RISK-BASED AREA OF REVIEW (AOR) ESTIMATION TO SUPPORT INJECTION WELL STORAGE FACILITY PERMIT REQUIREMENTS FOR CO_2 STORAGE PROJECTS
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ABSTRACT

This paper by the Energy & Environmental Research Center presents a workflow for delineating a risk-based area of review (AOR) to support a U.S. Environmental Protection Agency (EPA) Class VI permit for a carbon dioxide (CO_2) storage project. The approach combines semianalytical solutions for estimating the formation fluid leakage through a hypothetical leaky wellbore with the results of numerical reservoir simulations. The workflow is demonstrated using a case study for a 180,000-metric-ton-per-year storage project located in the PCOR (Plains CO_2 Reduction) Partnership region. Under the scenario where the leaky wellbore is open to a saline aquifer (thief zone) between the overlying seal (cap rock) and the underground sources of drinking water (USDW), the risk-based AOR collapses to the areal extent of the CO_2 plume in the storage reservoir because the pressure buildup in the storage reservoir beyond the CO_2 plume is insufficient to drive formation fluids up a hypothetical leaky wellbore into the USDW. However, even under the conservative assumption that the leaky wellbore is not open to a thief zone, beyond the areal extent of the CO_2 plume, the incremental leakage is less than 400 m^3 over 20 years, which represents ~0.0001% or less of the total volume of water contained within the USDW rock volume. The approach outlined in this paper is designed to be protective of USDWs and comply with the Safe Drinking Water Act requirements and provisions for the U.S. EPA Class VI Underground Injection Control (UIC) Program (Class VI Rule) and North Dakota Administrative Code Chapter 43-05-01.

TABLE OF CONTENTS

RISK-BASED AREA OF REVIEW (AOR) ESTIMATION TO SUPPORT INJECTION WELL STORAGE FACILITY PERMIT REQUIREMENTS FOR CO_2 STORAGE PROJECTS

EXECUTIVE SUMMARY

This paper by the Energy & Environmental Research Center presents a workflow and modeling approach for delineating a risk-based area of review (AOR) to support a U.S. Environmental Protection Agency (EPA) Class VI permit for a carbon dioxide (CO_2) storage project. The approach combines semianalytical solutions for estimating formation fluid leakage through a hypothetical leaky wellbore with the results of numerical reservoir simulations to define the AOR.

The modeling utilizes 1) semianalytical solutions from the peer-reviewed literature for formation fluid leakage through abandoned wellbores by Raven (1990) and Avci (1994), 2) a FORTRAN model compiled and described in Cihan et al. (2011, 2012) called ASLMA (Analytical Solution for Leakage in Multilayered Aquifers), and 3) a computational framework for estimating a risk-based AOR first proposed by Oldenburg et al. (2014, 2016). Therefore, the approach builds upon well-established research and underlying hydrogeological principles that have been upheld for nearly three decades. Moreover, the ASLMA model has been broadly applied to an array of storage projects. The work presented herein extends these earlier works using a custom wrapper written in the software environment, R (R Core Team, 2020), which was developed to perform multiple runs of the ASLMA model using given ranges for one or more input parameters. In addition, the current work simulates the pressure buildup within the storage reservoir in response to CO_2 injection using a compositional simulator to better accommodate the temporospatial evolution of pressure buildup within the storage reservoir that is more accurately modeled using a heterogeneous geologic model and a compositional simulator that accounts for the multiphase interactions.

The workflow is demonstrated using a case study for a 180,000-metric-ton-per-year storage project located in the PCOR (Plains CO_2 Reduction) Partnership region. For the storage project evaluated here, under the scenario where the leaky wellbore is open to a saline aquifer (thief zone) between the overlying seal (cap rock) and the underground sources of drinking water (USDW), the risk-based AOR essentially collapses to the areal extent of the CO_2 plume in the storage reservoir because the pressure buildup in the storage reservoir beyond the CO_2 plume is insufficient to drive formation fluids up a hypothetical leaky wellbore into the USDW. However, even under the conservative assumption that the leaky wellbore is not open to a thief zone, beyond the areal extent of the CO_2 plume, the incremental leakage is less than 400 m^3 over 20 years, which represents ~0.0001% or less of the total volume of water contained within the USDW rock volume. As discussed in the text, the threshold criterion for defining the risk-based AOR is site-specific and should be informed by the results of the sensitivity analysis and available site characterization data.

The approach outlined in this paper is designed to be protective of USDWs and, therefore, comply with the Safe Drinking Water Act requirements and provisions for the U.S. EPA Class VI Underground Injection Control (UIC) Program (Class VI Rule) and North Dakota Administrative Code Chapter 43-05-01.

NOTES ON DELIVERABLE D14

This deliverable has been formatted as a journal article that will eventually be submitted to a peer-reviewed journal. Because of the nature of peer-reviewed literature, the final version of this document will be modified based on reviewer comments and the specific formatting guidelines of the publishing journal. The final version of the paper will be submitted to the U.S. Department of Energy project manager.

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APPENDIX A

RISK-BASED AREA OF REVIEW ESTIMATION TO SUPPORT INJECTION WELL STORAGE FACILITY PERMIT REQUIREMENTS FOR CO_2 STORAGE PROJECTS JOURNAL ARTICLE

LONG TITLE: Risk-Based Area of Review (AOR) Estimation to Support Injection Well Storage Facility Permit Requirements for CO_2 Storage Projects

SHORT TITLE: Risk-Based Area of Review (AOR) Estimation for CO_2 Storage Projects

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ABSTRACT

This paper presents a workflow for delineating a risk-based area of review (AOR) to support a U.S. Environmental Protection Agency (EPA) Class VI permit for a carbon dioxide (CO_2) storage project. The approach combines semianalytical solutions for estimating formation fluid leakage through a hypothetical leaky wellbore with the results of numerical reservoir simulations. The workflow is demonstrated using a case study for a 180,000-metric-ton-per-year storage project located in the PCOR (Plains CO_2 Reduction) Partnership region. Under the scenario where the leaky wellbore is open to a saline aquifer (thief zone) between the overlying seal (cap rock) and the underground sources of drinking water (USDW), the risk-based AOR collapses to the areal extent of the CO_2 plume in the storage reservoir because the pressure buildup in the storage reservoir beyond the CO_2 plume is insufficient to drive formation fluids up a hypothetical leaky wellbore into the USDW. However, even under the conservative assumption that the leaky wellbore is not open to a thief zone, beyond the areal extent of the CO_2 plume, the incremental leakage is less than 400 m^3 over 20 years, which represents ~0.0001% or less of the total volume of water contained within the USDW rock volume. The approach outlined in this paper is designed to be protective of USDWs and comply with the Safe Drinking Water Act requirements and provisions for the U.S. EPA Class VI Underground Injection Control (UIC) Program (Class VI Rule) and North Dakota Administrative Code Chapter 43-05-01.

KEYWORDS: Area of Review (AOR), Class VI Rule, Storage Facility Permit, CCS

1.0 INTRODUCTION

Carbon capture and storage (CCS) is a process whereby carbon dioxide (CO_2) is captured from an industrial facility, preventing its release to the atmosphere, and injected via one or more injection wells into a deep geologic reservoir for permanent storage. CCS is a key technology option to mitigate CO_2 emissions while allowing the full range of economic and societal benefits derived from fossil fuels. The PCOR (Plains CO_2 Reduction) Partnership, funded by the U.S. Department of Energy (DOE), the North Dakota Industrial Commission (NDIC), and participating member organizations, is fostering the deployment of CCS in the PCOR Partnership region. The PCOR Partnership region covers the central interior of North America and includes all or part of ten states (Alaska, Iowa, Minnesota, Missouri, Montana, Nebraska, North Dakota, South Dakota, Wisconsin, and Wyoming) and four Canadian provinces (Alberta, British Columbia, Manitoba, and Saskatchewan). The Energy & Environmental Research Center (EERC) leads the PCOR Partnership Initiative, with support from the University of Wyoming and the University of Alaska at Fairbanks.

In the United States, the U.S. Environmental Protection Agency (EPA) regulates the construction, operation, permitting, and closure of injection wells used to place fluids underground for storage. The federal regulations for the Underground Injection Control (UIC) Program are found in Title 40 of the Code of Federal Regulations. The Safe Drinking Water Act (SDWA) establishes requirements and provisions for the UIC Program (EPA, 2020). Regulations for CCS fall under the Class VI Rule of the UIC Program – *Wells Used for Geologic Sequestration of* CO_2. The Class VI Rule requirements are designed to protect underground sources of drinking water (USDWs). On April 24, 2018, EPA approved an application from the state of North Dakota under the SDWA to implement a UIC Program for Class VI injection wells located within the state, except within Indian lands. Therefore, in the state of North Dakota, Class VI injection wells and the associated storage facility permit for the storage project are managed under the North Dakota Century Code (Chapter 38-22, Carbon Dioxide Underground Storage) and the North Dakota Administrative Code Chapter 43-05-01 (*Geologic Storage of Carbon Dioxide*).

A CO_2 storage project (hereafter "*storage project*") comprises a *storage facility* (an area on the ground surface, defined by the operator and/or regulatory agency, where CO_2 injection facilities are developed and storage activities, including monitoring, take place) and a *storage complex* (a subsurface geological system comprising a storage unit and primary and possibly secondary seal(s), extending laterally to the defined limits of the CO_2 storage operation or operations) (Canadian Standards Association [CSA], 2012). The primary regulatory permit for a *storage project* is the *storage facility permit,* a major technical component of which is the delineation of the *area of review* (AOR). The AOR is defined as the region surrounding the *storage project* where underground sources of drinking water may be endangered by the injection activity (40 CFR 146.84 and North Dakota Administrative Code Section 43-05-01-05.1. *Area of review and corrective action*). EPA (2013) guidance for AOR evaluation includes several computational methods for estimating the pressure buildup in the storage reservoir in response to CO_2 injection and the resultant areal extent of pressure buildup above a "critical pressure" that could potentially drive higher salinity formation fluids from the storage reservoir up an open conduit to the lowermost USDW. The methods described in EPA (2013) for estimating the AOR under the Class VI Rule were developed assuming that the storage reservoirs would be in hydrostatic equilibrium with overlying aquifers. However, in the state of North Dakota, and potentially elsewhere around the United States, candidate storage reservoirs are already overpressurized relative to overlying aquifers and thus subject to potential vertical formation fluid migration from the storage reservoir to the lowermost USDW even prior to the planned storage project. Consequently, applying EPA (2013) methods to these geological situations essentially results in an infinite AOR, which makes regulatory compliance infeasible.

Several researchers have recognized the need for alternative methods for estimating the AOR for locations that are already overpressurized relative to overlying aquifers. For example, Birkholzer et al. (2014) described the unnecessary conservatism in the EPA's definition of the critical pressure, which could lead to a heavy burden on storage facility permit applicants. As an alternative, the authors proposed a risk-based reinterpretation of this framework that would allow for a reduction in the AOR while ensuring protection of drinking water resources. A computational framework for estimating a risk-based AOR was proposed by Oldenburg et al. (2014, 2016), who compared formation fluid leakage through a hypothetical open flow path in the baseline scenario (no CO_2 injection) to the incrementally larger leakage that would occur in the CO_2 injection case. The modeling for the risk-based AOR used semianalytical solutions to single-phase flow equations to model reservoir pressurization and vertical migration through leaky wells. These semianalytical solutions were extensions of earlier work for formation fluid leakage through abandoned wellbores by Raven (1990) and Avci (1994), which were creatively solved, coded, and compiled in FORTRAN under the name, ASLMA (Analytical Solution for Leakage in Multilayered Aquifers) and extensively described in Cihan et al. (2011, 2012) (hereafter "ASLMA Model"). Recently, White et al. (2020) outlined a similar risk-based approach for evaluating the AOR using the National Risk Assessment Partnership (NRAP) Integrated Assessment Model for Carbon Storage (NRAP-IAM-CS). However, the NRAP-IAM-CS and the subsequent open-sourced version (NRAP-Open-IAM) are constrained to the assumption that the storage reservoir is in hydrostatic equilibrium with overlying aquifers and, therefore, may not accurately estimate the AOR for storage projects located in regions where the storage reservoir is overpressurized relative to overlying aquifers.

