Understanding Induced Seismicity with a Discrete Fracture Network and Matrix Model with Mohr-Coulomb Failure and Nonlinear Hydraulic Diffusivity

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Abstract

Injection-induced seismicity (IIS) typically occurs when pressure diffuses from a sedimentary target formation down into fractured and faulted, low-permeability, critically-stressed basement rock. Previous studies of IIS have used basin-scale models of pressure diffusion that rely on an equivalent porous medium (EPM) approach to assign hydraulic diffusivity and a triggering pressure (TP) criteria for seismic initiation. We show that these models employed unrealistically-large values of hydraulic diffusivity, usually by neglecting the compressibility of the fractures in the specific storage coefficient, to result in pressure diffusion to seismogenic depths ([?]2 km into the basement). The EPM-TP approach does not explicitly represent the mechanical and hydrologic behavior of fractures and faults, and it fails to explain why relatively few disposal wells are associated with IIS. We develop a parallelized, partially-coupled, hydro-mechanical, discrete fracture network and matrix model (DFNM) model with thousands of fractures and the capability to calculate Mohr-Coulomb (MC) failure to indicate seismicity and alter hydraulic diffusivity. In consistent comparisons, DFNM-MC simulations allow for deeper, more heterogeneous pressure diffusion than EPM-TP simulations, and they do not need to employ unrealistic diffusivity values to result in pressure diffusion to seismogenic depths. A sensitivity analysis shows that small deviations in fault orientation ([?]2 degrees from optimal) and fracture network density outside an intermediate range can drastically decrease the likelihood of IIS, potentially explaining why only a small fraction of disposal wells are associated with IIS. The EPM-TP approach is unsuitable to investigate IIS, but the DFNM-MC approach offers a promising, nuanced approach for further study.

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Key Points:

- We introduce a discrete fracture network and matrix model with Mohr-Coulomb for induced seismicity
- Previous equivalent porous media models employed unrealistically-large hydraulic diffusivity values
- Fracture network density and sub-optimal fault orientation explain why seismicity is rare

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Abstract

Injection-induced seismicity (IIS) typically occurs when pressure diffuses from a sedimentary target formation down into fractured and faulted, low-permeability, critically-stressed basement rock. Previous studies of IIS have used basin-scale models of pressure diffusion that rely on an equivalent porous medium (EPM) approach to assign hydraulic diffusivity and a triggering pressure (TP) criteria for seismic initiation. We show that these models employed unrealistically-large values of hydraulic diffusivity, usually by neglecting the compressibility of the fractures in the specific storage coefficient, to result in pressure diffusion to seismogenic depths (≥2 km into the basement). The EPM-TP approach does not explicitly represent the mechanical and hydrologic behavior of fractures and faults, and it fails to explain why relatively few disposal wells are associated with IIS. We develop a parallelized, partially-coupled, hydro-mechanical, discrete fracture network and matrix model (DFNM) model with thousands of fractures and the capability to calculate Mohr-Coulomb (MC) failure to indicate seismicity and alter hydraulic diffusivity. In consistent comparisons, DFNM-MC simulations allow for deeper, more heterogeneous pressure diffusion than EPM-TP simulations, and they do not need to employ unrealistic diffusivity values to result in pressure diffusion to seismogenic depths. A sensitivity analysis shows that small deviations in fault orientation ($\leq 2^{\circ}$ from optimal) and fracture network density outside an intermediate range can drastically decrease the likelihood of IIS, potentially explaining why only a small fraction of disposal wells are associated with IIS. The EPM-TP approach is unsuitable to investigate IIS, but the DFNM-MC approach offers a promising, nuanced approach for further study.

Plain Language Summary

Wastewater from the oil and gas industry is often injected into deep disposal wells far below groundwater aquifers. Injected fluids can migrate to deep faults via permeable fractures, where even small pressure changes can lead to human-caused earthquakes (HCEs). This suggests that most disposal wells should cause earthquakes, but only a small fraction actually do. Many previous studies of HCEs ignored fractures and faults, causing them to use unrealistic rock properties in their computer models, which led to misunderstandings about HCEs. We create a computer model that calculates how the fluid pressure moves rapidly through permeable fractures and causes earthquakes on faults. The results explain why HCEs only occur near a small fraction of disposal wells: first, fluid pressure can only reach a fault if the fractures form a connected hydraulic pathway to the fault, and second, even if fluid pressure reaches a fault, an earthquake only occurs for a narrow range of fault orientations. Scientists should stop using the old computer models that ignore fractures and faults to assess HCEs. To reduce HCEs, fluid should not be injected near: (a) permeable fracture networks with long-range connectivity, and (b) faults whose orientation is within the range that could produce earthquakes.

1 Introduction

Injection-induced seismicity (IIS) was first observed in Denver in the 1960s (Healy et al., 1968) and has become much more prevalent in the Central USA in the past decade (Ellsworth, 2013; Weingarten et al., 2015). In the USA, IIS can occur when wastewater, which is co-produced with oil and gas (O&G), is injected into disposal wells near basement rock. Since much of the crust is critically-stressed (Townend & Zoback, 2000), even slight perturbations in the pore pressure or stress state can lead to seismicity. Despite this fact, only a small fraction of wastewater disposal wells are spatio-temporally associated with IIS (Ellsworth, 2013; Nicholson & Wesson, 1992; Weingarten et al., 2015). The likelihood of IIS depends on the type of rock that underlies the disposal well, which is hypothesized to reflect the influence of fractures and faults that channel and focus fluid pressure in some rock types and not in others (Shah & Keller, 2017).

IIS is thought to occur when pore pressure diffuses down from the injection formation to underlying basement faults, thereby destabilizing them according to the Mohr-Coulomb (MC) shear failure criteria. The MC criteria depends on the in-situ stress state, the pore pressure, and the orientation and mechanical parameters of the fracture or fault (National Research Council, 2013). Most IIS occurs at depths $\geq$2 km below the top of the basement (BTB), which could be because the stress state and/or rheology of rock at that depth is more favorable for hosting earthquakes than shallower rock (Vilarrasa & Carrera, 2015). A hydraulic pathway composed of fractures and faults is required to bring elevated pressure to these seismogenic depths. The ability of these fractures and faults to act as a hydraulic pathway depends not only on their network topology, but also on the deformation of individual fractures and faults; increased pore pressure and shear failure (i.e. earthquakes) can dilate fractures and increase their permeability.

Much of the three-dimensional, reservoir- to basin-scale modeling efforts to understand IIS have relied on an equivalent porous media approach (EPM) to assign permeability and a triggering pressure (TP) approach for earthquake initiation. The EPM approach averages out the hydraulic effect of fractures, faults, and intact rock over large regions of the computational domain. The TP approach employs a single value of pressure increment, $\Delta P = TP$, to be associated with earthquake initiation. There are several important limitations to the EPM-TP approach. Firstly, the EPM-TP models have generally been used in an a posteriori sense, with the hydraulic diffusivity being calibrated to produce pressure at seismogenic depths. We suggest below that many of these studies employed unrealistically-large hydraulic diffusivity values, which calls their conclusions into question (see Sec. 2). Secondly, the EPM-TP models cannot explain why only localized regions of the basement exhibit IIS, even though they predict widespread continuous regions of elevated pressure in the basement. Thirdly, the EPM-TP approach cannot be used to forecast IIS because both the TP and the hydraulic diffusivity depend on properties of the fracture network, fault orientations, and geomechanics that the EPM-TP approach does not include.

In this paper we introduce a discrete fracture network and matrix (DFNM) model designed to understand how pore pressure diffuses through both matrix and fractures to seismogenic depths ($\geq$ 2 km BTB) in the context of IIS. It incorporates partial hydro-mechanical coupling, which allows alteration of hydraulic properties by normal and shear deformation of fractures, and calculation of MC failure. Although it is possible for shear failure to be aseismic in some cases (National Research Council, 2013), we assume that MC failure is an indicator of seismicity in this work. With its parallelization and simplifying mechanical assumptions, our model can simulate thousands of fractures and faults over large 3D domains, which is a step forward in the state of the art for modeling IIS at the reservoir to basin scale. It allows us to investigate some key research questions such as:

1. How exactly does fluid pressure diffuse through >2 km of fractured, low-permeability basement rock, and what is the effective hydraulic diffusivity of the *combined* fracture/matrix system?
2. How important are the deformation-induced changes on hydraulic diffusivity to the propagation of pressure?
3. Why are only a small percentage of disposal wells associated with IIS (Ellsworth, 2013; Nicholson & Wesson, 1992; Weingarten et al., 2015)? We would expect that the majority of disposal wells would be associated with IIS, since the entire crust is critically stressed (Townend & Zoback, 2000) and EPM-TP models show that pore pressure from deep disposal wells regularly diffuses to large regions of the basement (e.g. Keranen et al. (2014); Brown et al. (2017)).

Sec. 2 gives more background about wastewater disposal sites, previous approaches to modeling IIS, and the hydraulic diffusivity of fractured basement rock. Sec. 3 describes our DFNM-MC approach. Sec. 4 describes our conceptual and numerical model of an IIS site that is inspired by Greeley, Colorado. Sec. 5.1 shows results that highlight the differences between the EPM-TP approach and the DFNM-MC approach, and Sec. 5.2 explores the importance of fracture intensity, fault orientation, and deformation-enhanced hydraulic diffusivity in a sensitivity analysis. Sec. 6 provides a discussion of our approach in context of other IIS modeling efforts, and the major conclusions.

