TITLE:

Pressure management via brine extraction in geological CO₂ storage: adaptive optimization strategies under poorly characterized reservoir conditions

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1	Pressure Management via Brine Extraction in Geological CO ₂ Storage:
2	Adaptive Optimization Strategies under Poorly Characterized Reservoir
3	Conditions
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19	Abstract
20	Industrial-scale injection of CO ₂ into the subsurface increases the fluid pressure in the reservoir,
21	which if not properly controlled can potentially lead to geomechanical damage (i.e., fracturing of
22	the caprock or reactivation of faults) and subsequent CO ₂ leakage. Brine extraction is one approach

23 for managing formation pressure, effective stress, and plume movement in response to CO_2 24 injection. The management of the extracted brine can be expensive (i.e., due to transportation, 25 treatment, disposal, or re-injection), with added cost to the carbon capture and sequestration 26 (CCS); thus, minimizing the volume of extraction brine is of great importance to ensure that the 27 economics of CCS are favorable. The main objective of this study is to demonstrate the use of 28 adaptive optimization methods in the planning of brine extraction and to investigate how the 29 quality of initial site characterization data and the use of newly acquired monitoring data (e.g. 30 pressure at observation wells) impact the optimization performance. We apply an adaptive 31 management approach that integrates monitoring, calibration, and optimization of brine extraction 32 rates to achieve pre-defined pressure constraints. Our results show that reservoir pressure 33 management can be extremely benefited by early and high frequency pressure monitoring during 34 early injection times, especially for poor initial reservoir characterization. Low frequencies of 35 model calibration and optimization with monitoring data may lead to optimization problems, 36 because either pressure buildup constraints are violated or excessively high extraction rates are 37 proposed. The adaptive pressure management approach may constitute an effective tool to manage 38 pressure buildup under uncertain reservoir conditions by minimizing the volumes of extracted 39 brine while controlling pressure buildup.

40 Keywords: CO₂ storage, pressure management, fault activation, caprock fracturing, parameter
41 uncertainty, brine extraction

42 **1 Introduction**

Injection of CO_2 into the subsurface at industrial scale can result in significant fluid pressure increase in a reservoir, which can be a limiting factor for sequestration capacity in saline aquifers (Zhou and Birkholzer, 2011; Thibeau et al., 2014). The possibility of distant pressure46 related impacts need to be considered, which if not properly controlled can lead to potential 47 environmental impacts (Zhou and Birkholzer, 2011). These potential environmental concerns 48 include groundwater contamination (Apps et al., 2010; Birkholzer et al., 2009) stemming from 49 pressure-driven brine leakage through conductive pathways, such as improperly plugged 50 abandoned wells or distant faults (Metz et al., 2005), and the potential for fault reactivation and 51 possibly seal breaching (Morris et al., 2011; Rutqvist et al., 2007). Large areas with pressure 52 increases can also require more complex and costly site characterization and monitoring (US EPA, 53 2008; Oldenburg et al., 2016).

54 Concerns about local- or regional-scale pressurization have motivated research on 55 engineering approaches for subsurface pressure control, usually involving some strategies of 56 extracting resident brines from a storage reservoir while CO₂ is injected. The potential benefits of 57 employing brine extraction wells to manage pressure in the reservoir include reduced stress on the 58 sealing formation, reduced risk of brine and CO₂ intrusion into other formations, increased storage 59 capacity, and reduced area of review for regulatory assessment (Birkholzer and Zhou, 2009). In 60 recent years, pressure management approaches via brine extraction have been studied in generic 61 modeling exercises to demonstrate the proof of concept and feasibility (e.g. Bergmo et al., 2011), 62 but so far brine extraction has not been used in actual geological carbon storage (GCS) projects, 63 mainly because the currently injected CO₂ volume are limited and large-scale pressure increases 64 are rare. However, for large-scale projects expected in future GCS deployment, modeling analyses 65 reveal that brine extraction can be very beneficial and in some cases necessary, enhancing storage capacity and injectivity (Buscheck et al., 2012; Buscheck et al., 2014; Pongtepupathum et al., 66 67 2017; Ziemkiewicz et al., 2016) and reducing risk of environmental impacts and induced 68 seismicity (Birkholzer et al., 2012). For example, the industrial-scale Gorgon CO₂ storage project

69 in Australia considered the possibility of brine extraction through four wells located to the west of 70 the site (Flett et al., 2008; Greig et al., 2016; Liu et al., 2013).

71

Ensuring safety and robustness against failure is critical and must be integrated into actual 72 GCS projects (Harp et al., 2017). 'A factor of safety' is a concept applied in all engineering 73 applications. In our work we assumed that the threshold values for critical pressures already 74 include the factor of safety. The main goal of this study is to investigate the influence of two factors 75 on the extraction rates of brine for pressure management. These two factors are i) the quality of data of the initial site characterization, and ii) the frequency of model calibration and optimization 76 77 calculations based on newly acquired monitoring data.

78 In preparation for deployment of future large-scale GCS projects, the U.S. Department of 79 Energy (DOE) created the Brine Extraction and Storage Test (DOE-BEST) program to evaluate 80 the technical feasibility of managing subsurface pressures associated with large-scale CO₂ 81 injection volumes and to assess the cost and effectiveness of desalination technologies for saline 82 waters containing high total dissolved solids (TDS). Two projects funded under this program are 83 currently in the final planning and design phase. The projects will demonstrate management of 84 reservoir pressure through brine extraction in actual field settings and test desalination approaches 85 for the utilization of the extracted brines (DOE, 2016).

