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Publication Date

2016-09-01

DOI

10.1016/j.ijggc.2016.06.015

Peer reviewed

The National Risk Assessment Partnership's integrated assessment model for carbon storage: A tool to support decision making amidst uncertainty

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Highlights

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We provide an overview of NRAP's Integrated Assessment Model (NRAP-IAM-CS) for quantification of risks at geologic CO₂ storage sites.

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Integrated assessment modeling approach can be effective in predicting long-term performance of an entire geologic CO₂ storage system.

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NRAP-IAM-CS can be used to compute risk profiles as well as help inform decision making process.

-

NRAP-IAM-CS can be used to perform multi-variate analysis taking into consideration uncertain variables in geologic CO₂ storage system.

Abstract

The US DOE-funded National Risk Assessment Partnership (NRAP) has developed an integrated assessment model (NRAP-IAM-CS) that can be used to simulate carbon dioxide (CO₂) injection, migration, and associated impacts at a geologic carbon storage site. The model, NRAP-IAM-CS, incorporates a system-modeling-based approach while taking into account the full subsurface system from the storage reservoir to groundwater aquifers and the atmosphere. The approach utilizes reduced order models (ROMs) that allow fast computations of entire system performance even for periods of hundreds to thousands of years. The ROMs are run in Monte Carlo mode allowing estimation of uncertainties of the entire system without requiring long computational times. The NRAP-IAM-CS incorporates ROMs that realistically represent several key processes and properties of storage reservoirs, wells, seals, and groundwater aquifers. Results from the NRAP-IAM-CS model are used to quantify risk profiles for selected parameter

distributions of reservoir properties, seal properties, numbers of wells, well properties, thief zones, and groundwater aquifer properties. A series of examples is used to illustrate how the risk under different storage conditions evolves over time, both during injection, in the near-term post injection period, and over the long term. It is also shown how results from NRAP-IAM-CS can be used to investigate the importance of different parameters on risk of leakage and risk of groundwater contamination under different storage conditions.

Keywords

Risk assessment

Risk quantification

CO₂ sequestration

Risk profiles

Integrated assessment model

Reduced order models

NRAP

1. Introduction

The fundamental premise of Geologic Carbon Sequestration (GCS) as a climate-change mitigation strategy is that captured CO₂ can be injected into and contained within geologic structures ([IPCC, 2005](#)).

Potential for leakage of CO₂ and brine due to CO₂ injection is a primary concern to multiple stakeholders. Concern for environmental impacts is largely focused on potential contamination of potable groundwater, either by the injected CO₂ or by displaced brine migrating through any potential man-made or natural leakage pathways ([IPCC, 2005](#)).

The United States Environmental Protection Agency (US-EPA) has primary responsibility for protecting underground sources of drinking water (USDW) within the US under the Safe Drinking Water Act and regulates subsurface fluid injection under the Underground Injection Control (UIC) program. The US-EPA has established a new class of wells (Class VI) expressly for regulating GCS-related injections ([US EPA, 2008](#)).

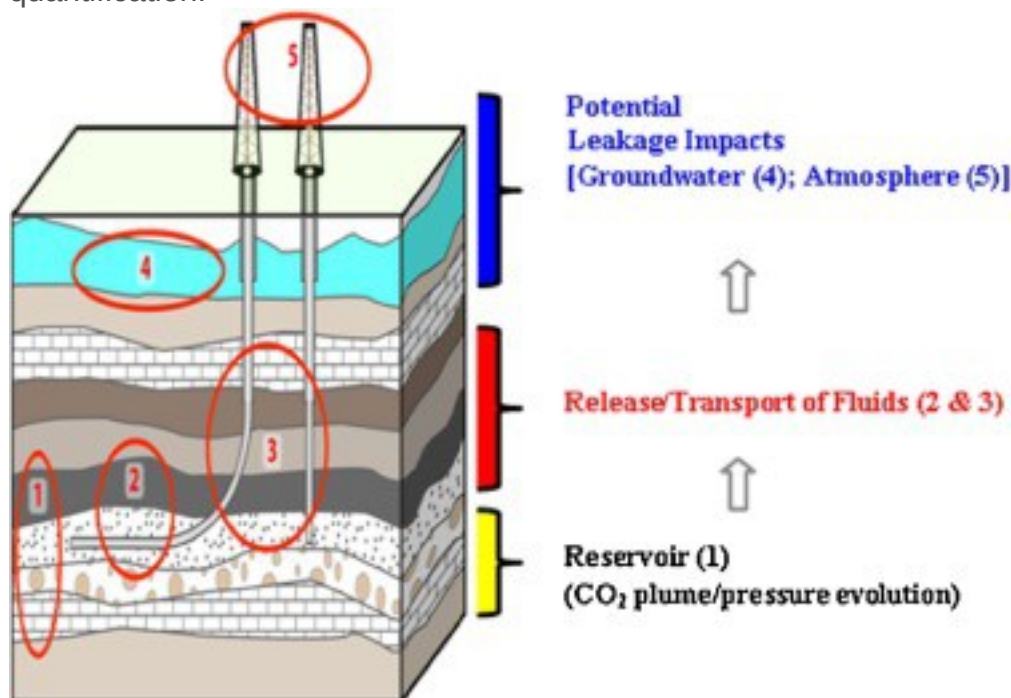
Favorable locations for GCS sites will have one or more layers of low-permeability caprocks (typically shale) which provide a natural barrier to diminish the likelihood of surface leakage of CO₂ (leakage to the atmosphere) and leakage of both CO₂ and displaced brine into groundwater resources. Typically the candidate GCS reservoirs will be deep, making the likelihood of surface leakage of CO₂ through natural flow pathways (faults/fractures) very low. In contrast, improperly sealed wellbores have a greater

likelihood to be leakage pathways for migration of CO₂ and brine ([Gasda et al., 2004](#)) and have been the focus of extensive studies. A secondary requirement of GCS is that the environmental impacts of injecting CO₂ are small enough to be within approved permit conditions. From the perspective of USDW quality, leakage of CO₂ and brine can potentially change groundwater quality to levels that may violate drinking water standards ([Keating et al., 2012](#), [Zheng et al., 2012](#)). A third concern about GCS is the potential of large-scale injection to cause pressure rise in reservoirs ([Birkholzer et al., 2015](#)), resulting in induced seismicity that is a public nuisance and potentially a safety hazard through effects on buildings and structures ([Pawar et al., 2015](#), [White and Foxall, 2014](#), [Mazzoldi et al., 2012](#)).

In some states within the United States, regulation of subsurface fluid injection is carried out by the state regulatory agency in which case the state has characterization, well-construction, and monitoring requirements that may or may not be the same as the US-EPA's. California, for example, is currently developing policy and procedures for GCS monitoring, verification, and accounting that will be consistent with the needs of its cap and trade rule, and serve the dual purpose of understanding environmental performance and awarding appropriate monetary value for stored CO₂. Operators of GCS sites have all of the usual concerns attending any industrial operation, e.g., about worker safety (mostly from surface operations) and impacts to nearby neighbors, as well as concerns about short- and long-term liability of the injected CO₂ after the injection operation is completed. Finally, large-scale surface leakage of CO₂ would represent a profound failure of GCS through the wasted energy and capital spent on capture, compression, and transportation of CO₂ to the GCS site. As for brine leakage, the public faces loss or diminished quality of its precious groundwater resources, which are becoming increasingly more valuable as population expands into areas reliant on groundwater for drinking and agriculture.

Quantifying risks to build stakeholder confidence in GCS and informing risk management and mitigation decision-making requires credible predictions of long-term performance of the entire CO₂ storage site. Gaining confidence that assessed risks are acceptable and manageable requires that the long-term performance predictions use a sound scientific basis that takes into account the underlying physical and chemical interactions. Development of science-based predictive tools for GCS risk assessment is challenging given the scale and complexity of those sites. An individual storage site may have a footprint on the order of hundreds of km² ([Birkholzer et al., 2009](#)) such that, considering the response of the entire CO₂ storage system (from sequestration reservoir to potential receptors; [Fig. 1](#)) could represent volumes on the order of 10³ km³, or

greater. Considering that these simulations need to address coupled hydrological, thermal and chemical processes at multiple length scales, it becomes clear that developing a single computational model to predict field-scale behavior of a complex engineered natural system is quite challenging. The approach of fully coupling complex models involves significant computational cost. Meanwhile, uncertainty in subsurface systems demands that a large number (often many thousands) of realizations of the systems be modeled to bracket and quantify the uncertainty associated with impacts, likelihoods, and therefore risk. Both of these issues point to the need for models that bring together different key processes and are computationally fast for uncertainty quantification.



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Fig. 1. Schematic diagram of various parts of the coupled engineered geologic CO₂ storage system that need to be considered for risk assessment and management, including storage reservoir, caprock, sealing layer, wells, overlying groundwater formations, and the near-surface atmosphere.

In recent years multiple approaches have been proposed for predicting long-term performance of GCS systems. [Viswanathan et al. \(2008\)](#), [LeNeveu \(2008\)](#), and [Meyer et al. \(2009\)](#) have applied system-modeling approaches to compute leakage through wellbores. [Celia et al. \(2011\)](#) demonstrated application of a semi-analytical approach to compute risk of CO₂ and brine leakage through multiple wells during the injection period.

This approach combines a set of semi-analytical and analytical solutions developed for CO₂ injection and leakage along abandoned wells ([Nordbotten et al., 2005](#), [Celia and Nordbotten, 2009](#)). Finally, models for entire GCS systems based on system-modeling approaches have been developed, including, CO₂-PENS by [Stauffer et al. \(2009\)](#), Certification Framework by [Oldenburg et al. \(2009\)](#), QPAC-CO₂ by [Metcalf et al. \(2013\)](#), and a system model developed by [Zhang et al. \(2007\)](#).

System-modeling approaches have been applied extensively for quantitative environmental risk assessment for a range of subsurface energy applications. This approach treats the overall site as a group of coupled subsystems, each of which embodies a unique set of physical and chemical characteristics and processes. This approach assumes that the subsystems can be treated without implicit coupling (i.e., they can be treated independently, addressing subsystem coupling explicitly by an integrated model). Such models are analogous to predicting the behavior of a multi-component system (e.g., an industrial facility) by independently predicting the behavior of individual components that are linked via an engineering system model. For predicting their performance, GCS sites can be broken into the following subsystems as illustrated in [Fig. 1](#): storage reservoir; potential release pathways such as wellbores; and potential receptors (or impact categories).

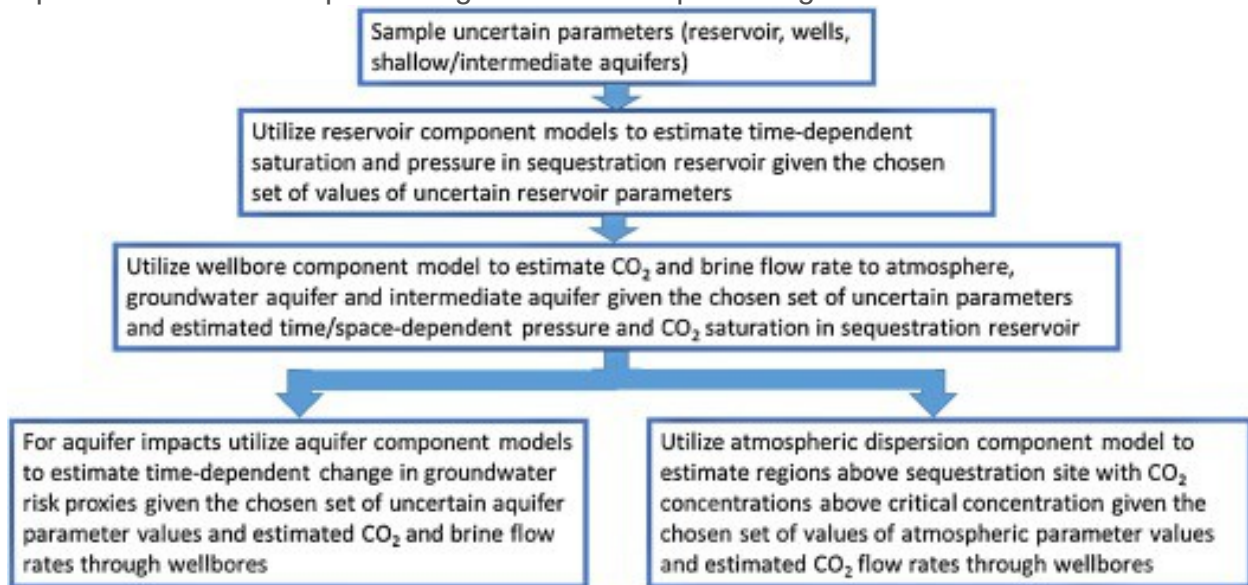
In order to quantitatively assess risks related to CO₂ and brine leakage, as well as induced seismicity, the U.S. Department of Energy (US-DOE) has been funding a project aimed at developing tools and approaches that can be used to inform decisions related to long-term GCS risks. This project, called the National Risk Assessment Partnership (NRAP), is a collaborative effort by five National Laboratories (Lawrence Berkeley, LBNL; Lawrence Livermore, LLNL; Los Alamos, LANL; National Energy Technology Laboratory, NETL and Pacific Northwest, PNNL). Research teams from each National Laboratory are building on decades of experience with subsurface systems (e.g., geothermal systems, nuclear waste disposal, hydrocarbon production) and harnessing National Laboratory computational power to build robust tools to help stakeholders address key questions about the long term performance of GCS sites, taking into account system complexities and uncertainties.