2 Background

2.1 Description of Wastewater Disposal Sites

Information about disposal wells, geology of the target formation, and statistical observations of IIS are relatively abundant. US EPA Class II injection wells are permitted to inject waste fluids from O&G operations, and their regulations are focused on protecting underground sources of drinking water (i.e. relatively shallow, non-saline aquifers) (Zhang et al., 2013; Ellsworth, 2013). This means that wastewater disposal must take place in deep saline aquifers, which are usually thick, permeable, porous sedimentary rock, near basement rock. There are over 44,000 wastewater disposal wells in the U.S. (U.S. EPA, 2018), but only a small fraction of them are associated spatio-temporally with IIS (Ellsworth, 2013; Nicholson & Wesson, 1992; Weingarten et al., 2015). High-rate injection wells are more likely to be associated with IIS than low-rate injection wells (Weingarten et al., 2015), but there is also evidence that cumulative injection across many wells can cause IIS (Brown et al., 2017; Peterie et al., 2018; Langenbruch & Zoback, 2016). If the target formation sits atop a thick sedimentary unit or an extrusive rock, then IIS is less likely than if it sits atop fractured intrusive basement rock, which is hypothesized to be because flow is confined to fractures in intrusive rock, causing larger pressures (Shah & Keller, 2017). The importance of fractures in propagating pressure to seismogenic depths is a key feature that we explore in this paper.

Information about the crystalline basement rock, which hosts the majority of IIS hypocenters, is more difficult to find. Across Oklahoma, Colorado, and much of the Midwest, wastewater disposal often takes place in close proximity to crystalline basement rock (Shah & Keller, 2017; W. L. Yeck et al., 2016; Peterie et al., 2018; Zhang et al., 2013). Intact basement rock has very low in-situ hydraulic diffusivity, so fractures and faults are thought to act as the primary hydraulic pathways through the basement. The locations of large faults are sometimes already known from public maps and observations of previous seismicity, or can be mapped with gravity- and magnetic-based geophysical techniques (Shah & Keller, 2017), but the location of smaller basement faults and fractures are typically unknown or are proprietary data. Furthermore, many parameters that are relevant to understanding IIS (e.g. fracture orientation, mechanical properties, and hydrologic properties) are unknown for these fractures and faults. Nevertheless, it is possible to collect statistics of fracture properties, orientation, and density, which can be useful in modeling pressure diffusion (e.g. SKB (2011); Hyman et al. (2015)). Across Colorado, Oklahoma, New Mexico, and southern Kansas, most of the IIS is observed at least 2 km BTB and can be seen all the way to 8 km BTB (Nakai et al., 2017; W. L. Yeck et al., 2016; Schoenball & Ellsworth, 2017).

IIS occurs in the basement because it has a more favorable stress state and rheology to host seismicity than the shallower sedimentary rock. Most of the earth's crust is critically-stressed (Townend & Zoback, 2000), but the shallow, sedimentary rock tends not to be (Vilarrasa & Carrera, 2015). In fact, evidence from numerical modeling and frequency-depth distributions of natural earthquakes suggest that the crust may be most critically stressed at 5-6 km depth, which corresponds to ≥ 2 km BTB in many areas, depending on the thickness of sedimentary cover (Vilarrasa & Carrera, 2015). Furthermore, crystalline basement rock tends to deform in a brittle fashion, which encourages earthquakes, whereas sedimentary rock is softer and deforms in a more ductile fashion, reducing the potential for earthquakes (Vilarrasa & Carrera, 2015). Finally, earthquakes tend to have larger magnitudes with greater depth, and there are concerns that density-driven flow due to brine injection will continue to diffuse pressure downward even as injection rates slow or stop (Pollyea et al., 2019), which further underscores the importance of understanding how pressure diffuses thorough basement rock to seismogenic depths.

While some studies have investigated how poroelastic stress changes or Coulomb static stress transfer can lead to induced seismicity (Goebel et al., 2017; Brown & Ge, 2018), the most prominent conceptual model of IIS posits that fluid pressure diffuses down into the basement faults, thereby destabilizing the faults and causing MC failure (Brown et al., 2017; National Research Council, 2013; Keranen et al., 2014; Langenbruch et al., 2018; Zhang et al., 2013; Nakai et al., 2017; Healy et al., 1968). There are at least two reasons why this pressure-diffusion conceptual model is popular. Firstly, increased pore pressure always destabilizes a fault, whereas poroelastic stress changes and Coulomb static stress transfer could act to destabilize *or* stabilize a fault, depending on the fault orientation and location. Secondly, poroelastic stress changes propagate very rapidly (at the speed of sound in rock), and therefore are inconsistent with the observation that there is usually a time lag between the beginning of injection and the onset of seismicity, suggesting a pore pressure diffusion process (Shapiro & Dinske, 2009). Since we are focused on the diffusion of pore pressure through kilometers of fractured, low-permeability, crystalline rock, we need to understand the hydraulic diffusivity of the combined fracture/matrix system, which is discussed in the next section.

2.2 Hydraulic Di usivity

Hydraulic diffusivity is a rock property that describes how pore pressure diffuses through porous media. Based on the classical groundwater flow equation in porous media, which forms the basis for EPM models, the hydraulic diffusivity is defined as

$$c = \frac{K}{S_s} = \frac{k}{\mu(\phi\beta_w + \beta_m)} \tag{1}$$

where $K = k\rho g/\mu$ is the hydraulic conductivity, $S_s = \rho g(\phi\beta_w + \beta_m)$ is the specific storage, k is the permeability, ρ is the fluid density, g is gravity, μ is the dynamic viscosity of the fluid, ϕ is the porosity, β_w is the fluid compressibility, and β_m is the porous medium compressibility.

There are some subtleties in understanding and measuring hydraulic diffusivity in basement rock because it is composed of fractures and intact crystalline rock matrix. The permeability is dominated by fractures and faults, while the intact crystalline rock has very-low permeability. Faults can be either transmissive, sealing, or a combination thereof, and in this study we consider them as transmissive features. Furthermore, the hydraulic diffusivity of fractures is also a function of geomechanical deformation. Fractures that are held open, for example by high pore pressures, are more permeable and store more fluid than closed fractures. The permeability of the combined fracture/matrix rock decreases with depth (Manning & Ingebritsen, 1999), and one of the contributing factors could be the increased lithostatic stress that forces fractures closed. Shear dilation after MC failure can also alter the permeability and fluid storage within a fracture.

Hydraulic diffusivity depends on the scale over which it is measured (Townend & Zoback, 2000). At the core scale, permeability of crystalline rock can vary from 10^{-24}–10^{-17} m^2, and it decreases with depth and confining pressure (Freeze & Cherry, 1979; Morrow & Lockner, 1997). The compressibility of unfractured granite is $\sim 10^{-11}$ Pa^{-1} (De Marsily, 1986), and porosity is $\leq$0.05 (Freeze & Cherry, 1979). Using these parameters, the hydraulic diffusivity for an unfractured granite at the core scale is $10^{-10} \leq c_{core} \leq 10^{-4}$ m^2/s. At the reservoir scales over which IIS is observed (1 – 10 km), estimates of c are larger. The bulk compressibility of jointed rock ranges from 10^{-10} – 10^{-8} Pa^{-1} (Freeze & Cherry, 1979). The bulk permeability of fractured basement rock depends on the fracture network, but has been estimated to be $10^{-17} - 10^{-16}$ m^2 (Townend & Zoback, 2000). Using these parameters, the hydraulic diffusivity for bulk, fractured, reservoir-scale rock is expected to range between $10^{-6} \leq c_{bulk} \leq 10^{-3}$ m^2/s.

Hydraulic diffusivity has also been estimated based on space-time patterns of seismic clouds following injection or reservoir impoundment. Talwani et al. (2007) used this approach to infer an apparent "seismogenic diffusivity" in the range $0.1 < c_{sT} < 10.0$ m^2/s. We use the notation c_{sT} to denote seismogenic diffusivity in the sense of Talwani. However, it is unclear whether the seismogenic diffusivity is the same as the hydraulic diffusivity. Shapiro and Dinske (2009) interpret estimates of c following an EPM interpretation, but the EPM hydraulic diffusivity derived from a seismic cloud can be an overestimation of the actual EPM hydraulic diffusivity, when permeable fractures are embedded within a low-permeability matrix (Haagenson et al., 2018a, 2018b). Talwani et al. (2007) interpret c_{sT} as the hydraulic diffusivity associated with induced seismicity, assuming single linear fractures connect the fluid source with the hypocentral location. The hydraulic diffusivity of a parallel-plate fracture using the cubic law for permeability can be approximated as (Murphy et al., 2004):

$$c = \frac{b^2}{12\mu(\beta_w + \beta_f)} \tag{2}$$

where b is the hydraulic aperture, $\beta_f = b^{-1}(db/d\sigma_n^{'})$ is the fracture compressibility, and $\sigma_n^{'}$ is the effective normal stress. However Talwani et al.'s analysis neglect leakoff from fractures and tortuosity of fracture flow paths, both of which lead to slower pressure diffusion. Therefore, we expect that the inferred c_{sT} values are smaller than the true hydraulic diffusivity of the fractures. Table 1 shows the values of basement hydraulic diffusivity at the core and reservoir scale, the seismogenic diffusivity, and the values of hydraulic diffusivity employed by several EPM-TP modeling studies. These values are important to keep in mind when considering conceptual and numerical models of pore pressure diffusion in the context of IIS.

2.3 Previous Approaches to Modeling Pressure Di usion That Causes IIS

In general, models of IIS should couple the equations of pressure diffusion and geomechanics (i.e. employ a hydro-mechanical approach) for a rock mass containing discontinuities in the form of fractures and faults. However, hydro-mechanical equations are challenging to solve on scales of the order of tens of kilometers even assuming the rock mass behaves as a continuum. Proper treatment of discontinuous displacements across fractures and faults makes the problem even more challenging. Although fully coupled hydro-mechanical models have been presented, which qualitatively reproduce the phenomenology of IIS, they have largely been demonstrated either without explicit consideration of fractures and faults (e.g. Shirzaei et al. (2016)) or in limited 2D domains (e.g. Jin and Zoback (2017, 2018)).

