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## Dynamic Risk Assessment for Geologic CO<sub>2</sub> Sequestration

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**Abstract:** At a geologic CO<sub>2</sub> sequestration (GCS) site, geologic uncertainty usually leads to large uncertainty in the predictions of properties that influence metrics for leakage risk assessment, such as CO<sub>2</sub> saturations and pressures in potentially leaky wellbores, CO<sub>2</sub>/brine leakage rates, and leakage consequences such as changes in drinking water quality in groundwater aquifers. The large uncertainty in these risk-related system properties and risk metrics can lead to over-conservative risk management decisions to ensure safe operations of GCS sites. The objective of this work is to develop a novel approach based on dynamic risk assessment to effectively reduce the uncertainty in the predicted risk-related system properties and risk metrics. We demonstrate our framework for dynamic risk assessment on two case studies: a 3D synthetic example and a synthetic field example based on the Rock Springs Uplift (RSU) storage site in Wyoming, USA. Results show that the U.S. National Risk Assessment Partnership's Open Source Integrated Assessment Model (NRAP-Open-IAM) coupled with a conformance evaluation can be used to effectively quantify and reduce the uncertainty in the predictions of risk-related system properties and risk metrics in GCS.

**Keywords:** Geological CO<sub>2</sub> sequestration; Dynamic risk assessment; Integrated assessment model; Data assimilation; Uncertainty quantification

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## 30 **1. Introduction**

31 One of the main concerns with geologic CO<sub>2</sub> sequestration (GCS) projects is the risk of leakage  
32 of CO<sub>2</sub> and brine to overlying resources (e.g., underground sources of drinking water (USDW),  
33 hydrocarbon and mineral resources) (Benson and Myer, 2003; Harp et al., 2016; Xiao et al., 2020).  
34 To build the confidence of stakeholders, a scientific approach is needed to quantitatively manage  
35 this risk and to provide accurate predictions of long-term risks of CO<sub>2</sub> sequestration systems  
36 (Condor et al., 2011; De Lary et al., 2015; Li and Liu, 2016; Pawar et al., 2013; Pawar et al., 2016).

37 Numerous studies have demonstrated application of quantitative approaches for risk assessment.  
38 Stauffer et al. (2009) developed CO<sub>2</sub>- Predicting Engineered Natural Systems (CO<sub>2</sub>-PENS) for  
39 GCS performance assessment and risk analysis. The design of CO<sub>2</sub>-PENS is for the purpose of  
40 performing probabilistic simulations of CO<sub>2</sub> capture, transport, storage, and leakage to overlying  
41 aquifers and ultimately the atmosphere. Zhang et al. (2011) developed a CO<sub>2</sub> sequestration module  
42 on the basis of the CQUESTRA (Carbon dioxide seQUESTRAtion) model for probabilistic risk  
43 assessment. They showed that significant CO<sub>2</sub> leakage is not likely for a site with a single injection  
44 well, while multiple potentially leaky wells present the risk of measurable leakage. Nicot et al.  
45 (2013) leveraged the certification framework (CF) (Oldenburg et al., 2009) to assess the risks of  
46 CO<sub>2</sub> and brine leakage from a storage reservoir to various overlying components such as USDWs  
47 and near-surface environments. The utilization of the CF approach to the Southeast Regional  
48 Carbon Sequestration Partnership (SECARB) Phase III CO<sub>2</sub> injection site indicated that the risks  
49 for CO<sub>2</sub> and brine leakage are both low. The U.S. Department of Energy's National Risk

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50 Assessment Partnership (NRAP) developed a scientific prediction tool for risk assessment called  
51 the Integrated Assessment Model for Carbon Sequestration (NRAP-IAM-CS) (Pawar et al., 2013;  
52 Pawar et al., 2016), and the CO<sub>2</sub>-PENS model was utilized as a foundation for developing this tool.  
53 The NRAP-IAM-CS separates a GCS operation into its key components (e.g., geologic reservoir,  
54 leakage pathway, groundwater aquifers) and simulates the physical processes within each  
55 component separately. Onishi et al. (2019) applied the NRAP-IAM-CS tool to assess GCS risk for  
56 a carbonate reservoir, specifically, Kevin Dome in Montana. They found that the potential amount  
57 of CO<sub>2</sub> leaked is affected by permeability, residual CO<sub>2</sub> saturation, CO<sub>2</sub> relative permeability  
58 hysteresis, confining rock permeability, and capillary pressure. Xiao et al. (2020) conducted risk  
59 assessment for an active CO<sub>2</sub> enhanced oil recovery (EOR) field, The Farnsworth Unit in Texas.  
60 The CO<sub>2</sub> and brine leakage risks to the overlying USDW were quantified with a proxy modeling  
61 approach. Most recently, NRAP has developed a Python-based open-source IAM (NRAP-Open-  
62 IAM) to help address questions about a potential GCS site's ability to effectively contain injected  
63 CO<sub>2</sub> and protect groundwater and other overlying environmentally sensitive receptors from CO<sub>2</sub>  
64 and brine leakage, and facilitate stakeholder decision-making about the safety and effectiveness of  
65 GCS. NRAP-Open-IAM has a collection of reduced order models (ROMs) for each potential  
66 system component in a CO<sub>2</sub> storage site, and a number of tools that can be used for risk assessment.  
67 A core capability of the NRAP-Open-IAM is to allow a user to execute stochastic and dynamic  
68 simulation of whole GCS system performance and leakage risk assessment very quickly  
69 (Vasylykivska et al., 2021).

70 The prior GCS risk assessment efforts mentioned above did not formally investigate the value  
71 of information of monitoring data (e.g., pressure, temperature and CO<sub>2</sub> saturation data) collected  
72 from monitoring wells during the operation of CO<sub>2</sub> storage. It has been demonstrated by several

73 studies that monitoring data can contribute to reducing the uncertainty of predicted risk-related  
74 system properties and risk metrics (i.e., narrowing of uncertainty bands). Oladyshkin et al. (2013)  
75 developed a workflow using bootstrap filtering and ROMs to integrate pressure measurements into  
76 reservoir models and evaluate the reduction of uncertainty in CO<sub>2</sub> leakage rate at a sequestration  
77 site. Several uncertain parameters, namely, wellbore permeability, reservoir permeability, and  
78 reservoir porosity were considered in their work. Chen et al. (2018) presented a methodology based  
79 on a filter-based data assimilation method and a proxy model to conduct network design of CO<sub>2</sub>  
80 monitoring. The optimal monitoring solution was chosen by reducing the uncertainty in the  
81 forecast of the total amount of CO<sub>2</sub> leakage. Although the methods proposed by Chen et al. and  
82 Oladyshkin et al. for assimilation of monitoring data are computationally efficient, their  
83 approaches are limited to situations involving only a limited set of uncertain parameters. Sun and  
84 Durlofsky (2019) proposed an approach using data-space inversion (DSI) to quantify uncertainty  
85 in the predictions of CO<sub>2</sub> plume locations. In the DSI approach, the distributions of CO<sub>2</sub> saturation  
86 are predicted using simulation results based on prior models together with monitoring data. It is  
87 worth mentioning that posterior models (updated models) conditional to observations were not  
88 generated in the DSI approach. This is different from the traditional data assimilation approaches  
89 such as the well-known ensemble-based methods (e.g., Ensemble Kalman Filter). Recently, Chen  
90 et al. (2020) demonstrated how uncertainty in the predictions of risks can be reduced by conducting  
91 assimilation of monitoring data, where the data assimilation is performed by using an advanced  
92 version of a state-of-the-art data assimilation approach, namely the Ensemble Smoother with  
93 Multiple Data Assimilation (ES-MDA) (Emerick and Reynolds, 2013). The risk assessment  
94 considered in their work mainly focuses on the quantification of risk-related system properties in  
95 the reservoir (e.g., pressure and CO<sub>2</sub> saturation and plume areas). High-fidelity numerical

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96 simulations of a hypothetical reservoir undergoing CO<sub>2</sub> injection and the corresponding virtual  
97 monitoring data over time, along with a series of increasingly accurate operational models  
98 developed over time during a hypothetical GCS project, were used to show reductions in the  
99 uncertainty of predictions of pressure and saturation during the period of operation of the GCS  
100 project (Doughty and Oldenburg, 2020). In this paper, we extend the work of Chen et al. (2020)  
101 and conduct a more comprehensive dynamic risk assessment where the risk can originate not only  
102 from the reservoir but also from wellbores and groundwater aquifers.

103 This paper proceeds as follows: first, we present the proposed framework for dynamic risk  
104 assessment and then we describe the two major components of the framework, i.e., conformance  
105 evaluation and risk assessment. Next, we demonstrate the proposed framework for dynamic risk  
106 assessment with two case studies: a 3D synthetic example and a synthetic field example based on  
107 the RSU site in Wyoming, USA. Finally, we present the conclusions of this paper.

