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Computational Tools and Workflows for Quantitative Risk Assessment and Decision Support for Geologic Carbon Storage Sites: Progress and Insights from the U.S. DOE's National Risk Assessment Partnership

Robert M. Dilmore[a], Delphine Appriou[b], Diana H. Bacon[b], Christopher F. Brown[b], Abdullah Cihan[c], Erika Gasperikova[c], Kayla Kroll[d], Curtis M. Oldenburg[c], Rajesh J. Pawar[e], Megan M. Smith[d], Brian R. Strazisar[a], Dennise Templeton[d], R. Burt Thomas[a], Veronika S. Vasylkivska[a,f], Joshua A. White[d]

[a] *National Energy Technology Laboratory, Research & Innovation Center, 626 Cochrans Mill Road, P.O. Box 10940, Pittsburgh, PA 15236*
[b] *Pacific Northwest National Laboratory, Earth Systems Science Division, 902 Battelle Blvd, Richland, WA 99354*
[c] *Lawrence Berkeley National Laboratory, Earth & Environmental Sciences Area, 1 Cyclotron Road, Berkeley, CA 94720*
[d] *Lawrence Livermore National Laboratory, Atmospheric, Earth and Energy Division, 7000 East Ave., Livermore, CA 94550-9234*
[e] *Los Alamos National Laboratory, Earth and Environmental Sciences Division, P.O. Box 1663, Los Alamos, NM 87545*
[f] NETL Support Contractor, P.O. Box 10940, Pittsburgh, PA 15236

Abstract

The 2005 Intergovernmental Panel on Climate Change (IPCC) Special Report on CCS raised the profile of CO_2 capture and storage (CCS) as an important technology for reducing greenhouse gas (GHG) emissions. CCS is now recognized as a key component of most climate change mitigation scenarios. Since publication of that report the international research, development, and deployment (RD&D) community has advanced key technical aspects, clarified regulatory requirements, explored value chain and infrastructure solutions, and developed incentive paradigms to enable and promote large-scale deployment of CCS. These efforts have included research to better characterize geologic storage resources, to improve injection performance and storage efficiency, to assess and manage subsurface environmental risks, and to advance monitoring technologies to assure system conformance. These efforts have helped to build confidence in the viability of geologic carbon storage (GCS), but stakeholder concerns about long-term risks and liability associated with GCS remain a hurdle to broad acceptance and large-scale deployment of CCS.

Since 2010, the U.S. DOE's National Risk Assessment Partnership (NRAP) – a research collaboration between five contributing national laboratories – has worked to establish and demonstrate methods and tools to quantify and manage the subsurface environmental risks associated with GCS, amidst uncertainty. This work supports the Office of Fossil Energy and Carbon Management Carbon Transport and Storage Program's goal of advancing safe and secure commercial-scale GCS deployment. To address the technical challenge of simulating the physical response of the GCS site to large-scale CO_2 injection, NRAP has adopted an approach that relies on coupling computationally efficient reduced-order and/or data-driven proxy models of important system components (i.e., storage reservoir, sealing caprock, leakage pathways, intermediate formations, overlying groundwater aquifers, and the atmosphere) in an integrated assessment framework. That integrated model of the physical system is complemented with fit-for purpose functionality to support site characterization and risk-related decisions. The recently released NRAP Phase II toolset includes the Open-Source Integrated Assessment Model (NRAP-Open-IAM) for evaluation of trends in leakage risk and potential impact, tools to support monitoring design optimization (Designs for Risk Evaluation and Management – DREAM v3.0 and Passive Seismic Monitoring Tool - PSMT), and tools for state of stress evaluation (State-of-Stress Analysis Tool - SOSAT) and forecasting induced seismicity risk. The NRAP team has also released a pair of reports describing conceptual workflows to incorporate physics-based, quantitative risk assessment into many of the design, planning, operation, and closure decisions for GCS projects. An online catalogue highlights published studies where these tools and methods are demonstrated. In this presentation, the utility of these products to assess risks and address key stakeholder questions will be highlighted through examples, and related insights about the safety and security of geologic carbon storage in qualified storage sites will be discussed.