The model used in NRAP to quantify leakage risk is an Integrated Assessment Model (IAM) based on the system modeling approach. The purpose of this article is to describe the IAM developed by NRAP which we call the NRAP-IAM-CS for GCS site performance predictions, and to demonstrate how it can be used to quantify leakage risks, including leakage of CO₂ and brine to the atmosphere and groundwater, through multiple examples. The paper also demonstrates how NRAP-IAM-CS can be used to

inform various decisions related to site effectiveness and site operations. A description of NRAP-IAM-CS is provided and four examples are detailed to demonstrate the model's application and utility.

2. Integrated assessment model (NRAP-IAM-CS)

IAMs are mechanistic computational models of processes that occur within and among various components of a complex system; in the context of GCS, that system is composed of the CO₂ injector, storage reservoir, active or plugged and abandoned wells, USDW, atmosphere and any permeable formations that may lie between the USDW and sequestration reservoir. IAMs model the couplings of processes from the point of injection through to the arrival of leaking CO₂ or brine into USDW or the atmosphere. Within the NRAP-IAM-CS, the system components are connected in a manner to represent the various inter-component connectivity and interactions at a CO₂ storage site. For example, the component model for the sequestration reservoir is connected to the component model for a wellbore and the component model for the wellbore is connected to that for the shallow aquifer and so on. The inter-component connections are used to capture the CO₂ and/or brine movement between model components. [Fig. 2](#) shows how various component models are used while simulating leakage scenarios which include injection of CO₂ in the reservoir, CO₂ and brine leakage through wellbores and subsequent migration to the atmosphere or to a groundwater aquifer which leads to potential geochemical impacts to groundwater.



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Fig. 2. A schematic diagram depicting how various component models of the NRAP-IAM-CS are linked to simulate performance of the coupled GCS system.

While this approach is effective in efficiently simulating a complex system, it assumes that the coupling between different component models is one-way and forward moving. This does limit accounting for any feedback that may exist between two components.

To calculate the impact or consequences part of the risk equation, NRAP uses what are referred to as risk proxies to avoid unnecessary ambiguity and complexity in risk assessment. For example, instead of modeling and calculating an exposure of humans to and health impacts from groundwater contaminated with a heavy metal such as lead that arose either from dissolution of natural minerals in the groundwater aquifer due to carbonic acid produced by leaked CO₂ or due to transport by leaked brine, NRAP models only the geochemical changes in the groundwater or flow rate of CO₂ entering the aquifer. In this case, this CO₂ leakage into aquifer is a proxy for the eventual dissolution of minerals containing lead, and potential consumption by humans. The advantage of the risk-proxy approach is that the NRAP team can select an objective and relatively easily modeled quantity relative to an end-point human-exposure quantity, the modeling of which would bring up issues of human characteristics and behavior (e.g., body weight, amount of groundwater consumed, etc.). The leakage risk proxies currently used by NRAP are as follows: (1) pH in the shallow aquifer (a direct function of dissolved CO₂ concentration) as proxy for amount of dissolved CO₂ in groundwater; (2) TDS in the shallow aquifer (a direct function of brine and CO₂ concentration) as proxy for salinization of groundwater; (3) Concentration of heavy metals in the shallow aquifer including Arsenic (As), Lead (Pb), Cadmium (Cd) and Barium (Ba) as proxy for contamination by mineral dissolution; (4) Concentration of organics in the shallow aquifer including Naphthalene, Benzene, and Phenol as proxy for mobilization and/or intrusion of brines from deeper formations; and (5) Flow rate of CO₂ into the atmosphere through a leakage pathway such as a leaky well as a proxy for storage effectiveness and surface leakage hazard. NRAP is also considering induced seismicity risk, measured by proxy calculations of ground motion. In this paper we focus on CO₂ and brine leakage risk for groundwater resources.

NRAP's IAM is built on the CO₂-PENS model structure ([Stauffer et al., 2009](#)) which was developed with the GoldSim® software package ([GoldSim Technology Group, 2014](#)). GoldSim® is a commercially available system-modeling package tailored for the unique needs of engineered geologic systems, particularly those with large uncertainties and heterogeneities. Various approaches can be used to build and implement models for

system components that can be integrated using GoldSim®, including mathematical expressions, look-up tables, and dynamic link libraries for external executables including process-level models such as reservoir simulators. Goldsim® also provides a convenient framework to control time-stepping and sampling of uncertain variables in Monte Carlo-type stochastic modeling applications, and incorporates functionality for uncertainty quantification.

2.1. NRAP-IAM-CS component models

The central part of the NRAP-IAM-CS comprises the component models for the various sub-systems that make up a sequestration system. The component models are intended to capture the physical and chemical interactions that take place as a result of CO₂ injection or migration within each individual component. To meet both the requirements of modeling coupled processes and carrying out possibly thousands of realizations to quantify the effect of uncertainty in the system and input parameters, NRAP is developing and using Reduced Order Models (ROMs) which are approximations of high-fidelity, complex models but with much less computational cost. ROMs are required to capture the essential behavior of the system while being much more computationally efficient. Various approaches can be used to develop component ROMs ranging from functions built using complex numerical simulations ([Sun et al., 2013](#), [Keating et al., 2016](#), [Harp et al., 2016](#), [Hou et al., 2014](#), [Wainwright et al., 2013](#), [Carroll et al., 2014](#), [Zhang et al., 2016a](#)) to direct incorporation of numerical simulation results as look-up tables. The component models implemented within NRAP-IAM-CS are summarized in [Table 1](#) and the details are provided below.

Table 1. Component ROMs used in the NRAP-IAM-CS.

Component	ROM Methodology	Uncertain Parameters	References
Reservoir	ROM integrating vertically integrated analytical model for saturation and statistical correlation based on complex MC simulations for pressure	Reservoir Porosity, Reservoir Permeability, Depth, Reservoir Thickness, Injection Rate	Nordbotten et al., 2005 (only for saturation ROM)
	Look-up Tables of reservoir simulation results	Reservoir Porosity, Reservoir Permeability, Caprock Permeability	Wainwright et al., 2013
Wellbore	Cemented Wells: MARS Response Surface	Cement Permeability, Reservoir Pressure, Reservoir Saturation, Depth, Intermediate Aquifer Depth	Harp et al., 2016
	Open Wells: Look-up Tables	Reservoir Pressure, Reservoir Saturation, Depth	Pan and Oldenburg, 2014

Component	ROM Methodology	Uncertain Parameters	References
Groundwater Aquifer	Unconfined Carbonate: MARS Response Surface with linking function	Aquifer Thickness, Aquifer Permeability, Aquifer Porosity, Background Flow, Sequestration Reservoir Brine Molality, Calcite surface area, Decay constants for organics (Benzene, Phenol, Napthalene), Partition coefficient (kd) for organics.	Keating et al., 2016
	Confined Alluvium: MARS Response Surface with linking function	Aquifer Thickness, Aquifer Permeability, Aquifer Porosity, Background Flow, Sequestration Reservoir Brine Molality, Calcite surface area, Decay constants for organics (Benzene, Phenol, Napthalene), Partition coefficient (kd) for organics.	Carroll et al., 2014

2.1.1.1. CO₂ storage reservoir

The component model for the storage reservoir is used to predict dynamic reservoir pressure and saturation as a result of CO₂ injection. Various approaches can be used to predict the pressures and saturations in the reservoir, including analytical or semi-analytical models, ROMs developed using complex reservoir simulations, directly importing results of reservoir simulations, or directly linking reservoir simulators. Each of these approaches has advantages and disadvantages. Directly linking a reservoir simulator provides the best fidelity to complex reservoir simulations but this approach can be computationally demanding if it is used to perform Monte-Carlo studies with multiple realizations. The analytical/semi-analytical or ROMs are computationally efficient but have lower fidelity compared to the approach of directly linking reservoir simulators. Directly importing results of reservoir simulations as look-up tables has the dual advantage of being computationally efficient and maintaining the fidelity of reservoir simulations.

Currently, the NRAP-IAM-CS uses two different approaches for reservoir component models, (1) a look-up table approach for site-specific applications, and (2) a ROM approach for generic reservoirs with homogeneous properties. In the look-up table approach, predictions of site-specific reservoir simulations (reservoir pressures and saturations) at multiple time-steps can be read in and stored as look-up tables. These look-up tables are interpolated to calculate pressures and saturations at any location of interest in the reservoir at any time of interest during NRAP-IAM-CS simulations. This approach can take advantage of site-specific reservoir simulations that include one or multiple simulation runs. In Section 3, an example application of the lookup-table

approach is demonstrated using TOUGH2 reservoir simulation results for a site in California. The ROM approach implemented in the NRAP-IAM-CS combines a ROM to predict dynamic reservoir pressure and an analytical model developed by [Nordbotten et al. \(2005\)](#) to predict CO₂ saturation. The ROM to predict pressure was developed using results of Monte-Carlo (MC) simulations of CO₂ injection in a reservoir and resulting pressure changes with LANL's FEHM multi-phase reservoir simulator. The reservoir simulations were performed for the injection period as well as a post-injection period during which reservoir pressure could dissipate. The MC simulations were performed by varying a number of uncertain parameters ([Table 1](#)). Statistical correlations were developed for time- and space-dependent reservoir pressure as a function of variable parameters using dimensional analysis approach. The analytical model used for predicting time- and space-dependent CO₂ saturation was based on the model for time-dependent CO₂ plume radius developed by [Nordbotten et al. \(2005\)](#). One of the limitations of the Nordbotten et al. model is that it is applicable only during the injection period. In order to predict the CO₂ plume evolution during the post-injection period we use an approach that computes CO₂ plume velocity based on the Darcy velocity calculated with the ROM for pressure. This combined ROM for predicting reservoir behavior can be applied to any generic reservoir where site-specific data for reservoir properties are available.

2.1.2. Wellbores

The component model for wellbore is used to calculate the CO₂ and brine flow rates through cemented as well as open wellbores that penetrate through the primary seal and into the storage reservoir. Calculated flow rates are dependent on driving forces such as pressure increase and saturation at the reservoir-wellbore intersection as well as effective wellbore permeability for the cemented wellbores. For cemented wellbores a ROM in the form of a response surface is used to predict CO₂ and brine flow rates ([Harp et al., 2016](#)) while in the case of open wellbores flow rates are predicted using a multi-dimensional look-up table approach. Each of the models was developed independently. The cemented wellbore ROM was developed using numerical simulations of CO₂ injection and subsequent migration of CO₂ and brine using a model that included a sequestration reservoir and a wellbore that extended from the sequestration reservoir to the ground surface as well as to two intermediate aquifers, one of which represented a shallow groundwater aquifer, between the sequestration reservoir and the ground surface. Approximately 1500 simulations were performed varying multiple parameters ([Table 1](#)). The predicted CO₂ and brine leakage rates into

the intermediate aquifer, shallow groundwater aquifer, and atmosphere were used in the statistical analysis software R ([Venables et al., 2015](#)) to generate higher resolution response surfaces using a MARS (Multi-variate Adaptive Regression Spline) fitting scheme. For open wellbores, numerical simulations of CO₂ leakage through open wellbores were performed using the drift-flux model implemented in LBNL's T2Well simulator ([Pan and Oldenburg, 2014](#), [Hu et al., 2012](#)). Over 500 simulation runs were performed by varying wellbore-reservoir intersection pressure, saturation and wellbore depth. The simulated CO₂ and brine leakage rates from these runs were converted into a three-dimensional look-up table. It should be noted that both the FEHM and T2Well simulations took into account the complexities of CO₂ phase change during leakage from deeper reservoirs (where CO₂ typically exists in super-critical state) to shallow aquifer or atmosphere (where CO₂ typically exists in gaseous state).

