

Plains CO, Reduction (PCOR) Partnership

Energy & Environmental Research Center (EERC)



NATIONAL RISK ASSESSMENT PARTNERSHIP (NRAP) TESTING AND VALIDATION: PART 2 – NRAP OPEN-SOURCE INTEGRATED ASSESSMENT MODEL (OPEN-IAM)

Plains CO₂ Reduction (PCOR) Partnership Task 3 – Deliverable D10 – Part 2

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NATIONAL RISK ASSESSMENT PARTNERSHIP (NRAP) TESTING AND VALIDATION: PART 1 – NRAP OPEN-SOURCE INTEGRATED ASSESSMENT MODEL (OPEN-IAM)

EXECUTIVE SUMMARY

The Energy & Environmental Research Center conducted extensive testing of the National Risk Assessment Partnership (NRAP) Open-Source Integrated Assessment Model (Open-IAM) under Subtask 3.2 (NRAP Validation) of Task 3 (Data Collection, Sharing, and Analysis) of the Plains CO₂ Reduction Partnership Initiative to Accelerate Carbon Capture, Utilization, and Storage Deployment (hereafter "PCOR Partnership"). A previous study by Mahmood and others (2021) summarized detailed testing and validation of the NRAP-Open-IAM. The current study extends the previous work and was also conducted under Subtask 3.2 of the PCOR Partnership.

The goal of the current study was to compare NRAP-Open-IAM and the Lawrence Berkeley National Laboratory Analytical Solution for Leakage in Multilayered Aquifers (ASLMA) Model results for the same set of inputs and the same set of legacy wellbores located beyond the estimated CO₂ plume extent but within the area of review (AOR). The objectives of this study were to i) use both the NRAP-Open-IAM and ASLMA Model to evaluate a commercial-scale (3.5–4.0 million metric tons of CO₂ injected per year over 20 years) storage project injecting CO₂ into a storage unit with properties that are representative of the Broom Creek Formation in central North Dakota, ii) generate outputs from both tools of simulated formation fluid leakage from the storage unit to the lowermost underground source of drinking water (USDW) for three legacy wellbores located beyond the estimated CO₂ plume extent but within the AOR, iii) quantify the similarities and differences between the outputs of each tool, and iv) provide recommendations for evaluating potential legacy wellbore leakage using the NRAP-Open-IAM and ASLMA Model to assist practitioners supporting the Class VI injection well permitting process and associated groundwater monitoring plans.

The testing resulted in the following key findings:

• Site characterization data that include site-specific measurements of depth, thickness, initial pressure, temperature, porosity, permeability, and salinity are essential to properly estimating wellbore leakage risks to USDWs. The current work underscores the importance of site-specific initial pressure measurements to the NRAP-Open-IAM formation fluid leakage calculations.

- While the single-phase flow assumptions in the ASLMA Model have been shown to be applicable for far-field pressure changes beyond the CO₂ plume, the current work shows that the ASLMA Model overestimated pressure buildup at the end of 20 years as compared to numerical reservoir simulation. Therefore, utilizing the pressure buildup derived from numerical reservoir simulation may provide more accurate inputs to the NRAP-Open-IAM.
- For storage units that do not conform to the freshwater pressure gradient assumption (0.433 psi/ft), using the observed (actual) initial pressure will result in NRAP-Open-IAM overestimating the formation fluid leakage. Adjusting the NRAP-Open-IAM outputs by either modifying the initial pressure or subtracting a baseline case provide solutions that are more comparable between the NRAP-Open-IAM and ASLMA Model and likely more accurate estimates of the incremental wellbore leakage risk to USDWs.



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NATIONAL RISK ASSESSMENT PARTNERSHIP (NRAP) TESTING AND VALIDATION: PART 2 – NRAP OPEN-SOURCE INTEGRATED ASSESSMENT MODEL (OPEN-IAM)

INTRODUCTION

CCS Projects and the Area of Review

Carbon capture and storage (CCS) is a process that captures carbon dioxide (CO₂) from an anthropogenic point source or extracts CO₂ directly from the atmosphere and injects the CO₂ via one or more injection wells into a deep geologic formation (storage unit) for permanent storage. 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 (CFR, Parts 124, and 144–47). The Safe Drinking Water Act (SDWA) establishes requirements and provisions for the UIC Program. Regulations for CCS fall under the Class VI rule of the UIC Program: Wells Used for Geologic Sequestration of CO₂. Two states—North Dakota and Wyoming—have primary enforcement authority (primacy, i.e., recognized by EPA) under the SDWA to implement a UIC program for Class VI injection wells located within their states, except within Indian lands. Storage project operators in the remaining 48 states must work with EPA to permit Class VI injection wells.

A major technical component of the Class VI injection well permitting process and associated groundwater monitoring plan is the delineation of an area of review (AOR). The AOR is defined as the region surrounding the storage project where underground sources of drinking water (USDWs) may be endangered by the injection activity (40 CFR 146.84 and North Dakota Administrative Code Section 43-05-01-05.1. AOR and corrective action). The AOR is used to delineate the areal extent of highest risk of leakage of formation fluid (brine) or CO₂ to USDWs along a legacy wellbore or other permeable pathways such as a transmissive fault, which can, therefore, be used to guide monitoring plans and, if warranted, corrective actions. The areal extent of the anticipated pressure buildup above a critical pressure due to injection of CO₂ can be used to delineate the AOR (U.S. Environmental Protection Agency, 2013). The critical pressure is the minimum pressure within the storage unit that can cause fluid flow from the storage unit into the formation matrix of a USDW through a hypothetical conduit (e.g., artificial penetration) at a known geographic location that is open in both intervals. If the pressure buildup in the storage unit exceeds the critical pressure and a leakage pathway exists, then there is a potential risk of endangering a USDW. Because storage unit and USDW characteristics vary over an area of interest, the critical pressure may also vary. For simplicity, this document refers to "a critical pressure" at a known location. The AOR may also be delineated using a risk-based approach to

define the areal extent beyond which no significant leakage would occur from the storage unit to the lowermost USDW via a hypothetical conduit. Only the region inside of this areal extent is a risk-based AOR. The risk-based approach differs from the simplified examples in EPA guidance that presume that all locations where the storage unit pressure is above the critical pressure pose a potential leakage risk and must, therefore, be included in the AOR (White and others, 2020; Burton-Kelly and others, 2021). Nevertheless, risk-based approaches are consistent with EPA guidance (U.S. Environmental Protection Agency, 2013) and the UIC program requirements designed to ensure USDW protection from endangerment (Title 40 of the CFR Parts 124 and 144–47).