The current work applies the ASLMA Model to a potential storage project in the PCOR Partnership region to illustrate how the workflow described by Oldenburg et al. (2014, 2016) can be used for risk-based AOR estimation to support a Class VI storage facility permit. The proposed workflow extends the ASLMA Model with custom scripting to include broader uncertainty quantification and combines the results from numerical reservoir simulations to estimate the risk-based AOR. In addition, this work examines the effect of an intermediary saline aquifer between the storage reservoir and USDW, which acts as a “thief zone” because the loss of fluid into the saline aquifer lowers the vertical hydraulic head gradient with increasing vertical location in a leaky wellbore, thereby decreasing or nearly eliminating vertical fluid migration above the saline aquifer to the USDW. The thief zone phenomenon was described by Nordbotten et al. (2004) as an ‘‘elevator model,’’ by analogy with an elevator full of people on the main floor, who then get off at various floors as the elevator moves up, such that only very few people ride all the way to the top floor. The workflow and tools described in this paper provide a detailed workplan for delineating the AOR for a proposed storage project and to periodically reevaluate the delineation.

2.0 METHODS

2.1 Risk-Based AOR Workflow

Figure 1 summarizes the workflow used in this study to develop a risk-based AOR for a storage facility permit. The methods described in the remainder of this section describe each step in the workflow and refer to Supporting Information for additional details.

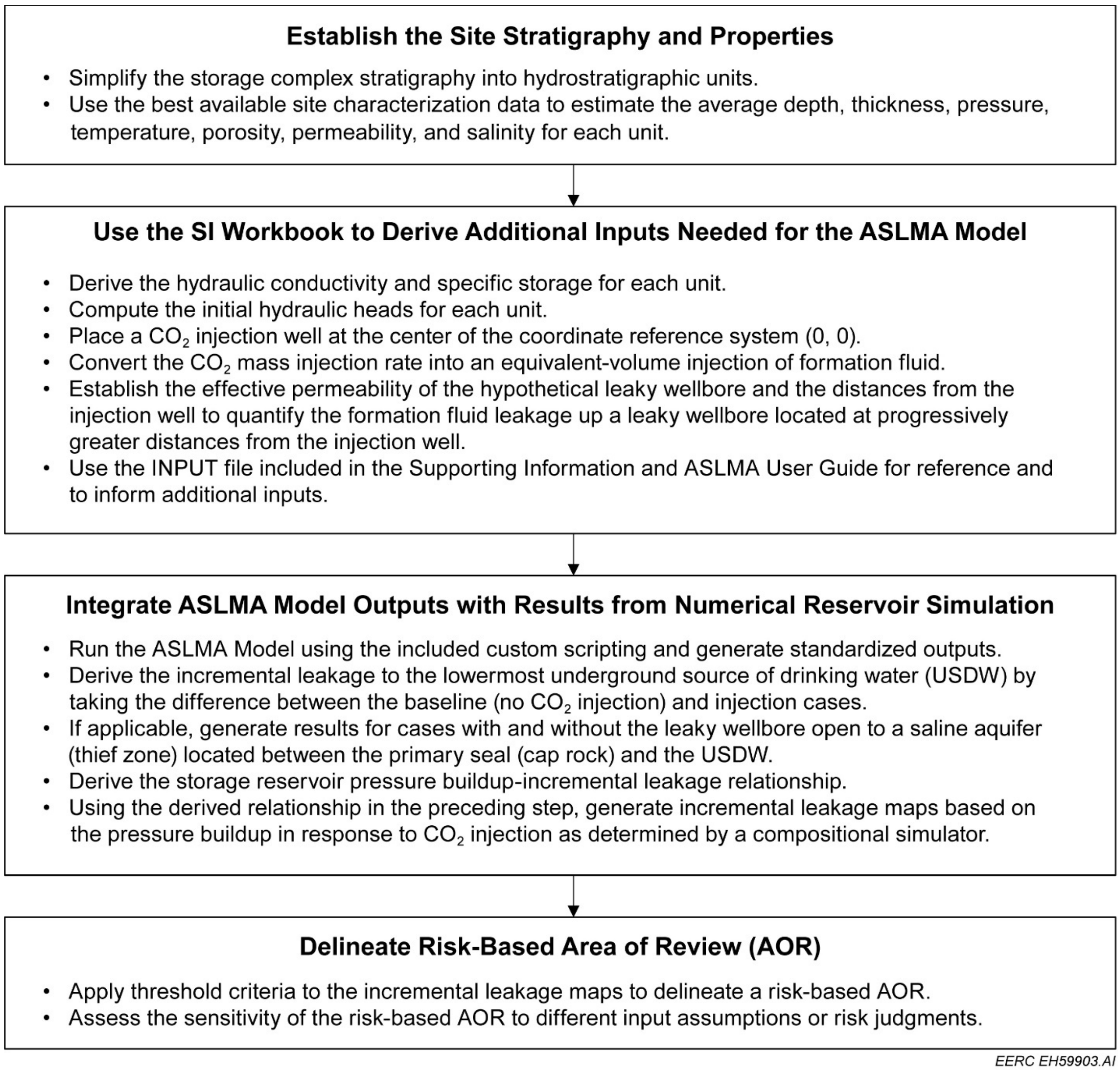

Figure 1. Workflow for delineating a risk-based AOR for a storage facility permit.

2.2 Storage Complex Stratigraphy and Properties

The risk-based AOR workflow begins with simplifying the storage complex stratigraphy into hydrostratigraphic units and using the best available site characterization data to estimate the average properties of each unit. Figure 2 illustrates the stratigraphy and average properties used to represent the storage complex in this study. These properties are averaged from available wireline log and drill core data from regional oil and gas wells and project-specific characterization wells. Individual geologic members are grouped to simplify the stratigraphy into hydrostratigraphic units with similar hydrologic characteristics related to fluid flow. The resultant stratigraphy consists of a deep saline formation storage reservoir (Aquifer 1 – Broom Creek formation, 1938 m deep, 96 m thick), an overlying aquitard that serves as the primary seal or cap rock (Aquitard 1 – Swift-Broom Creek, 1604 m deep, 334 m thick), an intermediate saline aquifer (Aquifer 2 – Inyan Kara Group, 1462 deep, 142 m thick [thief zone]), a second set of aquitards that act as additional seals (Aquitard 2 – Pierre-Inyan Kara, 562 m deep, 900 m thick), and a shallow USDW (Aquifer 3 – Fox Hills sandstone, 473 m deep, 88 m thick). The units from the Fox Hills sandstone to the ground surface are not directly modeled; however, the thicknesses of these units are implicit in the baseline pressures for the underlying units. The average properties for each hydrostratigraphic unit define the reference (nominal) case for the ASLMA Model.

Hydrostratigraphic Unit	Depth* (m)	Thickness (m)	Pressure (MPa)	Temperature (°C)	Porosity (%)	Permeability (m^2)	Salinity (ppm)	Equivalent Fresh-Water Head (m)
Overlying Units to Ground Surface (not directly modeled)		473						
Aquifer 3 (USDW - Fox Hills sandstone)	473	88	5.2	21.2	34	2.76E-13	1,800	760
Aquitard 2 (Pierre-Inyan Kara) (additional seals)	562	900	10.0	35.6	10	9.87E-17	5,800	761
Aquifer 2 (Thief Zone - Inyan Kara Group)	1,462	142	15.1	50.8	20	3.95E-13	10,000	762
Aquitard 1 (Swift-Broom Creek) (primary seal or cap rock)	1,604	334	17.5	57.7	10	9.87E-17	40,000	760
Aquifer 1 (Storage Reservoir - Broom Creek Formation)	1,938	96	22.0	64.0	25	3.33E-13	65,000	1,010

* Ground surface elevation 750 m amsl.

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Figure 2. Simplified stratigraphy and average properties used to represent the storage complex.

2.3 ASLMA Model

The storage facility permit requires that the operator "predict, using existing site characterization, monitoring and operational data, and computational modeling, the projected lateral and vertical migration of the CO_2 plume and its associated pressure front in the subsurface from the commencement of injection activities until the plume movement ceases, or until the end of a fixed time period as determined by the commission" (North Dakota Administrative Code Section 43-05-01-05.1 *Area of review and corrective action*). However, the associated pressure front (pressure buildup in the storage reservoir) caused by CO_2 injection typically extends beyond the CO_2 plume (and 1-mile buffer region) and, consequently, drives the delineation of the AOR. Therefore, delineation of the AOR typically focuses on pressure buildup in the storage reservoir.

Building a geologic model in a commercial-grade software platform like Schlumberger Petrel and running fluid flow simulations using numerical reservoir simulation in a commercial-grade software platform like Computer Modelling Group's compositional simulator, GEM (CMG-GEM), provide the "gold standard" for estimating pressure buildup in response to CO_2 injection (e.g., Bosshart et al., 2018). However, these numerical reservoir simulations are typically limited to the storage reservoir and primary seal formation (cap rock) and do not include the geologic units overlying the cap rock because of the computational burden of conducting such a complex simulation. In addition, geologic modeling of the overlying units may add a substantial amount of time and effort during prefeasibility-phase projects that is unwarranted given the amount of uncertainty that may be present if a few nearby wells can be used for characterization activities. Earlier studies (e.g., Nicot, 2008; Birkholzer et al., 2009; Bandilla et al., 2012; Cihan et al., 2011, 2012) have shown that far-field fluid pressure changes outside of the CO_2 plume domain can be reasonably well described by a single-phase flow calculation by representing CO_2 injection as an equivalent-volume injection of brine (Oldenburg et al., 2014). The semianalytical solutions embedded within the ASLMA Model have been shown to compare well with the numerical model, TOUGH2-ECO2-N, and provided accurate results for pressures beyond the CO_2 plume zone (Birkholzer et al., 2009; Cihan et al., 2011, 2012). Therefore, the proposed workflow for delineating a risk-based AOR uses the ASLMA Model to examine pressure buildup in the storage reservoir and the resultant effects of this buildup on the vertical migration of formation fluid via (single) leaky wellbores located at progressively greater distances from the injection well. The ASLMA Model has been extensively described in Cihan et al. (2011, 2012), so only the parameterization of the model inputs is described here. After establishing the site stratigraphy and average properties (Figure 2), the next step in the risk-based AOR workflow is to generate the set of input parameters needed to implement the ASLMA Model. A macro-enabled Microsoft Excel workbook with built-in Visual Basic Application (VBA) functions is included in Supporting Information of this paper, which provides the calculations needed to execute the ASLMA Model (SI Workbook).