86 Recognizing the potential management cost of extracted brine (Harto and Veil, 2011), 87 recent work by Birkholzer et al. (2012) and Cihan et al. (2015) aimed to develop flexible 88 optimization methods for pressure control, with the goal of minimizing the volume of extracted 89 brine while maximizing CO₂ storage and meeting other constraints needed for safe and efficient 90 GCS operations. For given pressure constraints, such as the maximum allowable pore pressure 91 along a critically stressed fault, the optimization algorithm finds optimal solutions for placement

92 of extraction wells and transient pumping rates. Example applications of optimization algorithms 93 to hypothetical CO_2 storage scenarios in realistic field settings demonstrate that strategic extraction 94 can achieve a significant reductions in the total volume of extracted brine while limiting pressure 95 increases (Cihan et al., 2015).

The knowledge of subsurface properties is always incomplete. Especially during the 96 97 planning stages of CO₂ projects, site characterization data are often quite limited and there are 98 large uncertainties in rock properties. Thus, predictive models for the reservoir conditions upon 99 CO₂ injection are initially associated with large model uncertainties. These models can be 100 improved through calibration using monitoring data obtained during the operation of the projects. 101 Based on new data received and subsequent improvement of the existing models, optimization 102 calculations may then need to be revised and operational decisions for controlling and managing 103 subsurface pressurization may need to be updated. The oil industry commonly uses the so-called 104 "closed-loop" approach, which includes optimization and model-updating algorithms for reservoir 105 management (Aitokhuehi and Durlofsky, 2005; Sarma et al., 2006). Observations such as well-log 106 measurements, production rates (oil, gas, and water), and 4D seismic data are collected to improve 107 knowledge of uncertain parameters and then used to improve the prediction of reservoir simulation 108 models (Evensen et al., 2007; Nævdal et al., 2005; Skjervheim et al., 2005).

The goal of this study is to apply an adaptive management approach that combines monitoring + inversion + optimization in an integrated framework for pressure control in GCS applications. We use this framework to develop and implement a pressure management strategy at a hypothetical site. In terms of geological setting and well configurations, the hypothetical example resembles one of the DOE-BEST projects, which will provide a testbed for demonstrating adaptive pressure management. However, the spatial and temporal scales of the hypothetical scenario

investigated in this study are much larger than the planned field test scenario in this DOE-BEST project. It is important to note that the actual DOE -BEST project demonstration site has no known faults, whereas the hypothetical scenario reported here includes a critically stressed hypothetical fault which needs to be protected from hypothetical reservoir pressure increases.

119 Using the hypothetical injection application as an example case, we focus on testing and 120 demonstrating an adaptive management approach to understand the influence of two factors on the 121 optimized extraction rates for pressure management. These factors are: 1) the quality of data 122 obtained during the initial site characterization such as hydraulic properties of the reservoir system, 123 and 2) the frequency of model calibration and optimization calculations based on newly acquired 124 monitoring data. Our objective is to demonstrate that adaptive management can effectively manage 125 pressure effects associated with fluid injection, such as the potential for inducing seismic events 126 and leakage along hypothetical faults, and that it can do so under realistic conditions where 127 reservoir data are uncertain. The management strategy that we use for the hypothetical site 128 combines two complementary brine extraction methods: (1) "active" extraction of brine from the 129 injection reservoir to the surface with optimized time-varying pumping rates, and (2) "passive" 130 pressure relief, which relies on the pressure increase in the injection reservoir to provide the driving 131 force for resident brine to flow through a relief well; in this case, transferring fluids into suitable 132 deeper geological layers than the injection layer (Figure 1). The advantage of "passive" pressure 133 relief is that once a relief well is drilled and completed there are no additional costs for brine 134 pumping or handling, in contrast to "active" extraction. The disadvantage is that "passive" brine 135 extraction cannot be optimized to the project needs; the brine volume transferred out of the storage 136 reservoir into other formations is a function of their pressure differentials. For this same reason,

137 "passive" brine extraction requires that the receiving units are not overpressurized to the point138 where they cannot passively receive the brine.



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Figure 1. Schematic showing the pressure management strategy in this study to reduce risk of caprock failure and risk of fault reactivation. The schematic shows the five top aquitards as well as the five top aquifers of Table 1(from 22 to 18). Injection of CO₂ occurs into two reservoir layers (aquifers 22 and 21 in Table 1). Brines are extracted from two wells, one of them "actively" pumping to the surface, the other "passively" moving brines into deeper layers. The back of the schematic figure shows a hypothetical critically stressed fault, for which a maximum allowable pressure change has been defined. Another pressure limit is defined to avoid caprock damage.

The paper is organized as follows. Section 2 presents brief descriptions of the adaptive management methodology, the reservoir modeling approaches, the optimization and calibration problem solved, and selected scenarios of the adaptive management approach. In section 3 and section 4, the results of the sensitivity analysis of site characterization are presented and discussed. Section 5 summarizes the main conclusions of this study.

153 **2** Adaptive management approach

Adaptive management involves (1) analysis and interpretation of monitoring data acquired during the field test, (2) reservoir model testing, (3) updating of model parameters using inverse modeling methods, and (4) revised optimization plus, if necessary, modification of reservoir management schemes (i.e., time-dependent extraction rates, changes in extraction schemes) based on the updated reservoir model predictions. In this study, we use a computer algorithm that automatically accomplishes the steps above at a selected frequency to estimate future minimum extraction rates based on the existing reservoir model.