The confining system of a CO₂ storage unit comprises low-permeability geologic layers immediately overlying the storage unit (primary seal or cap rock) and secondary barriers to CO₂ or brine leakage that can include additional low-permeability geologic layers and/or saline aquifers between the primary seal and overlying USDWs that prevent vertical migration of the injected CO₂ stream and displaced formation fluids. Legacy wellbores are potential pathways for fluid leakage from the storage unit to overlying aquifers because these artificial penetrations breach the confining system and can, therefore, connect the storage unit to USDWs (International Organization for Standardization, 2017). Therefore, risk-based AOR methods generally evaluate the leakage potential of hypothetical legacy wellbores under a range of input assumptions and use those results to delineate the risk-based AOR. For example, in a recent storage facility permit for Minnkota Power Cooperative, Inc.'s Milton R. Young Station targeting the Broom Creek Formation in Oliver County, North Dakota (Case No. 29029, Order No. 31583 – approved January 2022), the applicant successfully used the risk-based AOR methodology of Burton-Kelly and others (2021) to delineate a risk-based AOR. Therefore, the risk-based AOR was established as the minimum AOR extent required under North Dakota regulations, which is the storage facility area (essentially the CO₂ plume boundary in the storage unit) plus a 1-mile buffer (Department of Mineral Resources, 2022). The areal extent of pressure buildup in the storage unit is typically much larger than the estimated extent of the CO₂ plume in the storage unit. Because the minimum AOR will always include the estimated extent of the CO₂ plume but might not include the full extent of the pressure buildup, evaluating the endangerment to USDWs from CO₂ injection and the associated AOR generally focuses on the relationships between pressure buildup in the storage unit, legacy wellbores, and the potential for leakage of formation fluids from the storage unit to the lowermost USDW for wells located beyond the estimated extent of the CO₂ plume.

Reduced-Order Models for Delineating a Risk-Based AOR

Building a heterogeneous geologic model using a commercial-grade software platform like Schlumberger's 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), is an industry-standard approach for estimating pressure buildup in the storage unit in response to CO₂ injection (Bosshart and others, 2018). These commercial-grade tools also provide a broad set of parameters that can be tested for their influence on the simulated fluid flow within the storage unit. Storage project development (i.e., permitting Class VI injection wells) focuses primarily on characterizing and modeling the storage unit and lower portion of the sealing unit immediately above the storage unit (sometimes called the "cap rock" or "primary seal"). For computational efficiency, secondary seals or overlying aquifers are rarely incorporated into

geologic models. Instead, analytical or semianalytical solutions (sometimes called "reduced-order models" or "ROMs") that make simplifying assumptions about the properties of the confining system are used to quantitatively evaluate potential leakage scenarios of formation fluids or CO₂ above the cap rock. ROMs can accelerate the process of understanding potential endangerment to USDWs from leakage of formation fluid caused by CO₂ injection, and these results can be used to better inform decisions about the risk-based AOR and groundwater monitoring. Two such solutions are packaged as software tools to estimate the potential amount of leakage from the storage unit to overlying USDWs via legacy wellbores: i) the National Risk Assessment Partnership (NRAP) Open-Source Integrated Assessment Model (hereafter "NRAP-Open-IAM" Vasylkivska and others, 2022) and ii) the Lawrence Berkeley National Laboratory (LBNL) Analytical Solution for Leakage in Multilayered Aquifers (hereafter "ASLMA Model," Cihan and others, 2011, 2012).

NRAP-Open-IAM is an integrated assessment model developed to perform quantitative risk assessment for CO₂ storage projects (Vasylkivska and others, 2022). The tool is based on multiple ROMs that integrate the components of a storage site, including the storage unit, overlying stratigraphy (primary seal, intermediate aquifers, additional seals, and lowermost USDW), and additional modules for estimating CO₂ or formation fluid leakage through legacy wells and resultant impacts to aquifers.

The ASLMA Model has been extensively described in Cihan and others (2011, 2012). The solution assumes single-phase flow in a multilayered system of aquifers and aquitards, which has been shown to be applicable for far-field pressure changes beyond the CO₂ plume (Cihan and others, 2011, 2012; Nicot, 2008; Birkholzer and others, 2009; Bandilla and others, 2012). Because the ASLMA Model is a single-phase model, multiphase processes are not incorporated into the solution. However, when CO₂ injection rates are converted to the equivalent volumes of singlephase fluid (brine), the ASLMA Model provides accurate pressure buildup and leakage results for areas beyond the CO2 plume according to the numerical model TOUGH2-ECO2N (Cihan and others, 2011, 2012; Birkholzer and others, 2009). The ASLMA Model includes several assumptions in the calculations. For example, all aquifers and aquitards are assumed to be homogeneous and isotropic, with uniform thickness and infinite radial extent. Fluid flow is horizontal in the aquifers and vertical in the aquitards. The equations of horizontal groundwater flow in the aquifers are coupled to the vertical-flow equations in the vertical leakage pathways and aguitards. Unlike NRAP-Open-IAM, the ASLMA Model outputs are specific to formation fluid leakage and do not include CO2 leakage because the tool is designed to investigate far-field pressure and legacy wellbores located beyond the CO₂ plume extent. LBNL has recently published an extension of the solutions for nonhydrostatic multilayered subsurface systems coded in the ASLMA Model to include hydraulic storage and Darcy flow in aquitards; over- or underpressurization rates in aquifers and aquitards; and multiple injection, extraction, and leaky wells. The ASLMA Model code with these enhancements is now called SALSA (Semi-Analytical Leakage Solutions for Aquifers) (Cihan and others, 2022). However, the current work used the ASLMA Model, which provided a sufficient tool for the study goals and objectives.