The prospect of rapid, large-scale deployment of GCS technology to aggressively reduce anthropogenic CO_2 emissions requires careful consideration of interference between multiple commercial-scale storage projects within a basin. Going forward, NRAP is expanding and adapting site-scale risk quantification tools and methods to enable assessment of risks and inform management decisions for basin-scale deployment. Increasingly, this work will leverage next-generation approaches for surrogate modelling, fast prediction, and advanced visualization enabled by machine learning and artificial intelligence to promote virtual learning, scenario evaluation, and augment risk-based decision making.

Keywords: quantitative risk assessment, geologic carbon storage, carbon capture and storage, uncertainty, monitoring, integrated assessment modeling, leakage, induced seismicity

Nomenclature

AoR	Area of Review
CCS	Carbon capture and storage
DOE	Department of Energy
GCS	Geologic carbon storage
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
NETL	National Energy Technology Laboratory
NRAP	National Risk Assessment Partnership
PISC	Post-Injection Site Care
PNNL	Pacific Northwest National Laboratory

1. Introduction

Carbon capture and storage (CCS) is recognized as an important technology in many climate change mitigation scenarios [1]–[4]. To enable large-scale implementation, the international CCS community has been advancing and demonstrating key technical aspects of this technology across the value chain [5]–[7]. These include developing efficient and cost-effective CO_2 capture technology [8]–[11], identifying requirements and addressing logistical challenges for transportation infrastructure [12]–[15], and building the science base, regulatory frameworks, incentive structures, and resource capacity to safely and permanently store meaningful quantities of CO_2 [3], [7], [16], [17]. Additionally, there remains a critical need to build confidence among the public and other stakeholders that geologic CO_2 storage (GCS) is a safe and reliable technology [7]. To meet this need, the CCS community needs to effectively translate the substantial existing scientific and engineering knowledge from research, field demonstration, and analogous industrial experience into tools and protocols to promote risk communication between stakeholders and support risk-related decision making.

It is generally accepted that the risks for a GCS project can be expected to increase through the period of active injection, peak near the end of injection, and diminish thereafter [18]. Temporal and spatial evolution and magnitude of those risks will be governed by the laws of physics but will vary as a function of site-specific geologic characteristics, site development history disposition, and operator decisions. To effectively assess and manage subsurface risks, therefore, requires development of physics-based, site-specific quantitative risk assessment methods and tools that can effectively communicate about risks and inform decision making amidst uncertainty [19]. This need has motivated a substantial body of research [20], [21].

