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TOUGH-RFPA: Coupled Thermal-Hydraulic-Mechanical Rock Failure Process Analysis with Application to Deep Geothermal Wells

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ABSTRACT

This paper presents a coupled thermal-hydraulic-mechanical (THM) model for simulating failure processes in geological media. The coupling between stress/strain and heat transfer describing how thermal expansion affects stress is based on the theory of thermo-elasticity. Additionally, the coupling between stress/strain and fluid flow describing how pore-pressure affects stress is governed by Biot's consolidation theory. Stress/strain-dependent porosity/permeability/capillary-pressure defines the influence of stress on fluid flow and thermal fields. The THM model is implemented in the solver module that links the multiphase, multicomponent fluid flow simulator TOUGH2 with the geomechanical simulator RFPA (Rock Failure Process Analysis), which is based on the concept that heterogeneity leads to non-linearity and progressive failure behavior. Capability of TOUGH-RFPA simulator was verified by two benchmark problems related to hydraulic-mechanical and thermal-mechanical response in a hollow cylinder. Then the applicability of TOUGH-RFPA was demonstrated for modeling cooling-induced damage around a very deep geothermal well with mesoscopic heterogeneous properties, which showed complex damage evolution and fracturing during well cooling and fluid pressurization.

Keywords: Thermal-hydraulic-mechanical modeling, Geothermal well, Cooling, Stimulation, Hydraulic fracturing

List of symbols

Symbol	Unit	Property
c_R	$\text{J kg}^{-1}\text{K}^{-1}$	Specific heat of rock grains
D	-	Damage variable
D_v	$\text{m}^2 \text{s}^{-1}$	Effective molecular diffusion
e_β	J kg^{-1}	Specific internal energy per unit mass of phase β
E	Pa	Young's modulus
E_0	Pa	Mean mesoscopic Young's modulus
E_i	Pa	Young's modulus of an elastic element
E_d	Pa	Young's modulus of a damaged element
$\mathbf{f}$	Pa	Body force
$f(x)$	Pa^{-1}	Distribution density
$\mathbf{F}^h$	$\text{J m}^{-2}\text{s}^{-1}$	Specific heat flux
$\mathbf{F}^\kappa$	$\text{kg m}^{-2}\text{s}^{-1}$	Flux density for mass of component κ
F_β^κ	$\text{kg m}^{-2}\text{s}^{-1}$	Flux density for mass of component κ in phase β
g	m s^{-2}	Acceleration of gravity
G	Pa	Shear modulus
h_β^κ	J kg^{-1}	Enthalpy (energy per unit mass) of component κ in phase β
k	m^2	Permeability
k_0	m^2	Initial intrinsic permeability

Symbol	Unit	Property
k_d	m ²	Permeability of a damaged element
k_e	m ²	Permeability of an elastic element
k_f	m ²	Permeability of a failure element
$k_{r\beta}$	-	Relative permeability for flow in phase β
K	Pa	Bulk modulus
l	m	Side length of an element
m	-	Homogeneity index
M^h	J m ⁻³	Specific heat
M^κ	kg m ⁻³	Mass of component κ per unit volume
p	Pa	Pore-pressure
P_c	Pa	Capillary pressure
P_{c0}	Pa	Initial capillary pressure
P_β	Pa	Fluid pressure in phase β
q^h	J m ⁻³ s ⁻¹	Heat source
q^κ	kg m ⁻³ s ⁻¹	Specific mass sink/source
S_h	Pa	Minimum horizontal stress
S_H	Pa	Maximum horizontal stress
S_v	Pa	Vertical stress
S_β	-	Saturation of phase β
t	S	Time
T	K	Temperature
ΔT	K	Temperature change
$\mathbf{u}$	m	Displacement vector
V	m ³	Volume of an element
ΔV	m ³	Volume change of an element
w	m	Fracture aperture of a conceptual fractured element
w_f	m	Equivalent diameter of the section in a failure element
x		Experimental material parameters
x_0		Mean value of material parameters put into numerical simulation program
X_β^κ	-	Mass fraction of component κ in phase β
y		Variable
z	m	Elevation
α	-	Biot coefficient
α_d	-	Biot coefficient of a damaged element
α_v	K ⁻¹	Volumetric expansion coefficient
β	-	Phase symbol
$\boldsymbol{\varepsilon}$	-	Strain tensor

Symbol	Unit	Property
$\bar{\epsilon}$	-	Equivalent principal strain
ϵ_1	-	Maximum principal strain
ϵ_2	-	Intermediate principal strain
ϵ_3	-	Minimum principal strain
ϵ_c	-	Critical stain under peak compressive stress
ϵ_{cu}	-	Ultimate compression strain
ϵ_t	-	Threshold strain
ϵ_m	-	Ultimate tensile strain
ϵ_v	-	Volumetric strain
μ_β	Pa s	Fluid dynamic viscosity of phase β
ν	-	Poisson ratio
ρ_R	kg m ⁻³	Density of rock
ρ_β	kg m ⁻³	Density of phase β
σ	Pa	Stress tensor
σ_1	Pa	Maximum principal stress
σ'_1	Pa	Effective maximum principal stress
σ_3	Pa	Minimum principal stress
σ'_3	Pa	Effective minimum principal stress
σ_c	Pa	Uniaxial compressive strength
σ_{c0}	Pa	Mean mesoscopic uniaxial compressive strength
σ_h	Pa	Projection of the minimum horizontal stress on the plane vertical to the borehole
σ_H	Pa	Projection of the maximum horizontal stress on the plane vertical to the borehole
σ_{rt}	Pa	Residual tensile stress
σ_{rc}	Pa	Residual compressive stress
σ_{t0}	Pa	Uniaxial tensile strength
ϕ	-	Porosity
ϕ_0	-	Initial porosity
λ_m	J s ⁻¹ m ⁻¹ K ⁻¹	Apparent macroscopic (over all phases) thermal conductivity
λ_R	J s ⁻¹ m ⁻¹ K ⁻¹	Thermal conductivity of rock
λ_β	J s ⁻¹ m ⁻¹ K ⁻¹	Thermal conductivity of phase β
θ	-	Friction angle