There are several notable differences between NRAP-Open-IAM and ASLMA Model with respect to simulating formation fluid leakage from legacy wellbores located beyond the CO₂ plume. First, the inputs of pressure buildup and CO₂ saturation in the storage unit for NRAP-Open-

IAM are derived from a geologic model and numerical reservoir simulator, therefore accounting for the heterogeneities of the storage unit geology and the complexities of multiphase (formation fluid and CO₂) interactions. In contrast, the ASLMA Model uses a semianalytical solution to the pressure buildup equations, using the injection of a single-phase fluid (formation fluid) at a rate volumetrically equivalent to that of the prescribed CO₂ injection. In essence, NRAP-Open-IAM uses pressure and CO2 saturation inputs from a third-party software while the ALSMA Model derives its own pressure buildup estimates and does not incorporate CO2 as a separate phase. Second, the Multisegmented Wellbore ROM within NRAP-Open-IAM assumes that the stratigraphic units are in hydrostratigraphic equilibrium and does not consider the storage unit being under- or overpressured with respect to the overlying aquifers. In contrast, the ASLMA Model can accommodate under- or overpressured storage units (Oldenburg and others, 2014, 2016). For the example used in this study, the storage unit is overpressured relative to overlying aquifers and thus subject to potential vertical formation fluid migration from the storage unit to the lowermost USDW, even without injection occurring. Lastly, NRAP-Open-IAM allows the user to define uncertain input parameters for some variables and apply Latin hypercube sampling to perform stochastic analyses, whereas the ASLMA Model is limited to discrete inputs and requires customized programming outside of the tool to examine the effects of uncertainty on the simulated formation fluid leakage (Burton-Kelly and others, 2021; Mahmood and others, 2021).

Study Goals and Objectives

A previous study by Mahmood and others (2021) summarized detailed testing and validation of the NRAP-Open-IAM, which was conducted under Subtask 3.2 (NRAP Validation) of Task 3 (Data Collection, Sharing, and Analysis) of the Plains CO2 Reduction Partnership Initiative to Accelerate Carbon Capture, Utilization, and Storage Deployment (hereafter "PCOR Partnership"). The current study extends the previous work and was also conducted under Subtask 3.2 of the PCOR Partnership. The goal of the current study is to compare NRAP-Open-IAM and ASLMA Model results for the same set of inputs and the same set of legacy wellbores located beyond the estimated CO₂ plume extent but within the AOR. The objectives of this study are to i) use both the NRAP-Open-IAM and ASLMA Model to evaluate a commercial-scale storage project injecting CO₂ into a storage unit with properties that are representative of the Broom Creek Formation in central North Dakota, ii) generate outputs from both tools of simulated formation fluid leakage from the storage unit to the lowermost USDW for three legacy wellbores located beyond the estimated CO₂ plume extent but within the AOR, iii) quantify the similarities and differences between the outputs of each tool, and iv) provide recommendations for evaluating potential legacy wellbore leakage using the NRAP-Open-IAM and ASLMA Model to assist practitioners supporting the Class VI injection well permitting process and associated groundwater monitoring plans.

METHODS

Storage Site Description

The reference geologic stratigraphy used in this study is based on a section of the Williston Basin of North Dakota (Figure 1). Table 1 shows the reference geologic stratigraphy used for this

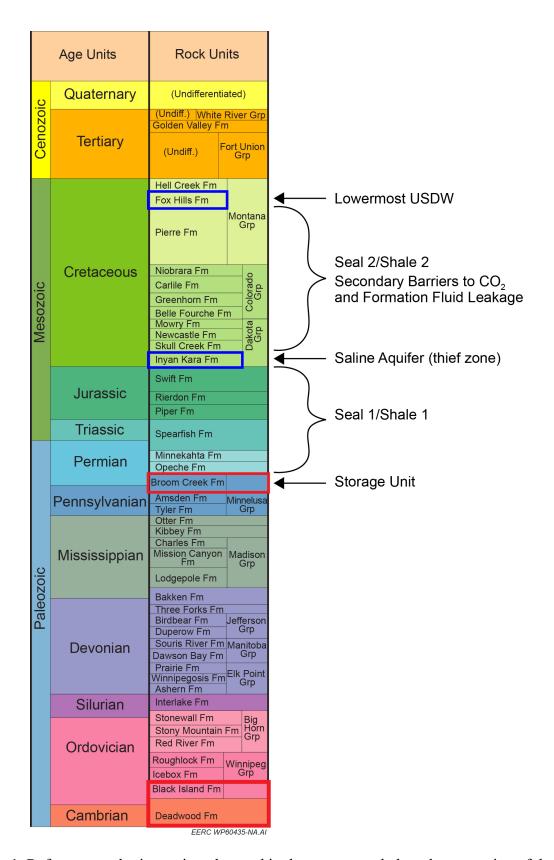


Figure 1. Reference geologic stratigraphy used in the current study based on a section of the Williston Basin of North Dakota.

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Table 1. Storage Project Stratigraphy with Average Properties of the Study Site Used in the NRAP-Open-IAM and ASLMA Model Testing

					Initial					Total
	Nome	nclature ^a	Depth ^b	Thickness	Pressure	Temperature	Porosity	Permeability	Salinity	Head
Hydrostratigraphic	ASLMA	NRAP-	m	m	MPa	°C		log ₁₀ (m ²)		m
Unit	Model	Open-IAM	(ft)	(ft)	(psi)	(°F)	%	(mD)	ppm	(ft)
Seal/Shale 3	N/A	Shale 3	0	224	N/A ^c	N/A	N/A	N/A	N/A	N/A
Overlying Units to				(735)						
Ground Surface										
Aquifer 2	AQ3	Aquifer 2	224	126	2.9	14.5	34	-12.6	1800	618
USDW			(735)	(413)	(421)	(58.1)		(280)		(2028)
(Fox Hills Fm)										
Seal/Shale 2	AQT2	Shale 2	351	773	7.3	27.6	2	-19.0	5800	617
Additional Seals			(1152)	(2536)	(1059)	(81.7)		(0.00011)		(2024)
(Pierre–Inyan Kara Fm)										
Aquifer 1	AQ2	Aquifer 1	1123	55	10.8	48.1	13	-13.4	3365	562
Thief Zone			(3684)	(180)	(1566)	(118.6)		(36.4)		(1844)
(Inyan Kara Fm)										
Seal/Shale 1	AQT1	Shale 1	1178	267	12.9	51.5	2	-19.0	40,000	587
Primary Seal/Cap Rock			(3884)	(876)	(1871)	(124.7)		(0.00011)		(1926)
(Swift–Broom Creek Fm)										
Storage Unit	AQ1	Storage unit	1445	71	16.4	57.4	12.84	-13.7	49,350	762
(Broom Creek Fm)			(4741)	(233)	(2383)	(135.3)		(22)		(2500)

^a ASLMA Model and NRAP-Open-IAM use different nomenclature to identify the storage unit, sealing formations, and aquifers.

^b Depth to the top of the formation. Ground surface elevation is 609 m (1998 ft) above mean sea level.

