

NRAP Toolkit Screening for CarbonSAFE Illinois – Macon County

Nicolas Huerta^a, Diana Bacon^a, Carl Carman^b, Christopher Brown^a

^aPacific Northwest National Laboratory, PO Box 999, Richland, WA, 99352

*^bUniversity of Illinois, Illinois State Geological Survey, 615 E. Peabody Dr.,
Champaign, IL, 61820, USA*

This report was prepared for:
CarbonSAFE Macon County
US DOE 00029381

Principal Investigator: Dr. Steve Whittaker
Illinois State Geological Survey
615 E. Peabody Dr.
Champaign, IL, 61820-7406

I ILLINOIS
Illinois State Geological Survey
PRAIRIE RESEARCH INSTITUTE



**Pacific
Northwest**
NATIONAL LABORATORY

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, or manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Executive Summary

Geologic carbon storage (GCS) is one of several technologies being developed to mitigate climate change by reducing the emission of carbon dioxide to the atmosphere from industrial point sources, like coal-fired powerplants or ethanol production plants. Through the U.S. Department of Energy's (DOE) CarbonSAFE program the Illinois State Geologic Survey is leading a multi-stage project to identify, characterize, develop, and operate an industrial-scale GCS project that would capture, transport, and inject 50 million metric tons (Mt) of CO₂ into the Mt. Simon Sandstone formation.

As part of the characterization and development effort, an iterative risk assessment is being developed as site-specific information becomes available. This risk assessment will facilitate permitting of the injection well, inform monitoring technology deployment, estimate the fluid and pressure plumes' movement, and capture project risk for insurance and operational decisions. This study employs tools being developed by the National Risk Assessment Partnership (NRAP), another U.S. DOE program that is quantifying the science underpinning the risks associated with GCS operations. These tools are being improved by application to field projects, like those within the CarbonSAFE program, with the overall programmatic goal of both efforts to accelerate the commercial deployment of GCS.

In this report we take stratigraphic data from the ISGS-led Macon County Phase 2 CarbonSAFE's proposed site in Christian County, Illinois, and conduct reservoir simulations to generate pressure and CO₂ saturation plume data as a function of time. We then use this plume data along with the stratigraphic data as inputs to the NRAP Open-source Integrated Assessment Model (NRAP-Open-IAM) to evaluate project risks. For this report we focus on the probabilistic risk associated with hypothetical leakage of CO₂ and brine along the injection well and one monitoring well. We also study the resulting impact to two overlying aquifers, which could be used to inform monitoring technology selection.

Our results indicate that for all realizations and for both hypothetical wells, the modeled leak rate into the aquifers is low and the total amount is far below the 1% leakage value commonly cited as the acceptable criteria for fluid leakage in GCS. Both the injection well and the monitoring well had CO₂ and brine leaks along their pathway and into overlying aquifers. As expected, the leak rate would be highest if it occurred along the injection well. Change to the overlying aquifer was observed for all three metrics studied (pH, pressure, and TDS). However, impacts were generally localized around a very small (meter-scale) radius for a given well. The notable exception was for an impact to pH in the St. Peter aquifer, which was projected to extend for 10's of meters away from the leaky well.

Results of this exercise are being used to improve the NRAP risk assessment models for eventual use in the EPA's Class VI injection well permitting processes and to inform Phase 3 CarbonSAFE projects as they further develop monitoring strategies and expand the subsurface risk assessments for their sites.

Acronyms and Abbreviations

AZMI	Above Zone Monitoring Intervals
CarbonSAFE	Carbon Storage Assurance Facility Enterprise
DOE	Department of Energy
DREAM	Designs for Risk Evaluation and Management
GCS	Geologic Carbon Storage
IAM	Integrated Assessment Model
ISGS	Illinois State Geological Survey
NRAP	National Risk Assessment Partnership
NRAP-Open-IAM	NRAP Open Integrated Assessment Model
PNNL	Pacific Northwest National Laboratory
STOMP	Subsurface Transport Over Multiple Phases
TDS	Total Dissolved Solids
USDW	Underground Source of Drinking Water
ROM	Reduced Order Model

Contents

Executive Summary	2
Acronyms and Abbreviations.....	33
Contents	4
1.0 Introduction	6
2.0 Methods.....	7
2.1 Workflow.....	7
2.2 Geologic and reservoir model.....	8
2.3 Subsurface Transport Over Multiple Phases (STOMP) reservoir simulations	11
2.3.1 Initial and boundary conditions	Error! Bookmark not defined.
2.4 NRAP Open Integrated Assessment Model (NRAP-Open-IAM).....	12
3.0 Results.....	14
3.1 Reservoir simulations: Pressure and saturation evolution	14
3.2 NRAP-Open-IAM risk forecasting.....	18
3.2.1 Leakage flux.....	18
3.2.2 Leak impact.....	20
3.2.3 Monitoring recommendations	24
4.0 Discussion and Conclusions	24
5.0 References	26

Figures

<i>Figure 1 – General workflow for assessing the subsurface risks associated with the injection of carbon dioxide.....</i>	<i>7</i>
<i>Figure 2 – Domain map showing T. R. McMillen as a hypothetical injection well, and a hypothetical monitoring well 2.5 km to the east.....</i>	<i>8</i>
<i>Figure 3 – Stratigraphic model for the Christian County site and simplified geologic model used in the STOMP reservoir simulations and in the NRAP-Open-IAM analysis.</i>	<i>10</i>
<i>Figure 4 – Reservoir simulation results showing the grid used (a.) and the CO₂ saturation iso-surface ($S_{CO_2} > 0.01$) at (b.) 5 years, (c.) 10 years, (d.) 30 years, (e.) 40 years, and (f.) 60 years. Note that the x-axis and y-axis are at different scales than the z-axis.</i>	<i>14</i>
<i>Figure 5 – Reservoir simulation results showing an x-axis slice at 8,500 m (across the injection well location). Plotted on the images is the pressure differential in MPa from time 0 years to (a.) 1 year, (b.) 5 years, (c.) 10 years, (d.) 30 years, (e.) 40 years, and (f.) 60 years.</i>	<i>15</i>
<i>Figure 6 – Reservoir simulation results showing an x-axis slice at 8,500 m (across the injection well location). Plotted on the images is the CO₂ saturation at time (a.) 1 year, (b.) 5 years, (c.) 10 years, (d.) 30 years, (e.) 40 years, and (f.) 60 years.</i>	<i>16</i>

<i>Figure 7 – Reservoir simulation results for the top of Layer B (z-node 36) at a depth of -1,821.2 m. The black contours show the fluid pressure in MPa and the red contour shows the CO₂ saturation of 0.01 at times: (a.) 1 year, (b.) 5 years, (c.) 10 years, (d.) 35 years, (e.) 40 years, and (f.) 60 years.</i>	17
<i>Figure 8 – Reservoir simulation results for the top of Layer B (z-node 36) at a depth of -1,821.2 m. The red line shows the contour for CO₂ saturation at 0.01. The black contours show the change in pressure in MPa from the initial time to the following times: (a.) 1 year, (b.) 5 years, (c.) 10 years, (d.) 35 years, (e.) 40 years, and (f.) 60 years.</i>	17
<i>Figure 9 – Stochastic realizations (n = 50) for leak rates (top) and cumulate mass leaked (bottom) of brine and CO₂ up the injection well. Mass rates are shown for leakage into the atmosphere, St. Peter aquifer, and the Ironton-Galesville aquifer (top to bottom respectively). Cumulative mass is shown for the St. Peter aquifer and Ironton-Galesville (top to bottom respectively).</i>	19
<i>Figure 10 – Stochastic realizations (n = 50) for leak rates (top) and cumulate mass leaked (bottom) of brine and CO₂ up the monitoring well. Mass rates are shown for leakage into the atmosphere, St. Peter aquifer, and the Ironton-Galesville aquifer (top to bottom respectively). Cumulative mass is shown for the St. Peter aquifer and Ironton-Galesville (top to bottom respectively).</i>	20
<i>Figure 11 – Stochastic realizations (n = 50) for impacts to the St. Peter aquifer and Ironton-Galesville aquifer at the injection well. (left column) Volume of the aquifers impacted by a perturbation in pressure (top), pH (middle), and TDS (bottom). (right column) Radius of the aquifers impacted by a perturbation in pressure (top), pH (middle), and TDS (right).</i>	22
<i>Figure 12 – Stochastic realizations (n = 50) for impacts to the St. Peter aquifer and Ironton-Galesville aquifer at the monitoring well. (left column) Volume of the aquifers impacted by a perturbation in pressure (top), pH (middle), and TDS (bottom). (right column) Radius of the aquifers impacted by a perturbation in pressure (top), pH (middle), and TDS (right).</i>	23

Tables

Table 1 – Reservoir initial and boundary conditions.	11
Table 2 - Properties for the Mt. Simon Layers used in STOMP simulations.	12
Table 3 – Stochastic and deterministic parameters used in the NRAP-Open-IAM analysis.	13

Introduction

Geologic carbon storage (GCS) is one technology being developed to reduce anthropogenic atmospheric emissions of carbon dioxide from industrial plants. Fully deploying this technology will contribute to the United States maintaining its energy independence and security. To accelerate this technology, the U.S. Department of Energy's Office of Fossil Energy is leading an initiative called the Carbon Storage Assurance Facility Enterprise (CarbonSAFE) (U.S. DOEa) to provide funding for the development of GCS sites that can be used to store 50+ million metric tons of CO₂ from industrial sources. As part of the CarbonSAFE initiative, the Illinois State Geological Survey (ISGS) is leading a project to develop a storage site in central Illinois. This project is officially identified as CarbonSAFE Illinois Macon County (FE0029381) (U.S. DOEb), which was the original target location. During execution of the project, neighboring Christian County was identified as a more attractive candidate site due to more optimal storage conditions.