1. INTRODUCTION

Coupled processes are vital in reservoir engineering during both reservoir stimulation and subsequent energy production (e.g., geothermal, oil and gas reservoirs) [1-9]. Complex thermal-hydraulic-mechanical (THM) processes, including heat transfer, fluid flow, and rock deformations occur simultaneously and are affected by many non-linear processes [8, 10, 11]. Therefore, numerical modeling is recognized as an expedite and low-cost approach to simulate and analyze the multiphysics processes [11-13]. A vast amount of progress has been made in the past two decades in thermal-hydraulic-mechanical modeling, including those related to nuclear waste disposal research within the international DECOVALEX project [14, 15]. Utilizing numerical methods, such as the finite element method, THM models have been implemented for research tools such as ROCMAS, opensource initiatives such as OpenGeosys, and commercial software such as COMSOL Multiphysics [14, 16-18]. Another approach is to link existing reservoir simulators to geomechanical models, such a work done with the TOUGH-FLAC simulator, and other TOUGH-based multiphase flow and geomechanical simulators [19-24]. In addition, some other codes based on the finite volume method (FEM), control volume finite element method (CVFE), displacement discontinuity method (DDM), numerical manifold method (NMM) and discrete element method (DEM) help in understanding the parameter variation and evaluating the performance of reservoir [8, 25-30].

The combinations of space discretization methods have been developed and widely applied for modeling fracture processes in rock materials. The main types of hybrid models are the hybrid Finite Element Method-Discrete Element Method (FEM-DEM), the hybrid Finite Element Method-Boundary Element Method (FEM-BEM), the hybrid Finite Element-Meshfree Method-Finite Volume Method (FEMM-FVM), the hybrid Finite Volume Method- Discrete Element Method (FVM-DEM), and the hybrid Embedded Discrete Fracture Method-Extended Finite Element Method (XFEM-EDFM) models [31-35]. However, for complex large-scale 3D problems of arbitrary fracturing orientation, the computational efficiency for millions, even billions of elements and the computational accuracy of fracture geometry are challenging at this stage.

Numerical modeling of coupled processes in fractured media involves several components: modeling of fluid flow in fractures, modeling of mechanics of fractures, and modeling of fluid flow and mechanics in porous rocks. Depending on geometric representation of fractures, different fluid flow models are developed, such as BEM, FEM, NMM, DEM, FVM-FDM, FVM-FEM [27, 36-40]. These can be categorized into n-dimensional, n-1 dimensional and zero-dimensional models [27, 28]. For mechanical analysis of fractures, there are two types of models typically: continuous models where fractures are represented with the same dimension as the dimension of rock matrix, and discontinuous models where fractures are discontinuous boundaries of rock matrix. The BEM allows lower-dimensional boundary discretization to analyze fracture problems [36], but its applications to heterogeneous systems with great numbers of fractures are rarely seen to the authors' knowledge. In a hybrid-dimensional FEM model, a fracture is simulated as discontinuous boundaries of rock matrix, thus in, no additional degrees of freedom are introduced for fractures [37]. NMM utilizes three different types of geometry to represent fractures at different scales, including porous nonlinear domain, discrete fracture networks, and rough fracture

surfaces at the discontinuum asperity scale [27]. However, 3D modeling for discrete fractures with the capabilities to address coupled THM processes remains challenging. Fractured material is represented by assembled independent blocks with contacts or interfaces between them in DEM, which was fulfilled in 3DEC [38]. Its ability to model micro-cracks has been recognized, but high computational cost limits its application. Other 3D models include TOUGH-FLAC as an application of FVM-FDM where 3D fractures are represented as solid continuum elements [39]. TReactMech [40] and TOUGH-FEMM [35] by linking TOUGH code to other finite element codes where in both models fractures are represented as discontinuities.

In order to rigorously capture dynamic changes of fractures as a result of coupled THM process, we integrated the advantages of TOUGH2 [41] for modeling multiphase fluid flow and heat transport based on the FVM with the geomechanics code Rock Failure Process Analysis (RFPA) [42] for modeling deformation and failure based on the FEM. RFPA can simulate the failure process of heterogeneous rock without special fracture elements or predefined fracture paths [42-44]. Accurate modeling of rock failure and the growth of discrete fractures is required, because rock failure and fractures influence the fluid flow transmissivity and heat transfer [25, 45-48]. Moreover, mechanical properties and thermo-physical properties may be spatially heterogeneous and evolve with system temperature, pressure, and mechanical stress [21, 49, 50]. For geothermal and hydrocarbon reservoir management, both coupled THM processes and thermo-physical fluid property variations under phase changes have to be considered as these systems usually involve high temperature and pressure [9, 15, 51]. The TOUGH-RFPA combination is ideal for investigating such spatial heterogeneity impact in reservoir managements, from the wellbore stimulation volume to the large-scale reservoirs. TOUGH-RFPA can calculate millions of elements at this stage. However, for modeling an engineering scale model of hundreds of cubic meters, the mesh size is much greater than mineral grain size. Therefore, the TOUGH-RFPA offers fine-grained simulation for laboratory-scale models and coarse-grained simulation for field-scale models. Potentially, billions of elements can be calculated in the future when RFPA is linked to TOUGH3 [52], which is an upgraded version of TOUGH2 with parallelization and optimized memory allocation.

In the present work, we present a coupled THM model for simulating the rock failure process in geological media. The THM model is implemented in a solver module that links the TOUGH2 multiphase fluid flow simulator with RFPA. The linked simulator TOUGH-RFPA takes advantage of the capability to calculate multiphase and multicomponent flow using TOUGH2, and the ability to analyzing rock damage using RFPA. The heterogeneity of rock is realized by assigning the thermal, hydraulic and mechanical parameters of elements according to distribution functions, such as the Weibull distribution [53, 54]. Then, two benchmark problems are simulated to verify the capability of the TOUGH-RFPA simulator in terms of thermal-elastic and poroelastic stress. At last, a case study concerning the cold-water injection process of a geothermal well with conditions derived from the International Deep Drilling Projects (IDDP-2) geothermal well in Iceland is simulated to demonstrate the applicability of TOUGH-RFPA to model cooling-induced damage around a well considering heterogeneous mesoscopic mechanical properties.