2.1.3. Shallow aquifers

The component model for groundwater is used to predict changes in groundwater chemical composition due to CO₂ and brine leakage and subsequent aqueous geochemical interactions. As mentioned earlier, NRAP uses multiple risk proxies for assessing impacts to groundwater including pH, TDS, concentrations of heavy metals (Pb, As, Cd, Ba) and concentrations of organics (Naphthalene, Benzene, Phenol). The groundwater model uses ROMs to predict the time-dependent volume of the aquifer where values of the above mentioned risk proxies exceed certain thresholds. The cutoffs are, pH < 6.5, TDS and concentrations above MCL (Maximum Contaminant Level) or no impact thresholds ([Last et al., 2013](#)). Two separate sets of ROMs are currently implemented, one for mineralogy representative of a confined alluvium aquifer and the second for that of an unconfined carbonate aquifer. The confined alluvium aquifer ROMs were developed using the High Plains Aquifer as a proxy ([Carroll et al., 2014](#)) while the ones for carbonate aquifer were developed using the Edwards Aquifer as a proxy ([Bacon et al., 2016](#), [Keating et al., 2016](#)). The ROMs were developed to account for hydrologic as well as geochemical processes and used a linking function approach to effectively combine them ([Bianchi et al., 2016](#)). Both set of ROMs have the form of a multi-dimensional response surface and are functions of multiple uncertain parameters ([Table 1](#)), including, hydraulic parameters and geochemical parameters. Similar to the wellbore ROMs, the aquifer ROMs were developed using Monte-Carlo computations of numerical reservoir simulations of CO₂ and brine leakage and subsequent flow and geochemical interactions.

2.1.4. Atmospheric dispersion

The atmospheric dispersion ROM is used to predict regions where CO₂ concentrations are above a critical concentration level in the immediate region above the leakage source ([Zhang et al., 2016b](#)). The ROM is an adaptation of the empirical correlations developed by [Britter and McQuaid \(1988\)](#) who distilled field trials of dispersion of dense gases into a nomograph. The Britter and McQuaid (B&M) approach uses general correlations developed from careful measurements in field experiments and consolidates the model input into dimensionless groups based on the gas of interest and the fundamental gas flow equations. The method is simple and does not include time-dependent or dynamic aspects, but it produces results that agree well with steady-state simulations of plume extent and concentration variations based on rigorous flow and dispersion equations ([Zhang et al., 2016b](#)). The Britter and McQuaid method was developed for single source ground-level releases of dense gas, either instantaneous or continuous, but it has been adapted to handle multiple-source releases (such as leakage from multiple wellbores) for the NRAP-IAM-CS.

2.2. Accounting for site parameter uncertainties

One of the challenges in predicting long-term behavior of subsurface reservoirs is that there is limited knowledge of subsurface characteristics and conditions which leads to uncertainties in predictions. For greenfield saline reservoirs (i.e., those that have not been exploited for oil and gas) characterization data may not be as extensive as for oil and gas reservoirs or saline aquifers that contain them. Effective risk assessment and site management decision making requires employment of approaches that take into account parameter uncertainties and their overall impact ([Pawar et al., 2015](#)). To account for uncertainties and understand their impacts, both short-term and long-term site performance predictions should be made by sampling the probable range of values of uncertain parameters.

NRAP-IAM-CS is developed such that key uncertain parameters can be specified as distributions or as single deterministic values. These parameters primarily include hydrologic and geochemical parameters specific to different parts of the overall system. The uncertain parameters included in the current version of the NRAP-IAM-CS are limited to those that were used to develop the component models and the inputs to the ROMs within them. For example, the ROM for the groundwater aquifer has multiple uncertain parameters including, hydrologic parameters such as permeability, thickness, hydraulic gradient, and geochemical parameters such as calcite surface area, decay constants for organics (Benzene, Phenol, Napthalene), and partition coefficient (kd) for organics.

One of the most uncertain parameters in estimating wellbore leakage risks is effective wellbore permeability ([Carey, 2013](#)). There are very few direct measurements of wellbore cement permeability. [Carey \(2013\)](#) demonstrates NRAP's approach to develop distributions of effective wellbore permeability that were inferred from field data on sustained casing pressure or vent flow. These distributions have been incorporated in the NRAP-IAM-CS and can be used as analogs where direct observations do not exist. Additionally, the user can also specify wellbore permeability either as distributions or single values based on observations or expert elicitation.

2.3. NRAP-IAM-CS computations

NRAP-IAM-CS can be used to perform stochastic MC simulation while sampling the user-specified uncertain parameters. The parameter values are sampled using a Latin Hypercube Sampling (LHS) approach. During sampling, each parameter's probability distribution is divided into as many strata as the number of realizations and the parameter value is picked for each realization from each stratum randomly. This approach is built into GoldSim and ensures that a uniform spanning sampling is achieved. Multiple quantities are computed during an NRAP-IAM-CS simulation, including, time-dependent leakage rates of CO₂ and brine through wellbores into intermediate aquifers, groundwater, and to the atmosphere as well as time-dependent volumes of aquifer with pH < 6.5, TDS and concentrations of heavy metals (As, Pb, Cd, Ba), and organics (Naphthalene, Benzene, Phenol) above MCLs or background threshold values. These outputs can be used to quantify overall risks, to aid the decision-making process related to site operations and site effectiveness, and to show the evolution of those risks through time given system uncertainty (risk profiles, or probabilistic plots of risk proxies as a function of time).

3. Examples of NRAP-IAM-CS applications

In this section we demonstrate applicability of the NRAP-IAM-CS through multiple illustrative examples. The NRAP-IAM-CS can be used to simulate long-term performance of any CO₂ storage site and explore a wide range of leakage scenarios with the primary focus being leakage through wellbores. The example applications below demonstrate how NRAP-IAM-CS-computed results can be used to quantify environmental risk profiles (using risk proxies) as well as to inform decisions related to operation and long-term management of a storage site. [Table 2](#) summarizes the examples including the scenario and computed results.

Table 2. Examples of scenarios and corresponding MC simulations.

Example	Section	Scenario/Set-up	Computed Results
Quantification of risk profile of atmospheric CO₂ leakage	3.1	Scenario: Direct leakage of CO ₂ from storage reservoir to atmosphere through cemented wellbores	Time-dependent CO ₂ leak rate to the atmosphere
		Set-up: Monte-Carlo simulation with 1000 realizations,	
Assess impact of legacy well and site operations on containment goals during injection stage	3.2	a) 200 years total simulation time (50 years injection followed by 150 years post-injection).	Time-dependent CO ₂ leak rate to the atmosphere
		b) 1000 years total simulation time (50 years injection followed by 950 years post-injection).	
Assess impact of CO₂ and/or brine leakage on groundwater quality	3.3	IAM-Component Models: Reservoir (Lookup Table Approach), Cemented Wellbore ROM	CO ₂ leakage rate to atmosphere
		Uncertain Parameters: Reservoir porosity, Reservoir permeability, Residual CO ₂ saturation, Wellbore cement permeability, Wellbore location	
Assess impact of legacy well and site operations on containment goals during injection stage	3.2	Scenario: Direct leakage of CO ₂ from storage reservoir to atmosphere through a single wellbore	CO ₂ leakage rate to atmosphere
		Set-up: Simulation with one realization, 50 years total simulation time (50 years injection).	
Assess impact of CO₂ and/or brine leakage on groundwater quality	3.3	IAM-Component Models: Reservoir (ROM), Wellbore ROM	Volume of pH < 6.5 plume & TDS > MCL in groundwater aquifer
		Uncertain Parameters: Wellbore quality (open, cemented with variable cement quality), CO ₂ injection rate	
Assess impact of CO₂ and/or brine leakage on groundwater quality	3.3	Scenario: Leakage of CO ₂ and brine from storage reservoir to groundwater aquifer through cemented wellbores	Volume of pH < 6.5 plume & TDS > MCL in groundwater aquifer
		Set-up: Monte-Carlo simulation with 1000 realizations, 200 years total simulation time (50 years injection followed by 150 years post-injection).	
Assess impact of CO₂ and/or brine leakage on groundwater quality	3.3	IAM-Component Models: Reservoir (Lookup Table Approach), Cemented Wellbore ROM, Unconfined carbonate groundwater aquifer ROM	Volume of pH < 6.5 plume & TDS > MCL in groundwater aquifer

Example	Section	Scenario/Set-up	Computed Results
		Uncertain Parameters: Reservoir porosity, Reservoir permeability, Residual CO ₂ saturation, Wellbore cement permeability, Wellbore location, Groundwater aquifer thickness	

3.1. NRAP-IAM-CS application to quantification of risk profiles

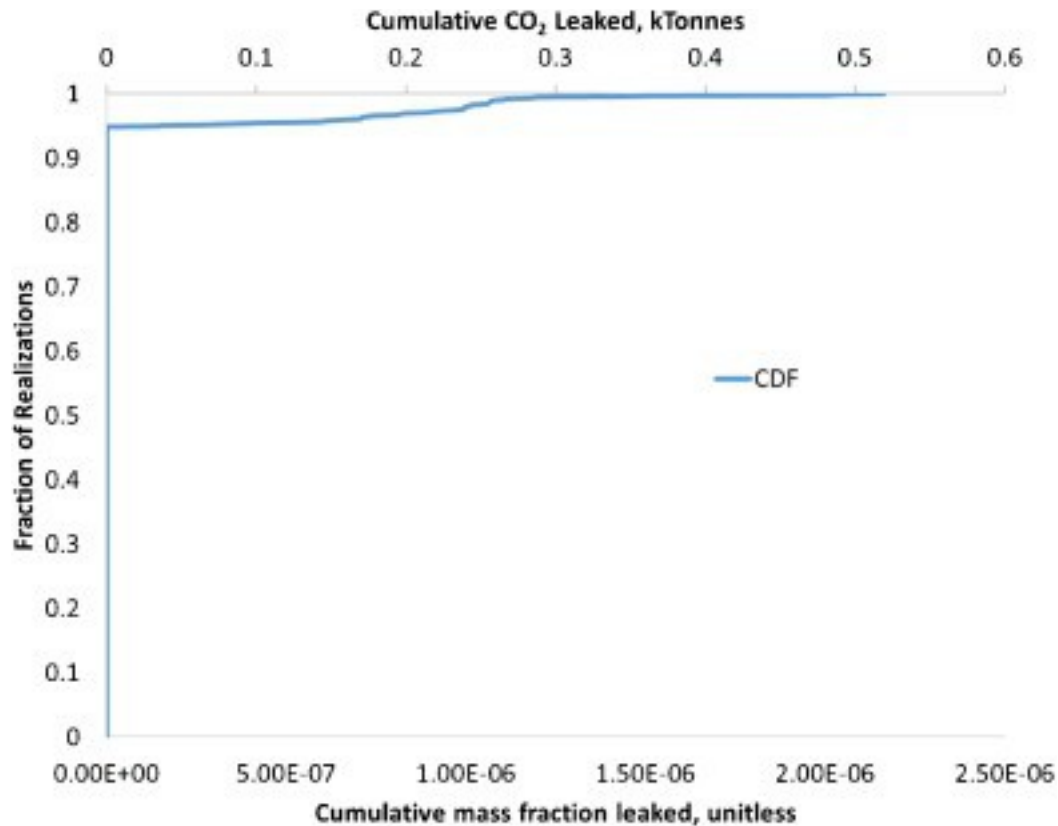
The concept of environmental risk profiles for GCS sites was introduced by [Benson \(2007\)](#) to demonstrate that environmental risks evolve with time. The risk profiles introduced by Benson were primarily qualitative in nature and have been used effectively to communicate time-dependence of risks expected by experts in the GCS community. Yet, over the past years it has become increasingly apparent that a number of stakeholders require quantitative assessment of risks to make decisions related to effectiveness and management of GCS sites ([Wilson et al., 2007](#)).

