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Authors

Bacon, Diana Holford
Locke II, Randall A
Keating, Elizabeth
et al.

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Application of the Aquifer Impact Model to support decisions at a CO_2 sequestration site

Diana Holford Bacon , Pacific Northwest National Laboratory, Richland, WA, USA

Randall A. Locke II , University of Illinois, Illinois State Geological Survey, Champaign, IL, USA

Elizabeth Keating, Los Alamos National Laboratory, Los Alamos, NM, USA

Susan Carroll, Lawrence Livermore National Laboratory, Livermore, CA, USA

Abbas Iranmanesh, University of Illinois, Illinois State Geological Survey, Champaign, IL, USA

Kayyum Mansoor, Lawrence Livermore National Laboratory, Livermore, CA, USA

Bracken Wimmer, University of Illinois, Illinois State Geological Survey, Champaign, IL, USA

Liange Zheng , Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Hongbo Shao and Sallie E. Greenberg, University of Illinois, Illinois State Geological Survey, Champaign, IL, USA

Correspondence to: Diana Bacon, Pacific Northwest National Laboratory, P.O. Box 999, MSIN P7-54, Richland, WA 99352, USA. E-mail: diana.bacon@pnnl.gov

Abstract

The National Risk Assessment Partnership (NRAP) has developed a suite of tools to assess and manage risk at CO_2 sequestration sites. The NRAP tool suite includes the Aquifer Impact Model (AIM), which evaluates the potential for groundwater impacts from leaks of CO_2 and brine through abandoned wellbores. There are two aquifer reduced-order models (ROMs) included with the AIM tool, a confined alluvium aquifer, and an unconfined carbonate aquifer. The models accept aquifer parameters as a range of variable inputs so they may have broad applicability. The generic aquifer models may be used at the early stages of site selection, when site-specific data is not available. Guidelines have been developed for determining when the generic ROMs might be applicable to a new site. This paper considers the application of the AIM to predicting the impact of CO_2 or brine leakage were it to occur at the Illinois Basin Decatur Project (IBDP). Results of the model sensitivity analysis can help guide characterization efforts; the hydraulic parameters and leakage source term magnitude are more sensitive than clay fraction or cation exchange capacity. Sand permeability was the only hydraulic parameter measured at the IBDP site. More information on the other hydraulic parameters could reduce uncertainty in risk estimates. Some non-adjustable parameters are significantly different for the ROM than for the observations at the IBDP site. The generic ROMs could be made more useful

to a wider range of sites if the initial conditions and no-impact threshold values were adjustable parameters.

Keywords: carbon sequestration; risk analysis; groundwater; brine; carbon dioxide; leakage

Introduction

Geological carbon sequestration (GCS) is a global carbon emission reduction strategy involving the capture of CO_2 emitted from fossil fuel burning power plants, and the subsequent injection of the captured CO_2 into deep saline aquifers or depleted oil and gas reservoirs. A critical question that arises from the proposed GCS is the potential impacts of CO_2 injection on the quality of drinking water systems overlying CO_2 sequestration storage sites.

Although storage reservoirs are evaluated and selected based on their ability to safely and securely store emplaced fluids, leakage of CO_2 from storage reservoirs is a primary risk factor and potential barrier to the widespread acceptance of geologic CO_2 sequestration.[1-3] Therefore, a systematic understanding of how CO_2 leakage would affect the geochemistry of potable aquifers, and subsequently control or affect elemental and contaminant release via sequential and/or simultaneous abiotic and biotic processes and reactions is vital. Field-scale experiments have been carried out around the world to identify CO_2 leakage and to investigate effects on groundwater quality in shallow aquifers.[4] However, these experimental leaks are of shorter duration and smaller size than might occur at an industrial-scale carbon storage site. Even larger leaks may be difficult to detect using current monitoring techniques.[5]

The National Risk Assessment Partnership (NRAP) has developed a suite of tools to assess and manage risk at CO_2 sequestration sites.[6] This quantification approach is based on simulating coupled physical and chemical processes to predict how the natural system behaves over time, and it explicitly includes uncertainty quantification. In order to probabilistically address uncertainty, NRAP is developing efficient, reduced-order models (ROMs) as part of its approach. These ROMs are built from detailed, physics-based process models to provide confidence in the predictions over a range of conditions.[7] However, the ROMs are designed to accurately reproduce the predictions from the computationally intensive process models at a fraction of the computational time, thereby allowing the utilization of Monte Carlo methods to probe variability in key parameters and their impact on leakage impacts.

The NRAP tool suite includes the Aquifer Impact Model (AIM), which currently consists of two polynomial or look-up table-based ROMs that predict the impact of CO_2 and brine leaks through abandoned wellbores on overlying aquifers. The generic ROMs were are based on data from two aquifers, a confined siliciclastic alluvium aquifer[8] and an unconfined carbonate aquifer,[9] but the models accept aquifer characteristics as a range of variable

inputs so that they may have broader applicability. These aquifer ROMs are also included in the NRAP Integrated Assessment Model, NRAP-IAM-CS, which couples ROMs of geologic carbon sequestration, wellbore leakage, and groundwater impacts. Previous studies have concluded that pH and TDS impact predictions from the AIM are the most transferable to other aquifers.[10] Guidelines have been developed for determining when the generic ROMs could be applied at a new site.[11]

Part of the motivation for including adjustable input parameters in AIM was so that these ROMs could be applied to aquifers with different hydrogeologic or geochemical characteristics than the alluvium or carbonate aquifers used to develop them. In principle, this generality could allow the ROMs to be applied broadly to other aquifers. However, there are some aspects of the models from which the ROMs were derived that are intrinsic and non-adjustable. These include background groundwater chemistry (both average values and variability), the type of permeability heterogeneity, and the nature of the upper boundary (confined or unconfined). These less obvious factors should be considered when deciding whether to apply existing ROMs to a new site, or whether to build a new site-specific ROM. If an aquifer overlying a proposed CO_2 sequestration site was substantially different than the alluvium or carbonate aquifer reference cases in one or more of these intrinsic characteristics, these ROMs should only be applied with caution, or not at all (Fig. 1).