2. METHODOLOGY

2.1 Basic assumptions

TOUGH-RFPA is developed with the following assumptions [55]:

- Eight-node isoparametric hexahedral element is used as the basic element in RFPA [44].
- Fractures are represented as solid elements (i.e., equidimensional as the rock matrix). Therefore, fractured porous rocks are assumed to be a heterogeneous, nonisothermal, deformable porous medium. Its heterogeneity is considered by assuming that the geomechanical and geophysical properties conform to the Weibull distribution (specified by the Weibull distribution parameters) [53, 56].
- A multiphase and multicomponent system is considered where the porous rock and fractures might be filled with different phases of fluids (liquid, gaseous, supercritical) or different components of fluids. [19].
- Coexisting fluid and solid components are assumed to be in local thermal equilibrium [41].
- The heat diffusion in the porous media is governed by Fourier's law, and the coupled process between stress/strain and heat transfer in the deforming porous media is based on thermo-elastic consolidation theory.
- At the elemental scale, the rock mass is treated as an elastobrittle material with a residual strength. Its mechanical behavior is modeled by an elastic damage constitutive law, and the residual strain/deformation upon unloading is not considered [56-58].
- Mechanical damage of an element can be initiated based on the Mohr-Coulomb failure criterion combined with a maximum tensile stress criterion [56-58].
- The fluid flow in the porous and fractured media is governed by Darcy's law. The hydraulic behavior responds to changes in the stress field by considering effective stress and by porosity and permeability variation [41, 56-58].

2.2 Static mechanical equations

In this section, the stress and strain are negative in compression and positive in tension. In the geomechanical model, elastic mechanics for an isotropic linear poroelastic medium is used to describe rock deformation at the elemental scale before damage [59], including the following constitutive relations:

$$\boldsymbol{\sigma} = 2G\boldsymbol{\varepsilon} + \frac{2\nu G}{1-2\nu} \text{tr}(\boldsymbol{\varepsilon})\mathbf{I} - \alpha P\mathbf{I} - K\alpha_v \Delta T\mathbf{I} \quad (1)$$

$$P = \sum_{\beta} S_{\beta} P_{\beta} \quad (2)$$

While the equations of equilibrium and the strain-displacement relation can be expressed as:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = 0 \quad (3)$$

and

$$\boldsymbol{\varepsilon} = \frac{1}{2}((\nabla \mathbf{u})^T + \nabla \mathbf{u}) \quad (4)$$

2.3 Mass balance equations

The mass balance equation for a multiphase-multicomponent system in TOUGH-RFPA is governed by [19, 41]:

$$\frac{\partial M^\kappa}{\partial t} - q^\kappa = -\nabla \cdot \mathbf{F}^\kappa \quad (5)$$

Eq. (5) considers the movement of the matrix relative to a fixed control volume.

The mass per unit volume of component κ is determined by [41]:

$$M^\kappa = \phi \sum_{\beta} S_{\beta} \rho_{\beta} X_{\beta}^{\kappa} \quad (6)$$

The coupling of TH with M is implemented through a porosity correction and permeability variation. The porosity of an element for the next iteration typically varies as functions of the differential pressure, the differential temperature, and the differential total stress [60]:

$$\phi^{(n+1)} = \phi^{(n)} + \left(\frac{\alpha - (1 - \alpha)\phi^{(n)}}{K} \right) dP + \alpha_v \phi^{(n)} dT + \frac{\alpha}{K} d\sigma \quad (7)$$

The mass flux of component κ is computed by Darcy's Law and Fick's law as follows [19]:

$$\mathbf{F}^\kappa = -\sum_{\beta} X_{\beta}^{\kappa} \left(k \frac{k_{r\beta} \rho_{\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} \mathbf{g}) \right) - \sum_{\beta} \rho_{\beta} D_v \mathbf{I} \nabla X_{\beta}^{\kappa} \quad (8)$$

2.4 Energy conservation equation (Heat Balance Equation)

According to the assumption of thermal equilibrium between the fluid and solid phases, energy conservation equation in TOUGH neglecting the terms representing the interconvertibility of thermal and mechanical energy is governed by [19, 41]:

$$\frac{\partial M^h}{\partial t} - q^h = -\nabla \cdot \mathbf{F}^h \quad (9)$$

The format of this equation is the same as the Eq. (5). The specific heat is determined by [41]:

$$M^h = (1 - \phi) \rho_R c_R T + \phi \sum_{\beta} S_{\beta} \rho_{\beta} e_{\beta} \quad (10)$$

The heat flux of component κ is computed by [41]:

$$\mathbf{F}^h = \sum_{\beta} \sum_{\kappa} h_{\beta}^{\kappa} F_{\beta}^{\kappa} - \lambda_m \nabla T \quad (11)$$

Where λ_m is the thermal conductivity of filled unsaturated medium and computed by the following equation [41]:

$$\lambda_m = (1 - \phi) \lambda_R + \phi \sum_{\beta} S_{\beta} \lambda_{\beta} \quad (12)$$

2.5 Heterogeneity distribution function of elements

Mechanical properties and thermo-physical characteristics of minerals are different. They lead to great spatial heterogeneity in mesoscopic properties of rock [44]. In TOUGH-RFPA modeling, the rock is composed of a large

number of elements where material parameters are commonly assumed to follow a Weibull function with threshold values [53], as:

$$f(x) = \frac{m}{x_0} \left(\frac{x}{x_0} \right)^{m-1} \exp \left(- \frac{x}{x_0} \right)^m \quad (13)$$

2.6 Damage evolution of elements

An element has only one failure mode. The failure criteria (including the Mohr-Coulomb failure criterion, and the maximum stress criterion) are expressed as following equations [43]:

$$\begin{cases} \sigma'_1 \geq \sigma_t & (\sigma'_3 \geq \frac{1+\sin \theta}{1-\sin \theta} \sigma_t - \sigma_c) \\ \sigma'_3 - \frac{1+\sin \theta}{1-\sin \theta} \sigma'_1 \leq -\sigma_c & (\sigma'_3 < \frac{1+\sin \theta}{1-\sin \theta} \sigma_t - \sigma_c) \end{cases} \quad (14)$$

When an element's effective stress satisfies any one of the criteria, the element begins to accumulate damage. Based on the assumption of equivalent strain principle in damage mechanics, the Young's modulus of the damaged element is given by:

$$E_d = (1 - D) E_i \quad (15)$$

When $D=1$, $E_d = e^{-12}$ MPa is given to avoid an ill-conditioned stiffness matrix.

