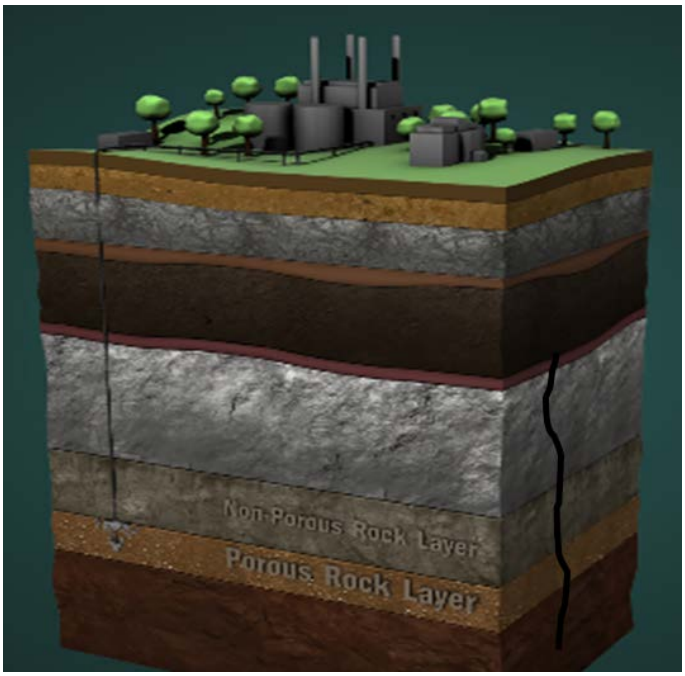

National Risk Assessment Partnership (NRAP) Phase I Accomplishments 2011–2016

10 November 2016

Office of Fossil Energy

NRAP-TRS-I-020-2016

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Cover Illustration: Artist rendition of a CO_2 storage reservoir and surrounding geologic system.

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NRAP Phase I Accomplishments 2011–2016

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Level I Technical Report Series

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Acronyms, Abbreviations, and Symbols

Term	Description
1D	One dimension
3D	Three dimensional
AIM	Aquifer Impact Model
AoR	Area of Review
CCS	Carbon capture and storage
CO_2	Carbon dioxide
DAS	Detailed area study
DOE	U.S. Department of Energy
DREAM	Designs for Risk Evaluation and Management
EM	Electromagnetic methods
EPA	U.S. Environmental Protection Agency
ERT	Electrical resistivity tomography
FEHM	Finite Element Heat and Mass
GCS	Geologic carbon storage
GMPEs	Ground Motion Prediction Equations
GMPIS	Ground Motion Prediction applications to potential Induced Seismicity
GUI	Graphical user interface
IAM	Integrated assessment model
IPCC	Intergovernmental Panel on Climate Change
InSaR	Interferometric Synthetic Aperture Radar
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
LUT	Look-up table
MSLR	Multiple Source Leakage Reduced-order model
NETL	National Energy Technology Laboratory
NL	National laboratory
NRAP	National Risk Assessment Partnership
NRAP-IAM-CS	NRAP Integrated Assessment Model-Carbon Storage
NSealR	NRAP Seal barrier Reduced-order model
PCE	Polynomial chaos expansion

Acronyms, Abbreviations, Symbols (cont.)

Term	Description
PISC	Post-injection site care
PNNL	Pacific Northwest National Laboratory
PSRA	Probabilistic Seismic Risk Assessment
RCRA	Resource Conservation and Recovery Act
ROM	Reduced-order model
RCSP	Regional Carbon Sequestration Partnership
REV	Reservoir Evaluation & Visualization
RROM-Gen	Reservoir Reduced-Order Model Generator
$scCO_2$	Supercritical CO_2
SCC	Strategic Center for Coal
SECARB	Southeast Carbon Sequestration Partnership
SRM	Surrogate reservoir model
STSF	Short-Term Seismic Forecasting
TDS	Total dissolved solids
TRS	Technical Report Series
U.S.	United States
USDW	Underground sources of drinking water
VOI	Value of information
VSP	Vertical seismic profile
WG	Working Group
WLAT	Wellbore Leakage Analysis

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EXECUTIVE SUMMARY

The National Risk Assessment Partnership (NRAP) brings together scientists and engineers from five U.S. Department of Energy's (DOE) national laboratories (NL), to develop insights into the environmental risk behavior of long-term carbon dioxide (CO_2) storage in geologic formations. Through stakeholder involvement, the NRAP program also benefits from the perspective of industry, government, non-government organizations, and academia regarding research needs on this topic. Phase I of the NRAP effort has recently concluded and this report summarizes the results of this 6-year effort. Phase I was focused on quantification of risk and related uncertainties, using the approach detailed in this report, and summarized in Figure 1, below.

