



HAL
open science

Three-dimensional Modeling of Cracking with Thermo-hydromechanical Process by Considering Rock Heterogeneity

Zhan Yu, Jianfu Shao, Yue Sun, Minh-Ngoc Vu, Carlos Plua, Gilles Armand

► **To cite this version:**

Zhan Yu, Jianfu Shao, Yue Sun, Minh-Ngoc Vu, Carlos Plua, et al.. Three-dimensional Modeling of Cracking with Thermo-hydromechanical Process by Considering Rock Heterogeneity. *Rock Mechanics and Rock Engineering*, In press, 10.1007/s00603-023-03536-4 . hal-04364465

HAL Id: hal-04364465

<https://hal.science/hal-04364465>

Submitted on 30 Dec 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/373772893>

Three-dimensional Modeling of Cracking with Thermo-hydromechanical Process by Considering Rock Heterogeneity

Article in *Rock Mechanics and Rock Engineering* · September 2023

DOI: 10.1007/s00603-023-03536-4

CITATIONS

0

READS

212

6 authors, including:



Zhan Yu

Université de Lille

18 PUBLICATIONS 74 CITATIONS

SEE PROFILE



Sun Yue

Université de Lille

13 PUBLICATIONS 128 CITATIONS

SEE PROFILE



Ngoc Minh Vu

French National Radioactive Waste Management Agency (Andra)

211 PUBLICATIONS 1,651 CITATIONS

SEE PROFILE



Carlos Plua

Andra

30 PUBLICATIONS 223 CITATIONS

SEE PROFILE

Three-dimensional modeling of cracking with thermo-hydromechanical process by considering rock heterogeneity

Zhan YU^{a,b}, Jianfu SHAO^{b,c,*}, Yue SUN^b, Minh-ngoc VU^d, Carlos PLUA^d, Gilles ARMAND^d

^a*Key Laboratory of Ministry of Education on Safe Mining of Deep Metal Mines, College of Resources and Civil Engineering, Northeastern University, Shenyang, 110819, China*

^b*University of Lille, CNRS, EC Lille, LaMcube, UMR9013, 59000 Lille, France*

^c*Institut Universitaire de France (IUF), France*

^d*Andra, Chatenay Malabry, France*

Abstract

This study is part of numerical simulations performed on an in-situ heating test conducted by the French National Radioactive Waste Management Agency (Andra) at the Meuse/Haute-Marne Underground Research Laboratory (URL) to study the thermo-hydromechanical behavior of the host Callovo-Oxfordian COx claystone in quasi real conditions, through the international research project DECOVALEX. We present a numerical study of damage and cracking process in saturated claystone subjected to thermo-hydromechanical coupling by considering material heterogeneity distribution. For this purpose, a macroscopic elastic model is first determined by using two steps of homogenization by taking into account the effects of porosity and mineral inclusions. This model is implemented into a finite element code devoted to solving thermo-hydromechanical coupling problems. The nucleation and propagation of cracks are described by using an extended phase-field method, considering the effects of temperature and fluid pressure on the evolution of phase-field. The proposed model is applied to the numerical analysis of cracking process due to excavation and heating around a group of boreholes (CRQ). The numerical results of the 3D simulation are compared with in-situ measurements of temperature and pore pressure distribution. The excavation damage zone and heating fracture is reproduced and analysed according to the structure of the heating position and the heterogeneity of the rock.

Keywords: Hydro-thermal cracking, material anisotropy, heterogeneous rocks, claystone,

Highlights

- A phase-field model is developed with thermo-hydromechanical processes;
- Both tensile and shear cracks are taken into account;
- Crack nucleation is emphasized by spatial heterogeneity of material properties;
- Cracking processes due to thermal-hydraulic interaction are analyzed in three-dimensional conditions.

1. Introduction

Clayey rocks are considered in France as a potential geological barrier for underground disposal of radioactive waste. In this context, it is necessary to investigate thermo-hydromechanical (THM) properties of such rocks and other materials involved in the storage facilities. For this purpose, under the coordination of the French National Agency for radioactive waste management (Andra), a series of in-situ experiments have been and are being carried out at the Bure Underground Research Laboratory (MHM URL). Detailed presentations of some experiments can be found in [1, 2, 3]. The main objective of those experiments is to investigate thermo-hydromechanical responses of the host Callovo-Oxfordian (COx) claystone and other components during excavation, heating, and gas injection. The results obtained from these experiments are used for the validation of numerical models developed for the analysis and design of the future geological storage project known as Cigeo.

In order to foster international collaboration in research on the geological disposal of radioactive waste, an active and long-standing international project called DECOVALEX has been established. Various topics and benchmark modeling studies have been investigated and performed [4, 5, 6].

*Corresponding author: jian-fu.shao@polytech-lille.fr

17 In the phase of DECOVALEX-2023, the task A1 has been proposed to improve the
18 numerical models' ability to predict the mechanisms and processes of fracture initiation and
19 growth in clayey rocks due to heating induced fluid pressure variation. In the task, the
20 step 1.2 is to reproduce the THM responses of an in-situ heating experiment performed by
21 Andra at the MHM URL in June 2019, called "Representative THM Behavior of a high-level
22 waste (HLW) Cell" (CRQ). This experiment involved two heating phases, lasting two and
23 one months respectively, separated by a cooling phase. It is an accelerated heating scenario
24 with the aim of replicating an effective stress evolution path which is expected to close to
25 that in the area around a HLW cell in the Cigeo project in a short period of time. The
26 rock is quickly heated until the pore fluid pressure reaches a critical value for the possible
27 creation of fractures.

28 Therefore, for the feasibility study of geological disposal of nuclear waste, the nucleation
29 and evolution of cracks is an essential issue. Such cracks can be initiated during gallery
30 excavation, temperature increase due to waste heat production, and gas pressure rise. They
31 are also expected to progressively [close](#) due to self-sealing and healing [process](#). During the
32 last decades, different types of numerical methods have been developed for modeling cracking
33 process. Without giving an exhaustive review, we can mention for instance enriched finite
34 element methods [7] and extended finite element methods (XFEM) [8, 9, 10]. In those
35 methods, it is needed to define specific criteria to describe the onset and propagation of
36 cracks. Other types of methods, including various discrete element methods, have also been
37 developed and can be used for modeling cracking processes. However, the description of
38 progressive transition from diffuse deformation to localized cracking is still a pending issue.
39 The analysis of three-dimensional multiple cracks is also a hard task.

40 Based on the variational principle for fracture mechanics [11], the so-called phase-field
41 method has been developed [12, 13]. By the approximation of sharp cracks by a regular-
42 ized crack density function and the minimization of a total energy functional, the phase-field
43 method is particularly efficient to deal with the progressive nucleation of localized cracks un-
44 der complex three dimensional problems. It is applied to modeling dynamic brittle fracture
45 [14], extended to multi-physics problems [15], and plastic materials [16, 17], etc..

46 In many previous studies, the accent was put on tensile cracks. For rocks subjected
 47 to compressive stresses as in most rock engineering problems, shear cracks represent an
 48 essential mechanism. Some extensions have been proposed [18, 19], generally using a specific
 49 decomposition of energy functional into a tensile part and a shear part. However, some
 50 critical issues should still be addressed. Under compressive stresses, complex mixed cracking
 51 modes can be observed [20, 21]. The propagation of frictional shear cracks is not only
 52 effected by deviatoric stress but also by confining pressure. Different types of extensions have
 53 been proposed considering frictional contact of cracks [22, 23, 24, 25]. Another interesting
 54 approach is to introduce two independent phase fields, respectively representing the tensile
 55 and shear cracks [26, 27].

56 In the present study, the concept of two phase fields developed in our previous work [26]
 57 is adopted for modeling tensile and shear cracks. It is further extended to three-dimensional
 58 coupled thermo-hydromechanical problems. In particular, the influence of fluid pressure
 59 due to heating process on the initiation and propagation of cracks is taken into account.
 60 Moreover, the effect of material heterogeneity due to spatial variability of mineralogical
 61 composition of clayey rocks is also investigated. The numerical results are compared with
 62 experimental data obtained from in-situ experiments.

63 **2. Phase-field method for thermo-hydromechanical problems**

64 In this work, a saturated porous medium is assumed to occupy the volume Ω with
 65 the external boundary $\partial\Omega$. Three physical fields are considered to describe the thermo-
 66 hydromechanical behavior of this material: i) In the mechanical field, it has the body force
 67 \mathbf{f}_b in Ω , the surface force \mathbf{t}_N on the part of external boundary $\partial\Omega_f$ and the prescribed
 68 displacement $\bar{\mathbf{u}}$ on the complementary part external boundary $\partial\Omega_u$; ii) In the pore fluid
 69 pressure field, it has the fluid flux \bar{w} on the external boundary $\partial\Omega_w$ and to the prescribed
 70 fluid pressure \bar{p} on the external boundary $\partial\Omega_p$; iii) In the temperature field, it has the heat
 71 flux $\bar{\mathbf{q}}$ on the external boundary $\partial\Omega_q$ and the prescribed temperature change $\bar{\theta}$ on the external
 72 boundary $\partial\Omega_\theta$. In addition, in this THM problem the process of onset and propagation of
 73 crack is taken into account by using phase-field method.

74 Since it has been seen many times in the literature, it is the author choice to keep the
 75 writing as light and simple as possible, emphasizing only the several strong assumptions
 76 made and their consequences, for the sake of the reading.

77 2.1. Variational framework

78 Based on the spirit of Griffith theory, [11] proposed a variation approach for quasi-
 79 static brittle fracture. The nucleation and propagation of quasi-static cracking process are
 80 considered as the minimisation of energy function that comprises stored energy and energy
 81 necessary for crack formation. This variational framework is suitable to extended to consider
 82 the crack process on the mentioned saturated porous material subjected to THM loads. In
 83 this way, the total energy functional is developed as:

$$E(\boldsymbol{\varepsilon}^e, m, \theta, \Gamma) = E_e(\boldsymbol{\varepsilon}^e, m, \theta, \Gamma) + E_c(\Gamma) \quad (1)$$

84 where $E_c(\Gamma)$ is the fracture surface energy and $E_e(\boldsymbol{\varepsilon}^e, m, \theta, \Gamma)$ denotes the elastic strain
 85 energy of cracked material, which is a function of elastic strain tensor $\boldsymbol{\varepsilon}^e$, fluid mass change
 86 per unit initial volume m and variation of temperature θ , as well as the set of crack Γ .

87 2.1.1. Phase field model

88 Following the regularization strategy proposed by [12], the crack can be represented by
 89 the scalar phase field variable d , which has the range from 0 (intact material) to 1 (fully
 90 broken). Furthermore, in order to easily deal with mixed-mode cracks of rock-like material,
 91 a so-called double phase field method [28] is considered to introduce tensile damage d^t and
 92 shear damage d^s . In this way, the approximated crack surface area can be represented as:

$$A_\Gamma \approx A_\Gamma^t(d^t) + A_\Gamma^s(d^s) = \int_\Omega \{\gamma^t(d^t, \nabla d^t) + \gamma^s(d^s, \nabla d^s)\} d\Omega \quad (2)$$

93 where total surface area of sharp crack A_Γ is approximated by the volumetric integration of a
 94 crack density function for tensile crack $\gamma^t(d^t, \nabla d^t)$ and shear crack $\gamma^s(d^s, \nabla d^s)$. Among three
 95 commonly employed phase-field models proposed by [12, 29, 30], we adopt the formulation
 96 presented by [29], which can be expressed as follows:

$$\gamma^\alpha(d^\alpha, \nabla d^\alpha) = \frac{1}{2} \left\{ \frac{1}{l_d} (d^\alpha)^2 + l_d \nabla d^\alpha \cdot \nabla d^\alpha \right\} \quad ; \quad \alpha = t, s \quad (3)$$

97 where l_d denotes a length scale parameter which is in relation with the width of smeared
 98 cracks. The crack density functions, denoted as $\gamma^\alpha(d^\alpha, \nabla d^\alpha)$, are dependent on both the
 99 damage variables d^α and their gradients ∇d^α . This non-local formulation enables the regu-
 100 larization of damage localization issues. With the help of the approximation work, Equation
 101 (1) can be rewritten as:

$$E(\boldsymbol{\varepsilon}^e, m, \theta, d^t, d^s) = \int_{\Omega} w_e(\boldsymbol{\varepsilon}^e, m, \theta, d^t, d^s) d\Omega + \int_{\Omega} w_c(d^t, d^s, \nabla d^t, \nabla d^s) d\Omega \quad (4)$$

102 with elastic strain energy of cracked material w_e , and the energy density per unit volume
 103 requested to create the crack w_c :

$$w_c(d^t, d^s, \nabla d^t, \nabla d^s) = g_c^t \gamma^t(d^t, \nabla d^t) + g_c^s \gamma^s(d^s, \nabla d^s) \quad (5)$$

104 2.1.2. Elastic free energy

105 For an intact saturated porous medium, the constitutive relations due to thermo-poroelastic
 106 theory [31, 32] can be expressed as:

$$\boldsymbol{\sigma} - \boldsymbol{\sigma}^0 = \mathbb{C}_b^0 : \boldsymbol{\varepsilon}^e - b\mathbf{I}(p - p^0) - 3K_b\alpha_b\mathbf{I}\theta \quad (6)$$

$$p - p_0 = M(-b\mathbf{I} : \boldsymbol{\varepsilon}^e + \frac{m}{\rho_f^0}) + 3\alpha_m M\theta \quad (7)$$

$$s - s_0 = s_m^0 m + \alpha_b \mathbf{I} : (\boldsymbol{\sigma} - \boldsymbol{\sigma}^0) - (3\alpha_m - b\alpha_b \mathbf{I})(p - p_0) + \frac{C_\sigma^b}{T_0} \theta \quad (8)$$