The damage variable of elements failing in tensile mode can be expressed as [43, 44]:

$$D = \begin{cases} 0 & \bar{\varepsilon} < \varepsilon_t \\ 1 - \frac{\sigma_{rt}}{\bar{\varepsilon} E_i} & \varepsilon_t \leq \bar{\varepsilon} < \varepsilon_{tu} \\ 1 & \bar{\varepsilon} \geq \varepsilon_{tu} \end{cases} \quad (16)$$

$$\varepsilon_{tu} = \eta \varepsilon_t \quad (17)$$

where $\bar{\varepsilon}$ is an equivalent principal strain. It is defined as follows [61]:

$$\bar{\varepsilon} = \sqrt{\langle \varepsilon_1 \rangle^2 + \langle \varepsilon_2 \rangle^2 + \langle \varepsilon_3 \rangle^2} \quad (18)$$

where ε_1 , ε_2 and ε_3 are principal strains and $\langle \rangle$ is a function defined as follows:

$$\langle y \rangle = \begin{cases} y & y \geq 0 \\ 0 & y < 0 \end{cases} \quad (19)$$

The damage variable of elements failing in shear mode can be expressed as [43, 44]:

$$D = \begin{cases} 0 & \varepsilon_3 > \varepsilon_c \\ 1 + \frac{\sigma_{rc}}{\varepsilon_3 E_i} & \varepsilon_3 \leq \varepsilon_c \end{cases} \quad (20)$$

In TOUGH-RFPA, elements can be classified by the damage variable D into three kinds. They are elastic elements ($D=0$), damaged (fractured) elements ($0 < D < 1$) with residual strength and failed elements ($D=1$) which lose all strength.

2.7 Permeability variation of elements

The permeability of an element varies as a function of the porosity during elastic deformation, increases according to a strain-dependent law when the element is damaged and obeys the assumption of pipe laminar flow after failure [56-58].

2.7.1 Porosity-dependent permeability of elastic elements

During elastic deformation, the permeability variation with porosity for an elastic element can be described based on the Kozeny–Carman equation by [62-64]:

$$k_e = k_0 \frac{\phi^3 (1 - \phi_0^2)}{\phi_0^3 (1 - \phi^2)} \quad (21)$$

2.7.2 Strain-dependent permeability of damaged elements

For elements failing in shear, the rearrangement of grains and pores due to shear slip affects permeability slightly [65] with the permeability changes assumed to still obeys Eq. (21).

When an element exceeds its strength, we can consider the degradation of Young's modulus to be physically manifested as the development of fractures [66]. Thus, we assume that a damaged element can conceptually be represented hydraulically as a unit of rock containing three orthogonal fractures with smooth parallel sides [56, 58].

We assume that the total volume of fractures equal to the volume change. The aperture w of the conceptual fractured element determined by its volumetric strain can be expressed as follows:

$$w = \frac{\Delta V}{3l^2} = \frac{V}{3\sqrt[3]{V^2}} \varepsilon_v = \frac{\sqrt[3]{V}}{3} \varepsilon_v \quad (22)$$

The damaged permeability for the next step is calculated based on cubic law as [66]:

$$k_d^{n+1} = \frac{w^2}{12} = \frac{\sqrt[3]{V^2}}{108} (\varepsilon_v^n)^2 \quad (23)$$

So, permeability for a damaged element is uniquely defined by volumetric strain, which is supported by experimental observations [67-70].

2.7.3 Mesh-dependent permeability of failure elements

The fluid flowing through a failed element is conceptualized by using the assumption of pipe laminar flow. Therefore, permeability of a failed element can be determined as follows [71]:

$$k_f = \frac{w_f^2}{32} \quad (24)$$

The equivalent diameter w_f is calculated by side length of the element by $w_f^2 = \frac{4l^2}{\pi}$, where l is the relevant element length.

1 For damaged elements and failed elements, adjustment of the permeability by an amplification factor is an
2 alternative. Then the permeability is calculated through the following equations:

$$3 \quad k_d = \alpha_d k_0 \quad (25)$$

$$4 \quad k_f = \alpha_f k_0 \quad (26)$$

5 Typically, α_d and α_f are determined by experimental data and empirical parameters.
6

Figure 1 Computation schematic of TOUGH-RFPA

Figure 2 Data transfer between TOUGH and RFPA

Figure 3 Data interpolation in TOUGH-RFPA (blue dots represent RFPA nodes, orange dots represent TOUGH nodes)

2.8 Coupling approach between TOUGH and RFPA

The above equations are utilized in the TOUGH-RFPA using the computational scheme shown in Figure 1. The codes consist of four modules, which are the preprocessing module, calculation module, damage analysis module, and postprocessing module [55]. Among them, the calculation module is written in FORTRAN, while the others are implemented using Visual C++ [72]. TOUGH-RFPA is fully coupled for thermal-hydraulic process and sequentially coupled for mechanical process in every iteration. TOUGH and RFPA solve equations separately and transfer data to each other through subroutines and data files. Figure 2 shows the data transfer processes within every iteration and between each step. Green lines represent transferring data by data files to the next time step. The updated mechanical parameters and permeability are determined in the damage analysis module. Red lines represent transferring parameters and returning values between subroutines. Porosity correction determined by the differential pressure, the differential temperature, and the differential effective stress is updated every iteration. Because a TOUGH mesh uses one node within each element, and RFPA nodes are located in element corners as

shown in Figure 3, temperature and pressure have to be interpolated from the body center to corners [19]. Elements that share the same corner node contribute to the value of that node, such as the solid blue dot in Figure 3.

3. VERIFICATION

3.1 Hydraulic fracturing of a hollow cylinder

In this section, a 2D model of a hollow cylinder with fluid pressure applied on the inner wall is employed to verify the hydro-mechanical calculation capabilities of TOUGH-RFPA. Based on the plane strain assumption, the numerical model was built with 80,000 elements, as shown in Figure 4. Parameters related to this verification example is listed in Table 1. The inner pressure is 3 MPa.