Most large-scale modeling studies of IIS are based on the groundwater flow equation, simulate pressure diffusion from an injection well, and assume that seismicity is associated with exceedance of a critical threshold pressure, which we refer to as TP. These EPM-TP models typically neglect the large disparity in permeability between connected fractures and the surrounding low-permeability basement rock, and assume a homogeneous EPM. These models have been employed a-posteriori to demonstrate TP at locations of IIS in several studies (Keranen et al., 2014; Brown et al., 2017; Nakai et al., 2017; Shirzaei et al., 2016). However, most of these studies assume unrealistically-large values of hydraulic diffusivity, in order to achieve rapid pressure diffusion to the location of seismicity (see Table 1). EPM-TP models also are unable to explain why IIS does not occur at all sites where the pressure exceeds TP. In the subsections below, we describe the EPM-TP models and fully-coupled hydro-mechanical models that include flow

Table 1. The crystalline-basement rock hydraulic diffusivity observed experimentally and used in several modeling studies. The first three table entries are experimental- or field-determined values for different length scales and techniques. The next five entries show the hydraulic diffusivity employed in EPM modeling studies, which are larger than c_{bulk}. The next five entries show studies that use an EPM model with a permeable fault. They generally employ smaller c for the intact basement, but in most cases it is still larger than c_{bulk}. The final two entries show the hydraulic diffusivity used in our comparison between a DFNM model and a corresponding EPM model with permeability assigned from a numerical permeameter test on the DFNM (see Sec. 4.4 and 5.1).

Experiment or Study	Basement Rock c (m^2/s)	Fracture or Fault c (m^2/s)
Unfractured granite at core scale (c_{core})	$10^{-10} - 10^{-4}$	N/A
Fractured granite at reservoir scale (c_{bulk})	$10^{-6} - 10^{-3}$	N/A
Seismogenic fractures (c_{sT})	N/A	$10^{-1} - 10^{1}$
Brown et al. (2017)[a]	$10^{-3} - 4 \cdot 10^{0}$	N/A
Keranen et al. (2014)	$10^{-2} - 10^{-1}$	N/A
Langenbruch et al. (2018)[d]	$2 \cdot 10^{-1}$	N/A
Pollyea et al. (2019)[b]	$10^{-3} - 10^{-1}$	N/A
Shirzaei et al. (2016)[a]	$10^{-2} - 10^{-1}$	N/A
Nakai et al. (2017)[a,d]	$10^{-4} - 10^{-2}$	10^{-1}
Hearn et al. (2018)	10^{-7}	$3 \cdot 10^{0} - 3 \cdot 10^{1}$
Zhang et al. (2013)	$2 \cdot 10^{-3}$	10^{1}
Ogwari et al. (2018)[d]	10^{-7}	$10^{-2} - 10^{-1}$
Schoenball et al. (2018)[c]	Not Reported	Not Reported
DFNM model (Sec. 5.1)	10^{-5}	$\sim 5 \cdot 10^{3}$
Scenario EPM1 (Sec. 5.1)	$\sim 2 \cdot 10^{-4}$	N/A

[a]Basement hydraulic diffusivity decreases with depth.
[b]Dual continua model, c calculated from reported volume-weighted k and ϕ.
[c]Compressibility is not reported, so hydraulic diffusivity cannot be calculated.
[d]Hydraulic diffusivity is calculated with assumed fluid properties: $\rho = 1000$ kg/m^3 and $\mu = 0.001$ Pa-s.

in discrete fracture(s) or fault(s). Tables S1 and S2 summarize the physics of the models that are discussed in this section.

2.3.1 EPM-TP and Similar Models

EPM models have generally employed unrealistically large (often by a few orders of magnitude) values of hydraulic diffusivity to propagate pressure to seismogenic locations. For EPM models, c should equal c_{bulk}, but all of the EPM studies (Keranen et al., 2014; Brown et al., 2017; Langenbruch et al., 2018; Shirzaei et al., 2016; Pollyea et al., 2019) have used significantly larger values (see Table 1). For models that include one or two faults (Nakai et al., 2017; Hearn et al., 2018; Zhang et al., 2013; Ogwari et al., 2018; Schoenball et al., 2018), it could be argued that c in the unfaulted part should be assigned to c_{bulk} (if one assumes that the basement away from the fault is highly fractured), or to c_{core} (if one assumes that the unfaulted basement is minimally fractured). But many of these studies employ values of c in the unfaulted basement that are larger than, or at the upper end of the range for c_{bulk} and c_{core}. In many cases, the problem in the employed value of c comes from the assignment of the specific storage ($S_s < 10^{-6}$ m^{-1}) or, equivalently, the compressibility ($\beta_m < 10^{-10}$ Pa-1), both of which ignore the compressibility of basement fractures and inflate the value of c (see Eq. 1) (e.g. Brown et al. (2017); Langenbruch et al. (2018); Nakai et al. (2017); Pollyea et al. (2019)). Not only do the EPM models employ incorrect values of c, some follow logic that leads to questionable conclusions. For example, they calibrate c to encourage pressure increment $> TP$ at locations of observed seismic clouds, and then they conclude that pressure diffusion is a plausible causative mechanism of seismicity (Keranen et al., 2014; Brown et al., 2017)). We show in Sec. 5.1 that an EPM model with realistic values of c would actually show the opposite - that pressure diffusion is not a plausible mechanism of earthquake triggering. Only fracture-based models seem to be able to explain pressure propagation to seismogenic depths, and only in small, localized regions of the basement (Sec. 5).

Another problem with the EPM-TP approach is that it cannot explain why earthquakes *do not* occur at some locations. The EPM approach results in very smooth pressure profiles, which are probably unrealistic given the heterogeneity that fractures and faults introduce, wherein $\Delta P > TP$ in regions of the basement that are much larger than the seismic regions (e.g. Brown et al. (2017) Fig. 4d). There are several reasons why seismicity may not occur in these regions: (a) pressure has not actually diffused there, (b) there are no favorably-oriented faults there, or (c) the stress state is less critical, but the EPM-TP cannot evaluate which may be the case. This is illustrated in Fig. 4D of Keranen et al. (2014), where the average pressure upon failure is 0.07 MPa, but ranges from 0.04 to >0.4 MPa. We show in Sec. 5.2 that very small variations in fault orientation and triggering pressure (as low as 2° and 0.13 MPa, respectively) can drastically reduce the likelihood of an earthquake. Finally, we note that some of the studies cited in this section may incorporate more advanced triggering mechanisms (Zhang et al., 2013; Schoenball et al., 2018), mechanical coupling (Shirzaei et al., 2016), a hybrid physical-statistical model (Langenbruch et al., 2018), or a dual continua approximation (Pollyea et al., 2019) (see Table S1), but they are still EPM-TP models or have similar drawbacks to the EPM-TP models.

2.3.2 Hydro-Mechanical, MC, Fracture and Matrix Models

There is another class of models that includes much more of the relevant physics for understanding IIS. These models solve the fully-coupled hydro-mechanical equations, include fracture(s)/fault(s), calculate Mohr-Coulomb failure, and account for the changes in hydraulic properties due to mechanical deformations (Jin & Zoback, 2018, 2017; Jha & Juanes, 2014; Ucar et al., 2018; Rinaldi et al., 2014; Kelkar et al., 2014; Chang & Segall, 2016). Many of these studies also account for even more advanced earthquake physics such as strain-softening (Rinaldi et al., 2014; Jha & Juanes, 2014), or multiple failure events on a given fracture (Jin & Zoback, 2018). They would be ideal tools to investigate pressure diffusion related to IIS, but they are computationally expensive and therefore limited to small spatial scales, limited number of fractures/faults, and/or 2D domains. Furthermore, these models have not been used to investigate how pressure propagates from a disposal well into the deep basement (> 2 km BTB), either because they focus on geothermal energy (Ucar et al., 2018; Kelkar et al., 2014) and carbon sequestration (Rinaldi et al., 2014; Jha & Juanes, 2014), or because the simulation is focused on pressure diffusion near the wellbore, rather than to seismogenic depths (Jin & Zoback, 2018, 2017; Chang & Segall, 2016). There are other studies that do not fall neatly into the EPM/TP category of Sec. 2.3.1 or the hydro-mechanical, MC, fracture models of this section. Some models use a rate-and-state seismicity model, as an alternative to the MC criteria, and couple to pressure diffusion models to predict the rise and fall of seismicity rates (Dempsey & Riffault, 2019; Riffault et al., 2018; Norbeck & Rubinstein, 2018). Others perform a partial hydro-mechanical coupling and calculate MC failure on seed points that represent potential earthquake hypocenters (Rinaldi & Nespoli, 2017).

3 DFNM-MC Modeling Approach

Our goal is to present a modeling approach that improves significantly upon the EPM-TP approach, while facilitating computational tractability for 3D simulations on scales of the order of tens of km with thousands of fractures and faults. We follow the approach of previous hydro-mechanical, MC, fracture-matrix models (see Sec. 2.3.2), but we introduce some simplifying assumptions to decrease computational cost. The salient features of our approach are:

1. Discrete fractures and faults are explicitly represented, and their properties are assigned in a physically consistent manner. Fracture orientations are variable. Fluid flow in both the fracture and rock matrix are represented.
2. The rock matrix properties are consistently within accepted ranges for properties of basement rock.
3. The model allows rapid pressure diffusion along connected fractures without resorting to unrealistically low values for medium compressibility.
4. A partially coupled approach, wherein the fracture hydraulic diffusivity is allowed to evolve as a function of effective normal stress on a fracture plane, and in response to slip events. The approach is only partially coupled because the initial stress state is specified and is assumed to be time-invariant. However, the time variation of effective stress due to pressure diffusion is captured in this approach.
5. Although rapid pressure diffusion through a connected network of fractures occurs, seismic events occur only when the MC failure criterion is satisfied along a fracture or a fault. Thus, failure events only occur along favorably oriented fractures/faults. The model can thus provide an explanation for why IIS occurs only at a small fraction of deep wastewater injection sites.