In the first example considered, the NRAP-IAM-CS is exercised to quantify risk profiles for atmospheric CO₂ release. We consider a scenario of CO₂ leakage to the atmosphere through a single cemented well at a hypothetical CO₂ storage site. We assume that the location and the effective permeability of the well are both uncertain. Our objective is to compute the likelihood that CO₂ leakage through the well directly to the atmosphere will exceed certain concentration cutoffs. We assume that there is no monitoring deployed and no mitigation applied to stop the leakage making it a very conservative risk calculation. During any actual field operation, if leakage is detected its impact will be evaluated and action will be taken if mitigation is deemed necessary, so this scenario represents an extreme case in which the leak cannot be detected and/or is not remediated. For this scenario a Monte Carlo (MC) simulation with 1000 realizations of the NRAP-IAM-CS was performed utilizing the reservoir and wellbore component models. For the reservoir we used the look-up table approach described in Section [2.1](#). Results of numerical simulations of industrial scale CO₂ injection at the Kimberlina reservoir in the San Joaquin Valley in Southern California were used to represent the storage reservoir and its response to CO₂ injection and long-term storage ([Wainwright et al., 2013](#)). We emphasize that this is a hypothetical scenario as there is no current CO₂ injection in progress or planned at the Kimberlina reservoir. Multiple simulations of large-scale CO₂ injection in the Kimberlina reservoir at 5 million tonnes/year for 50 years were performed using LBNL's TOUGH2 simulator. Each of the reservoir simulation runs was performed for 200 years which included a 150 year post-injection period. In all, 300 simulation runs were performed to capture the effect of variability in three reservoir

parameters including porosity and permeability of the target reservoir and permeability of caprock. Sensitivity analysis on these parameters was used to reduce the 300 runs to 54 representative runs that captured the effect of variability in the reservoir parameters. The time and space-dependent reservoir pressure and saturation results for these 54 runs were brought into the NRAP-IAM-CS as look-up tables. Each one of these 54 runs was associated with a representative reservoir permeability, reservoir porosity, and caprock permeability value, such that during the MC simulation of the NRAP-IAM-CS a specific reservoir simulation run could be selected based on a set of the values of uncertain reservoir parameters selected for the realization. As mentioned earlier, for this scenario it was assumed that there is one legacy well which penetrates the storage reservoir but its location and integrity are not known. In order to simulate the uncertainty in location of the wellbore, the location of the well was randomly varied from one MC simulation run to the next within a 12 km² area around the injection well. For effective wellbore permeability, one of the built-in distributions was used that has been inferred from the vent flow observations in wells in Alberta, Canada ([Carey, 2013](#)).

During each realization of the MC simulation, 200 years of total site performance was simulated which included 50 years of active CO₂ injection followed by 150 years of post-injection. The NRAP-IAM-CS-predicted direct CO₂ leakage to the atmosphere is considered in the following analysis.

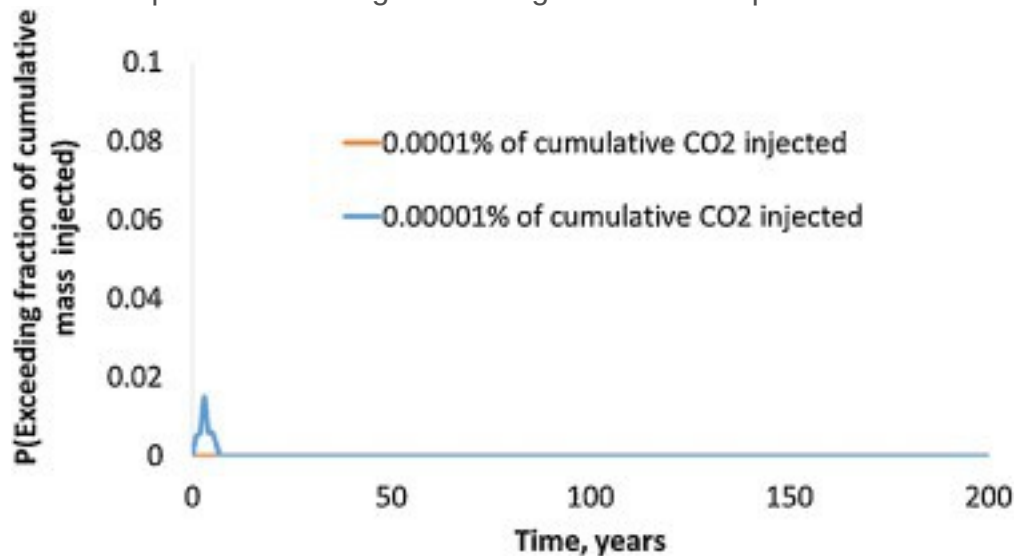
Results of the MC simulation ([Fig. 3](#)) show that few (only about 5%) of the calculated realizations exhibit non-zero leakage to the atmosphere over 200 years of performance. Of the subset of realizations with predicted leakage to the atmosphere, none showed cumulative fractions of the total mass leaked greater than 2.1×10^{-6} of the total 250 million tonnes of CO₂ injected (or about 50,000 tonnes of CO₂) over 200 years of total predicted performance.



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Fig. 3. Cumulative distribution function (CDF) of cumulative mass of CO₂ leaked in absolute and fractional terms to the atmosphere over 200 years of site performance. The time-dependent leakage rates from this 1000-realization MC simulation were also used to calculate risk profiles quantified as the probability of exceeding different selected thresholds for leakage rate (CO₂ leaked in each year divided by the cumulative CO₂ injected to that time). Probability in the NRAP-IAM-CS is the likelihood of exceeding a proxy threshold, e.g., number of times a risk proxy threshold is exceeded in a given year. Given that currently there are no regulations related to acceptable CO₂ leak rates, multiple hypothetical cutoffs were used for demonstration purposes. As shown in [Fig. 4](#), the computed risk profiles (for the simulated scenario for this hypothetical site) show that overall the probability of exceeding the hypothetical thresholds is negligible for all but the very smallest (nominally inconsequential) selected leakage thresholds. As mentioned earlier, we had assumed that no monitoring and leakage mitigation was applied during this scenario. In mitigation scenarios, the computed risk profiles will be different from those shown in [Fig. 4](#) depending on when the leak is detected and mitigation is deployed. Similar to computing the risk profiles for atmospheric CO₂ leakage

as demonstrated here NRAP-IAM-CS can also be used to compute risk profiles for other risk proxies including those for groundwater impacts.



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Fig. 4. Time-dependent risk profiles computed as the probability of annual mass leakage rate exceeding various cutoffs of fraction of cumulative mass of CO₂ injected – as calculated for a hypothetical scenario.

As mentioned earlier, one of the main advantages of using the system-modeling approach is uncertainty quantification and the ability to identify how uncertainty in various uncertain parameters drives the overall site performance uncertainties. This is a critical component of probabilistic risk assessment. The results of uncertainty quantification are used to identify approaches, including monitoring or additional characterization, through which the site performance uncertainty can be reduced. The NRAP-IAM-CS includes functionality to explore how uncertain parameters (independent variables that are treated stochastically in the IAM) impact system performance for key outputs. The NRAP-IAM-CS stochastic modeling framework (GoldSim®) incorporates functionality to calculate a series of metrics to characterize model uncertainty including correlation matrices (with or without assumed independence between input variables), regression coefficients, and an importance measure – a normalized value representing the fraction of the result variance that is explained by each variable – that is useful for identifying nonlinear, non-monotonic relationships between input variables and a result ([Saltelli and Tarantola, 2002](#)). The importance measure is a variance-based sensitivity measure.

We used results of the MC simulation to perform uncertainty quantification. For this purpose the output of interest is the predicted flow rate of CO₂ to the atmosphere, while the uncertain input parameters include permeability of the storage interval, porosity of the storage interval, permeability of the primary caprock, and weighted wellbore permeability. All of these variables are assumed to be uncorrelated. We use a weighted wellbore permeability value instead of directly using all the wellbore permeability values sampled during the MC run. The weighted wellbore permeability is a normalized composite parameter that takes into account the fraction of time that each well is in contact with the free-phase CO₂ plume and the effective permeability of the well. This approach ensures that proper weights are given to the effective wellbore permeability based on its exposure to CO₂ or lack of it. Results ([Table 3](#)) show that the single most important uncertain variable (the variable with the highest importance measure value) is the weighted wellbore permeability value. This indicates that, for the scenario considered, the well permeability and the time during which that well is contacted by free-phase CO₂, rather than attributes of the storage interval or primary seal, drive the predicted leakage response.

Table 3. Results of multi-variate analysis showing the influence of various uncertain parameters on CO₂ flow rate to the atmosphere.

Model Parameter	Importance Measure
Weighted wellbore effective permeability	0.457
Storage reservoir permeability	0.01
Storage reservoir porosity	0.001
Caprock permeability	0.002

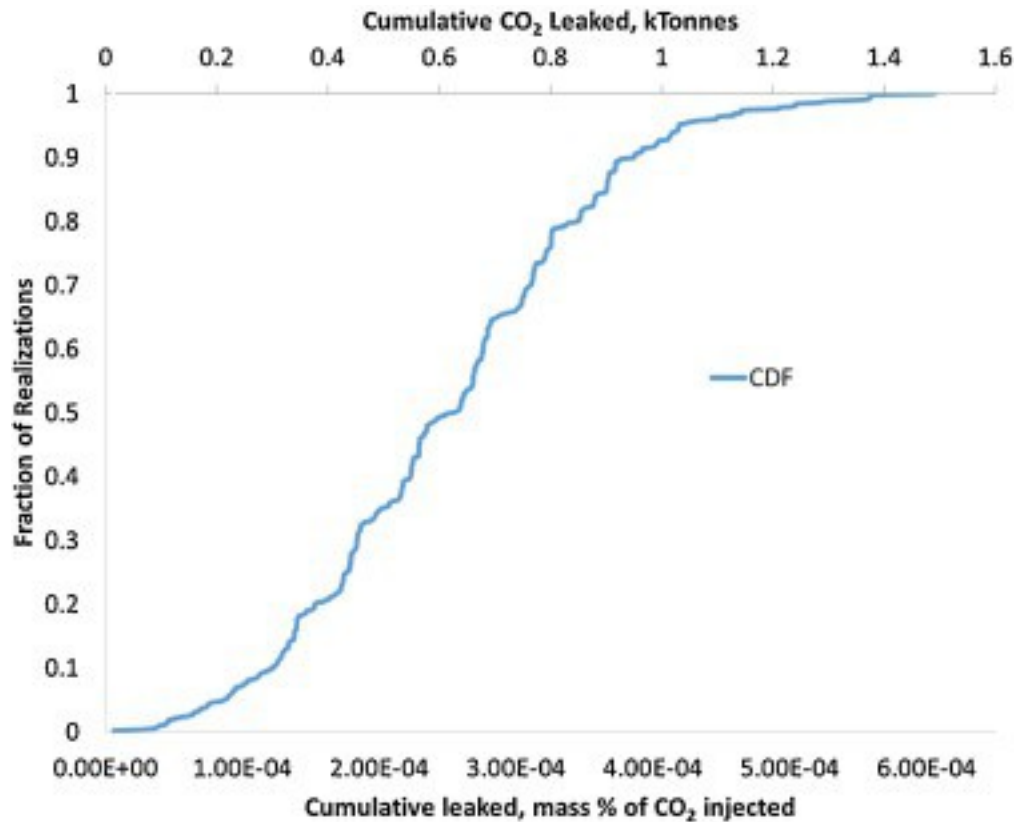
It should be noted that these reported observations are specific to the scenario and uncertain parameters considered in this example, and simulations for scenarios with different characteristics and underlying assumptions would be expected to result in different predicted performance. This example shows the value of considering uncertainty in key characteristics of realistic geologic storage scenarios, and using systems-level modeling to understand the likely performance of these complex engineered geologic systems in the context of that uncertainty.

3.1.1. Example NRAP-IAM-CS application to quantify risk profiles for leakage through multiple wellbores and effect of residual trapping on leakage

In this example we extend the NRAP-IAM-CS application to a scenario with added complexities compared to the previously discussed example. For this scenario three significant differences were incorporated: (1) rather than a single cemented well it was

assumed that there are multiple wells distributed at a spatial density of 10 wells/km² over the same 12 km² area around the CO₂ injection location; (2) a residual free phase CO₂ saturation of 0.2 was assumed in the storage reservoir, and (3) a longer simulation time of 1000 years (50 years of total injection followed by 950 years post-injection) compared to 200 years as in the previous scenario was considered. The first of these scenario choices represents a brownfield or depleted oil and gas reservoir setting where the CO₂ plume in the storage reservoir has the potential to contact multiple wells. The non-zero residual CO₂ saturation may reduce the significant fraction of the CO₂ contacting the wells as it is immobile and therefore unavailable to ultimately migrate out of the storage reservoir. The third scenario choice will extend the modeled site performance to include a considerably longer period of post-injection site care. We set up the NRAP-IAM-CS assuming the same Kimberlina-like reservoir scenario as mentioned in the previous example. Similarly, we also assumed that the wellbore permeability was unknown and used the same Alberta-type effective permeability distribution to assign them.

[Fig. 5](#) shows a cumulative distribution function for total CO₂ leakage to the atmosphere after 1000 years of total site-scale performance. This result shows that, for the scenarios considered, all of the realizations result in a small amount of CO₂ leakage to the atmosphere over 1000 years, but the maximum predicted leakage is only about $6 \times 10^{-4}\%$ of the total CO₂ injected (250 million tonnes). The distribution of total predicted leakage is of the same order of magnitude as the cumulative mass leaked after 200 years in the previous example. While the increased number of cemented wells may result in higher probability of the injected CO₂ plume contacting a well, it appears that the residual trapping in the storage reservoir may be limiting the CO₂ available for migration through the wellbores resulting in reduced total leakage.



