Original Research Article

GREENHOUSE GASES SCIENCE AND TECHNOLOGY

Evaluating probability of containment effectiveness at a GCS site using integrated assessment modeling approach with Bayesian decision network

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Abstract: Improved scientific and engineering understanding of the behavior of geologic CO_2 storage together with established regulatory framework and incentive structures raise the prospects for accelerated, large-scale deployment of this greenhouse gas emissions reduction approach. Incentive structures call for the establishment of appropriate verification and accounting approaches to support claims of the integrity of a geologic storage complex and to justify taking credit for long-term storage. In this study, we present a framework for assessing the probability of containment effectiveness over the lifetime of a geologic carbon storage site (e.g., after 70 years of injection and postinjection site performance) using forward stochastic model realizations based on site characterization data and using a monitoring-informed Bayesian network based on hypothetical detectability from surface seismic surveys over the site injection and post-injection phases. The National Risk Assessment Partnership's open-source Integrated Assessment Model (NRAP-Open-IAM) was utilized to develop an ensemble of 10,000 a priori stochastic forecasts of CO_2 containment. Those simulations were used to train the Bayesian network model to estimate the prior probabilities of the CO_2 leakage mass into overlying, monitorable aquifers considering the uncertainties in the reservoir properties, permeability of potentially leaky wells and the overlying aquifers. The conditional probabilities in the Bayesian network were either learned from the NRAP-Open-IAM simulations or derived from the predefined detection thresholds for the monitoring method. Observations obtained from monitoring, over time during the site operation phases were then used to generate updated posterior probabilities of containment (and any loss from containment) in the Bayesian network by propagating the prior probabilities through the conditional

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probabilities. We demonstrate how to construct and use the Bayesian network for verifying the long-term storage complex effectiveness informed by monitoring based on the NRAP-Open-IAM simulations previously developed for the FutureGen 2.0 site. This approach may have relevance for stake holders to demonstrate secure geologic storage, provide a defensible, probabilistic approach to claim credit for geologic storage, and to estimate the likelihood that any fraction of the claimed credit may need to be refunded to the creditor based on available monitoring information. © 2021 Society of Chemical Industry and John Wiley & Sons, Ltd.

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Keywords: Bayesian network; carbon sequestration; monitoring; NRAP-Open-IAM; risk assessment

Introduction

Carbon capture, utilization, and sequestration (CCUS) is being pursued by the international research, development, and deployment community as a means to stabilize and reduce the atmospheric concentration of carbon dioxide (CO_2), to partially mitigate global warming. Together with CCUS technology advances and established regulatory framework, creation of incentive programs will raise the prospects for accelerated deployment of CCUS.[1,2] To promote the practical applicability of storage, credit-based incentive programs, appropriate verification, and accounting approaches are needed to adequately account for the integrity of a geologic storage complex and to justify taking credit for long-term storage. In addition, practical storage requires an integrated scheme for the forecasting of the storage complex performance over the appropriate time interval (the injection period plus a predefined postinjection period), monitoring to verify that expected storage performance is met, quantification of any potential migration outside of containment, and a means of verifying and accurately evaluating long-term storage effectiveness.[3]

Stochastically forecasting the time-varying performance of full-scale injection and storage at a geologic carbon storage (GCS) site can be quite computationally expensive. The National Risk Assessment Partnership (NRAP) developed reduced-order and/or data-driven proxy models for important system components,[4] including the storage reservoir, the leakage pathways (e.g., wellbores), the groundwater aquifers, and the atmosphere, and then coupled these component models, which allows for fast forecasting and quantification of risks over time.[5] These component models, referred to here as NRAP-Open-IAM tools, are either analytical models or trained using detailed multiphase flow and transport simulations. For example, two approaches are used to develop the component models for the storage reservoir. One is a look-up table approach that utilizes reservoir pressures and saturations from site-specific reservoir simulations. Another approach is a simplified physical model based on work of Nordbotten *et al.*[6,7] For the methods and principles that the system model and each component model are based on, the readers are referred to Pawar *et al.* and the NRAP-Open-IAM user's manual.[8,5] The inputs and outputs of each component model are described in the NRAP-Open-IAM user's manual.[8] The NRAP-Open-IAM tools have been used to perform probabilistic simulations for analysis of long-term CO_2 storage at geologic carbon sequestration sites.[9] Some example applications of the NRAP-Open-IAM tools can be found on the NRAP-Open-IAM tool website.[4] There have been other methods for developing reduced-order models. For example, Jin and Durlofsky[10] extended an existing reduced-order modeling framework to simulate and optimize the CO_2 storage operations. Tian *et al.*[11] used statistical approaches to reproduce the cumulative distribution functions of the CO_2 breakthrough time and the total mass from Monte Carlo simulations.

Monitoring methods are required to be implemented at sequestration sites for tracking the plume migration in the deep subsurface and for demonstrating the long-term secure storage of CO_2.[12,13] The monitoring method may include direct point measurements (such as pressure monitoring and fluid sampling) and indirect geophysical monitoring (such as seismic monitoring, gravity monitoring, electrical resistivity tomography, and magnetotelluric monitoring). Some monitoring methods are well-based and can provide local point measurements of the target parameters. And others, such as the surface seismic surveys, can provide a broad image of the subsurface property changes, which is a combined effect of changes in multiple subsurface properties. The surface seismic surveys have been widely used at carbon sequestration sites for tracking the CO_2 plume migration and estimating the total injected CO_2 amount for concordance evaluation.[14–16] Large uncertainties are associated with interpretation of the surface seismic data and the inverted CO_2 plume properties (such as the extent, the volume and the mass of the CO_2 plume).

There is a necessity for workflow/methodology to incorporate monitoring data into the assessment of the secure geologic storage. Assessing the potential CO_2 leakage risks into overlying aquifer layers above the caprock, given observations from monitoring method is important for verifying the long-term storage complex effectiveness. In this study, we employed Bayesian networks to update the initial evaluation of the probability of containment based on monitoring observations and mitigation activities conducted during site operation.

A Bayesian network is a statistical model that represents probability distributions of system variables (represented as network nodes) and their conditional relationships (represented as directional arrows) in a concise and graphical way.[17] For each node in the Bayesian network, the conditional probabilities of the possible states of the node, given all the combinations of the states of its parent nodes must be defined. Bayesian networks have been applied to various decision making problems.[18–21] Bobbio *et al.*[22] compared the fault tree analysis with Bayesian networks in the area of dependability analysis. Gerstenberger *et al.*[23] applied Bayesian networks to risk assessment in CCUS. Bayesian networks were applied to inferring CO_2 leakage from near-surface soil CO_2 flux measurements and near-surface tracer monitoring[24] and combining interpretation of different monitoring information to enhance detectability of leakage at GCS sites.[25] The Bayesian approaches have also been used to infer CO_2 leakage from pressure measurements.[26] Namhata *et al.*[27] applied Bayesian inference to updating of fractured seal characterization using observations of pressure change in above zone monitoring interval. Jenkins[28] reviewed statistical methods for testing leakage and no leakage models using monitoring data in the context of CCUS and emphasized the importance of Bayesian methods in addressing stakeholders' questions and dealing with multiple models.