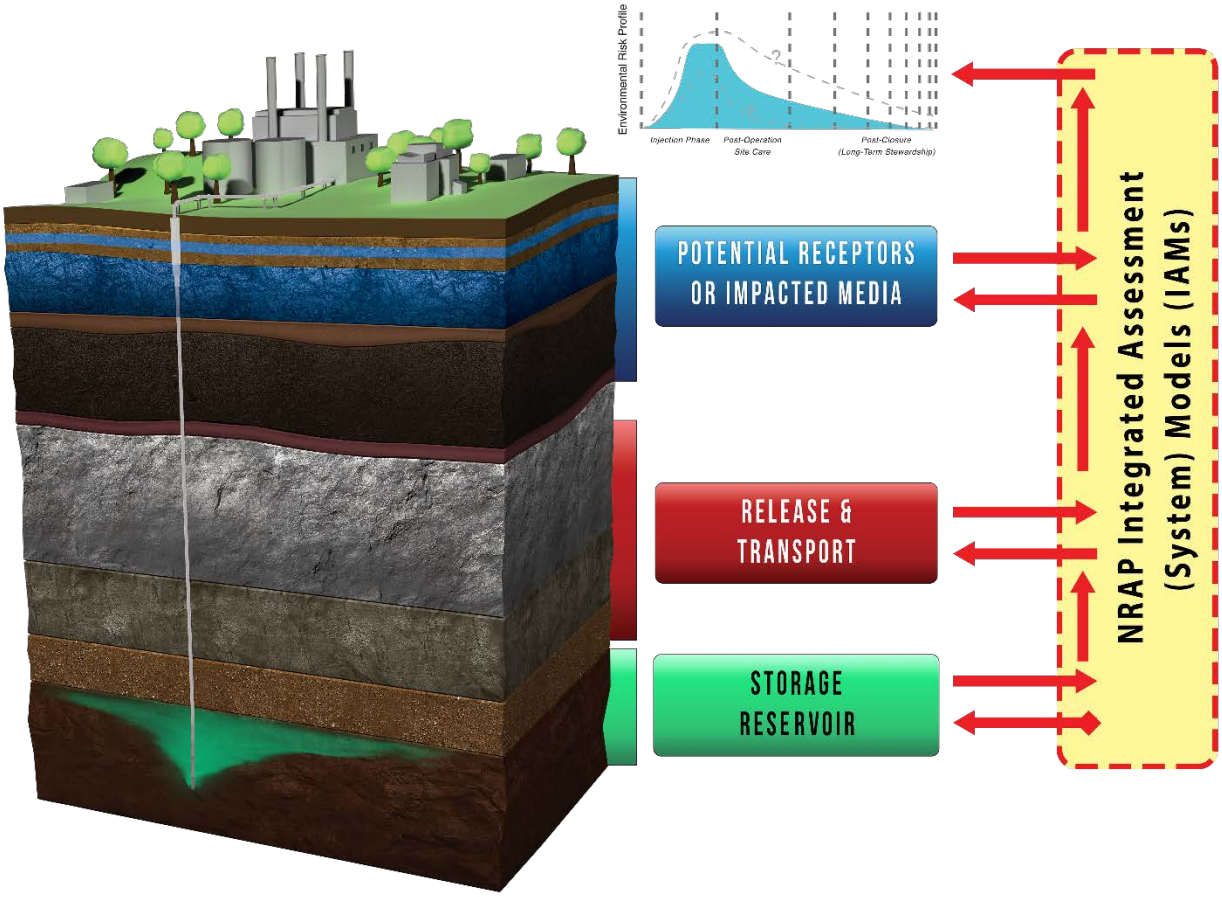

Figure 1: In the NRAP approach to quantitative risk assessment, sets of full-complexity numerical simulations of key system components (e.g., reservoir, potential leakage pathways, and overlying receptors) are used as the basis from which to build computationally-efficient reduced-order models (ROMs). Those ROMs can then be exercised to understand component behavior, or coupled in an integrated assessment framework with Monte Carlo-type analysis used to explore full-system risk performance through time, in the context of system uncertainties.

Improving the science base to build confidence for long-term CO_2 storage decisions was another key aspect that was studied by the project personnel. The main results for this part of the effort are:

- Development of physics based models of geologic carbon storage (GCS), systems and system components
- Demonstration of the validity and limitations of reduced complexity models, and integrated assessments models
- Computational and experimental analysis to address key system uncertainties
- Simulation of long term carbon storage system performance, in the context of those uncertainties

An important set of products from NRAP's Phase I effort is the set of tools that can be used to explore environmental risk behavior at CO_2 storage sites. The NRAP toolset is comprised of ten simulation tools representing important components of the engineered geologic system related to understanding the risk for and associated with potential fluid migration and induced seismicity. The tools, described in greater detail in the body of this report, are summarized below.