When the hydraulic gradient is steady as shown in Figure 5(a), the stresses are determined by the internal pore-pressure. Therefore, the radial and tangential stresses induced by the hydraulic pressure at any point are formulated by Zhan et al. [73] as follows:

$$P = P_a - \frac{\ln r/a}{\ln b/a} P_a \quad (27)$$

$$\sigma_r^P = \frac{-P_a}{\ln b/a} \frac{(1+\nu)(ab)^2}{2(b^2 - a^2)} \left(\frac{\ln b/a}{r^2} + \frac{\ln r/b}{a^2} - \frac{\ln r/a}{b^2} \right) \quad (28)$$

$$\sigma_\theta^P = \frac{-P_a}{\ln b/a} \frac{(1+\nu)(ab)^2}{2(b^2 - a^2)} \left(-\frac{\ln b/a}{r^2} + \frac{\ln r/b}{a^2} - \frac{\ln r/a}{b^2} \right) + \frac{P_a}{\ln b/a} \frac{1-\nu}{2} \quad (29)$$

Figure 4 The cross-section of the hollow cylinder validation model

Table 1 Mechanical and physical parameters of the hollow cylinder model

Parameters	Value
Poisson ratio ν	0.25
Permeability k	$1 \times 10^{-12} \text{ m}^2$
Biot coefficient α	1

Figure 5 Distribution of pore-pressure in the numerical model calculated by TOUGH-RFPA (a) Contour plot of the pore-pressure; (b) Comparison between numerical results and analytical results of pore-pressure.

Two simulations with different material homogeneities ($m=1000$ and $m=3$) are performed. Stress contours (supposing compression is positive) obtained from the numerical simulation are shown in Figure 6. Inhomogeneity induces larger effective stress in some elements.

Figure 6 Distribution of effective minimum compressive principal stress in the numerical models calculated by TOUGH-

RFPA (a) Homogenous model (MPa); (b) Heterogeneous model (MPa). Positive stress values signify compressive stress.

Figure 7 shows the analytically and numerically obtained radial and tangential stress (supposing tension is positive) variation with radius at $\theta=0$. The analytical stress values are calculated from Eq. (28) and Eq. (29). As can be seen from the line graph, the tangential stress is the largest at the wall of the hole. The radial stress firstly increases then decreases with radius. By comparing simulated results with different homogeneities, it is found that the experimental results are in close agreement with the analytical solution. However, the result curves of the low homogeneity ($m=3$) model fluctuate around the curves of high homogeneity ($m=1000$), affecting the damage evolution path in further simulation.

Figure 7 Comparison between numerical results and analytical results of effective radial and tangential stresses at $\theta=0$. Positive values signify tension.

3.2 Heating of a quarter hollow cylinder

In this section, a 2D model of a quarter hollow cylinder with constant temperature applied on the inner wall is employed to verify the thermal-mechanical calculation of TOUGH-RFPA. Based on the plane strain assumption, the numerical model was built with 80,000 elements as shown in Figure 8, whereas material parameters are listed in Table 2. The initial temperature of the entire model is 20 °C. The inner boundary temperature is 70 °C and the outer boundary temperature is 20 °C.

Table 2 Mechanical and physical parameters of the hollow cylinder model

Parameters	Value
Poisson ratio ν	0.25
Biot coefficient α	1
Young's modulus E	40 GPa
Thermal conductivity λ_R	4.2 W/m°C
Volumetric thermal expansion coefficient α_v	2.4 E-5 /°C

Figure 8 Cross-section of heating hollow cylinder model

The solutions to this problem under steady-state are formulated by Nowacki [74], as described in Eq. (30) through (33):

$$T = \frac{\ln(b/r)}{\ln(b/a)} T_a + \frac{\ln(a/r)}{\ln(a/b)} T_b \quad (30)$$

$$\sigma_r^T = \frac{E\alpha_v}{6(1-\nu)} \frac{T_a - T_b}{\ln(b/a)} \left[-\ln \frac{b}{r} + \frac{a^2}{b^2 - a^2} \left(\frac{b^2}{r^2} - 1 \right) \ln \frac{b}{a} \right] \quad (31)$$

$$\sigma_\theta^T = \frac{E\alpha_v}{6(1-\nu)} \frac{T_a - T_b}{\ln(b/a)} \left[1 - \ln \frac{b}{r} - \frac{a^2}{b^2 - a^2} \left(\frac{b^2}{r^2} - 1 \right) \ln \frac{b}{a} \right] \quad (32)$$

$$\sigma_a^T = \frac{-E\alpha_v}{6(1-\nu)} \frac{T_a - T_b}{\ln(b/a)} \left[2 \ln \frac{b}{r} - \nu + \frac{2\nu}{1+2\nu} \frac{2a^2}{b^2 - a^2} \ln \frac{b}{a} \right] \quad (33)$$

Contour plots of temperature and the minimum principal stress (supposing compression is positive) are presented in Figure 9(a) and Figure 10. The highest stress concentration occurs close to the heated hole where the temperature is the highest, whereas tensile stress occurs close to the outer boundary. The maximum magnitude of the minimum stress in heterogeneous model is more sparsely distributed than the homogenous one.

The comparison between numerical and analytical results of temperature and stress are shown in Figure 9(b) and Figure 11. The stress results in Figure 11 are shown for radial, tangential and axial stress (supposing tension is positive) components, including the analytical stress values calculated from Eq. (31) to Eq. (33). It is found that the radial and tangential stress curves intersect at $r=0.00919$ m and the radial and axial stress curves intersect at $r=0.0208$ m, which means that the principal stresses rotate at these two positions. At the outer boundary ($r=0.025$ m), where the tensile stress reaches its largest value, tensile failure could most easily occur. The largest compressive stress and the largest variation in stress occur in the heterogeneous model for axial stress towards the inner part. This variation in thermal stress is a result of the variation in elastic modulus. The numerical and analytic results are in good agreement, though some minor differences can be observed that could be related to mesh discretization using eight-node isoparametric hexahedral elements. A coarser mesh with larger element size can also provide a reasonable accurate result, but a finer mesh with smaller element size leads to more accurate results, especially for model simulations involving arc-shaped boundaries.