The Bayesian network (BN) method is based on Bayes' rule of conditional probability (Eqn 1),[29] which allows all the probabilities in the network to be updated as new observations are obtained (entered as new findings in the network). The conditional relationships are shown as directed arrows on the BN graph.

$$Prob\{B_i|A\} = \frac{Prob\{A \cap B_i\}}{Prob\{A\}} = \frac{Prob\{A|B_i\} * Prob\{B_i\}}{\sum_{j=1}^{n} Prob\{A|B_j\} * Prob\{B_j\}} \quad (1)$$

where $Prob\{B_i|A\}$ is the posterior probability of B_i, $Prob\{A|B_i\}$ is the likelihood of A occurs when B_i is known to occur, $Prob\{B_i\}$ is the prior probability of B_i, $Prob\{A \cap B_i\}$ is the probability of both A and B_i occur, and $Prob\{A\}$ is the marginal probability of A (i.e., total probability of A). A and B represent nodes on the BN graph.

The objective of this study is to develop a framework for assessing the probability of containment effectiveness over the lifetime of a geologic carbon storage site lifetime (e.g., after 70 years of total site performance) using forward stochastic model realizations based on site characterization data and using Bayesian networks given monitoring observations (e.g., surface seismic surveys) at time t ($t < 70$ years). The National Risk Assessment Partnership's open-source Integrated Assessment Model (NRAP-Open-IAM) was utilized to develop initial forecast of CO_2 geologic containment effectiveness before injection operations begin and to train the Bayesian network model to estimate the prior probabilities of the CO_2 leakage mass into overlying aquifers as a function of important uncertainties (in reservoir properties, permeability of potentially leaky wells, and permeability of the overlying aquifers). Conditional probabilities used in the Bayesian network are either learned from the NRAP-Open-IAM simulations or derived from the predefined detection thresholds for the monitoring method. We describe how the Bayesian network was constructed to verify long-term effectiveness of the storage complex given leakage monitoring information—using NRAP-Open-IAM simulations previously developed

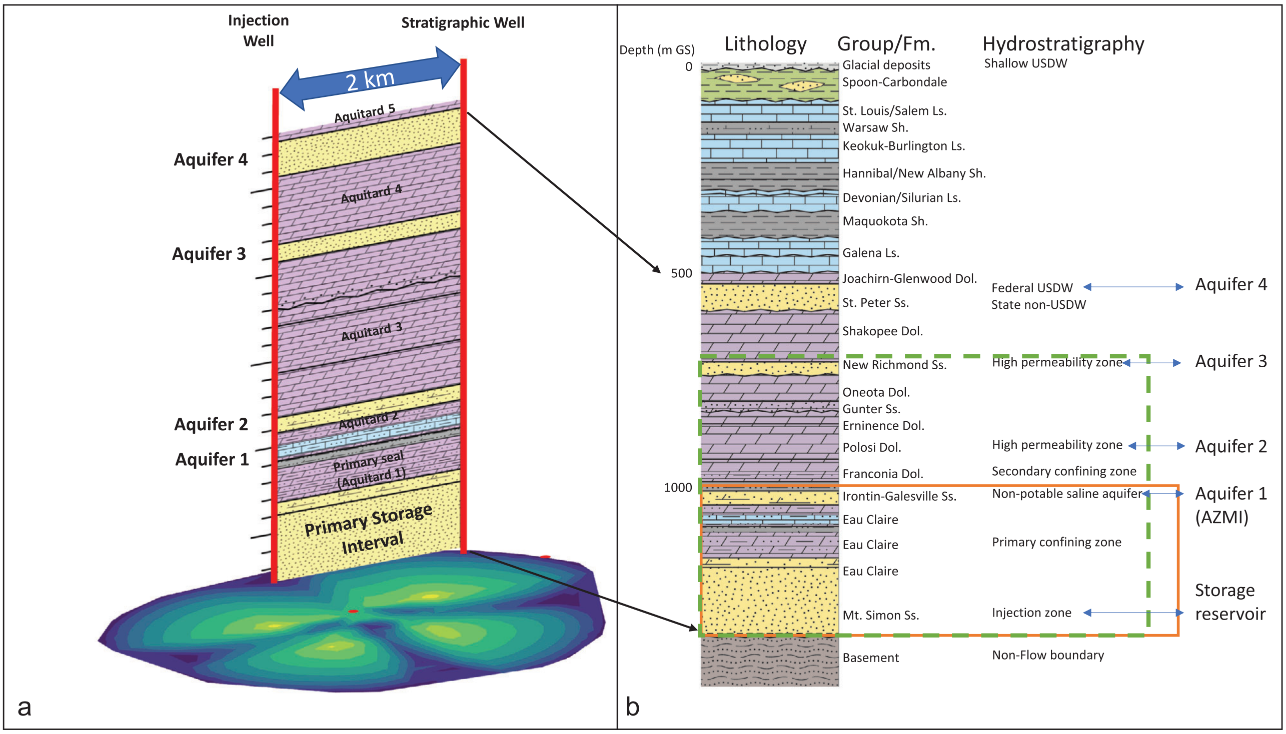

Figure 1. (a) Schematic diagram of the system model; and (b) Stratigraphy and hydrostratigraphy at the FutureGen 2.0 site, depths are given in meters. The storage reservoir and the four aquifer layers in the composite CO_2 storage system model are denoted on the figure. The green and the orange rectangles illustrate the defined larger containment envelope and the smaller containment envelope, respectively. Please note that Aquitard 5 shown in Fig. 1a includes everything from the Joachem–Glenwood Dolomite (Jaochem–Glenwood Dol in Fig. 1b) to the surface.

for hypothetical CO_2 storage case at the FutureGen 2.0 site.

In the second section, we summarize the leakage simulations used for quantifying the long-term storage complex effectiveness, and describe the methods used for initial evaluation of site performance (without considering monitoring), and for updated evaluations that consider monitoring information and mitigation activities. Results of the evaluations are presented in the third section and discussed in the fourth and fifth sections.

Methods and supporting simulations

Leakage simulations

For this work we generate 10 000 realizations of potential leakage from the geologic carbon storage complex based on modeled storage performance at the formerly proposed FutureGen 2.0 site.[30] These simulations were developed using the NRAP-Open-IAM[8] by linking a lookup table representation of the storage site's primary storage reservoir component and an analytical model of a multisegmented well to simulate potential brine and CO_2 leakage through the CO_2 injection well and one stratigraphic well. Based on proposed geography of the FutureGen 2.0 site,[9] the distance between the injection well and stratigraphic well is assumed to be approximately 2 km. The composite CO_2 storage system model consists of the storage reservoir, four aquifer layers and five aquitards with interbedded porous and permeable intervals. The layers are numbered from the bottom to the top with aquitard 1 being the primary sealing caprock above the storage reservoir and aquitard five being the aquitard directly above the lowermost groundwater aquifer (Fig. 1a). The four aquifer layers (i.e., aquifer 1–4) in the system model are at the depths of 1044, 936, 742, and 592 m, corresponding to the Ironton–Galesville (the porous and permeable interval directly above the primary seal—sometimes referred to as the above-zone monitoring interval, or AZMI), Potosi, New Richmond, and St Peter formations (the lowermost