We call this the discrete fracture network and matrix with Mohr Coulomb failure (DFNM-MC) approach – it allows for flow in a discrete fracture network (DFN) and the surrounding rock matrix. The pressure at which MC failure occurs on a fracture of fault depends on its orientation and the local stress state. The most favorable orientation corresponding to the minimum pressure is determined by the initial stress state.

Within this DFNM-MC framework, there is no distinction between a fracture and a fault other than the size of the feature. This DFNM-MC approach has been validated against analytical and numerical solutions in previous work (Birdsell, Rajaram, & Karra, 2018; Birdsell, 2018). In Sec. 3.1 we discuss and justify the partially-coupled hydro-mechanical approach, which allows us to simulate important mechanical processes without resorting to the higher complexity and computational cost of a fully-coupled hydro-mechanical approach. In Sec. 3.2, we describe the equations of flow in porous media and in fractures/faults and we show how the constitutive relationships for porosity and permeability can be altered in fractured grid cells so that the simulator can consistently solve for both fracture and matrix flow in a single domain. In Sec. 3.3, we describe how the hydraulic diffusivity is treated as a function of normal and shear deformation.

3.1 Framework of Partially-Coupled Hydro-Mechanical Approach

Our numerical model is focused primarily on pore pressure diffusion, but it is partially coupled to geomechanics to capture some of the physics that are relevant to IIS. The aspects of IIS that require geomechanical coupling include: (a) evaluation of the MC failure criteria, and (b) the influence of mechanical deformations on the hydraulic diffusivity of fractures. We assume that the in-situ stress state is a function of space but is frozen in time. This may seem like an oversimplification, but it captures many of the physical complexities that the EPM-TP approach does not. For example, fractures that are subject to a large compressive normal stress are forced closed and therefore less permeable; such behavior is readily captured within the framework of the partially coupled approach. Furthermore, MC failure criteria depends on fracture orientation, which is also explicitly represented in a DFNM framework. This partially-coupled approach dramatically reduces computational expense in comparison to fully coupled approaches, while still honoring fundamental aspects of geomechanics as they relate to IIS.

The normal stress on a fracture/fault is calculated as $\sigma_n(\boldsymbol{x}) = (\boldsymbol{\sigma}(\boldsymbol{x})\boldsymbol{n})\cdot\boldsymbol{n}$ where $\boldsymbol{\sigma}(\boldsymbol{x})$ is the second-order stress tensor as a function of the position vector, $\boldsymbol{x}$, describing the location in the domain, and $\boldsymbol{n}$ is the unit vector normal to the fracture plane. The magnitude of the shear stress is calculated as $|\boldsymbol{\tau}| = |(\boldsymbol{\sigma}(\boldsymbol{x})\boldsymbol{n}) \times \boldsymbol{n}|$. The code is capable of resolving the entire stress tensor $\boldsymbol{\sigma}$, but we assume that the principal components of stress are vertical and horizontal in all of the simulations presented in this paper, which is representative for much of the subsurface (Zoback, 2010), and we use the principal coordinate system so that there are no shear stresses in the stress tensor. The vertical stress, the maximum principal horizontal stress, and the minimum principal horizontal stress are denoted by σ_v, $\sigma_{H,max}$, and $\sigma_{h,min}$, respectively. We assume that the horizontal stresses take the following form: $\sigma_{H,max} = \alpha_1\sigma_v$, and $\sigma_{h,min} = \alpha_2\sigma_v$ where α_1 and α_2 are constants such that $\alpha_1 \geq \alpha_2$. With this definition of stress, the effective normal stress is a function of space and time $\sigma_n'(\boldsymbol{x}, t) = \sigma_n(\boldsymbol{x}) + P(\boldsymbol{x}, t)$, where the normal stress is a function of space and fracture orientation but is frozen in time, and pressure $P(x, t)$ varies with both space and time. Using this sign convention, the effective stress is negative (i.e. compressive), and effective normal stress increases towards a value of zero as the pore pressure increases towards a value of $-\sigma_n$. This formulation falls short of fully-coupled hydro-mechanics, but is still useful in tracking when the MC criteria is satisfied and the evolution of hydraulic diffusivity as a function of stress and pressure.

3.2 Flow in Porous Matrix and Fractures

Single-phase flow through the porous matrix is governed by the groundwater flow equation, which can be written as:

$$\frac{\partial(\rho\phi)}{\partial t} - \nabla\cdot\left(\frac{\rho k}{\mu}\nabla(P + \rho g z)\right) = Q_m \tag{3}$$

where P, z, and Q_m represent fluid pressure, the elevation, and fluid sources/sinks in the matrix, respectively.

Flow through a parallel-plate fracture can be described using the local cubic law for transmissivity (Zimmerman & Bodvarsson, 1996; Murphy et al., 2004; Chaudhuri et al., 2013):

$$\frac{\partial(\rho b)}{\partial t} - \nabla \cdot \left(\frac{\rho b^3}{12 f \mu} \nabla(P + \rho g z) \right) = Q_f - L_{m-f} \tag{4}$$

where f is a coefficient that is generally greater than or equal to unity that accounts for fracture roughness (Witherspoon et al., 1980), Q_f is a source/sink term normalized by fracture height, and L_{m-f} is the leakoff mass flux per unit area from the fracture to the matrix. Eq. 4 is a 2D representation of the conservation of mass per unit fracture width, perpendicular to the direction of flow and the aperture. In an approach where the fracture and matrix are treated as separate domains, the pressure from the fracture domain would be treated as a boundary condition to the matrix domain, and the pressures within the matrix domain would be used to calculate the leakoff flux as a function of the local pressure difference across the fracture-matrix interface. The leakoff flux would need to be represented as a sink term in the fracture domain.

PFLOTRAN is a massively-parallel, control-volume, subsurface flow and transport code that solves Eq. 3. We take advantage of PFLOTRAN's (Lichtner et al., 2019a; Hammond et al., 2014; Lichtner et al., 2019b) parallel features and robust computational algorithms to simulate large domains with large property contrasts, which requires that we treat the fractures and matrix as a single domain rather than two. With such an approach, a single computational grid is employed encompassing fracture and matrix blocks. The conditions at fracture-matrix interfaces are automatically accounted for consistently in a finite volume approach that represents fluxes across adjacent nodes based on local pressure gradients. Leakoff fluxes are thus naturally calculated based on the local pressure gradients across interfaces between fracture and matrix blocks, and do not need to be represented explicitly as a sink term. To correctly capture the physics of fracture flow within the formulation employed by PFLOTRAN, the following fracture relationships can be introduced for porosity and permeability (Birdsell et al., 2015; Chaudhuri et al., 2013; Pandey et al., 2017; Bower & Zyvoloski, 1997):

$$\phi = \frac{b}{b_p} \phi_\tau \tag{5}$$

$$k = \frac{b^3}{12 b_p f} k_\tau \tag{6}$$

where b_p is the grid block dimension in the direction normal to the fracture, ϕ_τ and k_τ are porosity and permeability multipliers that are equal to 1 prior to shear failure and experience a step change when MC shear failure occurs along a fracture or fault. Eq. 5 assumes that the change in fluid storage within the grid block is primarily due to fracture deformation. Eq. 6 assumes that the grid block permeability is dominated by fractures. These assumptions are valid for flow in basement fractures because they are much more permeable and compressible than the intact crystalline rock (especially for low-compressibility rock and with small values of b_p). When Eq. 5 and 6 are brought into Eq. 3, and a single-domain computational approach is employed, the modified flow equation for fractures is:

$$\frac{1}{b_p}\frac{\partial(\rho b)}{\partial t} - \nabla \cdot \left(\frac{\rho b^3}{12 b_p f \mu} \nabla(P + \rho g z) \right) = Q_m \tag{7}$$

which is identical to Eq. 4 divided by the grid block dimension (b_p) and adjusted to a 3D feature so that Q_m is used instead of Q_f and L_{m-f} is not explicitly included because leakoff is naturally calculated in the single domain approach. This approach has been employed in several previous works (Birdsell et al., 2015; Chaudhuri et al., 2013; Pandey et al., 2017).

We solve the equations of flow in the matrix (Eq. 3) and fractures (Eq. 7) using PFLOTRAN by utilizing the traditional definitions of porosity and permeability in the matrix grid blocks and Eq. 5 and 6 in the fracture grid blocks. This approach correctly captures the physics of flow within fractures, leakoff to matrix, and flow within the matrix. The fluid properties (i.e. ρ and μ) and the porosity in the storage term are functions of pressure and are updated iteratively within a Newton-Krylov iteration employed by PFLOTRAN in each time step. The porosity in the fracture block is defined in Eq. 5, while the porosity in the matrix is defined as $\phi = \beta_m(P - P_o) + \phi_o$ where β_m is the matrix compressibility, ϕ_o is the porosity at the reference pressure P_o (Birdsell, Karra, & Rajaram, 2018). Note that fracture deformation, i.e. variation in b as a function of effective stress, is described in Sec. 3.3. For implementation reasons, the permeability term shown in Eq. 6 is lagged by one time step in the fracture grid blocks, and it is important to take small enough time-steps that this lagging does not affect the results. To ensure that the time step size employed in Sec. 5 is appropriate, we carried out convergence studies showing that results were unchanged with smaller time steps. The DFNM approach consistently represents the physics of fracture and matrix flow, including leakoff, while taking advantage of an existing, efficient subsurface flow code. Additionally, it allows the hydraulic diffusivity to be updated as mechanical deformations alter b, as discussed in the next section.