Figure 9 Distribution of temperature in the numerical model calculated by TOUGH-RFPA (a) Contour plot of temperature($^{\circ}\text{C}$); (b) Comparison between numerical results and analytical results of temperature.

Figure 10 Distribution of minimum compressive principal stress in the numerical models calculated by TOUGH-RFPA (a) Homogenous model (MPa); (b) Heterogeneous model (MPa), Positive stress values signify compressive stress.

Figure 11 Comparison between numerical results and analytical results of principal stresses at $\theta=0$. Positive values signify tension.

4. APPLICATION OF TOUGH-RFPA TO COOLING PROCESS IN A GEOTHERMAL WELL

The capability of TOUGH-RFPA is demonstrated by simulating cooling-induced wellbore damage in a deep geothermal well considering in situ conditions derived from the International Deep Dripping Project well IDDP-2 at Reykjanes, Iceland [26]. At IDDP-2, relatively cool water is injected at 4500 m depth where the ambient temperature is over 400 °C and it is important to investigate what kind of damage such cooling may induce to the well. A coupled THM simulation of this well was conducted by Peter-Boirs et al. [26] using a particle code model,

i.e., the grains are simulated with rigid spheres connected with springs at contact points. Here, the TOUGH-RFPA is applied considering heterogeneous rock properties at the mesoscale. Similarly to Peter-Boirs et al. [26], a representative rock of fine-grained dolerite with the rock composition of 40% pyroxene, 55% plagioclase, and titanomagnetite 5% [75] is considered. The range of the thermal, hydraulic, and mechanical parameters of this representative rock are listed in Table 3, according to a literature review on the properties of minerals [26, 76-80]. In addition, uniaxial compression experiments of the representative rock are modeled with comparison of simulated and experimental macroscopic stress-strain evolution to further calibrate the mesoscopic parameters of the heterogeneous rock matrix.

Table 3 The range of values of the thermal, hydraulic, and mechanical properties

Parameter	Symbol	Value	Unit
Depth	z	4560	m
Vertical stress	S_v	134	MPa
Horizontal stress	S_H, S_h	60-180	MPa
Macroscopic Young's modulus	E	88±2.5	GPa
Uniaxial compressive strength	σ_c	226±11	MPa
Tensile strength	σ_T	11.5±0.9	MPa
Friction angle	φ	43	°
Poisson's ratio	ν	0.21±0.03	-
Permeability	k	E-18	m ²
Porosity	n	0.1~3.6	%
Volumetric thermal expansion coefficient	α_v	2.4E-5	/°C
Thermal conductivity	λ	2.3	W/m°C
Specific heat	C_R	1000	J/kg°C

4.1 Simulation of the uniaxial compression experiment through RFPA3D

The mean mesoscopic Young's modulus E_0 and strength σ_{c0} , which are used in the cooling simulation of the geothermal well were estimated through modeling of uniaxial compression. First, the approximate mesoscopic values are gained from the following regression equations [81]:

$$\frac{\sigma_c}{\sigma_{c0}} = 0.2602 \ln m + 0.0233 \quad (1.2 \leq m \leq 50) \quad (34)$$

$$\frac{E}{E_0} = 0.1412 \ln m + 0.6476 \quad (1.2 \leq m \leq 10) \quad (35)$$

Then, those values are adjusted based on comparing the simulated stress-strain curve with the laboratory one. Similarly to Peter-Boirs et al. [26], because of a lack of core sample mechanical data from the site, a representative

rock of fine-grained gabbro [80] with similar mineral composition to the IDDP-2 rock samples [75], is regarded as the reference experiment samples. Specimens (Ga3, Ga4, and Ga10) with a 70 mm diameter and 140 mm length were under constant strain rate conditions (3 to 4×10^{-3} mm/s) to get the uniaxial compressive strength (UCS) [80].

The dimension of the uniaxial compressive numerical model was the same as the experimental specimens. It was meshed by elements with a side length of 1 mm. The numerical model was loaded from the top by a constant displacement rate of 0.004mm/step. After simulation tests, the mesoscopic mechanical parameters used in the geothermal well cooling simulation are shown in Table 4. The stress-strain curves and failure types of representative gabbro [80] specimens and the numerical model with homogeneity index $m=3$ are shown in Figure 12 and Figure 13, respectively.

Table 4 Macroscopic, mesoscopic and simulated mechanical parameters

Parameter	Symbol	Value ¹⁾	Unit
Macroscopic Young's modulus	E	$88 \pm 2.5^{1)}$	GPa
Macroscopic strength	σ_c	$226 \pm 11^{1)}$	MPa
Homogeneity index	m	3	-
Mean mesoscopic Young's modulus	E_0	120	GPa
Mean mesoscopic strength	σ_{c0}	750	MPa
Numerical output Young's modulus	E_n	91	GPa
Numerical output strength	σ_{cn}	221	MPa

1) The macroscopic values according to [80]

Figure 12 Strain-stress curves of the numerical uniaxial compression model and data for gabbro specimens from [80]

Figure 13 Failure shapes of the numerical uniaxial compression model and the representative gabbro specimens [80]

4.2 Simulation of the cooling process through TOUGH-RFPA

We use 2D plane strain assumption with initial vertical stress to simplify the rock domain as shown in Figure 14. The direction perpendicular to the plane is the direction of the well axis. The numerical model is $0.88 \text{ m} \times 0.88 \text{ m} \times 0.0088 \text{ m}$, meshed by $200 \times 200 \times 2$ elements. The mesh size is 4.4 mm which approaches the rock grain size of about 3 mm. We considered an initial temperature of 375°C , that is the upper temperature limit for the thermo-physical fluid property, equation-of-state module, EOS1 in TOUGH2, while the initial rock pore pressure is 34 MPa. Constant stresses are applied to the outer boundaries with the possibility of applying a shear stress to be able to rotate the principal stress field in the horizontal plane. From time step 6, the temperature is fixed to 30°C at 34 MPa inside the borehole to represent a sudden cooling due to cold water injection, similar to the models by Peter-Boirs et al. [26]. The other parameters we used in TOUGH-RFPA cooling simulation are shown in Table 5 [26, 80, 82]. The average computational time by PC is 5 hours to simulate 85 minutes of cooling.