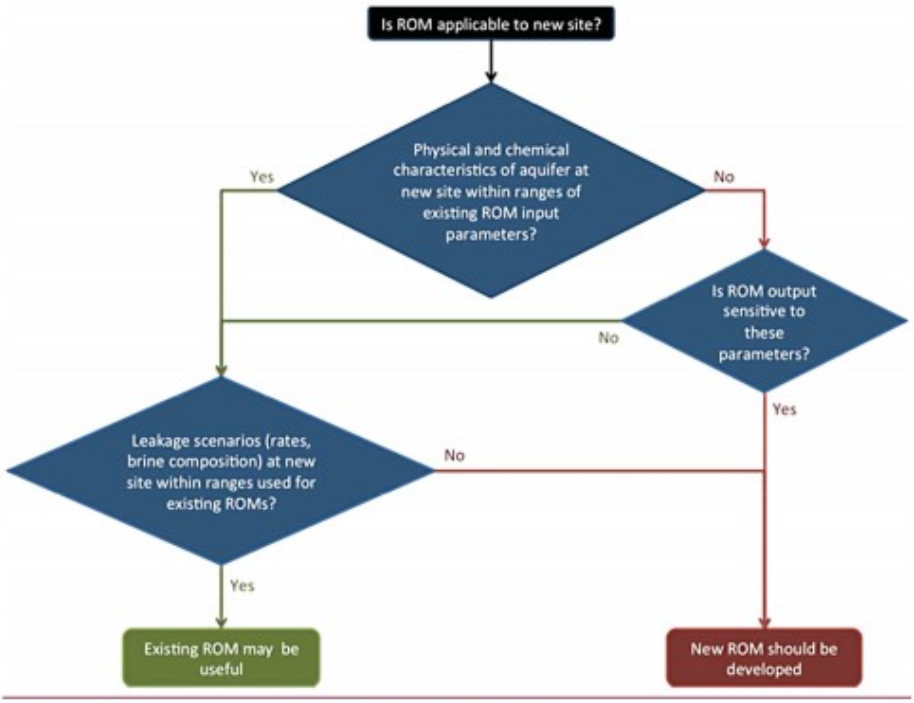

Figure 1. Criteria for Application of AIM to a new site.

This paper considers the applicability of the aquifer models in AIM to predicting the impact of CO_2 or brine leaks at the Illinois Basin - Decatur Project (IBDP) if such a leak occurred. Because there are no known abandoned wellbores at the site that penetrate the injection reservoir, this analysis is not meant to predict actual risk at the IBDP site. The goal is to assess whether the ranges of characteristic parameters at the site fall within the ranges of the aquifer models in AIM, or whether a site-specific aquifer model would be more appropriate. A further goal is to demonstrate how the tool could be used at early stages of a carbon storage project to guide site characterization efforts.

Methods

NRAP AIM

The NRAP AIM tool predicts the volume of groundwater in shallow aquifers impacted by point-source CO_2 and/or brine leaks introduced at the base of the aquifer. The input parameters are (i) the location and number of point-source leaks, (ii) flow rate of CO_2 and brine at each point source, and (iii) hydrogeologic and geochemical characteristics of the aquifer. The output variables are plume sizes for each of nine water quality metrics and the flux of CO_2 across the water table. If the user is interested in predicting impacts due to time-varying sequences of flow rates (hereafter called leakage scenarios), the AIM will be called at each time in the sequence. For each point in time, the AIM inputs will be the instantaneous CO_2 and brine flow rate (kg/s) and the cumulative mass of CO_2 and brine leaked since the start of the leakage scenario. In principle, hydrogeologic and geochemical characteristics of the aquifer could also change in time; however, this functionality has not been tested.

The size of impact plumes are calculated by the AIM using two alternative definitions of ‘impact’, which the user selects: (i) changes that cause an exceedance of a drinking water standard or maximum contaminant level (MCL); and (ii) changes that are above and beyond natural background variability in the aquifer, referred to hereafter as no-impact threshold values.[12] For specific values used in AIM development, see Table 1. The latter no-impact threshold definition is aligned with the proposed Environmental Protection Agency (EPA) Class VI Rule for CO_2 injection well permitting.[13] Nine water-quality metrics are considered: pH, total dissolved solids (TDS), four trace metals (As, Ba, Cd, Pb), and three organic compounds (Benzene, Naphthalene, and Phenol). The user of the toolset can select one or more outputs to calculate. The metrics pH and TDS were found to be most applicable to other sites, based on a comparison of ranges of values measured in a number of aquifers in the United States.[11]

Table 1. Initial aquifer concentrations used in the simulations, no-impact[12] and MCL[22] thresholds.