109 For the sake of readability, the mentioned symbols are explained in nomenclature. In this
 110 study, though the initial anisotropy of elastic properties of COx claystone is taken into ac-
 111 count, for the sake of simplicity, the tensors of Biot coefficients, thermal dilation coefficients
 112 and drained thermo-elastic coupling coefficients are taken as isotropic ones. In order to deal
 113 with anisotropic elastic materials, the so-called Reuss equivalent bulk modulus is here used:
 114 $K_b = k_{Reuss}(d^t, d^s)$. The Biot modulus is accordingly given by $1/M = (b - \phi)/K_m + \phi/K_f$.
 115 The differential thermal coefficient is given by $\alpha_m = (b - \phi)\alpha_b + \phi\alpha_f$. By using these
 116 constitutive relations, the elastic free energy of an intact material can be determined as:

$$w_e^0(\boldsymbol{\varepsilon}^e, p, \theta) = \frac{1}{2} \boldsymbol{\sigma}_b : \boldsymbol{\varepsilon}^e + \frac{1}{2} \frac{(p - p_0)^2}{M} - \frac{1}{2} \frac{C_\sigma^b}{T_0} \theta^2 \quad (9)$$

117 with Biot effective stress tensor σ_b :

$$\sigma^b = (\sigma - \sigma^0) + \mathbf{B}(p - p_0) \quad (10)$$

118 Given that the effective stress plays an important role in the onset and propagation of
 119 cracking process for saturated rock-like material, we decompose the Biot effective stress into
 120 a tensile part and a compressive part:

$$\begin{cases} \sigma^{b+} = \mathbb{P}_\sigma^+ : \sigma^b \\ \sigma^{b-} = \mathbb{P}_\sigma^- : \sigma^b \end{cases} \quad (11)$$

121 with the operators for spectral decomposition of stress tensor \mathbb{P}_σ^\pm proposed in [33, 34]. As-
 122 suming the extension behavior is affected by tensile crack and the compression behavior is
 123 mainly influenced by shear crack, the elastic free energy of the damaged material can be
 124 expressed as:

$$w_e(\boldsymbol{\varepsilon}^e, p, \theta, d^t, d^s) = h_t(d^t)w_e^{0+} + h_s(d^s)w_e^{0-} + \frac{1}{2} \frac{(p - p_0)^2}{M} - \frac{1}{2} \frac{C_\sigma^b}{T_0} \theta^2 \quad (12)$$

125 with

$$\begin{cases} w_e^{0+} = \frac{1}{2} \sigma^{b+} : \boldsymbol{\varepsilon}^e \\ w_e^{0-} = \frac{1}{2} \sigma^{b-} : \boldsymbol{\varepsilon}^e \end{cases} \quad (13)$$

126 The decomposition of Biot effective stress tensor is due to the operators \mathbb{P}_σ^\pm (see the detail
 127 of old study [35]). A common form $h_\alpha(d^\alpha) = (1 - k)(1 - d^\alpha)^2 + k$ with $\alpha = t, s$ is used to
 128 represent the degradation of failure process. In this study, $k = 1 \times 10^{-9}$ is applied to avoid
 129 the calculating error after the material is fully broken ($d^\alpha = 1$).

130 2.1.3. Evolution of crack fields

131 Given that all the terms of total energy functional are obtained and introduced, the
 132 governing equations for tensile crack d^t and shear crack d^s can be determined by solving the

133 minimization problem of Equation (4):

$$\left\{ \begin{array}{l} -\frac{\partial w_e}{\partial d^\alpha} - g_c^\alpha \delta_{d^\alpha} \gamma^\alpha = 0 \quad , \quad \dot{d}^\alpha > 0 \quad , \quad \text{in } \Omega \\ -\frac{\partial w_e}{\partial d^\alpha} - g_c^\alpha \delta_{d^\alpha} \gamma^\alpha \leq 0 \quad , \quad \dot{d}^\alpha = 0 \quad , \quad \text{in } \Omega \\ \frac{\partial \gamma}{\partial \nabla d^\alpha} \cdot \mathbf{n} = 0 \quad , \quad \text{on } \delta\Omega \end{array} \right. \quad (14)$$

134 More precisely, the evolution of two crack fields are described by the following equations:

$$\left\{ \begin{array}{l} -h'_t(d^t)w_{e+}^0 - g_c^t \left\{ \frac{1}{l_d} d^t - l_d \Delta d^t \right\} = 0 \quad , \quad \dot{d}^t > 0 \\ -h'_s(d^s)w_{e-}^0 - g_c^s \left\{ \frac{1}{l_d} d^s - l_d \Delta d^s \right\} = 0 \quad , \quad \dot{d}^s > 0 \end{array} \right. \quad (15)$$

135 where the two elastic energy of intact material w_e^{0+} and w_e^{0-} are represented in Equation
 136 (13). It is reasonable to define the tensile crack evolution is driven by the positive part of
 137 elastic energy w_e^{0+} . On the other hand, given that the pure compression behavior can not
 138 contribute to create the shear crack, only a part of negative part of elastic energy w_e^{0-} can
 139 be seen as the driving quantity for compressive-shear crack (see [28] for detail):

$$w_-^s = \frac{1}{2G} \left\langle \frac{\langle \sigma_1^t \rangle_- - \langle \sigma_3^t \rangle_-}{2 \cos \varphi} + \frac{\langle \sigma_1^t \rangle_- + \langle \sigma_3^t \rangle_-}{2} \tan \varphi - c \right\rangle_+^2 \quad (16)$$

140 with the bracket $\langle \cdot \rangle_\pm$ such as:

$$\left\{ \begin{array}{l} \langle a \rangle_+ = a, \quad \langle a \rangle_- = 0, \quad a \geq 0 \\ \langle a \rangle_+ = 0, \quad \langle a \rangle_- = a, \quad a < 0 \end{array} \right. \quad (17)$$

141 with cohesion c and friction angle φ of material. The major and minor Terzaghi effective
 142 principal stress σ_1^t and σ_3^t are considered according to the study [36, 37]. By substituting
 143 the physically-based driving energy into (15), w_{e-}^0 can be replaced by w_-^s . Finally, based on
 144 the concept of [13], two energy history functionals are defined as follows:

$$\left\{ \begin{array}{l} \mathcal{H}^t(t) = \max[w_{e+}^0(\tau)]_{\tau \in [0,t]} \\ \mathcal{H}_-^s(t) = \max[w_-^s(\tau)]_{\tau \in [0,t]} \end{array} \right. \quad (18)$$

145 Given that the history functionals H^t and H_-^s are used instead of w_{e+}^0 and w_-^s in the
 146 evolution equation of tensile and shear crack respectively, the irreversibility of cracking
 147 process is taken into account.

148 3. Numerical implementation in finite element method

149 The THM problem considering tensile and shear crack can be solved by using the frame-
 150 work of finite element method. According to Equations (6), (7), (8) and (15), the weak
 151 forms for five unknown fields are expressed as:

$$\int_{\Omega} \delta \boldsymbol{\varepsilon} : \mathbb{C}^b(d^t, d^s) : \boldsymbol{\varepsilon} dV - \int_{\Omega} \delta \boldsymbol{\varepsilon} : (\delta p) \mathbf{I} dV - \int_{\Omega} \delta \boldsymbol{\varepsilon} : (3\alpha_b K_b(d^t, d^s) T) \mathbf{I} dV = \int_{\Omega_f} \mathbf{t} \cdot \delta \mathbf{u} dS \quad (19)$$

$$\begin{aligned} \int_{\Omega} \frac{\mathbf{k}(d^t)}{\mu} \nabla p \cdot \nabla (\delta p) dV &= \int_{\Omega_{\omega}} \frac{\mathbf{k}(d^t)}{\mu} \delta p \cdot \nabla p \bar{n} dS - \int_{\Omega} \frac{1}{M} \frac{\partial p}{\partial t} \delta p dV \\ &\quad - \int_{\Omega} b \frac{\partial \varepsilon_{kk}}{\partial t} \delta p dV + \int_{\Omega} 3\alpha_m \frac{\partial \theta}{\partial t} \delta p dV \end{aligned} \quad (20)$$

$$\begin{aligned} \int_{\Omega} \lambda \nabla T \cdot \nabla (\delta \theta) dV &= \int_{\Omega_q} \lambda \delta T \nabla T \cdot \bar{n} dS - \int_{\Omega} C_{\varepsilon}^b \frac{\partial \theta}{\partial t} \delta \theta dV - \int_{\Omega} (3\alpha_b K_b(d^t, d^s) T_0) \frac{\partial \varepsilon_{kk}}{\partial t} \delta \theta dV \\ &\quad + \int_{\Omega} (3\alpha_m T_0) \frac{\partial p}{\partial t} \delta \theta dV + \int_{\Omega} \frac{\mathbf{k}(d^t)}{\mu} \nabla p \cdot (C_p \nabla \theta) \delta \theta dV \end{aligned} \quad (21)$$

$$\int_{\Omega} \{ (g_c^t / l_d + 2\mathcal{H}_t) d^t \delta d^t + g_c^t \nabla d^t \cdot \nabla (\partial d^t) \} dV = \int_{\Omega} 2\mathcal{H}_t \partial d^t dV \quad (22)$$

$$\int_{\Omega} \{ (g_c^s / l_d + 2\mathcal{H}_-^s) d^s \delta d^s + g_c^s \nabla d^s \cdot \nabla (\partial d^s) \} dV = \int_{\Omega} 2\mathcal{H}_-^s \partial d^s dV \quad (23)$$

152 Among these relations, the effect of damage is mainly realized on mechanical field and
 153 pore pressure field according to the elastic stiffness of undamaged material:

$$\mathbb{C}_b(d^t, d^s) = \{ h_t(d^t) \mathbb{P}_{\sigma}^+ + h_s(d^s) \mathbb{P}_{\sigma}^- \} : \mathbb{C}_b^0 \quad (24)$$

154 and the permeability tensor of cracked porous medium:

$$\mathbf{k}(d^t, d^s) = \mathbf{k}_0 \exp(\eta_k \max(d^t, d^s)) \quad (25)$$

155 with the elastic stiffness of undamaged material \mathbb{C}_b^0 , evolution rate of permeability η_k and
156 the initial permeability tensor of intact porous medium \mathbf{k}_0 . The drained bulk modulus
157 $K_b(d^t, d^s)$ can be calculated according to obtained $\mathbb{C}_b(d^t, d^s)$. The damage effect for thermal
158 parameters of the material is ignored in this study.

159 In the framework of the finite element method, following the previous work, the THM
160 coupling problem formulation [26] and the formulation of the tensile and shear crack prob-
161 lem [28] can be solved. Considering the physical characteristic of the rock material, the
162 temperature field is solved by an explicit decoupled algorithm, as it is not sensitive to the
163 effects of the mechanical field, the pore pressure field and the damage fields. In order to
164 save the computation memory and time, the fixed stress iteration [38] is used to solve the
165 hydromechanical coupling. And the so-called Alternate Minimization (AM) solver proposed
166 in [12, 39] is used to couple the displacement field and phase fields because of its good
167 robustness performance.

168 4. Consideration of material heterogeneity

169 In rock-like materials, cracks often start due to variations in the material, such as at
170 interfaces between stiff inclusions and a weak matrix, or in weak zones with high porosity.
171 Previous studies have used a numerical trick of placing weak elements in the material to
172 facilitate crack initiation and propagation. However, in this work, we use a micro-mechanics
173 based approach to more accurately reflect the effect of material heterogeneity on mechanical
174 properties. Specifically, we use an analytical homogenization method to determine macro-
175 scopic elastic properties as explicit functions of porosity and inclusion volume fraction at
176 the microscopic scale.

177 For this study, we focus on the Callovo-Oxfordian (COx) claystone, which has been
178 widely studied in France for its potential use in storing radioactive waste. Previous research
179 [40] has identified two main scales of interest for this material: at the mesoscopic scale,
180 mineral particles like quartz, calcite, and pyrite are randomly distributed in a clay matrix;
181 at the microscopic scale, the majority of pores are found inside the clay matrix.

182 In order to determine the macroscopic elastic properties, two steps of linear homoge-
 183 nization is performed considering two micro-structure parameters: the porosity of the clay
 184 matrix f_p and the volume fraction of mineral inclusions f_i , one gets:

$$f_p = \frac{\Omega_p}{\Omega_p + \Omega_m} \quad (26)$$

$$f_i = \frac{\Omega_i}{\Omega_i + \Omega_p + \Omega_m} \quad (27)$$

186 Ω is the volume of representative volume element, while Ω_p , Ω_i and Ω_m are respectively the
 187 volumes occupied by pores, inclusions and solid clay matrix. To account for the inclusion-
 188 matrix morphology, we use the standard Mori-Tanaka scheme for each homogenization step
 189 [41]. In the first step, we determine the effective elastic tensor of the porous matrix (\mathbb{C}^{mp})
 190 by considering the effect of porosity. One gets:

$$\mathbb{C}^{mp} = (1 - f_p)\mathbb{C}^m : [(1 - f_p)\mathbb{I} + f_p(\mathbb{I} - \mathbb{P}^p : \mathbb{C}^m)^{-1}]^{-1} \quad (28)$$

191 $\mathbb{P}^p(\mathbb{C}^m)$ is the fourth order Hill tensor for ellipsoidal pores [42, 43], \mathbb{C}^m is the elastic tensor
 192 of solid matrix, and \mathbb{I} is the fourth order unit tensor. At the mesoscopic step of homoge-
 193 nization, the macroscopic elastic tensor of heterogeneous rocks is determined after including
 194 the influence of mineral inclusions:

$$\mathbb{C}^{hom} = \mathbb{C}^{mp} + [f_i(\mathbb{C}^{in} - \mathbb{C}^{mp}) : \mathbb{D}^{in}] : [\mathbb{I} + f_i(\mathbb{C}^{in} - \mathbb{I})]^{-1} \quad (29)$$

195 with

$$\mathbb{D}^{in} = [\mathbb{I} + \mathbb{P}^i : (\mathbb{C}^{in} - \mathbb{C}^{mp})]^{-1} \quad (30)$$

196 $\mathbb{P}^i(\mathbb{C}^{mp})$ is the Hill tensor for spherical inclusions [42, 43]. It is worth noting that, we combine
 197 different families of mineral particles into a single equivalent inclusion phase, and represent
 198 its elastic stiffness tensor as \mathbb{C}^{in} .