3.3 Hydraulic Di usivity as a Function of Fracture Deformation

The hydraulic diffusivity of fractured rock changes as fractures experience mechanical deformations (Sec. 2.2). There are at least two ways that hydraulic diffusivity can be altered in the context of IIS. The first is via normal deformation on fractures/faults, which alters b and therefore ϕ and k (Eq. 5 and 6). The second is via shear deformation, which can have a range of effects on porosity and permeability, which are modeled by ϕ_τ and k_τ in Eq. 5 and 6. This section presents the relationships used to model the influence of normal and shear deformation on the hydraulic diffusivity of fractures within the DFNM-MC approach.

3.3.1 The Influence of Normal Deformation on Hydraulic Diffusivity

We use the Bandis et al. (1983) constitutive relationship to relate the fracture aperture to the effective normal stress:

$$b = b_{max} + \frac{A\sigma_n^{'}}{1 - B\sigma_n^{'}} \tag{8}$$

where b_{max} is the aperture when $\sigma_n^{'} = 0$ and A and B are parameters. $\sigma_n^{'}$ is negative at the depths of IIS because the magnitude of compressive normal stress is larger than the magnitude of pore pressure (see Sec. 3.1). A is the inverse of the initial fracture stiffness, K_{ni}, at $\sigma_n^{'} = 0$ (i.e. $1/A = K_{ni} = \partial\sigma_n^{'}/\partial b$). $A/B = b_{max} - b_{min}$ where b_{min} is the fracture aperture as $\sigma_n^{'} \to -\infty$. As originally measured in the lab, the Bandis model applies to the mechanical fracture aperture, but it has also been used to describe hydraulic aperture (Murphy et al., 2004; Pandey et al., 2017). In our partially-coupled hydro-mechanical model, the stress is a function of space and the pore pressure is a function of space and time. Therefore the Bandis relationship implies an initial aperture field based on the stress state, the initial pressure, and the fracture orientation. Subsequently, the aperture field can evolve with time as the pore pressure changes throughout the simulation, and fractures are pressurized.

3.3.2 The Influence of Shear Deformation on Hydraulic Diffusivity

In addition to deforming in the normal direction, fractures and faults can fail in shear. One model that describes when shear failure will occur is the MC failure criterion:

$$c_0 - \mu_f\sigma_n^{'} - |\boldsymbol{\tau}| \leq 0 \tag{9}$$

where c_0 is the fault cohesion and μ_f is the coefficient of friction. Fracture and fault ermeability can be enhanced by up to two orders of magnitude due to shear failure (Evans et al., 2005; Rutqvist et al., 2007; Kelkar et al., 2014). Studies of asperity-scale shear processes suggest that the permeability enhancement within the fracture may be anisotropic (Mallikamas & Rajaram, 2005; Lang et al., 2018), but we follow previous reservoir-scale work in assuming that the permeability enhancement within the fracture is isotropic (Kelkar et al., 2014). Even though porosity may change due to shear failure, it is likely to be much smaller than the change in permeability because the increase in permeability after shearing is at least partially due to changes in the aperture correlation structure, which has a smaller influence on porosity (Mallikamas & Rajaram, 2005). In our model, we assume that permeability increases as a step change after Mohr-Coulomb failure, without a change in porosity (i.e. $k_\tau \geq 1.0$ and $\phi_\tau = 1.0$ after Mohr-Coulomb failure in Eq. 5 and 6). These assumptions have also been made by previous modeling studies (Rutqvist et al., 2007; Kelkar et al., 2011).

4 Conceptual and Numerical Model

In this section, we describe the conceptual and numerical model, the fracture generation algorithm, the initial and boundary conditions, and the simulation scenarios that are presented in the results section (Sec. 5). We chose our conceptual and numerical model based on an approximate representation of the IIS site near Greeley, CO. There are two reasons for doing this: (a) because it allows us to compare a DFNM-MC model to a previous EPM-TP study at a well-characterized site, and (b) because the Greeley site has many similarities with other IIS sites in the U.S., and therefore the results will be representative of many areas of IIS.

4.1 Greeley, Colorado IIS

Our conceptual and numerical model is shown in Fig. 1. While there are many disposal wells near the Greeley swarm, the NGL-C4A well has received the most attention due to its large injection volumes and its spatio-temporal correlation with the seismicity (Brown et al., 2017; W. L. Yeck et al., 2016). It is drilled into a 500-m thick group of formations that are primarily permeable sandstone with lesser amounts of carbonate and shale, which are overlain by a mudstone confining layer and underlain by critically-stressed crystalline basement. The NGL-C4A well started injecting approximately one year prior to the M_w 3.2 earthquake in June 2014 at an average rate of $\sim 5{\cdot}10^5$ m^3/yr. After the earthquake, injection was briefly halted and remedial cement was added in the hope that it would hydraulically isolate the well from the basement. Seismicity was monitored as the injection rate was increased to near the pre-earthquake value. Nevertheless, another felt sequence occurred in August 2016, approximately 3 years after injection originally began.

Some parameters at the Greeley site are well known. For example, the injection formation permeability has been measured at the core scale and the field scale (Brown et al., 2017). General estimates of the matrix compressibility (β_m) and porosity (ϕ), which affect the hydraulic diffusivity by contributing to the storage term, are available for sandstone, mudstone, and fractured crystalline rock (Freeze & Cherry, 1979). The injection formation is fractured toward the bottom. These fractures could hydraulically connect the injection formation to the basement, which is also fractured (W. Yeck et al., 2016). The most uncertain parameter in this hydrologic system is the permeability of the basement fracture/matrix system. The uncertainty in basement permeability is due to uncertainty in the number, size, connectivity, and hydraulic properties of basement fractures and faults, which dominate the permeability. Due to the uncertainties in fracture properties, fractures are randomly generated (see Sec. 4.2). There is also uncertainty in the permeability of the unfractured basement rock, and we assume a value at the upper-

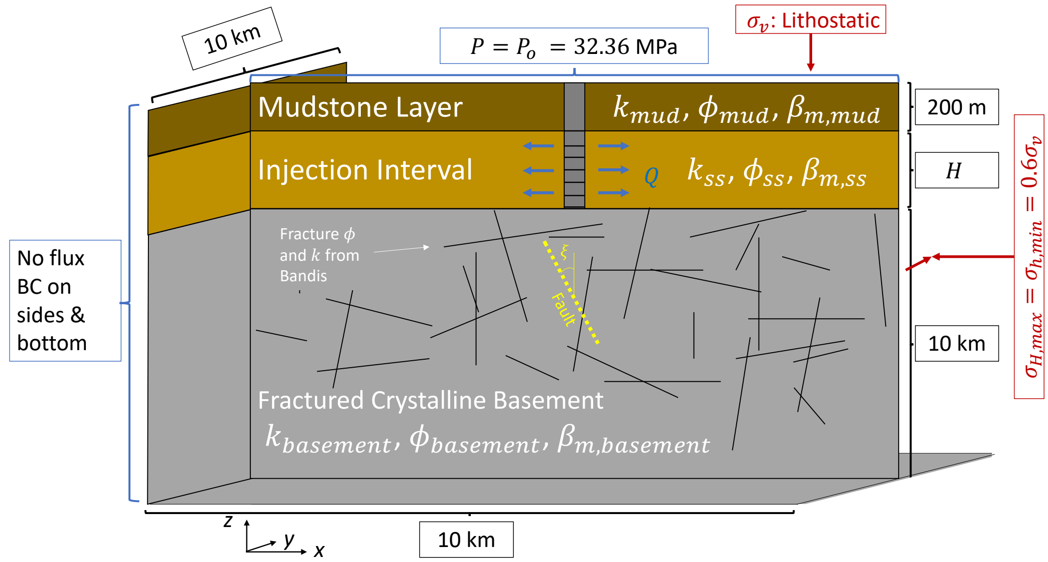

Figure 1. Conceptual model and boundary conditions. The domain size is 10 km in the x and y directions and $(10.2 + H)$ km in the z direction. H is the aquifer height and equals 0.5 km for the simulations in Sec. 5.1 and 0.4 m in Sec. 5.2. Hydrologic boundary conditions and the well source term are illustrated in blue. Injection takes place at $x = y = 5.0$ km, $10.0 \leq z \leq 10.0 + H$ km. The stress state is illustrated in red. Rock properties are indicated on the figure with subscripts "mud", "ss", and "basement" for the mudstone confining layer, the sandstone injection interval, and the in-tact basement rock, respectively. Fractures are indicated schematically with black lines. Fractures (and the fault in Sec. 5.2) are assigned porosity, permeability, and aperture based on Eq. 5, 6, and 8, respectively. The yellow dashed line illustrates a deterministically-located fault that is used in the sensitivity analysis in Sec. 5.2. ξ is the angle between the maximum principal stress (i.e. the vertical stress σ_v) and the fault, which is selected so that the fault is optimally- or suboptimally-oriented. Figure is modified from Birdsell, Rajaram, and Karra (2018).

end of unfractured metamorphic and igneous rocks (Freeze & Cherry, 1979). The parameters used in the DFNM-MC simulations in Sec. 5 are reported in Table 2.

4.2 Fracture Generation Algorithm

Given the uncertainties in fracture locations and properties, fractures are generated from statistical distributions. The distance between subsequently-generated fracture centers is taken from a power law distribution, and the direction between subsequently-generated fracture centers is randomly chosen. If the entire fracture falls outside of the domain, a new fracture location is randomly chosen within the basement. We generate fracture orientations from three equally-probable fracture families that point north-south, east-west, and horizontally. Within each family, there is also variation in the orientation according to a von Mises-Fisher distribution (Wood, 1994). Fractures are idealized as circles of radius r which are generated from a truncated power law distribution (Hyman et al., 2015)

$$r = r_o \left[1 - u + u\left(\frac{r_o}{r_u}\right)^{\alpha_r}\right] \tag{10}$$

Table 2. Simulation parameters for the DFNM-MC simulations presented in Sec. 5.1. Note that the fracture permeability and porosity are not directly reported in this table, but can be calculated from the effective stress, the parameters in this table, and Eq. 5 and 6. The parameters in scenarios EPM1, EPM2, and EPM3 in Sec. 5.1 are the same as in this table except for $k_{basement}$ and $\beta_{m,basement}$, which were adjusted to account for the equivalent permeability and compressibility (see Table 3). Most of the parameters remain the same in the sensitivity analysis (Sec. 5.2), except: (a) the grid dimension, b_p, is increased to 200 m and the aquifer thickness, H, is reduced to 400 m to decrease computational cost; (b) the simulation duration, t, is increased to 10 yr to investigate longer-term disposal; and (c) the number of fractures is varied in the sensitivity analysis.