2.3.1 Aquifer- and Aquitard-Derived Properties

The ASLMA Model assumes homogeneous properties within each hydrostratigraphic unit. For each unit shown in Figure 2, pressure, temperature, porosity, permeability, and salinity are used to derive two key inputs for the ASLMA Model: hydraulic conductivity (HCON) and specific storage (SS). VBA functions included in the SI Workbook are used to estimate the formation fluid density and viscosity from the aquifer or aquitard pressure, temperature, and salinity inputs, which are then used to estimate the HCON and SS. The estimated reference case HCON for the storage reservoir (Aquifer 1), thief zone (Aquifer 2), and USDW (Aquifer 3) are

0.576, 0.606, and 0.240 m/d, respectively, and the estimated SS for these units is 2.05E-06, 1.64E-06, and 2.70E-06 (1/m), respectively. Details about the HCON and SS derivations are provided in Supporting Information.

2.3.2 Initial Hydraulic Heads

The original ASLMA Model initially assumed hydrostatic pressure distributions in the entire system. The current work uses a modified version of the ASLMA Model to simulate pressure perturbations and leakage rates when there are initial head differences in the aquifers (Oldenburg et al., 2014). The initial hydraulic heads are calculated assuming an equivalent fresh-water head based on the unit-specific elevations and pressures. The equivalent freshwater heads are entered into the ASLMA Model and establish the initial pressure conditions for the storage complex prior to CO_2 injection. For example, the initial reference case equivalent freshwater heads for the storage reservoir (Aquifer 1), thief zone (Aquifer 2), and USDW (Aquifer 3) are 1010, 762, and 760 m, respectively, which illustrates the state of overpressure in the storage complex, as both Aquifers 1 and 2 have a greater initial hydraulic head relative to Aquifer 3. Therefore, the storage complex requires different treatment than the default AOR calculations described in EPA (2013). Details on the calculations of initial hydraulic head are provided in the Supporting Information.

2.3.3 CO_2 Injection Parameters

The storage project being modeled in the reference case has a relatively small target CO_2 injection rate of 180,000 metric tons CO_2 per year for 20 years. A single injector is placed at the center of the ASLMA model grid at an x,y-location of (0,0) in the coordinate reference system. The ASLMA Model requires the CO_2 injection rate to be converted into an equivalent-volume injection of formation fluid in units of cubic meters per day. VBA functions included in the SI

Workbook are used to estimate the CO_2 density from the storage reservoir pressure and temperature, which results in an estimated density of 730 kg/m^3 in the reference case. The CO_2 mass injection rate and CO_2 density are then used to derive the daily equivalent-volume injection rate of approximately 675 m^3 per day. Details of these calculations are provided in Supporting Information and the SI Workbook.

2.3.4 Hypothetical Leaky Wellbore

In our storage project example, no wellbores are known to exist that penetrate the primary seal (cap rock) within the study area. However, for heuristic, what-if scenario modeling, which is needed to generate the data for delineating a risk-based AOR, a hypothetical leaky wellbore is inserted into the ASLMA Model at 1, 2, …, 100 km from the CO_2 injection well. The pressure buildup in the storage reservoir at each distance, along with the recorded cumulative volume of formation fluid vertically migrating through the leaky wellbore from the storage reservoir to the USDW (i.e., from Aquifer 1 to Aquifer 3) throughout the 20-year injection period, provide the data set needed to derive the risk-based AOR.

Published ranges for the effective permeability of a leaky wellbore have included an "open wellbore" with an effective permeability as high as 10^{-5} m^2 to values more representative of leakage through a wellbore annulus of 10^{-10} to 10^{-12} m^2 (Watson and Bachu, 2008, 2009; Celia et al., 2011). Carey (2017) provides probability distributions for the effective permeability of potentially leaking wells at CO_2 storage sites and estimated a wide range from 10^{-10} to 10^{-20} m^2. For the reference case ASLMA Model, the effectively permeability of the leaky wellbore is set to 10^{-10} m^2, which is a relatively conservative (highly permeable) value near the top of the published range for the effective permeability of potentially leaking wells at CO_2 storage sites. Additional cases are evaluated to quantify the effect of the leaky wellbore effective permeability on the risk-based AOR. Details regarding the leaky wellbore properties are provided in Supporting Information.

The current work uses the ASLMA Model Type 1 feature (focused leakage only) for the nominal model response, which makes the conservative assumption that the aquitards are impermeable. This assumption prevents the pressure from diffusing into the overlying aquitards, resulting in a greater pressure buildup in the storage reservoir and a commensurately greater amount of formation fluid vertically migrating from the storage reservoir through the leaky wellbore. The conservative assumption of Model Type 1 rather than Model Type 3 (coupled focused and diffuse leakage) provides an added level of protection to the delineation of a risk-based AOR by projecting a larger pressure buildup in the storage reservoir and, therefore, a greater leakage of formation fluid up the leaky wellbore.

2.3.5 Saline Aquifer Thief Zone

As shown in Figure 2, a saline aquifer (Aquifer 2) exists between the primary seal above the storage reservoir and the USDW (Aquifer 3). Formation fluid migrating up a leaky wellbore that is open to Aquifer 2 will preferentially flow into Aquifer 2, and the continued flow up the wellbore and into the USDW will be reduced. Therefore, the presence of Aquifer 2 acts as a thief zone and reduces the potential for formation fluid impacts to groundwater. The term “thief zone” is also used in the oil and gas industry to describe a formation encountered during drilling into which circulating fluids can be lost. As described in Supporting Information, models with and without opening the leaky wellbore to Aquifer 2 are run and evaluated to quantify the effect of a thief zone on the risk-based AOR.

2.4 Customized R Code for Multiple Model Runs

A custom wrapper written in the software environment, R (R Core Team, 2020), was developed to perform multiple runs of the ASLMA Model using given ranges for one or more input parameters. The input text file for the ASLMA Model was modified to include an "@R variable name" token for the inputs that were going to vary across model runs. While all inputs could be programmed to accept variable ranges, the current work focuses on the following: 1) CO_2 injection rate, 2) opening or closing the aquifer-wellbore segment to the Aquifer 2 thief zone, 3) hydraulic conductivity of the aquifers, 4) specific storage, and 5) hydraulic conductivity of the leaky well-aquifer segments.

The custom R wrapper consists of two parts: 1) a package containing the ASLMA Model FORTRAN code and R functions to read tokenized input files (Figure 3), replace tokens with given parameter values, write new input files, call the ASLMA Model executable, and capture the resulting "BUILDUP_AQ" and "FLOW_LW" output files as R data frames and 2) a script that calls the functions in the R package and handles parameter preprocessing and output data postprocessing. Inputs to the R script are the tokenized ASLMA Model input file, parameter token names, and values with which to replace those token names in the input file.

In addition, to generate multiple runs more readily, the customized R code standardizes the ASLMA Model outputs across multiple runs, expediting the analysis and graphing within the R programming environment or other software programs.

Figure 3 ASLMA Model input file with variable tokens - Notepad

File Edit Format View Help

```
*TITLE: ASLMA MODEL FOR R
*-----------------------------------------------------------------------*
* Model Selection
* Model Type=1 : Focused Leakage Only
* Model Type=2 : Diffuse Leakage Only
* Model Type=3 : Coupled Focused and Diffuse Leakage
* Enter Model Type
    1

*-----------------------------------------------------------------------*
* 1- RESERVOIR DESCRIPTION
* 1.1. Layer types at bottom and top
* AQUIFER = 1,  AQUITARD = 0
* BOTTOM OF THE DOMAIN, BL
  1

* TOP OF THE DOMAIN; TL
  1

* 1.2: Number of Aquifers, NAQ
  3

* 1.3: Aquifer Properties
* Listed from bottom (aquifer 1, top line) to top (aquifer 6, bottom line)
* BAQ   HCONX       ANSR    SS    HEAD_INIT
* Aquifer 1 (Storage Reservoir, Broom Creek)
  96    @aq1_hconx    1.  @aq1_ss    1010
* Aquifer 2 (Thief Zone, Inyan Kara)
  142   @aq2_hconx    1.  @aq2_ss    762
* Aquifer 3 (USDW, Fox Hills)
  88    2.40E-01    1.  2.70E-06    760
```

Ln 32, Col 1 | 100% | Unix (LF) | UTF-8

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Figure 3. Example portion of ASLMA Model input file with variable tokens.

2.5 Calculating the Potential Incremental Leakage to the USDW

As previously noted, several candidate storage reservoirs within North Dakota (and likely elsewhere around the world) are already overpressurized relative to overlying aquifers and thus subject to potential vertical fluid migration from the storage reservoir to the lowermost USDW even prior to the planned storage project. Stated differently, were a hypothetical leaky wellbore to exist that connects the storage reservoir to the USDW, then even in the absence of CO_2 injection, there would be an existing flow of formation fluids from the storage reservoir to the USDW. This pressure situation is important since the relative change in the storage reservoir pressure buildup and formation fluid flow to the USDW (incremental leakage) between the baseline scenario (no CO_2 injection) and the CO_2 injection scenario is a critical input for assessing endangerment for the purpose of defining a risk-based AOR.

The following approach is adapted from Oldenburg et al. (2014) and the sequence of steps is as follows:

1. Run the baseline scenario (no CO_2 injection) ASLMA Model to estimate the cumulative flow (leakage) of formation fluid from the storage reservoir to overlying aquifers via hypothetical wellbores. Multiple leaky wellbores at progressively greater distances are not needed for the baseline case because there is no injection occurring. Record the pressure in the storage reservoir and cumulative flow of formation fluid into Aquifer 3 (USDW). For the baseline case with the leaky wellbore open to Aquifer 2 (thief zone), record the pressure in the storage reservoir and cumulative flow of formation fluid into both Aquifer 2 (thief zone) and Aquifer 3 (USDW) at each leaky wellbore distance. The outputs from this step are the storage reservoir pressure buildup and cumulative flows attributable to the intrinsic relative overpressure condition and not to CO_2 injection. The modeling work done for the current study writes outputs for 20 years of CO_2 injection; however, the time steps should mirror the site-specific CO_2 injection operations.
2. Run the CO_2 injection scenario ASLMA Model to estimate the cumulative flow (leakage) of formation fluid from the storage reservoir to overlying aquifers under CO_2 injection. Record the pressure and cumulative flow of formation fluid into Aquifer 3 (USDW) at each leaky wellbore distance. For the CO_2 injection case with the leaky wellbore open to Aquifer 2 (thief zone), record the pressure in the storage reservoir and

cumulative flow of formation fluid into both Aquifer 2 (thief zone) and Aquifer 3 (USDW) at each leaky wellbore distance. The outputs from this step are the storage reservoir pressure buildup and cumulative flows attributable to both the intrinsic relative overpressure condition and CO_2 injection.