199 Since the spatial variability of macroscopic elastic properties in COx claystone is at-
 200 tributed to the non-uniform distribution of porosity and inclusion concentration, in this
 201 study, we assume a random distribution of porosity (f_p) and volumetric fraction of mineral
 202 inclusions (f_i) using the standard Weibull distribution function:

$$\xi_\alpha = \frac{m_\alpha}{\beta_\alpha} \left(\frac{f_\alpha}{\beta_\alpha} \right)^{m_\alpha - 1} \exp\left[-\left(\frac{f_\alpha}{\beta_\alpha}\right)^{m_\alpha}\right], \alpha = p, i \quad (31)$$

203 where f_α is the volume fraction of pores ($\alpha = p$) and mineral inclusions ($\alpha = i$). β_α is the
204 scale parameter of the distribution which represents the mean value of random variable. m_α
205 is the homogeneity index of the material.

206 In this study, we have adopted an elastic-damage model. Plastic deformation is neglected.
207 Moreover, there exist theoretical homogenization models for predicting macroscopic elastic
208 properties with mineral compositions and porosity. Therefore, it seems to be a good choice
209 to consider effect of material heterogeneity on elastic properties.

210 5. Numerical simulation

211 In this section, the proposed THM modeling, which takes into account the double phase
212 field method, is applied to simulate the results of the in-situ CRQ test performed at Andra's
213 Underground Research Laboratory (URL) [44]. The simulation focuses on capturing the
214 thermo-hydromechanical responses and failure behavior of COx claystone during excavation
215 and heating-cooling processes.

216 5.1. General presentation of CRQ test

217 Figure 1 provides a partial view of the Andra URL, which is situated at a depth of -490
218 m. The study focuses on the GCS gallery located within the COx claystone layer. The
219 CRQ (Representative THM Behavior of a HLW Cell) in-situ experiment was performed in
220 the GCS gallery, as shown in Figure 1 (right). The experiment involved drilling ten 20
221 m long heater boreholes (CRQ1701-CRQ1710) horizontally from the GCS drift wall, with
222 the heaters installed in the last 10 m. In addition, sixteen sensors were positioned in four
223 additional boreholes (CRQ1720-CRQ1723) to monitor temperature and pore pressure. The
224 aim of the experiment was to examine the cracking process resulting from the THM behavior
225 of the rock, with the anticipated fracture location being between the two central boreholes
226 and 15 m from the GCS drift wall, which is at the mid-plane of the heater devices.

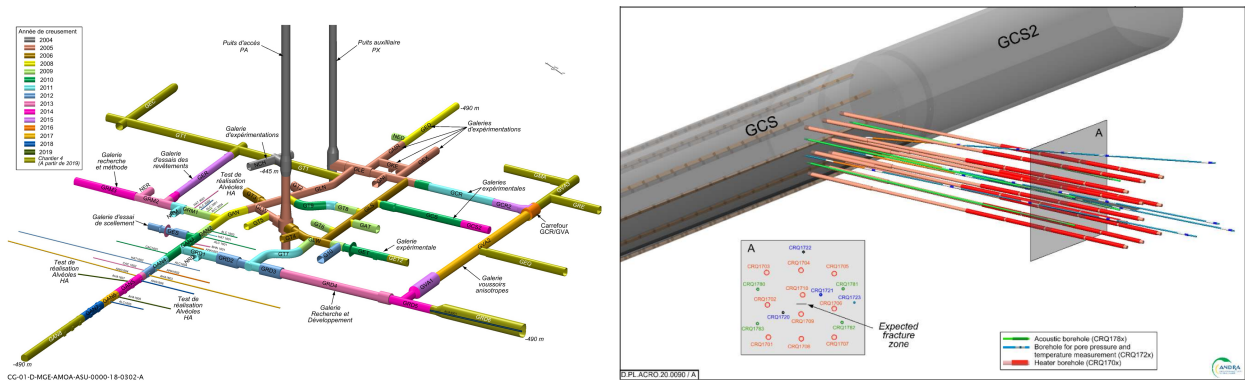


Figure 1: Partial view of Andra URL [44] (left) and view of CRQ heating test (right)

227 Two heating phases were performed using the mentioned heaters, and the heat power
 228 applied is shown in Figure 2. It is worth noting that the heater devised in CRQ1704 was
 229 damaged after the first heating phase. Therefore, the second heating phase was only heated
 230 by the remaining nine heater devices.

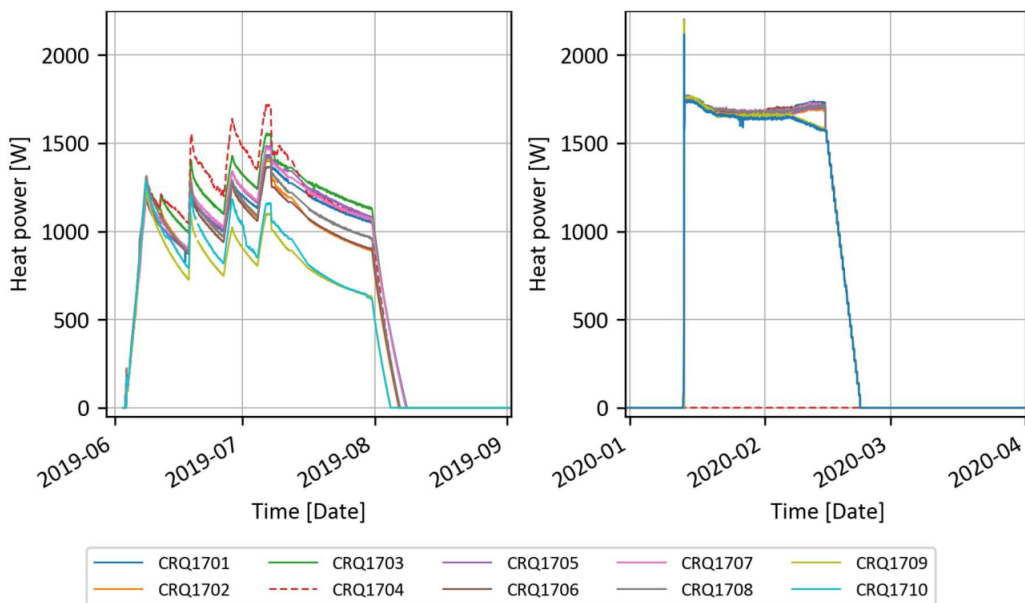


Figure 2: Timeline of the CRQ experiment with evolution of the heat power history of each heater device: (Left) first heating phase and (Right) second heating phase (provided by task specification)

231 *5.2. Input data of modeling*

232 As shown in Figure 3 (left), the studied 3D domain consists of a cube with dimensions of
233 50 m \times 50 m \times 50 m in order to represent the far field. On one surface of the studied cube,
234 half of the GCS drift with 5.2 m diameter is located. Ten heater boreholes with a diameter
235 of 0.172 m and a length of 20 m are placed on the wall of the GCS drift. The detailed
236 coordinates of these ten heater boreholes are shown in the appendix. For simplicity, the
237 four boreholes with sensors are not included. In this way, 883,232 tetrahedral elements with
238 148,807 nodes are used to mesh the studied domain, as shown in Figure 3 (right). Since the
239 rock around the heaters is expected to be damaged, the finest mesh is defined for this heater
240 part, which is 10-20 m deep from the GCS drift wall. This is balanced choice between a fine
241 description of damaged zones and computation costs such as computing memory and time
242 used.

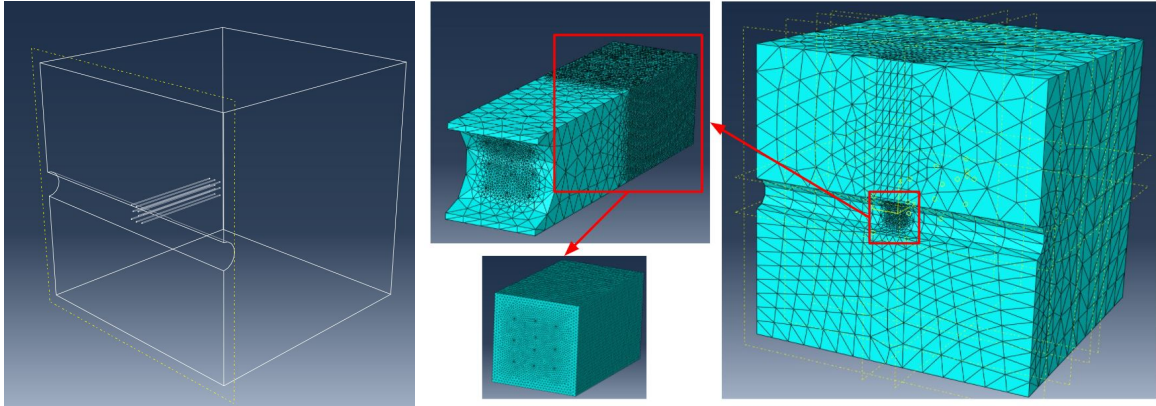


Figure 3: Geometry and mesh of CRQ simulation

243 Based on the study of [1, 45], the initial stress state of the studied domain is defined as
244 follows: i) the minimum principal stress σ_h is -12.4 MPa (parallel to the heater boreholes);
245 ii) the maximum principal stress σ_H is -16.1 MPa (parallel to the GCS gallery); and iii) the
246 vertical principal stress σ_v is -12.7 MPa (perpendicular to the heater boreholes and GCS
247 gallery). The initial temperature and pore pressure of the whole domain are assumed to be
248 uniform, with $T_0 = 22^\circ\text{C}$ and $p_0=4.7$ MPa, which are the values at a depth of -490 m from
249 the ground.

250 The boundary conditions are defined as shown in Table 1. The lateral faces are considered
 251 to have symmetrical conditions for all THM fields. The top and bottom faces are permeable
 252 to heat flux and fluid flux. After excavation of the GCS gallery, the drift wall is not fixed
 253 for displacement but is fixed for pore pressure at 0.1 MPa. The temperature of the gallery is
 254 applied based on the values measured during the experiment. The boundary conditions for
 255 the boreholes is changed while the heating phase begins. The surface of the drift changes
 256 from permeable to impermeable due to the installation of the resin.

Table 1: Boundary conditions of the CRQ simulation

Boundary	Thermal	Hydraulic	Mechanical
Lateral faces	Free surface	Free surface	Zero normal displacement
Top face	$22^{\circ}C$	4.7 MPa	-12.7 MPa
Bottom face	$22^{\circ}C$	4.7 MPa	Zero normal displacement
GCS drift wall	T(t)	0.1 MPa	Free surface
Borehole wall (before heating)	Free surface	0.1 MPa	Free surface
Borehole wall (during heating)	Free surface	Free surface	Free surface

257 According to previous studies [46], the COx claystone is considered to be a transversely
 258 isotropic material with regards to elastic modulus, failure strength, thermal, and hydraulic
 259 properties. For simplicity, only the initial anisotropy of elastic properties, permeability, and
 260 thermal conductivity is considered, while the other parameters are assumed to be isotropic.
 261 Following the previous experiment [47] and simulation work [48] for a laboratory-scale heat-
 262 ing test on the same rock, material parameters are provided as shown in Table 2. It is
 263 important to highlight that the measured parameters in the experiment can be influenced
 264 by several factors, including potential variable discrepancies and inherent variability among
 265 individual rock samples. The material parameters employed in this simulation have been
 266 carefully calibrated, taking into account the distinctions between laboratory-scale and in-
 267 situ tests. This calibration falls within an appropriate range, informed by the accumulated
 268 knowledge of COx claystone from ANDRA's experience.

269 The regular parameters of water are used in this work. For simplicity, the following
 270 parameters are considered as constant: bulk modulus of water $K_f = 2.2$ GPa, density of
 271 water $\rho_f = 1000$ kg/m³, heat capacity of water $C_f = 4180$ J/kg/K. The water dynamic
 272 viscosity μ_f (Pa·s) is due to temperature ($^{\circ}C$), it has:

$$\mu_f(T) = 4.2844 \times 10^{-5} + (0.157(T + 64.993)^2 - 91.296)^{-1} \quad (32)$$

273 And the volumetric thermal expansion of water ($1/^{\circ}C$) is also dependent on temperature
 274 ($^{\circ}C$):

$$\alpha_f(T) = -6T^4 + 1660T^3 - 197796T^2 + 16862446T - 64319951 \quad (33)$$

275 It is worth noting that, for the reason of comparison between different teams which
 276 worked on this simulation of in-situ test, Andra proposed that these two parameters are the
 277 most sensitive ones to temperature variation.

278 Furthermore, since the phase field method is applied to describe the cracking process
 279 in this study, the parameters defined in this numerical method should be chosen carefully
 280 as shown in Table 3. Although scale length l_d is a defined parameter which controls the
 281 width of localized damage, it also serves as a material property within phase-field modeling.
 282 This is due to the fact that the peak stress of a material is determined by the scale length
 283 in conjunction with the toughness parameter and elasticity parameters [16, 49]. For the
 284 evolution of tensile damage, one gets:

$$\sigma_t = \sqrt{g_c^t \frac{E_{eq}}{3l_d}} \quad (34)$$

285 with the average value of uniaxial tensile strength for COx claystone $\sigma_t = 3$ MPa, and the
 286 equivalent isotropic elastic modulus $E_{eq} = (E_{\parallel} \times E_{\parallel} \times E_{\perp})^{1/3}$. Following the work of [13], a
 287 scale length is defined according to the element size h used in the area predicted to formation
 288 of damage: $l_d = 2h$. On the other hand, according to Equation (15), the evolution of shear
 289 damage zone is due to three parameters: toughness coefficient of shear damage g_c^s , friction
 290 angle φ and cohesion c . It is noticed that although the physical significance of the friction and
 291 cohesion is the same as that widely adopted, their values in the context of phase-field model
 292 are generally different with those used in classical Mohr-Coulomb criterion. Their value are

293 chosen so that one obtains reasonable values of uniaxial compression strength and tensile
294 strength. The detailed explanation of the choice of these parameters for COx claystone is
295 presented in the previous study [35]. Moreover, the scale length l_d , which controls the width
296 of localized damage, is determined by the element size. In this study, the value used is twice
297 the element size of the predicted damaged area. The permeability variation coefficient η_k ,
298 defined in Equation (25), is identified with the help of experimental work [50], and it has
299 worked well in previous numerical studies [35] that considered 2D problems for the same
300 rock.