Figure 14 The model sketch of the domain near the borehole based on plane strain assumption. (a) boundary conditions for time step 1~5; (b) boundary conditions after time step 6; (c) Young's modulus distribution

The stress state of 4500 m depth at the IDPP-2 well is not known and is therefore varied in a sensitivity study using ranges of in situ stresses as shown in Figure 15. The fluid pressure of 34 MPa was measured at the bottom of the well [83], and the coefficient of friction was set to 0.6. The vertical stress is set to 134 MPa, as estimated from the weight of the overburden by Peter-Boirs et al. [26]. In Iceland, a strike-slip regime is dominant near the surface [84, 85]. The normal faulting regime prevails with a further increase in depth [84, 85]. Therefore, only the strike-slip faulting zone and normal faulting zone are plotted in Figure 15. Four cases (CASE-NF1, CASE-NF2, CASE-NF/SS, CASE-SS) are chosen for this modeling. The direction of the wellbore dip direction is N210°E and the deviation from the vertical is approximated at 28° [82, 86]. Moreover, the mean maximum horizontal stress (σ_H) azimuth is 47°, according to the drilling-induced fractures (DIFs) data from borehole RN-34 in Reykjanes [84]. The stress states at the modeled wellbore cross-section of the four cases are listed in Table 6. This will allow for the investigation of the different damage patterns that could occur for different stress states.

Table 5 The mechanical and physical parameters used in TOUGH-RFPA cooling simulation

Parameter	Symbol	Value	Unit
Borehole diameter	d	0.22	m
Poisson's ratio	ν	0.21	-
Friction angle	φ	43	°
Compression-tension ratio	-	19.65	-
Residual strength coefficient	λ	0.1	-
Ultimate tensile strain coefficient	η_t	5	-
Ultimate compressive strain coefficient	η_c	200	-
Permeability	k	1×10^{-19}	m ²
Porosity	n	3	%
Biot coefficient	α	0.001	-
Biot coefficient of a damaged element	α_d	0.99	-
Volumetric thermal expansion coefficient	α_v	2.4×10^{-5}	/°C
Thermal conductivity	λ	2.3	W/m°C
Specific heat	C_R	1000	J/kg°C

Figure 15 Polygons which define possible stress magnitudes at 4500 m for pore pressure of 34 MPa

Table 6 Cases of different in-situ stresses

Case No.	S_H (MPa)	S_h (MPa)	S_v (MPa)	σ_x (MPa)	σ_y (MPa)	τ_{xy} (MPa)	σ_z (MPa)
CASE-NF1	70	70	134	70	88	0	120
CASE-NF2	90	90	134	90	104	0	124
CASE-NF/SS	134	66	134	128	89	17	120
CASE-SS	150	71	134	143	94	20	122

Figure 16 The variation of temperature and pore pressure of elements a, b, and c with time in CASE-NF2 (the solid lines

represent temperature, and the dashed lines represent pore-pressure)

The temperature and pore pressure evolutions for CASE-NF2 are shown in Figure 16. Three typical elements (a, b, and c) at $r=0.1166$ m (at the borehole wall and marked by the blue lines), $r=0.1606$ m (about 0.05 m from the borehole wall and marked by the red lines), and $r=0.4378$ m (near the outer model boundary and marked by the green lines) were chosen. Figure 16 shows that the green (solid) temperature line is horizontal, signifying constant temperature, while the green (dashed) pressure line changes after $t=1070$ s, which shows that the heat conduction is much slower than fluid pressure diffusion. Temperature curves of both element a and element b decrease with the cooling process. The blue curve drops sharply during the first 500s due to the high gradient near the borehole wall. Then its variation rate becomes slower. The red curve decreases gradually during the entire calculation period. It illustrates a general temperature decreases with the cooling of the borehole. Comparing the three (dashed) pressure curves, we found that the closer the element is to the inner boundary, the faster the pressure declines. This pressure decline is caused by cooling contraction of the fluid within the low permeability rock. When $t=1070$ s, the green dashed line starts to decline, meaning that the pressure field reaches the outer boundary. Simultaneously, the pressure near the inner boundary (near the borehole wall) starts to increase slightly because of pressure diffusion from the constant pressure boundary at the borehole wall.

Figure 17 The variation of x-stress and y-stress with x-coordinate from along line $y=0.44$ m for time step 5 (the solid lines represent x-stress, and the dashed lines represent y-stress), (a) x-stress; (b) y-stress. Positive stress values signify tensile stress.

The variation of x-stress and y-stress with x-coordinate along line $y=0.44$ m for time step 5 of four cases are presented in Figure 17. At this moment, the temperature and injection fluid has not been applied to the boundary, so the stress distribution is solely controlled by the in-situ stress. The stresses fluctuate greatly due to the heterogeneity. By comparing CASE-NF1 with CASE-NF2, both of the x-stress and y-stress in CASE-NF2 is smaller than in CASE-NF1. As a result, the magnitude of the compressive stress near the wellbore in CASE-NF2

is higher than that in CASE-NF1. The y-stress near the wellbore in CASE-NF/SS and CASE-SS are much smaller than in CASE-NF1 and CASE-NF2, because the deflection of x-direction away from the minimum horizontal stress (σ_h) is large as shown in Figure 18. Figure 18 demonstrates that the main failure mode is compression during drilling before the injection of cooling water. Comparing the four cases in the figure, the damaged elements mainly distribute along the direction of minimum horizontal stress, when a large number of elements are damaged as CASE-SS. However, when little visible damage is observed, the position of damaged elements is more random as CASE-NF1, CASE-NF2 and CASE-NF/SS. The maximum compressive stress in CASE-NF1, CASE-NF2 and CASE-NF/SS is large enough to break some elements with lower strength while the stress is lower than the strength of elements with higher strength. The position of elements with low strength and elastic modulus is random, so the damage location is random. The four cases have a same strength distribution, so some of the damage elements have the same locations. The randomness can be seen in the micro-resistivity imaging (SMI) of well RN-15/IDDP2 in Figure 19 [87].