3. Calculate the ratio and difference between the cumulative flow of formation fluid for each aquifer/leaky wellbore distance under the CO_2 injection scenario (Step 2) to the cumulative flow of formation fluid for each aquifer/leaky wellbore distance under the baseline (no CO_2 injection) scenario (Step 1) to quantify the relative change in cumulative flow attributable to CO_2 injection (i.e., the incremental leakage that occurs due to the storage project). This approach is analogous to Normalization Method 2 in Oldenburg et al. (2014), which does not account for the additional cumulative leakage into Aquifer 3 that may have occurred along any hypothetical leaky wellbore that existed prior to the start of CO_2 injection and provides a more conservative estimate, i.e., results in a larger incremental leakage. Steps 1, 2, and 3 use the cumulative flow rather than the leakage rate because the leakage rate does not provide an overall indication of long-term total impact to the USDW.
4. Calculate the incremental storage reservoir pressure buildup for each aquifer/leaky wellbore distance by subtracting the reservoir pressure buildup in the baseline (no CO_2 injection) scenario from the reservoir pressure buildup under the CO_2 injection scenario. The incremental reservoir pressure buildup rather than the absolute pressure buildup under the CO_2 injection scenario is used because, under some combinations of input parameters, there is a reduction in pressure in the reservoir at the leaky well location in both the baseline and CO_2 injection scenarios. Relate the incremental

pressure buildup in the storage reservoir at the end of 20 years to the incremental leakage to Aquifer 3 (USDW) at the end of 20 years using derived functions or linear interpolations for both the case with and without the leaky wellbore open to Aquifer 2 (thief zone). The mathematical relationship derived in this step informs the subsequent mapping in Step 6.

5. Simulate the pressure buildup within the storage reservoir in response to CO_2 injection using a compositional simulator (e.g., CMG-GEM). While this step could be omitted and the workflow could go directly to Step 6, the reason for using CMG-GEM is to better accommodate the temporospatial evolution of pressure buildup within the storage reservoir that is more accurately modeled using a heterogeneous geologic model and a compositional simulator that accounts for the multiphase interactions.
6. Using the compositional simulator output, apply the incremental pressure buildup-incremental leakage relationship derived in Step 4 to an areal map of reservoir pressure buildup from the compositional simulator (e.g., the model layer with the maximum pressure buildup at the end of simulation) to produce a map of potential incremental leakage to Aquifer 3 (USDW). Delineate a risk-based AOR whose two-dimensional (2D) extent encompasses a specified threshold incremental leakage. The choice of threshold incremental leakage is discussed later in the manuscript.
7. Quantify the sensitivity of the incremental leakage (and, by extension, the risk-based AOR) to variation in petrophysical properties of the storage reservoir and overlying units, wellbore properties, and the presence of a thief zone between the primary seal (cap rock) and the USDW.

Table 1 summarizes the set of four ASLMA Model runs (case matrix) for executing the above combinations of scenarios for Steps 1–6.

Table 1. ASLMA Model Case Matrix Showing Reference Case Parameters for Estimating the Risk-Based AOR

Case Number	Case Name	Injection Rate (metric tons per year)	Thief Zone (Aquifer 2)
Case 1	Baseline (no CO_2 injection)	0	Off
Case 2	Baseline (no CO_2 injection)	0	On
Case 3	Nominal case	180,000	Off
Case 4	Nominal case	180,000	On

2.6 Sensitivity Analysis

Our understanding or prediction of geologic systems is always uncertain. For example, uncertainty exists in both the random and systematic errors used to measure fundamental rock properties, as well as in the assumptions used to estimate the parameters from theoretical models, such as estimating permeability from well test data (Horne, 1995; Ramaswami et al., 2005). However, there is also environmental variability over space for these parameters. This variability is inherent to the storage complex, and unlike uncertainty, it cannot be reduced through additional measurements (Gilbert, 1987; Ramaswami et al., 2005). In this paper, the hydrostratigraphic unit properties shown in Figure 2 and the ASLMA Model inputs derived in the SI Workbook represent the *average values*. Therefore, the ASLMA Model results using these average values represent the nominal (i.e., reference-case) response, and the risk-based AOR derived from the nominal response represents the most likely outcome (i.e., the best estimated value of the output, incremental leakage, corresponding to the best estimated values of the inputs). The sensitivity analysis focuses the effect of the ASLMA Model input variables on the incremental leakage and, therefore, the estimated risk-based AOR of the nominal response.

While each of the input variables contribute to the output, the sensitivity analysis focuses on the variation in four inputs: HCON of Aquifer 1 (storage reservoir) and Aquifer 2 (thief zone), SS of Aquifers 1 and 2, hydraulic conductivity of the leaky wellbore, and CO_2 injection rate. HCON and SS for each aquifer depend on the underlying properties used to derive them and are not independent. Therefore, a one-at-a-time sensitivity analysis holding one of the two inputs constant while varying the other would be invalid. Instead, the sensitivity analysis approach derives a joint-probability region for HCON and SS and then explores the ASLMA Model outputs as the input variables move from lower to higher HCON/SS, covering the region between approximately the 30th and 70th percentiles of the joint distribution.

The sensitivity analysis for the leaky wellbore assumes that the quality of materials in each well is uniform along the entire well, which means that the effective permeability values for each wellbore-aquifer and wellbore-aquitard segment are completely correlated. In other words, one value of effective permeability is chosen, and that value is assigned to all leaky wellbore segments (Celia et al., 2011). The sensitivity analysis explores a range of leaky wellbore effective permeabilities from 10^{-9} to 10^{-13} m^2, using log-order increments (i.e., 10^{-9}, 10^{-10}, …, 10^{-13} m^2), or one order-of-magnitude higher permeability than the nominal case to three orders-of-magnitude lower permeability than the nominal case.

The nominal CO_2 mass injection rate is 180,000 metric tons per year, which reflects the expected injection rate of the example storage project. However, two additional injection rates are included in the sensitivity analysis: 500,000 and 1,000,000 metric tons per year.

Varying the HCON and SS of Aquifers 1 and 2, the hydraulic conductivity of the leaky wellbore and the CO_2 mass injection rate, provides a sensitivity analysis test matrix of 16 additional ASLMA Model runs (one nominal case [Test Case No. 1] plus 16 additional runs, i.e., 17 runs total). Details about the formulation of the sensitivity analysis test matrix are provided in Supporting Information (Table S-1).

3.0 RESULTS

The workflow described above produces two sets of results: 1) an isotropic prediction of potential incremental total cumulative leakage based on distance from a single injection well using only the ASLMA Model and 2) an anisotropic prediction map of potential incremental total cumulative leakage using a combination of the relationship between reservoir buildup and leakage derived from the ASLMA Model and reservoir buildup results from compositional simulation of the geocellular model.

3.1 Incremental Total Cumulative Leakage from ASLMA Model

Figure 4a shows the results of the nominal ASLMA Model with the incremental leakage expressed as a ratio (percent) for both the scenario with and without the leaky wellbore being open to Aquifer 2 (thief zone). Figure 4b shows the results expressed as a volume (m^3). The incremental leakage is a function of both distance from the injection well and time, as a leaky wellbore located closer to the injection well is subjected to greater pressure buildup over the injection period and, therefore, commensurately greater incremental leakage.

For a leaky wellbore located 2 km from the injection well and the case when the leaky wellbore is closed to Aquifer 2 (thief zone), the incremental leakage to Aquifer 3 (USDW) at the end of 20 years is approximately 2.4% above the baseline (no CO_2 injection) (*y*-axis of 1.024 in Figure 4a, top left panel). However, when the leaky wellbore located 2 km from the injection well is open to Aquifer 2, the incremental leakage to Aquifer 3 at the end of 20 years is essentially zero (0.2%, *y*-axis of 1.002 in Figure 4a, top right panel). Thus the presence of a thief zone significantly reduces the incremental leakage, which is consistent with the "elevator model" described by Nordbotten et al. (2004) and other published modeling studies that have included a thief zone (e.g., Cihan et al., 2012; Birkholzer et al., 2014; Huerta and Vasylkivska, 2016).

At leaky wellbores located farther from the injection well, the incremental leakage at the end of 20 years decreases substantially. For example, for leaky wellbores located 4, 8, and 15 km from the injection well, the incremental leakage into Aquifer 3 at the end of 20 years is approximately 1.8% (1.018 on the *y*-axis), 1.3% (1.013 on the *y*-axis), and 0.8% (1.008 on the *y*-axis), respectively, above the baseline (no CO_2 injection) case when the leaky wellbore is closed to Aquifer 2. When the leaky wellbore is open to Aquifer 2, the incremental leakage to Aquifer 3 at the end of 20 years for these distances is essentially zero (all less than 0.2%).

The incremental leakage expressed as a volume helps place the results into the broader hydrogeological context with respect to assessing endangerment to the USDW. For example, for the leaky wellbore located 2 km from the injection well, the 2.4% increase above baseline (no CO_2 injection) equates to a cumulative volume of only 381 m^3 at the end of 20 years (*y*-axis of 222 in Figure 4b, top left panel). Aquifer 3 is 88 m thick; therefore, within a cylinder of radius 2 km and using the average porosity of 34%, Aquifer 3 contains approximately 376 million m^3 of water [$\pi(2000\ m)^2(88\ m)(0.34)$]. Thus an incremental leakage of 381 m^3 of formation fluid over

20 years equates to about 0.0001% of the total volume of water contained within that rock volume. The incremental leakage at distances beyond 2 km equate to less than 0.0001% of the total volume of water contained within that rock volume.

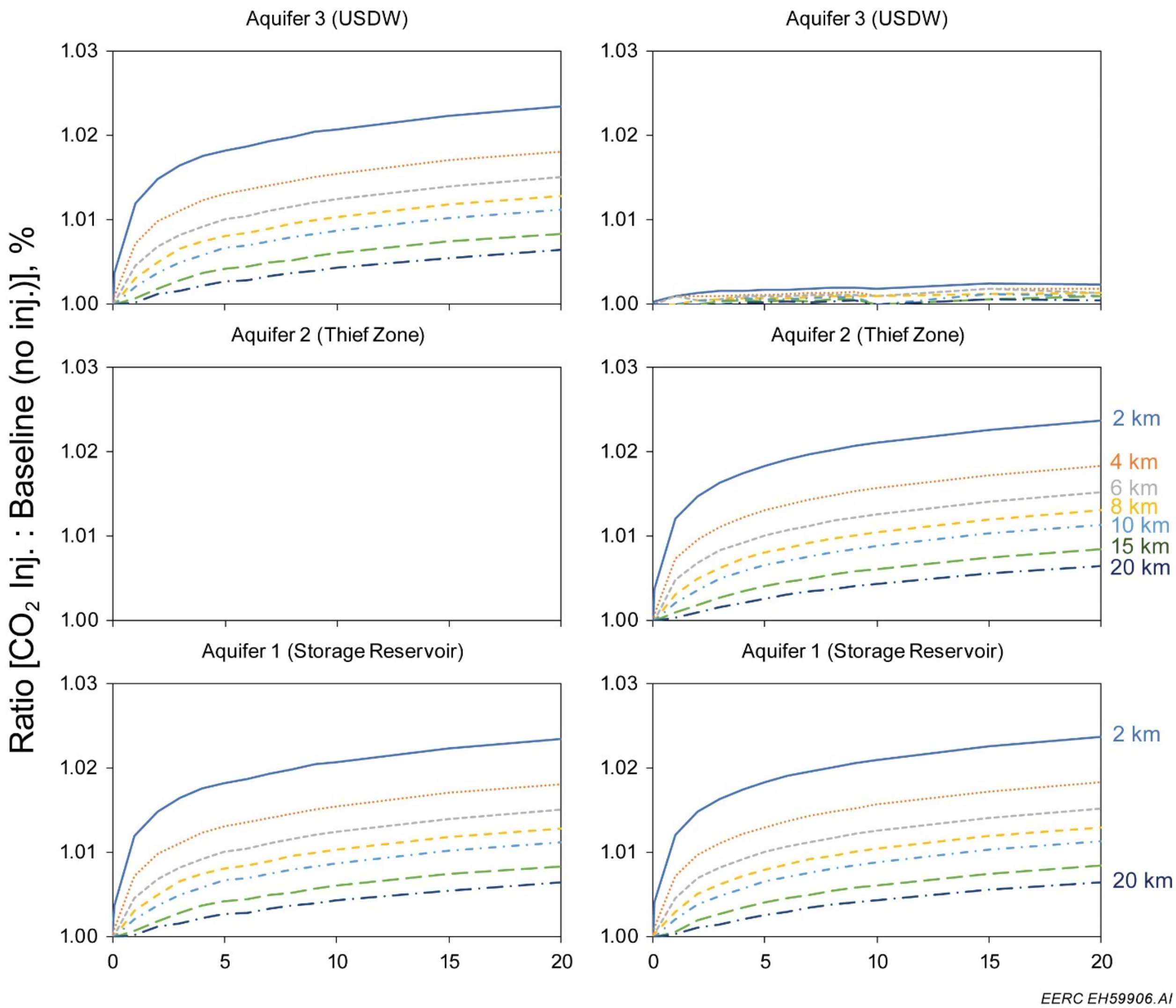


Figure 4a. Results of the ASLMA Model for leaky well distances from 2 to 20 km with the incremental total cumulative leakage expressed as a ratio. The left column of panels shows the scenario where the leaky wellbore is closed to Aquifer 2 (thief zone), and the right column of panels shows the scenario where the leaky wellbore is open to Aquifer 2.