	Unconfined Carbonate Aquifer (Edwards)		Confined Unconsolidated Sands Aquifer (High Plains)		U.S. EPA Regulatory Standard
Analyte	Initial Model[a]	No-Impact Threshold[b]	Initial Model[c]	No-Impact Threshold[b]	MCL Threshold
pH	6.9	6.6	7.6	6.625[d]	6.5
Total Dissolved Solids	330	420 mg L^{-1}	570 mg L^{-1}	1300 mg L^{-1}[e]	500 mg L^{-1}
Arsenic	0.31	0.55 μg L^{-1}	1.5 μg L^{-1}	9.3 μg L^{-1}	10 μg L^{-1}
Cadmium	0.00	0.04 μg L^{-1}	0.059 μg L^{-1}	0.25 μg L^{-1}	5 μg L^{-1}
Lead	0.06	0.15 μg L^{-1}	.086 μg L^{-1}	0.63 μg L^{-1}	15 μg L^{-1}

[a]Initial values from Lindgren *et al.*,[23] Lindgren,[24] and Musgrove *et al.*[25]
[b]95%-confidence, 95%-coverage tolerance limit based on log values except for pH, which is already a log value.
[c]Initial values from Nativ and Smith[26] and McMahon *et al.*[27]
[d]Value is about 0.5 pH units lower than no-impact threshold estimated by Last *et al.*[12] because ROMs at higher threshold produced non-physical results.
[e]Threshold value exceeds regulatory standard.

As described in Carroll *et al.*[10] two aquifer ROMs were included in the NRAP AIM: a confined alluvium aquifer and an unconfined carbonate aquifer. These were selected because they represent key aquifer types overlying potential storage reservoirs within the continental United States and there was ample reference information available for each aquifer type to enable construction of reactive-transport simulations.

AIM requires three types of information outlined in Table 2:

- Brine and CO_2 leak rates
- Concentration of solutes in the leaking brine
- Shallow aquifer hydrology and geochemistry

Table 2. AIM input parameters and their ranges.

Type		Parameter	Min	Max	Units
Confined Alluvium Aquifer					
Aquifer	Hydraulic	Sand fraction	0.35	0.65	–
		Correlation length X	200	2,500	m
		Correlation length Z	0.5	25	m
		Permeability sand	−14	−10	$\log_{10}(m^2)$
		Permeability clay	−18	−15	$\log_{10}(m^2)$
		Porosity sand	0.375	0.375	–
		Density sand	2,500	2,500	kg/m^3
		van Genuchten_m Sand	0.66	0.66	–
		van Genuchten_alpha Sand	−4.25	−4.25	–
	Chem1	Goethite[a]	0	0.15	–
		Illite[a]	0	0.2	–
		Kaolinite[a]	0	0.15	–
		Smectite[a]	0	0.3	–
		Cation exchange capacity	0.1	40	meq/100g
	Chem2	Benzene K_d	−4.5	0.69	$\log_{10}$ (L/kg)
		Benzene decay constant	−10	−6.1	$\log_{10}$ (1/s)
		PAH[b] K_d	−3.1	1.98	$\log_{10}$ (L/kg)
		PAH decay constant	−10	−6.45	$\log_{10}$ (1/s)
		Phenol K_d	−6	0.15	$\log_{10}$ (L/kg)
		Phenol decay constant	−10	−5.63	$\log_{10}$ (1/s)
Leak Rate		Mitigation time	25[c]	200	yr
		CO_2_flow	0	0.5	kg/s
		Brine_flow	0	0.075	kg/s
		CO_2 mass	2.23	9.058	$\log_{10}$ (kg)
		Brine mass	4.5	8.124	$\log_{10}$ (kg)
		Time	25[2]	200	yr
Brine Composition		[Na] = [Cl]	−2	0.73	$\log_{10}$ (Molality)
		[Pb]	−8.5	−5	$\log_{10}$ (Molality)
		[Benzene]	−8.8927	−4.8927	$\log_{10}$ (Molality)
		[As]	−9	−5	$\log_{10}$ (Molality)
		[Ba]	−5.1	−2.3	$\log_{10}$ (Molality)
		[Cd]	−9	−6	$\log_{10}$ (Molality)
		[PAH]	−10	−4.1	$\log_{10}$ (Molality)
		[Phenol]	−10	−3.7	$\log_{10}$ (Molality)
Unconfined Carbonate Aquifer					
Aquifer	Hydraulic	Permeability variance	0.017	1.89	–
		Correlation length	1	3.95	km
		Kx/Kz	1.1	49.1	–
		Mean permeability	−13.8	−10.6	$\log10(m^2)$
		Aquifer thickness	100	500	m

(*Continued*)

Table 2. Continued

Type	Parameter	Min	Max	Units
	Horizontal hydraulic gradient	2.88E-4	1.89E-2	–
Geochemistry	Calcite surface area	0	0.01	m^2/g
	Organic carbon volume fraction	0	0.01	–
	Benzene K_d	1.49	1.73	log (Koc)
	Benzene decay	0.15	2.84	log (day)
	PAH K_d	2.78	3.18	log (Koc)
	PAH decay constant	−0.85	2.04	log (day)
	Phenol K_d	1.21	1.48	log (Koc)
	Phenol decay constant	−1.22	2.06	log (day)
Leak Rate	CO_2_flow	0	500	g/s
	Brine_flow	0	75	g/s
	CO_2 mass	0	500	kTon
	Brine mass	0	100	kTon
	Time	0	200	yr
Brine Composition	[Cl][d]	−1	0.78	$\log_{10}$(Molality))

[a]Volume fraction of reactive minerals, calcite volume fraction is 0.2
[b]PAH = Polycyclic Aromatic Hydrocarbon
[c]Poor fidelity at times less than 25 years
[d]Only used for chemical scaling factor

The AIM tool will not allow the input parameters in Table 2 to be exceeded because they represent the range of parameters used in the reactive transport simulations that the ROMs are based on.