As part of this Phase 2 CarbonSAFE effort, the ISGS and Pacific Northwest National Laboratory (PNNL) have conducted an initial assessment of the technical feasibility of storing CO₂ at the site and identified the subsurface risks associated with such operations. This feasibility study includes conducting a reservoir simulation using preliminary data from stratigraphic wells in the area. The results from the reservoir simulations are used as inputs to the NRAP Open-source Integrated Assessment Model (NRAP-Open-IAM). The NRAP-Open-IAM is a python-based, publicly available systems-level model that can be used to stochastically simulate risk at a GCS. The NRAP-Open-IAM takes in the reservoir simulation results, along with data on the stratigraphy, well leak properties, fluid properties, and utilizes component modules to conduct an analysis to estimate risk over time. Risk in this exercise focuses on brine and/or CO₂ leakage into aquifers from the two wells that will be used in the GCS operation, the injection well and a single monitoring well. In addition to leak rates for brine and CO₂, the NRAP-Open-IAM analysis looks at the impact of this leakage on three metrics (pressure, Total Dissolved Solids (TDS), and pH) that are indicators of changes to aquifer quality and are also used as monitoring metrics to detect leaks. The results of this work will inform CarbonSAFE decisions and help to improve the NRAP tools for eventual deployment during Phase 3 CarbonSAFE efforts.

Methods

Workflow

The overall tool application workflow created by NRAP is under further development and is being informed by application to the CarbonSAFE projects. In this project we considered a workflow consisting of four sequential steps (Figure 1). The first step is to define the system using available data. Specific components of this include the geometry, geology, and properties of the subsurface system. This data is needed to construct the stratigraphic model, reservoir model, and to provide parameters used in subsequent steps. The second step is to conduct reservoir simulations using STOMP and the operational parameters defined for the storage project. The output of these simulations provides the reservoir pressure and CO₂ saturation plumes in time and space. These parameters are the key risk drivers and are used as inputs to the subsequent steps. The third step is using the NRAP-Open-IAM to conduct a risk assessment to forecast leak rates of brine and CO₂ into overlying aquifers and assess the impact of leakage on the aquifers. In addition to leak rates and impacts, the NRAP-Open-IAM results act as inputs for the final step, application of NRAP's Designs for Risk Evaluation And Management (DREAM) tool, which uses the time-to-first-detect maps and produces data to inform where monitoring deployment will be most impactful (Bacon et al., 2019; Yonkofski et al., 2019). As will be discussed in Section 4.0, results from application of the DREAM tool were ultimately not presented in this report but remain as a critical component to the eventual NRAP workflow and capabilities. The following sub-sections give more details about the implementation of each step.

Risk assessment workflow for CarbonSAFE Macon (Christian Co.)

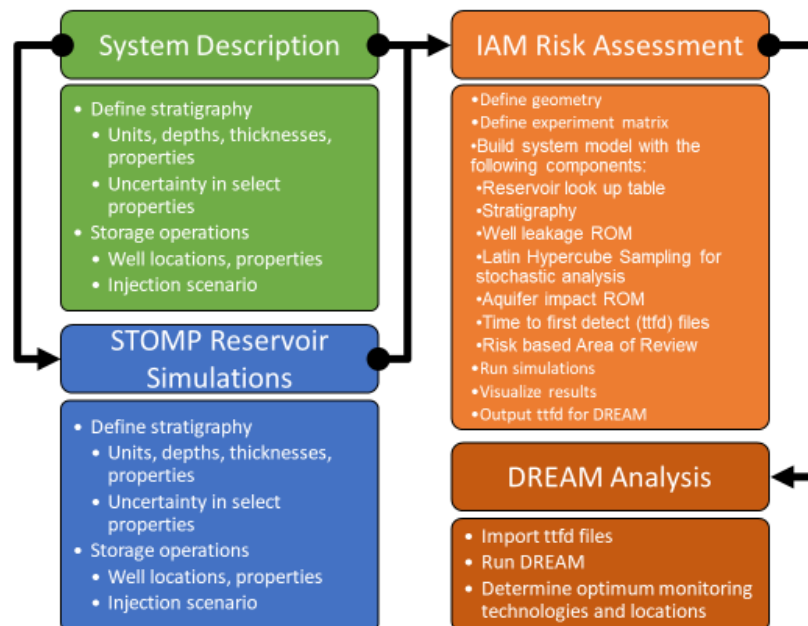


Figure 1 – General workflow for assessing the subsurface risks associated with the injection of carbon dioxide.

Geologic and Reservoir Model

T.R. McMillen No. 2 was drilled as part of the CarbonSAFE program and provides information regarding formation tops (Whittaker and Freiburg, 2018) and subsurface properties in the vicinity (Figure 2). Figure 3 shows the full stratigraphy observed from the well and the simplified stratigraphy used in this study. For this work we define the Mt. Simon Sandstone as the storage reservoir, which is divided into five distinct layers labeled

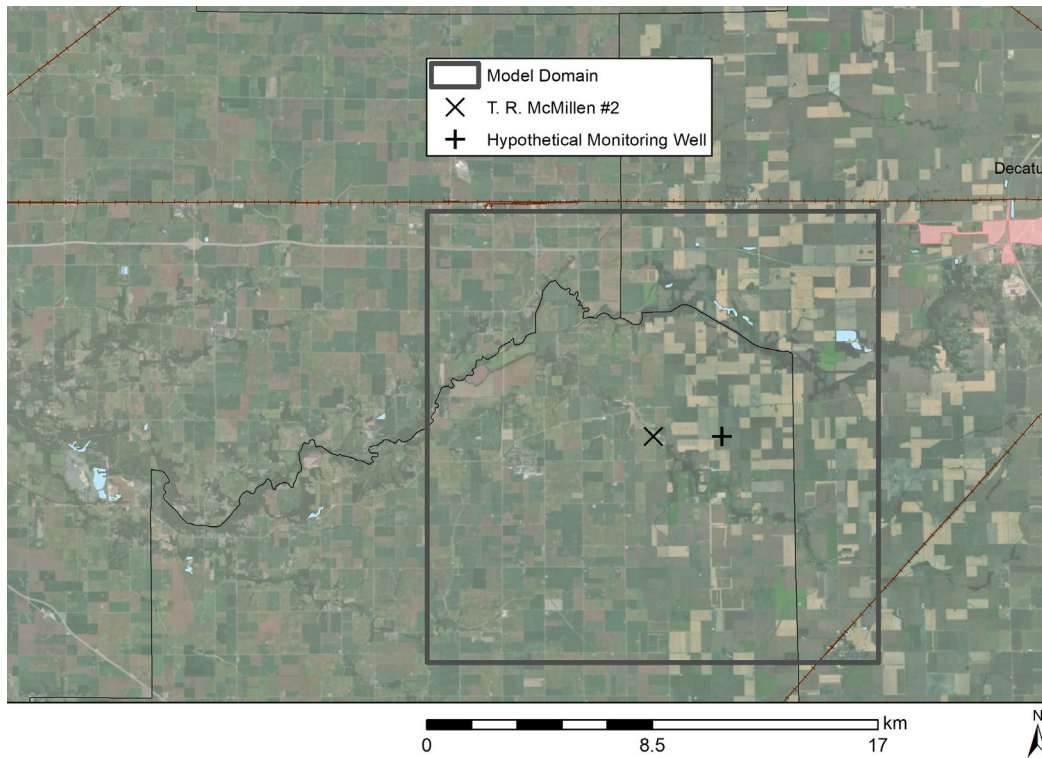


Figure 2 – Domain map showing T. R. McMillen as a hypothetical injection well, and a hypothetical monitoring well 2.5 km to the east.

Layer A to Layer E from the bottom to top of the formation. Overlying the reservoir are five units that are alternating “shales” and “aquifers.” Note that the shales are generally a grouping of several distinct formations that are not necessarily shales but are characterized by their relatively low permeabilities and are assumed to be non-transmissive for this exercise. The aquifers are individual formations that have sufficient permeability to act as Above Zone Monitoring Intervals (AZMIs) or have Total Dissolved Solids (TDS) low enough to be considered an Underground Source of Drinking Water (USDW) by regulators. The two aquifers included in our simulations are the Ironton-Galesville formation, an AZMI just above the Shale 1 overlying the injection reservoir, and the shallower St. Peter Sandstone, the lowermost USDW at the site.

The domain size used is 17 km north-to-south and 17 km east-to-west. Depth to the top of the Mt. Simon is 1,565.15 m which is 355.09 m thick at the site. The injection well is located at 8,502 m in the x-direction and 8,502 m in the y-direction. The monitoring well is placed within the expected

CO₂ plume footprint at 11,000 m in the x-direction and 8,502 m in the y-direction. Thus, the wells are placed 2,498 m apart.

For the STOMP reservoir simulations only the Mt. Simon Sandstone was used. The reservoir grids were generated using GRIDDER software (Los Alamos National Laboratory, 2016). While there can be a dip in the Illinois Basin's Mt. Simon formation, the dip and dip direction had not been quantified for the proposed site, so for this exercise a flat "layer cake" model was used. This unit was gridded into 58,500 total cells (30 in the x-direction, 30 in the y-direction, and 65 in the z-direction). The x-direction and y-direction had variable sized gridding ranging from 3,190.27 m to 4.43 m, with finer resolution towards the middle of the model domain (and near the injection well). For the z-direction the A to E Layers were gridded with uniform sized grids within a given layer. The grid size for each Layer is: A. 5.21 m; B. 1.88 m; C. 8.82 m; D. 8.26 m; E 8.23 m).