Variable	Description	Value	Unit
H	Aquifer thickness[a]	500	m
b_p	Grid block size[a]	100	m
k_{mud}	Permeability of confining layer	10^{-17}	m^2
k_{ss}	Permeability of injection interval	$4 \cdot 10^{-14}$	m^2
$k_{basement}$	Permeability of basement matrix	10^{-17}	m^2
ϕ_{mud}	Porosity of confining layer	0.2	
ϕ_{ss}	Porosity of injection interval	0.25	
$\phi_{basement}$	Porosity of basement matrix	0.05	
$\beta_{m,mud}$	Confining layer compressibility	10^{-8}	Pa^{-1}
$\beta_{m,ss}$	Injection interval compressibility	10^{-8}	Pa^{-1}
β_f	Fluid compressibility	$4.4 \cdot 10^{-10}$	Pa^{-1}
μ	Fluid viscosity	$8.9 \cdot 10^{-4}$	Pa-s
P_o	Reference pressure (Eq. 12-14; Fig. 1)	32.36	MPa
$\rho_{f,o}$	Reference density (Eq. 12-14)	1100	kg/m^3
d_o	Reference depth (Eq. 12-14)	3000	m
$\sigma_{v,o}$	Vertical stress at top of domain	-73.55	MPa
$\rho_{s,o}$	Rock density at top of domain	2500	kg/m^3
β_s	Compressibility of solid rock grains	$1.8 \cdot 10^{-10}$	Pa^{-1}
Q	Injection rate	$5 \cdot 10^8$	kg/yr
-	Injection location	$x = y = 5.0,\ 10.0 \leq z \leq 10.5$	km
t	Injection and simulation duration[b]	3	yr
n_{frac}	Number of fractures[c]	2000	
f	Fracture coefficient (Eq. 6)	1	
r_o	Minimum fracture radius (Eq. 10)	300	m
r_u	Maximum fracture radius (Eq. 10)	1000	m
α_r	Power law exponent (Eq. 10)	2.5	
A	Bandis parameter (Eq. 8)	10^{-11}	m/Pa
b_{min}	Minimum fracture aperture	$2 \cdot 10^{-4}$	m
$\Delta b_{max,range}$	Range of maximum aperture (Eq. 11)	$2 \cdot 10^{-4}$	m
$b_{max,o}$	Reference maximum aperture (Eq. 11)	$3 \cdot 10^{-4}$	m
α_1	Multiplier for $\sigma_{H,max}$ (Sec. 3.1)	0.6	
α_2	Multiplier for $\sigma_{h,min}$ (Sec. 3.1)	0.6	
c_0	Fault cohesion (Eq. 9)	0.0	Pa
μ_f	Coefficient of friction (Eq. 9)	0.67	

[a]Altered in Sec. 5.2 to reduce computational cost.
[b]Altered in Sec. 5.2 to investigate longer injection.
[c] $n_{frac} = 1000$ for base case in Sec. 5.2.

where r_o is the minimum radius, r_u is the maximum radius, α_r is the power-law exponent, and u is a uniform random variable between 0 and 1. The maximum fracture aperture, b_{max} in Eq. 8, is correlated to the fracture radius according to Eq. 11

$$b_{max} = b_{max,o} + \frac{r - r_o}{r_u - r_o} \Delta b_{max,range} \tag{11}$$

where $b_{max,o}$ is the maximum aperture for a fracture of length r_o and $\Delta b_{max,range}$ is the range over which b_{max} can vary. We assume fixed values for A and b_{min}, calculate b_{max} for each fracture with Eq. 11, and set $B = A/(b_{max} - b_{min})$.

To work with the DFNM-MC approach, fractures and their properties are mapped to the continuum grid. To capture the permeability anisotropy of fractures, so that flow goes more readily along fractures than perpendicular to them, it is important that $r_o > b_p$ and that the fracture permeability is much, much larger than the matrix permeability. (Both of these criteria are satisfied for the simulations presented in this paper.) Under these assumptions, we can assign an isotropic permeability value to the fractured grid blocks and trust that the fracture/matrix system heterogeneity will generate anisotropic behavior. We acknowledge that approaches using lower-dimensional fracture elements reproduce the fracture permeability anisotropy better than our approach (e.g. Jin and Zoback (2017, 2018); Ucar et al. (2018); Jha and Juanes (2014)), but note that our approach still allows for leakoff into the surrounding matrix, and is a relatively good approximation of the permeability tensor of a fracture/matrix system (see Supplementary Text S1 and Fig. S1). At grid cells where multiple fractures intersect, the properties of the fracture that is most favorably-oriented for MC failure are used. This ensures that the model will experience seismicity at the value of ΔP that corresponds to the smallest ΔP_c of the fractures within the grid block.

4.3 Initial and Boundary Conditions Corresponding to a Critically-Stressed Basement

In this study, we interpret a critically-stressed rock to be one in which the critical pressure increment required for MC failure *on an optimally-oriented fracture* is less than or equal to 0.1 MPa, while the majority of fractures will require a larger pressure increase to experience MC failure. Therefore we refer to the "minimum critical pressure" ($\Delta P_{c,min}$) as the pressure increase that is required to cause an earthquake on an optimally-oriented fracture. In reality, the initial conditions of stress and pressure: (1) increase with depth so that $\Delta P_{c,min}$ may be a function of depth, and (2) vary horizontally at a given depth so that $\Delta P_{c,min}$ may also vary horizontally. We assume that there are no variations in the horizontal initial conditions so that $\Delta P_{c,min}$ is a function of depth but not lateral position. As discussed in the following paragraphs, we select initial conditions and material parameters such that $\Delta P_{c,min} = 0.05$ MPa at the top of the basement, increases to a maximum of 0.1 MPa at 4 km BTB, and slowly decreases at greater depths. We refer to these minimum and maximum values of minimum critical pressure as $\Delta P_{c,min1} = 0.05$ MPa and $\Delta P_{c,min2} = 0.1$ MPa, respectively. The in-situ stress state, initial pressure, and material parameters are chosen carefully so that the basement is critically stressed initially, which allows our DFNM-MC simulation results to be compared to previous EPM-TP models that assumed $TP \approx 0.1$ MPa.

The initial pore pressure is assumed hydrostatic, which for a compressible fluid can be described as:

$$P(d) = P_o + \int_{d_o}^{d} \rho_f(d) g dz \tag{12}$$

$$P_o = \rho_{f,o} g d_o \tag{13}$$

$$\rho_f(d) = \rho_{f,o} \exp\left(\beta_f(P(d) - P_o)\right) \tag{14}$$

where d is the depth below ground surface, $\rho_{f,o}$ is the reference fluid density (assumed to be 1100 kg/m^3), and P_o is the reference fluid pressure at the reference depth d_o = 3000 m, which is taken as the top of the domain. The vertical stress is similarly assumed to follow a lithostatic stress profile:

$$\sigma_v(d) = \sigma_{v,o} + \int_{d_o}^{d} \rho_s(d) g dz \tag{15}$$

$$\sigma_{v,o} = \rho_{s,o} g d_o \tag{16}$$

$$\rho_s(d) = \sigma_{v,o} \exp \beta_s(\sigma_v(d) - \sigma_{v,o}) \tag{17}$$

where ρ_s is the solid rock grain density, $\rho_{s,o}$ and $\sigma_{v,o}$ are the reference rock density and vertical stress at the top of the domain, and β_s is the compressibility of the solid rock grains. Eq. 17 was chosen for convenience, but solid density could be expressed more generally in terms of all three principal components of stress (i.e. σ_v, $\sigma_{H,max}$, and $\sigma_{h,min}$), and it could also account for the different rock types (e.g. mudstone, sandstone, and basement rock). Nevertheless since the horizontal stresses are also a function of the vertical stress, the use of Eq. 17 is a reasonable approximation, and the mudstone and sandstone layers are thin enough that including different rock types would have a small effect on the stress state. For the simulations presented in this paper, we assume that the multipliers for the horizontal stresses are $\alpha_1 = \alpha_2 = 0.6$ (see Sec. 3.1), which is consistent with the apparent normal faulting regime near Greeley, CO (Brown et al., 2017). By calculating $\Delta P_{c,min}$ as a function of depth at many combinations of parameter values, we selected parameter values as: $\mu_f = 0.67$, $\rho_{s,o} = 2500$ kg/m^3, and $\beta_s = 1.8 \cdot 10^{-10}$ Pa^{-1}. The values of μ_f and $\rho_{s,o}$ fall within their accepted ranges, and β_s is approximately ten times larger than for perfectly intact granite rock (De Marsily, 1986). These rock and fault parameter values, along with the assumed values for hydrostatic pressure, ensure that our definition of a critically-stressed basement is satisfied (i.e. $\Delta P_{c,min} \leq$ 0.1 MPa). Even though the value of β_s is larger than the literature value, and the combination of fault, stress, and pressure parameters are not unique, Eq. 12-17 create an initial pressure and stress condition that allows for comparison to previous EPM-TP modeling studies that assumed $TP \approx 0.1$ MPa as an earthquake-triggering condition. Note that the compressibility of the solid rock grains is typically much, much smaller than the matrix compressibility (i.e. $\beta_s << \beta_m$) and has a minimal contribution to the hydraulic diffusivity, which is why Eq. 1 can be written without β_s (Birdsell, Karra, & Rajaram, 2018). For this same reason, our selected value of β_s does not alter the hydraulic diffusivity to an unrealistic value, and the value of β_s is only relevant to specify an initial stress condition.