In some sense, every aquifer in the world is unique and no two aquifers would respond exactly the same way to a brine or CO_2 leak. However, it may be possible for generic models to be tuned for application to specific sites. The AIM is generic in the sense that many aquifer characteristics have variable input parameters and so could be applied to a new site by setting input parameters appropriately. As shown in Table 2, the AIM accepts a fairly wide range of permeabilities, background hydrologic gradients, thicknesses, and mineral content. Many aquifers in the United States have characteristics falling within these ranges. However, some aspects of the simulations from which the AIM was derived are intrinsic and non-adjustable. These include initial water chemistry and threshold impact values (Table 1), the geochemical reaction network used in the simulations, the type of permeability heterogeneity, and the nature of the upper boundary (closed or open). If an aquifer overlying a proposed CO_2 sequestration site was substantially different than the High Plains or Edwards Aquifer in one of these intrinsic characteristics, the AIM tool should only be applied with caution or not at all. For a more detailed discussion of these issues, see Keating *et al*.[11]

Leak rates

A *leakage scenario* is a time series of brine and CO_2 leak rates at a point source at the base of the aquifer. The ROM requires a leak-rate file containing one or more leakage scenarios to analyze. The user can create this type of file using a text editor or spreadsheet program. Alternatively, the user can use an NRAP tool bundled within AIM to create idealized, hypothetical leakage scenarios for analysis.[14] The heuristic leak scenario builder tool generates leakage scenarios as shown in Fig. 2.

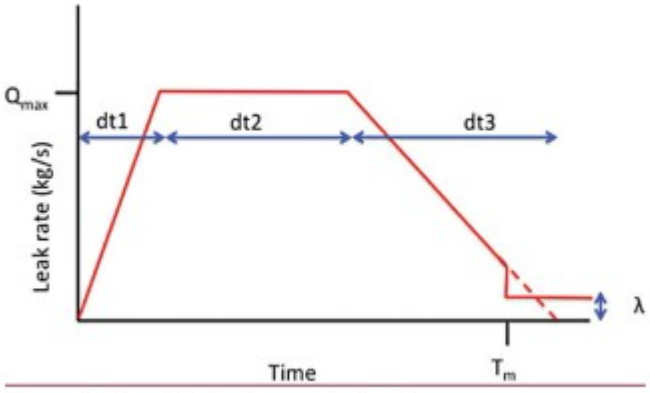

Figure 2. Heuristic leak scenario builder.

Detailed wellbore and fault leakage scenarios have been developed previously, for examples see Nordbotten *et al*.[15] and Jordan *et al*.[16] The AIM is designed to accept wellbore leakage scenarios generated by any method, as long as leak rates are within the ranges shown in Table 2. For simplicity, a heuristic leakage model is provided along with the groundwater impact model so that the user can easily generate 'what if' scenarios for planning purposes. This simple model has six parameters (Table 3) for each leaking fluid (CO_2 and brine).

Table 3. Leak rate model parameters.

Parameter	Definition
Qmax	maximum leak rate (kg/s)
dt1	time for rise to maximum (years)
dt2	time leak is at maximum rate (years)
dt3	time for leak rate to decline to minimum (years)
Lambda, λ	minimum leak rate (fraction of maximum)
T_m	Leak mitigation time (years)

Solute concentrations in leaking brine

The unconfined carbonate aquifer accepts chloride concentration (moles/kg) in the leaking brine as input. Accepted ranges are 0.1–6 moles/kg.

Concentrations of trace metals and organics in the brine are automatically scaled according to chloride concentration, using factors detailed in Bacon *et al*.[17] The confined alluvium aquifer ROM accepts trace metal concentrations that are independent from chloride concentrations.

Aquifer parameters

The *unconfined carbonate* and *confined alluvium* tools of the AIM have 20 and 35 input parameters, respectively. Most of the parameters describe hydrogeologic and geochemical characteristics of the aquifer; a smaller number are related to the leaking CO_2/brine. The parameters and their acceptable input ranges are listed in Table 2. In principle, these parameters could be estimated from available published data, new site-specific characterization activities, or treated as uncertain parameters in a probabilistic framework. Although many of the aquifer parameters may ultimately be fairly well-known at a site, the time-varying flow rates of CO_2 and/or brine in potential leak scenarios are likely to remain uncertain. Therefore, it is not expected that these models would ever be applied in a deterministic context.

Selected shallow monitoring well information from the Illinois Basin – Decatur Project

The Midwest Geological Sequestration Consortium (MGSC) has developed the Illinois Basin - Decatur Project (IBDP) at the Archer Daniels Midland Company (ADM) ethanol production facility in Decatur, IL, USA.[18] The objective of the project is to validate the capacity, injectivity, and containment of the Mount Simon Sandstone which is the reservoir with the greatest estimated carbon storage capacity in the Illinois Basin and Midwest region. Injection operations in well CCS1 began on November 4, 2011 and were completed successfully on November 26, 2014 with a total mass of 999,215 tonnes stored in the deep saline reservoir. The IBDP has developed an extensive Monitoring, Validation, and Accounting (MVA) program that uses different techniques to monitor the injection zone, sub surface, surface, and atmosphere. IBDP environmental monitoring began in 2009, and shallow groundwater monitoring was initiated in August 2010. The project is currently in the post-injection phase and monitoring will be continued as specified in the federal Underground Injection Control Program Class VI permit that was issued for the project.

