and tensile failure criteria. New fractures were created at 424 s and propagated to the 542 monitoring points by approximately 430 s. The injection flow rate after failure was primarily influenced 543 by elastic and plastic aperture enhancements. Therefore, the injection flow rate evidently increased with 544 decreasing normal stiffness and increasing creation aperture size.

⁵⁴⁵ The anchor displacement in the elastic stage was influenced by the normal stiffness and fault

direction. The magnitude decreased with increasing normal stiffness, and the direction exactly corresponded to the normal direction of the fault. The effects were evident in the numerical model, and thus it was possible to better match the field data by adjusting the influencing parameters. However, choices of the parameters were limited, because they also affected the elastic hydraulic aperture and the onset of fracture failure, resulting in different injection flow rate and pressure response.

551 After the occurrence of fracture failure, the anchor displacement was dominated by fault shear and 552 normal displacements. In particular, the fault shear displacement controlled the vertical component of 553 the relative displacement between the anchors. With a large shear displacement, the vertical component 554 fell below zero, which means that upper anchor moved downward relative to the lower anchor due to 555 fault slip. In other words, for a more reasonable representation of anchor displacement curves, the shear 556 displacement should be limited. In our model, the most influential factor on the shear displacement was 557 the initial shear stress acting along a fault. We attempted to minimize the initial shear stress by adjusting 558 the principal stresses in a range of 6.0 - 7.0, which was given in the literature^{41, 42}, but even the 559 simulation with the smallest minimum initial shear stress exhibited a large shear displacement.

560 Figs. 23, 24, and 25 show the comparisons between the numerical results of Case 2 and field 561 experimental results for injection flow rate, pressure at monitoring point, and relative displacement of 562 the upper anchor to lower anchor. In terms of the injection flow rate and pressure response, Case 2 under 563 the maximum principal stress of 7.0 MPa showed better agreement with field data than Case 1. However, 564 the fault reactivation produced shear displacement of hundreds of micrometers, and consequently 565 anchor displacement at the site was poorly represented. In Case 1, which showed the best match, the 566 maximum principal stress was chosen as 5.1 MPa so that the fault could have a minor value of the initial 567 shear stress, 0.032 MPa. As shown in Figs. 21 and 22, the fault slip was small, and the vertical anchor 568 movement was more reasonably reproduced. From these findings, it can be inferred that the hydraulic 569 aperture at the site was associated with tensile opening rather than hydro-shearing. Guglielmi et al.³⁹ 570 indicated that the in-situ stress condition of the research site might be different from that reported by 571 Martin and Lanvon⁴¹ and Yong et al.⁴² because of the excavation followed by stress redistribution. The 572 simple assumption for vertical and horizontal principal directions taken in this study might also impede 573 the calibration.

574 Although the emphasis is placed on representing the hydro-mechanical responses associated with 575 fault reactivation in the present study, the proposed model can be used for the prediction of induced 576 seismicity. For example, the seismic moment can be estimated from the simulation results of the fault 577 shear displacement and failure zone shown in Fig. 26. Based on the rock mass shear modulus, average 578 slip (the area-weighted average of shear displacements over failed interface elements) and slip area, a 579 seismic moment, M_o , of 1.57×10^5 Nm is predicted. The relation between seismic moment and 580 magnitude reported by Hanks and Karnamori⁴⁴ gives a moment magnitude, $M_{\rm W}$, of -2.6. Since we used 581 a simple elastic-perfectly plastic model for the fault frictional process, the estimate of seismic moment

may be inaccurate. With the appropriate selection of the properties and behavior models based on
 laboratory and field experiments, a better accuracy can be achieved in a further study.

584 **5. Summary and conclusions**

⁵⁸⁵ In the present study, we have numerically simulated the water injection into a fault and examined the ⁵⁸⁶ coupled hydro-mechanical processes along the fault and the surrounding rock. We proposed a modeling ⁵⁸⁷ approach using the TOUGH-FLAC simulator through benchmark calculations for well-defined models, ⁵⁸⁸ and demonstrated its applicability by reproducing field experiment results obtained at the Mont Terri ⁵⁸⁹ Rock Laboratory in Switzerland.