Subsurface Transport Over Multiple Phases (STOMP) Reservoir Simulations

To conduct reservoir simulations, STOMP-CO₂e (version 1290) was used with the Lis solver (version 2.0). This version solves for four coupled conservation equations: water mass, CO₂ mass, salt mass, and thermal energy and includes aqueous and gas mobile phases and a solid phase consisting of precipitated salt (White et al., 2012).

Initial and boundary conditions were defined in the model for the parameters (P): pressure, temperature, and salinity. ISGS provided data from an analog reservoir (Table 1), which was used to fit a simple linear curve to determine the value for a given P at a depth (D) from the respective gradient (G) and offset (O). Table 1 shows the gradient and offset for each parameter. The equation is:

$$P = G \times D + O$$

Table 1 – Reservoir initial and boundary conditions.

Temperature		Pressure		Salinity	
Gradient, °C/m	0.0172	Gradient, MPa/m	0.00947	Gradient, -/m	0.000124
Surface, °C	15.13	Offset, MPa	0.893	Offset, -	-0.103

STOMP uses the value at a point and the gradient for a given parameter as initial conditions. The hydrostatic option triggers the generation of hydrostatic pressure conditions for all active grid cells, from a reference aqueous pressure and x, y, and z location in space; reference temperature, z location in space, and geothermal gradient; reference dissolved salt concentration, z location in space, and geosalinity gradient. Additional geometric, petrophysical and state variable properties for the Mt. Simon are shown in Table 2.

Across all boundaries, energy was held at the geothermal gradient. The boundary conditions at the top and the bottom of the model domain were zero flux for both fluids and for salt. The model domain’s sides were held to the initial condition for fluid pressures and zero flux for salt.

The total simulation time was 60 years, with 30 years of CO₂ injection and 30 years of post-injection. Injection was invoked using the “Coupled Well Card” and was defined over the Lower (B) Layer. The injection rate was 1.67 Mt/yr and the maximum injection pressure was set at 25 MPa. The maximum injection pressure was calculated to be below an assumed fracture pressure at the top of the Lower (B) Layer. The fracture pressure was assumed from the FutureGen 2.0 Class VI well permit and was 0.65 psi/ft (FutureGen Alliance, 2013). The pressure gradient for our study is 0.61 psi/ft.

For this exercise there was no available relative permeability data from the site, so we used simplified models to estimate the multiphase flow behavior. The saturation function “Brooks and Corey” was used with non-wetting phase entry head at 0.1 m, and Lambda value of 2.0. The aqueous and gas relative permeability model was “Burdine”, which required no input parameters. It is expected that these models will be replaced with more accurate, site-specific empirical relationships once more data becomes available.

Table 2 - Properties for the Mt. Simon Layers used in STOMP simulations.

Mt. Simon Sandstone	Depth to Unit Top, m	Thickness, m	Porosity, -	(X, Y) Permeability, m ²	(Z) Permeability, m ²	Temp, C	Press, MPa	Salinity, -
Upper (E)	1,565.15	41.15	0.1	6.40×10 ⁻¹⁶	6.40×10 ⁻¹⁷	42.05	15.71	0.0911
Middle (D)	1,606.30	82.60	0.13	3.50×10 ⁻¹⁴	3.50×10 ⁻¹⁵	42.76	16.10	0.0962
Middle (C)	1,688.90	132.28	0.14	9.80×10 ⁻¹⁵	9.80×10 ⁻¹⁶	44.18	16.89	0.1064
Lower (B)	1,821.18	46.94	0.2	1.50×10 ⁻¹³	1.50×10 ⁻¹⁴	46.45	18.14	0.1228
Lower (A)	1,868.12	52.1	0.15	2.80×10 ⁻¹⁵	2.80×10 ⁻¹⁶	47.26	18.58	0.1286
Reservoir bottom	1,920.24							

NRAP Open Integrated Assessment Model (NRAP-Open-IAM)

For the risk assessment component, the NRAP-Open-IAM (version a1.1.2) was used as part of an initial assessment and implemented using the python scripting approach. This is a key design feature of the NRAP-Open-IAM. The NRAP-Open-IAM allows for the inclusion of different component modules and can be run in various modes depending on the objective of the study. This approach was adapted from Bacon et al. (2019).

For this study we used the following component modules: Reservoir Lookup Table, Stratigraphy, Multisegmented Well Model, FutureGen2 AZMI ROM, Stochastic Simulations, and a leakage impact calculator. The Reservoir Lookup Table module is used to import and sample pressure and CO₂ saturation over time from the STOMP results. The Stratigraphy module is used to define the layers used in the system and is a convenient way to link the modules. The Multisegmented Well Model module is used to simulate fluid leakage from the reservoir into the aquifers. The FutureGen2 AZMI ROM module is used to take the fluid leakage rates and estimate changes to the aquifers, this ROM was built specifically for rocks in the Illinois basin. The Stochastic Simulations uses Latin Hypercube Sampling to run realizations over using the stochastic properties of the system. Finally, the leakage impact calculator determines the measurable distance of impact to the aquifer (for a given monitoring metric) from the leaky well.

Table 3 shows stratigraphic and petrophysical properties used by the model. Additional parameters are a leaking well radius of 0.1143 m (~4.5 inch), a brine density of 1,030.9 kg/m³, a brine viscosity of 7.5×10⁻⁴ Pa-s, a CO₂ density of 775 kg/m³, a CO₂ viscosity of 6.6×10⁻⁵ Pa-s. To stochastically simulate different leakage scenarios, we used 50 realizations and varied the well leak permeability (seen as the permeability value for “Shale” in Table 3) and aquifer permeability using a uniform distribution between the parameters in Table 3 that have a value range. To estimate leak impact and monitoring detectability the FutureGen2 AZMI ROM uses the following thresholds: a relative pressure change of 0.00065 psi, a relative TDS change of 0.1 mg/L, and an absolute pH change of 0.2 (Bacon et al., 2019).

Table 3 – Stochastic and deterministic parameters used in the NRAP-Open-IAM analysis.

Unit name	Depth to top, m	Thickness, m	Porosity, -	Permeability, m ²	Anisotropy	Relative volume fraction of calcite, -
Shale 3	0	873.25	-	1.0×10^{-17}	-	-
St Peter	873.25	78.03	0.18	3.80×10^{-13} to 3.80×10^{-12}	0.3	0.1
Shale 2	951.28	423.98	-	1.0×10^{-16} to 1.0×10^{-13}	-	-
Ironton- Galesville	1,375.26	30.48	0.118	2.57×10^{-14} to 1.29×10^{-13}	0.3	0.1
Shale 1	1,405.74	159.41	-	1.0×10^{-16} to 1.0×10^{-13}	-	-
Mt. Simon	1,565.15	355.09	-	-	-	-

Results

Reservoir simulations: Pressure and saturation evolution

Results of the STOMP simulations indicate that the planned injection of 50 Mt over 30 years can be achieved and that the fracture pressure was not exceeded. Figure 4 shows the evolution of the CO₂ plume in the reservoir during injection at 5, 10, and 30 years (Figure 4b -d). During this time the plume spreads laterally and vertically, though vertical exaggeration and local gridding refinement overstate the vertical spread. Lateral movement of CO₂ occurs primarily in the injection interval (Layer B), which is the more finely gridded horizontal unit in Figure 4a. After injection stops, the CO₂ plume continues to spread laterally but vertical migration becomes dominant (Figure 4e and f). From a risk perspective, the buoyant CO₂ continues to remain mobile at 60 years (Figure 4f) but has yet to reach the top of the Mt. Simon reservoir.

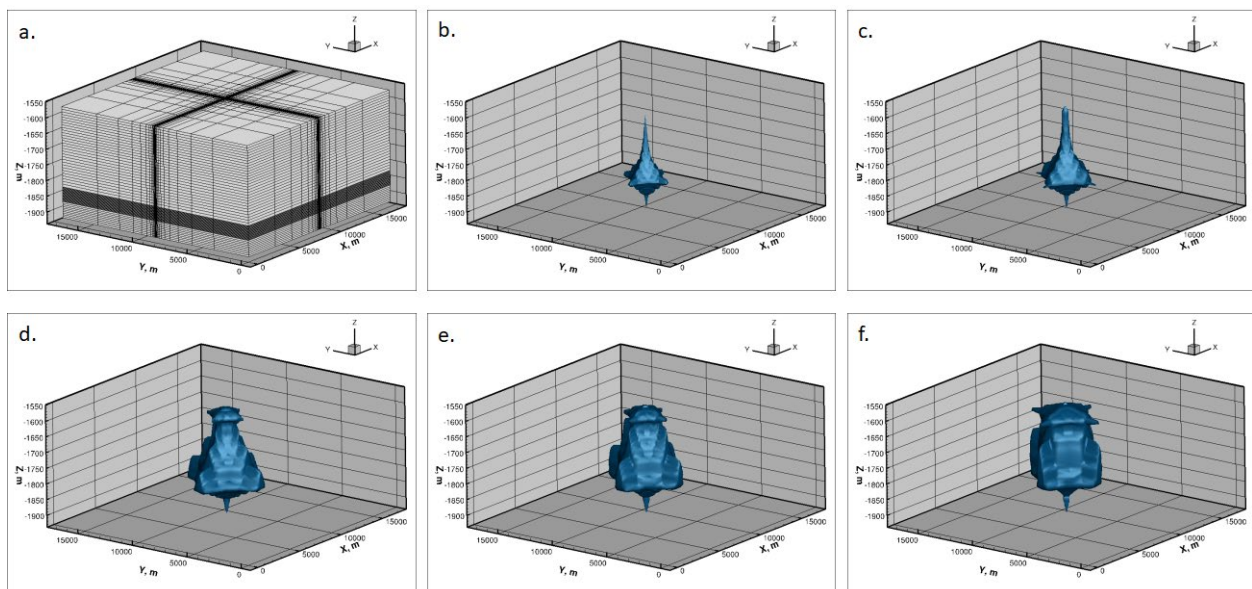


Figure 4 – Reservoir simulation results showing the grid used (a.) and the CO₂ saturation iso-surface ($S_{CO_2} > 0.01$) at (b.) 5 years, (c.) 10 years, (d.) 30 years, (e.) 40 years, and (f.) 60 years. Note that the x-axis and y-axis are at different scales than the z-axis.