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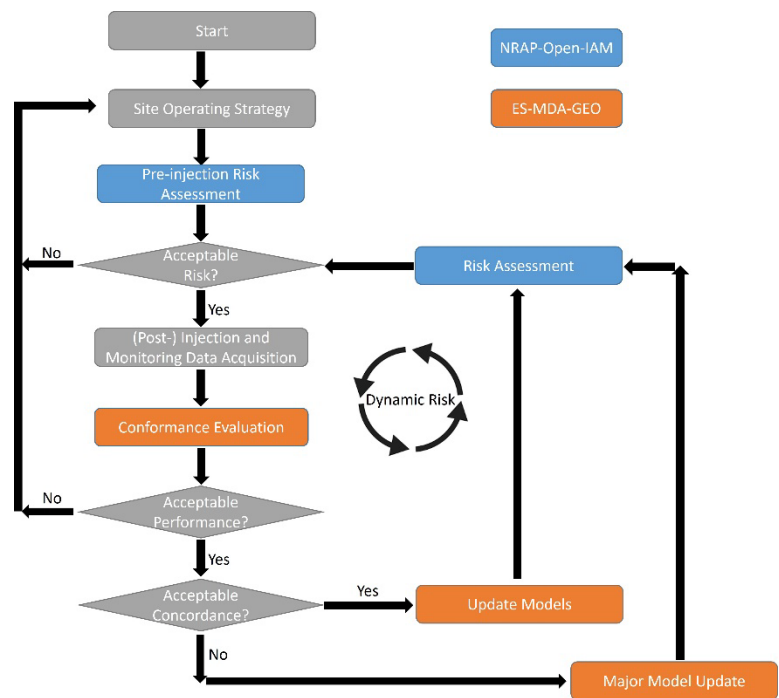
## 109 **2. Methodology**

### 110 **2.1. Dynamic risk assessment**

111 The proposed framework for dynamic risk assessment is presented in Figure 1. As can be  
112 observed from Figure 1, two main components are included in this framework, i.e., conformance  
113 evaluation and risk assessment. The conformance of a CO<sub>2</sub> sequestration system is defined as the  
114 condition under which there is acceptable past and current concordance and acceptable forecasted  
115 performance (Oldenburg, 2018). Concordance quantifies the agreement between observations and  
116 simulations, while performance indicates that the GCS operation is working to specifications, e.g.,  
117 CO<sub>2</sub> and brine leakage rates below acceptable thresholds. Risk assessment for GCS is the overall

118 process of identifying, analyzing, and quantifying risks, i.e., the product of the likelihood and  
119 consequences of possible failure scenarios. Risk assessment is part of a risk management strategy  
120 utilized to quantify potential failures of GCS such as leakage during the injection and post-  
121 injection phases. Here, dynamic risk assessment is defined as the process of iteratively identifying  
122 and evaluating GCS risks when observational data or measurements become available from a  
123 storage site. This goal of the dynamic process is to reduce the uncertainty in the predictions of risk-  
124 related system properties and risk metrics in GCS. Next, we give a brief summary of the proposed  
125 framework for dynamic risk assessment.

126



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128

129

Figure 1. The framework for dynamic risk assessment in geologic CO<sub>2</sub> sequestration.

130

131

**Step 1.** Design storage site operating strategy. With an identified CO<sub>2</sub> storage site, the site operating strategy including the number and locations of injection/monitoring wells and CO<sub>2</sub>

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132 injection schedule will be determined. Numerous studies have been conducted to identify the  
133 optimal site operating strategy (e.g., Zhang and Agarwal (2013), Yonkofski et al. (2016),  
134 Sambandam (2018), Chen et al. (2018), González-Nicolás et al. (2019)). Note the design of the  
135 site operating strategy is not the scope of this paper, and we assume the initial operating strategy  
136 is pre-determined.

137 **Step 2.** Perform pre-injection risk assessment. Prior to CO<sub>2</sub> injection, a risk assessment can be  
138 conducted using NRAP-Open-IAM or other GCS risk assessment tools to determine whether  
139 specific risks (e.g., CO<sub>2</sub>/brine leakage risks) are acceptable. If the assessed risks are not acceptable,  
140 then one needs to go back to Step 1 and adjust the site operating strategy until all the assessed risks  
141 are within the acceptable threshold.

142 **Step 3.** Start CO<sub>2</sub> injection and monitoring data acquisition. After CO<sub>2</sub> injection gets started,  
143 measurements such as pressure and CO<sub>2</sub> saturation in monitoring wells will become available.  
144 These measurements are usually collected with a particular frequency. Here, we use the data  
145 collected once per month, although they may be collected at a higher frequency. The collected  
146 monitoring measurements will be integrated into reservoir models for conformance evaluation in  
147 the next step.

148 **Step 4.** Conduct conformance evaluation and update reservoir models. In the conformance  
149 evaluation, the forecasted performance (i.e., GCS operation is working to specifications) needs to  
150 be evaluated first. If the current and forecasted GCS performance is acceptable, the next part of  
151 conformance can be evaluated, namely the agreement between observations (i.e., monitoring  
152 measurements) and reservoir simulation predictions. If there are minor discrepancies between  
153 observations and predictions made by the reservoir models, updates to the models will be made  
154 using ES-MDA-GEO, which is the most advanced version of the state-of-the-art data assimilation



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155 approach ES-MDA (Rafiee and Reynolds, 2017). Note that when there is a large discrepancy  
156 between observations and simulated results, a process of major model update by incorporating  
157 more measurements such as geophysical monitoring data and seismic data may be required (Luo  
158 et al., 2017).

159 **Step 5.** Re-calculate the predicted risk with the updated reservoir models. With the updated  
160 reservoir models, we can make more accurate predictions, with less uncertainty in risk-related  
161 system properties such as pressure ( $P$ ) and CO<sub>2</sub> saturation ( $S$ ) plumes, and P/S in monitoring and  
162 legacy wells. These improvements can also improve the accuracy of integrated assessment  
163 modeling and the predictive accuracy in the risk-related metrics or quantities, e.g., CO<sub>2</sub> and brine  
164 leakage rates and groundwater aquifer volumes with pH/TDS change. The risk assessment will be  
165 conducted periodically until no significant uncertainty reduction can be observed in the risk  
166 assessment by incorporating measurements from monitoring wells.

167 Next, more technical details about conformance evaluation and risk assessment will be  
168 provided.

## 169 **2.2. Conformance evaluation**

170 In this study, the conformance evaluation was performed using a data assimilation approach  
171 called ES-MDA with *geometric* inflation factors (ES-MDA-GEO) (Rafiee and Reynolds, 2017).  
172 It has been demonstrated that ES-MDA is superior over EnKF (Ensemble Kalman Filter) for data  
173 assimilation or history matching (Emerick and Reynolds, 2013). Although the original ES-MDA  
174 has already been shown to be an effective approach for assimilating various types of data collected  
175 from subsurface (Emerick, 2018; Evensen, 2018; Kim et al., 2018; Silva et al., 2017; Zhang et al.,  
176 2020; Zhao et al., 2017), the major drawback of the original ES-MDA algorithm is that in each  
177 data assimilation step, the inflation factors must be predetermined before the process of data

178 assimilation. To resolve this critical issue with the application of the original ES-MDA algorithm  
179 for data assimilation, Le et al. (2016) developed an adaptive approach to iteratively update the  
180 inflation factors at each step of ES-MDA data assimilation. Although this adaptive approach has  
181 reasonably improved the performance of the original version of ES-MDA algorithm, it usually  
182 needs a large number of data assimilation steps to converge, which may be computationally  
183 prohibited for large-scale field cases. Rafiee and Reynolds (2017) developed an effective and  
184 efficient approach to compute the inflation factor used at each step for data assimilation, which  
185 allows users to specify the total number of steps to be used in the process of data assimilation  
186 based on the available computing resources, while at the same time allowing enough changes in  
187 the reservoir models at each data assimilation step to control the issue of over- and under-shooting  
188 that can lead to inaccurate inversion or updating of reservoir geological models. This version of  
189 the ES-MDA algorithm is called ES-MDA-GEO and was utilized in this work for assimilating data  
190 collected from monitoring wells during sequestration operations. The major steps for the  
191 implementation of ES-MDA-GEO are shown below. Refer to Rafiee and Reynolds (2017) for  
192 more details on the implementation and theoretical derivation of this algorithm.

193

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### 194 **Pseudo-code for the implementation of ES-MDA-GEO:**

---

195 Step 1. Generate prior reservoir models denoted by  $\{m_j^{a,0}\}_{j=1}^{N_e}$  using geostatistical conditional simulation.

196 Step 2. Determine the total number of steps for data assimilation,  $N_a$ .

197 Step 3. For  $i = 1$  to  $N_a$ :

- 198 • Set  $m_j^{f,i} = m_j^{a,i-1}$  for  $j = 1, 2, \dots, N_e$ .
- 199 • Run the ensemble models from time zero.
- 200 • Calculate  $\Delta M^i$  and  $\Delta D^i$  using Eqs. 1 and 2, respectively.
- 201 • Calculate  $G_D^i$  using  $G_D^i = C_D^{-1/2} \Delta D^i$ .
- 202 • If ( $i = 1$ ) then
  - 203 • Set  $\alpha_1 = \max\{\bar{\lambda}, N_a\}$ , where  $\bar{\lambda}$  is average singular value of  $G_D^i$ .