161 The initial reservoir model, based on available site characterization data, is used to estimate 162 the initial and future minimum extraction rates that provide acceptable pressure conditions. These 163 acceptable conditions, or pressure constraints need to be defined before the start of the 164 optimization. An optimization algorithm coupled to the reservoir model then generates optimal 165 extraction rates that may vary during the project period (Stage 1). Depending on the reservoir 166 conditions, extraction may not need to start at the beginning of injection in most cases. However, 167 if the initially estimated values are not zero, the extraction well(s) start pumping using the 168 calculated initial extraction rate(s). As soon as newly acquired data become available during the 169 operation (e.g., pressure changes at the observation wells, geophysical measurements), the model

170 predictions are compared against the observations (Stage 2). If the model predictions are 171 significantly different from the observations, which is typically the case, especially during early 172 operation, then the reservoir model is updated or recalibrated with the new data using an inverse 173 modeling tool (Stage 3). After the model calibration process, the algorithm goes back to Stage 1 174 to estimate new optimal extraction rates at the current and future times that satisfy the constraints 175 based on the predictions with the existing model. The extraction well(s) continue operating at the 176 current extraction rate until new data are analyzed and the model and extraction rates are updated. 177 The adaptive management algorithm may continue to be used throughout the injection and perhaps 178 post-injection phase to ensure that the extraction rates are minimized and pressure constraints are 179 met.

180 **2.1 Reservoir flow model**

181 For this study, a multilayered reservoir model was constructed using the existing well logs, 182 lithologic logs, sidewall core data, and well test data gathered from an existing well near the DOE-183 BEST project field site. The targeted reservoir system is a thick (about 700 m) sequence of very 184 porous and permeable fluvial and fluvial deltaic sandstones alternating with shale. Injection occurs 185 only into the upper two sandstone layers at a total rate of $1,090 \text{ m}^3/\text{d}$ (~ equivalent to about 0.3 Mt 186 of CO₂ injection) over 30 years. We assume that there is a concern about caprock fracturing and 187 potential fault slip due to increased pressures near the injection well and along a hypothetical fault 188 which is a few kilometers away from the injection well. We furthermore assume that the critical 189 pressure changes for caprock fracturing and fault slip are $\Delta P_{crt,c} = 8$ MPa and $\Delta P_{crt,f} = 0.4$ MPa, 190 respectively. As mentioned before, the pressure management strategy involves a passive relief 191 well and an active extraction well to control pressure changes (see Figure 1).

192 To efficiently simulate the fluid flow and pressure changes in the reservoir system, we 193 employ a semi-analytical model for single-phase flow in multilayered systems that has capabilities 194 to represent multiple injection/extraction and leaky wells, diffuse flow through aquifer-aquitard 195 interfaces, and focused brine leakage or flow through leaky wells (Cihan et al. 2011). We 196 approximate the target reservoir with its sandstone and shale layers as aquifers and aquitards, 197 respectively, where fluid flow is assumed horizontal in the aquifers and vertical in the aquitards. 198 Initially, hydrostatic pressure is assumed for the whole system of aquifers and aquitards. Each 199 aquifer and aquitard may have different hydraulic properties and thicknesses; however, within each 200 aquifer and aquitard, properties and thickness remain uniform. Leaky wells are represented as 201 Darcy-type flow pathways with segment-wise property variations (e.g., well radii, permeability, 202 screened/cased in well-aquifer segments, plugged/unplugged in well-aquitard segments). The 203 segments correspond to intersections of each well with individual layers of the multilayered 204 system. Further details of the semi-analytical solution approach and a description of the computer 205 program to compute the solution in terms of pressure changes can be found in Cihan et al. (2011). 206 The leaky well feature of the semi-analytical model is particularly useful for this study to represent 207 the passive relief well in our hypothetical scenario. Table 1 lists the identified 22 aquifer and 22 208 aquitard layers (from bottom to top) of the target reservoir system with their hydraulic properties 209 including thickness, hydraulic conductivity and specific storativity. Aquifer Layers 21 and 22 (top 210 two aquifer layers) are the injection layers.

211

Aquifers				Aquitards				
Layer	Thickness	$K = K_{xx}$	$S=S_s$	Layer	Thickness	$K' = K_{zz}$	$S' = S_s$	
	(m)	(m/d)	(m^{-1})		(m)	(m/d)	(m ⁻¹)	
1 (bot)	42.062	0.176	1.856E-06	1	6.706	4.729E-04	1.065E-06	
2	18.288	0.207	2.025E-06	2	6.096	1.537E-03	1.081E-06	
3	10.973	0.674	2.025E-06	3	6.706	4.032E-03	1.452E-06	
4	29.261	0.237	1.940E-06	4	7.925	6.706E-04	1.162E-06	
5	8.534	0.144	1.856E-06	5	18.593	1.889E-03	1.065E-06	
6	30.785	0.182	1.680E-06	6	10.973	1.548E-03	1.743E-06	
7	15.850	0.670	2.000E-06	7	9.449	3.124E-03	1.355E-06	
8	23.470	0.498	2.001E-06	8	14.021	1.809E-03	1.150E-06	
9	13.106	0.871	1.990E-06	9	5.791	1.059E-03	1.162E-06	
10	16.459	0.447	2.025E-06	10	9.144	3.859E-03	1.452E-06	
11	9.144	0.321	2.025E-06	11	8.534	4.960E-03	1.020E-06	
12	3.048	0.826	1.940E-06	12	7.315	2.301E-03	1.258E-06	
13	23.165	0.284	1.940E-06	13	1.829	1.462E-03	1.162E-06	
14	10.973	0.338	2.025E-06	14	4.572	1.896E-03	1.646E-06	
15	34.138	0.720	3.122E-06	15	12.192	5.159E-04	5.808E-07	
16	55.778	0.195	2.025E-06	16	9.449	1.032E-03	1.936E-06	
17	3.962	1.032	3.037E-06	17	2.438	6.190E-04	1.452E-06	
18	14.021	0.037	2.278E-06	18	12.192	5.732E-03	2.420E-06	
19	46.634	0.273	2.607E-06	19	3.962	5.159E-05	8.713E-07	
20	23.165	0.403	2.563E-06	20	7.620	1.032E-03	1.646E-06	
21	10.668	0.503	2.244E-06	21	2.438	2.053E-09	8.713E-07	
22	3.048	0.375	2.306E-06	22 (top)	86.563	4.769E-04	1.258E-06	

Table 1. Reference ('true') hydraulic property values of reservoir layers containing aquifers alternating with aquitards. The bottom layer is an aquifer, and the top layer is an aquitard.