301 Only the excavation damage zone (EDZ) around the GCS drift is considered. The EDZ
302 is located in the area with a depth of 2.6 m from the GCS drift wall. The permeability is
303 increased by 10 times the initial value in this zone. In this way, after the excavation of the
304 GCS gallery, there is a gradient of pore pressure close to the drift wall due to the seepage
305 phenomenon. Comparing the pore pressure measured by the sensor around the GCS gallery
306 on 2018/7/31, as shown in Figure 4, the numerical results show good agreement with the
307 effect of the EDZ. It is indeed worth noting that the main feature of the pore pressure
308 distribution that needs to be reproduced is influenced by the EDZ of the GCS gallery.
309 However, it's important to acknowledge that the modeling of GCS excavation in this study
310 has certain limitations. For example, the mesh around the GCS may not be fine enough,
311 and the time-dependent behavior during the excavation process is not taken into account.

Table 2: Material parameters for COx claystone from [47]

Parameters	Unit	Notation	Value
Young's modulus (parallel to bedding)	10^9 Pa	E_{\parallel}	6.0
Young's modulus (perpendicular to bedding)	10^9 Pa	E_{\perp}	4.0
Poisson ratio (Parallel to bedding)	-	$\mu_{\parallel\parallel}$	0.3
Poisson ratio (Perpendicular to bedding)	-	$\mu_{\perp\parallel}$	0.3
Shear modulus (Perpendicular to bedding)	10^9 Pa	$G_{\perp\parallel}$	1.7
Density of solid grains	kg/m^3	ρ_s	2770
Biot coefficient	-	b	0.8
Porosity	-	ϕ	0.18
Initial permeability (parallel to bedding)	10^{-20} m^2	k_{\parallel}^0	4.0
Initial permeability (perpendicular to bedding)	10^{-20} m^2	k_{\perp}^0	1.33
Equivalent thermal conductivity (parallel to bedding)	W/m/K	λ_{\parallel}	2.1
Equivalent thermal conductivity (perpendicular to bedding)	W/m/K	λ_{\perp}	1.28
Heat capacity of porous medium	J/kg/K	C_p	1050
Volumetric thermal expansion of solid grains	10^{-5} 1/K	α_s	4.5

Table 3: Parameter of phase field model for CRQ simulation

Parameters	Value
Material toughness	$g_c^t=4500$ N/m; $g_c^s=500$ N/m
Friction angle	$\varphi=15^\circ$
Cohesion	$c=0.1$ MPa
Scale length	$l_d=0.18$ m
Permeability variation	$\eta_k=40$

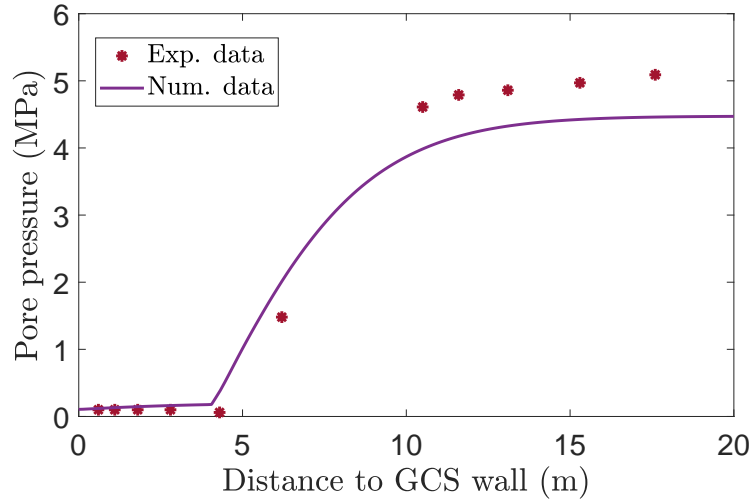


Figure 4: Pore pressure evolution around the GCS drift at 2018/7/31, comparing the experimental result and numerical result

312 The simulation is applied from the excavation of the GCS gallery to the end of the second
 313 cooling phase. The detailed dates of the main operations are shown in the appendix. For
 314 better readability, in the following numerical presentations, the dates are replaced by days,
 315 where day $t=0$ is defined as the day before the excavation of the GCS gallery.

316 5.3. Simulation results

317 Figure 5 shows the variation of temperature over time at the sixteen sensor points located
 318 in four boreholes: CRQ1720-1723. The two peaks in the figure correspond to the end of
 319 the first heating phase and the second heating phase. By comparing the experimental and
 320 numerical results, it is clear that the tendencies are well-reproduced and the peak values are
 321 almost identical. The peak values of the second heating are higher than the peak values of
 322 the first heating, except for the points on CRQ1722. This is because the heater CRQ1704
 323 was damaged during the second heating phase, and CRQ1722 is the closest borehole to
 324 the damaged heater. Nevertheless, it should be noted that reproducing the temperature
 325 evolution in the in-situ test scale is relatively straightforward due to the fact that the heat
 326 transfer process in the rock-like material remains unaffected by initial fracture or crack
 327 nucleation.

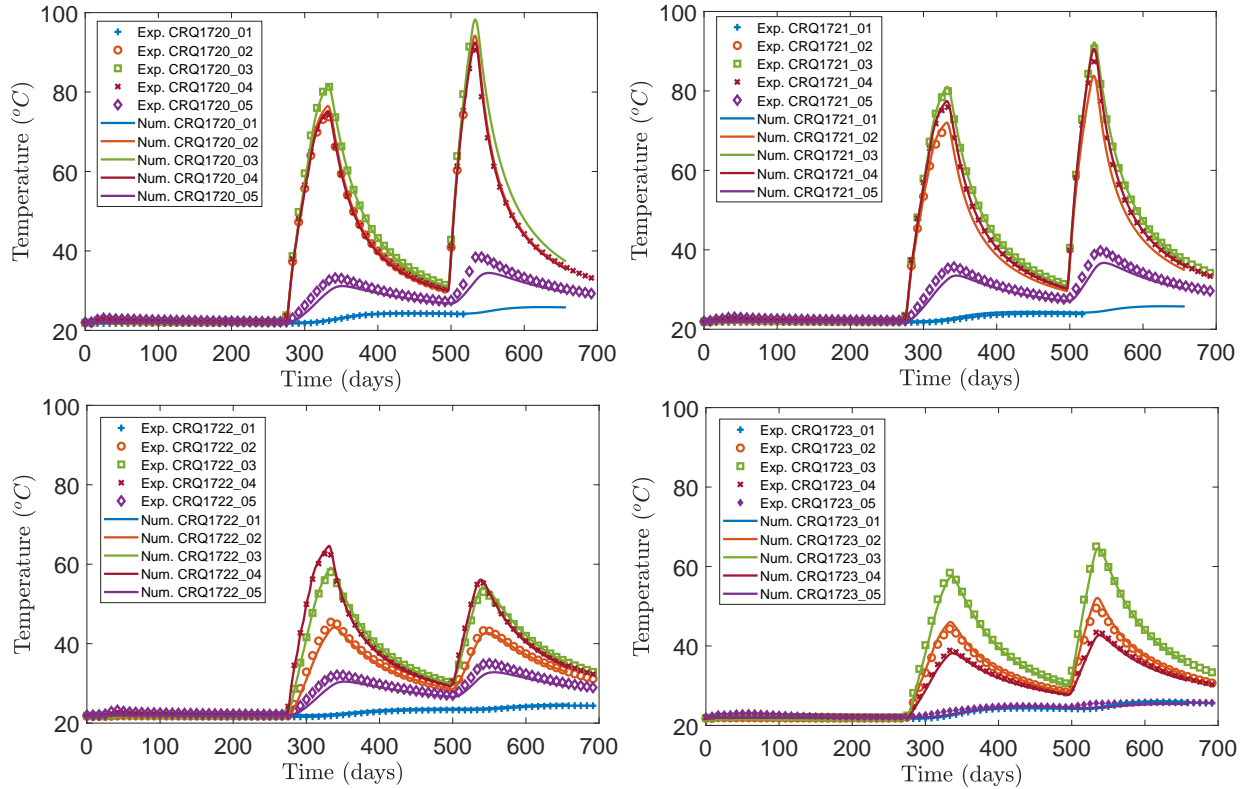


Figure 5: Evolution of temperature at the sensor points of CRQ 1720-1723, comparing the experimental results and numerical results

328 Figure 6 illustrates the temperature distributions at the end of the first heating phase
 329 and the end of the second heating phase. The temperature concentration area plays an
 330 important role to study the thermal damage. The middle plane of the heating section is
 331 expected to exhibit the highest temperatures. Hence, this plane is selected to analyze the
 332 THM coupling behavior resulting from heating. After the completion of the first heating
 333 phase, it is evident that the region with the highest temperature is concentrated around
 334 the two middle boreholes, namely CRQ1709 and CRQ1710. However, at the end of the
 335 second heating phase, a shift in the position of the zone with the highest temperature can
 336 be observed. This change is attributed to the damage sustained by the heater in CRQ1704
 337 (the top center borehole), causing the zone of elevated temperature to relocate towards the
 338 lower of the two central boreholes, as depicted in the isothermal map.

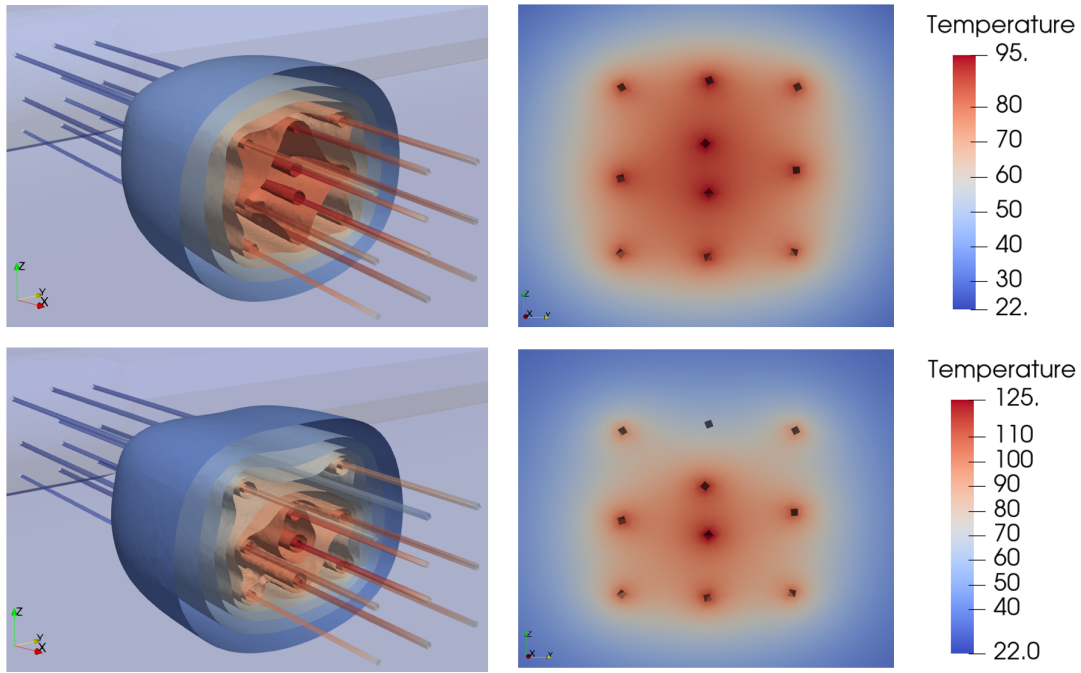


Figure 6: Distribution of temperature ($^{\circ}\text{C}$) at the end of the first heating phase (top) and the end of second heating phase (bottom)

339 The onset of damage is mainly caused by the operation of excavation and heating during
 340 the CRQ test. As shown in Figure 7, the damage due to the excavation of boreholes is
 341 reproduced as the shear damage. This damage creates what is known as a borehole damaged
 342 zone (BDZ), a phenomenon commonly observed in in-situ experiments with CO_x claystone.
 343 The maximum value of the shear damage variable d^s is about 0.23, which indicates that only
 344 micro-cracking occurs around the boreholes, and not macro-cracking. These micro-cracks
 345 lead to increased permeability, which is a consequence of pores being connected by fractures,
 346 as described in Equation (25).

347 We visualize in Figure 8 the region with higher permeability due to the excavation, with
 348 elements having permeability values 10 times higher than the initial permeability being
 349 highlighted. It can be seen that these elements within the BDZ eventually form a tube
 350 that connects with the excavation damaged zone (EDZ) of the GCS gallery. As mentioned
 351 previously, the borehole walls are defined as impermeable due to the installation of the resin.
 352 As a result, water can easily flow to the GCS gallery through the connected high-permeability

353 zones. This phenomenon is verified in the in-situ test according to the observation of the
 354 seepage around the boreholes on the GCS drift wall.