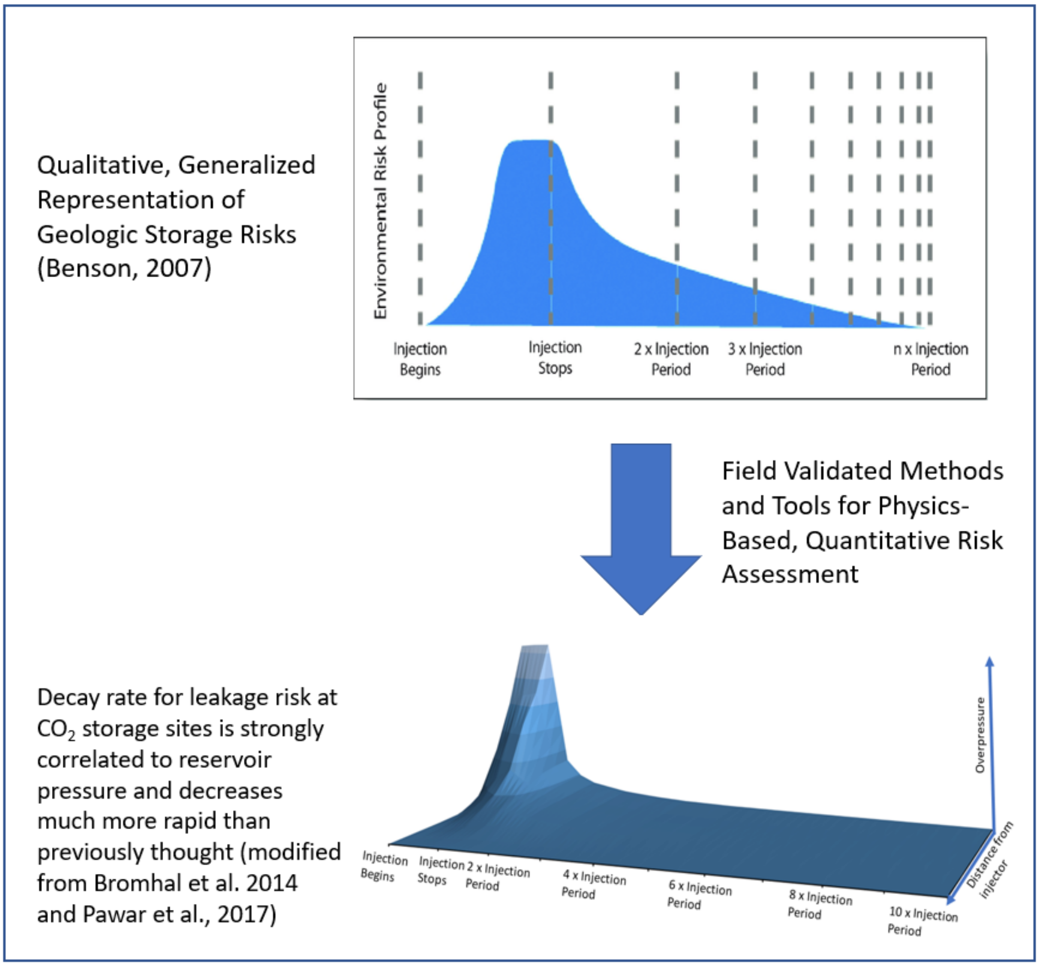

Figure 1. Representation of the evolution of the state of knowledge and ability to quantify time-varying subsurface environmental risks at a geologic carbon storage site (top from [18] ; bottom modified from [22], [23])

In 2010, the U.S. Department of Energy (DOE) Office of Fossil Energy (now the Office of Fossil Energy and Carbon Management) established the National Risk Assessment Partnership (NRAP) - a research collaboration among five national laboratories (Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), the National Energy Technology Laboratory (NETL), and Pacific Northwest National Laboratory (PNNL)), tasked with developing approaches to quantify and manage the subsurface environmental risks associated with GCS to aid in deployment of large-scale GCS. A first phase of NRAP (2010-2016) focused on establishing the science base and developing first-of-kind methods and prototype tools to quantitatively assess subsurface environmental risks at GCS sites, i.e., risks associated with potential unintended fluid migration and induced seismicity. Accomplishments from NRAP's Phase-I efforts [24] included:

- developing a computational integrated assessment framework to quantify potential leakage risks and groundwater impacts at GCS sites and generating the first quantitative risk profiles encompassing an entire GCS system [25];
- innovating reduced-order modeling approaches to rapidly quantify subsurface GCS site performance amidst uncertainty [26]–[33];
- identifying relevant probabilistic seismic risk analysis approaches [34] and creating the first comprehensive risk model for induced seismicity at GCS sites (Foxall et al., 2013);
- developing insights into reservoir-risk relationships [22], [35], [36] and well integrity for GCS sites [29], [37];
- establishing methods to determine statistically significant groundwater quality changes indicating impact [38], [39]; and
- providing preliminary insights into the utility of select monitoring approaches [40] and exploring the potential for optimization of monitoring design [41].

Phase-II work has been focused on refining risk assessment tools and methods to enable dynamic risk evaluation and uncertainty reduction, and support risk management decisions. This article is intended to provide a summary of the approach and accomplishments of NRAP Phase II research.