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In actual field demonstrations, higher-fidelity numerical models are typically more appropriate, but in this demonstration application, we prefer using the semi-analytical solution to be able to conduct ultrafast model calibration and optimization calculations within the adaptive management framework. Brine flow and pressure changes along the far-field fault and brine flow through the passive well outside the CO_2 plume zone can be described reasonably well by the single-phase flow models —without considering local two-phase and variable density effects simply by representing the injection of CO_2 as an equivalent volume of saline water (Nicot 2008; Cihan et al., 2013). However, Cihan et al. (2013) showed that the analytical solution for singlephase brine flow would slightly overpredict pressure buildup within the CO₂ plume zone, compared to the multiphase simulator TOUGH2/ECO₂N (Pruess 2005). This in turn leads to slightly higher brine extraction rates, calculated by the optimization algorithm, than actually required. Thus, we may consider the optimization results based on the analytical model to be on the conservative side.

229

230 2.2 Optimization

231 The specific goal of the optimization in this study is to minimize the volume of extracted 232 brine while effectively controlling pressure buildup such that (1) the caprock fracturing pressure 233 is not exceeded, and (2) reactivation along a hypothetical fault near the injection location can be 234 avoided. (These pressure constraints are a proxy for any other pressure constraints one may need 235 to define in a given project.) If the total volume of injected fluid is V_{inj} , and the total volume of 236 extracted fluid is V_{ext} , then the goal is to minimize the extraction ratio defined by V_{ext}/V_{inj} . Costs 237 associated with the pumping per volume of injected or produced fluid and treatment of extracted 238 brine are assumed to be proportional to the extraction ratio defined in Eq. (1). Formally, the 239 specific optimization problem that involves the objective function and the constraints, respectively, 240 can be expressed as:

Minimize
$$f(\mathbf{p}) = V_{ext}/V_{inj}$$

(1)

Subject to
$$g_1(\mathbf{p}) = max\{\Delta P(x_{obs}, t)\} - \Delta P_{crt,f} < 0,$$
 (2)
 $g_2(\mathbf{p}) = max\{\Delta P(x_{obs}, t)\} - \Delta P_{crt,c} < 0$

241 where p is the parameter vector that may include constant or time-dependent function parameters 242 for controlling extraction rates and, in the most general case, the number and locations of extraction 243 wells if one decides to have the algorithm select an optimal well design. For this study, we assume 244 that the location of extraction wells is known, and that the extraction rate(s) are optimized as piece-245 wise time-dependent parameters. The two constraints in Eq. (2) represent the pressure management 246 goal of keeping reservoir pressure increases in defined impact zones below critical pressure 247 buildup values (with respect to the pressure prior to the injection, $\Delta P(t)=P(t)-P(t=0)$). We assume 248 in the first constraint (g_1) that the fault slip risk becomes too high if the pressure buildup at any 249 location in the impact zone (hypothetical fault) exceeds $\Delta P_{crt,f}$. Pressure buildup along the impact 250 zone is recorded through a vector of observation points (\mathbf{x}_{obs}) , as many as required. In addition to 251 the pressure buildup constraint along the fault, we take into account the fracturing pressure 252 constraint (g₂) near the injection well ($\Delta P_{crt,c}$).

To solve the optimization problem, we apply a constrained differential evolution (CDE) algorithm modified from a differential evolution algorithm (Deb, 2000; Cihan et al., 2015) within each step of the adaptive management framework. The CDE algorithm is particularly useful for solving global optimization problems involving well placement and dynamic injection/extraction control (e.g., Cihan et al., 2015). As mentioned above, we assume in this study that the well locations are known, and we employ CDE to solve only the problem of dynamic extraction control.

259 2.3 Calibration

The specific goal of the calibration in this study is to minimize the error between pressure measurements observed and pressure measurements generated with the simulations (Equation 3). For the inverse estimations conducted at each step of the adaptive algorithm, we use the same method (CDE) as in Stage 1 to inversely estimate unknown reservoir properties using observed hydraulic pressure buildups. With regards to monitoring data available in our hypothetical example, we assume that pressure measurements are made at each aquifer (22 aquifers) and at three locations: in the injection well, the active extraction well, and the passive relief well.

Minimize
$$h(\boldsymbol{q}) = \sum_{1}^{N_{Obs}} \sum_{1}^{N_{Time}} \left(\frac{P(\boldsymbol{x},t) - P(\boldsymbol{x}_{obs},t)}{P(\boldsymbol{x}_{obs},t)} \right)$$
 (3)

where *q* is the parameter vector that include the aquifer and aquitards properties to be calibrated, N_{Obs} is the equal to the number of locations (66 = 22*3), and N_{Time} is the number of observations along time.

The observation values are generated by using the true model with the reference properties in Table 1 and then these are compared with the observation values generated by the properties of the model.