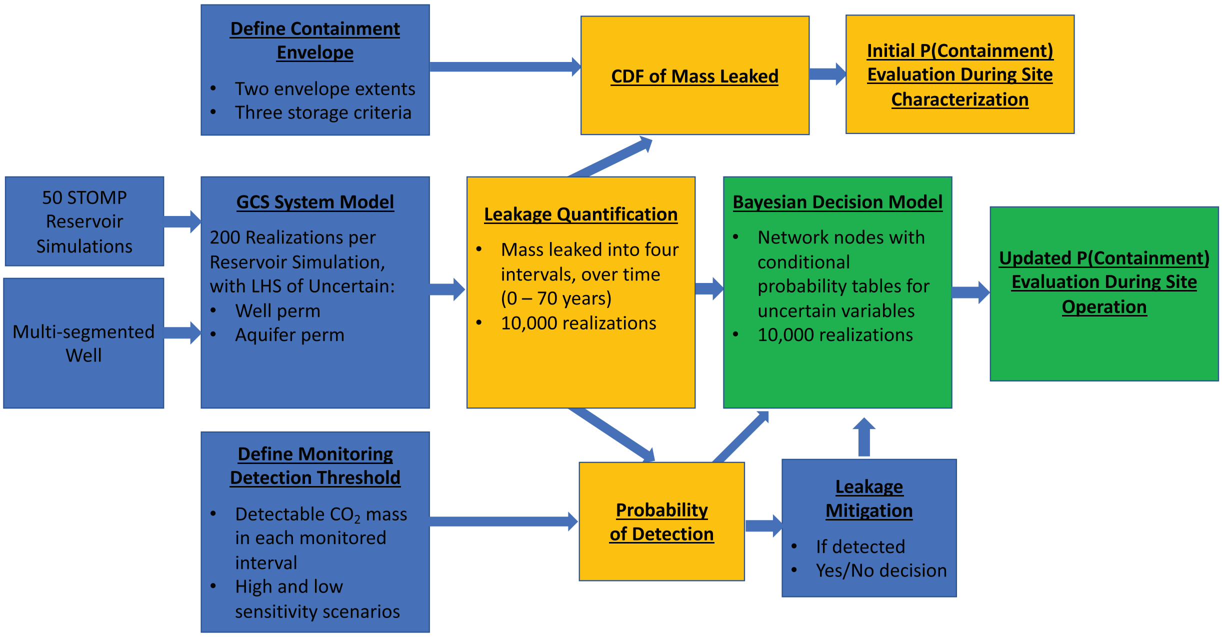

Figure 2. Flowchart showing the simulation and evaluation steps.

groundwater aquifer) at the FutureGen 2.0 site, respectively. Figure 1a shows a simplified representation of the stratigraphy at the FutureGen 2.0 site; the storage reservoir and the four aquifer layers in the system model are denoted in Fig. 1b. The 10 000 leakage realizations were generated based on an earlier study by Bacon and colleagues[9] with parameter ranges selected based on information specific to the FutureGen 2.0 site. The same parameter ranges are used in the present study.

The lookup table reservoir component in NRAP-Open-IAM was derived from full-physics reservoir simulations and uses interpolation in time and space to calculate pressure and CO_2 saturation at the interface between the storage reservoir and the primary sealing caprock (aquitard 1). One thousand multiphase flow reservoir simulations were previously conducted by Bacon and colleagues[9] using the STOMP simulator,[31] considering the uncertainty in the permeability for each of the 31 computational reservoir model layers. Each simulation run considers a 20-year injection at a rate of 1.1 million metric tons (MMT) CO_2 per year, and a 50-year postinjection period; the cumulative mass of CO_2 injected is 22 MMT. The multisegmented well component is used to calculate CO_2 and brine mass flux to the four overlying aquifer layers. The range of well permeabilities assumed (Table 2, from[9]) were relatively high, as compared to values by Carey.[32]

Fifty STOMP reservoir simulations were randomly sampled and each selected simulation was used as the basis to run 200 NRAP-Open-IAM simulations, resulting in 10 000 (= 50 × 200) realizations. Leakage through wells and into the four overlying aquifer layers considered uncertainty in well permeability and the permeability of the four aquifer layers, with uncertain parameter values generated by Latin hypercube sampling. Each system model realization had 15-time steps, calculated at five-year intervals throughout the 70 years of simulated performance. Figure 2 shows the simulation steps and the outputs used for evaluation of the containment effectiveness for CO_2 storage at the site, as well as the methodology employed for evaluating the probability of containment.

Initial evaluation

During site characterization, initial evaluation of the probability of containment at a site was calculated using NRAP-Open-IAM simulation results. To quantify the storage complex effectiveness, the spatial envelope of the storage complex was first defined. In this study, we considered two scenarios for the storage complex envelope (see Fig. 1b). The larger containment envelope was defined as the reservoir interval and the three overlying aquifer layers (i.e., the Ironton–Galesville, the Potosi, and the New Richmond formations) above the reservoir at the FutureGen 2.0 site. The smaller containment envelope was defined as

Table 1. A description of assumptions in evaluating the long-term storage complex effectiveness.

Assumption	Description
Larger containment envelope	Storage reservoir and aquifers 1, 2, and 3
Smaller containment envelope	Storage reservoir and aquifer 1
99.9% storage criterion	Maximum allowed leakage mass out of the containment envelope is 22 000 metric tons
99.99% storage criterion	Maximum allowed leakage mass out of the containment envelope is 2 200 metric tons
99.999% storage criterion	Maximum allowed leakage mass out of the containment envelope is 220 metric tons

the reservoir interval and aquifer 1 (i.e., the Ironton–Galesville formation), which corresponds to the containment envelope definition assumed for the Future Gen 2.0 Class VI injection well permit application.[33] The defined envelope of the storage complex does not affect the physical behavior of the system but including additional overlying aquifers (aquifers 2 and 3) represents a more permissive containment envelope scenario. Because aquifer 4 (i.e., the St Peter formation) is the lowermost groundwater aquifer at the site, that interval is considered outside even the larger containment envelope., and calculated fluid migration outside of this larger containment envelope also represents leakage to the groundwater aquifer.

After the containment envelope is defined, the targeted CO_2 storage permanence criterion for claiming storage credit was selected. Here, we compared the evaluation results using three different storage permanence thresholds—99.9% storage, 99.99% storage, and 99.999% storage. Because the total mass of CO_2 injected at the FutureGen 2.0 site for the hypothetical scenario considered is 22 MMT, the maximum allowed leakage mass out of the containment envelope is 22 000 metric tons for the 99.9% storage criterion or 2200 tons for the 99.99% storage criterion or 220 tons for the 99.999% storage criterion. Table 1 summarizes the scenarios used in evaluating the long-term storage complex effectiveness.

Based on the 10 000 realizations of forward leakage simulations of the FutureGen 2 site developed using the NRAP-Open-IAM described above, the probability of containment is calculated. Cumulative density function (CDF) of the total CO_2 mass leakage out of the defined containment envelope after 70 years were generated (probability that the cumulative leakage mass is lower than the maximum allowed leakage mass for the specified storage criterion). Descriptive statistics (mean, median, and percentiles) of the leakage mass from each well into the four aquifers as a function of site operation time were also calculated.