204                   • Solve  $\frac{1-(1/\beta)^{N_a-1}}{1-(1/\beta)} = \alpha_1$  for  $\beta$ .  
 205           Else  
 206                   • Set  $\alpha_i = \beta^{i-1}\alpha_1$ .  
 207           End If  
 208       • For  $j = 1$  to  $N_e$   
 209                   • For each ensemble number, perturb the observation vector using  $d_{uc,j}^i = d_{obs} + \sqrt{\alpha_i}C_D^{1/2}z_j$ ,  
 210                   where  $z_j \sim \mathcal{N}(0, I_{N_d})$ .  
 211                   • Update the ensemble using the following equation  $m_j^{a,i} = m_j^{f,i} + \Delta M^i (G_D^i)^T [G_D^i (G_D^i)^T +$   
 212                    $\alpha_i I_{N_d}]^{-1} C_D^{-1/2} (d_{uc,j}^i - d_j^{f,i})$ .  
 213           End For  
 214   End For

---

215  
 216 where  $m$  denotes the vector of model parameters; superscripts  $a$  and  $f$  denote analysis and  
 217 forecast, respectively;  $N_e$  refers to the total number of model realizations;  $N_a$  denotes the  
 218 predefined number of data assimilation steps;  $\Delta M^i$  and  $\Delta D^i$  denote the model square root matrix  
 219 and data square root matrix, respectively, and are defined as

$$220 \quad \Delta M^i = \frac{1}{\sqrt{N_e-1}} [m_1^{f,i} - \bar{m}^{f,i}, \dots, m_{N_e}^{f,i} - \bar{m}^{f,i}], \quad (1)$$

$$221 \quad \Delta D^i = \frac{1}{\sqrt{N_e-1}} [d_1^{f,i} - \bar{d}^{f,i}, \dots, d_{N_e}^{f,i} - \bar{d}^{f,i}], \quad (2)$$

222 where

$$223 \quad \bar{m}^{f,i} = \frac{1}{N_e} \sum_{j=1}^{N_e} m_j^{f,i}, \quad (3)$$

$$224 \quad \bar{d}^{f,i} = \frac{1}{N_e} \sum_{j=1}^{N_e} d_j^{f,i}; \quad (4)$$

225  $G_D^i$  is the dimensionless sensitivity matrix;  $C_D$  is the covariance matrix of observed data  
 226 measurement errors;  $\alpha_i$  is the measurement error inflation factor at the  $i$ th data assimilation step;  
 227  $d_{obs}$  is the vector of observed data;  $d_{uc,j}^i$  is a sample from the normal distribution  $\mathcal{N}(d_{obs}, \alpha_i C_D)$ ;  
 228  $d_j^{f,i}$  denotes the forecast data obtained from the forward model evaluated at  $m_j^{f,i}$ .

229 Through conformance evaluation via ES-MDA-GEO-based data assimilation, temporal CO<sub>2</sub>  
230 sequestration site-monitoring data can be integrated into geological models. The uncertainty in  
231 reservoir parameters such as a heterogeneous permeability field can subsequently be reduced.

### 232 **2.3. Risk assessment**

233 The risk assessment for GCS was conducted using an open source integrated assessment model  
234 (NRAP-Open-IAM) developed by the U.S. Department of Energy's National Risk Assessment  
235 Partnership (NRAP) (Vasylykivska et al., 2021). The NRAP-Open-IAM has been developed to  
236 perform stochastic simulation of whole GCS system performance, leakage risk assessment and  
237 uncertainty quantification. NRAP-Open-IAM is more user-friendly (e.g., open source and  
238 customizable by its users) and has a number of new features and capabilities (e.g., uncertainty  
239 reduction and risk management) relative to its predecessor, NRAP-IAM-CS. There are three major  
240 component model types in NRAP-Open-IAM: reservoir, leakage pathways, and receptors (see  
241 Figure 2). Component models in NRAP-Open-IAM are coupled such that the outputs of one  
242 component provide inputs to the other component models.

243 By coupling different components of a GCS system in the integrated assessment modeling, the  
244 uncertainty in the predictions of different risk metrics, e.g., such as CO<sub>2</sub> and brine leakage rates  
245 and pH and TDS plume size, can be effectively quantified. By combining the conformance  
246 evaluation process with the risk assessment tool NRAP-Open-IAM, we can dynamically quantify  
247 the impact of utilizing monitoring measurements on reducing uncertainty in the predictions of  
248 different risk-related system properties such as saturation and pressure in leaking wellbores, CO<sub>2</sub>  
249 and brine leakage rates from wellbores, and risk metrics for groundwater aquifer impact such as  
250 pH and TDS plume size.

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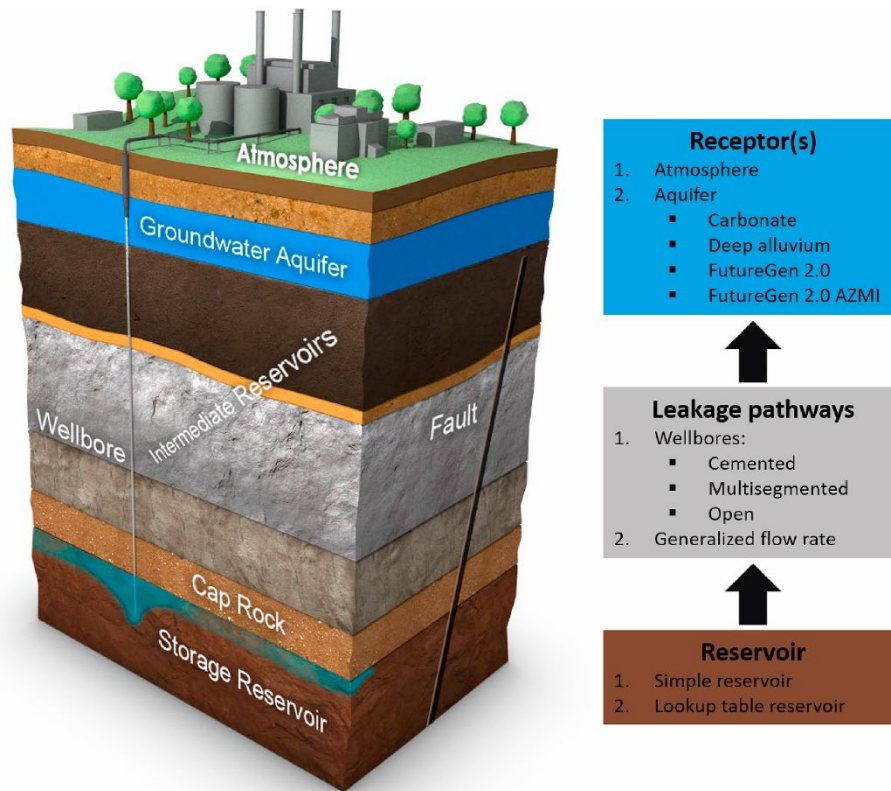


Figure 2. Base component models of NRAP-Open-IAM (Vasylykivska et al., 2021).

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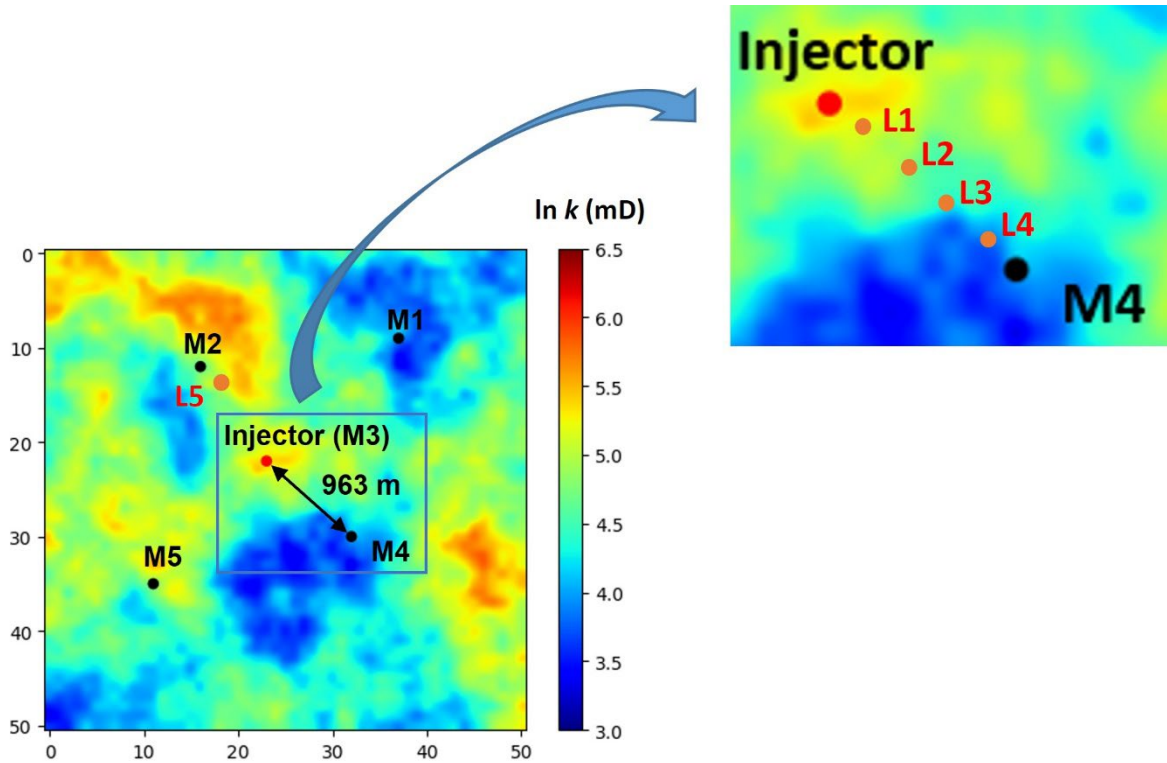
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### 255 3. Example 1: 3D Synthetic Case