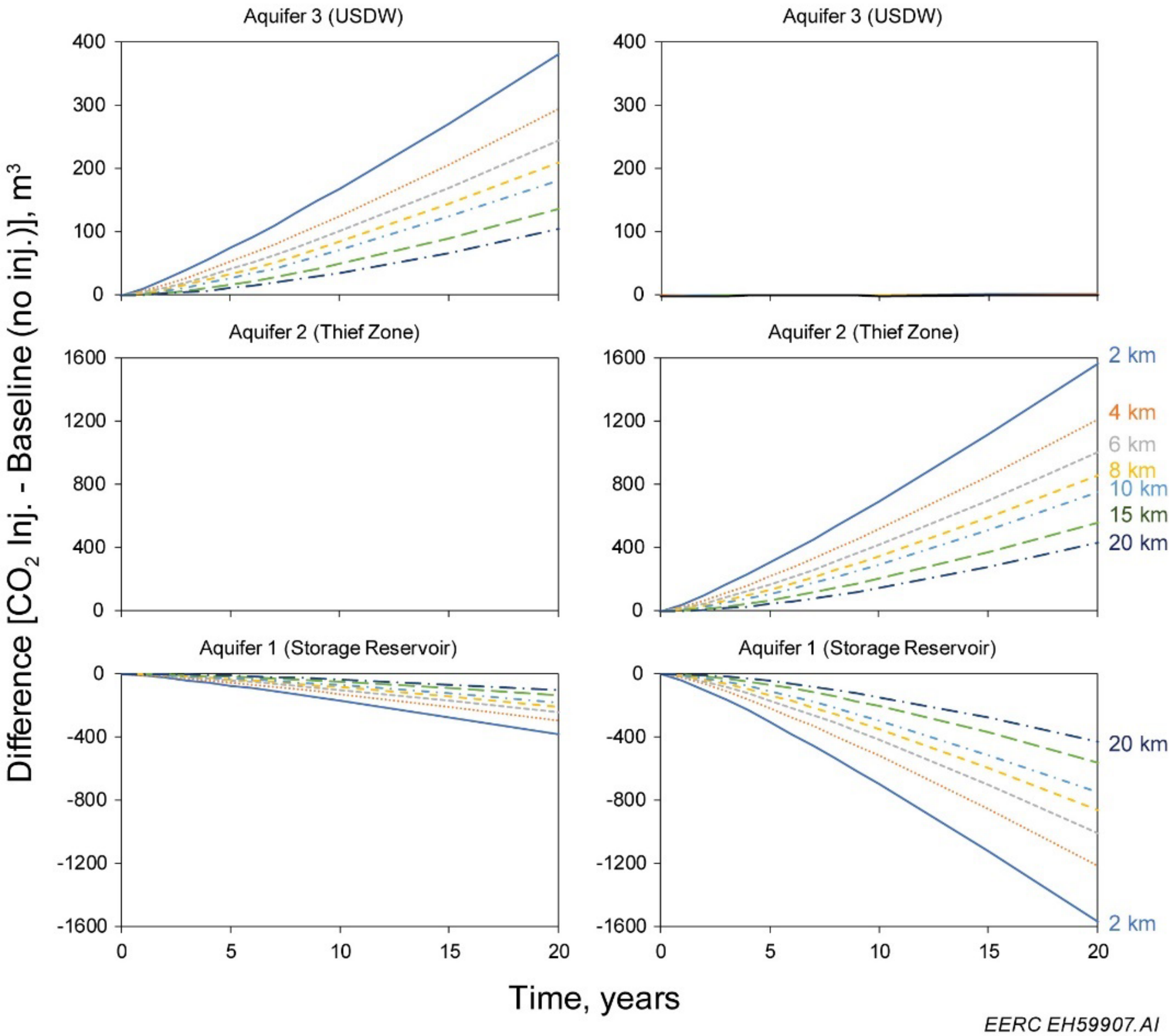


Figure 4b. Results of the ASLMA Model for leaky well distances from 2 to 20 km with the incremental total cumulative leakage expressed as a volume. The left column of panels shows the scenario where the leaky wellbore is closed to Aquifer 2 (thief zone), and the right column of panels shows the scenario where the leaky wellbore is open to Aquifer 2.

3.2 Relating Pressure Buildup to Incremental Leakage with ASLMA Model and Compositional Simulation

Figure 5 shows the relationship between maximum pressure buildup in the storage reservoir and the incremental leakage to Aquifer 3 (USDW) at each hypothetical leaky wellbore location at the end of 20 years for both the cases with and without the leaky wellbore open to Aquifer 2 (thief zone). In the case where the leaky wellbore is closed to Aquifer 2 (thief zone = off), there is no incremental leakage to Aquifer 2 (the incremental leakage to Aquifer 2 is not used for delineating the risk-based AOR and is provided only for reference). The curvilinear relationship between pressure buildup in the storage reservoir and the incremental leakage to Aquifer 3 is used to predict incremental leakage from the pressure buildup map produced by compositional simulation of the geocellular model. The maximum simulated pressure buildup in the reservoir (generally the top layer of the simulation model) is represented by a raster map of pressure buildup values. For each raster value, the relationship between pressure buildup and incremental leakage is used to predict incremental leakage using linear interpolation between the points making up the USDW curve, both with and without a thief zone. As shown in the figure, when the leaky wellbore is open to Aquifer 2, it decreases the incremental total cumulative leakage to Aquifer 3 by one to two orders of magnitude for any given pressure.

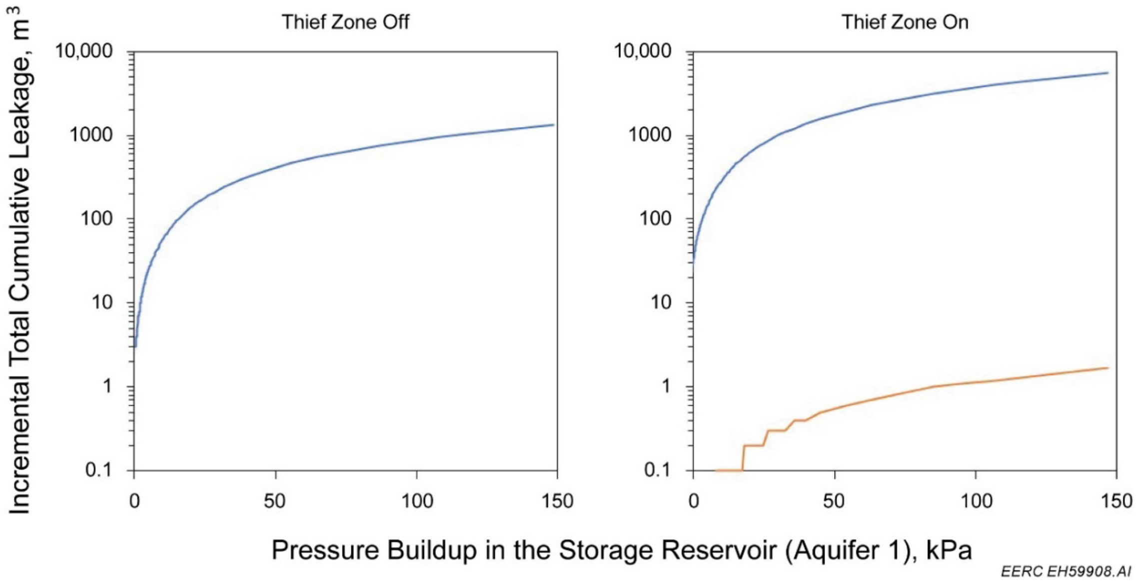


Figure 5. Relationship between pressure buildup in the storage reservoir (*x*-axis, kPa) and incremental total cumulative leakage (*y*-axis, m^3) for Aquifer 2 (thief zone, red dashed line) and Aquifer 3 (USDW, blue line). The left panel shows the scenario where the leaky wellbore is closed to Aquifer 2 (Thief Zone = Off) and the right panel shows the scenario where the leaky wellbore is open to Aquifer 2 (Thief Zone = On).

3.2.1 Incremental Leakage Maps

The pressure buildup-incremental leakage relationships in Figure 5 result in the incremental leakage maps shown in Figure 6, which show the estimated total cumulative incremental leakage potential from a hypothetical leaky well into Aquifer 3 (USDW) over the entire 20-year period. For the case where the leaky wellbore is closed to Aquifer 2 (thief zone), the areal extent of the CO_2 plume in the storage reservoir plus half-mile buffer (as determined using a compositional simulator and the site-specific geological model) corresponds to an incremental leakage potential of approximately 350 m^3 (Figure 6a). In contrast, when the leaky

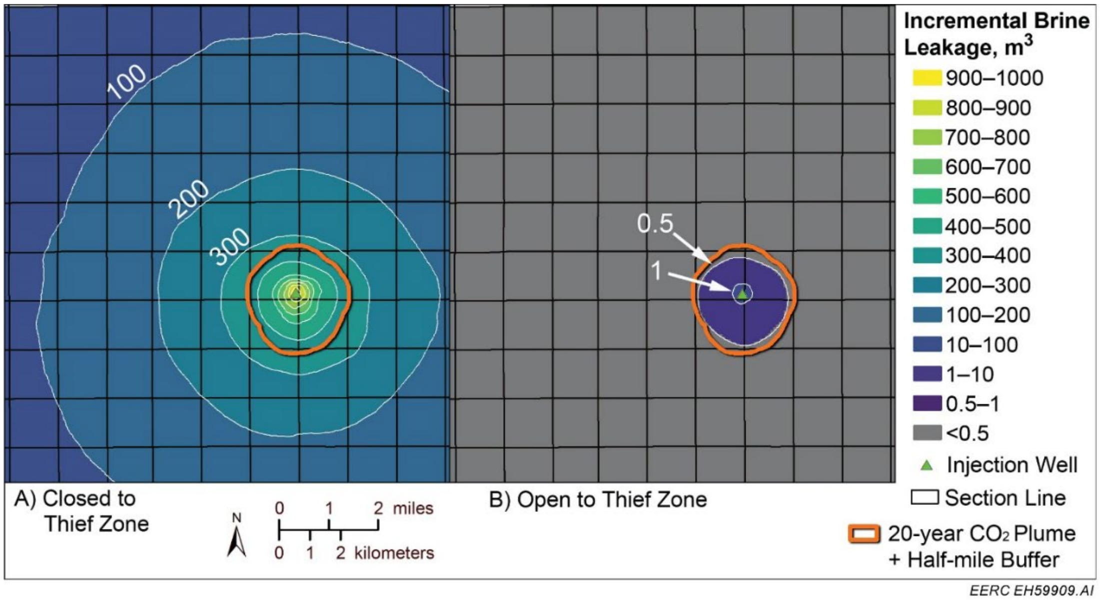


Figure 6. Incremental leakage maps at the end of 20 years of CO_2 injection for the scenario where the leaky wellbore is closed to Aquifer 2 (thief zone) (a) or open to Aquifer 2 (b). The white polygon in both panels denotes the areal extent of the CO_2 plume in the storage reservoir plus half-mile buffer at the end of 20 years of CO_2 injection as determined using a compositional simulator and the site-specific geological model.

wellbore is open to Aquifer 2, there is essentially no incremental leakage to Aquifer 3, and the areal extent of measurable incremental leakage is less than the extent of the CO_2 plume in the storage reservoir plus half-mile buffer (Figure 6b). The final step of the risk-based AOR workflow is to apply a threshold criterion to the incremental leakage maps to delineate a risk-based AOR, as discussed below.