^c N/A (not applicable) means that the parameter is undefined in either software or not defined in the current study.

study and illustrates key terms needed for understanding the subsequent equations and discussions. Individual geologic members are grouped to simplify the stratigraphy into hydrostratigraphic units. In the context of this study, a hydrostratigraphic unit is a geologic formation or group of formations that are hydraulically connected and exhibit similar characteristics with respect to the transmission of fluids. In this example, the storage unit is the Broom Creek Formation, a deep saline formation approximately 1445 m (4741 ft) deep and 71 m (233 ft) thick. The primary sealing unit (Seal 1/Shale 1) is the interval from the top of the Broom Creek Formation to the top of the Swift Formation, comprising a series of shales approximately 267 m (876 ft) thick. The remaining overburden of geologic units above the primary sealing unit include another saline aquifer (Inyan Kara Formation – Aquifer 1), a secondary set of sealing units (interval from the top of the Inyan Kara Formation to the top of the Pierre Formation – Seal 2/Shale 2), a freshwater aguifer that is the lowermost USDW (Fox Hills Formation – Aquifer 2), and overburden that includes additional seals that extend to the surface (Seal 3/Shale 3). The combination of the Broom Creek Formation storage unit and the first overlying seal (top of the Broom Creek Formation to the top of the Swift Formation) comprise the storage complex. The saline aquifer (Inyan Kara Formation – Aquifer 1) is designated as a "thief zone" because vertically migrating fluid is lost to this saline aquifer, thereby lowering the vertical hydraulic head gradient with increasing vertical location in a leaky wellbore, and thereby decreasing, or nearly eliminating, vertical fluid migration above the saline aquifer to the USDW (Burton-Kelly and others, 2021). The thief zone phenomenon was described by Nordbotten and others (2004) as an "elevator model," by analogy with an elevator full of people on the ground 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. Figure 2 illustrates the simplified stratigraphy used in the current study.

To evaluate fluid flow in the Broom Creek Formation in response to CO_2 injection, a heterogeneous geologic model was constructed using site-specific data for a 24×18 -km study area in North Dakota, USA, using Schlumberger's Petrel. CMG GEM compositional simulation software was used to simulate commercial-scale CO_2 injection into the Broom Creek Formation. CO_2 was injected into the Broom Creek Formation using two wells ~305 m (1000 ft) apart at a rate of 4 million metric tons (MMt) per year for the first 15 years and 3.5 MMt/year for the last 5 years, for a total injection of 77.5 MMt over a period of 20 years. Average depth, thickness, porosity, and permeability were extracted from the simulation model to produce the average properties for the storage unit in Table 1.

Figure 3 is a map of the study area showing the relative locations of the injection well (Well 1), monitoring well (Well 5), and three legacy oil and gas wells (Legacy Wellbores 2, 3, and 4) (Table 2). Only the injection well and the monitoring well are within the storage facility area defined by the stabilized CO₂ plume extent. For the purposes of this study, Wells 2, 3, and 4 were considered as leaky wells to compare leakage rates between the NRAP-Open-IAM and ASLMA Model.

Some areas of the Broom Creek Formation in North Dakota are overpressured with respect to the lowest USDW under preinjection conditions. This means that formation fluids would flow from the Broom Creek Formation to the lowermost USDW if a flow pathway existed, even if no injection were occurring. EPA (2013) includes a method by Thornhill and others (1982) to determine whether a formation is overpressured. The method estimates the increase in pressure that may be sustained in the storage unit, $\Delta P_{i,f}$, by comparing the hydraulic head of the storage unit

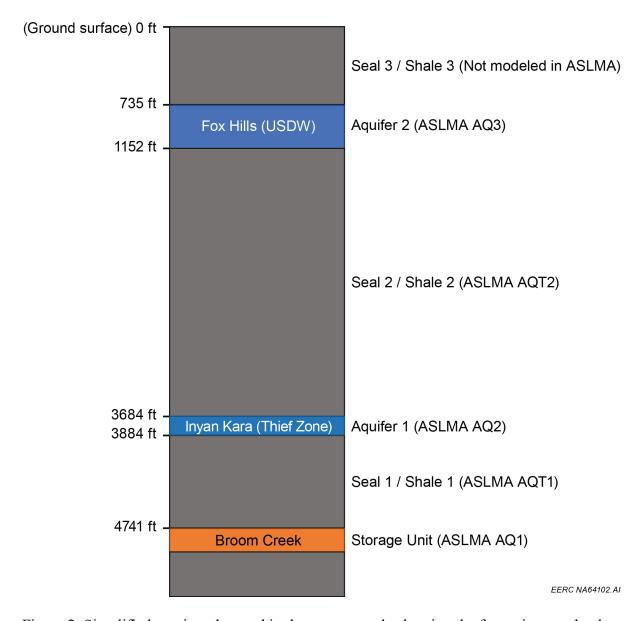


Figure 2. Simplified stratigraphy used in the current study showing the formation top depths, relative thicknesses of each hydrostratigraphic unit, and nomenclatures used for the NRAP-Open-IAM and ASLMA Model (in parenthesis).

to the hydraulic head of the lowermost USDW. In short, where $\Delta P_{i,f} < 0$, the storage unit is overpressured; i.e., the preinjection hydraulic head in the storage unit is greater than the hydraulic head of the lowermost USDW, resulting in upward flow from the storage unit to the USDW. At the injection well in the center of the study area (Well 1), $\Delta P_{i,f}$ is approximately -200 psi and, therefore, meets the definition of overpressured.

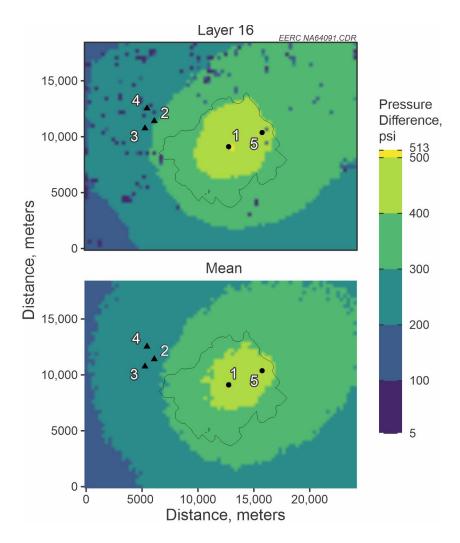


Figure 3. Map of the study area. The background color ramp shows CMG GEM simulated increase in storage unit pressure at the end of the injection period at reservoir model Layer 16, which is the topmost layer of the storage unit just below the cap rock (top) and vertically averaged over the reservoir model layers or the full thickness of the Broom Creek Formation (bottom). The polygon in each panel shows the CMG GEM simulated CO₂ plume extent (max. CO₂ saturation > 10%) at the end of the injection period. Points show locations of the injection well (1), monitoring well (5), and three distant wells to the west (2, 3, 4). Wells within the CO₂ plume extent are shown as circles; wells outside the CO₂ plume are shown as triangles. Small groups of cells with low pressure in Layer 16 indicate nonreservoir lithology (shale or anhydrite) where pressure changes did not propagate.