#### 256 3.1. Model description

257 We first considered a 3D synthetic reservoir model with a  $51 \times 51 \times 11$  mesh. The reservoir  
258 model is  $4 \text{ km} \times 4 \text{ km}$  in the horizontal direction, and 100 m thick. The reservoir is at 1 km depth.  
259 Given that this is a synthetic case, we generated monitoring data assuming a ground-truth reservoir  
260 model. Figure 3 shows the horizontal log-permeability distribution for the top layer for the ground-  
261 truth model and the locations for injection (M3), monitoring (M1, M2, M4 and M5) and legacy  
262 wells (L1, L2, ..., L5). The remaining 10 layers follow the same horizontal log-permeability  
263 distribution as the top layer. The  $\text{CO}_2$  injection rate is equal to 1 MM ( $10^6$ ) tons per year. The  
264 injection and post-injection periods are 5 years and 10 years, respectively. The data collected from

265 the monitoring wells and injection well are CO<sub>2</sub> saturation and pressure. The data collection  
266 frequency is once per month, resulting in 12 measurements per year for CO<sub>2</sub> saturation and  
267 pressure. The collected data are subsequently assimilated into the prior models to reduce  
268 uncertainty in the risk assessment. We generated 100 prior reservoir models using unconditional  
269 sequential Gaussian geostatistical simulations. The assimilation of monitoring data to calibrate  
270 reservoir models has already been presented in the earlier work of Chen et al. (2020). In this paper,  
271 we focus on the dynamic risk assessment using NRAP-Open-IAM based on the simulation results  
272 from the calibrated models.



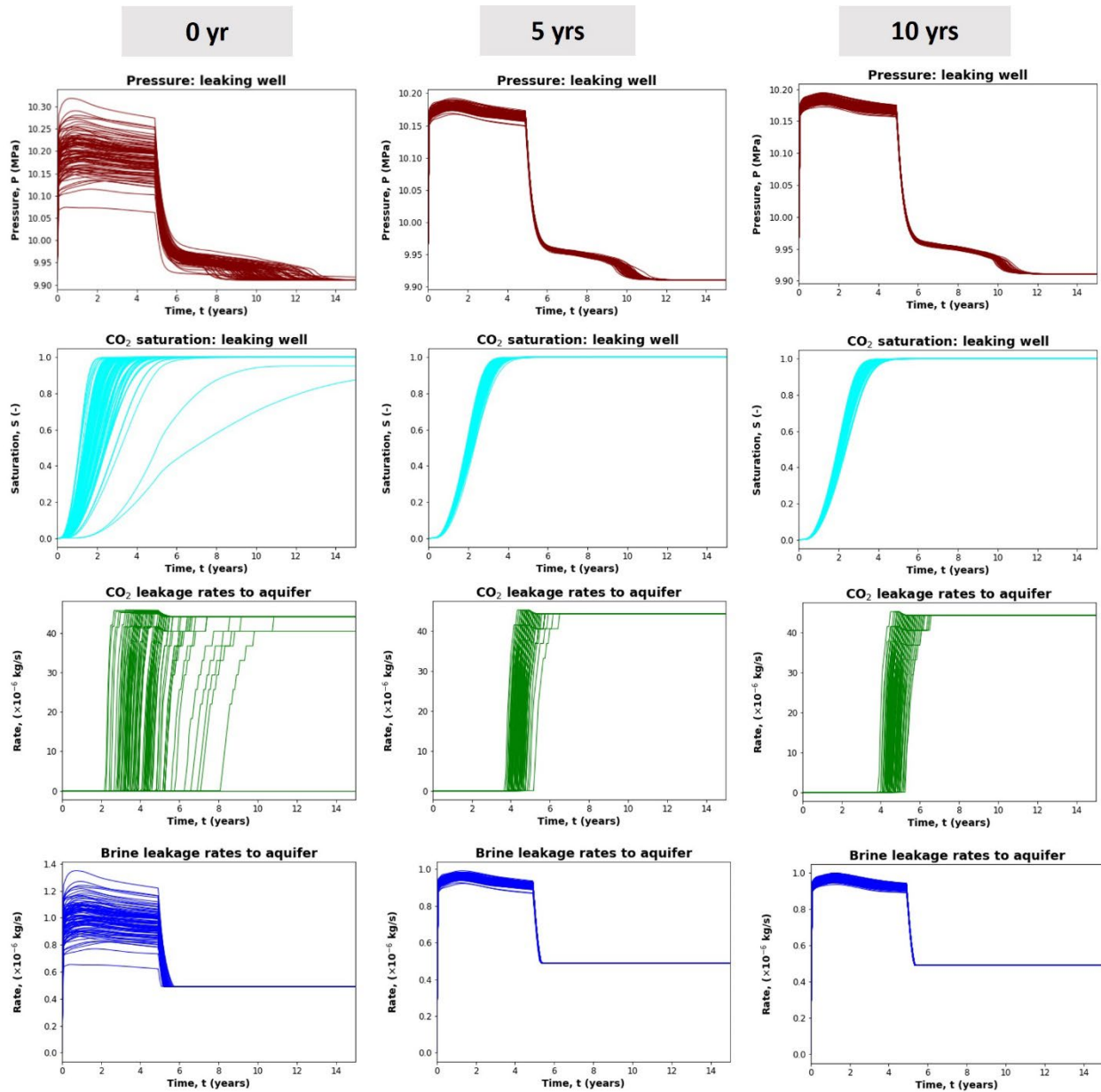
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274 **Figure 3. Horizontal log-permeability distribution for the top layer for the ground-true model and the locations**  
275 **for injector (M3), monitoring wells (M1, M2, M4, and M5) and legacy wells (L1, L2, L3, L4, and L5).**

## 276 **3.2. Results and analysis**

### 277 **3.2.1. Effect of monitoring durations**

278 To investigate the impact of monitoring durations on uncertainty reduction in the predictions of  
279 risk-related system properties and risk metrics, three different monitoring durations, namely, 0-  
280 year, 5-year and 10-year were considered. The legacy well L4 was chosen as the potentially leaky  
281 well for the dynamic risk assessment. The predictions of temporal pressure and CO<sub>2</sub> saturation in  
282 the legacy well L4 and CO<sub>2</sub> and brine leakage rates based on the prior models and the updated  
283 (posterior) models are presented in Figure 4. As shown in Figure 4, the uncertainties are relatively  
284 large in the predictions of pressure, saturation, and CO<sub>2</sub>/brine leakage rates based on the prior  
285 models (0-year monitoring; first column), whereas the uncertainties based on the predictions with  
286 updated models after assimilation of 5-year monitoring data are significantly reduced (second  
287 column). However, after 5 years (i.e., CO<sub>2</sub> injection stops), additional data collection and  
288 assimilation does not result in any further reduction in the uncertainty (third column). For instance,  
289 the time when CO<sub>2</sub> leakage to groundwater aquifer starts ranges from Year 2 to Year 8 based on  
290 the predictions with prior models that are not updated with monitoring data. This uncertainty is  
291 substantially reduced to a narrower range from 2.8 - 5.1 years through predictions with the model  
292 updated by assimilating 5 years of monitoring data. However, the range does not decrease further  
293 through predictions with the updated models by assimilating 10 years of monitoring data. It can  
294 also be observed from these figures that CO<sub>2</sub> and brine leakage rates remain constant during the  
295 post-injection period because the system properties, e.g., pressure and CO<sub>2</sub> saturation, reach a  
296 steady state, leading to constant leakage rates for CO<sub>2</sub> and brine.



297

298 **Figure 4.** The predictions of temporal pressure and CO<sub>2</sub> saturation in the legacy well L4 and CO<sub>2</sub> and brine  
299 leakage rates to aquifer based on the prior models (Column 1) and the updated models with 5 years (Column  
300 2) and 10 years (Column 3) of monitoring data.