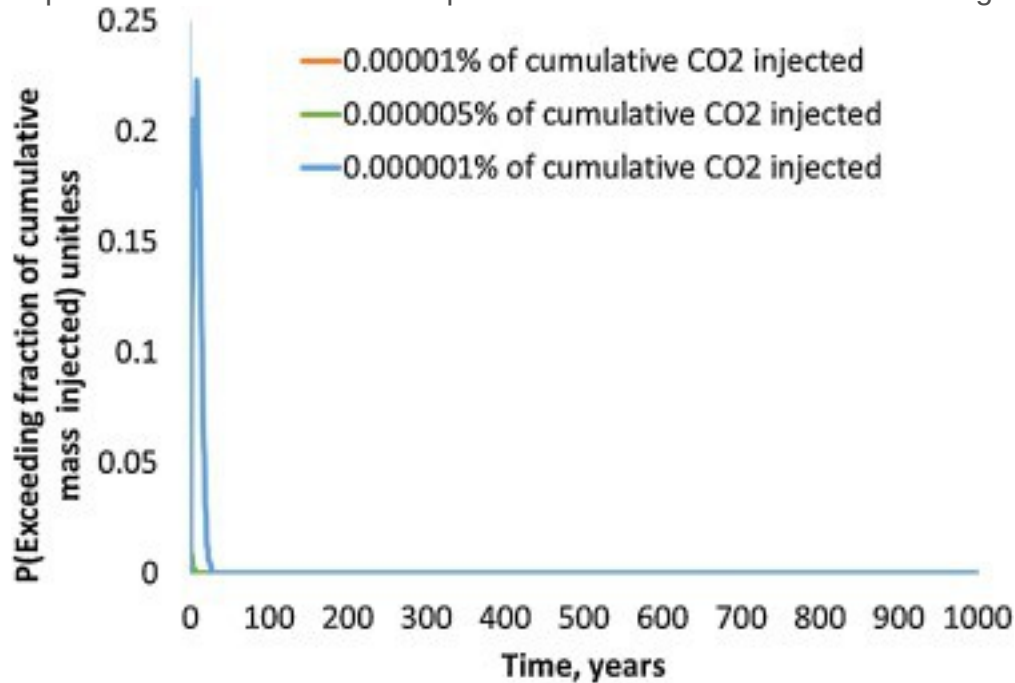
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Fig. 5. CDF of the cumulative mass of CO₂ leaked in absolute and fractional terms to the atmosphere over 1000 years of site performance for the scenario of multiple wells with effects of residual trapping.

As in the previous example, leakage-risk profiles were calculated for multiple cumulative leakage cutoffs (as mass percentages of cumulative stored CO₂ through each simulation year) and are plotted in [Fig. 6](#). Probabilities of exceeding leakage of $1 \times 10^{-5}\%$ (1×10^{-7} mass fraction) were zero for all simulation times and it was only by considering an even lower leakage threshold of $5 \times 10^{-6}\%$ that any exceedance was predicted.

These results are comparable to the ones shown in [Fig. 4](#) and illustrate the same temporal trend with probability of exceedance decreasing to zero. It should be noted that similar to the previous example, we assume a conservative scenario where there is no deployment of monitoring and mitigation technologies. Finally, as shown in [Table 4](#), the multi-variate uncertainty analysis showed similar trends relative to the previously-described scenario, with weighted wellbore effective permeability representing the most important uncertain parameter (most significantly affecting variance in the observed cumulative leakage). However, in this case, the storage reservoir permeability showed significantly higher importance than in the previous example. This is related to the

increased CO₂ saturation plume extent resulting from higher reservoir permeability, and exposure of more wells to that plume – which drives additional leakage.



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Fig. 6. Time-dependent risk profiles computed as the probability of annual mass leakage rate exceeding various cutoffs of fraction of cumulative mass of CO₂ injected, as calculated for a hypothetical scenario with multiple legacy wells at a CO₂ storage site.

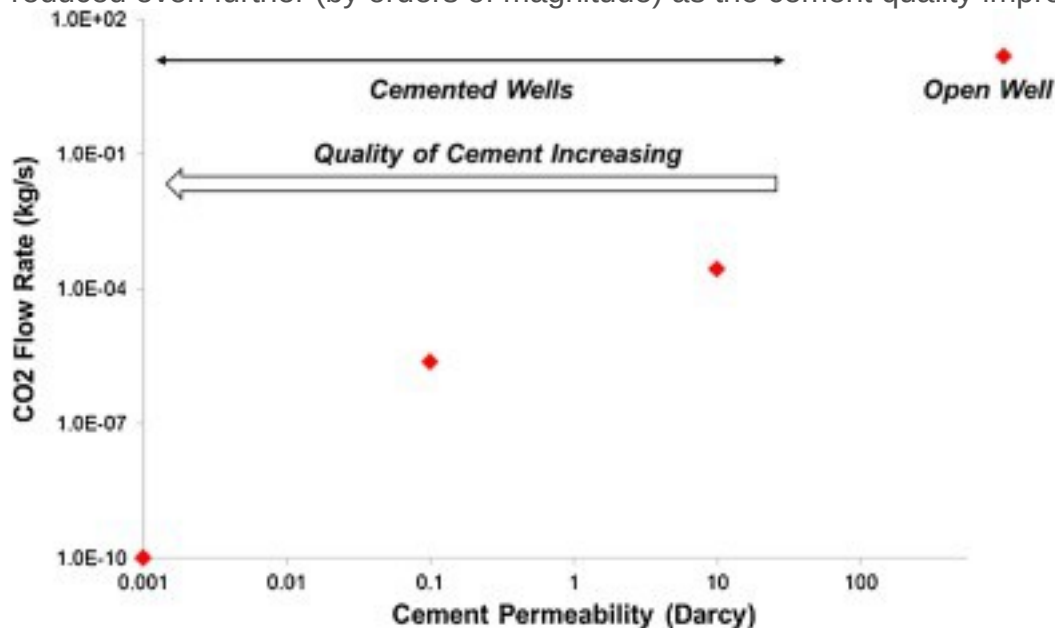
Table 4. Results of multi-variate analysis showing influence of various uncertain parameters on CO₂ flow rate to the atmosphere for a scenario with multiple wells in the presence of residual trapping.

Model Parameter	Importance Measure
Weighted wellbore effective permeability	0.578
Storage reservoir permeability	0.136
Storage reservoir porosity	0.016
Caprock permeability	0.006

In addition to quantifying risk profiles as demonstrated in the previous two examples, the NRAP-IAM-CS can also be used to inform various decisions related to storage site operations and performance taking into account underlying uncertainty as demonstrated by the following two examples.

3.2. Example NRAP-IAM-CS application to characterize impact of legacy well and site operations on containment goals

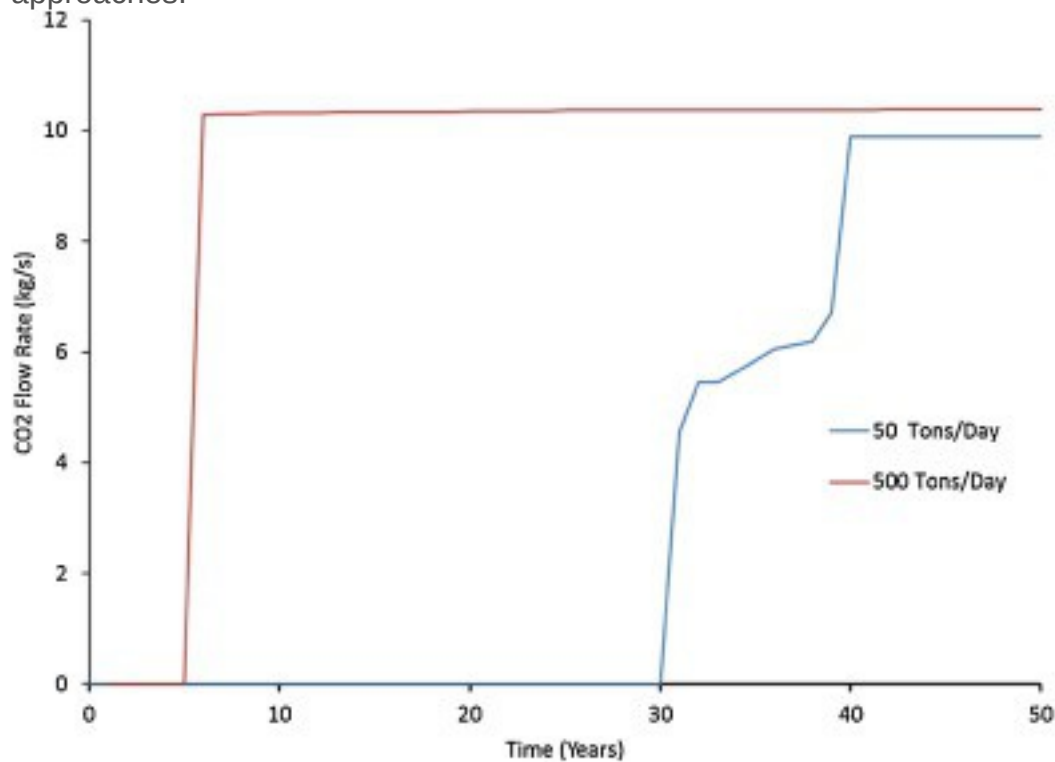
This example demonstrates how the NRAP-IAM-CS can be used to inform questions such as: How does the quality of a legacy well affect storage? And, How do operational parameters affect potential leakage through a legacy well at a greenfield saline reservoir? We consider a hypothetical CO₂ storage site with a saline storage reservoir and a legacy well. For this scenario we use the built-in reservoir ROM to predict pressure and saturation changes due to CO₂ injection and the wellbore ROM to predict CO₂ leakage rates. The storage reservoir is assumed to be homogeneous with a spatial extent of 10 km × 10 km, 3 Darcy permeability, 0.2 porosity and 20 m thickness. We assume that the CO₂ injector is located at the center of the storage reservoir and there is a legacy well present in the reservoir. For the first scenario it is assumed that the location of the wellbore is known but its seal integrity as controlled by cement quality is highly uncertain. We are interested in understanding how the wellbore cement quality affects potential CO₂ leakage. The wellbore is assumed to be at a distance of 1 km from the injector. In order to calculate CO₂ leakage through the wellbore, multiple runs of the NRAP-IAM-CS were performed assuming that the wellbore is open or cemented but with a range of effective permeability from 10 Darcy (representing bad cement quality) to 1 milliDarcy (representing good cement quality). Each of the NRAP-IAM-CS runs simulated a 50-year site performance with a CO₂ injection rate of 50 t/day. Fig. 7 shows how the maximum CO₂ flow rate through the wellbore changes with the wellbore quality (from an open well to well with good cement quality). As expected, the presence of any cement significantly reduces the CO₂ flow rate compared to an open well and it is reduced even further (by orders of magnitude) as the cement quality improves.



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Fig. 7. Predicted CO₂ flow rate through a wellbore at a hypothetical CO₂ storage site as a function of wellbore quality (effective cement permeability).

In the second scenario we are interested in knowing how site operational parameters affect the timing of CO₂ leakage through an open wellbore located at a distance of 1 km from the injector. Similar to the previous scenario, multiple runs of the NRAP-IAM-CS were performed by varying CO₂ injection rate while simulating 50-year performance of a hypothetical site. [Fig. 8](#) shows the plots of CO₂ leakage against time for two CO₂ injection rates. For the higher injection rate (500 t/day) leakage is observed much sooner than for the lower injection rate (50 t/day). While this result is qualitatively intuitive, quantitative predictions such as those shown in [Fig. 8](#) provide valuable information related to the site response as well as to design of monitoring and mitigation approaches.