Table 2. Model Well Locations and Distance from Injection Well

Well ID	X Location, m	Y Location, m	Distance from Injector, m
1 (injector)	12,744	9107	0
2	6097	11,407	7033
3	5261	10,755	7663
4	5442	12,536	8067
5 (monitor)	15,739	10,374	3251

NRAP-Open-IAM Inputs

The NRAP-Open-IAM is an "integrated assessment model" in the sense that it integrates outputs from different components under a single tool. While the current version of NRAP-Open-IAM includes 14 different components, the testing conducted herein utilized only four components needed to simulate wellbore leakage from the storage unit to the lowermost USDW:

- Model component
- Stratigraphy component
- Lookup table (LUT) reservoir component
- Multisegmented wellbore (MSW) component

A detailed description of each component was provided in Mahmood and others (2021), and only a summary is provided here. The current study used NRAP-Open-IAM version a2.2.0.

The model component allows the user to outline model parameters, including the simulation name, end time of the simulation, time step, type of simulation and/or analysis (forward modeling, LHS [Latin Hypercube Sampling], or Parstudy [Parameter Study Analysis]), and output directory. The end time was set to 20 years of CO₂ injection and with 1-year time steps, and only forward modeling was used in the present study.

The stratigraphy component allows the user to define the stratigraphy of the storage complex and includes the thickness of the storage unit and overlying hydrostratigraphic units. The stratigraphy component was constructed to match the hydrostratigraphic units and properties in Table 1 and Figure 2. The stratigraphic layers are numbered from the bottom to the top of the stratigraphy, such that the first shale layer overlying the storage unit (i.e., the primary seal or cap rock) is "Shale 1," the aquifer overlying Shale 1 is "Aquifer 1," etc., leading to the uppermost aquifer (Aquifer 2 – also the lowermost USDW) and uppermost shale layer (Shale 3).

The LUT reservoir component uses pressure and CO₂ saturation inputs predicted by compositional reservoir simulation software. The reservoir simulation output must be from a single, two-dimensional (2D) layer extracted from a three-dimensional (3D) reservoir model. The reservoir simulation output must include pressure and CO₂ saturation values for each model layer grid cell and time step from the start of CO₂ injection to the end time specified in the model component. Postprocessing routines described in Mahmood and others (2021) were used to extract pressure and CO₂ saturation from CMG GEM for two cases: i) reservoir model Layer 16 (the

storage unit—cap rock interface in the reservoir model) and ii) vertically averaged over the reservoir model layers (Figure 1).

The MSW component estimates the leakage rates of brine and CO₂ along wells with the presence of overlying aquifers or thief zones. The MSW component was used to place three leaky wellbores (Wells 2, 3, and 4) in the model domain at the x- and y-coordinates shown in Table 2. The properties assigned to these leaky wellbores are described under the case matrix section.

Open-IAM is written in Python programming language and has the capability to build and run simulations in multiple ways. The simplest way to build and run simulations is the graphical user interface (GUI). The other two ways are the text-based control file interface and Python scripts. This study primarily focused on using the control file interface to build and run deterministic (forward) simulation scenarios. The control file interface provided additional flexibility that was needed to develop a model in the NRAP-Open-IAM that was comparable to the ASLMA Model. For example, the GUI required that all aquifers had the same permeability whereas the control file allowed the user to define formation-specific permeability values. To mimic cases where no thief zone was present, the source code for the MSW component was slightly modified to reduce the allowed permeability range for each well-aquifer interface (Seunghwan Baek, Pacific Northwest National Laboratory, personal communication, 01/20/2023).

ASLMA Model Inputs

The ASLMA Model requires inputs of hydrogeologic properties for the storage unit and overlying formations. The stratigraphy was constructed to match the hydrostratigraphic units and properties in Table 1 and Figure 2. The average pressure, temperature, porosity, permeability, and salinity for each unit were used to derive two key ASLMA inputs: hydraulic conductivity (K) and specific storage (SS). Descriptions of these properties and calculations are provided in Burton-Kelly and others (2021). The stratigraphic layers are numbered from the bottom to the top of the stratigraphy, such that the storage unit is "Aquifer 1" (AQ1), the first shale layer overlying the storage unit (i.e., the primary seal or cap rock) is "Aquitard 1" (AQT1), etc., leading to the uppermost aquifer (Aquifer 3 [AQ3]), which is also the lowermost USDW. The ASLMA Model did not define a unit above AQ3. Therefore, AQ3 from the ASLMA Model (lowermost USDW) is equivalent to Aquifer 2 in the NRAP-Open-IAM, and AQ2 from the ASLMA Model (thief zone) is equivalent to Aquifer 1 in the NRAP-Open-IAM.

As previously discussed, in the CMG GEM reservoir simulation model, CO₂ was injected into the Broom Creek Formation using one well at a rate of 4 MMt per year for the first 15 years and 3.5 MMt/year for the last 5 years, for a total injection of 77.5 MMt over a period of 20 years. An assumed CO₂ density of 720 kg/m³ was used to derive the daily equivalent formation water volume injection rates of 15,221 m³/day and 13,318 m³/day, respectively (4,000,000,000 kg \div 720 kg/m³ \div 365 days = 15,221 m³/day). The CO₂ density is a representative reservoir simulation value from within the CO₂ plume near the injection well after several years of injection. For computational ease, changes in CO₂ density over the 20-year injection period were ignored.

Three leaky wellbores (Wells 2, 3, and 4) were placed in the ASLMA Model domain at the x- and y-coordinates shown in Table 2. The properties assigned to these leaky wellbores are described under the case matrix section.

Case Matrix

The same stratigraphy, petrophysical properties, and CO₂ injection schedule were used for all comparisons. An extensive case matrix of different NRAP-Open-IAM and ASLMA Model input parameter settings was explored as part of the testing; however, only a reduced case matrix is presented and described in this report. The reduced case matrix is used to illustrate key differences between the NRAP-Open-IAM and ASLMA Model relevant to practitioners supporting the Class VI injection well permitting process and associated groundwater monitoring plans (Table 3).