273 **2.4 Scenarios of the adaptive management framework**

274 We employ the adaptive optimization framework to optimize the frequency in which data 275 should be collected and how we could do to make this a better and safer site. For this purpose we 276 study the effects of two factors on the optimized volume of extracted brine: 1) the quality of data 277 obtained during the initial site characterization (e.g. hydraulic properties of the reservoir system), 278 and 2) the frequency of model calibration and optimization calculations based on the monitoring 279 data. Table 2 summarizes the different sensitivity scenarios for these two factors. By considering 280 several levels of uncertainty for the initial property data of the reservoir system (over or under-281 estimated), we study their effects on the calculated values of the optimal brine extraction ratios in 282 Eq. (1). Under uncertain initial reservoir conditions, we also investigate the effects of the frequency 283 of model updates a on the performance of adaptive optimization. In the section 4, we present 284 comparisons of the extraction rates calculated for 'true' reservoir properties versus the estimated

ratios for 'uncertain' reservoir properties, with different-level initial guesses and different-frequency model updates.

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Table 2. Scenarios considered for the adaptive management framework

Frequency of model under	Deviations from the actual hydraulic			
Frequency of model update	properties			
Fixed frequencies of 30yr, 10yr, 6yr, 5yr, 3yr,	Over and under-estimated properties at time=0:			
and variable frequency (from 3 days at very early times to 3yr at late times)	+20%, +40%, -20%, -40%			

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290 The uncertain hydraulic properties considered in this study are the hydraulic conductivity 291 and specific storage parameters of one of the injection aquifers (Aquifer Layer 22) and 292 corresponding overlying aquitard (Aquitard Layer 22). We select this layer because the pressure 293 changes are most sensitive to their properties. The reservoir properties of the other aquifer layers 294 (1-21) are tied to those of Aquifer Layer 22, and the properties of the other aquitard layers (1-21) 295 are tied to those of Aquitard Layer 22, which reduces the number of unknowns from 88 to 4. 296 Because of the petrological similarities of the aquitard layers, we can assume that the relative ratios 297 of the estimated parameters can be assumed reasonably accurate for all aquifer layers and all 298 aquitard layers, respectively. In other words, we can recalculate the reservoir properties of Aquifer 299 and Aquitard Layers 1-21 based on the inversely estimated properties of Layer 22 (K_{22} , K_{22} ', S_{s22} , 300 S_{s22}), assuming that parameter ratios are fixed (K_i/K_{22} , S_{si}/S_{s22} , K_i'/K_{22} ', S_{si}'/S_{s22} ', $i=1,\ldots,21$, 301 calculated using Table 1), where the prime sign indicates aquitard.

302 **3. Results**

303 3.1 Results without pressure management

304 We first present pressure results in the target reservoir for CO₂ injection without any 305 pressure management. Figure 2 shows maximum pressure changes as a function of time near the 306 well and along the fault in response to fluid injection at 1,090 m³/d (~ equivalent to about 0.3 Mt 307 of CO_2 injection) for 30 years into an injection zone at about 1,500 m depth from the surface. The 308 injection zone corresponds to Aquifer Layers 21 and 22. The total injection rate is distributed into 309 the two aquifer layers of the model proportionally according to their transmissivity values. 310 Significant differences can be observed between the five reservoir property cases (i.e., true, -40%, 311 -20%, +20%, +40%). In Figure 2a, the forward modeling results with under-estimated reservoir 312 properties (-20% and -40%) indicate that the caprock pressure buildup constraint of 8 MPa can be 313 reached very quickly as soon as the injection starts. The model results with over-estimated 314 reservoir properties (+20% and +40%) show no risk of caprock failure, while the true model shows 315 that the critical pressure buildup of fracturing the caprock is reached after about 22 years of 316 injection. Figure 2b shows that fault slip can occur within about three to twelve years of injection 317 for all reservoir property cases, under- or over-estimated. The estimated time for the constraint 318 violation (fault pressure above 0.4 MPa) decreases with decreasing aquifer hydraulic conductivity 319 values.



Figure 2. Profiles of maximum pressure buildup (in MPa) (a) at the caprock and (b) at the fault.
(Note that Cihan et al.'s computer program (2011) produces the results in terms of head in meters,
and to convert the head buildup to pressure buildup, we used a uniform brine density of 1126.026
kg/m³.)



327 **3.2 Results applying adaptive management approach**

328 Figure 3 shows pressure buildup contours for the +20% case in Aquifer Layer 22 where 329 the pressure buildup front has the largest extent compared to the other layers, for two pressure 330 management scenarios: Figure 3a shows a simulation where only the passive relief well operates, 331 which transfers brine from the injection reservoirs to deeper layers. Figure 3b shows results for a 332 case where passive relief and active extraction operate together. In the first case, there is no 333 optimization since the passive brine transfer depends only on the vertical pressure differential 334 between injection layers and deeper layers. In contrast, the active brine extraction rates in Figure 335 3b are optimized to meet the given pressure constraints.







Figure 3. Pressure buildup contours (in MPa) at time=30 years with (a) only passive extraction
and (b) passive and active extraction (updates every 3 years) for the +20% case in Layer 22.

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As seen in Figure 3a, passive pressure relief alone is not sufficient to reduce the injectioninduced pressure buildup below the desired critical value of 0.4 MPa near the hypothetical fault. Therefore, active brine extraction is needed to satisfy the pressure constraints, especially near the fault. With the objective of determining optimal dynamic extraction rates, we ran our automated adaptive optimization algorithm that starts with the different initial guesses of the reservoir properties (-40%, -20%, +20%, and +40%). For each of these cases, we also varied the model update frequency to understand its impact on the performance of the adaptive pressure management (Table 2). As a reminder, the monitoring data used for model calibration in this study are the pressure measurements at the top two aquifer layers of three wells (injection, passive relief, and extraction). We assume here that monitoring data collection and model update are conducted at the same frequency. In practice, monitoring data collection for pressure changes should be expected to be much more frequent than the model updates.