590 In our model, elements of aperture-sized thickness are used for the fluid flow analysis in TOUGH2, 591 whereas interface elements of zero-thickness are used for the mechanical calculation in FLAC3D. In 592 the coupling process, the geometrical features, hydrological properties, and effective stress are 593 continuously updated by the sequential executions of both codes and the data transfer between the 594 elements and interface elements. This modeling approach allowed the explicit representation of the fault, 595 preventing the involvement of many parameters and assumptions for equivalent thickness and fault 596 properties. Moreover, the merit of the interface element enabled us to observe how the tensile opening 597 and hydro-shearing played roles in hydraulic aperture in a direct manner. The transient responses of the 598 fault, including pressure response, injection flow rate, elastic behavior, fracture failure, and stepwise 599 pressurization were analyzed for two different fault models, FM1 and FM2. The two fault models 600 exhibited entirely different behaviors due to different pathway evolutions and the consequent pressure 601 build-up, which indicates the importance of appropriate descriptions of hydraulic aperture in fault 602 modeling.

603 The developed model was applied to the fault reactivation experiment conducted at the 'Main Fault' 604 intersecting the low permeability clay formation of the Mont Terri Rock Laboratory in Switzerland. We 605 used the model FM1 to reproduce the fracture opening and propagation processes and the hydro-606 mechanical characteristics observed at the site. With priority given to the reliable representation of 607 fracture failure, the numerical model was calibrated to the field data by adjusting the input parameters 608 in a trial-and-error manner. In this procedure, the effects of input parameters such as dip angle, dip 609 direction, shear and normal stiffnesses, cohesion, fault creation aperture size, and in-situ stress 610 conditions were discussed. In the best matching simulation, the results of flow rate and pressure build-611 up at high injection pressure were in good agreement with the field experimental results. The relative 612 displacement of anchors installed in proximity to the injection point showed a discrepancy between the 613 numerical and experimental results. Even though the vertical displacement was 3 - 4 times greater than 614 the experimental result, a fair agreement was obtained in the horizontal displacement and the overall 615 variation tendency.

616

It was found from the benchmark calculations and the simulation of field reactivation experiment

617 that the proposed model can capture the process of fracture opening and propagation, and thus provide 618 a reasonable prediction of the hydro-mechanical behavior associated with fault reactivation by fluid 619 injection. It is expected that this modeling approach can be applied to various fault hydraulic models 620 tailored to suit field observations. However, to ensure the applicability of the modeling approach to 621 field-scale problems there are a few technical problems that should be addressed in further study. In 622 particular, special attention should be paid when handling the interface elements and their contacts.²² 623 For example, the use of nonplanar interfaces, overlapping interfaces, and multiple intersecting 624 interfaces may cause some problems in detecting appropriate contacts and thus in calculating forces and 625 displacements. The numerical model will be enhanced by continuing collaboration and interaction with 626 other research teams of DECOLVAEX-2019 Task B and validated using available field data in further 627 studies.

628 Acknowledgments

629 The authors appreciate and thank the DECOVALEX-2019 Funding Organizations Andra, BGR/UFZ, 630 CNSC, US DOE, ENSI, JAEA, IRSN, KAERI, RWM, SÚRAO, SSM, and Taipower for their financial 631 and technical support of the work described in this paper. The statements made in the study are, however, 632 solely those of the authors and do not necessarily reflect those of the Funding Organizations. This 633 research was also supported by the Basic Research Project of the Korea Institute of Geoscience and 634 Mineral Resources (KIGAM, GP2020-010) funded by the Ministry of Science and ICT, Korea. LBNL's 635 funding was provided by the Spent Fuel and Waste Science and Technology, Office of Nuclear Energy, 636 of the U.S. Department of Energy under Contract Number DE-AC02-05CH11231 with Lawrence 637 Berkeley National Laboratory.