Table 3. Case Matrix Used to Compare the NRAP-Open-IAM and ASLMA Model

		Initial	Leaky Well	_		
Case		Pressure,	Permeability,	Thief	Pressure	CO_2
No.	ROM	MPa (psi)	$\log_{10}(\mathrm{m}^2)$	Zone	Model	Injection
1	MSW	16.4 (2381)	-9.0	On	Case 3 output	On
2	MSW	16.4 (2381)	-9.0	Off	Case 4 output	On
3	ASLMA	N/A*	-9.0	On	N/A*	On
4	ASLMA	N/A*	-9.0	Off	N/A*	On
5	MSW	14.5 (2103)	-9.0	On	Case 3 output	On
6	MSW	14.5 (2103)	-9.0	Off	Case 4 output	On
7	MSW	16.4 (2381)	-9.0	On	Constant (16.4 MPa)	Off
8	MSW	16.4 (2381)	-9.0	Off	Constant (16.4 MPa)	Off

^{*} N/A refers to the fact that the ASLMA Model derives its own pressure buildup and, therefore, does not require an input of initial pressure or pressure model input.

ROM

The ROM column in the case matrix refers to wellbore leakage estimates generated from either the NRAP-Open-IAM (specifically the MSW component within NRAP-Open-IAM: Cases 1, 2, and 5–8) or ASLMA Model (Cases 3 and 4) (Table 3).

Initial Pressure

The MSW component within NRAP-Open-IAM assumes a freshwater pressure gradient of 0.433 psi/ft, which results in a significantly different initial pressure for the storage unit than the observed (actual) initial pressure. For example, at the midpoint of the storage unit, the freshwater gradient assumption yields an estimated initial pressure of 4858 feet \times 0.433 psi/ft = 2103 psi (14.5 MPa). However, the observed formation pressure in the Broom Creek Formation in this region of central North Dakota is 2381 psi (16.4 MPa), with a pressure gradient of approximately 0.49 psi/ft. During the testing, it was observed that this difference in the initial pressures between

the two tools resulted in significantly different wellbore leakage estimates. Therefore, to illustrate the sensitivity of the NRAP-Open-IAM outputs to the initial pressure, the case matrix includes cases where the initial pressure at the injection well was set to the observed (actual) initial pressure of 16.4 MPa (2381 psi) (Cases 1, 2, 7, and 8) and to the initial pressure of 14.5 MPa (2103 psi), assuming a freshwater gradient (Cases 5 and 6) (Table 3).

Leaky Wellbore Effective Permeability

Both the NRAP-Open-IAM and ASLMA Model treat formation fluid leakage through wellbores as flow through porous media by using Darcy's law, which includes the i) cross-sectional area of flow between the wellbore casing and formation (annulus), ii) length of the wellbore (distance from the storage unit to the lowermost USDW), iii) hydraulic potential in the storage unit and USDW, and iv) effective permeability of the cemented annulus (Huerta and Vasylkivska, 2016). Since the cross-sectional area and length are constants and the hydraulic potential in the storage unit and USDW are derived from other inputs, the effective permeability of the cemented annulus is an important input variable for both tools.

Carey (2017) estimated a wide range of possible wellbore effective permeabilities from 10^{-10} to $10^{-20} \log_{10}(m^2)$ (101,325 to 10^{-5} mD). In the current study, a maximum leaky wellbore permeability of $10^{-9} \log_{10}(m^2)$ was used for all cases because it is the maximum value allowed by NRAP-Open-IAM (Vasylkivska and others, 2022). Moreover, additional testing (not presented here) showed that lower leaky wellbore effective permeability less than $10^{-9} \log_{10}(m^2)$ resulted in minimal to no significant leakage and, therefore, no comparative assessment (Table 3). While a leaky wellbore permeability of $10^{-9} \log_{10}(m^2)$ is orders-of-magnitude greater than values that might be observed at a real storage project, this maximum (worst-case) scenario allowed for more robust comparisons between the NRAP-Open-IAM and ASLMA Model.

Presence or Absence of a Thief Zone

The case matrix examines the effect of an intermediary saline aquifer (thief zone) between the storage unit and USDW. Cases where the leaky wellbore had access to the thief zone (thief zone on: Cases 1, 3, 5, and 7) or did not have access to the thief zone (thief zone off: Cases 2, 4, 6, and 8) were included in the case matrix (Table 3).

Pressure Model

As described above, the LUT reservoir component within NRAP-Open-IAM uses pressure inputs predicted by compositional reservoir simulation software whereas the ASLMA Model derives its own pressure buildup estimates using single-phase flow and several other simplifying assumptions. During the testing, it was observed that the simulated pressure buildup in the storage unit estimated by CMG GEM was significantly smaller than the pressure buildup estimated by the ASLMA Model. Since the pressure buildup in the storage unit is one of the primary drivers of the wellbore leakage estimates, the NRAP-Open-IAM and ASLMA Model outputs were not comparable.

As a solution to remove this pressure model effect from the comparative assessment, the ASLMA Model pressure outputs were used as inputs to the LUT reservoir component in lieu of the CMG GEM pressure outputs. Therefore, Cases 1 and 5 used the ALSMA Model pressure outputs from Case 3 as inputs to the LUT reservoir component, and Cases 2 and 6 used the ALSMA Model pressure outputs from Case 4 as inputs to the LUT reservoir component (Table 3).

Cases 7 and 8 used a constant pressure of 16.4 MPa across all time steps in the LUT reservoir component (Table 3). The reason for including these two cases in the case matrix was to generate baseline data for adjusting the results of NRAP-Open-IAM. During the testing, it was observed that inputs of formation pressure greater than the freshwater gradient assumption will generate leakage in NRAP-Open-IAM, even in the absence of CO₂ injection. Therefore, Cases 7 and 8 were used to calculate the leakage with no CO₂ injection, which was then used to adjust NRAP-Open-IAM cases with CO₂ injection to account for the fact that the leakage output represents total leakage or the sum of baseline leakage and additional leakage from increased pressure during CO₂ injection. In other words, the baseline leakage with no CO₂ injection was subtracted from the total leakage with CO₂ injection to derive the net leakage attributable to the relative pressure buildup in the storage unit and not the artifact of the MSW component freshwater gradient assumption.