2. Methods

NRAP's approach to quantifying GCS subsurface environmental risks relies on stochastic modeling for forecasting of full system behavior of a GCS site while taking into account site-specific uncertainty and variability. This system, as illustrated in Figure 2, includes not only the primary storage reservoir, but also potential migration pathways (wells, boreholes, faults, fractures), and receptors of concern (groundwater aquifers and the atmosphere). This research uses various fit-for-purpose computational approaches to enable rapid and credible characterization of important system attributes and behavior over time. These approaches describe performance in the context of uncertainty and can be used to constrain critical uncertainties, to improve understanding of likely site behavior, and support decision-making. These methods include:

- Full physics numerical simulation (e.g., [22], [42], [43]), reduced-order modeling; [44], [45]; and reduced-physics and analytical approaches [37], [46], [47] that describe the physical behavior and quantify effect of uncertainties in parameters on system behavior;
- Integrated assessment modeling that couples computationally efficient models of GCS system components to allow forecasting and uncertainty quantification of site-scale subsurface system behavior [48]–[52];
- Modeling of monitoring, including demonstration of approaches for full-physics and data-driven inversion of geophysical data to evaluate detectability of potential leakage from containment [53]–[59];
- Bayesian approaches to constrain uncertainty as new observational information becomes available [28], [57], [60], [61];
- Optimization approaches for design of effective monitoring [41], [53], [62];
- Approaches to identify useful site performance and risk metrics and trends, and build functionality for stakeholder decision support [22], [36], [63]–[68]; and
- Focused laboratory, simulation, and field experiments to constrain key uncertainties in GCS site performance and assessed leakage risks [69]–[75].

Methods and findings from these studies help to inform the development of open-source and publicly available computational tools and recommended practices for quantitative risk management and decision support.

A key technical challenge of GCS risk assessment is to simulate the physical response of a GCS site to full-scale injection and storage over time. Stochastic modeling of this complex system (Figure 2) with a single, internally coupled high-fidelity model is computationally intensive. To overcome this computational challenge, NRAP has adopted an integrated assessment modeling approach that relies on coupling of reduced-complexity and/or data-driven proxy models for important system components. The result is a coupled system model that enables the quantitative forecasting of risks as they evolve over time. By coupling computationally efficient reduced-order models with the integrated assessment framework, the stochastic forecasting of whole-system behavior is fast, making the integrated assessment model a useful tool for probabilistic risk quantification and decision support.