The evolution of pressure within the reservoir during and after injection is another critical risk driver for GCS. Figure 5 shows the pressure differential in MPa between the initial condition (0 years) and at three times during injection (a. 1 year, b. 5 years, c. 10 years), at injection stop (d. 30 years), and at two times post-injection (e. 40 years, and f. 60 years). The increase in pressure differential is highest during the beginning of the injection period (below 2.5 MPa) but declines during injection. Pressure returns to background values 5 years after injection ends. The vertical distribution in pressure is fairly uniform, with some small buildup at the base of the simulation domain early on.

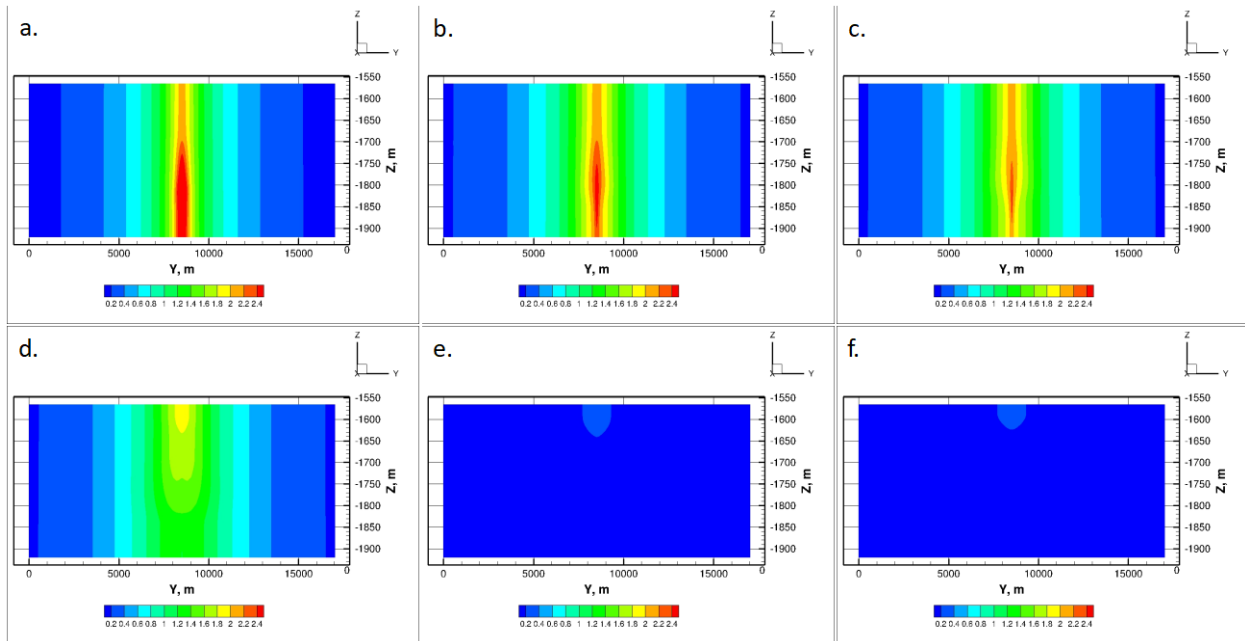


Figure 5 – Reservoir simulation results showing an x-axis slice at 8,500 m (across the injection well location). Plotted on the images is the pressure differential in MPa from time 0 years to (a.) 1 year, (b.) 5 years, (c.) 10 years, (d.) 30 years, (e.) 40 years, and (f.) 60 years.

Selection of the appropriate leakage source layer as input to the NRAP-Open-IAM depends on where and how the CO₂ and pressure plumes evolve during and after injection. From an operational perspective, we expect two likely candidates, namely the top of the reservoir and somewhere within the injection interval. Figure 5 shows that the pressure differential’s distribution in the vertical direction is essentially uniform. Thus, we use the CO₂ saturation distribution over time as the main guide for selecting the appropriate layer.

Figure 6 shows the CO₂ saturation at six timepoints for a slice in the x-direction at 8,500 m (roughly the center of the domain). There are three times during injection (a. 1 year, b. 5 years, and c. 10 years), one time at injection stop (d. 30 years), and two post-injection times (e. 40 years and f. 60 years). During injection the lateral spread of CO₂ is dominantly near the top of the injection interval (Layer B). After injection concludes, the CO₂ migrates towards the top of the reservoir but spreads laterally in layer D due to the relatively low vertical permeability of Layer E ($k_v = 3.2 \times 10^{-16} \text{ m}^2$). Because the pressure differential is largest during injection and based on where CO₂ is during this time, we selected z-axis node 36 (depth -1,821.2 m) within Layer B as the input layer for assessing risk using the NRAP Open-IAM.

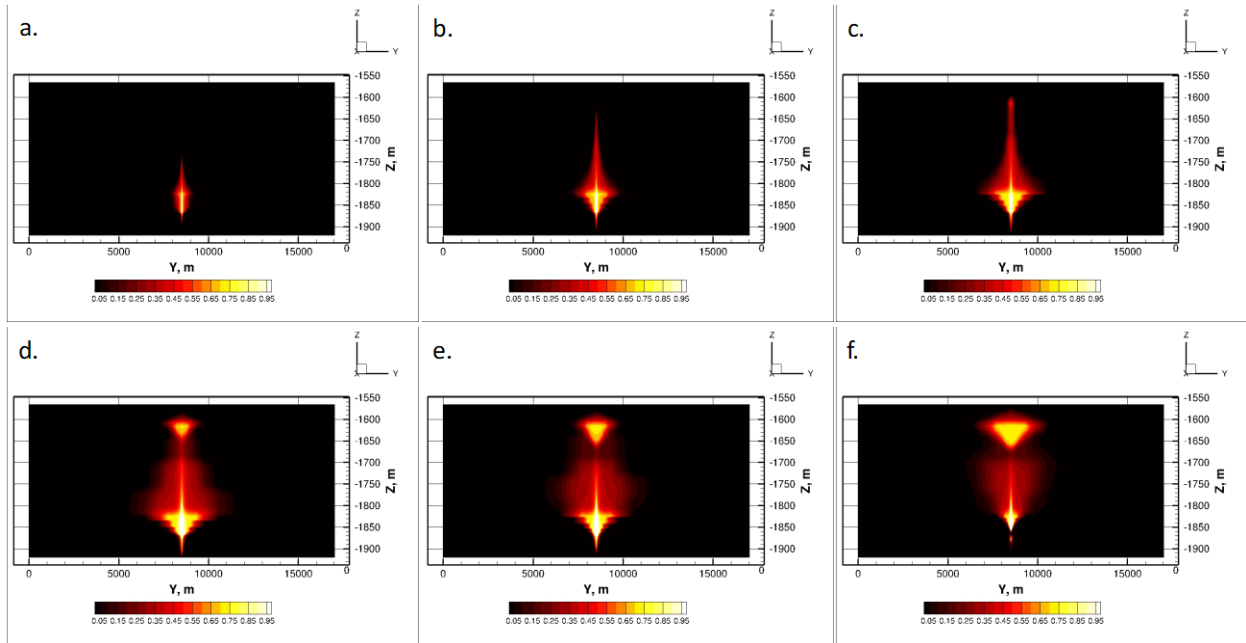


Figure 6 – Reservoir simulation results showing an x-axis slice at 8,500 m (across the injection well location). Plotted on the images is the CO₂ saturation at time (a.) 1 year, (b.) 5 years, (c.) 10 years, (d.) 30 years, (e.) 40 years, and (f.) 60 years.

Figure 7 shows the absolute pressure (black contours) and CO₂ saturation of 0.01 (red contour) for z-node 36 at six different times (a. 1 year, b. 5 years, c. 10 years, d. 35 years, e. 40 years, and f. 60 years). Figure 8 shows the pressure differential (black contours) and CO₂ saturation of 0.01 (red contour) for the same z-node at the same times. This data shows that the CO₂ spreads mostly laterally and is centered around the injection well. The CO₂ saturation decreases in this z-node after injection stops but CO₂ continues to move vertically out of this Z-node so that saturation is not actually decreasing overall in the reservoir. The pressure differential decreases significantly after injection stops (Figure 7, d to f), due to our assumption of a constant (hydrostatic) pressure boundary.