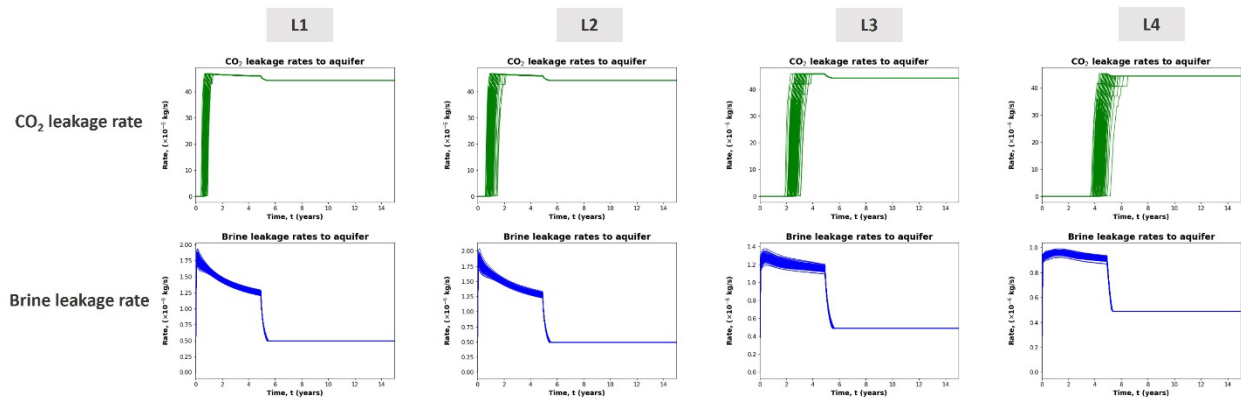
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### 302 3.2.2. Effect of legacy well locations

303 We investigated the effect of legacy well locations. We assumed four different locations  
304 between the injector and the monitoring well M4, named L1, L2, L3, and L4 on Figure 3. We



305 considered 5-year monitoring durations and used the updated models with assimilation of 5 years  
306 of monitoring data for predictions. The predictions of CO<sub>2</sub> and brine leakage rates to aquifer are  
307 shown in Figure 5. The figures show that the farther the legacy well is away from the injector, the  
308 later CO<sub>2</sub> leakage will be observed. Brine leakage is observed in the beginning of injection for all  
309 the legacy wells, but the magnitude is different. Note that the uncertainties in the predictions of  
310 CO<sub>2</sub> and brine leakage are very small. This is because all the predictions were made based on the  
311 updated models by assimilating 5 years of monitoring data. Taking L4 as an example, the reason  
312 why the observation of brine leakage is earlier than CO<sub>2</sub> leakage (see last column in Figure 5) is  
313 mainly because it takes a while for the transport of CO<sub>2</sub> from injection well to legacy well L4,  
314 while it does not take any significant time for brine to be produced from the legacy wells.



315  
316 **Figure 5. The predictions of CO<sub>2</sub> and brine leakage rates to aquifer at the legacy wells L1, L2, L3, and L4 based**  
317 **on the updated model with 5-year monitoring duration.**

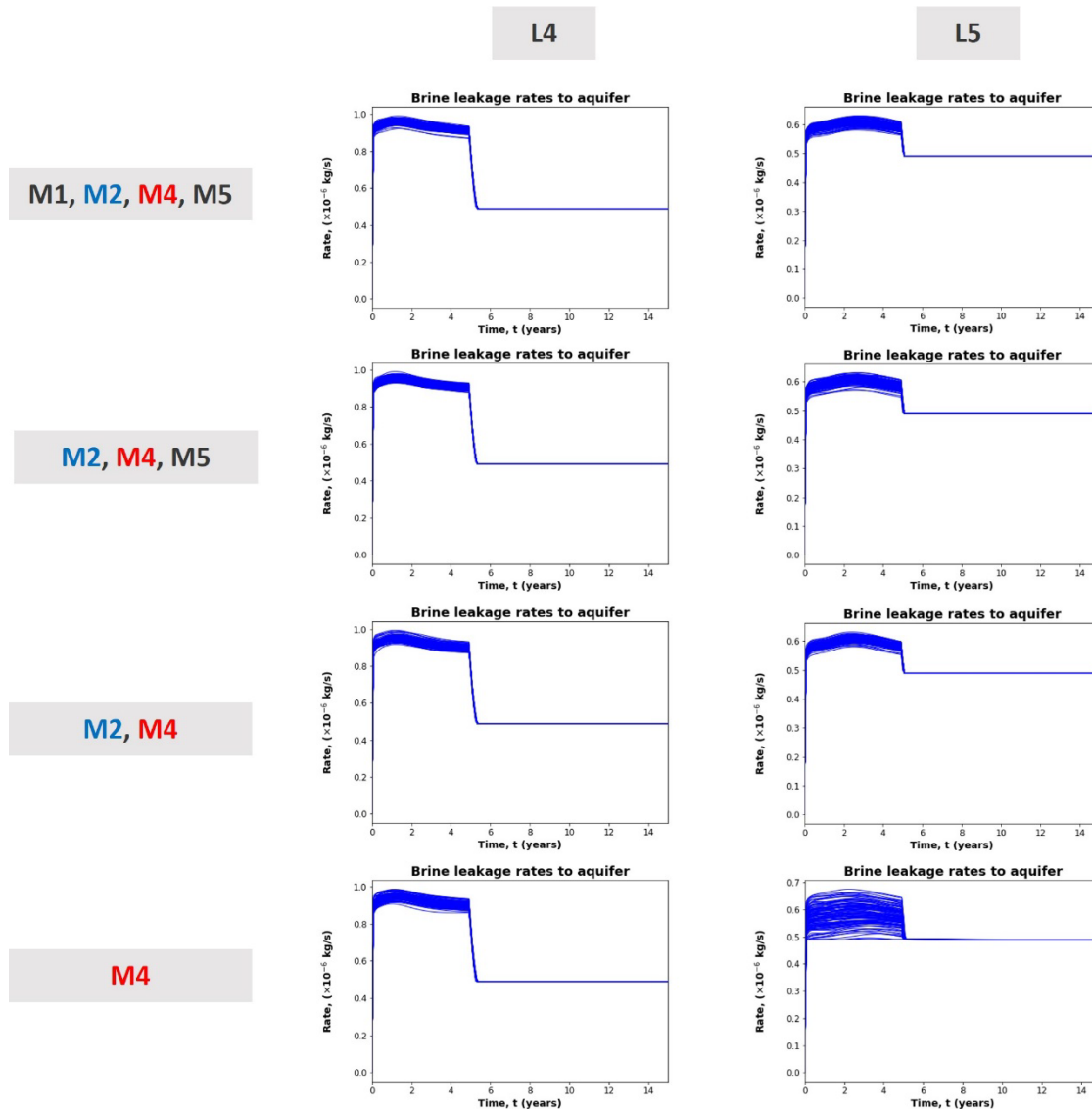
318

### 319 3.2.3. Effect of number of monitoring wells

320 In the work of Chen et al. (2020), we demonstrated that when more monitoring wells are placed  
321 in the reservoir, it usually leads to more significant improvement in reservoir models, i.e., the  
322 difference between the calibrated models and the ground-truth model is smaller. In this study, we

323 further investigated the impact of number of monitoring wells on uncertainty reduction in the  
324 predictions of risk metrics by sequentially eliminating monitoring wells M1, M5, and M2. M4  
325 remains in all scenarios. For this study, we chose legacy wells L4 and L5 as examples to  
326 demonstrate how to evaluate how much information each monitoring well contributes to reducing  
327 the uncertainty in leakage rate prediction. As can be observed from Figure 3, the location of the  
328 legacy well L4 is close to the monitoring well M4, while the location of the legacy well L5 is close  
329 to the monitoring well M2. Figure 6 presents the predictions of brine leakage rates through the  
330 legacy wells L4 and L5 based on the updated models with different number of monitoring wells.  
331 The first row of the figures corresponds to the predictions based on the updated models with all  
332 the monitoring wells (M1, M2, M4, and M5); the second row of the figures corresponds to the  
333 predictions based on the updated models with three monitoring wells (M2, M4, and M5); and the  
334 third and fourth rows of the figures correspond to the predictions based on the updated models  
335 with two (i.e., M2 and M4) and one (i.e., M4) monitoring wells, respectively. As we can see from  
336 Figure 6, we do not see any significant uncertainty reduction in the predictions of brine leakage  
337 rates when we reduce the monitoring wells M1 and M5 sequentially. This is mainly because both  
338 the legacy wells L4 and L5 have an adjacent monitoring well (M4 and M2, respectively) for the  
339 first three scenarios (i.e., cases with 4, 3 and 2 monitoring wells). The property (i.e., permeability)  
340 around L4 and L5 can be properly updated with the data collected from monitoring wells M4 and  
341 M2, so the uncertainty in the predictions such as leakage rates through L4 and L5 can be reasonably  
342 small. However, when monitoring well M2 is eliminated and only monitoring well M4 is  
343 remaining, only the permeability around well L4 can be properly updated via data assimilation,  
344 which can explain why we do not see any significant uncertainty change in the prediction of brine  
345 leakage through the legacy well L4, but the uncertainty in the prediction of brine leakage rate

346 through L5 during the injection period (0-5 year) has been significantly increased because no  
347 monitoring data are collected around L5. Similar findings have been observed for the prediction  
348 of CO<sub>2</sub> leakage rates which are not presented in this work. The results show M2 and M4 both  
349 contain information to reduce uncertainties in L5 prediction, whereas M4 contains mostly  
350 information for the prediction of leakage rate in L4.