638 **References**

- 639
 1. Bohloli B, Choi JC, Skurtveit E, Grande L, Park J, Vannest M. Criteria of fault geomechanical
 640 stability during a pressure build-up. 2015 IEAGHG report 2015/04. Cheltenham; 2015.
- 641
 2. Wiprut DJ, Zoback MD. Fault reactivation, leakage potential, and hydrocarbon column heights
 642 in the northern North Sea. In: Hydrocarbon Seal Quantification. Norwegian Petroleum Society
 643 Special Publication. 2002; 11: 203–219.
- Vidal-Gilbert S, Tenthorey E, Dewhurst D, Ennis-King J, Van Ruth P, Hillis R. Geomechanical
 analysis of the Naylor Field, Otway Basin, Australia: implications for CO2 injection and storage.
 International Journal of Greenhouse Gas Control. 2010; 4: 827–839.
- 647
 4. Rinaldi AP, Rutqvist J, Cappa F. Geomechanical effects on CO2 leakage through fault zones
 648
 649
 649
 2014; 20: 117–131.

650 5. Rutqvist J, Dobson PF, Garcia J, Hartline C, Jeanne P, Oldenburg CM, Vasco DW, Walters M. 651 The northwest Geysers EGS demonstration project, California: Pre-stimulation modeling and 652 interpretation of the stimulation. Mathematical Geosciences. 2015; 47: 3-29. 653 6. Nguyen TS, Guglielmi Y, Graupner B, Rutqvist J. Mathematical modelling of fault reactivation 654 induced by water injection. Minerals. 2019; 9: 282. 655 7. Rinaldi AP, Rutqvist J. Joint opening or hydroshearing? Analyzing a fracture zone stimulation 656 at Fenton Hill. Geothermics. 2019; 77: 83–98. 657 8. Vidal-Gilbert S, Nauroy JF, Brosse E. 3D geomechanical modelling for CO2 geologic storage 658 in the Dogger carbonates of the Paris Basin. International Journal of Greenhouse Gas Control. 659 2009; 3: 288–299. 660 9. Cuisiat F, Jostad HP, Andresen L, Skurtveit E, Skomedal E, Hettema M, Lyslo K. 661 Geomechanical integrity of sealing faults during depressurization of the Statfjord field. Journal 662 of Structural Geology. 2010; 32: 1754–1767. 663 10. Cappa F, Rutqvist J. Modeling of coupled deformation and permeability evolution during fault 664 reactivation induced by deep underground injection of CO2. International Journal of 665 Greenhouse Gas Control. 2011; 5: 336–346. 666 11. Morris JP, Hao Y, Foxall W, McNab W. A study of injection-induced mechanical deformation 667 at the In Salah CO2 storage project. International Journal of Greenhouse Gas Control. 2011; 668 5:270-280. 669 12. Orlic B, Heege J, Wassing B. Assessing the integrity of fault- and top seals at CO2 storage sites. 670 Energy Procedia. 2011; 4: 4798-4805. 671 13. Pirayehgar A, Dusseault MB. 2015, Numerical investigation of seismic events associated with 672 hydraulic fracturing. In: Proceedings of 13th ISRM International Symposium. Montreal, 673 Canada. 2015: ISRM-13CONGRESS-2015-168. 674 14. Zangeneh N, Eberhardt E, Bustin RM. Investigation of the influence of natural fractures and 675 in-situ stress on hydraulic fracture propagation using a distinct-element approach. Canadian 676 Geotechnical Journal. 2015; 52: 926-946. 677 15. Amini A, Eberhard E. Influence of tectonic stress regime on the magnitude distribution of 678 induced seismicity events related to hydraulic fracturing. Journal of Petroleum Science and 679 Engineering. 2019; 182: 106284. 680 16. Leijon B. Mechanical properties of fracture zones. SKB Technical Report TR 93-19; 1993. 681 17. Rutqvist J, Wu YS, Tsang CF, Bodvarsson G. A modeling approach for analysis of coupled 682 multiphase fluid flow, heat transfer, and deformation in fractured porous rock. International 683 Journal of Rock Mechanics and Mining Sciences. 2002; 39: 429-442. 684 18. Birkholzer JT, Tsang CF, Bond AE, Hudson JA, Jing L, Stephansson O. 25 years of 685 DECOVALEX - Scientific advances and lessons learned from an international research