Updated evaluation by monitoring

As monitoring data are gathered and interpreted during site operation, the initial estimation of ultimate probability of containment can be updated based on the monitoring observations. Separate Bayesian networks (BNs) were constructed for the defined larger containment envelope and the smaller containment envelope at the FutureGen 2.0 site to incorporate monitoring information in the workflow for evaluating and updating estimates for the probability of containment. These BNs were developed using the software package Netica.[34]

The BN model constructed for the larger containment envelope has eight nodes (see Fig. 4). The five nodes on the left (from the bottom to the top) represent the mass of CO_2 leaked into each of the four aquifers over time t ($t < 70$ years) and the total mass CO_2 leaked out of the defined containment envelope after 70 years. The prior probabilities and the conditional probability tables for these five nodes are trained using the estimated CO_2 mass leakage into the four aquifers based on the 10,000 NRAP-Open-IAM realizations at time steps before 70 years (i.e., in 5 year intervals from year 0 to year 65). The CO_2 mass leakage values are discretized into five functional classes (Table 2) to reduce the computational burden of conditional probability table development. The three nodes on the right of the graph denote surface seismic monitoring implemented at the site, mitigation activity that might be conducted and cumulative CO_2 mass leakage out of the defined containment envelope after 70 years of total site performance for scenarios with mitigation.

We considered a single monitoring method - surface seismic monitoring, though the approach can accommodate scenarios with multiple monitoring techniques and options for joint interpretation of

Table 2. Classes (i.e., states) of the leakage mass nodes in the Bayesian network and the corresponding intervals of the leakage mass values in metric tons.

Classes of leakage mass nodes	Intervals of leakage mass values (metric tons)
Negligible	[0, 10]
Low	(10, 100]
Medium	(100, 1 000]
High	(1 000, 10 000]
Very high	(10 000, 100 000)

Table 3. Two hypothetical scenarios for assumed minimum detectable CO_2 leakage masses (i.e., detection thresholds) for each monitored depth interval.

	Detection thresholds (CO_2 mass in metric tons)	
Aquifer (depth)	Low-threshold monitoring option(tons)	High-threshold monitoring option(tons)
1: Ironton–Galesville (1 044 m)	10 000	10 000
2: Potosi (936 m)	1 000	10 000
3: New Richmond (742 m)	100	1 000
4: St Peter (592 m)	10	100

those. The minimum CO_2 leakage mass that can be detected (i.e., the detection thresholds) by the surface seismic monitoring at the depths of each of the four aquifers were defined to derive the conditional probabilities for the monitoring node. Based on previous modeling work assessing the leak-detection capabilities of surface seismic monitoring using leakage simulations at the FutureGen 2.0 site,[35] it is estimated that 10 000 tons of CO_2 at the depth level of aquifer 1 (i.e., the Ironton–Galesville sandstone) can be detected by surface seismic monitoring using a high-density acquisition geometry if the signal-to-noise ratio of the seismic data is sufficiently high. For CO_2 plume at the depth levels of aquifers 2, 3, and 4, we assume the minimum detectable CO_2 leakage masses are 1000, 100, and 10 tons for the low-threshold monitoring option and 10 000, 1000, and 100 tons for the high-threshold monitoring option (Table 3).

In this study, mitigation is represented simply as an assumed instantaneous reduction in the effective permeability of the leaky wells to effectively zero. The conditional probability of the mitigation node is derived based on the assumption that if the monitoring observations suggest no CO_2 plume, mitigation will not be conducted; if the monitoring observations suggest there is CO_2 plume in any of the four aquifers, mitigation will be conducted in 90% of cases. This mitigation rate allows for cases such as CO_2 migration into deeper aquifers where decision makers may decide that mitigation is not warranted. The last node: CO_2 leakage mass out of the defined containment envelope after 70 years following mitigation is equal to the fifth node on the left of the graph (i.e., the simulated CO_2 leakage mass out of the defined containment envelope after 70 years using NRAP-Open-IAM without considering mitigation) in cases where no mitigation is conducted, but equal to the fourth node on the left (i.e., the simulated CO_2 leakage mass out of the defined containment envelope at time t using NRAP-Open-IAM) if mitigation has been conducted. The underlying assumption is that the mitigation activity will take the form of an engineering intervention to stop further CO_2 leakage out of the containment envelope, but the amount of CO_2 that has leaked out of the containment envelope up until the time of mitigation will remain the same after mitigation.

The BN model constructed for the smaller containment envelope is similar to that for the larger containment envelope, but has three nodes, instead of five nodes on the left of the graph. The leakage mass into aquifers 2, 3, and 4 is aggregated to represent the leakage mass out of the containment envelope.

The probabilities of the states in each node are calculated by propagating the prior probabilities downward through the conditional probability tables. Figure 4 shows the constructed Bayesian networks for the defined larger containment envelope and the smaller containment envelope for the initial model setup, based on the 10 000 NRAP-Open-IAM realizations. The probability of containment after considering monitoring and mitigation can be calculated from the distribution of the cumulative CO_2 leakage mass out of the defined containment envelope after 70 years following mitigation. For the 99.9% storage criterion, the maximum allowed leakage mass out of the containment envelope is 22 000 tons, which includes the negligible, the low, the medium and the high states in the leakage nodes on the Bayesian Networks. The probability of containment is calculated as:

$$\text{prob}\left(\text{containment}|99.9\%\ \text{storage}\right) = \text{prob}\left(\text{negligible}\right) + \text{prob}\left(\text{low}\right) + \text{prob}\left(\text{medium}\right) + \text{prob}\left(\text{high}\right)$$

For the 99.99% and the 99.999% storage criteria, the maximum allowed leakage masses are 2200 and 220 tons, respectively. The probability of containment for each storage criterion is calculated as:

$$\text{prob}\left(\text{containment}|99.99\%\ \text{storage}\right) = \text{prob}\left(\text{negligible}\right) + \text{prob}\left(\text{low}\right) + \text{prob}\left(\text{medium}\right)$$

$$\text{prob}\left(\text{containment}|99.999\%\ \text{storage}\right) = \text{prob}\left(\text{negligible}\right) + \text{prob}\left(\text{low}\right)$$

When monitoring observations are obtained during site operation, the new monitoring information can be entered in the Bayesian networks and the probabilities of the states of each node are updated based on the Bayes' rule. The updated probability of containment based on the monitoring observations can be calculated from the top node on the right of the BN graph.

We evaluated the probability of containment for different scenarios using 99.9, 99.99, and 99.999% as the respective containment effectiveness criteria and for each of the two defined monitoring scenarios to demonstrate the functionality of the constructed Bayesian networks. The initial model setup reflects results generated from the NRAP-Open-IAM realizations and the assumed detection thresholds for surface seismic monitoring based on scientific studies using the site characterization data. When repeated seismic monitoring observations are obtained during site operation, the evaluated probability of containment was updated in the Bayesian network by entering leakage detection findings for the relevant nodes. For example, if the monitoring observations suggest no CO_2 plume in any of the aquifers, the probability of the "not detected" state in the monitoring node will be changed to 100% (Fig. A3 in the Supporting Information Appendix) and if the monitoring observations suggest there is CO_2 plume in one or more of the monitored intervals, the probability of the "detected" state in the corresponding monitoring node will be changed to 100% (Fig. A4).

We demonstrate the updated probability of containment for scenarios in which (a) no CO_2 leakage plumes are found by surface seismic monitoring; (b) CO_2 leakage plumes are detected by surface seismic monitoring but no mitigation strategies are applied; and (c) CO_2 leakage plumes are detected by surface seismic monitoring and mitigation strategies are applied at the time of the plume detection.