Four regulatory compliance wells were drilled and constructed in April and May 2010 (Fig. 3). The monitoring horizon consists of several thin silty sandstone layers within a siltstone in the upper Pennsylvanian bedrock which is approximately 135–150 ft below land surface (bls), and was identified as an Underground Source of Drinking Water (USDW) by the Illinois EPA. The heterogeneity within the Pennsylvanian bedrock is exhibited by the variability of its mineral composition. The mineralogy within the most permeable zones used for monitoring ranges from 24–78% quartz, 0–4% dolomite, 0–2% calcite, 1–49% siderite, 10–20% feldspar, and 9–26% clay

content. Semi-quantitative mineralogical analyses were performed at the ISGS X-Ray Diffraction (XRD) Laboratory using randomly oriented XRD patterns.[19]

Figure 3. Location of shallow groundwater wells at the IBDP site (Aerial photography acquired April 30, 2015, by the Illinois Department of Transportation).

Table 4 contains coordinates for the four IBDP shallow groundwater monitoring wells (i.e., compliance wells), ADM-G101 through -G104. The original coordinates (from Berns, Clancy & Assoc.) included here are in the Illinois State Plane East (in feet), and Geographic (in decimal degrees) systems. The original coordinates are also converted to UTM Zone 16 (in meters, see the last two columns). All coordinate systems reference the 1983 North American Datum (NAD83). The wells are generally about 140 feet (43 m) deep with 10-foot (3 m) screened intervals installed in thin sandstone of Pennsylvanian-age bedrock. Table 5 shows the related well sampling data for pH and Total Dissolved Solids (TDS) between August 2010 and October 2015.

Table 4. Well locations.

Well	ADM-G101	ADM-G102	ADM-G103	ADM-G104
ELEVATION_FT	673.2	673.5	672.5	681.8
ELVREF	GROUND	GROUND	GROUND	GROUND
Date installed	5/6/10	5/11/10	4/27/10	5/24/10
SPE83_N_FT	1169622.8	1169624.7	1169774.7	1171119.0
SPE83_E_FT	827090.0	827036.8	826911.2	826003.9
LATDD83	39.877073	39.877077	39.877487	39.881161
LNGDD83	−88.893302	−88.893492	−88.893943	−88.897205
UTM16N83_X	338093.6	338077.4	338039.8	337769.4
UTM16N83_Y	4415829.1	4415829.9	4415876.2	4416290.0

Table 5. Quarterly pH and TDS data from IBDP compliance monitoring wells.

Date	G101_TDS	G102_TDS	G103_TDS	G104_TDS	G101_pH	G102_pH	G103_pH	G104_pH
8/12/10	1164	1212	1282	869	7.55	7.54	7.45	7.53
10/29/10	1145	1241	1339	869	7.30	7.36	7.40	7.32
1/19/11	1217	1226	1359	871	7.44	7.42	7.30	7.41
4/12/11	1172	1233	1366	866	7.24	7.18	7.15	7.16
7/7/11	1148	1221	1350	863	7.46	7.46	7.45	7.47
10/25/11	1177	1242	1353	863	6.76	6.73	7.09	7.23
1/17/12	1106	1216	1346	840	7.17	7.19	7.21	7.35
4/10/12	1145	1223	1373	869	7.40	7.36*	7.41	7.36
7/24/12	1172	1220	1347	858	7.72	7.51*	7.79	7.58
10/24/12	1150	1171	1340	859	7.38	7.41*	7.37	7.4
1/7/13	1152	1151	1357	849	7.03	7.25*	7.23	7.24
4/17/13	1145	1128	1365	871	7.23	7.39*	7.34	7.29
7/22/13	1126	1103	1359	864	7.40	7.71*	7.45	7.48
10/24/13	1120	1087	1341	843	7.46	7.71*	7.45	7.39
1/13/14	1144	1112	1342	847	7.38	8.03*	7.39	7.29
4/21/14	1127	1152	1353	876	7.37	8.04*	7.36	7.29
7/16/14	1162	1145	1355	876	7.39	8.04*	7.37	7.17
10/30/14	1122	1126	1348	833	7.25	7.88*	7.21	6.97
1/20/15	1150	1142	1363	827	7.22	7.86*	7.22	6.96
4/21/15	1121	1150	1348	835	7.28	8.01*	7.29	7.11
7/14/15	1120	1130	1349	850	7.18	7.73*	7.23	6.98
10/28/15	1085	1129	1343	828	7.41	7.91*	7.37	7.17

*While the pH values in most of the wells fluctuated between 6.7 and 7.8 units, an increasing trend was observed for well G102 after about January 2013. An increase in dissolved oxygen and sulfate concentrations has also been observed. These observed trends are not expected to be fully representative of natural in situ conditions and are attributed to a leak in the tubing of the sampling pump installed in that well, which enriched the oxygen content of the groundwater samples collected. The pump tubing has been repaired and pH values appear to be trending back to pre-January 2013 values.