The data for this slice is extracted from the STOMP plot file and converted to NRAP-Open-IAM .csv format by using a simple MATLAB script. The data extracted consists of node position, pressure, saturation, and time for fourteen timepoints (0, 1, 2, 3, 4, 5, 10, 15, 20, 25, 30, 35, 40, and 60 years).

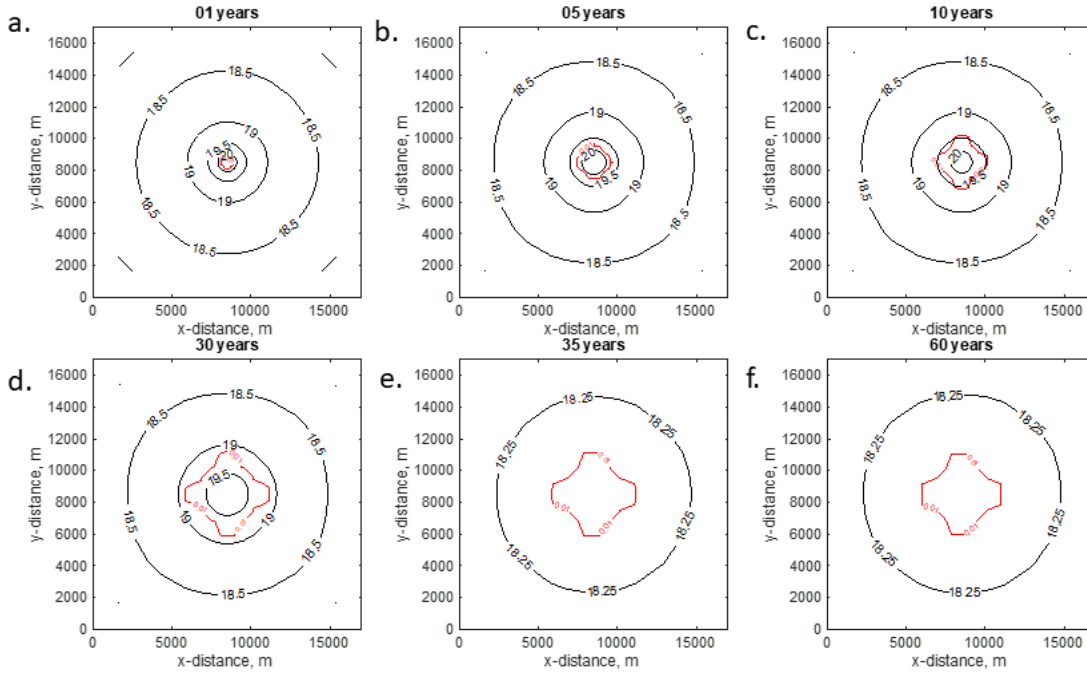


Figure 7 – Reservoir simulation results for the top of Layer B (z-node 36) at a depth of -1,821.2 m. The black contours show the fluid pressure in MPa and the red contour shows the CO₂ saturation of 0.01 at times: (a.) 1 year, (b.) 5 years, (c.) 10 years, (d.) 35 years, (e.) 40 years, and (f.) 60 years.

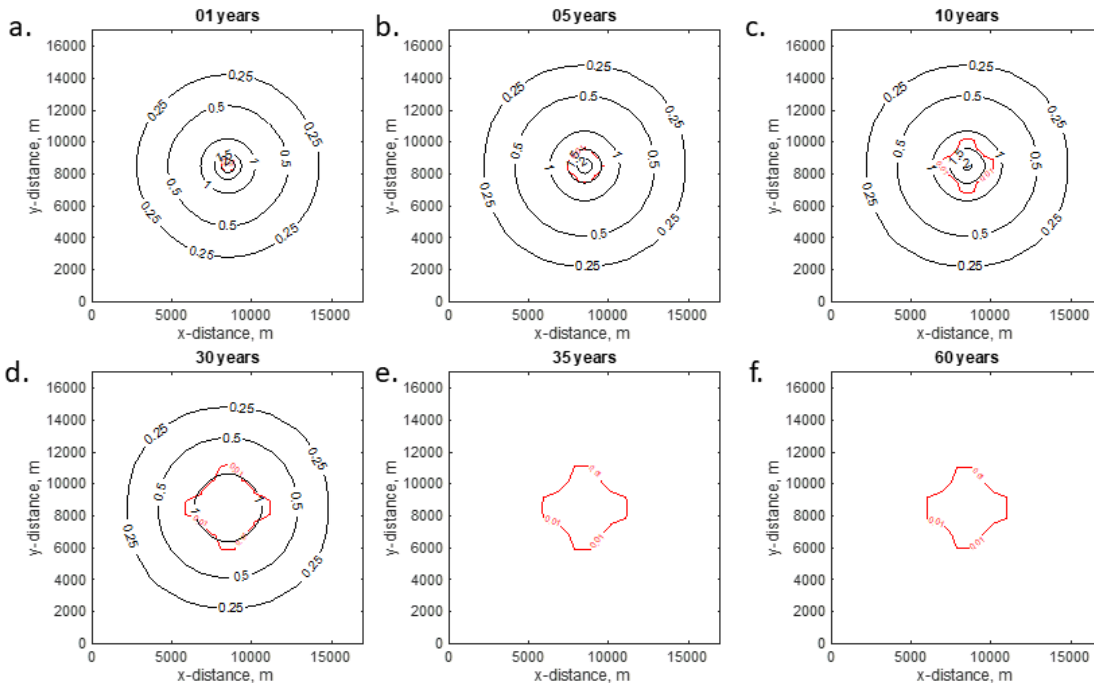


Figure 8 – Reservoir simulation results for the top of Layer B (z-node 36) at a depth of -1,821.2 m. The red line shows the contour for CO₂ saturation at 0.01. The black contours show the change in pressure in MPa from the initial time to the following times: (a.) 1 year, (b.) 5 years, (c.) 10 years, (d.) 35 years, (e.) 40 years, and (f.) 60 years.

NRAP-Open-IAM risk forecasting

This section presents results from combining the stratigraphic and geologic data for the site with the STOMP reservoir simulations to determine the risk for leakage along the injection well and one monitoring well. The leaks are then used to estimate the impact to the St. Peter and the Ironton-Galesville aquifers. Both results can be used to inform monitoring decisions.

Leakage flux

Figure 9 shows the leak rate (top row of three subplots) and cumulative fluid leaked (bottom row of two subplots) as a function of time for all 50 realizations along the injection well. The left column is for CO₂ and the right is brine. For leak rate the subplots are, from top to bottom respectively, leaks to the atmosphere, St. Peter, and Ironton-Galesville. For cumulative fluid leaked, the subplots are, from top to bottom respectively, leaks to the St. Peter and Ironton-Galesville. As expected, leakage to the atmosphere is minimal for both CO₂ (below 0.1 kg/yr) and brine (2×10^{-4} kg/yr). Leakage into the St. Peter is the largest for both CO₂ (above 3×10^4 kg/yr) and brine (below 60 kg/yr). These leak rates are continuous throughout the simulation. Leakage into the Ironton-Galesville occurs for the first few years but decreases to zero (or a negative value) after about 5 years. The negative flux is associated with fluid bypassing this aquifer to move into overlying units. Cumulatively, the mass of fluid moving into the St. Peter is small, by 60 years the worst-case leakage scenario has leaked less than 2,000 t of CO₂ and the worst-case for brine has leaked 3 t.

Figure 10 shows the leak rate (top row of three subplots) and cumulative fluid leaked (bottom row of two subplots) as a function of time for all 50 realization along the monitoring well. The left column is for CO₂ and the right is brine. For leak rate the subplots are, from top to bottom respectively, leaks to the atmosphere, St. Peter aquifer, and Ironton-Galesville aquifer. For cumulative fluid leaked, the subplots are, from top to bottom respectively, leaks to the St. Peter aquifer, and Ironton-Galesville aquifer. Leaks into the monitoring well are delayed by about a decade for all aquifers and fluids except brine leakage into the Ironton-Galesville. Similar to the injection well, leakage to the atmosphere is minimal for both CO₂ (below 0.1 kg/yr) and brine (2×10^{-4} kg/yr). Leakage into the St. Peter is the largest for both CO₂ (above 1×10^4 kg/yr for one case) and brine (at 6 kg/yr for one case). These leak rates are continuous throughout the simulation.

Leakage into the Ironton-Galesville along the monitoring well for CO₂ is characterized by a continuous increase from onset until the time injection stops (at 30 years) and then an asymptotic decrease over time. The peak value for CO₂ leakage is 600 kg/yr. Brine leakage into the Ironton-Galesville shows a maximum above 1,000 kg/yr with a gradually decreasing trend over time. Cumulatively, the mass of fluid moving into the St. Peter is small, by 60 years the worst-case leakage scenario has leaked less than 500 t of CO₂ and the worst case for brine has leaked less than 2.5 t. Cumulative brine leakage into the Ironton-Galesville is higher than at the injection well and is below 60 t at 60 years.

While a leak value in the 100's or 1,000's of tons of CO₂ may seem significant, it is important to cast these in terms of total amount of fluid injected, which is 50,000,000 t. The DOE guidance for storage assurance is 99% of the total amount injected, which corresponds to an allowable leakage of 500,000 t. Additionally, while these simulations show continuous leakage, it is expected that

the driving forces for leakage would diminish in time (e.g., the pressure drive in the reservoir and aquifers would reduce) and the CO₂ would become trapped by various mechanisms which would reduce the amount of free-phase fluid available for buoyant displacement. It is also important to realize that most of the simulation results shown in the figures were well below the values presented in this text, which were the upper bounds on leak rates and cumulative leak volumes. Finally, these values must be taken in the context of leak detectability and groundwater interactions. CO₂ and brine will be subject to geochemical reactions and dilution that will affect their concentrations and any monitoring signal we may want to use for leak detection. The following section studies this impact using additional modules in the NRAP-Open-IAM.