3.3 Sensitivity Analysis Results

Figure 7 shows the results of the sensitivity analysis for the four sets of input parameters. The horizontal lines are provided for reference and show the maximum incremental leakage to Aquifer 3 (USDW) at the end of 20 years for the nominal case with the leaky wellbore closed to

Aquifer 2 (thief zone off – 1340 m^3) and open to Aquifer 2 (thief zone on – 2 m^3), respectively (Figure 7e).

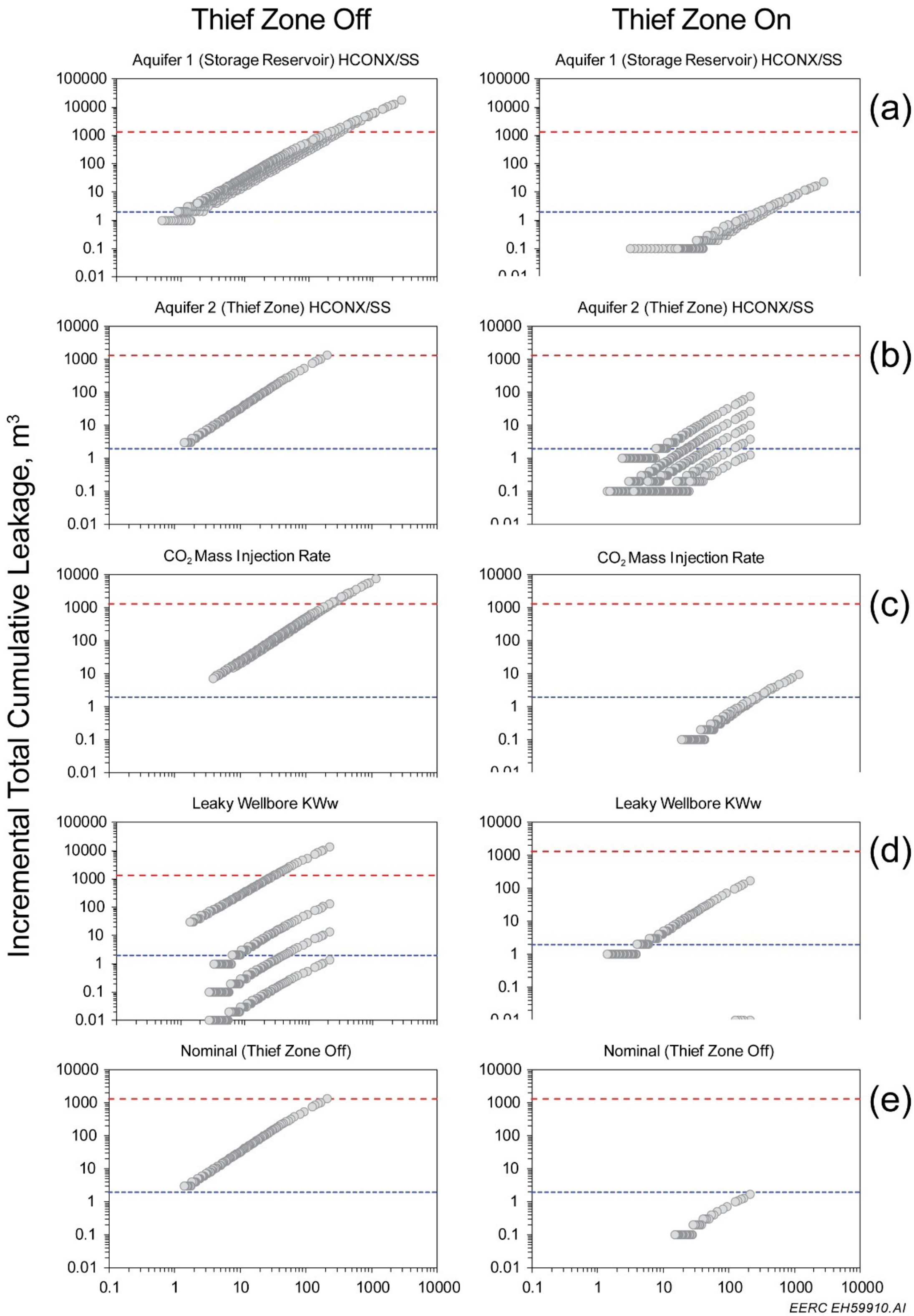
Lowering HCONX/SS of Aquifer 1 (storage reservoir) from the nominal case increases the pressure buildup in response to CO_2 injection and, therefore, increases the incremental leakage of formation fluids up the leaky wellbore to Aquifer 3. For example, for the same CO_2 injection rate as the nominal case, the lower HCON/SS of Aquifer 1 results in a maximum pressure buildup of 2760 kPa (1210% increase from the nominal value of 210 kPa) and a maximum incremental leakage of 17,330 m^3 (1190% increase from the nominal value of 1340 m^3). The result is slightly less pronounced for the case when the leaky wellbore is open to Aquifer 2, which results in a maximum pressure buildup of 2720 kPa (1200% increase from the nominal value of 201 kPa) and a maximum incremental leakage of 22 m^3 (1000% increase from the nominal value of 2 m^3) (Figure 7a).

Modifying the HCONX/SS of Aquifer 2 from the nominal case has no effect on the case when the leaky wellbore is closed to Aquifer 2. However, when the leaky wellbore is open to Aquifer 2, lowering HCONX/SS of Aquifer 2 from the nominal case increases the incremental leakage to Aquifer 3. For example, the maximum incremental leakage when the leaky wellbore is open to Aquifer 2 is 80 m^3 (3900% increase from the nominal value of 2 m^3) (Figure 7b). Therefore, the lower HCONX/SS of Aquifer 2 prevents the flow of formation fluids into Aquifer 2 from the leaky wellbore, and results in a greater incremental leakage to Aquifer 3. Conversely, increasing the HCONX/SS of Aquifer 2 from the nominal case decreases the incremental leakage to Aquifer 3, as shown in the bottom set of data points in Figure 7b.

The effect of increasing the CO_2 mass injection rate from the nominal case is analogous to lowering HCONX/SS of Aquifer 1: the higher injection rate increases the pressure buildup in

Aquifer 1 in response to CO_2 injection and, therefore, increases the incremental leakage of formation fluids up the leaky wellbore to Aquifer 3. The maximum incremental leakage with the leaky wellbore closed to Aquifer 2 is 7430 m^3 (450% increase from the nominal value of 1340 m^3) and maximum incremental leakage with the leaky wellbore open to Aquifer 2 is 10 m^3 (400% increase from the nominal value of 2 m^3) (Figure 7c).

Lastly, the effect of increasing the leaky wellbore effective permeability increases the incremental leakage to Aquifer 3; conversely, decreasing the leaky wellbore effective permeability decreases the incremental leakage to Aquifer 3 (Figure 7d). For example, the case with the greatest leaky wellbore effective permeability when the leaky wellbore is closed to Aquifer 2 results in a maximum incremental leakage of 13,250 m^3 (900% increase from the nominal value of 1340 m^3), while the case with the lowest leaky wellbore effective permeability when the leaky wellbore is closed to Aquifer 2 results in a maximum incremental leakage of 1 m^3 (–100% decrease from the nominal value of 1340 m^3). Similarly, the case with the greatest leaky wellbore effective permeability when the leaky wellbore is open to Aquifer 2 results in a maximum incremental leakage of 170 m^3 (8400% increase from nominal), while the case with the lowest leaky wellbore effective permeability when the leaky wellbore is open to Aquifer 2 results in a maximum incremental leakage of 0 m^3 (no measurable incremental leakage) (Figure 7d).



Thief Zone Off
Thief Zone On
Incremental Total Cumulative Leakage, m3
Aquifer 1 (Storage Reservoir) HCONX/SS
(a)
Aquifer 2 (Thief Zone) HCONX/SS
(b)
CO2 Mass Injection Rate
(c)
Leaky Wellbore KWw
(d)
Nominal (Thief Zone Off)
(e)
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536

Figure 7. Results of the sensitivity analysis showing pressure buildup in the storage reservoir (*x*-axis [$\log_{10}$-scale]) and the estimated incremental total cumulative leakage to Aquifer 3 (USDW) at the end of 20 years of CO_2 injection (*y*-axis [$\log_{10}$-scale]) as a function of varying four sets of input parameters: (a) HCONX/SS of Aquifer 1, (b) HCONX/SS of Aquifer 2, (c) CO_2 mass injection rate, and (d) leaky wellbore effective permeability, as compared to the reference (nominal) case (e). The horizontal lines at 1340 m^3 and 2 m^3 are provided for reference and show the maximum incremental leakage for the nominal case with the thief zone off and on, respectively.

The sensitivity analysis results show the importance of site characterization data to the delineation of the risk-based AOR, as the measurements of depth, pressure, temperature, salinity, porosity, and permeability affect the subsequent estimates of HCONX and SS for the hydrostratigraphic units. In addition, well integrity surveys provide invaluable data that can inform the potential wellbore leakage risk within the AOR.

4.0 DISCUSSION

The approach presented herein provides a defensible approach for generating an incremental leakage map using the combined results of the ASLMA Model and compositional simulation. These methods translate ASLMA Model-based pressure increase in the storage reservoir into expected incremental leakage into overlying aquifers according to average geometry and petrophysical properties. The approach builds upon well-established research and underlying hydrogeological principles. For example, the semianalytical solutions included in the ASLMA Model are extensions of earlier work for formation fluid leakage through abandoned wellbores by Raven (1990) and Avci (1994), which have been upheld for nearly three decades. In addition, the ASLMA Model (Cihan et al., 2011, 2012) has been broadly applied to an array of storage projects. However, the final step is to apply a threshold criterion to the incremental leakage maps to delineate a risk-based AOR. Ultimately, the specific criterion is a matter of risk judgment under uncertainty (Morgan et al., 1990).