Figure 18 The crack results of four cases under in-situ stress after drilling (dark blue dots represent compressive failure, red dots represent tensile failure).

Figure 19 Micro-resistivity imaging (SMI) of well RN-15/IDDP2 from 4455 m to 4457 m [87]

Figure 20 shows the temperature contour of four scenarios at $t=30$ minutes. It demonstrates that substantial damage has accumulated after 30 minutes of cooling from the borehole for all of the four cases. Damage is induced by both large temperature gradient and the anisotropic in-situ stress. The large temperature gradient causes progressive failure of elements around the borehole, which are induced mainly by effective tensile stress. The in-situ-stress first leads to damage accumulation along the direction of maximum compressive horizontal stress (σ_H).

1 Comparing CASE-NF1 with CASE-NF2, CASE-NF1 has more damages because of less resistance developed near
2 the borehole. The in-situ stress determined the resistance near the borehole. The vertical stresses of the two cases
3 are close, but the compressive stress ($3 \cdot S_H - S_H$) near the borehole induced by the horizontal stresses of CASE-NF2
4 was 40 MPa greater than that of CASE-NF1. The ratios of stress in y-direction to stress in x-direction in CASE-
5 NF1 and CASE-NF2 are 1.26 and 1.16, respectively. Therefore, the resistance of CASE-NF1 was smaller than
6 CASE-NF2 resulting in more damages. Damage zone geometries are quite different in these two cases. CASE-
7 NF/SS and CASE-SS have shear stress applied at the boundary, resulting in a rotation of the maximum horizontal
8 stress to be at an angle of about 11 degrees and 13 degrees relative to x-direction. As a result, the damages
9 preferable propagate along the same 11 degrees and 13 degrees directions, i.e., the direction parallel to the
10 maximum compressive horizontal stress. As can be seen from Figure 20, the damage propagates ahead of the
11 cooling in some elements. This is a result of stress redistribution ahead of failed elements. After an element fails,
12 it cannot hold any stress, so the stress in nearby elements increases dramatically, inducing new damaged elements
13 surrounding the cooled elements. The regardless of heat exchange between fluids in the wellbore and the
14 surrounding formation also influences the thermal field results.

Figure 20 The temperature contour (°C) and damaged elements for four cases at t=30 mins

Figure 21 presents the minimum stress field and the fractured damage zone of CASE-NF/SS after 1, 10, 30, 45, 60, and 85 mins of cooling from the borehole. Before injection, some compressive damage is observed near the borehole in the direction of minimum horizontal stress. When heat extraction starts and the time progresses, as the cooling and thermal stress is distributed in a radially symmetric pattern, the fractured zone develops along the direction of the minimum principal stress parallel to the maximum horizontal stress. From t=30 to 85 minutes, five major fractures are generated and keep growing in the direction of maximum horizontal stress. At the same time, some mesoscopic damage appears in the direction of minimum horizontal stress. Thus, the evolution of damage around the well progresses at different locations and different directions depending on the cooling time and is probably impacted by the history of damage evolution.

Figure 21 The change of the effective minimum principal compressive stress (MPa) and fractured development in CASE-NF/SS during cool water injection. Positive stress values signify compressive stress.

The influence of fluid injection pressures on fracture geometry in CASE-SS is shown in Figure 22. It is shown that injection pressure greatly affects the fracture number, fracture width, and fracture length. Comparing injection pressure of 34 MPa, 70 MPa and 90 MPa, the number of major fractures decrease from 6 to 3 and finally becomes 2. Under the pressure of 90 MPa and 96 MPa, only a pair of major fractures propagate along the direction of maximum horizontal stress. However, a larger damage zone is produced near the borehole in the model with 96 MPa, because of the great fluid pressure. Comparing the four scenarios at 30 minutes, the fracture aperture and fracture length increase with injection pressure. Moreover, the fracture propagates faster with a higher pressure. Thus, higher injection pressure produces long and wide fractures resulting in larger fluid loss into the formation, whereas lower injection pressure induces thin and complex fractures with less fluid loss.

Figure 22 Fluid pressure contours (MPa) showing the variation of hydraulic gradients for CASE-SS with different injection pressure at $t=30$ minutes.

The results indicated more major fractures than recently published modeling results on similarly deep geothermal well conditions [26]. This difference of the major fractures achieved in the TOUGH-RFPA maybe a result of different post-failure behavior. The RFPA considers damage and associated softening of the rock, whereas the particle code applied in previous studies considers the breakage of bonds between rigid particles,

meaning that the stress and strain redistribution along with the failure processes may be different. The breakage of bonds between rigid particles tends to induce more micro-fractures. More pervasive micro-fracturing can lead to stress release, which could possibly explain the smaller number of major fractures obtained in [26]. While the particle code model in [26] can model micro-crack developments between grains at high computational costs, the TOUGH-RFPA provides an alternative heterogeneous continuum damage model of much higher efficiency.

5. CONCLUDING REMARKS

We have developed, verified and demonstrated the applicability of the TOUGH-RFPA simulator for modeling thermal mechanical stress and damage evolution in heterogeneous rock. The simulator is built on linking the multiphase fluid flow and heat transport simulator TOUGH2 with RFPA3D (Rock Failure Process Analysis), which is based on the idea that heterogeneity leads to non-linearity and causes progressive failure behavior observed in brittle rock. TOUGH-RFPA is fully coupled for thermal-hydraulic process and sequentially coupled for mechanical process in every iteration. In this linked simulator, elastic damage mechanics describes the damage process of elements. During the damage evolution process, the physical properties (such as Young's modulus, permeability and porosity) vary with the stress or strain. The capability of TOUGH-RFPA simulator is verified by modeling poroelastic and thermal-mechanical responses in a hollow cylinder. Then the simulator was applied in simulating cooling-induced damage around a deep geothermal well, considering conditions derived from the International Deep Drilling Project, IDDP-2 well in Iceland. The result revealed a complex damage pattern development, extending preferentially along the direction parallel to the maximum compressive stress. Dedicated laboratory experiments of cooling-induced damage around wells would be proposed to study these processes in detail and to provide further validation of the numerical approach developed in this study.

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