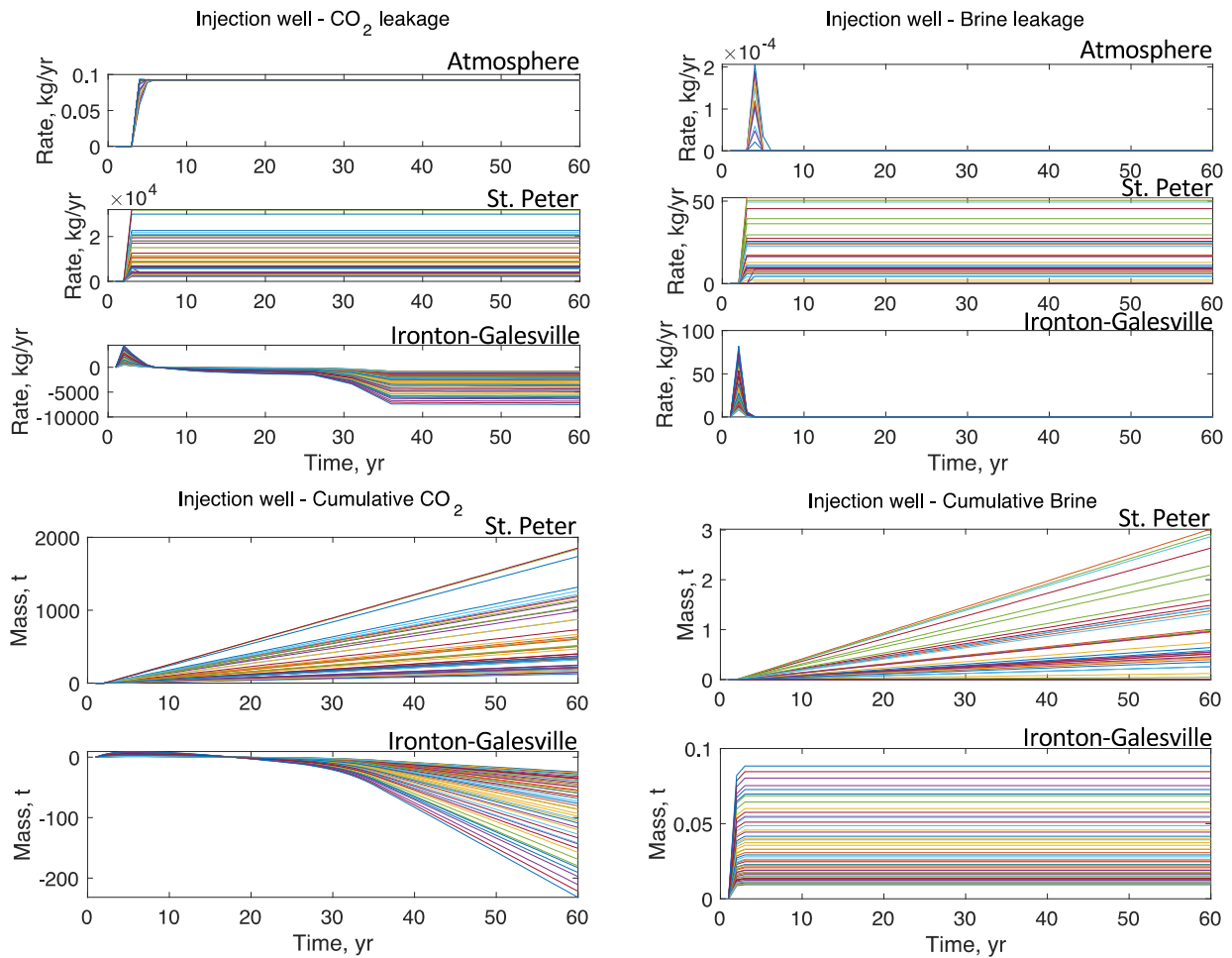


Figure 9 – Stochastic realizations ($n = 50$) for leak rates (top) and cumulate mass leaked (bottom) of brine and CO₂ up the injection well. Mass rates are shown for leakage into the atmosphere, St. Peter aquifer, and the Ironton-Galesville aquifer (top to bottom respectively). Cumulative mass is shown for the St. Peter aquifer and Ironton-Galesville (top to bottom respectively).

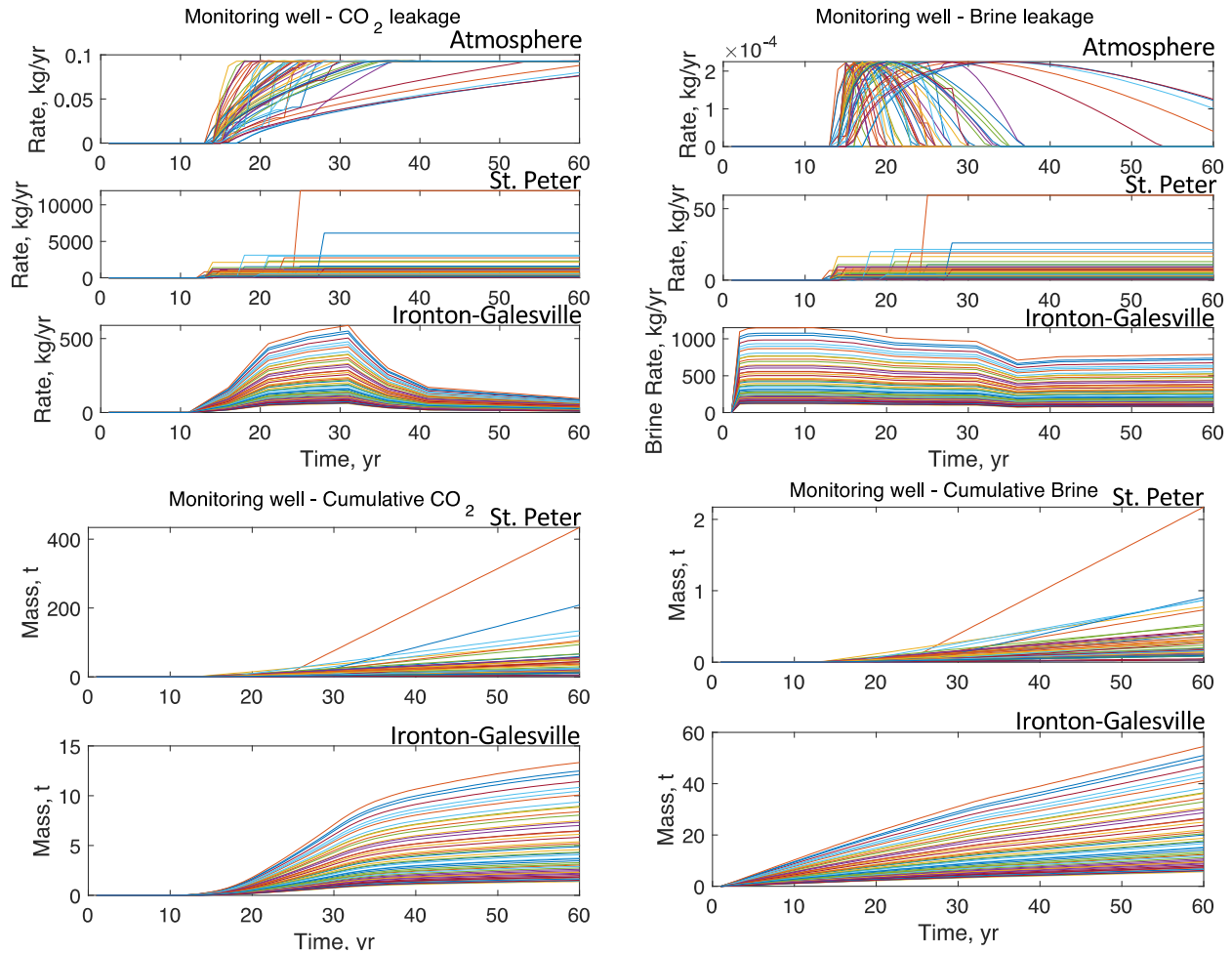


Figure 10 – Stochastic realizations ($n = 50$) for leak rates (top) and cumulate mass leaked (bottom) of brine and CO_2 up the monitoring well. Mass rates are shown for leakage into the atmosphere, St. Peter aquifer, and the Ironton-Galesville aquifer (top to bottom respectively). Cumulative mass is shown for the St. Peter aquifer and Ironton-Galesville (top to bottom respectively).

Leak impact

A thorough risk assessment needs to include not only an estimation for the flux of CO_2 and brine into the aquifers but also an assessment of the detectable impact or change to groundwater parameters that indicate potential degradation to a USDW. In addition to impact above a certain monitored threshold is the time-dependent volume and distance of that impact away from the leak source. The parameters used in this study are the change in pressure from initial aquifer pressure, the change in TDS, and the change in pH. An assessment for the impact was conducted for both aquifers and for leakage in both wells.