354 Figure 3b displays an example of a successful pressure management optimization for the 355 +20% case where updates of the monitoring, calibration, and optimization steps occur every three 356 years. When the adaptive management through active and passive extractions is applied, the 357 pressure buildup along the fault is controlled and does not exceed the maximum critical pressure 358 of 0.4 MPa at the end of the injection (time = 30 years). Despite the fact that the passive relief well 359 alone as a pressure control approach is not sufficient for this scenario, its use together with the 360 active extraction reduces the total volume of extracted brine by up to 20%. The benefit of using 361 passive relief wells in reducing brine extraction volumes can vary depending on the magnitudes of 362 the pressure buildup constraints and their distances from the injection well (Birkholzer et al., 363 2012).

Figure 4 summarizes the results of applying adaptive management to the different property and model calibration scenarios listed in Table 2. The figure shows the total extraction ratio (over the duration of the project) as a function of the model update and optimization frequency (Δt), starting with every three years up to 30 years. Cases that consider a model update frequency (Δt) of 30 years do not include monitoring or model update through calibration; they simply apply constant extraction rates optimized using the initial guesses.



371 **Figure 4.** Summary of the adaptive optimization results: Variation of the estimated brine 372 extraction ratio as a function of initial deviations from reservoir properties and model update 373 frequency (Δt).

374

375 Figure 4 shows that for the reference scenario ('true' model), more frequent updates 376 decrease the objective function from $V_{ext}/V_{inj}=12.8\%$ for $\Delta t=30$ years to $V_{ext}/V_{inj}=9.1\%$ for $\Delta t=3$ 377 years. In this case, a better optimization is achieved when the extraction rates are updated every 378 three years rather than operating with a constant extraction rate over 30 years. Optimization results 379 are more complicated for the scenarios involving uncertain initial model properties, in which case 380 the full monitoring + inversion + optimization cycle is conducted. For example, looking at the 381 cases with under-estimated initial parameters (-20% and -40%), the calculated optimal extraction 382 ratios are significantly higher than the actual optimal extraction ratios for all model update cases, 383 in particular if the model updates are conducted less frequently. This occurs because the reservoir

384 system is initially managed with a non-optimal model using the under-estimated reservoir 385 properties, and it takes several iteration cycles to estimate more reliable reservoir properties with 386 analyses of the monitoring pressure data. As the frequency of monitoring data analyses and model 387 updates increases (moving to the left on the time axis in Figure 4), the calculated extraction ratios 388 approach the true values. On the other hand, scenarios with over-estimated initial hydraulic 389 properties have a lower value of V_{ext}/V_{inj} than the reference scenario; in other words, the extracted 390 volume is under-estimated, specifically for cases with low frequency of updates (Δt >6 years); when the number of updates increases, the V_{ext}/V_{ini} approaches the true case. We show in Figure 391 392 5 that extracting less brine than necessary can result in *not* meeting the desired pressure constraints, 393 i.e., possibly causing failure of the caprock or activation of the fault, a result of the inaccurate 394 models used for optimization.

395 4 Discussion

396 **4.1 Influence of initial hydraulic properties uncertainty**

397 The potential impact of pressure management optimization with inaccurate models is 398 shown in Figure 5 for all the cases of over- and under-estimated reservoir properties and a model 399 calibration conducted every 10 years. This figure shows the evolution of the maximum pressure 400 buildup at the injection well (Figure 5a) and near the fault (Figure 5b), compared to the respective 401 pressure constraints for caprock failure and fault slip, respectively. Initially, the model prediction 402 of the pressure changes is not accurate due to incorrect hydraulic properties and insufficient data 403 collected. For the scenarios with under-estimated reservoir properties (-40% and -20%), the 404 extraction rates are over-estimated because the pressure buildup in the reservoir is over-estimated; 405 thus, the optimization assumes that more brine extraction is needed to stay below the caprock

fracturing pressure buildup at the injection well. As a result of these excessively high extraction 406 407 rates specifically within the first ten years, the reservoir pressure near the injection well remain 408 significantly lower than the pressure limit for caprock fracturing, a safe but also costly practice. In 409 contrast, for scenarios with over-estimated initial hydraulic properties (+20% and +40%), the 410 extraction rate calculated by the optimization is significantly under-estimated. As a result, the 411 observed pressure buildup at the fault exceeds the critical value (Figure 5b, results in blue), 412 potentially causing fault reactivation and leakage. In general, a low frequency of model updates 413 may produce excessive extraction volumes for under-estimated initial hydraulic properties, 414 whereas for over-estimated initial hydraulic properties, a violation of pressure buildup constraints 415 can occur affecting the robustness and safety of the GCS operation. The adaptive management 416 strategy can reduce the risk of failure due to the uncertainties in the reservoir properties, and 417 especially at early times frequent updates of the model are needed to increase the safety and the 418 confidence of the GCS operation over long injection periods. However, safety factors and the 419 associated uncertainties must be included when determining the optimization constraints (e.g., 420 Harp et al., 2017).

Although the 10-year frequency for the model update is an extreme case as generally one would not wait 10 years for incorporating new monitoring data for model calibration, the results point to the importance of conducting a pressure management optimization with adequately calibrated prediction models based on frequent model updates, in particular early in the project. At later project stages, since more data have been collected and used to estimate the reservoir properties during the calibration step, the algorithm calculates more reliable extraction rates for controlling the pressure in the reservoir system.