686 collaboration in coupled subsurface processes. International Journal of Rock Mechanics and 687 Mining Sciences. 2019; 122: 103995. 688 19. Rutqvist J, Graupner B, Guglielmi Y, Birkholzer J, Kim T, Maßmann J, Nguyen TS, Park JW, 689 Shiu W, Urpi L, Yoon JS, Ziefle G. An international simulation study of a controlled fault 690 activation experiment at Mont Terri Laboratory. International Journal of Rock Mechanics and 691 Mining Sciences. (this issue, to be submitted) 692 20. Guglielmi Y, Elsworth D, Cappa F, Henry P, Gout C, Dick P, Durand J. In situ observations on 693 the coupling between hydraulic diffusivity and displacements during fault reactivation in shales. 694 Journal of Geophysical Research: Solid Earth. 2015; 120: 7729-7748. 695 21. Pruess K, Oldenburg C, Moridis G. TOUGH2 User's guide, ver. 2.0. Lawrence Berkeley 696 National Laboratory (LBNL) Report LBL-43134. Berkeley: LBNL; 1999. 697 22. Itasca Consulting Group Inc. FLAC3D manual: Fast Lagrangian analysis of continua in 3 698 dimensions - ver. 5.0 manual. Minnesota: Itasca Consulting Group Inc; 2012. 699 23. Tsang CF, Birkholzer J, Rutqvist J. A comparative review of hydrologic issues involved in 700 geologic storage of CO2 and injection disposal of liquid waste. Environmental Geology. 2008; 701 54: 1723-1737. 702 24. Cappa F, Rutqvist J. Seismic rupture and ground accelerations induced by CO2 injection in the 703 shallow crust. Geophysical Journal International. 2012; 190: 1784–1789. 704 25. Kim HM, Rutqvist J, Ryu DW, Choi BH, Sunwoo C, Song WK. 2012. Exploring the concept 705 of compressed air energy storage (CAES) in lined rock caverns at shallow depth: A modeling 706 study of air tightness and energy balance. Applied Energy. 2012; 92: 653-667. 707 26. Rutqvist J. Status of the TOUGH-FLAC simulator and recent applications related to coupled 708 fluid flow and crustal deformations. Computers & Geosciences. 2012; 37: 739-750. 709 27. Rutqvist J, Dobson PF, Garcia J, Hartline C, Jeanne P, Oldenburg CM, Vasco DW, Walters M. 710 The northwest Gevsers EGS demonstration project, California: Pre-stimulation modeling and 711 interpretation of the stimulation. Mathematical Geosciences. 2015; 47: 3-29. 712 28. Park JW, Rutqvist J, Ryu DW, Park ES, Synn JH. Coupled thermal-hydrological-mechanical 713 behavior of rock mass surrounding a high-temperature thermal energy storage cavern at shallow 714 depth. International Journal of Rock Mechanics & Mining Sciences. 2016; 83: 149-161. 715 29. Zbinden D, Rinaldi AP, Urpi L, Wiemer S. On the physics-based processes behind production-716 induced seismicity in natural gas fields. Journal of Geophysical Research: Solid Earth. 2017; 717 122: 3792-3812. 718 30. Urpi L, Rinaldi AP, Rutqvist J, Wiemer S. Fault stability perturbation by thermal pressurization 719 and stress transfer around a deep geological repository in a clay formation. Journal of 720 Geophysical Research: Solid Earth. 2019; 124: 8506–8518. 721 31. Croucher AE, O'Sullivan MJ. Approaches to local grid refinement in TOUGH2 models. In:

722	Proceedings of 35th New Zealand Geothermal Workshop, Rotorua, New Zealand. 2013: 17-20.
723	32. Bonduà S, Battistelli A, Berry P, Bortolotti V, Consonni A, Cormio C, Geloni C, Vasini EM.
724	3D Voronoi grid dedicated software for modeling gas migration in deep layered sedimentary
725	formations with TOUGH2-TMGAS. Computers & Geosciences. 2017; 108: 50-55.
726	33. Witherspoon PA, Wang JSY, Iwai K, Gale JE. Validity of Cubic Law for Fluid Flow in a
727	Deformable Rock Fracture. Water Resources Research. 1980; 16: 1016–1024.
728	34. Freeze RA, Cherry JA. Groundwater. New Jersey: Prentice-Hall; 1979.
729	35. Rutqvist J, Tsang CF, Stephansson O. Determination of fracture storativity in hard rocks using
730	high pressure testing. Water Resources Research. 1998; 34: 2551-2560.
731	36. Biot MA, Willis DG. The elastic coefficients of the theory of consolidation. Journal of Applied
732	Mechanics. 1957; 24: 594–601.
733	37. Priest SD. Discontinuity analysis for rock engineering. New York: Chapman & Hall; 1993.
734	38. Bossart P, Bernier F, Birkholzer J, Bruggeman C, Connolly P, Dewonck S, Fukaya M, Herfort
735	M, Jensen M, Matray JM, Mayor JC, Moeri A, Oyama T, Schuster K, Shigeta N, Vietor T,
736	Wieczorek K. Mont Terri Rock Laboratory, 20 years of research: Introduction, site
737	characteristics and overview of experiments. Swiss Journal of Geosciences. 2017; 110: 3-22.
738	39. Guglielmi Y, Birkholzer J, Rutqvist J, Jeanne P, Nussbaum C. Can fault leakage occur before
739	or without reactivation? Results from an in situ fault reactivation experiment at Mont Terri.
740	Energy Procedia. 2017; 114: 3167–3174.
741	40. Guglielmi Y, Cappa F, Lancon H, Janowczyk J, Rutqvist J, Tsang CF, Wang JSY. ISRM
742	suggested method for step-rate injection method for fracture in-situ properties (SIMFIP): Using
743	a 3-components borehole deformation sensor. Rock Mechanics and Rock Engineering. 2017;
744	47: 303–311.
745	41. Martin CD, Lanyon GW. Measurement of in-situ stress in weak rocks at Mont Terri Rock
746	Laboratory, Switzerland. International Journal of Rock Mechanics & Mining Sciences. 2003;
747	40: 1077–1088.
748	42. Yong S, Kaiser PK, Loew S. Influence of tectonic shears on tunnel-induced fracturing.
749	International Journal of Rock Mechanics & Mining Sciences. 2010; 47: 894–907.
750	43. Jaeger JC, Cook NGW, Zimmerman RW. Fundamentals in rock mechanics. 4th edition. Oxford:
751	Blackwell publishing; 2007.
752	44. Hanks TC, Kanamori H. A moment magnitude scale. Journal of Geophysical Research: Solid
753	Earth. 1979; 84: 2348–2350.
754	
755	
756	
757	









Fig. 2. Model domain and numerical mesh in FLAC3D for benchmark calculations: (a) model
geometry and monitoring point locations, (b) host rock zone elements, and (c) fault interface
elements.

- 769
- 770
- 771





Fig. 5. Profiles of hydraulic aperture along the fault strike estimated at 100, 157, 420, 453, and 807 s
of water injection.



Fig. 6. Profiles of pressure along the fault strike estimated at 100, 157, 420, 453, and 807 s of water
injection.



Fig. 7. Variations in pressures monitored at P2 and P3; the red lines denote the results of FM1 and the
black lines denote the results of FM2.



791

792

Fig. 8. Variations in injection flow rate at P1; the red denotes the result of FM1 and the black denotes
the result of FM2.