For the storage project evaluated here, under the scenario where the leaky wellbore is open to a thief zone between the overlying seal and the USDW, the risk-based AOR essentially collapses to the areal extent of the CO_2 plume in the storage reservoir because the pressure buildup in the storage reservoir beyond the CO_2 plume is insufficient to drive formation fluids up a hypothetical leaky wellbore past the thief zone and into the USDW. However, even under the conservative assumption that the leaky wellbore is not open to the thief zone, at distances beyond the areal extent of the CO_2 plume, the incremental leakage is less than ~400 m^3 over 20 years (Figure 6) which represents ~0.0001% or less of the total volume of water contained within the USDW rock pore volume. Therefore, a risk-based AOR could be delineated based on a no-impact threshold (i.e., no incremental leakage) or a low- or nondetectable-threshold (i.e., a leakage volume so small that it either would not be detected by conventional analytical methods or otherwise have no measurable impact on the salinity of the USDW). The threshold criterion is site-specific and should be informed by the results of the sensitivity analysis and available site characterization data.

The example storage project presented in this paper represents a relatively small CO_2 injection rate of 180,000 metric tons per year. While the differences in the no-injection versus CO_2-injection comparisons are evident, they would be much more dramatic under larger injection volumes, such as those anticipated for a typical coal-fired power plant (1 million metric tons of CO_2 or more injected per year).

5.0 CONCLUSIONS

This paper presents a workflow and modeling approach for delineating a risk-based AOR to support an EPA Class VI storage facility permit for a CO_2 storage project. The approach combines semianalytical solutions for estimating the formation fluid leakage through a hypothetical leaky wellbore with the results of numerical reservoir simulations to define the AOR. For the storage project evaluated here, under the scenario where the leaky wellbore is open to a saline aquifer (thief zone) between the overlying seal (cap rock) and the USDW, the risk-based AOR essentially collapses to the areal extent of the CO_2 plume in the storage reservoir because the pressure buildup in the storage reservoir beyond the CO_2 plume is insufficient to drive formation fluids up a hypothetical leaky wellbore into the USDW. However, even under the conservative assumption that the leaky wellbore is not open to a thief zone, beyond the areal extent of the CO_2 plume, the incremental leakage is less than ~400 m^3 over 20 years (Figure 6) which represents ~0.0001% or less of the total volume of water contained within the USDW rock volume. The approach outlined in this paper is designed to be protective of USDWs and, therefore, comply with SDWA requirements and provisions for the U.S. EPA Class VI UIC program (Class VI Rule) and North Dakota Administrative Code Chapter 43-05-01.

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SUPPORTING INFORMATION

A macro-enabled Microsoft Excel workbook with built-in Visual Basic Application (VBA) functions is included in Supporting Information that provides the calculations needed to execute the ASLMA Model (SI Workbook). The remainder of this Supporting Information describes the calculations included in the SI Workbook.

S1.0 AQUIFER AND AQUITARD PROPERTIES

S1.1 Hydraulic Conductivity (HCON)

Hydraulic conductivity (HCON) is a function of fluid density, fluid viscosity, and the reservoir permeability, as shown in Equation S-1.

$$k = \kappa \frac{\rho g}{\mu} \qquad \text{[Equation S-1]}$$

Where:

k is hydraulic conductivity (m/d).

κ is permeability (m^2).

ρ is the fluid density (kg/m^3).

g is the acceleration due to gravity (9.81 m/s^2).

μ is the fluid viscosity (kg/m-s).

The fluid density and viscosity are a function of pressure, temperature, and salinity.

To estimate the brine density, the SI Workbook utilizes a VBA function, *BrineDen*, which uses inputs of temperature (T in units of °C), pressure (P in units of Pa), and salinity (XS as a dimensionless salt mass fraction). The *BrineDen* function was developed by Bandilla (2016a) based on the brine density solutions described in Haas (1976) and Battistelli et al. (1997).

To estimate brine viscosity, the SI Workbook utilizes a VBA function, *BrineVisc*, which also uses inputs of temperature (T in units of °C), pressure (P in units of Pa), and salinity (XS as a dimensionless salt mass fraction). The *BrineVisc* function was developed by Bandilla (2016b) based on the brine viscosity solutions described in Phillips et al. (1981).

The formation-specific pressure, temperature, and salinity values provide the inputs needed to estimate brine density via *BrineDen* and brine viscosity via *BrineVisc*, which, along with the formation-specific permeability, provide the inputs for estimating HCON for each unit via Equation S-1. For example, the pressure, temperature, and salinity for Aquifer 1 (Broom Creek Formation) are 22,019 Pa (3194 psi), 64.0°C (147.2°F), and 0.065 (65,000 ppm), respectively. These inputs result in an estimated brine density and viscosity of 1034 kg/m^3 and 5.06E-04 kg/m-s, respectively. The average permeability for Aquifer 1 is 3.33E-13 m^2 (337 md), which results in a HCON of 6.76E-01 m/d.

S1.2 Specific Storage (SS)

Specific storage (SS) is a function of fluid density, gravity, formation porosity, fluid compressibility, and pore compressibility, as shown in Equation S-2.

$$SS = \rho g \phi (\alpha + \beta) \qquad \text{[Equation S-2]}$$

Where:

ρ is the fluid density (kg/m^3).

g is the acceleration due to gravity (9.81 m/s^2).

ϕ is porosity (unitless).

α is the brine compressibility (1/Pa).

β is the pore compressibility (1/Pa).

Similar to the process for estimating HCON, the formation-specific pressure, temperature, and salinity values provide the inputs needed to estimate brine density via *BrineDen* and brine viscosity via *BrineVisc*, which, along with the formation-specific porosity, brine compressibility, and pore compressibility, provide the inputs for estimating SS for each unit via Equation S-2. The pore compressibility is assumed to be 4.5E-10 (1/Pa) for aquifers and 9.0E-10 (1/Pa) for aquitards, which is consistent with values used in Birkholzer et al. (2009) and representative of the site-specific lithology for the storage project. Users may change these inputs to reflect their site-specific values. An additional function is used to estimate pore compressibility. To estimate the brine compressibility, the SI Workbook utilizes a VBA function, *BrineComp*, which uses inputs of temperature (T in units of °C), pressure (P in units of Pa), and salinity (XS as a dimensionless salt mass fraction). The *BrineVisc* function was developed by Morgan (2016).

For example, the pressure, temperature, and salinity for Aquifer 1 (Broom Creek formation) are 22,019 Pa (3194 psi), 64.0°C (147.2°F), and 0.065 (65,000 ppm), respectively. These inputs result in an estimated brine density and viscosity of 1034 kg/m^3 and 5.06E-04 kg/m-s, respectively. Under these conditions, the brine compressibility is estimated to be 3.83E-10 (1/Pa) and the pore compressibility is assumed to be 4.5E-10 (1/Pa). Therefore, the estimated SS for Aquifer 1 is 2.05E-06 (1/m).

S2.0 INITIAL HYDRAULIC HEADS

The original ASLMA Model assumed initially hydrostatic pressure distributions in the entire system. The current work uses a modified version of the ASLMA Model to simulate pressure perturbations and leakage rates when there are initial head differences in the aquifers, i.e., preinjection relative overpressure (Oldenburg et al., 2014). The initial heads are calculated assuming an equivalent freshwater head based on the unit-specific elevations and pressures using Equation S-3 (Raven et al., 1990).

$$h_f = Z + \frac{p}{\rho_f g} \quad \text{[Equation S-3]}$$

Where:

h_f is the equivalent freshwater head (m).

Z is the elevation of the midpoint of the geologic unit (m).

p is the measured formation pressure (Pa).

ρ_f is the density of fresh water (1000 kg/m^3).

g is the acceleration due to gravity (9.81 m/s^2).

The equivalent freshwater heads are entered into the ASLMA Model parameter, HEAD_INIT, and establish the initial pressure conditions for the storage complex prior to CO_2 injection.

S3.0 CO_2 EQUIVALENT-VOLUME INJECTION OF BRINE

The target CO_2 injection rate for the storage project is 180,000 metric tons CO_2 per year for 20 years. Feasibility study and predesign investigations have concluded that one injection well will be sufficient for the injection operations. Therefore, a single injector is placed at the center of the ASLMA model grid at an x-y location of (0,0) in the coordinate reference system. The ASLMA Model requires the CO_2 injection rate to be converted into an equivalent-volume injection of brine in units of cubic meters per day. For estimating the CO_2 density, the SI Workbook utilizes a macro function, *CO2Den* (Burton-Kelly and Bosshart, 2020), which uses inputs of temperature (T in units of °C) and pressure (P in units of psi) of to estimate CO_2 density in the reservoir from correlations described in Ouyang (2011). The estimated CO_2 density is 730 kg/m^3, which results in a daily equivalent-volume injection rate of approximately 675 m^3 per day.

As CO_2 injection progresses throughout the 20-year operating period, the pressure in the storage reservoir will increase. Consequently, the CO_2 density will also increase, resulting in a lower equivalent-volume injection rate over time if the CO_2 mass injection rate is held constant at the surface. The current approach uses a constant equivalent-volume injection rate throughout the entire operational period, which results in overestimating pressure buildup in the storage reservoir over time. However, the ASLMA Model outputs are used to create a relationship between pressure buildup in the storage reservoir and the incremental total cumulative leakage that occurs because of the injection, not to delineate a distance-leakage relationship.

S4.0 HYPOTHETICAL LEAKY WELLBORE

In the ASLMA Model, wellbore leakage is treated as flow through porous media by using Darcy's law. As described in Cihan et al. (2011) and the ASLMA Model User's Guide, the leakage rate through the wellbore from an aquifer, up through the overlying well-aquitard segment, and into the next aquifer in succession depends on the hydraulic head difference between aquifers, the hydraulic conductivity of the well-aquitard segment, and the wellbore area. The brine that has migrated upward through the well-aquitard segment may be diverted into the overlying aquifer and/or may continue to migrate upward through the overlying well-aquitard segment, and beyond.

To solve the Darcy flow up the leaky wellbore, the ASLMA Model requires several sets of inputs to describe the properties of the wellbore, including the radii of the well at each well-aquifer segment (RwA), the hydraulic conductivity of each well-aquifer segment (KWw), the radii of the well at each well-aquitard segment (RW), and the hydraulic conductivity of each well-aquitard segment (KW).

For the current work, the wellbore radius is set to 0.15 m (5.9 inches) for all segments (RwA and RW). However, the user may change the wellbore radius to any plausible value for wellbores within the study area.

For the reference case ASLMA Model, the effectively permeability of the leaky wellbore is set to 10^{-10} m^2. The SI Workbook estimates the wellbore hydraulic conductivity for wellbore effective permeabilities from 10^{-9} to 10^{-13} m^2, which covers a range encompassing values that are representative of leakage through a wellbore annulus (10^{-10} to 10^{-12} m^2) (Watson and Bachu, 2008, 2009; Celia et al., 2011). Carey (2017) provides probability distributions for the effective permeability of potentially leaking wells at CO_2 storage sites, estimating a wider range from 10^{-10} to 10^{-20} m^2. The SI Workbook calculations assume a porosity of 35% and use the storage reservoir pressure, temperature, and fluid properties to estimate the hydraulic conductivity for all well-aquifer and well-aquitard segments (KWw and KW, respectively).