Results

Comparison of ROM parameter ranges and observed values

To determine whether the AIM is applicable to simulate hypothetical leakage at the IBDP site, the parameters of the ROM must be compared to the observations. As already described, four compliance wells at the site are screened in thin silty sandstone layers within a siltstone. The confined alluvium aquifer ROM assumed that the aquifer materials consisted of interbedded sand/gravel and clay. The rock type used to model the unconfined carbonate aquifer ROM was limestone consisting of almost pure calcite. The interbedded sand/gravel and clay layers of the confined alluvium aquifer ROM therefore seems most similar to the interbedded sandstone/siltstone layers at the IBDP site.

It is not clear how sensitive the impacts predicted by AIM are to the values assumed for initial conditions and the no-impact threshold values, which have fixed values. The initial conditions are based on average values of water quality metrics measured in groundwater, and the no-impact thresholds are based on upper 95th percentile values (or lower 5th percentile values in the case of pH). Table 6 shows that the average pH measured in the four wells ranged from 7.27 to 7.34, and the lower 5th percentile ranged from 6.87 to 7.15 (excluding samples from well G102 affected by the tubing leak). The confined alluvium ROM calculates impacted aquifer volumes based on an average pH of 7.6 and a no-impact threshold of 6.625. The no-impact threshold from the confined alluvium ROM and the mean of the lower 5th percentile values compare well. The average value of ~7.3 is slightly lower than the ROM average/initial value of 7.6. The impacted plume volume may be sensitive to the difference between the initial value of a water quality metric in the aquifer and the no-impact threshold. The larger the difference, the lower the chance that there will be an impact. This difference is greater in the confined alluvium ROM than it is in the IBDP site wells, indicating that the ROM may slightly under predict the impacted plume volume. These are not adjustable parameters in the model. However, given that the reactive transport simulations that the ROM is based on indicate that dissolved CO_2 in the aquifer will lower pH to a value of 3, much lower than the no-impact threshold value, a difference of 0.3 pH units in the average initial pH does not seem significant.

Table 6. Statistics for observed TDS (ppm) from IBDP site.

Date	G101_TDS	G102_TDS	G103_TDS	G104_TDS
Min	1085	1087	1282	827
Max	1217	1242	1373	876
Average	1144	1171	1349	856
95th percentile	1177	1241	1366	876

Table 7. Statistics for observed pH from IBDP site.

Date	G101_pH	G102_pH	G103_pH	G104_pH
Min	6.76	6.73	7.09	6.96
Max	7.72	7.54	7.79	7.58
Average	7.32	7.27	7.34	7.28
5th percentile	7.04	6.87	7.15	6.97

As shown in Table 1, the initial condition used for TDS in the confined alluvium ROM was 570 mg/L and the no-impact threshold value was 1300 mg/L. In the IBDP observation wells, the average value for TDS ranged between 856 and 1349, while the 95th percentile value ranged from 876 to 1366. So, the no-impact value is comparable to the highest 95th percentile value from the IBDP site, but the average values from the IBDP site are significantly higher than the observed average values for HPA used to create the ROM. The difference between the initial value and the no-impact value in the ROM is greater than the difference between the average and 95th percentile values in the observation wells. Depending on the salinity of the leaking brine, the ROM may under predict the impact to TDS in the aquifer. For high salinity brine leaks, the difference between the ROM and the site observations will not be significant.

The sand fraction in the confined alluvium ROM ranges from 0.35 to 0.65 (35% to 65%). All four compliance wells at the IBDP site are screened in a zone of interbedded thin shales and sandstones. The sand fraction at the IBDP site is unknown and so is treated as an uncertain parameter.

The horizontal (x) correlation lengths for the sand and gravel layers range from 200 to 2500 m and the vertical (z) correlation lengths for the sand and gravel layers range from 0.5 to 25 m in the confined alluvium ROM. The correlation length at the IBDP site is unknown and is treated as an uncertain parameter.

The intrinsic permeability of the Pennsylvanian-age USDW at the IBDP site is estimated to fall between 1.43×10^{-12} and 2.24×10^{-13} m^2, which falls within the range for sand layers in the alluvium ROM of 1×10^{-10} to 1×10^{-14} m^2. The permeability of the clay layers is not known, and is treated as an uncertain parameter with a range of 1×10^{-18} to 1×10^{-15} m^2.

The cation exchange capacity (CEC) at the monitoring well locations is uncertain, but the clay content ranges up to 4%. CEC is treated as an uncertain parameter in the confined alluvium ROM with a range of 0.1 to 40 meq/100g.

Sensitivity analysis

Once observations at the IBDP site were compared to the ROM parameters (step 1 in Fig. 1), a sensitivity analysis was conducted in order to determine which parameters were important (step 2 in Fig. 1). Selecting pH and TDS as the desired outputs, we first used the AIM tool to conduct a Monte Carlo (MC) uncertainty analysis and a global sensitivity analysis (SA).

The MC analysis was conducted using the parameters for the confined alluvium ROM, shown in blue font in Table 8. Default parameters were used where observations were not available for the IBDP site or where parameters were not adjustable. To accomplish the MC analysis, the tool first creates random parameter combinations within the user-specified parameter ranges.

The ROM is called for each parameter combination. The total number of parameter combinations, n, are determined as follows:

$$n = n_a \times n_l \times 200 \quad (1)$$

where n_a is the number of aquifer realizations, n_l is the number of leakage scenarios, and 200 is the timespan of each simulation, in years. We used the values of 100 for n_a and 100 for n_l.

Table 8. Comparison of Confined Alluvium ROM Parameters to IBDP site Observations (parameter ranges in blue are used in subsequent analysis).