- 27 -





Fig. 11. Fault normal displacement (u_n) and fault shear displacement in the fault dip direction (u_{sd}) estimated at (a) P1 and (b) P2; the red lines denote the results of FM1 and the black lines denote the results of FM2.

826

821 822

819

820





Fig. 13. Relative displacement of upper anchor to lower anchor; dz denotes the vertical displacement and dy denotes the displacement in the fault dip direction.







Fig. 16. Field experimental results for numerical simulation: (a) injection chamber pressure, pressure at monitoring point, and injection flow rate; (b) vertical and horizontal (northern and western) 859 components of relative displacement of upper anchor to lower anchor. 860



⁸⁶² Fig. 17. Numerical model including a fault plane with a dip direction of 135° and dip angle of 60°.



Fig. 18. Variation in injection flow rate (Case 1) – comparison between field experimental (black line)
and numerical (red line) results.

863

867





Fig. 21. Variations in relative displacement of upper anchor to lower anchor (Case 1) – comparison
 between field experimental (dashed lines) and best-matching numerical (solid lines) results.



Fig. 22. Comparison between anchor displacement and fault displacement (Case 1); u_n and u_s denote the normal and shear displacements of the fault monitored at injection point P1; d_n and d_s denote the components of anchors' relative displacement vector in fault normal and shear directions.

- 888
- 889



Fig. 23. Variation in injection flow rate (Case 2) – comparison between field experimental (black line)
 and numerical (red line) results.



Fig. 24. Variations in pressures at injection and monitoring points (Case 2) – comparison between
field experimental (dotted lines) and numerical (solid lines) results.





Fig. 25. Variations in relative displacement of upper anchor to lower anchor (Case 2) – comparison
 between field experimental (dashed lines) and numerical (solid lines) results.



904
905Fig. 26. Shear displacement and extent of shear failure zone estimated at 453 s of water injection with
injection pressure of 6.302 MPa (Case 1)

Material	Parameter	Value	
Host rock (Elastic)	Bulk modulus (GPa)	5.9	
	Shear modulus (GPa)	2.3	
	Bulk density (kg/m^3)	2450	
	Permeability	0	
Fluid	Density (kg/m ³)	1000	
	Compressibility (Pa ⁻¹)	4.4×10^{-1}	10
	Dynamic viscosity (Pa s)	1.0×10^{-2}	3
Fault (Elastic-perfectly plastic)	Fault model	FM1	FM2
	Normal stiffness (GPa/m)	20	20
	Shear stiffness (GPa/m)	20	20
	Cohesion (MPa)	0	0
	Static friction angle (°)	22	22
	Dilation angle (°)	0	10
	Tensile strength (MPa)	0	0
	Initial aperture (μ m)	0	10
	Initial creation aperture (μ m)	28	0

⁹¹⁵ Table 1. Input parameters of the host rock, fluid, and fault zone for benchmark calculations.

⁹¹⁸ Table 2. Input parameters of fault and in-situ stress used for the calibration process.

Parameter		Range	Case 1 (Best match)	Case 2 (Second-best match)
Fault	Dip direction (°) 120	120 - 150	140	135
	Dip angle (°)	50-70	70	60
	Shear stiffness (GPa/m)	20-100	60	55
	Shear stiffness (GPa/m)	20-100	30	22
	Cohesion (MPa)	0–2	0	0.2
	Creation aperture at rupture (μ m)	28-80	40	28
	Friction angle (°)	22 (Fixed)	22	22
	Dilation angle (°)	0 (Fixed)	0	0
	Tensile strength (MPa)	0 (Fixed)	0	0
In situ	Magnitude of principal stress (MPa)	$\sigma_1 = 5.0 - 7.0$	$\sigma_1 = 5.1$	$\sigma_1 = 7.0$
stress		$\sigma_2 = 4.0 - 5.0$	$\sigma_2 = 5.0$	$\sigma_2 = 5.0$
		$\sigma_3 = 0.6 - 3.0$	$\sigma_3 = 2.0$	$\sigma_3 = 3.0$