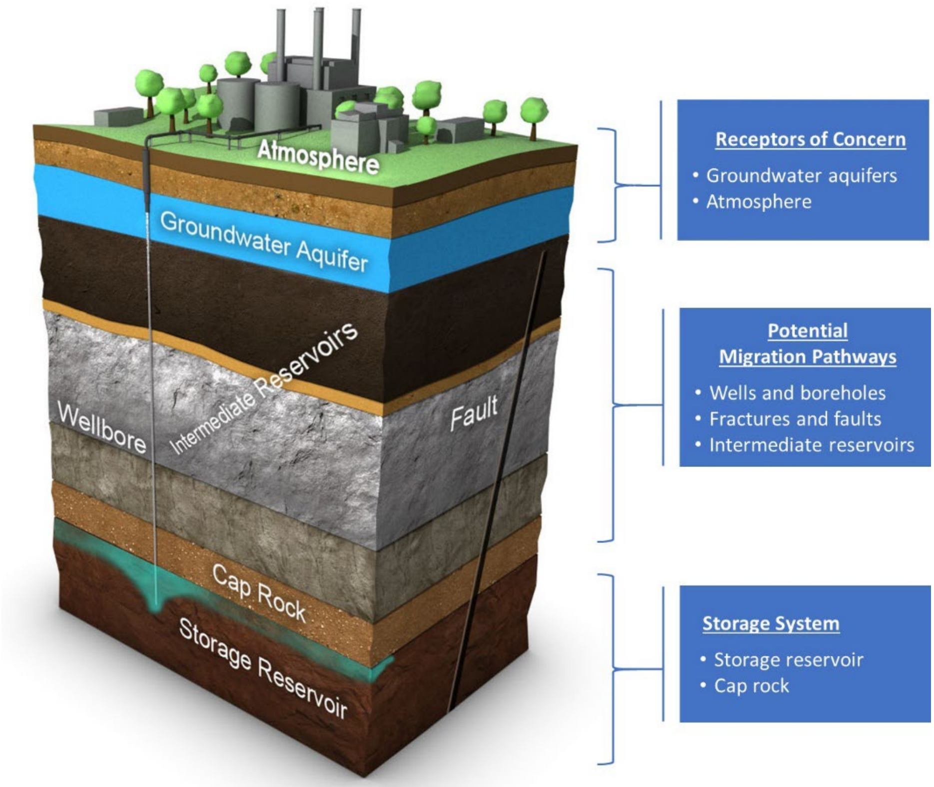

Fig. 2. Simplified schematic of geologic carbon storage site components considered in an integrated systems model for leakage risk assessment.

Concern about the potential to induce seismic activity at CO_2 storage sites in response to CO_2 injection represents a significant potential hurdle to successful large-scale deployment of GCS. Defensible, science-based tools to assess this risk and evaluate mitigation alternatives are needed to inform decision making for site selection, injection design, operations, and site closure. By developing methodologies and tools for probabilistic seismic hazard and risk assessment at CO_2 storage sites, researchers can explore the relationship between storage and induced seismicity and develop an understanding of the system uncertainties, the likelihood and impact of potential induced earthquakes, and identify injection practices and operational envelopes to effectively manage those risks. These tools also enable the evaluation of the effectiveness of select induced seismicity mitigation alternatives. Finally, development of hydrogeologic fault leakage models that are validated against field data can help to constrain uncertainties about the importance of faults as potential pathways for unwanted fluid migration.

NRAP's work related to GCS site monitoring is focused on design of adaptive, risk-based site monitoring to ensure containment, detect unwanted fluid migration, and ensure groundwater resource protection over the life of a project.

To accomplish this, NRAP has developed and demonstrated new methods for assessing the likelihood of various geophysical monitoring technologies to detect potential leakage through wells and faults. This approach calculates the monitoring signal for a large ensembles of numerical simulations of hypothetical leakage scenarios spanning varying geologic properties and leakage characteristics, and then assesses the likelihood of detection above noise for leaks of different size, composition, and depth [56], [57]. Novel research has also considered how machine learning and reduced-complexity approaches can be used for fast forecasting of geophysical signals and diagnosis of leakage. Other work has focused on designing risk-based and optimal site-scale monitoring networks that incorporate forward models of subsurface behavior (with uncertainty) and modeling of monitoring to maximize the probability of leak detection or to minimize time to detection and monitoring cost [41], [61], [76]. Finally, methods have been developed and demonstrated to use monitoring information to assess conformance of GCS operations with expected behavior and update forecasts forecasts of site performance [28], [65], [77], [78]. Future work will seek to refine these elements and incorporate them with the integrated risk assessment framework to support robust, risk-based monitoring design.

3. Results

The outcomes of NRAP research include a set of computational tools and workflows for risk management and decision support. These tools and workflows are being demonstrated with real and hypothetical case studies of increasing complexity to ensure their utility stakeholder for stakeholders.

3.1. NRAP Computational Tools for GCS Risk Assessment

The NRAP tools are intended to provide functionality for quantitative risk assessment and risk management decision support, amidst uncertainty in site performance. NRAP Phase II tools fall into three topic areas: (1) ensuring containment effectiveness/quantifying leakage risk, (2) managing induced seismicity, and (3) strategic monitoring design for uncertainty reduction. Table 1 is an index of the NRAP computational tools currently under development and refinement; a brief description of each of each tool is provided below. These tools are made freely available to the CCS research, development, and deployment community, and are largely open source. They are intended to be complementary to other commercial, regulatory, and research tools available to support site selection, permitting, and operational decisions [79].

Table 1. NRAP Phase II Tools and their functionality.