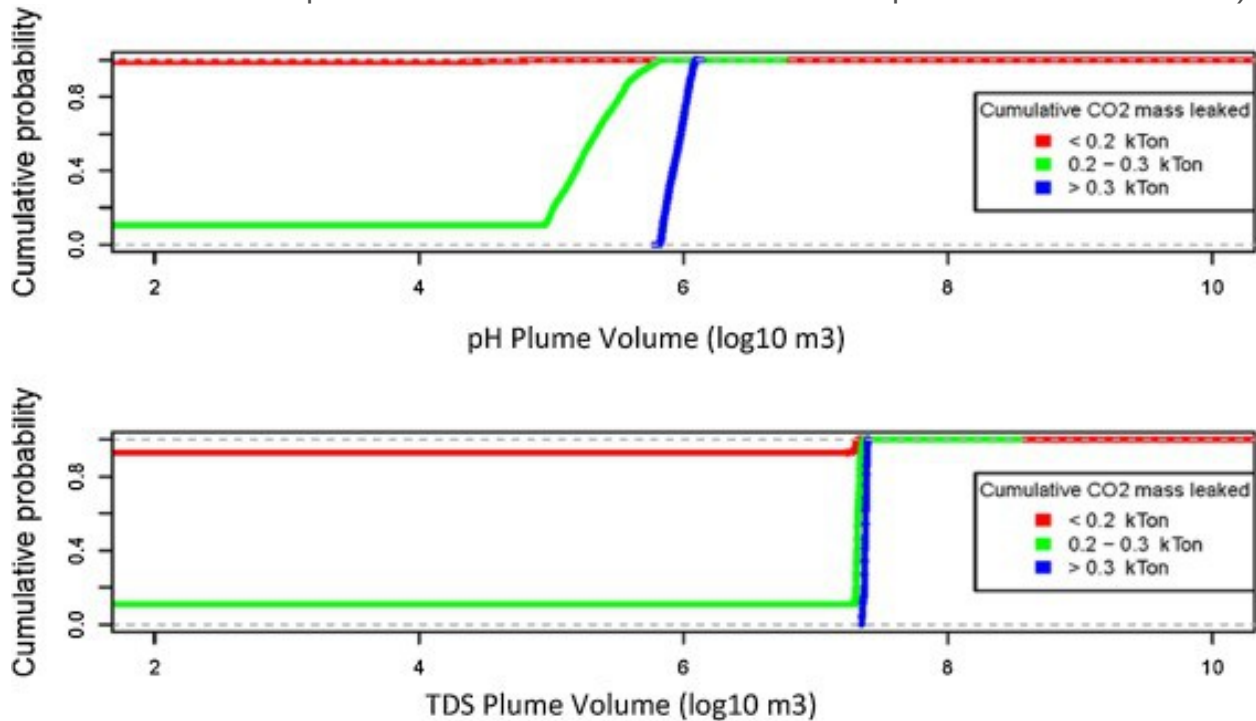
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Fig. 8. Comparison of CO₂ flow rate through an open well at a distance of 1 km from the injector for two different injection rates.

3.3. NRAP-IAM-CS application to quantify groundwater impacts

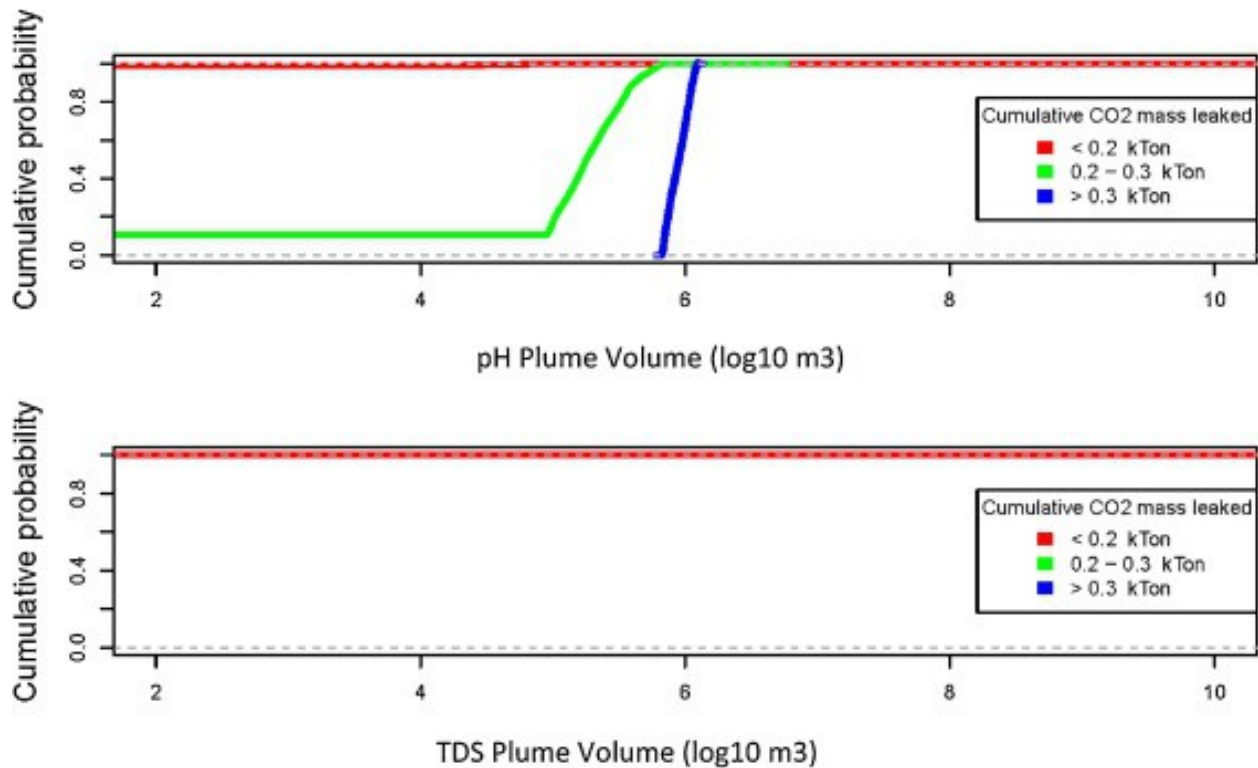
The previous examples focused on the risks of direct leakage to the atmosphere through the wellbores. As mentioned in Section [2.1](#), the NRAP-IAM-CS includes models for the groundwater aquifer and can be applied to simulate impacts of CO₂ and brine leakage into groundwater and associated impacts. The groundwater ROMs implemented in the NRAP-IAM-CS take into account hydrologic as well as geochemical processes. We demonstrate application of the NRAP-IAM-CS to compare responses to leakage of two sites with different groundwater characteristics. This example demonstrates how all of the different component models in the NRAP-IAM-CS including those for reservoir, wellbore and groundwater can be exercised together to simulate movement of CO₂ from injection to not only leakage through wellbores but also resulting response in groundwater quality. The hypothetical sites in question are assumed to have the same storage reservoir characteristics as the Kimberlina site used in previous applications. Both of the sites are assumed to have a single, abandoned legacy well present but the well location is assumed to be unknown. In addition, it is also assumed that the legacy well is plugged but the quality of cement and resulting effective wellbore permeability are unknown. The two sites are assumed to be overlain by a carbonate groundwater aquifer whose thicknesses are different with one being 100 m thick (with horizontal hydraulic gradient 2.88×10^{-4}) while the other 500 m thick (with horizontal hydraulic gradient 1.89×10^{-2}). The goal is to compare the two sites based on the groundwater response to leakage. Two scenarios of the NRAP-IAM-CS were set up with the only difference between the two being the groundwater aquifer thickness and horizontal hydraulic gradient. Each scenario simulated 200 years of site performance (50 years injection plus 150 years post-injection) through a MC simulation consisting of 1000 realizations. The uncertainty in well location was captured by varying the wellbore location in a 12 km² area around the injection well for different realizations. The uncertainty in well quality was captured by assigning it an effective permeability distribution based on the built-in permeability distribution based on the Alberta data mentioned in previous examples. To compare the performance of the two sites, the groundwater responses for the two risk proxies were compared, namely, pH < 6.5 plume volume and TDS > MCL plume volume. The plume volume results were used to calculate cdfs of plume volume for various cutoffs of cumulative CO₂ leakage. [Fig. 9](#), [Fig. 10](#) show the cdfs for groundwater aquifer thicknesses of 100 m and 500 m, respectively. The results demonstrate a number of interesting features. Both the hypothetical aquifers respond very similarly to leaks in that both show very small or non-existent plumes. While the pH response is similar between the two aquifers, the TDS response is different with the thicker aquifer exhibiting no change in TDS for the same magnitude of

leak. This may be due to the dilution effect of the thicker aquifer. The quantified volumes can also be used to determine monitoring strategies. The results show that any leak with a cumulative leaked mass smaller than 0.2 kt does not produce a “measurable” plume. For the leaks with cumulative leaked mass >0.3 kt the leak would only be detectable if groundwater monitoring wells were spaced closer than 80 m (the spacing is determined from the plume volume less than $1 \times 10^7 \text{ m}^3$ and aquifer thickness of 500 m).



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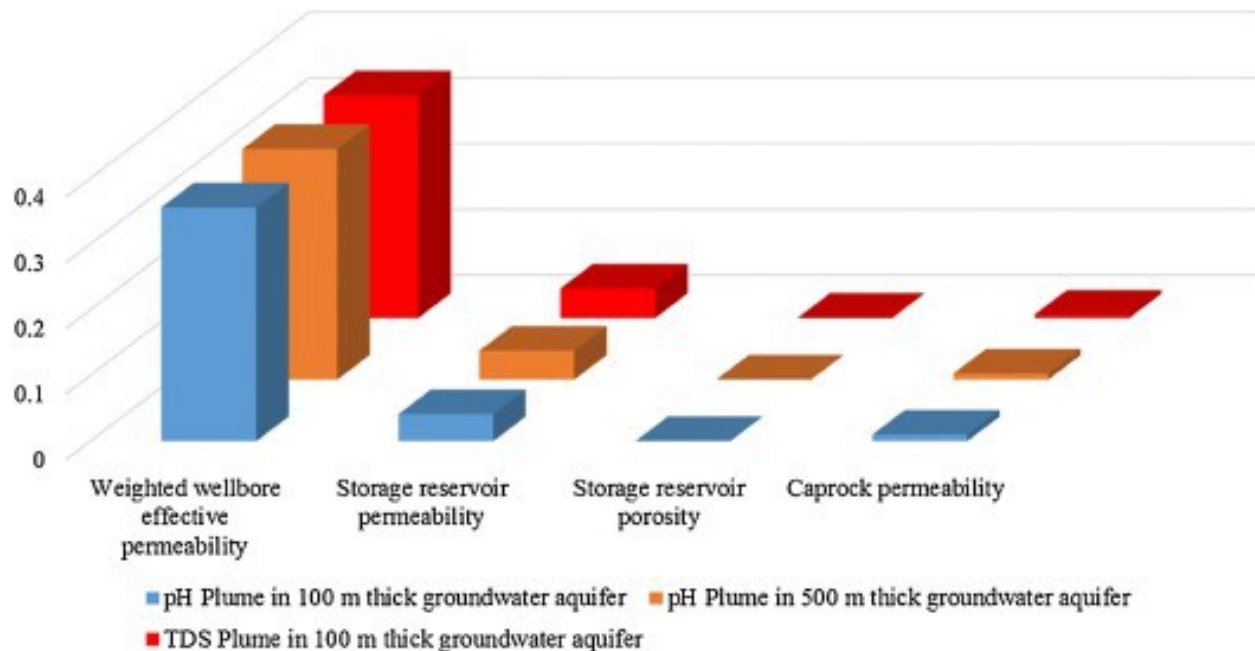
Fig. 9. Cumulative distribution function (CDF) of pH < 6.5 plume volume and TDS > MCL plume volume resulting from CO₂ and brine leakage in a 100 m-thick groundwater aquifer. The CDFs are calculated from a MC simulation with 1000 realizations and are plotted for three cutoff values of cumulative CO₂ leaked mass.



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Fig. 10. Cumulative distribution function (CDF) of pH < 6.5 plume volume and TDS > MCL plume volume resulting from CO₂ and brine leakage in a 500 m-thick groundwater aquifer. The CDFs are calculated from a MC simulation with 1000 realizations and are plotted for 3 cutoffs of cumulative CO₂ leaked mass.

The MC results were also used to identify important uncertain parameters through a multi-variate analysis. Note that even though the NRAP-IAM-CS can be used to incorporate uncertainty in a range of hydrologic and geochemical parameters for a groundwater aquifer, for this example application we assumed that all the groundwater aquifer parameters had a constant value that did not change from realization to realization. The storage reservoir permeability, storage reservoir porosity, caprock permeability and wellbore effective permeability were assumed to be uncertain. [Fig. 11](#) shows the calculated importance measures for the pH plume volume for both the aquifers and TDS plume volume for the 100 m thick aquifer (note that the TDS plume volumes were predicted to be zero for the 500 m thick aquifer). Similar to the previous examples it is apparent that the effective wellbore permeability is the most important parameter for all the computations.