S5.0 SALINE AQUIFER THIEF ZONE

A saline aquifer (Aquifer 2) exists between the primary seal above the storage reservoir and the USWD. Formation fluid migrating up a leaky wellbore that is open to Aquifer 2 will preferentially flow into Aquifer 2, and the continued flow up the wellbore and into the USDW will be reduced. Therefore, the presence of Aquifer 2 acts as a "thief zone" and reduces the potential for formation fluid impacts to groundwater. In addition to the leaky wellbore properties, the ASLMA Model allows the user to specify whether the status of an aquifer-wellbore segment (STAC) is closed (0) or open (1). If the status of the aquifer-wellbore segment is closed, then fluids migrating up the leaky wellbore cannot enter that geologic unit. To quantify the effect of the thief zone on the risk-based AOR, models with the leaky wellbore open to Aquifer 2 (STAC = 1) and with the leaky wellbore closed to Aquifer 2 (STAC = 0) are run and evaluated in both the injection and noninjection conditions.

S6.0 SENSITIVITY ANALYSIS

While each of the ASLMA Model input variables contribute to the output, the sensitivity analysis focuses on four inputs: hydraulic conductivity (HCONX) of Aquifer 1 (storage reservoir) and Aquifer 2 (thief zone), SS of Aquifers 1 and 2, hydraulic conductivity of the leaky wellbore, and CO_2 mass injection rate.

S6.1 HCON and SS Joint-Probability Region

HCON and SS for each aquifer depend on the underlying properties used to derive them and are not independent. Therefore, a one-at-a-time sensitivity analysis holding one of the two inputs constant while varying the other would be invalid. Instead, the sensitivity analysis approach derives a joint-probability region for HCON and SS and then explores the ASLMA Model outputs as the input variables move from lower HCON/SS to higher HCON/SS.

As shown in Equations S-1, HCONX for each aquifer is a function of aquifer temperature, pressure, and formation fluid salinity, which determine the formation fluid density and viscosity and aquifer permeability. Similarly, as shown in Equation S-2, SS for each aquifer is a function of aquifer temperature, pressure, and formation fluid salinity, which determine the formation fluid density and aquifer porosity. In addition, the calculation of SS also includes the fluid and pore compressibility terms. As a simplifying assumption, the sensitivity analysis assumes a constant aquifer temperature, pressure, and formation fluid salinity, i.e., a constant formation fluid density, viscosity, and compressibility. Therefore, variability in HCONX is solely attributable to the variation in permeability. The pore compressibility is derived from correlations published by Crawford et al. (2011); therefore, variability in SS is solely attributable to variation in porosity.

Site characterization data for Aquifer 2 show that the porosity distribution can be accurately described by a beta distribution with parameters $\alpha = 8.332$ and $\beta = 31.715$ and that the permeability can be accurately described by a lognormal distribution with parameters $\mu = 4.290$ and $\sigma = 4.076$. Analysis of porosity and permeability on paired samples provided a correlation coefficient of $\rho_{\text{porosity-permeability}} = 0.722$. Using these inputs and solving for HCONX via Equation S-1 and SS via Equation S-2 results in the joint-probability region for Aquifer 2 HCONX-SS shown in Figure S-1a.

Similarly, site characterization data for Aquifer 1 show that the porosity distribution can be accurately described by a beta distribution with parameters $\alpha = 4.070$ and $\beta = 18.589$ and that the permeability can be accurately described by a lognormal distribution with parameters $\mu = 4.623$ and $\sigma = 2.642$. Analysis of porosity and permeability on paired samples provided a correlation coefficient of $\rho_{\text{porosity-permeability}} = 0.634$. Using these inputs and solving for HCONX via Equation S-1 and SS via Equation S-2 results in the joint-probability region for Aquifer 1 HCONX-SS shown in Figure S-1b.

For Aquifers 2 and 1, the sensitivity analysis moves within a tolerance ellipse defined as the 30th and 70th percentiles from lower HCON/SS to higher HCON/SS in Figure S-1a and S-1b, respectively, and the test matrix includes five points for each aquifer.

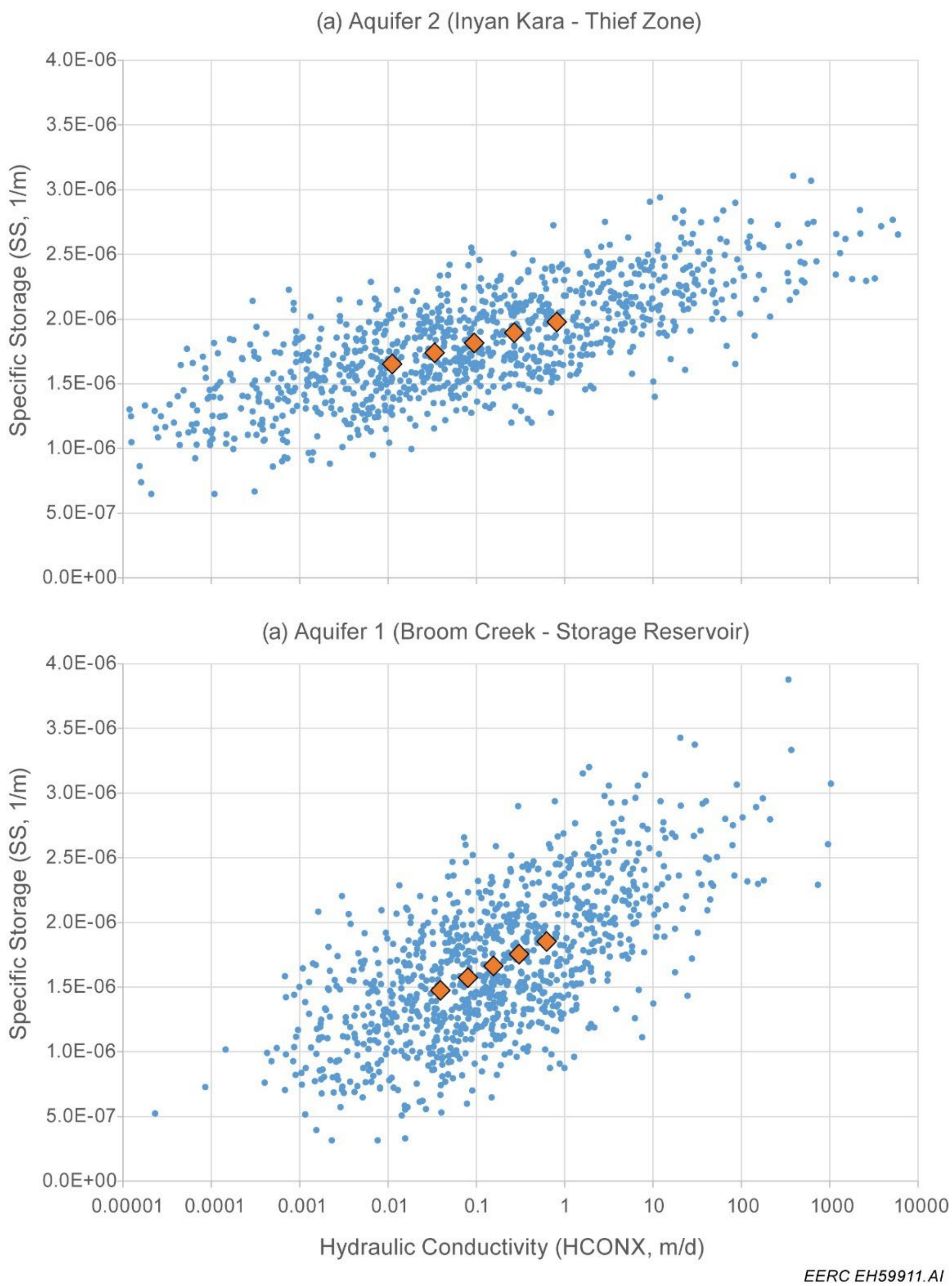

Figure S1. Joint-probability region for HCONX (*x*-axis) and SS (*y*-axis) for (a) Aquifer 2 (Inyan Kara – Thief Zone) and (b) Aquifer 1 (Broom Creek – Storage Reservoir) based on available site characterization data. The orange diamonds in each panel represent the sensitivity analysis test points listed in Table S-1.

S6.2 Leaky Wellbore Effective Permeability

The sensitivity analysis for the leaky wellbore assumes that the quality of materials in each well is uniform along the entire well, which means that the effective permeability values for each wellbore-aquifer and wellbore-aquitard segment are completely correlated. In other words, one value of effective permeability is chosen, and that value is assigned to all leaky wellbore segments (Celia et al., 2011). The sensitivity analysis explores a range of leaky wellbore effective permeabilities from 10^{-7} to 10^{-13} m^2, using log-order increments (i.e., 10^{-7}, 10^{-8}, …, 10^{-13} m^2) using the same calculation approach for KWw described previously. The test matrix includes seven runs for the leaky wellbore effective permeability range.

S6.3 CO_2 Mass Injection Rate

The nominal CO_2 mass injection rate is 180,000 metric tons per year, which reflects the expected injection rate of the planned storage project. However, two additional injection rates are included in the sensitivity analysis: 500,000 and 1,000,000 metric tons per year.

S6.4 Sensitivity Analysis Test Matrix

Varying the HCON and SS of Aquifers 1 and 2, the hydraulic conductivity of the leaky wellbore in log-order increments, and the CO_2 mass injection rate provides a sensitivity analysis test matrix of 16 additional ASLMA Model runs (one nominal case [Test Case No. 1] plus 16 additional runs, i.e., 17 runs total) (Table S-1).

Table S-1. Sensitivity Analysis Test Matrix. Yellow cells indicate the nominal input value.

Test Case No.	Aquifer 1 (Broom Creek - Storage Reservoir) HCONX (m/d)	Aquifer 1 (Broom Creek - Storage Reservoir) SS (1/m)	Aquifer 2 (Inyan Kara - Thief Zone) HCONX (m/d)	Aquifer 2 (Inyan Kara - Thief Zone) SS (1/m)	Leaky Wellbore Hydraulic Cond. KWw (m/d)	CO_2 Mass Injection Rate Q (metric tons per year)
1	5.76E-01	2.05E-06	6.06E-01	1.64E-06	1.73E+02	180,000
2	3.94E-02	1.47E-06	6.06E-01	1.64E-06	1.73E+02	180,000
3	8.07E-02	1.57E-06	6.06E-01	1.64E-06	1.73E+02	180,000
4	1.58E-01	1.66E-06	6.06E-01	1.64E-06	1.73E+02	180,000
5	3.08E-01	1.75E-06	6.06E-01	1.64E-06	1.73E+02	180,000
6	6.29E-01	1.85E-06	6.06E-01	1.64E-06	1.73E+02	180,000
7	5.76E-01	2.05E-06	1.12E-02	1.65E-06	1.73E+02	180,000
8	5.76E-01	2.05E-06	3.38E-02	1.74E-06	1.73E+02	180,000
9	5.76E-01	2.05E-06	9.54E-02	1.82E-06	1.73E+02	180,000
10	5.76E-01	2.05E-06	2.69E-01	1.89E-06	1.73E+02	180,000
11	5.76E-01	2.05E-06	8.17E-01	1.98E-06	1.73E+02	180,000
12	5.76E-01	2.05E-06	6.06E-01	1.64E-06	1.73E+03	180,000
13	5.76E-01	2.05E-06	6.06E-01	1.64E-06	1.73E+01	180,000
14	5.76E-01	2.05E-06	6.06E-01	1.64E-06	1.73E+00	180,000
15	5.76E-01	2.05E-06	6.06E-01	1.64E-06	1.73E-01	180,000
16	5.76E-01	2.05E-06	6.06E-01	1.64E-06	1.73E+02	1,000,000
17	5.76E-01	2.05E-06	6.06E-01	1.64E-06	1.73E+02	500,000

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