430 **Figure 5.** Maximum pressure buildup evolution registered from the observation points in response 431 to applied optimal extraction rates, produced by a scenario with low frequency of updates (Δt = 10 432 years): (a) at the caprock, and (b) along the fault.

433

434 **4.2 Influence of model update frequency at early times**

435 Concerns about inadequate optimization in both directions, either excessive extraction 436 rates (when properties are under-estimated) or potential pressure constraint violation (when 437 properties are over-estimated) can be eliminated if one conducts much more frequent model 438 updates, especially at early times. For example, we demonstrate below that for cases with under-439 estimated properties, frequent model updates at early times are highly beneficial to prevent the 440 excessive extractions. Considering the scenario with hydraulic properties under-estimated by 20%, 441 the pressure at the injection well reaches the critical pressure buildup for caprock fracturing within 442 50 days (without pressure management) and very high extraction rates are estimated with model 443 updates conducted infrequently (say every three or every ten years). In contrast, if model updates 444 are applied using daily pressure data during this time interval, the calculated optimal extraction 445 rates will be very close to those for the true model even if the initial reservoir properties are off. 446 Figure 6 shows that the root-mean-square error (RMSE) between predicted and observed pressure 447 significantly drops (by ~four orders of magnitude) within a month or so (after four updates), which 448 means that the calibrated hydraulic properties are similar to the true values. However, note that for 449 more complex reservoir systems, depending on the number and type of the observations, the 450 convergence of the model results to the observations may take much longer.



452
453 Figure 6. Scenario -20%: changes in the root-mean-square error (RMSE) between model
454 predicted heads and observed heads for high frequency updates between time =0-60 days.
455

456 Thus, inadequate optimization can be avoided if more updates of the reservoir properties 457 are included during the early stages of injection. Figure 7 illustrates that the optimized extraction 458 rates computed for scenario -20% are close to the true optimal extraction rates of the reference 459 case when we include model updates with monitoring data at a frequency of as low as 3 days 460 within the early injection period. In contrast, when no initial updates are applied at earlier times 461 (i.e., Δt is fixed and equal to 3 years), the extraction rate is strongly over-estimated during the first 462 three years (solid black line), because the initial hydraulic properties of the injection formations 463 are under-estimated and the model wrongly projects strong pressure buildup at the injection well. 464



Figure 7. Calculated extraction rates based on the scenario with initial hydraulic parameters deviated by -20% are compared with the actual optimal rates for the 'true' model. 'no model updates at early times' (solid black line) corresponds to a fixed model update frequency of three years, and 'frequent model updates at early times' (dashed black) corresponds to variable frequencies of model updates (changing from three days at very early times to three years at late times).

With more initial updates, profiles of the pressure buildup (Figure 8) oscillate near the critical value due to step-wise changes in the operational extraction rates, but they never exceed the critical pressure buildups of the caprock or the fault, keeping the maximum pressure under control. As expected, the impact of the high extraction rates during the first three years in the model without frequent updates at early times is manifested on the pressure profiles. This model presents lower pressure buildups near the fault and at the injection well in comparison to the model with more frequent updates at early times. As mentioned above, the model with no updates at early 480 times (solid line) over-estimates the extraction rate for the first period when hydraulic properties 481 have not been yet updated. This strongly decreases the pressure buildup and does not require new 482 extraction until time=12 years when pressure buildup at the fault approaches the maximum 483 pressure allowed. In contrast, the model with more frequent updates at early times requires 484 pumping, correctly, at a much earlier time (6 years). For the scenarios investigated here with 485 initially under-estimated hydraulic conductivity values and less frequent updates at early times, 486 our results show that the critical pressure buildup along the fault appears as the most stringent 487 constraint, because the maximum pressure changes along the caprock, near the injection well, 488 never comes too close to the critical pressure buildup value.



Figure 8. Maximum pressure changes 'observed' based on the 'true' model for the scenario with initial hydraulic parameters deviated by -20%. 'no model updates at early times' (solid black line) corresponds to a fixed model update frequency of three years, and 'frequent updates at early times' (dashed black) corresponds to variable frequencies of model updates (changing from three days at very early times to three years at late times): (a) Pressure buildup at the injection well, and (b) Pressure buildup along the fault.

4.3 Computational cost of the adaptive management approach

499 As already pointed out in Cihan et al. (2015), the number of forward calls required by the 500 CDE algorithm used in Stage 1 and Stage 3 of the approach is high. For the scenarios applied in 501 this study (Table 2), the maximum number of calls of the forward model for one observation time 502 is 1,010 for the optimization (Stage 1) and 3,020 for the calibration (Stage 3), corresponding to a 503 CPU time (or process time) of 45 minutes and 11 minutes, respectively. Note that simulations were 504 conducted in a regular desktop PC applying parallelization. These CPU times for both stages are 505 very affordable since we employ a semi-analytical model (Section 2.1) and obviously higher CPU 506 times are expected if a reservoir simulator is employed. However, the adaptive management 507 approach can easily be parallelized to work in a high performance computing cluster. We also 508 would like to highlight that simulations related to early observations, and consequently related to 509 better and safer results, are tied to short time of simulations (less than 15 days, Figure 8). Therefore, 510 CPU times of the forward simulations of the reservoir simulator should be much lower (order of 511 magnitudes) than for later stages of the injection.