NRAP Phase II Tool	Brief Description	Release Status	Reference
NRAP Open-Source Integrated Assessment Model (NRAP-Open-IAM)	An open-source platform to simulate long-term, full-system behavior (reservoir to aquifer/atmosphere) of GCS sites and support decision-making amidst uncertainties.	v2.6.0 8/2022	[49]
Designs for Risk Evaluation and Monitoring (DREAM)	Monitoring design optimization to minimize time to first detection and cost	v3.0 Expected 9/2022	[76], [80]
State of Stress Analysis Tool (SOSAT)	Estimate of the stress tensor to evaluate the geomechanical risks of unintentional fracturing and fault reactivation, with Bayesian updating	v2.0	[81]
Passive Seismic Monitoring Tool (PSMT)	Tool for optimal design of microseismic monitoring network using surface or borehole geophones	PSMT v.1.0 11/2016	[82]
Operational Forecasting of Induced Seismicity (ORION Toolkit)	Rapid seismic hazard assessment that uses field data (microseismic, well pressure, flow rate) calibrate field or basin models and identify conditions requiring operator intervention.	Expected 12/2022	-

The flagship tool of the NRAP toolset is the NRAP open-source integrated assessment model (NRAP-Open-IAM) – an open-source software that enables quantification of containment effectiveness and leakage risk at storage sites in the context of system uncertainties and variability [49]. NRAP-Open-IAM represents the next-generation in a line of systems-based computational models developed for quantitative GCS risk assessment [25], [50], [51]. The model comprises a set of reduced-order and analytical models of various components of the GCS system: storage reservoir, sealing caprock, potential leakage pathways including wells [31], [37], [44], [83], faults and fractures [84]–[87], receptors of concern including impact to groundwater resources [27], [29], [45], [88] and leakage to intermediate geologic intervals [89] and the atmosphere [46], a framework to support stochastic simulation, scenario evaluation, and uncertainty quantification. The of NRAP-Open-IAM includes functionality to generate quantitative, probabilistic, and time-dependent profiles of the evolution of risk at GCS sites and evaluate the influence of uncertain parameters on uncertainty in forecasted risk [25], [64], [68].

The Short-term Seismic Forecasting (STSF) tool uses site-specific catalogs of measured seismicity to forecast future event frequency over the short term. STSF tool uses a model developed for the decay of aftershocks of large seismic events to determine the event rate in future time bins [82]. The model is adapted with a term to modify the background seismicity rate above a pre-determined magnitude threshold as a function of injection-related parameters (e.g., injection rate or bottom-hole pressure). This injection-related seismicity forecasting capability can be a valuable tool to complement stoplight approaches for induced seismicity risk planning and permitting.

The injection of CO_2 and associated increase in pore pressure will alter the state of stress over the course of a GCS project. These changes could potentially affect fault stability or lead to unintended hydraulic fracturing – influencing risks related to induced seismicity and potential unwanted fluid migration, respectively. To avoid and manage these risks it is important to understand in-situ stresses. However, stress measurements are often sparse resulting in considerable uncertainty in the state of stress at GCS sites. The NRAP State of Stress Analysis Tool (SOSAT) embodies a Bayesian approach to calculating a distribution of in situ stress at specific locations at a GCS site based on commonly used measurements or relationships. SOSAT then uses calculated stress state probability distributions to estimate the probability of activating a critically oriented fault over a specified range of pore pressures [60], [81]. The SOSAT tool provides value during GCS site screening and characterization phases to target collection of specific additional data to constrain uncertainties in geomechanical risk and to help operators to make informed decisions during the operational phase [90]. The capability represented in SOSAT, therefore, helps build stakeholder confidence that geomechanical risks are understood and manageable.