351

352 Figure 6. The prediction of brine leakage rates through legacy wells L4 and L5 with different number of  
353 monitoring wells.

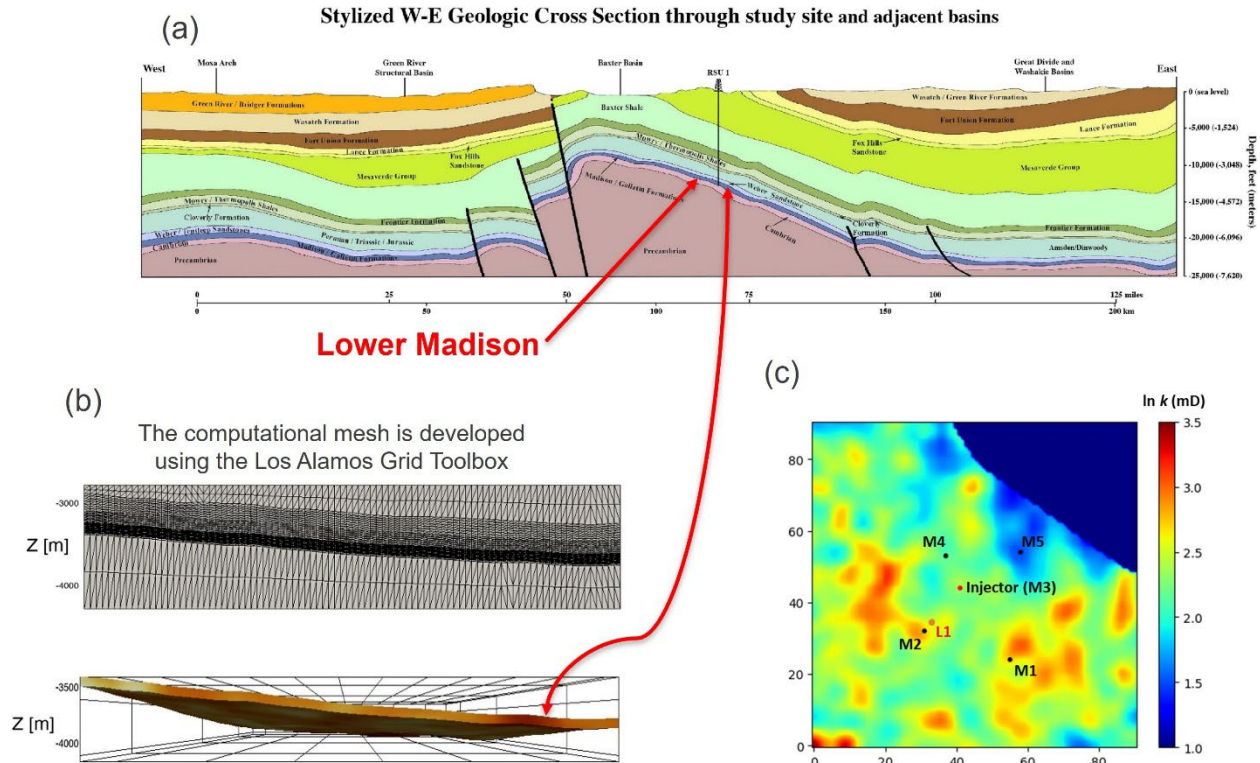
354

## 355 **4. Example 2: Rock Springs Uplift Storage Site**

### 356 **4.1. Site description**

357 The robustness of the proposed framework for dynamic risk assessment was re-evaluated using  
358 a hypothetical field site (synthetic case) based on the Rock Springs Uplift (RSU) in Wyoming,  
359 USA. The RSU site has been identified as a potential site for geologic CO<sub>2</sub> sequestration by the  
360 Wyoming Geological Survey (Surdam and Jiao, 2007). Figure 7(a) shows the geologic cross  
361 section through the site and the surrounding formations. The Lower Madison formation, as  
362 indicated by the red arrow, is one of the target storage reservoirs. The location for the exploratory  
363 well RSU 1 is chosen as the location of the CO<sub>2</sub> injection well for this study. The model dimension  
364 is 6 km × 6 km. The depth of storage reservoir (Lower Madison) ranges from 2.8 km to 4.3 km.  
365 The computational mesh of the storage reservoir shown in Figure 7(b) was developed using the  
366 Los Alamos Grid Toolbox (George et al., 1999). Figure 7(c) is the permeability distribution for  
367 the first layer in the hypothetical ground-truth model. We assume there is one injector (M3, same  
368 location as RSU 1) and four monitoring wells (M1, M2, M4, and M5), and here we consider one  
369 potential leaking well indicated by the orange dot labeled L1 in Figure 7(c). We consider the  
370 scenario where the monitoring measurements are pressures and CO<sub>2</sub> saturations. The monitoring  
371 data acquisition frequency is once per month. The CO<sub>2</sub> injection rate is 1 MM tons per year. We  
372 consider 10-year injection and 50-year post-injection periods. As with Example 1, the assimilation  
373 of monitoring data to calibrate reservoir models has already been presented in the work of Chen et  
374 al. (2020). In this study, we focus on how the risk is dynamically updated using NRAP-Open-IAM  
375 based on the simulation results from the calibrated models.

376



377  
 378 **Figure 7. RSU site description: (a) geologic cross section through the study site and adjacent basins; (b)**  
 379 **computational mesh for storage site; (c) ground-truth permeability distribution for the first layer. Geologic**  
 380 **cross section in (a) is from Surdam (2013).**

381

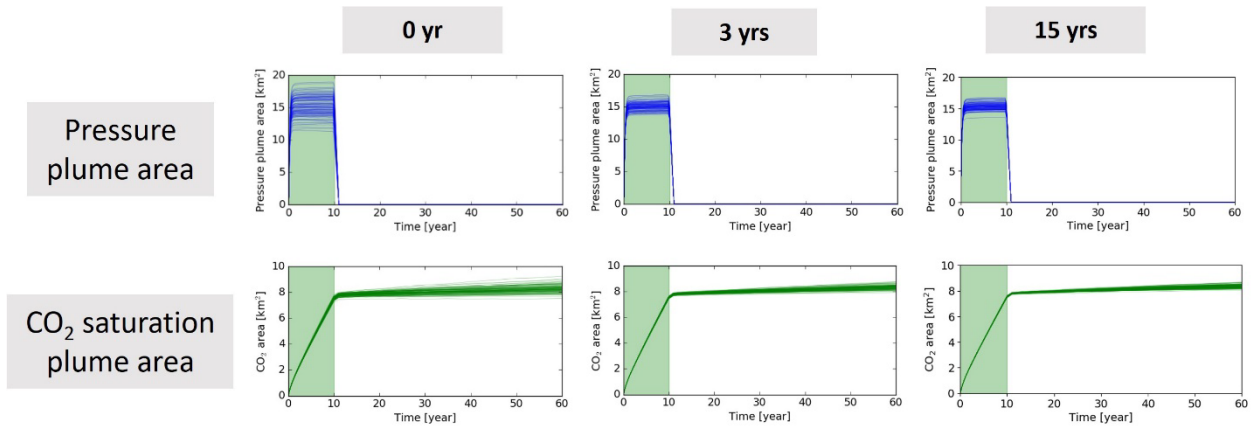
## 382 4.2. Results and analysis

383 Figure 8 and Figure 9 show the uncertainty in the predictions of pressure and CO<sub>2</sub> saturation  
 384 plume areas and other risk metrics, respectively, over increasing monitoring durations. As seen in  
 385 both figures, the predictions made using the models that have not been updated with monitoring  
 386 data have large uncertainty for both pressure plume area during the injection period (first 10 years)  
 387 and CO<sub>2</sub> saturation plume area during the post-injection period (first columns in Figure 8 and  
 388 Figure 9). However, with predictions based on updated models after assimilation of three years of  
 389 monitoring data, the uncertainty in the predictions of these quantities is significantly reduced  
 390 (second columns in Figure 8 and Figure 9). For the predictions based on the updated models with  
 391 the assimilation of 15 years of monitoring data, further uncertainty reduction was observed in the

392 predictions for some quantities, e.g., CO<sub>2</sub> saturation at legacy well (row 2 column 3 in Figure 9),  
393 CO<sub>2</sub> leakage rate to groundwater aquifer (row 3 column 3 in Figure 9) and the size of pH plume in  
394 groundwater aquifer (last row column 3 in Figure 9), but not for the remaining risk quantities. Note  
395 that the pressure plume area reduces to zero during the post-injection period (see first row in Figure  
396 8) because the side boundary condition for the reservoir model is set as a constant pressure  
397 boundary. The overpressure in the reservoir from CO<sub>2</sub> injection dissipates quickly after CO<sub>2</sub>  
398 injection stops, which is further demonstrated by the pressure change in the legacy well L1 (see  
399 first row in Figure 9). No significant change in the CO<sub>2</sub> saturation plume area was observed during  
400 the post-injection period because the pressure gradient between the injector and the side boundary  
401 substantially decreases after CO<sub>2</sub> injection stops and subsequently the movement of CO<sub>2</sub> towards  
402 the boundary slows down (see second row in Figure 8). The leakages of CO<sub>2</sub> and brine to aquifer  
403 reach a steady state during the post-injection period because the pressure and CO<sub>2</sub> saturation  
404 remain constant during the post-injection period. The pH plume volume reaches a pseudo steady  
405 state during the post-injection period because of the steady state leakage rate of CO<sub>2</sub> from reservoir  
406 through wellbore to aquifer (see last row in Figure 9).