RESULTS

Comparing Pressure Buildup Between CMG GEM and the ASLMA Model

Figure 4 shows time-series curves of the estimated pressure buildup in the storage unit at the locations of the three legacy wellbores (2, 3, and 4) from CMG GEM and two different types of ASLMA Model calculations: Type 1 (focused leakage only) and Type 3 (coupled focused and diffuse leakage). ALSMA Model Type 1 assumes that there is no pressure dissipation through the cap rock and, therefore, pressure leakage only occurs through wellbores (i.e., focused leakage), whereas ASLMA Model Type 3 allows for pressure leakage through wellbores and dissipation through the cap rock (i.e., coupled focused and diffuse leakage). Consequently, the pressure buildup calculated by ALSMA Model Type 3 is lower than the pressure buildup calculated by ALSMA Model Type 1. As shown in the figure, there were significant differences in the estimated pressure buildup in the storage unit between CMG GEM and both ASLMA Model types. For example, at Legacy Wellbore 2, the CMG GEM-estimated pressure buildup in the storage unit was 298 psi at the end of 20 years of CO₂ injection, whereas the ASLMA Model Type 1 and Type 3 estimates for the scenario with the thief zone on were 641 and 536 psi, respectively. The ASLMA Model Type 1 and Type 3, therefore, overestimated pressure buildup by 115% and 80%, respectively, as compared to CMG GEM. These differences are likely attributable to the combination of several factors, including i) the Petrel geologic model used for the reservoir simulation accounts for heterogeneity in porosity, permeability, and geologic structure, unlike the simplified assumptions within the ASLMA Model that the storage unit is homogeneous, isotropic, and horizontal; ii) CMG GEM accounts for multiphase processes within the CO₂ plume, which represent a large volume of the storage unit, with 77.5 MMt of CO₂ injected over a period of 20 years; and iii) the assumption of a constant CO₂ density to estimate the equivalent formation water volume injection in the ASLMA Model ignores changes in CO₂ density over the 20-year injection period, which could overestimate pressure buildup.

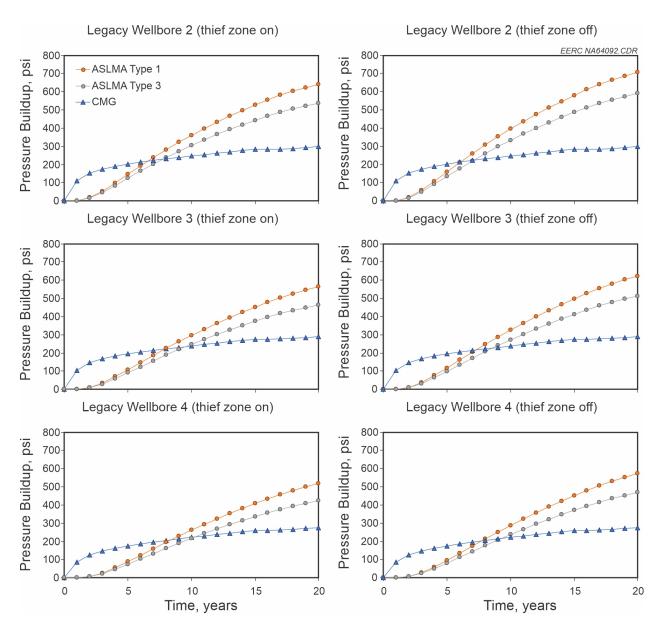


Figure 4. Time-series curves of the estimated pressure buildup in the storage unit at the locations of the three legacy wellbores (2, 3, and 4) from CMG GEM and two different types of ASLMA Model calculations: Type 1 (focused leakage only) and Type 3 (coupled focused and diffuse leakage). The left column shows the results for the ASLMA Model with the thief zone on, and the right column shows the results for the ASLMA Model with the thief zone off. The CMG curves are the same for all panels.

The CMG curves are the same for the left and right columns in Figure 4; however, the left column shows the results for the ASLMA Model with the thief zone on, and the right column shows the results for the ASLMA Model with the thief zone off. The differences in pressure buildup with and without a thief zone are significant. For example, at Legacy Wellbore 2, the ASLMA Model Type 1-estimated pressure buildup in the storage unit was 641 psi when the thief

zone was on (left column in Figure 4) and 708 psi when the thief zone was off (right column in Figure 4), for a difference of 10%. Therefore, greater formation fluid leakage from the storage unit to the lowermost USDW would be expected when the wellbore does not have access to a thief zone, i.e., thief zone off.

Comparing Formation Fluid Leakage at Legacy Wellbores

Figure 5 shows time-series curves of the cumulative formation fluid leakage to the lowermost USDW summed for all three legacy wellbores (2+3+4) for the case matrix (Table 3). As shown in the figure for the scenarios with the thief zone on (top panel in Figure 5), Case 1 resulted in significantly more cumulative formation fluid leakage at the end of 20 years (20,000 m³) compared to Case 3 (11,100 m³), Case 5 (11,500 m³), and Adjusted Case 1 (Case 1 minus Case 7) (11,900 m³). Case 1 used the NRAP-Open-IAM and the observed (actual) formation pressure of 2381 psi (16.4 MPa); therefore, the MSW component resulted in approximately 80% greater formation fluid leakage as compared to the ASLMA Model with the same inputs (i.e., Case 1 was 80% greater than Case 3). In contrast, Case 5 used the NRAP-Open-IAM and a freshwater pressure gradient assumption to assign an initial pressure of 2103 psi (14.5 MPa) to the storage unit, which resulted in more comparable formation fluid leakage between the NRAP-Open-IAM and the ASLMA Model (Case 5 was only 4% greater than Case 3). Finally, subtracting the baseline (no CO₂ injection) from Case 1 also resulted in more comparable formation fluid leakage between the NRAP-Open-IAM and the ASLMA Model, as Adjusted Case 1 (Case 1 minus Case 7) was only 7% greater than Case 3.

These results highlight the importance of the storage unit initial pressure to the formation fluid leakage estimates from the NRAP-Open-IAM and ASLMA Model. For storage complexes that do not adhere to the freshwater pressure gradient assumption of 0.433 psi/ft, the user cannot assume that the outputs from either tool are incremental leakage. Practitioners supporting the Class VI injection well permitting process and associated groundwater monitoring plans must, therefore, characterize the storage unit initial pressure and make the necessary adjustments to the NRAP-Open-IAM and ASLMA Model to properly quantify the wellbore leakage risk to USDWs. Essentially, there are four scenarios for running and comparing both tools:

- 1) Assuming a freshwater pressure gradient of 0.433 psi/ft and CO₂ injection, the NRAP-Open-IAM and ASLMA Model will yield equivalent results that represent *incremental leakage* attributable to CO₂ injection.
- 2) Assuming an overpressured storage unit initial pressure (e.g., 0.49 psi/ft like the example used here) and CO₂ injection, the NRAP-Open-IAM and ASLMA Model will generate higher leakage volumes and different results that reflect the sum of baseline leakage (prior to CO₂ injection) and incremental leakage (attributable to CO₂ injection), i.e., *total leakage*. This scenario would be the NRAP-Open-IAM with the observed (actual) initial pressure and the ASLMA Model with adjustments for initial head that were designed for overpressured storage units (Oldenburg and others, 2014, 2016).