Figure 11 shows the impact volume (top row) and impact radius (bottom row) for the three metrics studied at the injection well. These metrics are pressure (left column), TDS (middle column), and pH (right column). Within a row are subplots that show impact to the St. Peter aquifer (top subplot) and the Ironton-Galesville aquifer (bottom subplots). For the injection well, the volume and radius of impact is largest for the pH metric in both aquifers but larger in the St. Peter aquifer ($2.5 \times 10^6 \text{ m}^3$ and 100 m, respectively). While there is an impact to the pH at 12 m away from the injection

well, it only lasts for the first 5 years of the simulations. For pressure and TDS, the signal is so small that it does not have a detectable impact farther than 0.5 m away from the injection well.

Figure 12 shows the impact volume (top row) and impact radius (bottom row) for the three monitoring metrics studied at the monitoring well. These metrics are pressure (left column), TDS (middle column), and pH (right column). Within a row are subplots that show impact to the St. Peter aquifer (top subplot) and the Ironton-Galesville aquifer (bottom subplots). For the monitoring well, the volume of fluid impacted follows a similar trend as the injection well but at much lower volumes and distances impacted. The greatest impact is a change in pH in the St. Peter Aquifer with a volume below $5 \times 10^5 \text{ m}^3$ and a radius less than 50 m. This single realization is well above where most realizations cluster (impact volume below $2 \times 10^5 \text{ m}^3$ and a radius around 20 m). Impact in the Ironton-Galesville aquifer is small, at 3 m, and is only detectable for a decade between 10 and 20 years. The impact signal associated with a pressure or TDS change is only observable less than 0.5 m around the monitoring well.

All three metrics do show impacts, but some are so small or of short duration that they would be difficult to detect. Typically, in the risk assessment workflow we would generate time to first detection volume maps, which would be used as inputs to for the DREAM analysis but given the small impact for all but pH and the sensitivity of pH as a parameter it was concluded that general observations could be made on monitoring technology choices based on the aquifer impact simulations alone.

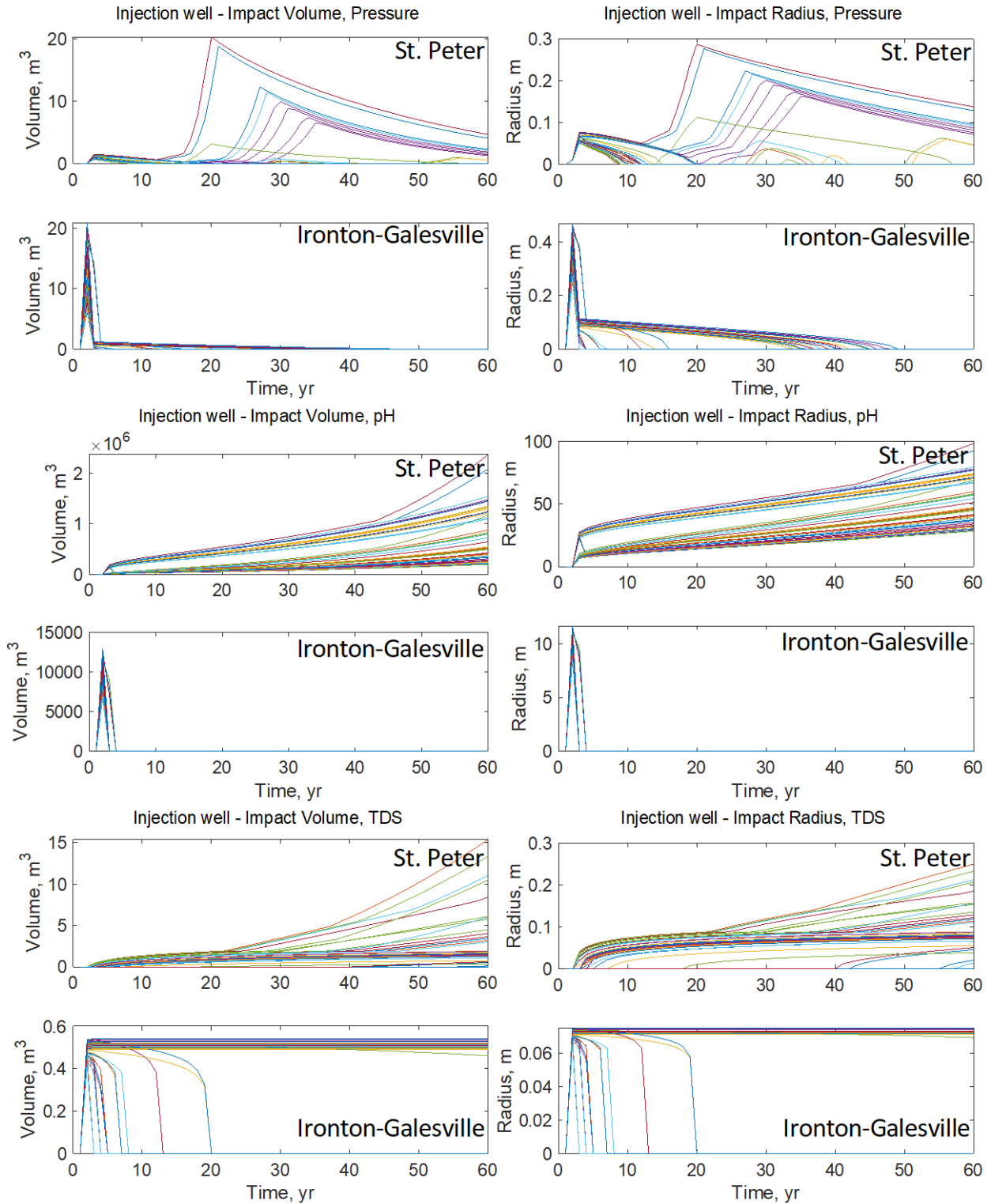


Figure 11 – Stochastic realizations ($n = 50$) for impacts to the St. Peter aquifer and Ironton-Galesville aquifer at the injection well. (left column) Volume of the aquifers impacted by a perturbation in pressure (top), pH (middle), and TDS (bottom). (right column) Radius of the aquifers impacted by a perturbation in pressure (top), pH (middle), and TDS (right).

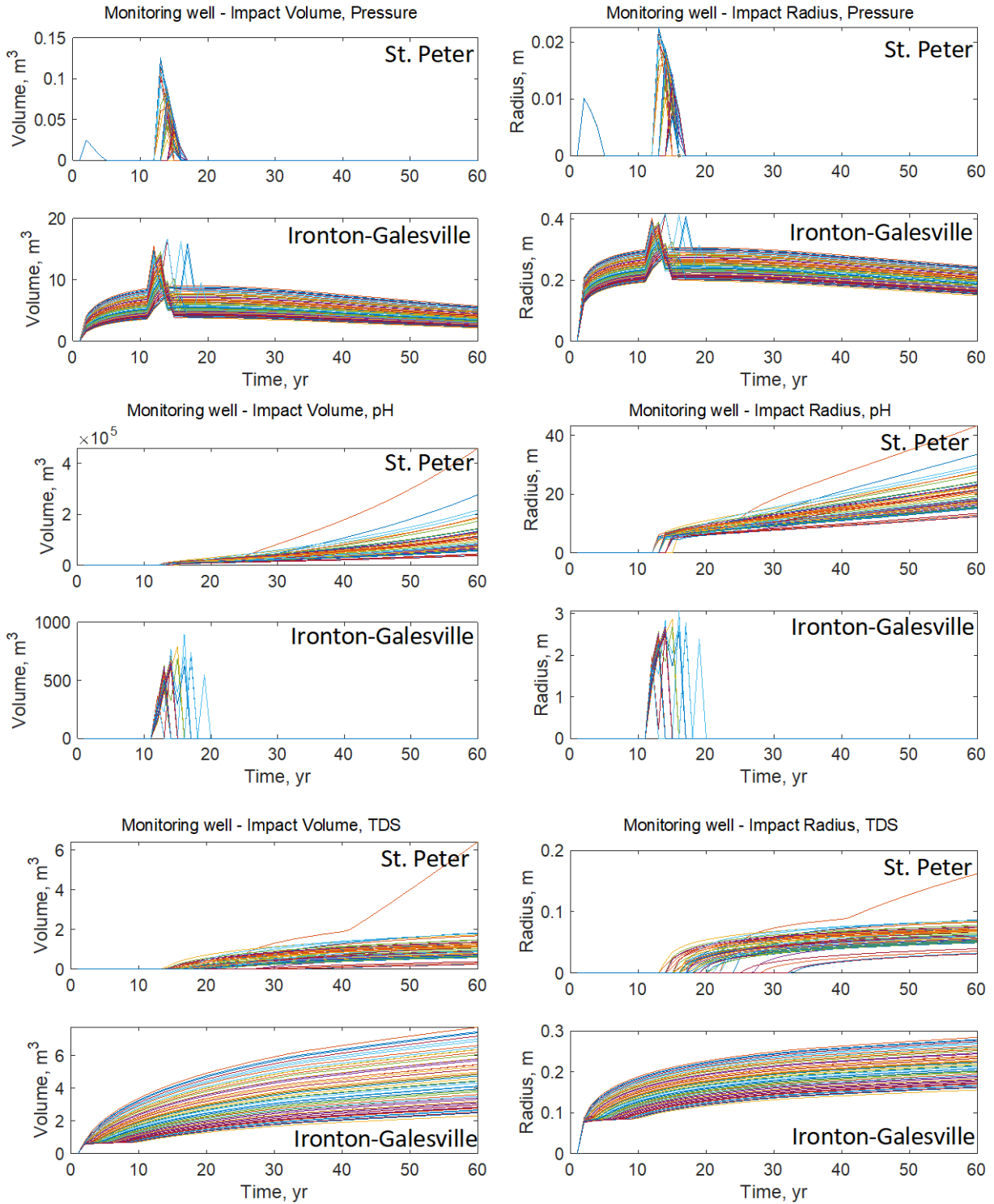


Figure 12 – Stochastic realizations ($n = 50$) for impacts to the St. Peter aquifer and Ironton-Galesville aquifer at the monitoring well. (left column) Volume of the aquifers impacted by a perturbation in pressure (top), pH (middle), and TDS (bottom). (right column) Radius of the aquifers impacted by a perturbation in pressure (top), pH (middle), and TDS (right).