407 It can also be observed that the monitoring data collected during injection period have more  
408 value of information than the data collected during post-injection period. The data collected during  
409 injection period leads to greater uncertainty reduction in risk-related system properties and risk  
410 metrics than the data collected during post-injection period. This is demonstrated with the two  
411 examples presented in this paper. In Example 1, most of the uncertainties in risk-related system  
412 properties and risk metrics were reduced during the injection period (first 5 years), while in  
413 Example 2, we can also see most of the uncertainties were reduced during the injection period

414 (first 3 years). This important observation can guide us when we should stop collecting data from  
415 monitoring wells for reducing uncertainty in predictions.

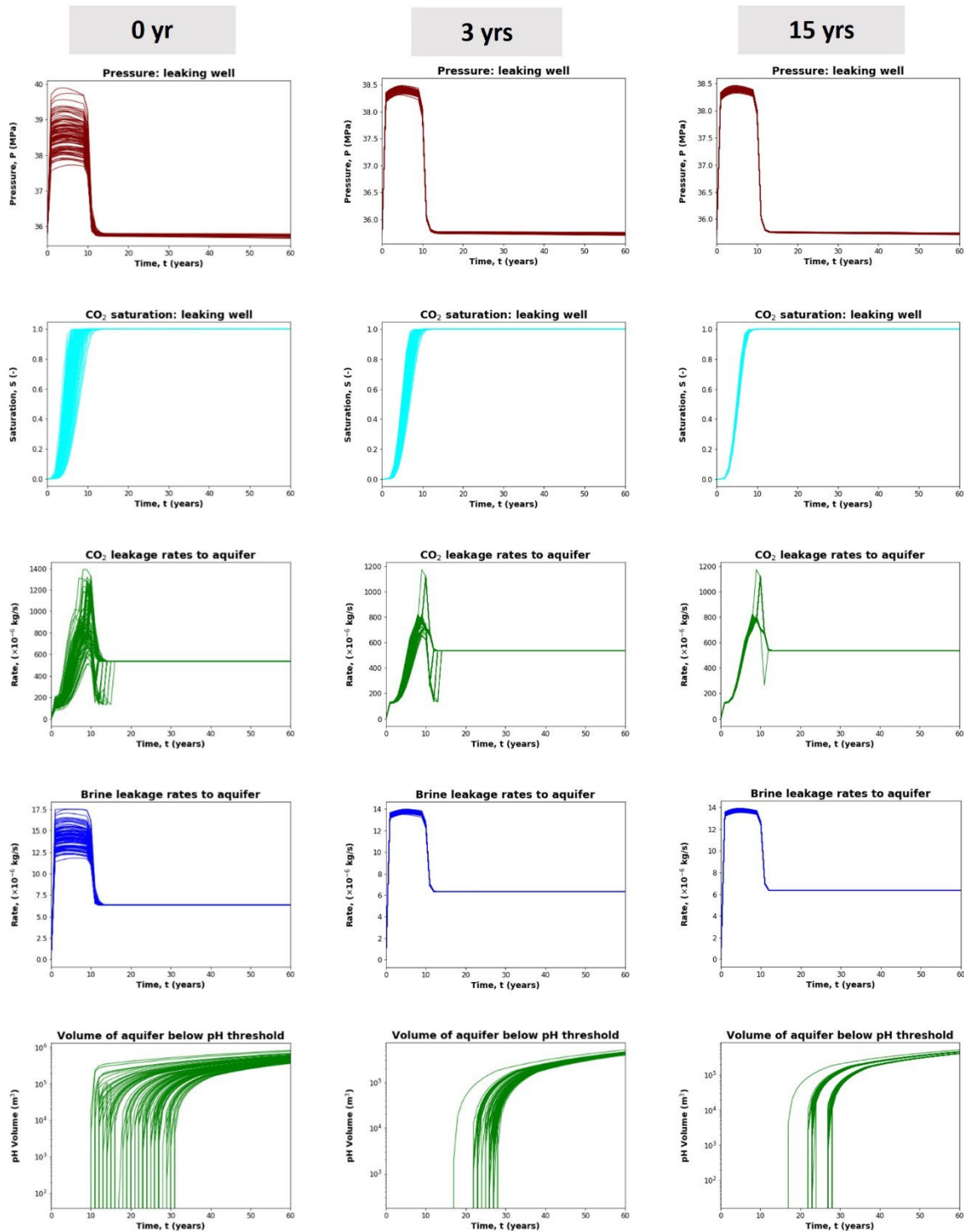


416

417

**Figure 8. Uncertainty in pressure/saturation plume areas over monitoring durations, RSU site.**

418



419  
 420 **Figure 9. Uncertainty in risk-related properties and risk metrics over the monitoring duration for the RSU site.**  
 421 **The first, second and third columns correspond to uncertainty in risk metrics or quantities based on prior**  
 422 **models, calibrated models with 3 years of monitoring data, and calibrated models with 15 years of monitoring**  
 423 **data, respectively. “leaking well” in the figures (first two rows) is hypothetical legacy well.**

424



## 425 **5. Conclusions**

426 We have demonstrated the effectiveness and robustness of the proposed framework based on  
427 coupling conformance evaluation with the NRAP-Open-IAM risk assessment tool for modeling  
428 dynamic risk with two case studies: a 3D synthetic example and a synthetic field-scale example  
429 based on the Rock Springs Uplift site in Wyoming, USA. The conformance evaluation of a GCS  
430 system was performed with a state-of-the-art ensemble-based data assimilation algorithm ES-  
431 MDA-GEO. It was observed that ES-MDA-GEO can be utilized to effectively and efficiently  
432 assimilate the monitoring measurements collected from CO<sub>2</sub> storage operations, and monitoring  
433 data assimilation can significantly reduce the uncertainties in predictions of risk-related system  
434 properties and risk metrics, e.g., pressure and CO<sub>2</sub> saturation plume areas, CO<sub>2</sub> and brine leakage  
435 rates, groundwater aquifer impact, etc. However, more data or measurements collected from  
436 monitoring wells cannot always guarantee more uncertainty reduction in the predictions of these  
437 risk-related system properties and risk metrics. We also observed that the monitoring data collected  
438 during the injection period have greater value of information than data collected during the post-  
439 injection period for uncertainty reduction.

440 It is important to note that only point data measurements from monitoring wells were considered  
441 in the conformance evaluation. This approach is consistent with the capabilities of borehole  
442 logging tools for measuring pressure and CO<sub>2</sub> saturation, and does not represent a limitation for  
443 pressure which tends to spread broadly making point measurements representative of larger-scale  
444 averages. On the other hand, for CO<sub>2</sub> saturation, it is important to note that local reservoir  
445 properties can control saturation and therefore such a local measurement does not provide the kind  
446 of integrated or large-scale measurement needed for accurate free-phase CO<sub>2</sub> plume delineation.  
447 In our future work, we will consider assimilation of spatial measurements, such as CO<sub>2</sub> saturation

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448 plume interpreted from 4D seismic in the conformance evaluation, and combine them with point  
449 measurements for a more comprehensive dynamic risk assessment.

450

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455

## 456 **References**

457 Benson, S.M., Myer, L., 2003. Monitoring to ensure safe and effective geologic sequestration of  
458 carbon dioxide, Workshop on carbon dioxide capture and storage.

459 Chen, B., Harp, D.R., Lin, Y., Keating, E.H., Pawar, R.J., 2018. Geologic CO<sub>2</sub> sequestration  
460 monitoring design: A machine learning and uncertainty quantification based approach. *Appl.*  
461 *Energy* 225, 332-345.

462 Chen, B., Harp, D.R., Lu, Z., Pawar, R.J., 2020. Reducing uncertainty in geologic CO<sub>2</sub>  
463 sequestration risk assessment by assimilating monitoring data. *Int. J. of Greenh. Gas Control* 94.

464 Condor, J., Unatrakarn, D., Wilson, M., Asghari, K., 2011. A comparative analysis of risk  
465 assessment methodologies for the geologic storage of carbon dioxide. *Energy Procedia* 4, 4036-  
466 4043.