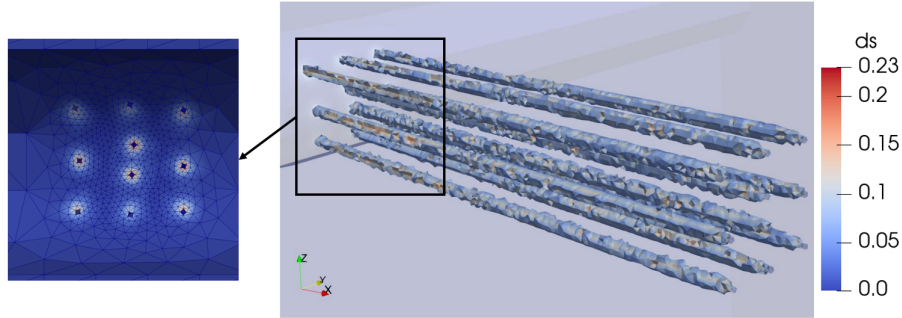


Figure 7: Distribution of the shear damage according to the excavation of heater boreholes

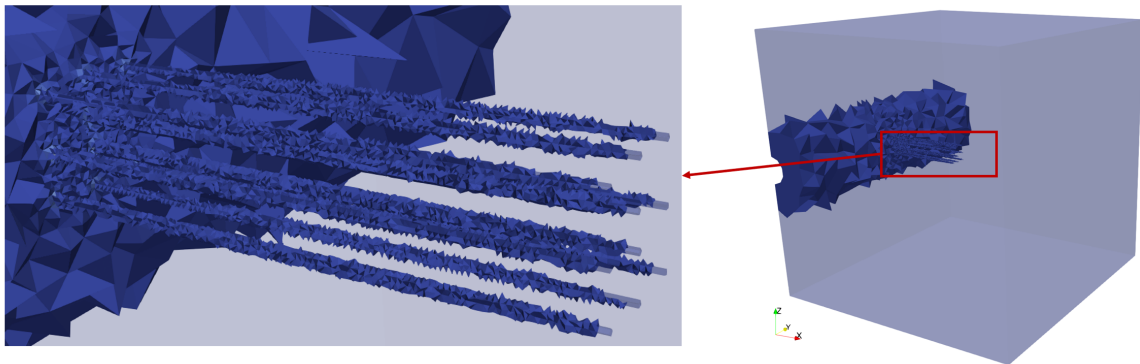


Figure 8: Distribution of the elements with greater than 10 times value higher than initial permeability k_0

355 By incorporating the seepage phenomenon, the numerical simulation results for pore
 356 pressure is depicted in Figure 9. The pore pressure has a reduction because of the borehole
 357 excavation at the beginning of the simulation. After the holding phase, the first heating
 358 phase begins at 273rd day. The simulation results closely align with the experimental findings
 359 for both the heating and cooling phases, with one exception. The data from sensors 01 and
 360 05, which are situated far from the heating section, exhibit some disparities. Regarding
 361 the reduction observed in the measured data from sensor 05 of CRQ1720 before the end of
 362 the first heating phase, it is likely attributable to a technical issue during the experiment.
 363 As for the 01 sensors, located at the deepest region approximately 5 meters below the end

364 of the boreholes, the measured pore pressure shows minimal impact from the two heating
 365 phases. This discrepancy, particularly evident in the sensors of CRQ1720, could indicate
 366 the presence of an initial fracture zone between the BDZ and sensor 01 of CRQ1720.

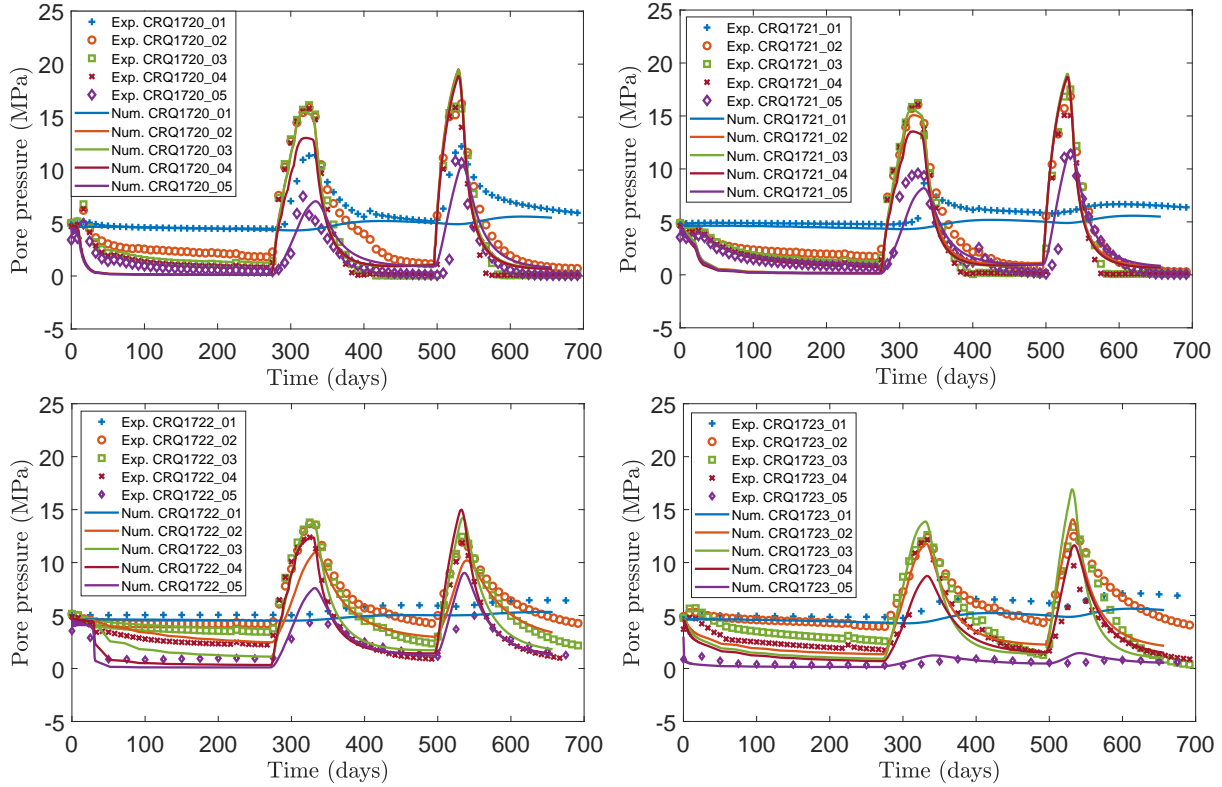


Figure 9: Evolution of pore pressure at the sensor points of CRQ 1720-1723, comparing the experimental results and numerical results

367 Of note, sensors 03 of four boreholes are located in the mid-plane of the heating area,
 368 which is considered the most important region to study failure behavior. As such, the
 369 evolution of pore pressure at the sensor 03 locations is presented together in Figure 10.
 370 The location of four sensor 03 are presented in the right figure with different colored icons.
 371 Among them, the sensors CRQ1720 and 1721 are located inside the square surrounded by
 372 ten heaters, while CRQ1722 and 1723 are located outside of it. It results in the blue and
 373 orange dotted curves of the pore pressure having higher peak values than the green and red
 374 ones. (The colors of the curves and icons are the same.) This feature is well reproduced in
 375 the numerical results. However, the simulation results have the limitation. Some features,

376 such as: i) the green dotted curve being slightly higher than the red one; ii) the green and
377 red dotted curves having a slower reduction than the blue and orange ones during the two
378 cooling phases, are not able to be reproduced in the simulation. The model used in this
379 work has its limitation. To improve the simulation and address these issues, considering the
380 elasto-plastic behavior of the material and incorporating an open-close crack function in the
381 numerical model could be beneficial. However, the reason about these differences between
382 experimental and numerical results may be complex. The evolution of pore pressure in the
383 in-situ test can indeed be influenced by various factors, including the leakage of resin or
384 the presence of initial fractures in the rock. These factors can introduce complexities and
385 uncertainties in the behavior of pore pressure.

386 To gain a deeper understanding of the damage effects observed during the in-situ heating
387 test, we present an additional set of numerical results depicted in Figure 11. These results are
388 obtained through a thermo-poro-elastic model simulation that does not take into account the
389 influence of damage. Similar to Figure 10, the numerical results of pore pressure is compared
390 with the experiment data of the sensors 03. While the trends of the curves are effectively
391 reproduced, the peak value in the numerical results is notably higher than that observed
392 in the experimental data. This discrepancy can be attributed to the absence of the BDZ,
393 where pore water is trapped due to the low permeability of COx claystone. Consequently,
394 the pore pressure in the numerical simulation increases to an unrealistic value during the
395 heating phases.

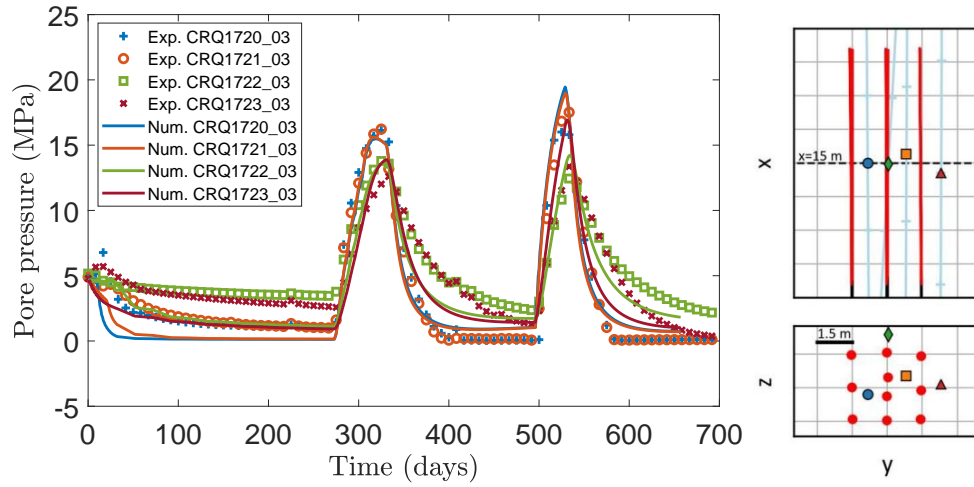


Figure 10: Evolution of pore pressure at the sensor points of sensor 03, comparing the experimental results and numerical results with considering damage effect

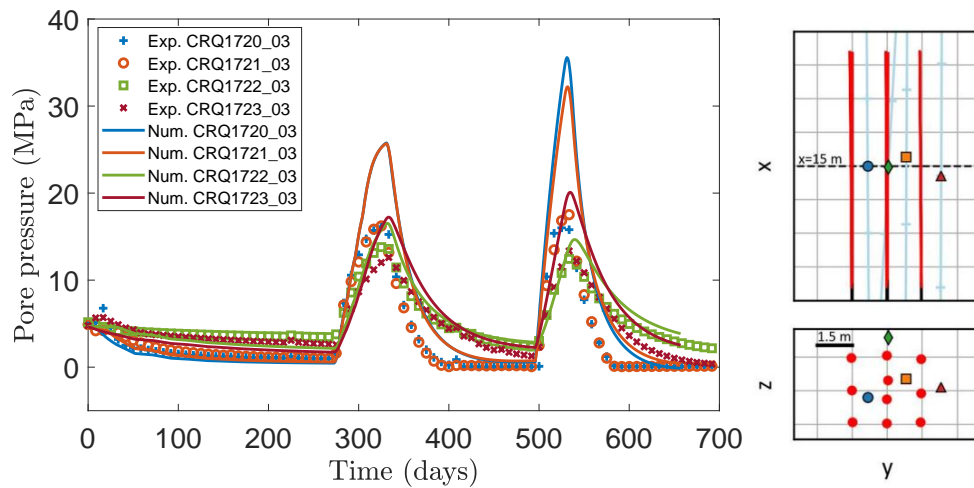


Figure 11: Evolution of pore pressure at the sensor points of sensor 03, comparing the experimental results and numerical results without considering damage effect

396 Furthermore, Figure 12 displays the distribution of pore pressure at the two ends of
 397 the heating phase, taking into account the damage effect. In contrast, Figure 13 represents
 398 the distribution of pore pressure in a simulation where the damage effect is not considered,
 399 allowing for a meaningful comparison between the two scenarios. Similar to the temperature
 400 results, the pore pressure induced by the second heating phase is higher compared to the
 401 pore pressure induced by the first heating phase. Additionally, due to the failure of the

402 heater, the overpressure zone that was previously observed around the three top boreholes
 403 is no longer present. In Figure 12, it is evident that the presence of the BDZ results in a
 404 reduction of pore pressure around the boreholes. On the other hand, unlike the overpressure
 405 zone is more concentrated in the case without damage consideration, the presence of the BDZ
 406 leads to a larger and more uniform overpressure zone. As a consequence, the distribution
 407 of pore pressure, which is influenced by the presence of the BDZ, can directly impact the
 408 formation of thermal damage.

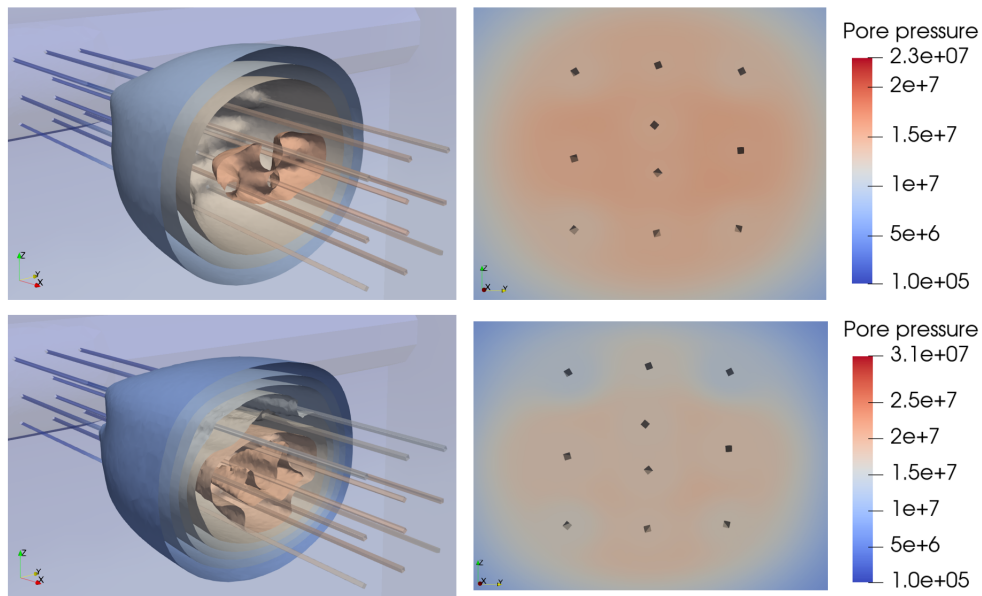


Figure 12: Distribution of pore pressure (Pa) at the end of the first heating phase (top) and the end of second heating phase (bottom), simulation with considering damage effect