In the base case, the monitoring nodes in the Bayesian network represent whether or not the CO_2 plume is detected by surface seismic monitoring. If additional information about the CO_2 plume, such as the interval into which CO_2 is leaked and the CO_2 mass of the plume, is obtained by inversion of the monitoring data, this additional information can be entered in the Bayesian network to further constrain the estimated distribution of CO_2 mass leakage out of the containment envelope and update the computed probability of containment after 70 years. We demonstrate how the additional information can be used in the Bayesian network for a single example scenario for the larger containment envelope, supposing the inversion results from the low-threshold monitoring option suggest there is CO_2 in aquifer 2 with an amount larger than 10 kt (i.e., the 'very high' class in the leakage mass node), and the amount of CO_2 in other aquifers is below the detection thresholds of the low-threshold monitoring option.

Results

Initial evaluation

The initial evaluation using the 10,000 NRAP-Open-IAM realizations shows that the probability of containment after 70 years for the larger containment envelope and the smaller containment envelope is 1.0 and 0.975 for the 99.9% storage criterion, 0.94 and 0.053 for the 99.99% storage criterion, and drops to 0.2 and 0 if the 99.999% storage criterion is chosen (Table 4), based on the empirical CDF of the simulated leakage mass out of the containment envelope after 70 years (Fig. 3). The results indicate that the defined storage envelope and the selected storage criterion can greatly influence the evaluation results of the storage complex effectiveness. Figure A1 of the Appendix shows the calculated descriptive statistics (mean, median, 75th, and 99th percentiles) from the 10 000 NRAP-Open-IAM realizations of the leakage mass from each leaky well into the four aquifers as a function of time since the injection starts. Simulated leakage from the injection well starts earlier and is greater in magnitude than that

Table 4. Initial site containment performance evaluation results based on results from 10 000 NRAP-Open-IAM system model realizations.

Storage criterion	Probability of containment: Larger containment envelope	Probability of containment: Smaller containment envelope
99.9% (allowed leakage = 22 000 tons CO_2 of 22 MMT total injected)	1	0.975
99.99% (allowed leakage = 2 200 tons CO_2 of 22 MMT total injected)	0.94	0.053
99.999% (allowed leakage = 220 tons CO_2 of 22 MMT total injected)	0.2	0

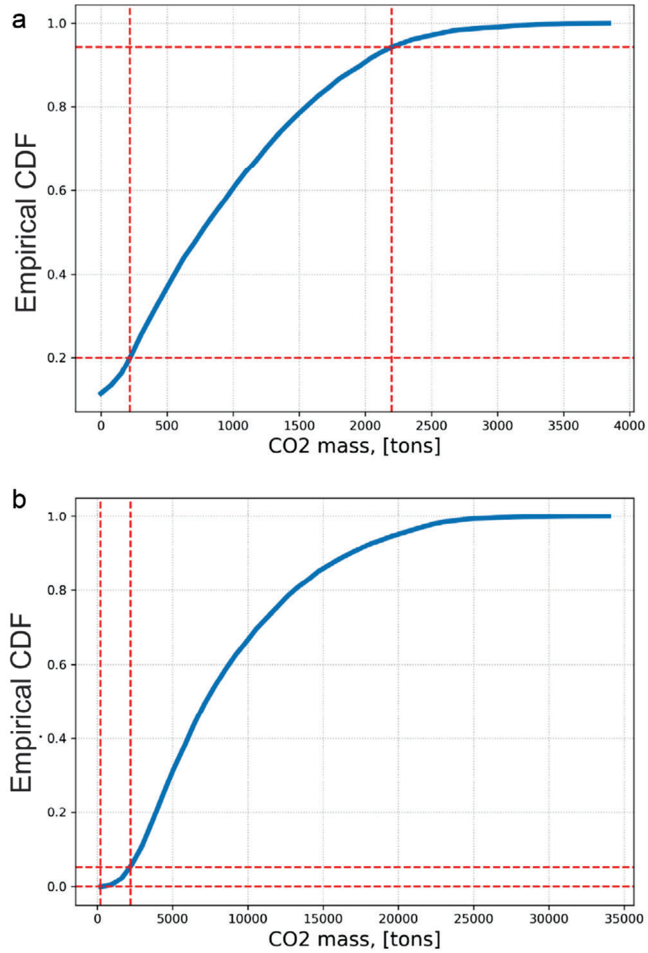

Figure 3. Empirical cumulative density function (CDF) of the simulated mass leakage out of (a) the defined larger containment envelope, which includes the storage reservoir and aquifers 1, 2, and 3; and (b) the defined smaller containment envelope, which includes the storage reservoir and aquifer 1, after 70 years based on 10 000 NRAP-Open-IAM realizations. The red dashed lines show how the probability of containment corresponding to each storage criterion is obtained from the empirical CDF for the defined containment envelope.

from the stratigraphic well. The largest amount of leakage reports to aquifer 2 (i.e., Potosi), followed by aquifer 4 (i.e., St Peter), aquifer 3 (i.e., New Richmond), and aquifer 1 (i.e., Ironton–Galesville). The 99th percentile values represent the simulated leakage magnitudes for unlikely leakage scenarios of greatest potential impact based on the characterized effective permeability for intact, leaky wells.

Updated evaluation by monitoring

Baseline scenario

The BN graphs of the defined containment envelope with the two monitoring options for the initial model setup are shown in Fig. 4 and Fig. A2 of the appendix, respectively. The baseline scenario does not consider monitoring and mitigation, which is calculated from the top left node on the BN graphs. The green bars in Fig. 5 shows the computed probability of containment at the defined larger containment envelope and the smaller containment envelope using 99.9%, 99.99%, and 99.999% storage criterion for the baseline scenario. For the 99.9% storage criterion, the probability of containment is 1 and 0.67 for the larger containment envelope and the smaller containment envelope, respectively. While for other higher storage criteria considered (i.e., 99.99% and 99.999%), the probability of containment for the smaller containment envelope quickly drops to a very low value and is much lower than that of the larger containment envelope. The chosen storage containment effectiveness criterion has a large effect on the evaluated probability of meeting containment objectives. For example, at the 99.9% storage criterion, the probability of containment for the larger containment envelope at the FutureGen 2.0 site is 1, while at 99.999% storage criterion, the probability of containment drops to 0.14. The estimated probability of containment using the Bayesian networks for the baseline scenario is lower than that in the initial evaluation using only NRAP-Open-IAM simulations due to the discretization of the leakage mass values in the Bayesian networks. Note that the