	Parameter	Confined Alluvium ROM Parameters	IBDP Pre-Injection Observations	Parameter vs. Observations
Non-adjustable	Initial pH	7.6	7.31 (average)	Higher
	pH No-Impact Threshold	6.625	6.81 (5^{th} percentile)	Lower
	Initial TDS	570 mg/L	1152 (average)	Lower
	TDS No-Impact Threshold	1300 mg/L	1358 (95^{th} percentile)	Similar
Adjustable	Sand fraction	0.35–0.65	–	Uncertain
	Correlation length X	200–2,500 m	–	Uncertain
	Correlation length Z	0.5–25 m	–	Uncertain
	Permeability sand	$10^{-14} - 10^{-10}$ m^2	$10^{-11.8} - 10^{-10.4}$ m^2	Within range
	Permeability clay	$10^{-18} - 10^{-15}$ m^2	–	Uncertain
	Goethite volume fraction	0–0.15	–	Uncertain
	Illite volume fraction	0–0.2	–	Uncertain
	Kaolinite volume fraction	0–0.15	–	Uncertain
	Smectite volume fraction	0–0.3	–	Uncertain
	Cation Exchange Capacity	0.1–40 meq/100 g	–	Uncertain

Selected results of the leakage scenarios are shown in Fig. 4. Only a random subset is shown so that individual lines are visible. Quartiles of plume size are shown in Fig. 5.

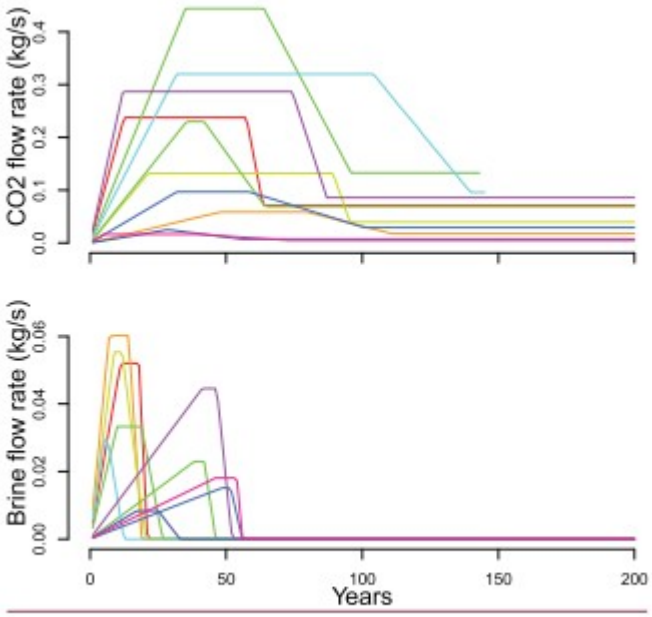

Figure 4. Subset of CO_2 and brine flow rate scenarios generated by the heuristic leak model in AIM

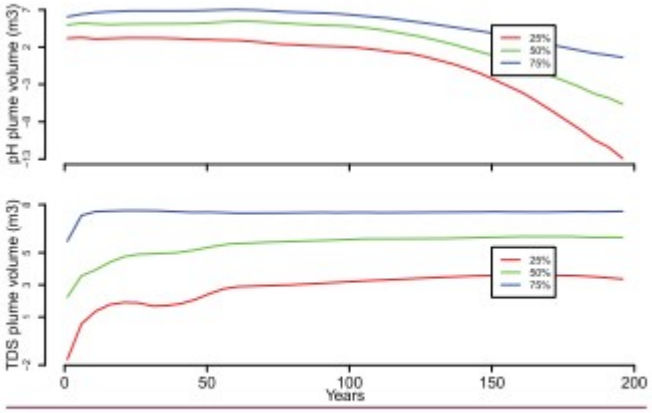

Figure 5. Quartiles for volume of aquifer below pH and above TDS impact thresholds by year using the sand permeability observed at the IBDP site.

To accomplish the SA, the sensitivity package for R was used[20] to define 1000 × m parameter combinations, where m is the total number of variable inputs (m = 29 for the confined alluvium ROM). The ROM was then called 1000 × m times, and afterwards the R software was used to calculate parameter sensitivities.

Figure 6 shows the results of a global sensitivity study on the two aquifer ROMs using the 'extended-FAST' method[21] as implemented in R Sensitivity Package.[20] This method allows the estimation of first order and total Sobol

indices for each model parameter. For pH plume size predictions, the most sensitive parameters were the fraction of sand (versus clay), permeability of sand and clay, and the CO_2 leakage rate and total amount leaked. For TDS plume size predictions, the most sensitive parameters were the fraction of sand, the x- (horizontal) and z-direction (vertical) correlation lengths, the sand and clay permeability, and the brine leakage rate and total amount of brine leaked.