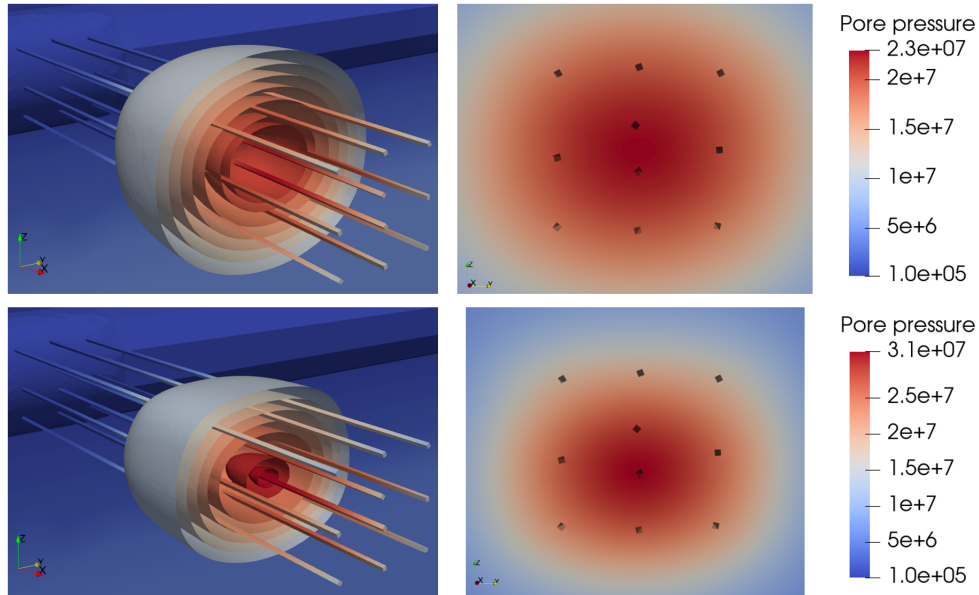


Figure 13: Distribution of pore pressure (Pa) at the end of the first heating phase (top) and the end of second heating phase (bottom), simulation without considering damage effect

409 After successfully reproducing the variation of pore pressure, the thermal damage evo-
 410 lution is now investigated. It is noticed that it is very difficult to quantitatively measure
 411 intensity of thermal damage in in-situ experiment. Only distributions of micro-cracks are
 412 characterized through drilled samples. Therefore, the comparison between modeling and
 413 experiment is mainly focused on the extent of cracked or damaged zone. Figure 14 shows
 414 the distribution of tensile damage due to the two heating phases. The distribution of shear
 415 damage is not shown here, since the shear damage is almost not changed during the heat-
 416 ing. The maximum value of tensile damage indicates that there is almost no hydro-thermal
 417 damage at the end of the first heating. A few damage appears due to the second heating,
 418 but no macro crack is predicted to see. The damaged zone is mainly located around the
 419 lower hole of the two center boreholes, because the highest pore pressure can be found in
 420 this area.

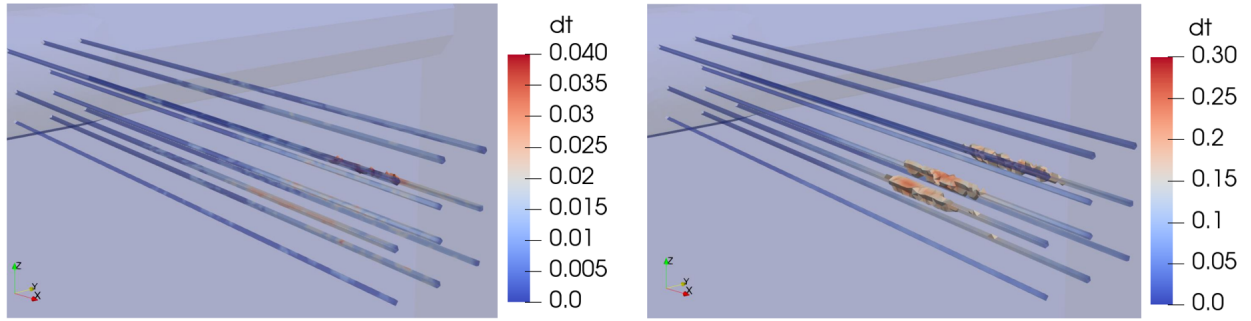


Figure 14: Distribution of the tensile damage according to the first heating phase (left) and second heating phase (right)

421 In this subsection, a simulation of the CRQ test is conducted by incorporating the
 422 consideration of damage. Both excavation-induced damage and heating-induced damage
 423 are reproduced using the proposed double phase field method. In addition, the effect of
 424 the BDZ on reducing the pore pressure in the over-pressure zone around the boreholes is
 425 taken into account. After successfully reproducing the peak value of the pore pressure,
 426 the simulation results can be used to predict the hydro-thermal fracture that occurs at the
 427 end of the simulation. Overall, this approach provides a convincing and effective result for
 428 predicting and studying the thermo-hydrmechanical behavior of claystone in the context
 429 of the CRQ test.

430 5.3.1. Study of material heterogeneity

431 As introduced before, given that material heterogeneity plays an important role during
 432 the cracking process of COx claystone, it should be considered in the simulation of CRQ test.
 433 According to the previous studies [51, 43], both the solid clay matrix and COx claystone are
 434 assumed to exhibit transversely isotropic elastic behavior, while the equivalent inclusion is
 435 assumed to be isotropic. The parameters used in this work for homogenization and random
 436 distribution are presented in detail in Table 4 based on the previous studies [52, 43]. It
 437 is worth noting that the elastic properties of constituent phase are identified by using an
 438 inverse optimization procedure by using the Equations (28) and (29). After taking typical
 439 values for calcite and quartz inclusions, the elastic parameters of clay matrix are calculated

440 from the measured macroscopic values for a given set of porosity and mineral composition.
 441 With these values, the homogenized elastic properties can be obtained: $E_{\parallel}^{hom} = 6.08$ GPa,
 442 $E_{\perp}^{hom} = 4.42$ GPa, $\nu_{\parallel}^{hom} = 0.28$, $\nu_{\parallel\perp}^{hom} = 0.33$ and $G_{\parallel\perp}^{hom} = 2.7$ GPa. These macroscopic elastic
 443 properties are suitable compare with the measured parameters of COx claystone from [51].

444 Based on previous simulation results that considered a uniform rock, it was observed
 445 that the critical failure behavior occurred in the vicinity of the heated part of boreholes.
 446 Consequently, we have limited our study of material heterogeneity to the area with a refined
 447 mesh, as illustrated in Figure 3. In this way, Figure 15 illustrates a representative example of
 448 the random distribution of porosity and volumetric fraction of inclusions. Since the Weibull
 449 distribution function is widely used in many situations, it is also adopted here. The involved
 450 parameters are chosen so that the variation of porosity and inclusion fraction correspond to
 451 typical variability of these parameters observed on COx claystone.

Table 4: Parameter of material heterogeneity for CRQ simulation

Parameters	Value
Young's modulus (solid matrix)	$E_{\parallel}^m = 3.6$ GPa, $E_{\perp}^m = 2.4$ GPa
Poisson's ratio (solid matrix)	$\nu_{\parallel}^m = 0.3$, $\nu_{\parallel\perp}^m = 0.3$
Shear modulus (solid matrix)	$G_{\parallel\perp}^m = 1.02$ GPa
Young's modulus (inclusion)	$E_i = 98$ GPa
Poisson's ratio (inclusion)	$\nu_i = 0.15$
Inclusion volume fraction	$\beta_i = 0.4$
Pore volume fraction	$\beta_p = 0.16$
Homogeneity index	$m_i = m_p = 1.5$

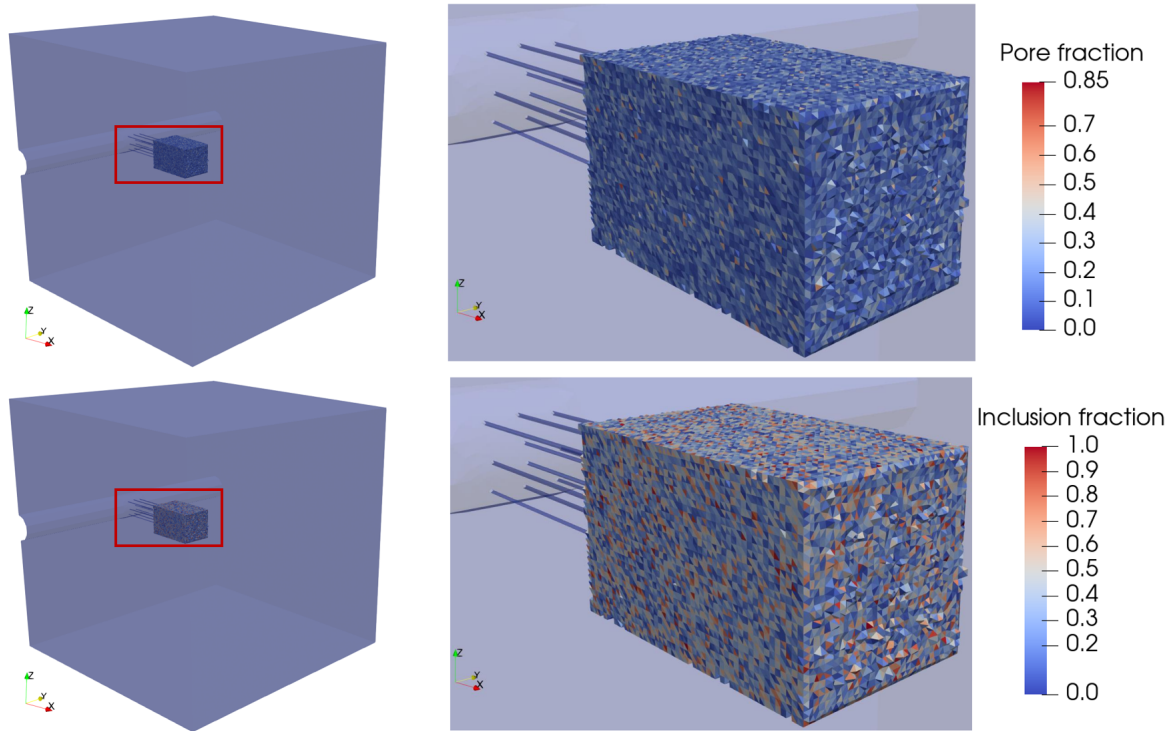


Figure 15: Distribution of pores volume fraction (top) and inclusion volume fraction (bottom)

452 Since we anticipate that the simulation outcomes will vary depending on the random
 453 distribution of pores and inclusions, we selected three simulations (denotes Num. 1, 2 and
 454 3) with different sets of random distribution for analysis. At first, Figure 16 shows the
 455 distribution of shear damage induced to excavation by using three different sets of random
 456 distribution. The maximum value of d^s differs among the three simulations due to variations
 457 in the homogenized elastic properties resulting from differences in porosity and inclusion
 458 volume fraction. However, the form of BDZ remains unchanged compared to the simulation
 459 results considering a uniform rock. Similarly, this BDZ leads to the mentioned seepage
 460 phenomenon, which can reduce the pore pressure at the study points as shown in Figure
 461 17. Even though the three simulations used different random distributions, the resulting
 462 numerical results are identical as depicted in Figure (a-c). For instance, the three curves of
 463 CRQ1720-03 are exactly coincided as shown in Figure (d).

464 Additionally, upon comparing the numerical results to the previous subsection, it is
 465 evident that the values are reduced, particularly during the cooling phases and at the end

466 of the second heating phase. To investigate this difference, a comparison of the distribution
 467 between the two simulations is provided in Figure 18. At the initial stage, the distribution of
 468 pore pressure does not show any non-uniform characteristics. Material heterogeneity is only
 469 taken into account for the stiffness matrix in the mechanical field, while major parameters
 470 in the pore pressure field, such as permeability, are not considered. In other words, the
 471 mechanical heterogeneity is not strong enough to significantly influence the pore pressure
 472 field.

473 However, the principal difference between the two simulation results lies in the pore
 474 pressure within the BDZ. Comparing the simulation with considering heterogeneity to the
 475 one without, there is a slightly greater reduction in pore pressure within the BDZ in the
 476 simulation that considers heterogeneity. This significant reduction improves the evolution
 477 of pore pressure during the cooling phases, bringing it closer to the experimental data. The
 478 reason for this reduction in the BDZ can be attributed to the presence of a larger BDZ due
 479 to the weak regions obtained through the random distribution of pores.