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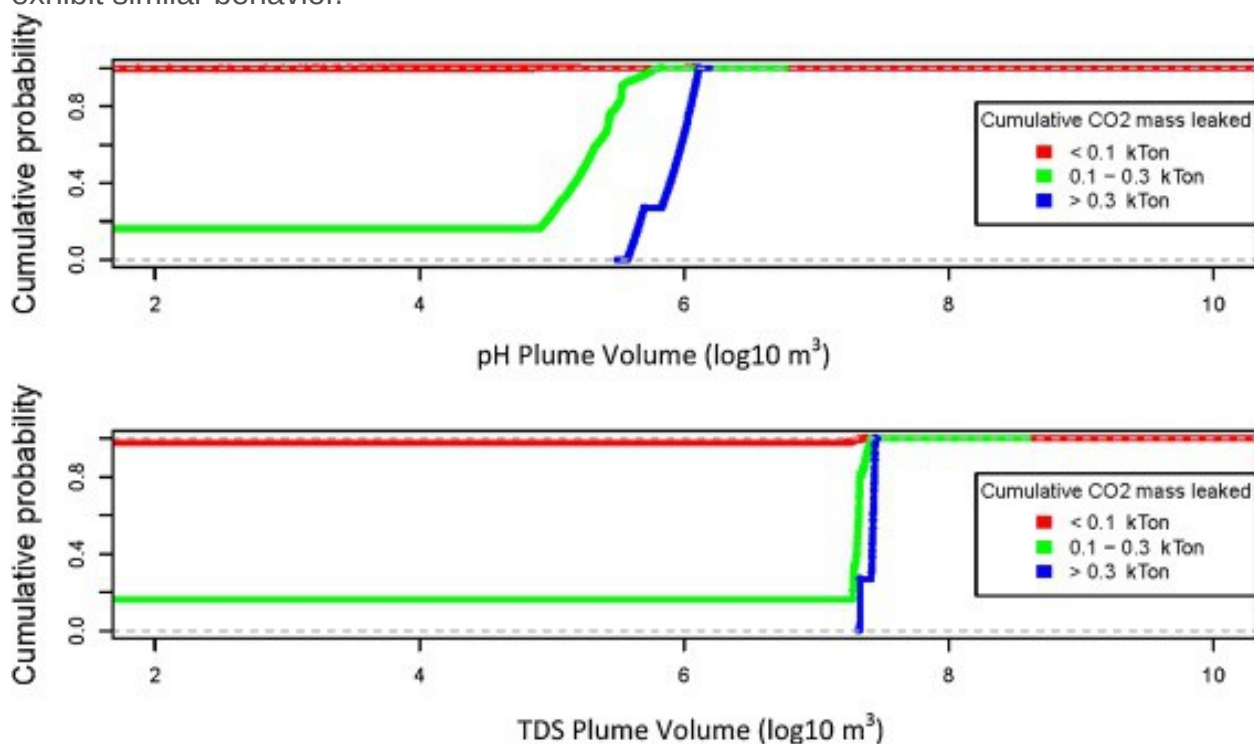
Fig. 11. Results of multi-variate analysis showing importance of uncertain wellbore and storage reservoir parameters on pH and TDS response in the groundwater aquifer due to CO₂ and brine leakage. The groundwater aquifer parameters were assumed to be constant for these simulations.

The example above demonstrated how multiple components at a geologic CO₂ storage site, including storage reservoir, leakage pathways and groundwater aquifer can be coupled to predict impact of leakage from storage reservoir into groundwater aquifer. We assumed that the storage reservoir and wellbore properties were uncertain but the groundwater aquifer parameters were not. One of the main advantages of NRAP-IAM-CS is the ability to explore the effect of uncertainties in multiple parameters for all the components. To demonstrate this capability we performed MC simulations with the same model setups used for assessing groundwater aquifer impacts as described above except assuming that the groundwater aquifer parameters are also uncertain. [Table 5](#) describes the various uncertain groundwater parameters and range of values for each of them sampled during the MC simulations. The uncertain parameters included not only hydrologic parameters but also geochemical parameters. We assumed that none of the uncertain parameters were correlated and all followed a uniform distribution. Finally, we assumed that while the two aquifers had different thicknesses (100 m, 500 m) both had the same set of uncertain parameters and parameter value ranges as listed in [Table 5](#).

Table 5. Table of uncertain groundwater aquifer hydrologic and geochemical parameters and range of values used for MC simulation of CO₂/brine leakage in groundwater aquifer and subsequent impacts.

Uncertain Parameter	Range
Mean aquifer permeability (Darcy)	0.01585–25.12
Aquifer permeability variance	0.017–1.89
Aquifer permeability correlation length (km)	1–3.95
Aquifer permeability anisotropy (horizontal/vertical)	1.1–49.1
Aquifer porosity	0.1–0.3
Storage reservoir brine molality	0.001–1
Calcite surface area	0–0.01

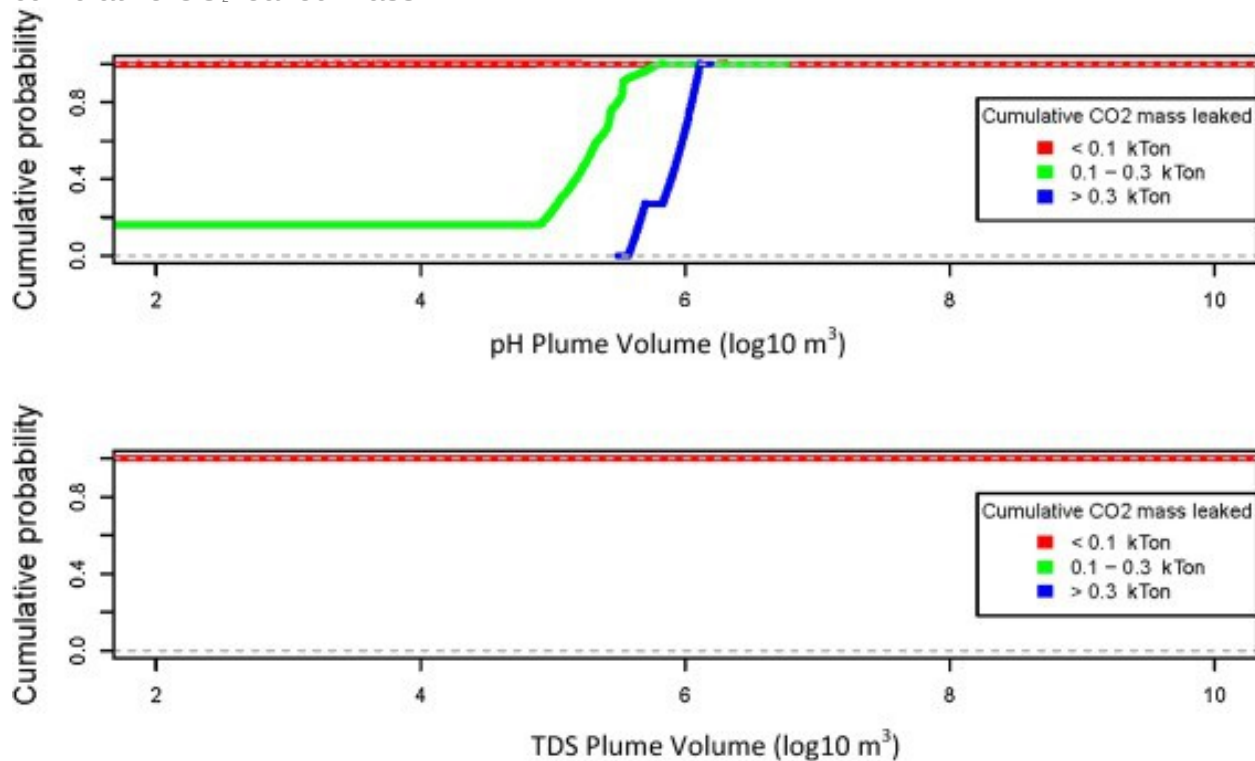
Similar to the previous problem set we performed two sets of MC simulations with 1000 realizations each while using LHS approach to sample from each uncertain variable. [Figs. 12 & 13](#) show results of the cdfs of pH < 6.5 and TDS > MCL plume volumes for the three cutoffs of cumulative CO₂ leaked mass for the two aquifers. While there are some differences in the nature of the cdfs compared to [Figs. 9 & 10](#), the overall trends are similar in that both exhibit very small or non-existent plumes and no change in TDS of the thicker aquifer. Given that the only difference between the two model setups is uncertainty in groundwater aquifer parameters, we expected the cdfs to exhibit similar behavior.



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Fig. 12. Cumulative distribution function (CDF) of pH < 6.5 plume volume and TDS > MCL plume volume resulting from CO₂ and brine leakage in a 100 m-thick groundwater aquifer with uncertain aquifer parameters. The CDFs are calculated from a MC simulation with 1000 realizations and are plotted for three cutoff values of cumulative CO₂ leaked mass.



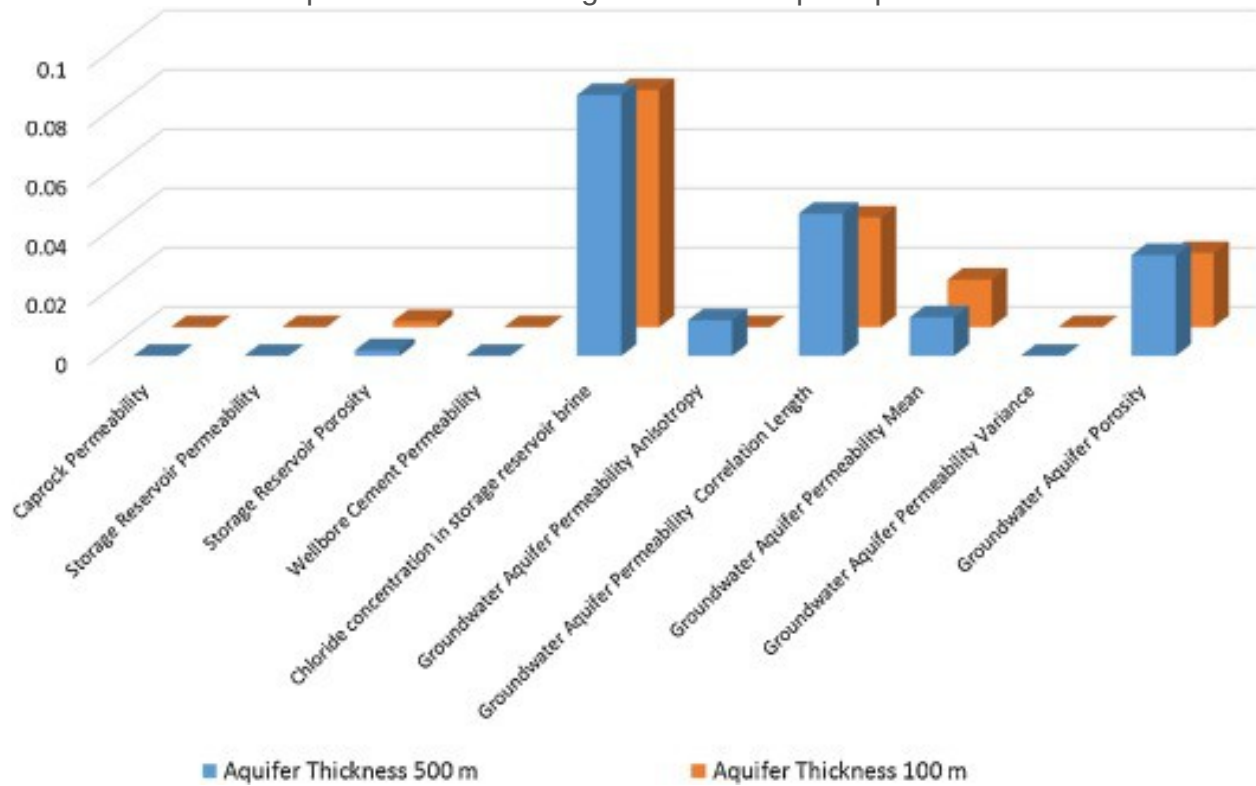
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Fig. 13. Cumulative distribution function (CDF) of pH < 6.5 plume volume and TDS > MCL plume volume resulting from CO₂ and brine leakage in a 500 m-thick groundwater aquifer with uncertain aquifer parameters. The CDFs are calculated from a MC simulation with 1000 realizations and are plotted for 3 cutoffs of cumulative CO₂ leaked mass.