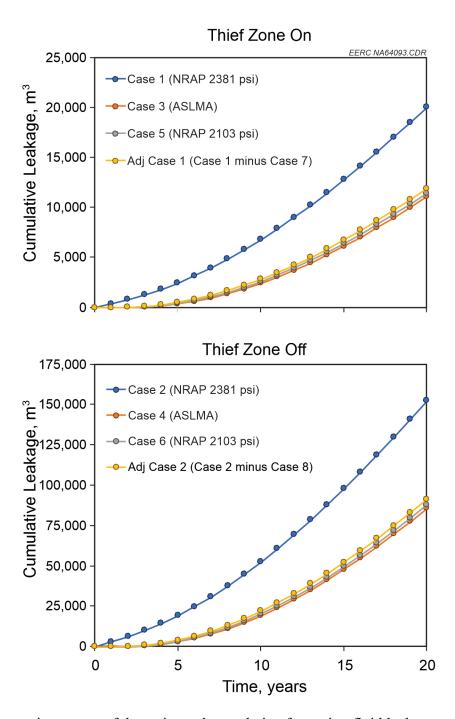


Figure 5. Time-series curves of the estimated cumulative formation fluid leakage to the lowermost USDW for all three legacy wellbores (2, 3, and 4) for Cases 1–6 and the adjusted Case 1 (Case 1 minus Case 7) and adjusted Case 2 (Case 2 minus Case 8). The top panel shows results for cases where the wellbore had access to a thief zone (thief zone on), and the bottom panel shows results for cases where the wellbore did not have access to a thief zone (thief zone off).

- 3) Assuming an overpressured storage unit initial pressure and no CO₂ injection will generate leakage volumes and different results that reflect the *baseline leakage* (prior to CO₂ injection). This scenario would be the NRAP-Open-IAM with the observed (actual) initial pressure set as a constant for all time steps and the ASLMA Model with adjustments for initial head also set as a constant for all time steps.
- 4) Subtracting baseline leakage (Scenario 3) from total leakage (Scenario 2) yields *incremental leakage*, which generates leakage volumes comparable to the freshwater pressure gradient assumption with CO₂ injection (Scenario 1).

Adjusting the NRAP-Open-IAM outputs by either modifying the initial pressure (Scenario 1) or subtracting a baseline case (Scenario 4) provides solutions that are more comparable between the NRAP-Open-IAM and ASLMA Model and likely more accurate estimates of the incremental wellbore leakage risk to USDWs.

The bottom panel of Figure 5 shows the scenarios with the thief zone off, meaning that the legacy wellbores connect the storage unit and the lowermost USDW without access to an intermediary saline aquifer in between. While the relative differences among Case 2, 4, 6, and (Case 2 minus Case 8) are like the preceding example, the magnitude of the cumulative formation fluid leakage is significantly greater. For example, the cumulative formation fluid leakage to the lowermost USDW at the end of 20 years for Cases 4, 6, and (Case 2 minus Case 8) was 85,900, 88,100, and 91,500 m³, respectively—nearly eight times greater than the scenarios with the thief zone on. These results underscore the importance of a thief zone to mitigating vertical fluid migration in leaky wellbores and the need to consider thief zones in estimating the wellbore leakage risk to USDWs.

Additional Considerations: GUI versus Control File

During testing, it was observed that when using the GUI to execute the NRAP-Open-IAM, the user inputs of aquifer permeability in the MSW component are overwritten with the default value of $-11 \log_{10}(m^2)$ due to the incorrect parameter name in the GUI source code. While this likely has a small effect on the wellbore leakage calculations, the text-based control file interface for running NRAP-Open-IAM is recommended. Moreover, the text-based control file interface provides greater control to the user for tailoring the input parameters to site-specific values.

KEY FINDINGS

The NRAP-Open-IAM testing generated the following list of key findings:

1. Site characterization data that include site-specific measurements of the properties listed in Table 1 (depth, thickness, initial pressure, temperature, porosity, permeability, and salinity) are essential to properly estimating wellbore leakage risks to USDWs. The current work underscores the importance of site-specific initial pressure measurements to the NRAP-Open-IAM formation fluid leakage calculations.

- 2. For storage units that do not conform to the freshwater pressure gradient assumption (0.433 psi/ft), using the observed (actual) initial pressure will result in NRAP-Open-IAM overestimating the formation fluid leakage. Adjusting the NRAP-Open-IAM outputs by either modifying the initial pressure or subtracting a baseline case provides solutions that are more comparable between the NRAP-Open-IAM and ASLMA Model and likely more accurate estimates of the incremental wellbore leakage risk to USDWs.
- 3. While the single-phase flow assumptions in the ASLMA Model have been shown to be applicable for far-field pressure changes beyond the CO₂ plume, the current work shows that the ASLMA Model Type 1 and Type 3, therefore, overestimated pressure buildup at the end of 20 years by 115% and 80%, respectively, as compared to CMG GEM. These differences are likely attributable to the combination of several factors, including i) the Petrel geologic model used for the reservoir simulation accounts for heterogeneity in porosity, permeability, and geologic structure, unlike the simplified assumptions within the ASLMA Model that the storage unit is homogeneous, isotropic, and horizontal; ii) CMG GEM accounts for multiphase processes within the CO₂ plume, which represents a large volume of the storage unit, with 77.5 MMt of CO₂ injected over a period of 20 years; and iii) the assumption of a constant CO₂ density to estimate the equivalent formation water volume injection in the ASLMA Model ignores changes in CO₂ density over the 20-year injection period, which could overestimate pressure buildup. Therefore, utilizing the pressure buildup derived from CMG GEM may provide more accurate inputs to the LUT reservoir component within the NRAP-Open-IAM. The current study only used the ASLMA Model pressure model to compare wellbore leakage results more effectively between the NRAP-Open-IAM and ASLMA Model.

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