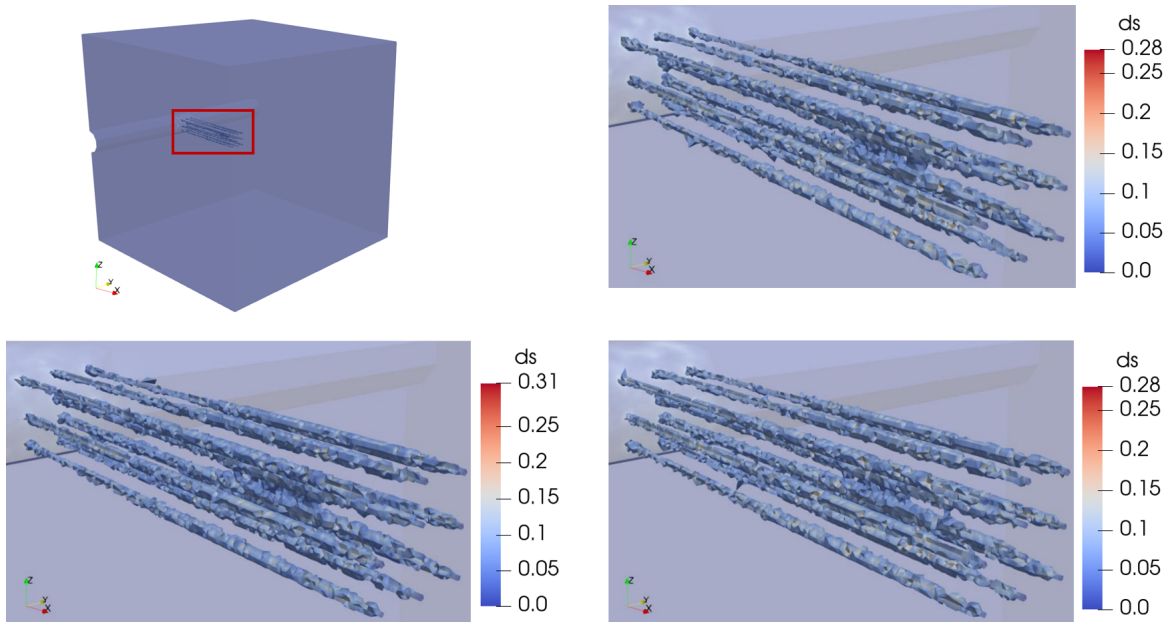


Figure 16: Distribution of shear damage induced by excavation, simulated by using different random distribution of pore and inclusion: Num. 1, 2 and 3

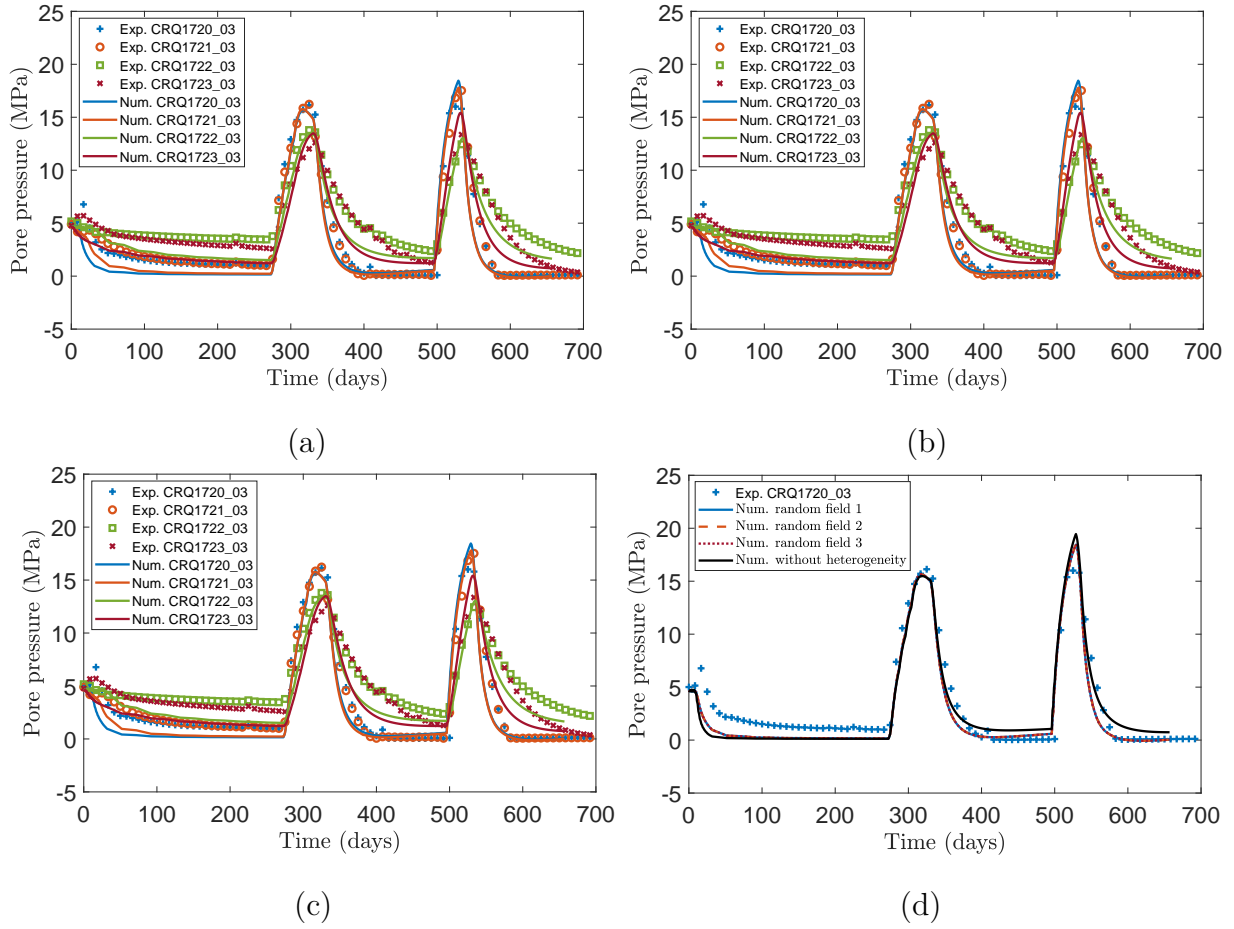


Figure 17: Evolution of pore pressure at sensor 03 of CRQ 1720-1723 for simulations using different distributions of pores and inclusions: Num. 1, 2 and 3 (a-c), and comparison of pore pressure evolution at sensor CRQ 1720-03 for simulations using different distributions of pores and inclusions: Num. 1, 2 and 3, as well as the simulation result without considering heterogeneity (d)

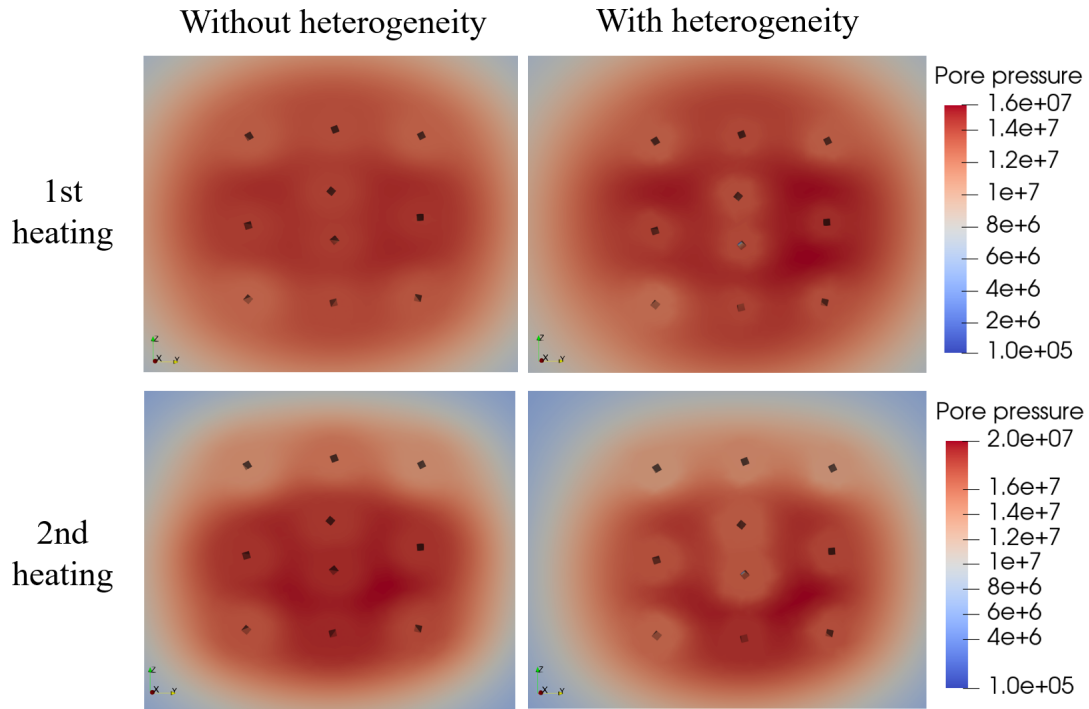


Figure 18: Distribution of pore pressure (Pa) at the end of the first and second heating: comparison between the simulation with and without considering damage effect

480 Figure 19 shows the distribution of tensile damage at the end of the second heating
 481 phase. It is worth noting that the tensile damage induced by the first heating phase is not
 482 shown since the maximum value of d^t is less than 0.1. It is reasonable to observe that the
 483 maximum values of d^t , which are 0.43, 0.79, and 0.83, respectively, are greater compared to
 484 the uniform simulation ($d^t = 0.3$) due to the presence of a weak region. The element with
 485 this maximum value is located between the two central boreholes as expected. Since there
 486 are no elements with high damage variables outside of this area in all three simulations, it
 487 appears that the results are consistent.

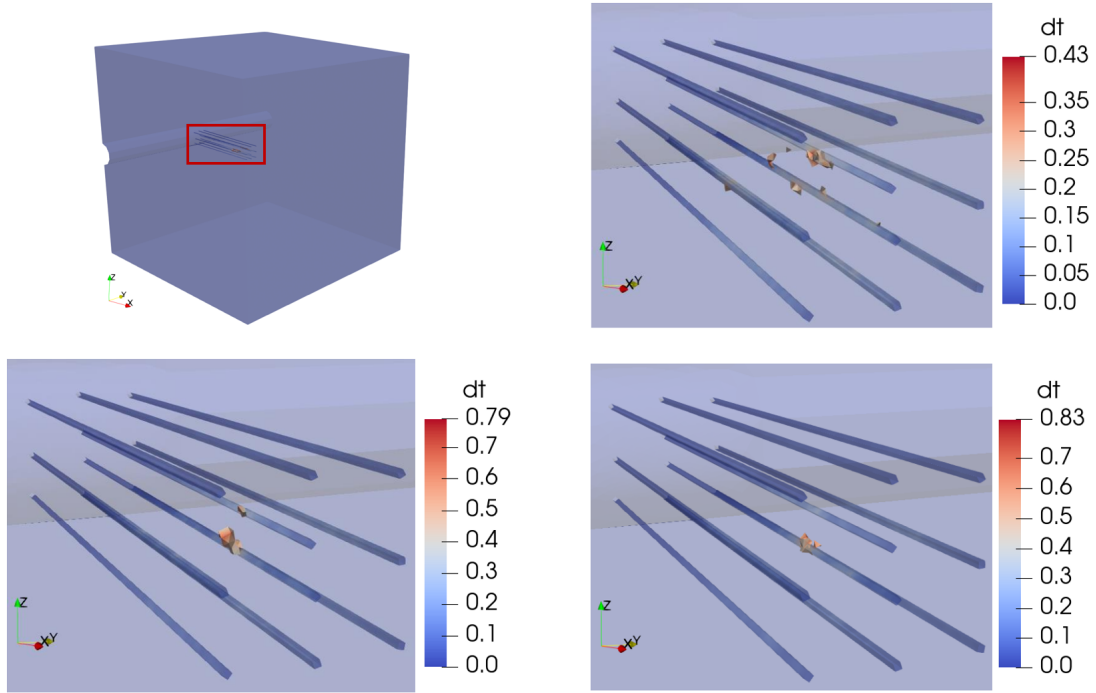


Figure 19: Distribution of tensile damage at end of second heating phase, simulated by using random distribution of pore and inclusion: Num. 1, 2 and 3

488 By considering the material heterogeneity, a more realistic representation of the rock
 489 behavior is achieved, and the simulation better captures the behavior of pore pressure in the
 490 BDZ, resulting in improved agreement with experimental data during the cooling phases.
 491 Additionally, the presence of weak regions in the rock, such as pores and inclusions, can
 492 influence the occurrence of thermal fractures.

493 However, it should be noted that the simulation considering material heterogeneity en-
 494 sures that the overall features of the thermal crack remain unchanged compared to the
 495 simulation without considering heterogeneity. Specifically, the thermal damage mainly ap-
 496 pears between the two center boreholes, and a macroscopic crack does not form (damage
 497 variable d^t or $d^s = 1$).

498 6. Conclusion

499 This study proposes a THM modeling approach that incorporates the phase-field method
 500 to account for damage effects. The model is capable of identifying both tensile and shear

501 cracks induced by THM coupling behavior. To test the model's effectiveness, it is applied
502 to simulate the CRQ test. The results show that the model accurately reproduces the
503 evolution of temperature and pore pressure at sensor points and the corresponding damage
504 zone. The study also finds that the THM coupling process is significantly affected by the
505 BDZ induced seepage phenomenon. The excavation and heating induced damage zone are
506 identified as shear and tensile damage, respectively. Moreover, the study verifies the model's
507 consistency with material heterogeneity. It is worth noticing that in the present study, the
508 mechanical properties are identified from typical laboratory tests such as triaxial compression
509 tests. The parameters related to fluid flow and heat diffusion are chosen by Andra, for
510 all the teams involved in the DECOVALEX project. There is no fitting of parameters
511 with respect to the in-situ experiment. Therefore, the numerical simulation presented here
512 represents an interesting phase of validation of the proposed numerical model. However,
513 further simulations of other experiments are still useful for a deep validation of the proposed
514 model. Moreover, other important features, such as the variation of critical fracture energy
515 with temperature change, should also be investigated.

516 **Acknowledgment:**

517 This work is jointly supported by the French National Agency for radioactive waste
518 management (ANDRA), the DECOVALEX project and the National Natural Science Foun-
519 dation of China (No. 12202099). DECOVALEX is an international research project com-
520 prising participants from industry, government and academia, focusing on development of
521 understanding, models and codes in complex coupled problems in sub-surface geological and
522 engineering applications. The authors appreciate and thank the DECOVALEX-2023 Fund-
523 ing Organizations for their financial and technical support of the work described in this
524 paper. The statements made in the paper are, however, solely those of the authors and do
525 not necessarily reflect those of the Funding Organizations.