The boundary conditions are simpler to specify than the initial conditions. The pore pressure along the top of the domain is fixed to $P = P_o = 32.26$ MPa. The remaining boundaries are no flux boundaries, and are sufficiently far from the injection well to minimize boundary effects. The well acts as a mass source of $Q = 5 \cdot 10^8$ kg/yr, based on the average injection rate of the NGL-C4A well. The stresses are specified everywhere within the domain initially, but mechanical boundary conditions do not need to be specified since the stresses and strains are not explicitly calculated in our partially-coupled approach (see Sec. 3.1).

4.4 Scenarios Simulated

The results are broken down into two parts in the next section: (a) Sec. 5.1 presents a comparison between DFNM-MC and EPM-TP modeling frameworks, and (b) Sec. 5.2 presents a sensitivity analysis using the DFNM-MC approach.

We follow the general simulation setup of Brown et al. (2017) in our comparison of the DFNM-MC approach and the EPM-TP approach, and we choose parameters for the DFNM-MC simulation to readily facilitate a comparison to Brown et al. (2017). We present one DFNM-MC simulation and three EPM-TP simulations. The DFNM-MC scenario has 2000 total fractures, with 1727 falling entirely within the domain and the remainder falling partially outside of the domain. The total fracture area is 10^9 m^2. The parameter differences between the three EPM scenarios in Sec. 5.1 are shown in Table 3. The first EPM scenario (EPM1) provides the most direct comparison to the DFNM simulation. It employs a value of basement compressibility that accounts for the compliant fractures ($\beta_m = 10^{-9}$ Pa^{-1}). It also employs an equivalent permeability that accounts for the presence of fractures in the DFNM simulation, wherein the principal components of the permeability tensor in the x, y, and z direction are $k_{eff,x} = 2.4 \cdot 10^{-16}$ m^2, $k_{eff,y} = 1.7 \cdot 10^{-16}$ m^2, and $k_{eff,z} = 3.4 \cdot 10^{-16}$ m^2, respectively. Note that we calculated the equivalent permeability using three numerical permeameter tests on the DFNM model. This was achieved by specifying a known pressure gradient at two opposing faces of the domain, numerically calculating the steady-state flow rate, and then back-calculating the relevant component of the permeability tensor using Darcy's equation. We assumed that the principal axes of the permeability tensor lined up with the x, y, and z directions. We note that the degree of anisotropy is relatively minor and can be explained by the randomness of the fracture network. The hydraulic diffusivity in EPM1 is $c \approx 2 \cdot 10^{-4}$ m^2/s, which falls within the range of c_{bulk} in Table 1. The second EPM scenario (EPM2) used the hydrologic parameters from Brown et al. (2017), including an exponentially-decreasing permeability and an incompressible basement rock matrix so that changes in fluid storage are only due to fluid compressibility. This corresponds to a hydraulic diffusivity value of $c \approx 2$ m^2/s at the top of the basement, which decreases with depth. The third EPM scenario (EPM3) uses the same permeability as Brown et al. (2017), with the compressibility of fractured basement rock as in the first EPM scenario (i.e. $\beta_m = 10^{-9}$ Pa^{-1}). In this scenario the hydraulic diffusivity $c \approx 0.04$ m^2/s. The simulation duration, t, is three years and involves injection at the average flow rate of the NGL-C4A well from the summer of 2013 to the summer of 2016 .

In Sec. 5.2, we present a sensitivity analysis to understand how fracture density, the orientation of a deterministically-located fault, and the nonlinear hydraulic diffusivity of fractures and faults affect the likelihood of IIS. This sensitivity analysis helps us understand how elevated pressure and seismicity can reach seismogenic depths (≥ 2 km BTB). We assume that there is a deterministically-located fault centered 2.0 km below the well (see Fig. 1) that is large enough to host a felt and potentially-damaging earthquake according to earthquake scaling laws and the Modified Mercalli Intensity scale. The fault radius is 1.5 km. The base-case scenario has 1000 fractures and an optimally-oriented fault. The minimum and maximum depth of the fault are 700 m and 3300 m BTB, respectively. To investigate fracture density, the number of fractures, n_{fracs}, is altered to be 100, 500, 1000, 2000, and 4000. Since fracture networks are generated randomly, simulations were performed on 20 realizations for each fracture density. To investigate the potential for optimally- and suboptimally-oriented faults to host IIS, several fault orientations are considered. Note the optimal orientation can be calculated in 2D since the horizontal components of stress are equal in our simulations. This is done by first calculating the friction angle from the coefficient of friction: $\kappa = \arctan(\mu_f) \cdot (180^{\circ}/\pi) = 33.8^{\circ}$, and then calculating the angle between $\sigma_1 = \sigma_v$ and the fault plane as: $\xi = 45^{\circ} - \kappa/2 = 28.1^{\circ}$ (see Fig. 1) (Einstein & Dershowitz, 1990). The calculation of optimal orientation can be expanded to 3D if the horizontal components of stress are

Table 3. The source and value of parameters used in the three EPM modeling scenarios investigated in Sec. 5.1. EPM1 represents the fairest comparison to the DFNM simulation because it uses permeability from a numerical permeameter test and a reasonable value of $\beta_{m,basement}$. EPM2 uses the Brown et al. (2017) parameters, including an unrealistically-small value of $\beta_{m,basement}$. EPM3 uses the Brown et al. (2017) permeability and a reasonable value of $\beta_{m,basement}$.

Variable	EPM1	EPM2	EPM3
$k_{basement}$ (m^2)	$\approx 2 \cdot 10^{-16}$	$4 \cdot 10^{-14} - 1 \cdot 10^{-18}$	$4 \cdot 10^{-14} - 1 \cdot 10^{-18}$
$k_{basement}$ source	Numerical permeameter	Brown et al. (2017)	Brown et al. (2017)
$\beta_{m,basement}$ (Pa^{-1})	10^{-9}	0	10^{-9}
$\beta_{m,basement}$ source	Freeze and Cherry (1979)	Brown et al. (2017)	Freeze and Cherry (1979)
c m^2/s	$\approx 2 \cdot 10^{-4}$	≈ 2, decreasing with depth	≈ 0.04, decreasing with depth

[a]Brown EPM model uses smaller β_m.

Table 4. Scenarios for the sensitivity analysis shown in Sec. 5.2.3. The sensitivity analysis explores the fracture/fault constitutive relationships that describe how deformations alter the hydraulic diffusivity. "MC-Bandis" includes permeability enhancement due to shear dilation after MC failure and permeability and porosity that are functions of normal deformation as described by the Bandis et al. (1983) constitutive relationship. "Bandis" turns off the permeability enhancement due to MC failure, and "Constant" turns off all the hydraulic diffusivity alterations due to MC and Bandis, although the Bandis relationship is used to assign the initial fracture parameters.

Variable	MC-Bandis	Bandis	Constant
k, fract.	Eq. 6	Eq. 6	Eq. 6 at I.C.
k_τ, after MC shear	10	1	N/A
ϕ, fract.	Eq. 5	Eq. 5	Eq. 5 at I.C.
ϕ_τ, after MC shear	1	1	N/A

not equal. The variation from optimal orientation, $\Delta\xi$, is altered in the sensitivity analysis by 0°, $\pm1^\circ$, and $\pm2^\circ$, where positive angles indicate that the fault is inclined further towards the horizontal. To investigate the importance of the hydraulic diffusivity constitutive relationships (i.e. Bandis and MC) on IIS, we simulate a scenario where MC shear failure and Bandis normal deformation alter the hydraulic diffusivity ("MC-Bandis"), one where only Bandis normal deformation alters the hydraulic diffusivity ("Bandis"), and one where the hydraulic diffusivity is invariant in time throughout the simulation ("Constant"). Note that for the invariant hydraulic diffusivity case, there is still a difference between c in the fractures and the matrix, but c in the fracture stays constant in time throughout the simulation. These three scenarios are summarized in Table 4. It is worth noting that in simulations where fault orientation and hydraulic diffusivity are altered, the same underlying fracture networks are used (i.e. the twenty sets of 1000 fractures that were generated to investigate fracture density were not re-generated). Some parameters in the sensitivity analysis are changed from their values in Sec. 5.1 and Table 2 to reduce computational costs and allow for hundreds of simulations. The grid block size is increased to $b_p = 200$ m, the aquifer thickness is reduced from $H = 500$ m to $H = 400$ m, and the injection and simulation duration, t, is increased to ten years to investigate longer-term pore pressure diffusion, which is relevant for many disposal wells.

5 Results

5.1 Comparison Between DFNM-MC and EPM-TP Approaches

This section focuses on evaluating the differences in behavior between the DFNM-MC approach and the EPM-TP approach as applied to the IIS near Greeley, CO (Sec. 4.1 and 4.4). Fig. 2(a) shows all the fractures in the DFNM-MC domain, colored by permeability. Fig. 2(b) shows a three-dimensional plot of fractures that experienced MC failure (i.e. seismicity) in the DFNM-MC simulation. The maximum depth of seismicity was only 900 m BTB, not ≥ 2000 m BTB that we would expect from field observations. However, $\Delta P_{c,min}$ did reach seismogenic depths as discussed in the next paragraph. In Sec. 5.2 we explore the factors that contribute to $\Delta P_{c,min}$ and seismicity at greater depths.