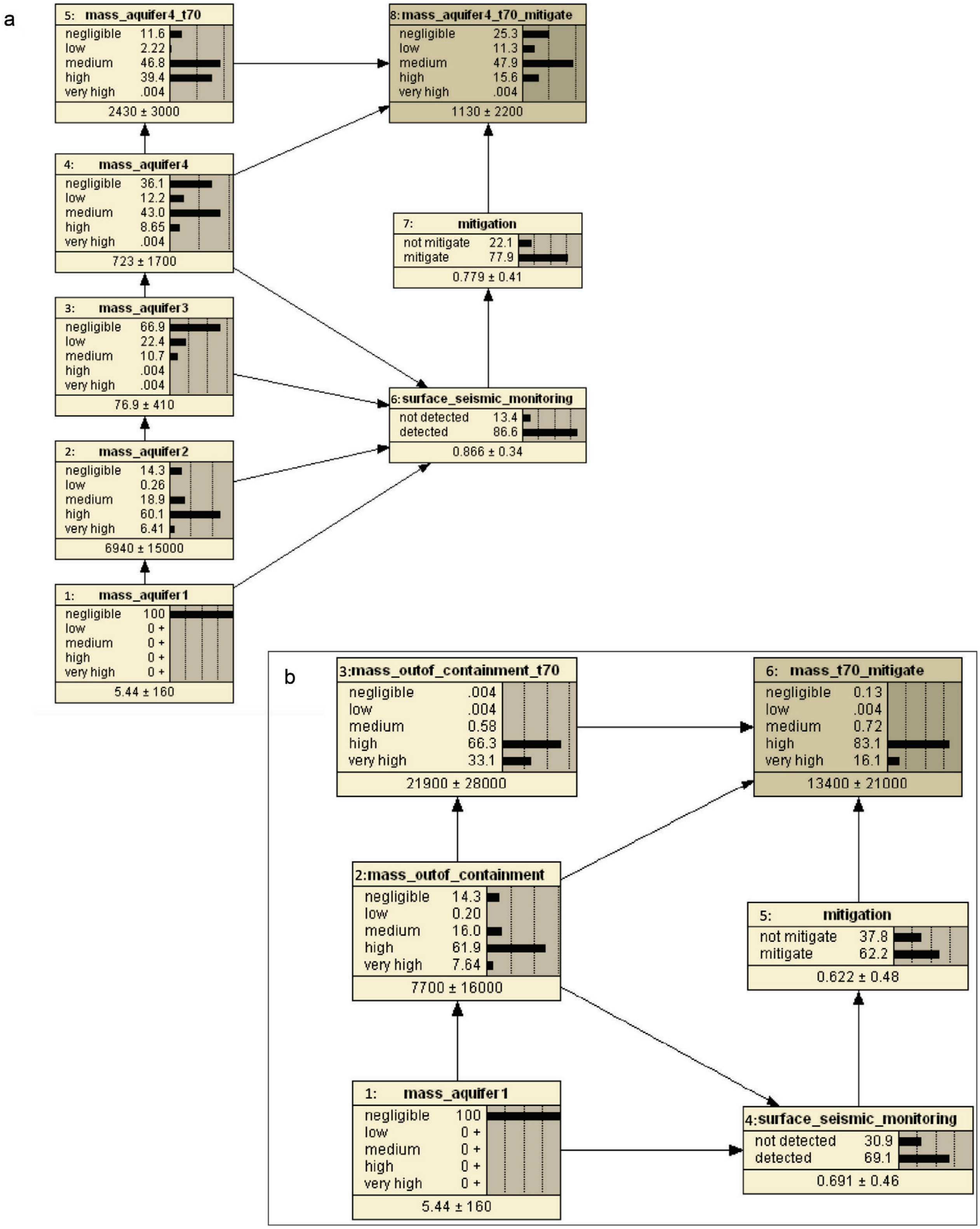

Figure 4. Bayesian network graphs of (a) the larger containment envelope and (b) the smaller containment envelope for the low-threshold monitoring option in the initial model setup. The larger containment envelope includes the storage reservoir and aquifers 1, 2, and 3; the smaller containment envelope includes the storage reservoir and aquifer 1.

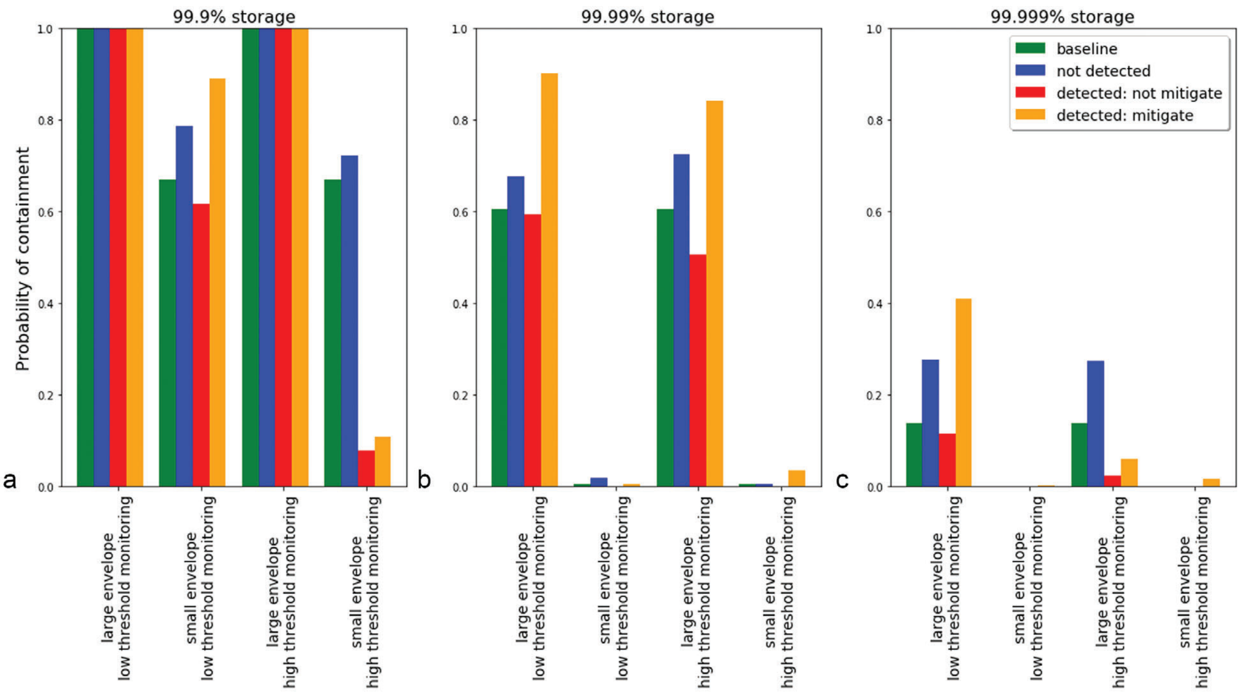

Figure 5. Probability of containment for the larger containment envelope and the smaller containment envelope using the low-threshold monitoring option and the high-threshold monitoring option for the baseline scenario, in which no monitoring and mitigation is considered; the 'not detected' scenario, where monitoring observations suggest no CO_2 plume; the 'detected: not mitigate' scenario, where monitoring observations suggest there is CO_2 plume but no mitigation is conducted; and the 'detected: mitigate' scenario, where monitoring observations suggest there is CO_2 plume and mitigation is conducted at the time of detection: (a) evaluated at the 99.9% storage criterion; (b) evaluated at the 99.99% storage criterion, and (c) evaluated at the 99.999% storage criterion.

assumed effective permeabilities of the two leaky wells were fairly high (ranging from 10^{-14} m^2 to 10^{-12} m^2) compared to other studies, so the estimated leakage risks are relatively high. The predicted most likely leakage class after 70 years is medium (i.e., between 100 and 1000 tons) and high (i.e., between 1000 and 10 000 tons) for the larger containment envelope and the smaller containment envelope, respectively.