526 **Appendix: Positions of sensors and dates of the heater boreholes drilling**

527 In order to identify the coordinates of the sensor points, the origin (0,0,0) of the model do-
528 main is located at the mid-distance between the heads of borehole CRQ1720 and CRQ1721.
529 In this way, the studied 3D domain of cube with a side length of 50 m vary between $x=-2.6$
530 m to 47.4 m (parallel to the heater boreholes); $y=-25.0$ m to 25.0 m (parallel to the GCS
531 gallery) and $z=-25$ m to 25 m (perpendicular to the heater boreholes and the GCS gallery).
532 In this defined coordinate system, the position of sensor points are shown as follows:

Table 5: The position of sensor points used in simulation of CRQ test

Sensor	Coordinate-x (m)	Coordinate-y (m)	Coordinate-z (m)
CRQ1720-01	24.99	0.91	-0.21
CRQ1720-02	17.99	0.86	-0.27
CRQ1720-03	15.00	0.84	-0.29
CRQ1720-04	12.00	0.82	-0.31
CRQ1720-05	8.00	0.79	-0.32
CRQ1721-01	25.39	-0.86	0.65
CRQ1721-02	18.38	-0.84	0.55
CRQ1721-03	15.38	-0.82	0.51
CRQ1721-04	12.38	-0.81	0.47
CRQ1721-05	8.38	-0.79	0.43
CRQ1722-01	24.92	-0.57	3.73
CRQ1722-02	17.90	-0.21	2.75
CRQ1722-03	14.93	-0.05	2.34
CRQ1722-04	11.97	0.10	1.94
CRQ1722-05	8.01	0.32	1.41
CRQ1723-01	24.57	-2.34	0.27
CRQ1723-02	19.56	-2.33	0.21
CRQ1723-03	14.56	-2.31	0.15
CRQ1723-04	9.57	-2.29	0.1
CRQ1723-05	4.57	-2.27	0.07

533 The detail date of the main operations during CRQ test is:

- 534 • The drift of GCS gallery: 15th September 2010
- 535 • The drift of heater boreholes: between 20th and 30th October 2017 (see Table)
- 536 • The first heating phase: between 3rd June and 31st July 2019

537

- The second heating phase: between 13th January and 14th February 2020

Table 6: Dates of the heater boreholes drilling for CRQ test

Borehole	Drilling date	Borehole	Drilling date
CRQ1701	14/09/2018	CRQ1706	03/09/2018
CRQ1702	13/09/2018	CRQ1707	05/09/2018
CRQ1703	27/09/2018	CRQ1708	07/09/2018
CRQ1704	02/10/2018	CRQ1709	11/09/2018
CRQ1705	04/10/2018	CRQ1710	24/09/2018

538

References

539

[1] G. Armand, F. Leveau, C. Nussbaum, R. deLaVaissiere, A. Noiret, D. Jaeggi, P. Landrein, C. Righini, Geometry and properties of the excavation induced fractures at the meuse-haute-marne url drifts., *Rock Mech. Rock Eng.* 47 (2014) 21–41.

542

[2] D. Seyedi, a. at, Upscaling thm modelling from small-scale to full-scale in-situ experiment in the callovo-oxfordian claystone., *Int. J. of Rock Mechanics and Mining Sciences* 144 (104582) (2021) 1365–1609.

543

544

[3] N. Conil, V. Manon, C. Plua, V. M. N., D. Seyedi, G. Armand, In situ investigation of the thm behavior of the callovo-oxfordian claystone., *Rock Mechanics and Rock Engineering online* (2020).

545

546

[4] C.-F. Tsang, O. Stephansson, L. Jing, F. Kautsky, Decovalex project: from 1992 to 2007, *Environmental Geology* 57 (6) (2009) 1221–1237.

547

548

[5] J. T. Birkholzer, A. E. Bond, J. A. Hudson, L. Jing, C.-F. Tsang, H. Shao, O. Kolditz, Decovalex-2015: an international collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (thmc) processes in geological systems (2018).

549

551

[6] J. T. Birkholzer, C.-F. Tsang, A. E. Bond, J. A. Hudson, L. Jing, O. Stephansson, 25 years of decovalex-scientific advances and lessons learned from an international research collaboration in coupled subsurface processes, *International Journal of Rock Mechanics and Mining Sciences* 122 (2019) 103995.

552

554

[7] J. Oliver, Modelling strong discontinuities in solid mechanics via strain softening constitutive equations, part 1: fundamentals, *Internat. J. Numer. Methods Engrg.* 39 (1996) 3575–3600.

555

556

[8] N. Moes, J. Dolbow, T. Belytschko, A finite element method for crack growth without remeshing, *Internat. J. Numer. Methods Engrg.* 46 (1999) 131–150.

557

558

[9] N. Moes, C. Stolz, N. Chevaugeon, P. E. Bernard, A level set based model for damage growth: The thick level set approach, *International Journal for Numerical Methods in Engineering* 86 (2010) 358–380.

559

- 560 [10] P. E. Bernard, N. Moes, N. Chevaugeon, Damage growth modeling using the thick level set (tls)
561 approach: Efficient discretization for quasi-static loadings, *Computer Methods in Applied Mechanics*
562 *and Engineering* 233-236 (2012) 11–27.
- 563 [11] G. A. Francfort, J.-J. Marigo, Revisiting brittle fracture as an energy minimization problem, *Journal*
564 *of the Mechanics and Physics of Solids* 46 (8) (1998) 1319–1342.
- 565 [12] B. Bourdin, G. A. Francfort, J.-J. Marigo, Numerical experiments in revisited brittle fracture, *Journal*
566 *of the Mechanics and Physics of Solids* 48 (4) (2000) 797–826.
- 567 [13] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation:
568 Robust algorithmic implementation based on operator splits, *Computer Methods in Applied Mechanics*
569 *and Engineering* 199 (45-48) (2010) 2765–2778.
- 570 [14] M. J. Borden, C. V. Verhoosel, M. A. Scott, T. J. Hughes, C. M. Landis, A phase-field description of
571 dynamic brittle fracture, *Computer Methods in Applied Mechanics and Engineering* 217 (2012) 77–95.
- 572 [15] C. Miehe, M. Hofacker, L.-M. Schänzel, F. Aldakheel, Phase field modeling of fracture in multi-physics
573 problems. part ii. coupled brittle-to-ductile failure criteria and crack propagation in thermo-elastic-
574 plastic solids, *Computer Methods in Applied Mechanics and Engineering* 294 (2015) 486–522.
- 575 [16] J. Choo, W. Sun, Coupled phase-field and plasticity modeling of geological materials: From brittle
576 fracture to ductile flow, *Computer Methods in Applied Mechanics and Engineering* 330 (2018) 1–32.
- 577 [17] J. Fang, C. Wu, J. Li, Q. Liu, C. Wu, G. Sun, L. Qing, Phase field fracture in elasto-plastic solids:
578 variational formulation for multi-surface plasticity and effects of plastic yield surfaces and hardening,
579 *International Journal of Mechanical Sciences* (2019).
- 580 [18] X. Zhang, S. W. Sloan, C. Vignes, D. Sheng, A modification of the phase-field model for mixed mode
581 crack propagation in rock-like materials, *Computer Methods in Applied Mechanics and Engineering*
582 322 (2017) 123–136.
- 583 [19] E. C. Bryant, W. Sun, A mixed-mode phase field fracture model in anisotropic rocks with consistent
584 kinematics, *Computer Methods in Applied Mechanics and Engineering* 342 (2018) 561–584.
- 585 [20] B. Evans, J. T. Fredrich, T.-F. Wong, The brittle-ductile transition in rocks: Recent experimental and
586 theoretical progress, *The Brittle-Ductile Transition in Rocks*, *Geophys. Monogr. Ser* 56 (1990) 1–20.
- 587 [21] T.-f. Wong, P. Baud, The brittle-ductile transition in porous rock: A review, *Journal of Structural*
588 *Geology* 44 (2012) 25–53.
- 589 [22] F. Fei, J. Choo, A phase-field method for modeling cracks with frictional contact, *International Journal*
590 *for Numerical Methods in Engineering* 121 (4) (2020) 740–762.
- 591 [23] F. Fei, J. Choo, A phase-field model of frictional shear fracture in geologic materials, *Computer Methods*
592 *in Applied Mechanics and Engineering* 369 (2020) 113265.
- 593 [24] J. Ulloa, J. Wambacq, R. Alessi, E. Samaniego, G. Degrande, S. François, A micromechanics-

- 594 based variational phase-field model for fracture in geomaterials with brittle-tensile and compressive-
595 ductile behavior, *Journal of the Mechanics and Physics of Solids* 159 (2022) 104684.
- 596 [25] T. You, H. Waisman, Q.-Z. Zhu, Brittle-ductile failure transition in geomaterials modeled by a modified
597 phase-field method with a varying damage-driving energy coefficient, *International Journal of Plasticity*
598 136 (2021) 102836.
- 599 [26] Z. Yu, J. F. Shao, M. N. Vu, G. Armand, Numerical study of thermo-hydro-mechanical responses of in
600 situ heating test with phase-field model., *International Journal of Rock Mechanics and Mining Sciences*
601 138 (2021) 104542.
- 602 [27] F. Fei, J. Choo, Double-phase-field formulation for mixed-mode fracture in rocks, *Computer Methods*
603 *in Applied Mechanics and Engineering* 376 (2021) 113655.
- 604 [28] Z. Yu, Y. Sun, M. N. Vu, J. F. Shao, Modeling of mixed cracks in rock-like brittle materials under
605 compressive stresses by a double-phase-field method, *Rock Mechanics and Rock Engineering* online
606 (2023).
- 607 [29] C. Miehe, F. Welschinger, M. Hofacker, Thermodynamically consistent phase-field models of fracture:
608 variational principles and multi-field fe implementations, *International Journal for Numerical Methods*
609 *in Engineering* 83 (10) (2010) 1273–1311.
- 610 [30] J.-Y. Wu, A unified phase-field theory for the mechanics of damage and quasi-brittle failure, *Journal*
611 *of the Mechanics and Physics of Solids* 103 (2017) 72–99.
- 612 [31] O. Coussy, *Poromechanics*, John Wiley & Sons, 2004.
- 613 [32] A. H.-D. Cheng, *Poroelasticity*, Vol. 27, Springer, 2016.
- 614 [33] V. Lubarda, D. Krajcinovic, S. Mastilovic, Damage model for brittle elastic solids with unequal tensile
615 and compressive strengths, *Engineering Fracture Mechanics* 49 (5) (1994) 681–697.
- 616 [34] S. Murakami, *Continuum damage mechanics: a continuum mechanics approach to the analysis of*
617 *damage and fracture*, Vol. 185, Springer Science & Business Media, 2012.
- 618 [35] Z. Yu, J. Shao, G. Duveau, M.-N. Vu, G. Armand, Numerical modeling of deformation and damage
619 around underground excavation by phase-field method with hydromechanical coupling, *Computers and*
620 *Geotechnics* 138 (2021) 104369.
- 621 [36] P. DeBuhan, L. Dormieux, On the validity of the effective stress concept for assessing the strength of
622 saturated porous materials: a homogenization approach, *J. Mech. Phys. Solids* 44 (1996) 1649–1677.
- 623 [37] D. Lydzba, J. F. Shao, Stress equivalence principle for saturated porous media, *Comptes Rendus*
624 *Mecanique* 330 (2002) 297–303.
- 625 [38] J. Kim, H. Tehelepi, R. Juanes, Stability and convergence of sequential methods for coupled flow
626 and geomechanics: Fixed-stress and fixed-strain splits, *Computer Methods in Applied Mechanics and*
627 *Engineering* 200 (2011) 1591–1606.

- 628 [39] B. Bourdin, G. A. Francfort, J.-J. Marigo, The variational approach to fracture, *Journal of elasticity*
629 91 (1-3) (2008) 5–148.
- 630 [40] J. C. Robinet, P. Sardini, D. Coelho, J. C. Parneix, D. Pret, S. Sammartino, E. Boller, S. Altmann,
631 Effects of mineral distribution at mesoscopic scale on solute diffusion in a clay-rich rock: Example of
632 the callovo-oxfordian mudstone (bure, france), *Water resources research* 48 (2012) W05554.
- 633 [41] T. Mori, K. Tanaka, Averages stress in matrix and average elastic energy of materials with misfitting
634 inclusions, *Acta Metall.* 21 (1973) 571–574.
- 635 [42] A. Giraud, Q. Huynh, D. Hoxha, D. Kondo, Application of results on eshelby tensor to the determination
636 of effective poroelastic properties of anisotropic rocks-like composites, *International Journal of Solids*
637 *and Structures* 44 (11) (2007) 3756–3772.
- 638 [43] J. J. Zhao, W. Q. Shen, Z. B. Shao, J. F. anc Liu, M. N. Vu, A constitutive model for anisotropic
639 clay-rich rocks considering micro-structural composition, *International Journal of Rock Mechanics and*
640 *Mining Sciences* 151 (2022) 105029.
- 641 [44] D. Seyedi, G. Armand, N. Conil, M. Vitel, M. N. Vu, On the thermo-hydro-mechanical pressurization
642 in callovo-oxfordian claystone under thermal loading., *Poromechanics VI 2017* (2017) 754–761.
- 643 [45] D. M. Seyedi, G. Armand, A. Noiret, “transverse action”—a model benchmark exercise for numerical
644 analysis of the callovo-oxfordian claystone hydromechanical response to excavation operations, *Com-*
645 *puters and Geotechnics* 85 (2017) 287–305.
- 646 [46] G. Armand, F. Bumbieler, N. Conil, R. delaVaissiere, J. M. Bosgiraud, M. N. Vu, Main outcomes
647 from in situ thermo-hydro-mechanical experiments programme to demonstrate feasibility of radioactive
648 high-level waste disposal in the callovo-oxfordian claystone., *J. of Rock Mechanics and Geotechnical*
649 *Engineering* 9 (2017) 415–427.
- 650 [47] P. Braun, Thermo-hydro-mechanical behavior of the callovo-oxfordian claystone: Effects of stress paths
651 and temperature changes, Ph.D. thesis, Université Paris-Est (2019).
- 652 [48] Z. Yu, J. Shao, Y. Sun, M. Wang, M. ngoc Vu, C. Plua, Numerical analysis of hydro-thermal fracturing
653 in saturated rocks by considering material anisotropy and micro-structural heterogeneity, *International*
654 *Journal of Rock Mechanics and Mining Sciences* 170 (2023) 105457.
- 655 [49] J.-Y. Wu, V. P. Nguyen, C. Thanh Nguyen, D. Sutula, S. Bordas, S. Sinaie, Phase field modelling of
656 fracture, *Advances in Applied Mechanics* 53 (2019) 1–183.
- 657 [50] R. de La Vaissiere, G. Armand, J. Talandier, Gas and water flow in an excavation-induced fracture
658 network around an underground drift: A case study for a radioactive waste repository in clay rock.,
659 *Journal of Hydrology* 521 (2015) 141–156.
- 660 [51] G. Armand, N. Conil, J. Talandier, D. M. Seyedi, Fundamental aspects of the hydromechanical be-
661 haviour of callovo-oxfordian claystone: from experimental studies to model calibration and validation,

662 Computers and Geotechnics 85 (2017) 277–286.

663 [52] F. Farhat, W. Shen, J. Shao, A micro-mechanics based viscoplastic model for clayey rocks, Computers
664 and Geotechnics 89 (2017) 92–102.