Fig. 3 shows a three-dimensional view of the extent of critical pressure propagation for the DFNM-MC and the EPM-TP simulations. Regions where $\Delta P < \Delta P_{c,min1} = 0.05$ MPa are removed from the figure because these regions cannot experience earthquakes. Regions where $\Delta P \geq \Delta P_{c,min2} = 0.10$ MPa are colored red. Optimally-oriented

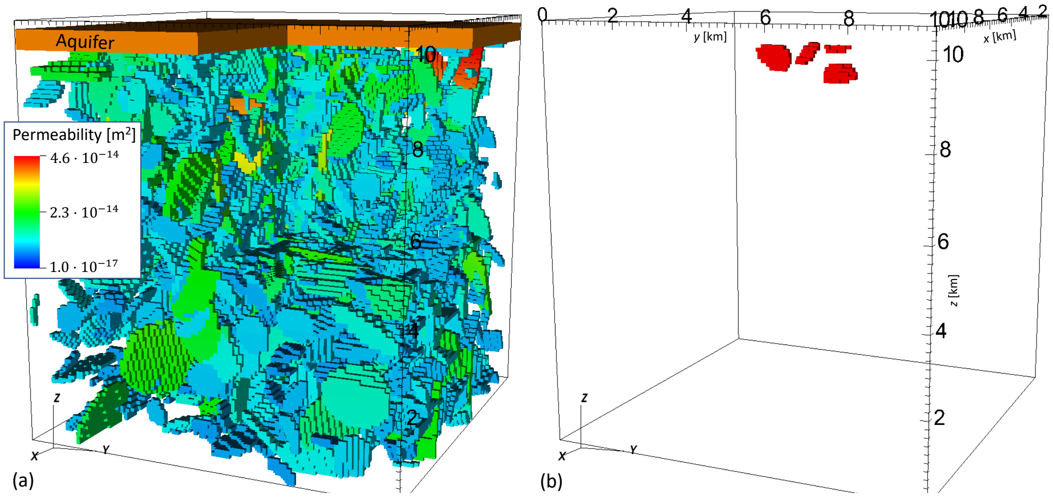

Figure 2. Illustration of the fracture network. Fig. (a) shows the initial permeability for all the regions within the domain that have $k > 10^{-17}$ m^2, which includes all the fractures and the sandstone aquifer near the top of the domain. The regions with $k \leq 10^{-17}$ m^2 (i.e. the unfractured basement and the overlying confining unit) are filtered out of the figure. There is a cutaway at $x = y = z = 5000$ m. Fig. (b) shows fractures that experienced Mohr-Coulomb failure, which is assumed to indicate seismicity.

fractures will experience MC failure between $\Delta P_{c,min1}$ and $\Delta P_{c,min2}$. Fig. 4 shows two-dimensional slice plots of pressure change through the $x-z$ plane at $y = 5$ km, in the plane of the well, and Fig. 5 shows slice plots of pressure change through the $x-y$ plane 2.0 km BTB. Fig. 3-5 clearly illustrate that the DFNM-MC model propagates critical pressure farther and more heterogeneously into the basement than the EPM1 scenario whose properties are consistent with the underlying DFNM domain. In fact, the maximum depth of $\Delta P_{c,min1}$ was 2150 m BTB for the DFNM model (Fig. 3(a)-5(a)) while only reaching 450 m for the EPM1 scenario (Fig. 3(b)-5(b)). Like EPM1, the EPM3 scenario (Fig. 3(d)-5(d)) does not propagate TP to depths $\geq$2 km BTB; only the EPM2 scenario (Fig. 3(c)-5(c)), which employs an unrealistically-large hydraulic diffusivity, results in TP below 2 km BTB. It is noteworthy that $\Delta P_{c,min1}$ propagates much deeper (2150 m BTB) than locations of MC failure (900 m BTB) for the DFNM-MC model (compare Figs. 2(b) and 3(a)). This is because only a small fraction of fractures are optimally oriented for MC failure. Other fractures require $\Delta P > \Delta P_{c,min}$ for failure, and therefore the $\Delta P_{c,min}$ front can propagate to greater depths than the seismic front.

5.2 DFNM Sensitivity Analysis

In this section, we perform a sensitivity analysis to understand the combination of parameters that can lead to critical pressure and MC failure at depths that are relevant to IIS (i.e. $\geq$2 km BTB). We vary three independent variables in the sensitivity analysis: the fracture density, the fault orientation, and the hydraulic diffusivity constitutive relationships for the fractures and faults, as discussed in Sec 4.4. We focus on three dependent variables in our results. First, we report the maximum depth that $\Delta P_{c,min1} = 0.05$ MPa reaches in each realization, which we call $d_{\Delta P_c}$. Second, we report the maximum depth of seismicity for each realization, $d_{seismicity}$. Third, we report the maximum depth of an earthquake on the fault (EOF) for each realization, d_{EOF}. Since we are interested in the probability of these occurrences as a function of depth, we define the probability of exceeding critical pressure at a given depth d as $P(d_{\Delta P_c} \geq d)$, the probabil-

Figure 3. Plot of pressure change for comparison of the extent of critical pressure propagation between the DFNM-MC and EPM-TP models (Sec. 5.1). Regions where $P < P_{c;min\ 1} = 0{:}05$ MPa are not shown because they cannot experience seismicity, and regions where $P > P_{c;min\ 2} = 0{:}1$ MPa are colored red. Fig. (a) is from the DFNM-MC scenario, (b) EPM1, (c) EPM2, and (d) EPM3. The hydraulic di usivity values in (b) - (d) were $2\ 10^{4}$, 2, and .04 m^2/s respectively (Table 3). Comparison between (a) and (b) shows that critical pressure propagates deeper and more heterogeneously in a DFNM-MC model than in an EPM-TP model where the equivalent permeability is based on the underlying DFNM. Comparison between (c) and (d) shows that critical pressure does not propagate as deep when realistic values of compressibility are used.

Figure 6. Fig. (a) shows the probability of exceeding critical pressure ($P_{c;min\ 1} = 0.05$ MPa) as a function of depth and the number of fractures, which is expressed by plotting $P(d_{P_c}$ d) versus d. The probability of exceeding critical pressure increased monotonically with the number of fractures at shallow depths, whereas at greater depths (2700 m BTB), the probability of exceeding critical pressure was largest for an intermediate number of fractures (i.e. 1000 or 2000 fractures). Similarly, Fig. (b) shows the probability of seismicity and EOF as a function of depth and number of fractures (i.e. $P(d_{seismicity}$ d) vs d and $P(d_{EOF}$ d) versus d). The probability of seismicity and EOF both increased with increasing number of fractures at shallow depths. At depths 2100 m BTB, the probability of seismicity and EOF was highest for an intermediate number of fractures (i.e. 1000 fractures). The figures also have dashed lines indicating 2 km BTB, where the fault is centered, and dotted lines indicating the top and bottom of the fault.

Fig. 9(a), the probability of exceeding critical pressure was unaffected by the choice of the hydraulic diffusivity relationship at depths shallower than 1300 m. At greater depths, the "Bandis" scenario resulted in a modest increase in the probability of critical pressure, when compared to the "Constant" scenario. The "MC-Bandis" scenario resulted in a considerably larger probability of critical pressure, especially at d 3300 m, compared to the "Constant" scenario. Fig. 9(b) shows the probability of seismicity as a function of depth and hydraulic diffusivity constitutive relationship. The probability of seismicity was larger for the "MC-Bandis" scenario than for the "Bandis" scenario, especially at the deeper parts of the fault (d 2500 m).

Why does the MC permeability enhancement seem to be important while the Bandis effect is less important? Firstly, MC failure enhances permeability, which increases the hydraulic diffusivity, whereas Bandis dilation increases the permeability and the porosity, which have competing effects on the hydraulic diffusivity (Eq. 1). Secondly, based on the Bandis model, fractures are forced almost entirely shut at the depths and lithostatic stresses commonly seen near IIS. As fractures are forced closed, their stiffness increases and asymptotes to infinity so that the stiffness of the fracture/matrix system approaches that of the matrix rock. Therefore, in the context of IIS, the fractures are unlikely to open very much as pore pressure is increased. Nevertheless, the Bandis dilation could prove to be more important in geologic settings where the effective normal stress is less compressive and fractures can open and close to a greater degree. It is clear that the MC permeability enhancement is an important factor in propagating critical pressure to 2 km.

events at the same location, update the hydraulic diffusivity as a function of fracture deformation, and include propagation of seismic waves and evaluation of the Coulomb stress change after MC failure. To our knowledge, this type of tool does not exist, and even simulators that do not propagate seismic waves are generally limited to 2D (Jin & Zoback, 2018, 2017) or a single fault (Jha & Juanes, 2014; Rinaldi et al., 2014; Kelkar et al., 2014) due to computational cost. For computational expediency, it may be possible to implement fracture and matrix simulators wherein the mechanical and hydrologic equations are fully coupled but the mechanical solution is not updated in every time step of the hydrologic calculation, but these have not been presented in the literature to our knowledge. Therefore, our partially-coupled DFNM-MC approach is especially attractive, because it can simulate large spatial scales with many fractures and faults. The DFNM-MC approach can contribute to probabilistic assessment of the risks of induced seismicity based on the datasets described in the previous paragraph. As demonstrated in Sec. 5.2, the DFNM-MC approach can be combined with Monte-Carlo simulations on multiple realizations of fracture networks across which fracture and fault locations, orientations, and properties are sampled from their respective probability density functions. The partially coupled nature and the parallelization of the DFNM-MC approach renders it computationally tractable for such probabilistic assessments. While forecasting IIS is still extremely difficult, a DFNM-MC model with all the relevant parameters could, in principle, offer a screening framework for forecasting before injection begins and/or during injection as part of an adaptive traffic light system (Wiemer et al., 2015; Király-Proag et al., 2016). One drawback of the partially-coupled DFNM-MC model is that it cannot evaluate poroelastic stress changes, earthquake-earthquake interactions, or allow for multiple failure events. Simulators that can evaluate these phenomena are computationally expensive, so the partially-coupled DFNM-MC approach could be used in a screening step to identify the most critical scenarios for further investigation with other, computationally-expensive simulators.

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