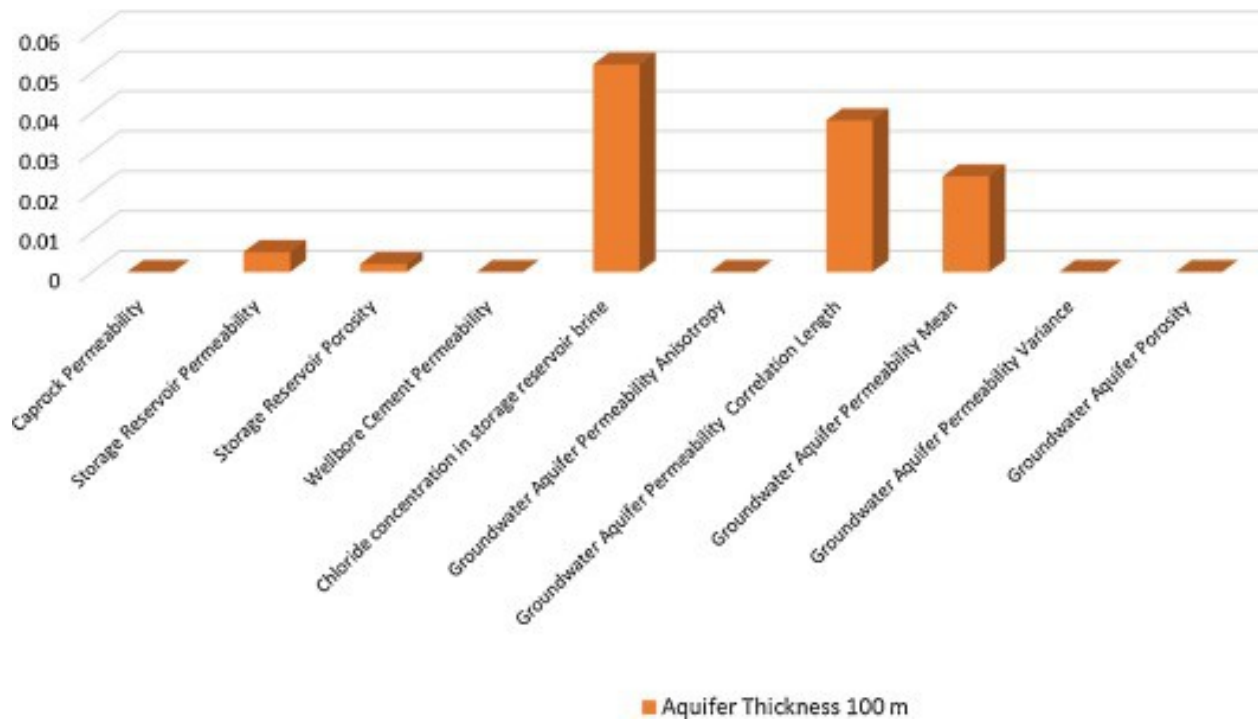
The most interesting aspect of the comparison is the effect of uncertainties on predicted pH and TDS changes. [Fig. 14](#), [Fig. 15](#) show the plots of computed importance measures for pH < 6.5 plume volumes for both the aquifers while [Fig. 16](#) shows the computed importance measures for TDS > MCL plume volumes for 100 m thick aquifer. Note that the computed importance of the uncertain variables is significantly different compared to the results shown in [Fig. 11](#) for the example where the groundwater aquifer parameters were not assumed to be uncertain. The results in [Fig. 14](#), [Fig. 15](#) show that

the groundwater aquifer parameters have more importance (variability in uncertain parameters resulting in variability in predictions) compared to the wellbore or storage reservoir parameters for this hypothetical scenario. This result is to be expected since the cumulative mass of leaked CO₂ is low (~kilotonnes) which leads to variability in aquifer parameters affecting variability in pH and TDS plumes more compared to the variability in parameters resulting in leakage. The result is consistent with the observations by [Keating et al. \(2016\)](#) who demonstrated that for large leaks variability in leak rates is more important than that in groundwater aquifer parameters.



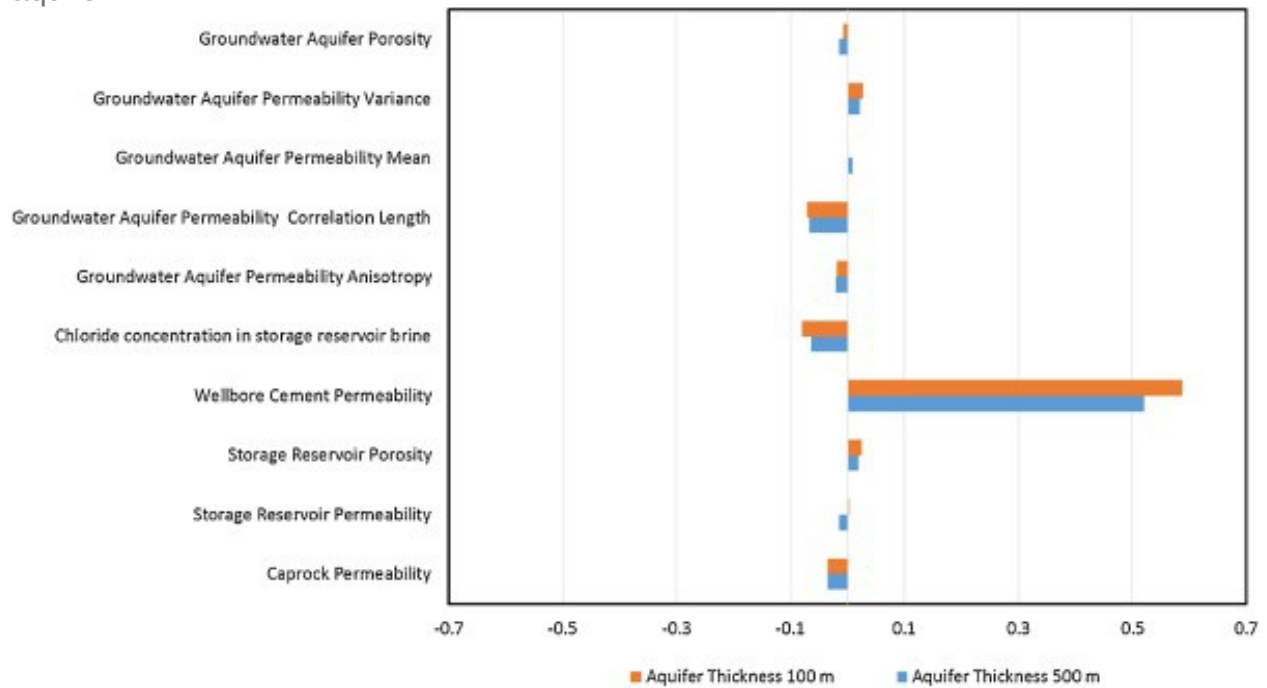
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Fig. 14. Results of multi-variate analysis showing importance of uncertain parameters on pH response in the groundwater aquifer due to CO₂ and brine leakage. The uncertain parameters included those for storage reservoir, wellbore and groundwater aquifer.



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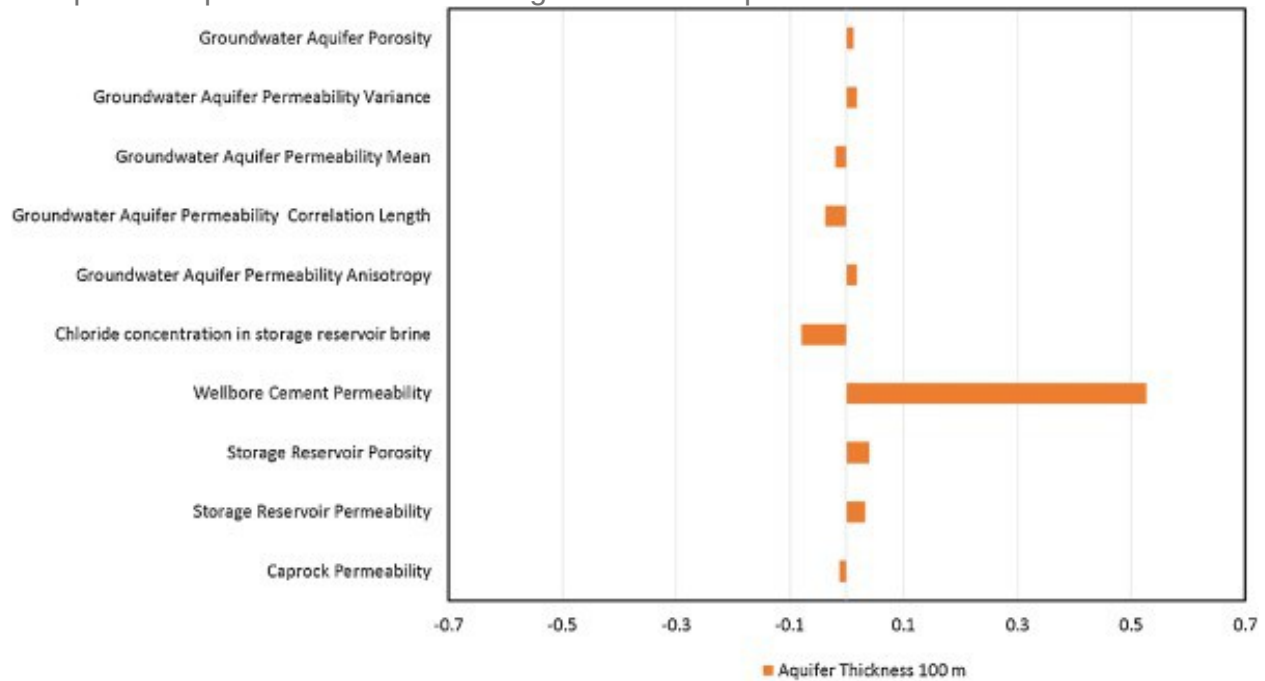
Fig. 15. Results of multi-variate analysis showing importance of uncertain parameters on TDS response in the groundwater aquifer due to CO₂ and brine leakage. The uncertain parameters included those for storage reservoir, wellbore and groundwater aquifer.



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Fig. 16. A tornado chart showing correlation coefficients between uncertain variables and pH < 6.5 plume volume for both groundwater aquifers.



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Fig. 17. A tornado chart showing correlation coefficients between uncertain variables and TDS > MCL plume volume for groundwater aquifer with 100 m thickness.

[Fig. 16](#), [Fig. 17](#) show tornado charts plotted with correlation coefficients for all the uncertain parameters. Compared to the importance measures ([Figs. 14 & 15](#)) the correlation coefficients ([Figs. 16 & 17](#)) demonstrate different trends where wellbore cement permeability has large and positive correlation coefficient value compared to other uncertain parameters. The correlation coefficients and importance measures are part of multi-variate sensitivity analysis that can be used to gain better understanding of effect of uncertain variables on computed results. The results presented here demonstrate the uncertainty quantification capabilities provided by NRAP-IAM-CS that can be used to estimate effect of uncertain parameters within the entire geologic CO₂ storage system.

4. Concluding remarks

There is broad interest among the GCS stakeholders, including site operators, regulators, insurers, policy makers, and the public to gain a credible, science-based quantitative understanding of long-term performance of geologic CO₂ storage sites

([Wilson et al., 2007](#)). The risk assessment applications to field projects to date have been qualitative ([Hnottavange-Telleen, 2013](#), [Gerstenberger et al., 2013](#), [Tucker et al., 2013](#)) as well as quantitative ([Metcalf et al., 2013](#), [Dodds et al., 2011](#)). To date none of the qualitative or quantitative risk assessment approaches have utilized predictions of long-term performance of geologic CO₂ storage sites primarily due to lack of available tools or approaches to perform the predictions. While it is challenging to simulate the long-term performance of an entire geologic CO₂ storage site (from storage reservoir to leakage pathways to shallow aquifers and atmosphere) and take into account key uncertain parameters, it has been shown to be technically feasible through the approach developed by NRAP. The examples and results discussed in Section 3 are intended to demonstrate how NRAP's Integrated Assessment Model (NRAP-IAM-CS) can be used to simulate long-term behavior of a CO₂ storage site in order to quantify risks as well as to inform decisions related to site operation and management to ensure long-term storage effectiveness. The science based approach used to develop NRAP-IAM-CS and its component ROMs ensures that the site performance predictions take into account the complex physical and chemical interactions that control CO₂ migration through a site. This is critical to ensure wider stakeholder confidence in predictions related to site effectiveness as well as site management decisions. Results of the example applications described above demonstrate how the processes and parameters in a coupled system affect behavior of connected components. Such quantifications help to identify the importance of uncertain parameters on overall performance metrics and to guide decisions related to focusing resources to reduce the uncertainty in order to improve overall performance. They can also be used to guide decisions related to site management and operations as well as designs for effective monitoring of leakage and related impacts.

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Acknowledgements

This work was completed as part of the National Risk Assessment Partnership (NRAP) project. Support for this project came from the U.S. Department of Energy's (DOE) Office of Fossil Energy's Crosscutting Research program. The authors wish to acknowledge Traci Rodosta and M. Kylee Rice (NETL Strategic Center for Coal) and Mark Ackiewicz (DOE Office of Fossil Energy) for programmatic guidance, direction, and support. The authors also wish to acknowledge contributions from researchers across the NRAP technical teams, who developed ROMs that are implemented in the NRAP-IAM-CS model.

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