Designs for Risk Evaluation and Management (DREAM) is a tool for leakage monitoring design and optimization at GCS sites. NRAP's DREAM tool was developed to assist in design of effective and efficient GCS leakage monitoring networks [41], [76], [91]. DREAM searches the solution space for ensembles of leakage simulations to find the optimal placement of monitoring devices to minimize the time to leak detection. To accomplish this, DREAM uses a computationally efficient simulated annealing approach that interactively mutates potential monitoring schemes. The tool can accept simulation output from full-physics numerical simulators, from reduced-order models, or from integrated assessment models. It can account for spatial and temporal monitoring constraints, monitoring technology detection capability, and budget constraints (cost or monitoring equipment availability). Recent demonstration of coupled application of DREAM and NRAP-Open-IAM highlights the value of effective monitoring design to build confidence in GCS containment effectiveness and to support justification for early site closure [92].

The ORION toolkit [93] will provide functionality to describe the relationship between fluid injection and seismic response in real-time and space at the site and basin-scale. ORION will provide estimates of the seismic hazard expressed by the seismic frequency, probability of exceedance, and the related ground motions. ORION will incorporate a set of specific forecasting models (eg., Epidemic Type Aftershock Sequence, Rate-and-State formulations, seismogenic index models) that apply before, during, and/or after injection begins, and provide capability for real-time estimation of an ongoing hazard (or a chosen proxy for hazard). Validity and applicability of the forecast models will be rigorously tested using CO_2 injection and analogous field data.

3.2. Workflows and Recommended Practices for GCS Risk Assessment

Complementary to the development of NRAP risk assessment framework and fit-for-purpose NRAP simulation tools, NRAP has established recommended practices detailing the conceptual approach for risk-based assessment and management of potential leakage and induced seismicity risks associated with GCS [94], [95]. These recommended practices were made available to the international CCS community for review and comment, and they will be revisited periodically to update and improve their content. Many of the steps in these recommended practices align with computational workflows and fit-for-purpose applications embodied in NRAP tools. Table 2 provides a summary of several of the workflows in the recommended practices that relate to GCS site decision support.

Table 2. NRAP Phase II workflows.

NRAP Toolset	NRAP Tools Used	Reference
State of Stress Assessment	SOSAT	[90]
Risk-Based Area of Review	NRAP-Open-IAM	[63], [66], [96]
Evaluating plume conformance		[28], [65], [78], [97]
Risk-based monitoring design	DREAM	[41], [61], [76], [92]
Probabilistic Accounting of Containment Assurance	NRAP-Open-IAM	[98]
Post-Injection Site Care Period Evaluation	NRAP-Open-IAM, DREAM	[64], [68], [92]
Risk Mitigation Scenario Evaluation	NRAP-Open-IAM	[99]
Seismic forecasting during injection operations	STSF	[82]
Managing injection-related seismicity risk		[67]

3.3. Testing and Application of NRAP Tools and Methods

Numerous studies describe applications of the NRAP tools and workflows to real and hypothetical GCS project scenarios – to test and verify their viability for decision support. NRAP tools are finding new application areas such as the offshore environment, e.g., where subsea CO_2 leakage incidents can lead to emissions at the sea surface and subsequent atmospheric dispersion [100]. A catalog summarizing those studies and linking to related resources is maintained as a resource for practitioners [101]. As commercial deployment of GCS ramps up over the next several years there will be increasing opportunity to validate NRAP methods and tools against field data and operator experience; the NRAP tool use catalog will be revised periodically to account for those applications.

4. Summary

The U.S. DOE's National Risk Assessment Partnership is advancing applied research to directly support the DOE's Office of Fossil Energy and Carbon Management's goal to enable safe and secure commercial GCS deployment. The NRAP team has developed, demonstrated the application of, and openly released computational tools that provide an engine for quantitative risk assessment that can be applied to support stakeholder decision making, amidst uncertainty, for site selection, injection operation design, and permitting. The NRAP approaches for risk-based decision making are distilled into recommended practices for assessment and management of leakage and induced seismicity risks. Going forward, NRAP will continue engage with industry and regulatory stakeholders to test and improve the NRAP tools and risk management workflows to ensure their utility for real-world applications. Future work will focus on linking risk quantification to forecasting of long-term GCS liability to inform investment and insurance decisions, and on extending the NRAP approach to assess basin-scale risks of many commercial GCS operations.

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