467 De Lary, L., Manceau, J.C., Loschetter, A., Rohmer, J., Bouc, O., Gravaud, I., Chiaberge, C.,  
468 Willaume, P., Yalamas, T., 2015. Quantitative risk assessment in the early stages of a CO<sub>2</sub>

This is the manuscript form of the published paper. Please see pg. 1 for how to cite this paper.

469 geological storage project: implementation of a practical approach in an uncertain context. *Greenh.*  
470 *Gases Sci. Technol.* 5, 50-63.

471 Doughty, C., Oldenburg, C.M., 2020. CO<sub>2</sub> plume evolution in a depleted natural gas reservoir:  
472 Modeling of conformance uncertainty reduction over time. *Int. J. of Greenh. Gas Control* 97,  
473 103026.

474 Emerick, A.A., 2018. Deterministic ensemble smoother with multiple data assimilation as an  
475 alternative for history-matching seismic data. *Comput. Geosci.* 22, 1175-1186.

476 Emerick, A.A., Reynolds, A.C., 2013. Ensemble smoother with multiple data assimilation.  
477 *Comput. Geosci.* 55, 3-15.

478 Evensen, G., 2018. Analysis of iterative ensemble smoothers for solving inverse problems.  
479 *Comput. Geosci.* 22, 885-908.

480 George, D., Kuprat, A., N. Carlson, Gable, C., 1999. LaGriT–Los Alamos Grid Toolbox.

481 González-Nicolás, A., Cihan, A., Petrusak, R., Zhou, Q., Trautz, R., Riestenberg, D., Godec, M.,  
482 Birkholzer, J.T., 2019. Pressure management via brine extraction in geological CO<sub>2</sub> storage:  
483 Adaptive optimization strategies under poorly characterized reservoir conditions. *Int. J. of Greenh.*  
484 *Gas Control* 83, 176-185.

485 Harp, D.R., Pawar, R., Carey, J.W., Gable, C.W., 2016. Reduced order models of transient CO<sub>2</sub>  
486 and brine leakage along abandoned wellbores from geologic carbon sequestration reservoirs. *Int.*  
487 *J. of Greenh. Gas Control* 45, 150-162.

488 Kim, S., Min, B., Lee, K., Jeong, H., 2018. Integration of an iterative update of sparse geologic  
489 dictionaries with ES-MDA for history matching of channelized reservoirs. *Geofluids* 2018.

490 Le, D.H., Emerick, A.A., Reynolds, A.C., 2016. An adaptive ensemble smoother with multiple  
491 data assimilation for assisted history matching. SPE J. 21, 195–207.

492 Li, Q., Liu, G., 2016. Risk assessment of the geological storage of CO<sub>2</sub>: A review, *Geologic  
493 Carbon Sequestration*. Springer, pp. 249-284.

494 Luo, X., Bhakta, T., Jakobsen, M., Nævdal, G., 2017. An ensemble 4D-seismic history-matching  
495 framework with sparse representation based on wavelet multiresolution analysis. SPE J. 22, 985-  
496 1010.

497 Nicot, J.-P., Oldenburg, C.M., Houseworth, J.E., Choi, J.-W., 2013. Analysis of potential leakage  
498 pathways at the Cranfield, MS, USA, CO<sub>2</sub> sequestration site. *Int. J. of Greenh. Gas Control* 18,  
499 388-400.

500 Oladyshkin, S., Class, H., Nowak, W., 2013. Bayesian updating via bootstrap filtering combined  
501 with data-driven polynomial chaos expansions: methodology and application to history matching  
502 for carbon dioxide storage in geological formations. *Comput. Geosci.* 17, 671-687.

503 Oldenburg, C.M., 2018. Are we all in concordance with the meaning of the word conformance,  
504 and is our definition in conformity with standard definitions? *Greenh. Gases Sci. Technol.* 8, 210-  
505 214.

506 Oldenburg, C.M., Bryant, S.L., Nicot, J.-P., 2009. Certification framework based on effective  
507 trapping for geologic carbon sequestration. *Int. J. of Greenh. Gas Control* 3, 444-457.

508 Onishi, T., Nguyen, M.C., Carey, J.W., Will, B., Zaluski, W., Bowen, D.W., Devault, B.C., Duguid,  
509 A., Zhou, Q., Fairweather, S.H., Spangler, L.H., Stauffer, P.H., 2019. Potential CO<sub>2</sub> and brine  
510 leakage through wellbore pathways for geologic CO<sub>2</sub> sequestration using the National Risk

This is the manuscript form of the published paper. Please see pg. 1 for how to cite this paper.

- 511 Assessment Partnership tools: Application to the Big Sky Regional Partnership. *Int. J. of Greenh.*  
512 *Gas Control* 81, 44-65.
- 513 Pawar, R., Bromhal, G., Dilmore, R., Foxall, B., Jones, E., Oldenburg, C., Stauffer, P., Unwin, S.,  
514 Guthrie, G., 2013. Quantification of Risk Profiles and Impacts of Uncertainties as part of US  
515 DOE's National Risk Assessment Partnership (NRAP), GHGT-11.
- 516 Pawar, R., Bromhal, G.S., Chu, S., Dilmore, R.M., Oldenburg, C.M., Stauffer, P.H., Zhang, Y.,  
517 Guthrie, G.D., 2016. The National Risk Assessment Partnership's integrated assessment model for  
518 carbon storage: A tool to support decision making amidst uncertainty. *Int. J. of Greenh. Gas*  
519 *Control* 52, 175-189.
- 520 Rafiee, J., Reynolds, A.C., 2017. Theoretical and efficient practical procedures for the generation  
521 of inflation factors for ES-MDA. *Inverse Problems* 33.
- 522 Sambandam, S.T., 2018. Optimization of CO<sub>2</sub> storage systems with constrained bottom-hole  
523 pressure injection. Master's Thesis, Stanford University, Department of Energy Resources  
524 Engineering.
- 525 Silva, V.L.S., Emerick, A.A., Couto, P., Alves, J.L.D., 2017. History matching and production  
526 optimization under uncertainties—Application of closed-loop reservoir management. *J. Petrol. Sci.*  
527 *Eng.* 157, 860-874.
- 528 Stauffer, P.H., Viswanathan, H.S., Pawar, R.J., Guthrie, G.D., 2009. A System Model for Geologic  
529 Sequestration of Carbon Dioxide. *Environ. Sci. Technol.* 43, 565-570.
- 530 Sun, W., Durlafsky, L.J., 2019. Data-space approaches for uncertainty quantification of CO<sub>2</sub>  
531 plume location in geological carbon storage. *Adv. Water Resour.* 123, 234-255.

- 532 Surdam, R.C., 2013. Geological CO<sub>2</sub> storage characterization: The key to deploying clean fossil  
533 energy technology. Springer Science & Business Media.
- 534 Surdam, R.C., Jiao, Z., 2007. The Rock Springs Uplift: An outstanding geological CO<sub>2</sub>  
535 sequestration site in southwest Wyoming. Wyoming State Geological Survey.
- 536 Vasylykivska, V., Dilmore, R., Lackey, G., Zhang, Y., King, S., Bacon, D., Chen, B., Mansoor, K.,  
537 Harp, D., 2021. NRAP-Open-IAM: A Flexible Open Source Integrated Assessment Model for  
538 Geologic Carbon Storage Risk Assessment and Management. Environ. Model. Softw. 143, 105114.
- 539 Xiao, T., McPherson, B., Esser, R., Jia, W., Dai, Z., Chu, S., Pan, F., Viswanathan, H., 2020.  
540 Chemical Impacts of Potential CO<sub>2</sub> and Brine Leakage on Ground water Quality with Quantitative  
541 Risk Assessment: A Case Study of the Farnsworth Unit. Energies 13, 6574.
- 542 Yonkofski, C.M., Gastelum, J.A., Porter, E.A., Rodriguez, L.R., Bacon, D.H., Brown, C.F., 2016.  
543 An optimization approach to design monitoring schemes for CO<sub>2</sub> leakage detection. Int. J. of  
544 Greenh. Gas Control 47, 233-239.
- 545 Zhang, Q., Jiang, S., Wu, X., Wang, Y., Meng, Q., 2020. Development and Calibration of a  
546 Semianalytic Model for Shale Wells with Nonuniform Distribution of Induced Fractures Based on  
547 ES-MDA Method. Energies 13, 3718.
- 548 Zhang, Y., Vouzis, P., Sahinidis, N.V., 2011. GPU simulations for risk assessment in CO<sub>2</sub>  
549 geologic sequestration. Comput. Chem. Eng. 35, 1631-1644.
- 550 Zhang, Z., Agarwal, R., 2013. Numerical simulation and optimization of CO<sub>2</sub> sequestration in  
551 saline aquifers. Comput. Fluids 80, 79-87.
- 552 Zhao, Y., Forouzanfar, F., Reynolds, A.C., 2017. History matching of multi-facies channelized  
553 reservoirs using ES-MDA with common basis DCT. Comput. Geosci. 21, 1343-1364.