512 **5 Conclusions**

513 Industrial scale injection of CO_2 into the subsurface can cause reservoir pressure increases 514 that can be properly controlled via pressure management schemes such as brine extraction. Such 515 control is important as excessive pressure buildup in a reservoir may result in groundwater 516 contamination stemming from leakage through conductive pathways, such as improperly plugged 517 abandoned wells or distant faults, or may trigger fault reactivation and possibly seal breaching. 518 Knowledge of the subsurface properties is always incomplete, especially during the planning 519 stages of CO₂ projects because of limited site characterization data and related uncertainties. Thus, 520 during the operation of a given project, the subsurface system behavior needs to be monitored 521 continuously, and the models and their predictions need to be frequently updated to effectively and
522 safely control reservoir pressure.

523 In this study, we developed and applied an automated adaptive pressure management 524 algorithm to understand primarily the effects of initial site characterization and frequency of model 525 updates (calibration) and optimization calculations on the accuracy and the success of managing a 526 subsurface reservoir system. Adaptive optimized management uses advanced automated 527 optimization algorithms and suitable process models. Adaptive management integrates 528 monitoring, forward modeling, inverse modeling and optimization in an iterative way. The 529 hypothetical scenario considered here assumes CO₂ injection into a deep aquifer-aquitard 530 (sandstone-shale) sequence, where pressure buildup from injection increases the risk of caprock 531 failure and fault activation. We designed and optimized a pressure management strategy involving 532 a passive relief well and an active brine extraction well to reduce pressure increases to avoid 533 caprock damage near the injection well and decrease the risk of activating a nearby fault.

534 Our results show that the success of adaptive pressure management depends strongly 535 on the frequency rate of model updates and calibration, particularly at early times. Less frequent 536 optimization + monitoring/testing + calibration cycles may lead to pressure buildups that exceed 537 constraints at initial times potentially resulting in excessively high extraction rates. These 538 conditions can be avoided or eliminated if optimization + monitoring/testing + calibration 539 calculations are conducted with greater frequency, especially during the early injection period. The 540 high extraction rates that the optimization algorithm finds initially for under-estimated hydraulic 541 properties can be decreased if more model updates are conducted at the onset of injection. 542 Similarly, early model improvement for cases with initial over-estimation of d hydraulic properties

avoids the risk of under-estimating the extraction rates during the first injection years, which could
result in a violation of the pressure constraints imposed for the optimization model.

545 We demonstrated the effectiveness of adaptive pressure management for a simple case of 546 a reservoir system with a limited set of monitoring data from three observation wells. This 547 framework could easily be expanded to include diverse data sets with observations made at other 548 locations and/or over large areas comprising different physical processes such as salinity, 549 temperature, geophysical or satellite deformation, etc. We conclude that adaptive management 550 constitutes an effective tool to manage subsurface pressure and plume control in application to 551 geological CO₂ storage which could be extended to other fields where injection of fluid takes place 552 (e.g., geothermal reservoirs).

553

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683 FIGURES

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685 Figure 1. Schematic showing the pressure management strategy in this study to reduce risk of 686 caprock failure and risk of fault reactivation. The schematic shows the five top aquitards as well 687 as the five top aquifers of Table 1 (from 22 to 18). Injection of CO₂ occurs into two reservoir layers 688 (aquifers 22 and 21 in Table 1). Brines are extracted from two wells, one of them "actively" 689 pumping to the surface, the other "passively" moving brines into deeper layers. The back of the 690 schematic figure shows a hypothetical critically stressed fault, for which a maximum allowable 691 pressure change has been defined. Another pressure limit is defined to avoid caprock damage. 692 693 Figure 2. Profiles of maximum pressure buildup (in MPa) (a) at the caprock and (b) at the fault. 694 (Note that Cihan et al.'s computer program (2011) produces the results in terms of head in meters, 695 and to convert the head buildup to pressure buildup, we used a uniform brine density of 1126.026 696 kg/m^3 .) 697 698 Figure 3. Pressure buildup contours (in MPa) at time=30 years with (a) only passive extraction and 699 (b) passive and active extraction (updates every 3 years) for the +20% case in Layer 22. 700 701 Figure 4. Summary of the adaptive optimization results: Variation of the estimated brine 702 extraction ratio as a function of initial deviations from reservoir properties and model update

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frequency (Δt).

Figure 5. Maximum pressure buildup evolution registered from the observation points in response to applied optimal extraction rates, produced by a scenario with low frequency of updates (Δt = 10 years): (a) at the caprock, and (b) along the fault.

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Figure 6. Scenario -20%: changes in the root-mean-square error (RMSE) between model

710 predicted heads and observed heads for high frequency updates between time =0-60 days.

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Figure 7. Calculated extraction rates based on the scenario with initial hydraulic parameters deviated by -20% are compared with the actual optimal rates for the 'true' model. 'no model updates at early times' (solid black line) corresponds to a fixed model update frequency of 3 years, and 'frequent model updates at early times' (dashed black) corresponds to variable frequencies of model updates (changing from 3 days at very early times to 3 years at late times).

Figure 8. Maximum pressure changes 'observed' based on the 'true' model for the scenario with initial hydraulic parameters deviated by -20%. 'no model updates at early times' (solid black line) corresponds to a fixed model update frequency of 3 years, and 'frequent updates at early times' (dashed black) corresponds to variable frequencies of model updates (changing from 3 days at very early times to 3 years at late times): (a) Pressure buildup at the injection well, and (b) Pressure buildup along the fault.

TABLES

- 727 Table 1. Reference ('true') hydraulic property values of reservoir layers containing aquifers
- alternating with aquitards. The bottom layer is an aquifer, and the top layer is an aquitard.

730 Table 2. Scenarios considered for the adaptive management framework