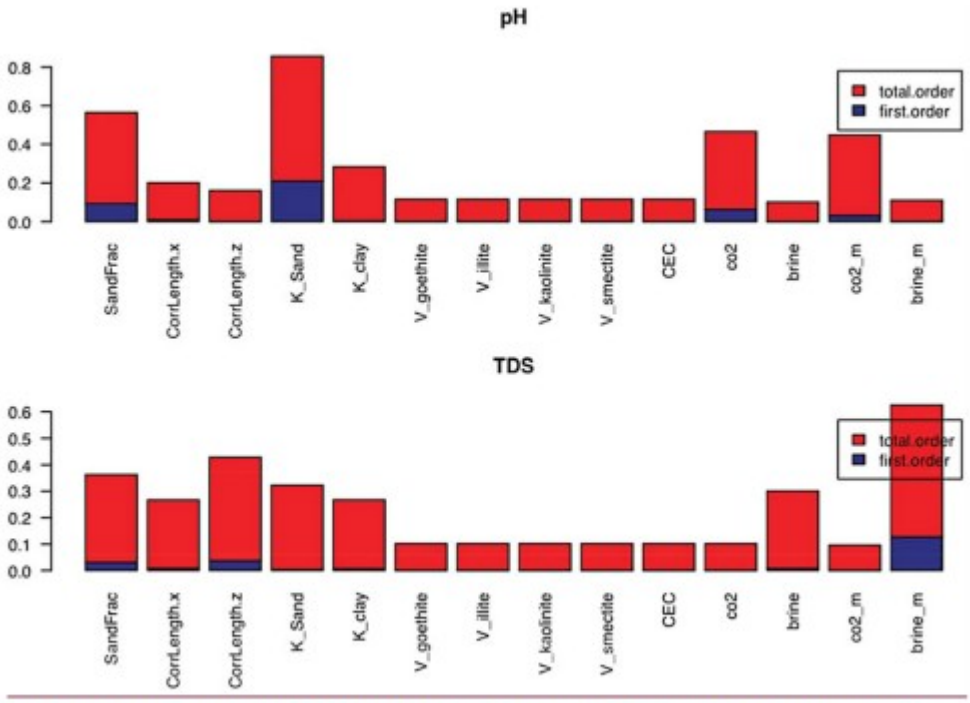

Figure 6. Sensitivity analysis using confined alluvium ROM using the sand permeability observed at IDBP site.

Conclusions

Based on the results of the sensitivity analysis for pH and TDS plume volume, the hydraulic parameters and source term magnitude are more sensitive parameters than geochemical parameters such as clay fraction or cation exchange capacity. This indicates that the generic confined alluvium ROM may be applicable to other sites if the hydraulic parameters fall within the default ranges.

More information on the other hydraulic parameters, such as sand fraction and sand/clay correlation lengths could possibly reduce uncertainty in risk estimates. The results of the sensitivity analysis are useful to an operator because they can use it to guide site characterization activities towards the most sensitive parameters. For example, the value of constraining the range of the sand fraction parameter can be explored. Figure 7 shows the pH plume and TDS plume size quartiles assuming that the sand permeability is constrained to the range for the IBDP site, and the remaining hydraulic

parameters are also constrained to a narrow upper range. Specifically, the sand fraction is constrained to 0.595–0.650, the X-direction correlation length to 2250–2500 m, the Z-direction correlation length to 22.5–25.0 m, and the clay permeability to 10^{-18} – 10^{-15} m^2. The difference between the 25th percentile and 75thpercentile pH and TDS plume sizes shown in Fig. 7 are smaller than in Fig. 5 where the other hydraulic parameters are unconstrained. This indicates that reducing uncertainty in the hydraulic parameters reduces uncertainty in the potential volume of aquifer impacted by a certain size of brine or CO_2 leak.

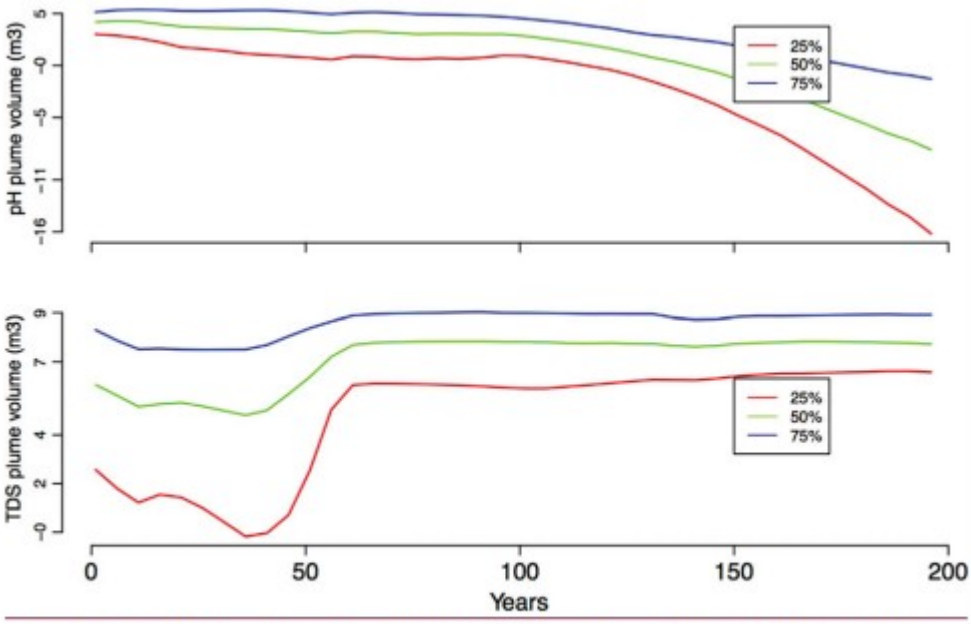

Figure 7. Quartiles for volume of aquifer below pH and above TDS impact thresholds by year with all hydraulic parameters constrained.

As shown in Table 8, some non-adjustable parameters, such as the initial pH and TDS and the pH no-impact threshold, are significantly different for the ROM than for the observations at the IBDP site. The reduced order model might be made more applicable to a wider range of sites if the initial conditions and no-impact threshold values were adjustable parameters, although the sensitivity of the risk predictions to these parameters remains to be investigated.

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