Scenarios of plume detection and mitigation

The updated probability of containment for various scenarios with monitoring observations entered is compared with the baseline scenario in Fig. 5. For all the scenarios evaluated, the probability of containment is close to 1 if the larger containment envelope and the 99.9% storage criterion are chosen (Fig. 5). For the defined smaller containment envelope, the probability of containment decreases greatly if the monitoring observations suggest there is CO_2 plume in aquifers out of the containment envelope, and the operator choose to not mitigate, especially for the high-threshold monitoring option. The probability of containment for the low-threshold monitoring option is higher than that for the high-threshold monitoring option, which is due to the lower detection thresholds (i.e., higher detection capabilities) assumed for the low-threshold monitoring option. This indicates that reducing the detection thresholds of the deployed surface seismic monitoring will increase the probability of the containment effectiveness at the site. The probability of containment for the 'not detected' scenario is always higher than that in the baseline scenario, suggesting that monitoring can improve our confidence in the estimated containment. If the monitoring observations suggest no CO_2 plume in the aquifers, it is more likely that CO_2 is contained in the storage complex and the probability of containment is higher than that of the 'detected: not mitigate' scenario, but may be lower than that of the 'detected: mitigate' scenario in some cases. The probability of containment for the smaller containment envelope is extremely low at the 99.99% and the 99.999% storage criterion for the scenarios considered. For the larger containment envelope, if the monitoring observations suggest there is CO_2 plume, but no mitigation is conducted, the posterior probability of containment after 70 years decreases at both the 99.99% and the 99.999% storage criterion. The decrease is larger for the high-threshold monitoring option than that for the low-threshold monitoring option due to the lower resolution (i.e., larger detection thresholds) of the high-threshold monitoring option, compared to that of the low-threshold monitoring option. If the high-threshold monitoring option detects the CO_2 plume, it is more likely that the amount of leakage mass has been larger. In cases where a decrease in the probability of containment below an a priori assumption is suggested by monitoring observations, some fraction of the credits that have been previously claimed for effective containment may need to be refunded (termed "recaptured" of credits in some instances). For example, at the 99.9% storage criterion, the probability of containment for the smaller containment envelope using the low-threshold monitoring option decreases from 0.67 in the baseline scenario to 0.08 when the high-threshold monitoring option detects the CO_2 plume and no mitigation is conducted. If the monitoring observations suggest there is CO_2 plume and mitigation strategies are applied at the time of detection to stop further leakage from the storage envelope, the probability of containment increases slightly compared to the baseline for the larger containment envelope at the 99.99% storage criterion, while decreases at the 99.999% storage criterion using the high-threshold monitoring option with lower resolution in detecting the CO_2 plume. In general, the probability of containment is much higher with mitigation, compared to monitoring without mitigation. The Bayesian network graphs for the monitoring and mitigation scenarios considered are included in the Supporting Information Appendix (Figs A3 and A4).

Effect of additional information from monitoring

In the previous section, the information used from surface seismic monitoring is whether there is CO_2 plume in the modeled system or not. In this example scenario, we assume that the low-threshold monitoring option is not only able to detect there is CO_2 plume in the modeled system, but also infer with confidence that the CO_2 plume is in aquifer 2 with the mass of larger than 10 kt. We further assume that the CO_2 mass in other aquifers is below the detection thresholds of the low-threshold monitoring option. The Bayesian network graph of the larger containment envelope for this example scenario is shown in Fig. 6. On the Bayesian network graph, in addition to changing the probability of the 'detected' state in the monitoring node to 100%, the probability of the 'very high' class in the node for leakage mass into aquifer 2 is also changed to 100% and the probabilities for classes higher than the detection thresholds of the low-threshold monitoring option in the nodes for leakage mass into aquifers 3 and 4 are changed to 0. Comparing the node "mass_aquifer4_t70" on the BN graph for the 'detected only' scenario (Fig. A4a) with that for the 'detected and located' scenario (Fig. 6) shows that the added depth interval and mass information about the CO_2 plume inferred from the monitoring method has significant effects on the distribution of the predicted CO_2 mass out of the containment envelope after 70 years, with the increased probabilities for relatively small mass values and decreased probabilities for relatively large mass values. Figure 7 compares the probability of containment after 70 years for the larger containment envelope using the low-threshold monitoring option at the 99.9%, 99.99%, and 99.999% storage criterion for the example scenario with depth interval and mass information inferred from the monitoring data vs. only knowing there is CO_2 plume in the modeled system from the monitoring method. The estimated probabilities of containment after 70 years at the 99.9%, 99.99%, and 99.999% storage criterion with the added information from monitoring are higher than those with only the information about detectability from the monitoring method (same as the red bars of the 'large envelope, low threshold monitoring' group in Fig. 5).

Discussion

The findings entered in the Bayesian network about the depth and the CO_2 mass observations require inversion from surface seismic data. At the current state of technology, relatively large uncertainty in the geophysical inversion results can exist, especially for quantitative inversion of the CO_2 plume.[14,36,37] Joint inversion or joint interpretation of data from multiple monitoring methods, including both the indirect geophysical monitoring data and the direct downhole measurements might improve the accuracy of the estimated depth interval and the CO_2 mass. Also, brine migration, which might be observable using some