Monitoring recommendations

The following observations and monitoring recommendations are made based on this preliminary investigation. Since this is a greenfield site with no existing wells and no significant faults identified, any new penetrations are primary sources of leakage risk. However, in addition to the injection well, we expect regulators to require at least one monitoring well in the injection interval. The placement of a monitoring well ~2.5 km away from the injection well would allow operators to observe CO₂ breakthrough in the reservoir by 12 years. The placement of more monitoring wells may be required, but that requirement should be balanced against the risk each new penetration presents.

The leakage monitoring metric that showed the largest radial impact was change in aquifer pH, which migrated several 10's of meters by the simulation end for both wells. Given the small radius of impact, placement of monitoring equipment in the injection and monitoring well would be one approach to detect leakage signals, although it would only detect leakage from the well itself and not from the other well. Conventional wisdom suggests that the more complex a well completion is, the greater chance there is to have well integrity issues and to require well intervention. However, there are no hard data to support which would be the best choice from a risk perspective. Nevertheless, the fewer penetrations there are in the system, the lower the chance for deleterious impacts to USDW and low risk to the project.

Discussion and Conclusions

This report summarizes work to deploy NRAP tools to a field site in support of the ISGS's Phase 2 CarbonSAFE project. Results indicate that there is a low probability for a high impact leak into either the St. Peter or the Ironton-Galesville aquifers. For all the realizations, the results showed leaked volumes were well within the acceptable thresholds. As expected, the highest risk occurs closest to the injection well and during injection. Simulations reveal that leakage impacts (and detectability) decrease after injection stops.

It is important to note that this exercise assumes the wells are leaking. However, it is expected that these new wells will be drilled using the latest technologies and thus will have a significantly lower probability to develop a leak than historical trends (Lackey et al., 2019). Thus, this risk assessment takes a very conservative approach. Further, this report joins a body of increasing literature that highlights the inherently low leakage risk at greenfield GCS sites (Anderson, 2017; Bacon, et al., 2019; Celia et al, 2015).

As the NRAP tools are in active development, there were several lessons learned which, when addressed by the NRAP program, will improve the next version of the tools.

- One lesson is to put better safeguards on running the aquifer impact ROM outside of the range it was developed for. As an example, in the Potosi Dolomite, which is a thin aquifer interval we did not study in this work, we attempted to estimate leakage, but the model returned unrealistic results for leakage impact. We identified that the Potosi was below the minimum aquifer thickness and was yielding erroneously high results. We are using these

observations to improve the NRAP aquifer impact ROM to expand its flexibility for use in future Illinois Basin applications.

- We have also observed that the leak rate, while small, often remains unchanged after injection has completed. We are currently testing the NRAP-Open-IAM to determine the source and validity of this unexpected result.
- It is critical that the reservoir simulations be conducted with the desired risk assessment in mind. For example, if the risk assessment is focused on the injection or post-injection time period then the time discretization and duration should span this range with sufficient resolution in time points to generate meaningful results in the NRAP-Open-IAM and not over interpolate. Another example is the choice of boundary conditions for the reservoir simulation. Specifically, an open or closed boundary condition without sufficient domain size may impact the pressure buildup and eventual decay, which are critical for assessing risk through the lifetime of a project. If the boundary conditions are uncertain than a sensitivity analysis should be conducted to determine an appropriate model domain and this uncertainty could be carried forward as stochastic simulations in the risk assessment itself.
- Scripts and codes were developed at various steps in the workflow to allow for data processing from one file format to another and for data analysis and presentation. These scripts could be annotated, generalized, and included as “helper” files in the NRAP toolset.

We anticipate that the one or more NRAP tools will be used to quantify the risks and assessments required for the EPA’s UIC Class VI well permit, which will be part of the CarbonSAFE Phase III effort. Once more accurate site-specific data is collected from a characterization well at the selected site, we will be able to iteratively generate reservoir simulations that use this additional data, plus uncertainty to create a number of reservoir simulations which are critical inputs to the NRAP models. Specifically, we would like to vary the assumptions about the boundary conditions, the heterogeneity, the saturation and relative permeability functions, and the dip of the reservoir. These parameters have an important impact on the CO₂ and pressure plume movement in time. With additional data we will also be able to deploy the DREAM tool and additional tools that characterize the subsurface stress state and induced seismicity risk (e.g., State of Stress Analysis Tool and RiskCat Tool).

With this stochastic input data and full deployment of tools, we can conduct a more robust uncertainty quantification using not only the reservoir realizations but additional data about the overlying aquifers to characterize leakage sensitivity of parameters like calcite volume fraction, porosity, permeability and aquifer thickness. With this data we will be able to generate Area of Review maps, risk-based Area of Review estimates, and to inform monitoring technology selection.

References

- Anderson, Steven T. “Risk, Liability, and Economic Issues with Long-Term CO₂ Storage—A Review.” *Natural Resources Research* 26, no. 1 (January 1, 2017): 89–112. <https://doi.org/10.1007/s11053-016-9303-6>.
- Bacon, Diana H., Catherine M. R. Yonkofski, Christopher F. Brown, Deniz I. Demirkanli, and Jonathan M. Whiting. “Risk-Based Post Injection Site Care and Monitoring for Commercial-Scale Carbon Storage: Reevaluation of the FutureGen 2.0 Site Using NRAP-Open-IAM and DREAM.” *International Journal of Greenhouse Gas Control* 90 (November 1, 2019): 102784. <https://doi.org/10.1016/j.ijggc.2019.102784>.
- Carroll, Susan A., Elizabeth Keating, Kayyum Mansoor, Zhenxue Dai, Yunwei Sun, Whitney Trainor-Guitton, Chris Brown, and Diana Bacon. “Key Factors for Determining Groundwater Impacts Due to Leakage from Geologic Carbon Sequestration Reservoirs.” *International Journal of Greenhouse Gas Control* 29 (October 2014): 153–68. <https://doi.org/10.1016/j.ijggc.2014.07.007>.
- Celia, M. A., S. Bachu, J. M. Nordbotten, and K. W. Bandilla. “Status of CO₂ Storage in Deep Saline Aquifers with Emphasis on Modeling Approaches and Practical Simulations.” *Water Resources Research* 51, no. 9 (2015): 6846–92. <https://doi.org/10.1002/2015WR017609>.
- FutureGen Industrial Alliance, I, 2013c. Underground Injection Control Permit Applications for FutureGen 2.0 Morgan County Class VI UIC Wells 1, 2, 3, and 4 –Chapter 3.0 Area of Review and Corrective Action Plan, FG-RPT-017-Revision 1. Jacksonville, Illinois. <https://archive.epa.gov/region5/water/uic/futuregen/web/pdf/futuregen-permitapp-201303.pdf>.
- Los Alamos National Laboratory. GRIDDER, grid generation tool. LA-CC-15-082, 2016 (<https://meshing.lanl.gov/gridder/gridder.html>, date accessed: 12/13/2019)
- Lackey, Greg, Veronika S. Vasylykivska, Nicolas J. Huerta, Seth King, and Robert M. Dilmore. “Managing Well Leakage Risks at a Geologic Carbon Storage Site with Many Wells.” *International Journal of Greenhouse Gas Control* 88 (September 1, 2019): 182–94. <https://doi.org/10.1016/j.ijggc.2019.06.011>.
- U.S. DOEa. “Carbon Storage Assurance Facility Enterprise (CarbonSAFE).” <https://www.netl.doe.gov/coal/carbon-storage/storage-infrastructure/carbonsafe> (retrieved: 2/05/2020)
- U.S. DOEb. “CarbonSAFE Illinois Macon County.” <https://www.netl.doe.gov/project-information?p=FE0029381> (retrieved: 2/05/2020)

White, Mark D., Bacon, Diana H., McGrail, B. Peter, Watson, David J., White, Signe K., and Zhang, Z. F. STOMP Subsurface Transport Over Multiple Phases: STOMP-CO₂ and STOMP-CO₂e Guide: Version 1.0. United States: N. p., 2012. Web. doi:10.2172/1059044.

Whittaker, S., Freiburg, J. “CarbonSAFE Illinois – Macon ~~Christian~~ County.” Presentation given at Mastering the Subsurface Through Technology Innovation, Partnerships and Collaboration: Carbon Storage and Oil and Natural Gas Technologies Review Meeting. August 13-16, 2018. <https://www.netl.doe.gov/sites/default/files/netl-file/S-Whittaker-CarbonSAFE.pdf> (retrieved: 2/13/2020)

Yonkofski, C., G. Tartakovsky, N. Huerta, and A. Wentworth. “Risk-Based Monitoring Designs for Detecting CO₂ Leakage through Abandoned Wellbores: An Application of NRAP’s WLAT and DREAM Tools.” *International Journal of Greenhouse Gas Control* 91 (December 1, 2019): 102807. <https://doi.org/10.1016/j.ijggc.2019.102807>.