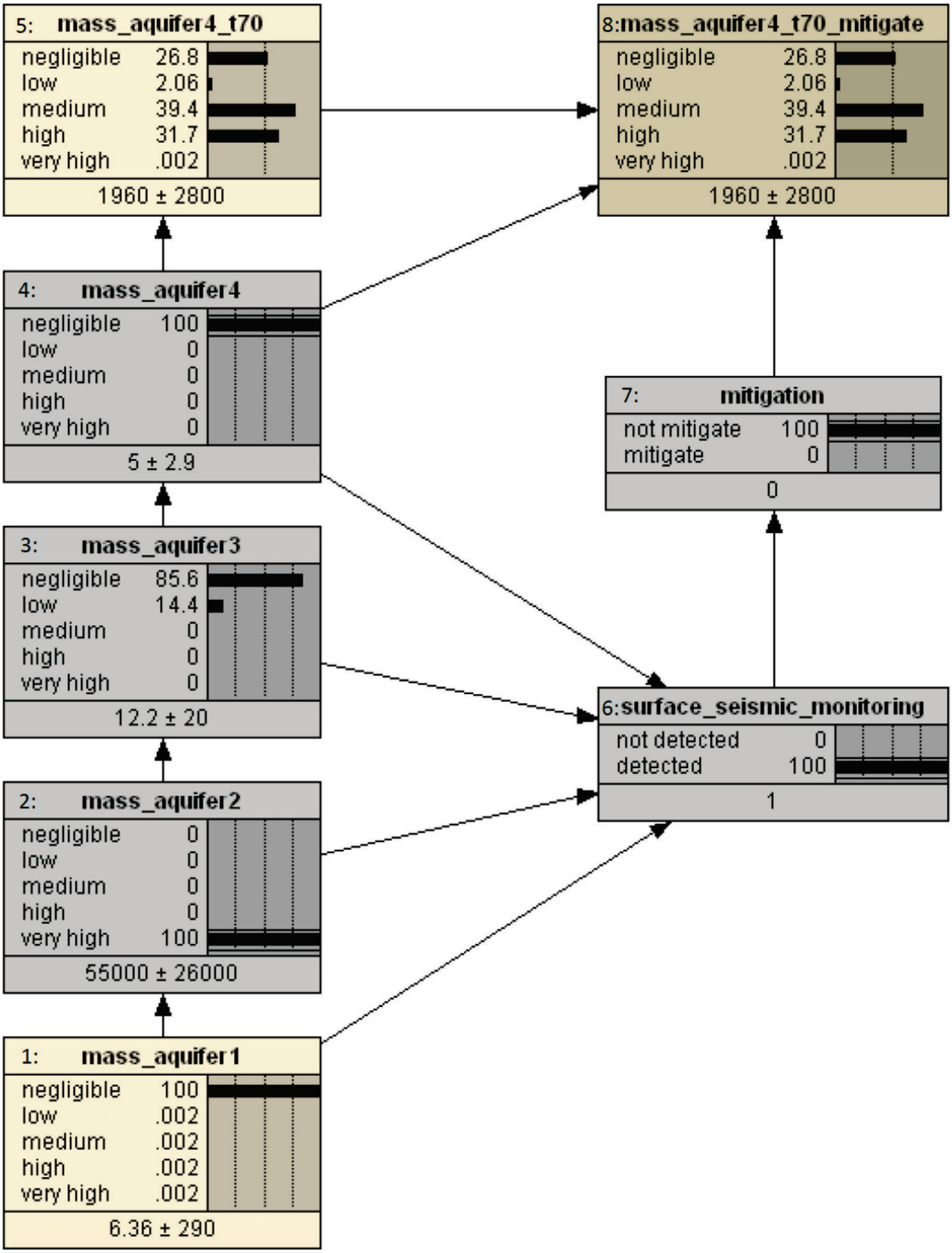

Figure 6. Bayesian network graph for the larger containment envelope with the low-threshold monitoring option for an example scenario showing the effect of additional information from the monitoring method.

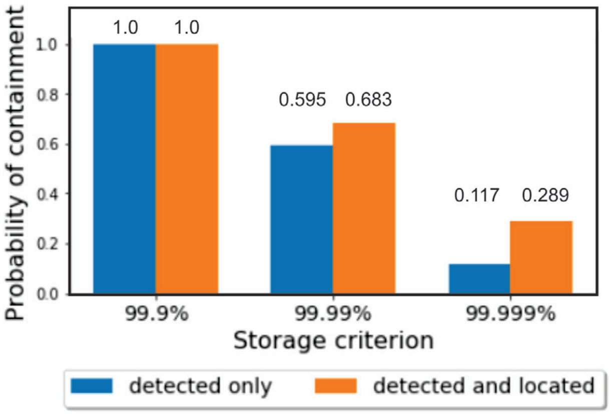

Figure 7. Comparison of the probability of containment after 70 years for the larger containment envelope using the low-threshold monitoring option between the example scenario with depth interval and mass information inferred from the monitoring data (denoted by 'detected and located') and the scenario only knowing there is CO_2 plume in the modeled system from the monitoring method (denoted by 'detected only', same as the red bars of the "large envelope, low threshold monitoring" group in Fig. 5).

geophysical techniques before CO_2 begins (e.g., electromagnetic conductivity) could be a useful means of early fluid migration and inference of future CO_2 migration. Recently, machine learning methods have been applied in various aspects related to seismic imaging and inversion.[38–42] For example, Zhou *et al*.[41] used convolutional neural networks to learn the relationship between simulated seismic data and the CO_2 mass based on flow simulations for a model storage site. If the monitoring method can more effectively provide information about the CO_2 plume (such as the detectability, the depth interval or the CO_2 mass) and also the probabilities associated with the observations (i.e., likelihood findings), these observations and the corresponding probabilities can be entered in the Bayesian network together to make probabilistic inferences and to further update the estimated probability of containment.

This study uses surface seismic monitoring as an example monitoring technique to demonstrate the usability of the Bayesian network. Nodes for other monitoring methods, such as the gravity monitoring, electrical resistivity tomography, or direct downhole pressure and TDS measurements, can be added to the Bayesian network when the detection thresholds and observations from these monitoring methods are available at the geologic carbon storage site. The Bayesian network method may have value for considering different monitoring alternatives, such as multiple monitoring techniques with joint interpretation/joint inversion, different array densities, for early leakage diagnosis and mitigation, and for supporting decisions about which monitoring technique to use at a site.

The performance of the Bayesian network largely depends on the training dataset, which requires thousands of realizations from physics-based simulations of geologic storage site performance. The NRAP-Open-IAM code enabled the calculation of several thousand realizations for the CO_2 storage system within a few hours on a desktop computer. The evaluation results presented in this study are based on 10 000 NRAP-Open-IAM realizations, but larger sets of realizations would be computationally accessible using this approach and would likely increase the stability and the prediction accuracy of the Bayesian network.

The current release of the NRAP-Open-IAM tool considers only wells as potential leakage pathways; functionality to support simulating leakage through faults or fractures otherwise low-permeability aquitard intervals is forthcoming. As mentioned in the leakage simulations section, the range of well permeabilities assumed for the leaky wells were relatively high, resulting in the relatively large mass leakage out of the containment envelope. Refinement of a priori well permeability estimates will improve forecasting and decision making around containment and leakage risk. Since our principal objective in this paper is to demonstrate the workflow for evaluating the probability of containment effectiveness using NRAP-Open-IAM and Bayesian networks, the multi-phase flow reservoir simulations over 70 years of total site performance were employed to train the reduced-order models in NRAP-Open-IAM. Further application of this workflow with simulations over much longer time (e.g., 1000 years) should allow the evaluation to be conducted with greater insight for real site application.

Future work could expand on the approach presented herein to use monitoring inversion results to update assumed distributions of uncertainty parameters used in forward simulations.[43] Consideration of additional mitigation alternatives and more detailed consideration of how monitoring information can be used to inform mitigation decisions is warranted. Finally, it would be valuable to test and extend the approach presented herein for brownfield cases (e.g., CO_2 enhanced oil recovery sites) with many potentially leaky wells.

Summary and conclusions

In this study, we have developed a workflow to evaluate the probability of containment effectiveness at a geologic carbon storage site using NRAP-Open-IAM and Bayesian networks. The initial evaluation is based on 10 000 NRAP-Open-IAM realizations designed for the FutureGen 2.0 site, forecasting the leakage risks at the injection well and at an offset stratigraphic well. Representations of site monitoring and mitigation through the site operation phase were then incorporated into the framework for assessing the probability of containment using Bayesian networks. Distinct BNs were constructed to represent different storage envelops that might be defined by the operator. Two scenarios for surface seismic monitoring detection thresholds were considered. We evaluated and compared the probability of containment for multiple scenarios at the 99.9%, 99.99%, and 99.999% storage criterion. Our results indicate that the defined containment envelope and the selected storage criterion greatly influence the estimated probability of containment. For all the scenarios evaluated, the probability of containment is close to 1 if the larger containment envelope and the 99.9% storage criterion are chosen. For the defined smaller containment envelope, the probability of containment is high at the 99.9% storage criterion but decreases greatly at the 99.99% and 99.999% storage criterion. Monitoring can improve our confidence in the estimated containment. In general, the probability of containment is much higher in scenarios where the decision to mitigate is enabled, as compared to monitoring without mitigation. This suggests the importance of considering mitigation in response to observed behavior (i.e., CO_2 plume detection) in the system to ensure effective containment (though there are many factors contributing to operator's decision making about mitigation). The estimated probability of containment can be further updated if monitoring method can provide information about the depth interval and the mass of the CO_2 plume, in addition to simply detecting the presence of a plume. This evaluation workflow provides a simple example of how GCS practitioners might use physics based, site-specific forecasting, and monitoring evidence within a probabilistic framework to support a justification for claiming credit for long-term CO_2 containment.

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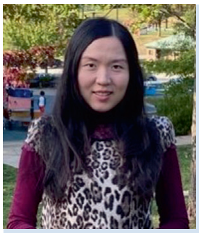

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