- The Reservoir Evaluation & Visualization (REV) tool generates pressure and CO_2 plumes sizes over time. It may be helpful for making Area of Review (AoR) determinations.
- The Reservoir Reduced-Order Model - Generator (RROM-Gen) tool generates reservoir look-up table reduced-order models (ROMs) from established reservoir simulations. It acts as a conversion tool which creates output that can be used directly by the NRAP Integrated Assessment Model-Carbon Storage (NRAP-IAM-CS).
- The Wellbore Leakage Analysis Tool (WLAT) evaluates existing wells for leakage potential. The tool also models migration of brine and/or CO_2 outside of storage reservoir and explores leakage response as a function of well disposition.
- NRAP Seal barrier Reduced-order model (NSealR) estimates leakage through a fractured seal and flux through a fractured or perforated seal. This tool computes two-phase (brine and supercritical CO_2) flux and includes fluid thermal/pressure dependence.
- The Aquifer Impact Model (AIM) tool gives a rapid probabilistic estimation of aquifer volume impacted by a potential leak. It distinguishes between CO_2 and brine leaks and is used to determine impact of threshold criteria.
- Multiple Source Leakage Reduced-order model (MSLR) determines the probability that the receptors are located within the radius of dense gas concentration that is above a given critical concentration. MSLR handles single- or multiple-source CO_2 leakage using a ROM.
- NRAP Integrated Assessment Model-Carbon Storage (NRAP-IAM-CS) simulates long-term full system behavior (from storage reservoir to aquifer/atmosphere). This tool provides results that can be used to compute risk profiles (time-lapse probability of leakage and groundwater impacts) and quantitative estimates of a storage site, with respect to system uncertainty.

- The prototype Designs for Risk Evaluation and Management (DREAM) monitoring optimization tool evaluates and selects the optimal monitoring design including subsurface monitoring design for a specific site. The tool also estimates the time to detection for the monitoring system.
- The Short Term Seismic Forecasting (STSF) tool forecasts seismic event frequency over the short term for a window of a few days using probabilistic methods and historical data. The tool can complement stoplight approach for induced seismicity planning and permitting.
- Ground Motion Prediction applications to potential Induced Seismicity (GMPIS) tool estimates ground motion at the surface that could result from potential induced earthquakes at CO_2 storage sites, providing useful information for use during the project planning and permitting stages.

These tools and supporting information can be accessed on the NRAP website https://edx.netl.doe.gov/nrap.

1. INTRODUCTION

Geologic carbon storage (GCS), the injection of carbon dioxide (CO_2) into permanent underground storage sites, is an important part of our nation's strategy for managing CO_2 emissions. Several pilot-to intermediate-scale carbon storage projects in the United States (U.S.) and across the world have demonstrated the technical feasibility of GCS. However, some technical, regulatory, and policy questions remain to be addressed before full-scale GCS can be implemented in the U.S. and internationally. Business and regulatory concerns still hinder its rapid commercial deployment. Industry investors worry about the uncertainties and potential liabilities inherent in owning an operation that must remain safe and secure for hundreds, if not thousands, of years. Regulators also need broad technical information to effectively address CO_2 storage.

"NRAP is comprised of the Nation's leading national laboratories in the areas of geosciences. This work, in turn, will provide an incredible toolset for the assessing, development, and management of geologic storage of CO_2 for its users. The development of this tool kit reflects the stakeholder collaborations with the labs resulting in practical and well researched applications."

~Michael Moore,
Executive Director NACCSA,
NRAP Stakeholder

Of particular relevance to making a business case for large-scale, long-term GCS is the development of quantitative, science-based methods for estimating long-term environmental risks related to potential leakage and induced seismicity. Such methods, and tools based on those methods, will help inform decision making with respect to two critical considerations for full scale carbon storage: 1) long-term liability and 2) cost of monitoring, particularly in the period of post-injection site care (PISC).

The U.S. Department of Energy's (DOE) Office of Fossil Energy and the National Energy Technology Laboratory (NETL) are conducting research to advance the science and engineering knowledge base for technologies that will accelerate the business case for large-scale CO_2 capture and storage, including prediction and quantification of risks. As part of this effort, NETL is leading a multi-laboratory effort that leverages broad technical capabilities across the DOE complex into a mission-focused platform to develop a critical science base and predictive tools that can be applied to risk assessment for long-term storage of CO_2: the National Risk Assessment Partnership (NRAP). NRAP brings together researchers from five DOE national laboratories: NETL, Los Alamos National Laboratory (LANL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), and Pacific Northwest National Laboratory (PNNL) to conduct integrated, collaborative, mission-driven research. This collaboration is strengthened even further by drawing on the expertise of academic and industry partners. Directed by multi-lab technical working groups (WGs), these research organizations conduct integrated, collaborative research.

The goal of NRAP is to develop defensible, science-based methodologies and tools for quantifying risks amidst system uncertainty and to better inform decision making for GCS sites. To achieve this goal, the NRAP project is being executed in two phases, each of which improves the science-based platform.

NRAP has completed Phase I activities (2011–2016), which focused on developing approaches to quantitatively assess site-scale risk performance. Phase I included efforts to build a critical science base to constrain key uncertainties in the behavior of important system components, develop methodologies and predictive tools for rapid estimation of long-term system performance and related uncertainties, and communicate the functionality and utility of those products to key GCS stakeholders. Through Phase I, NRAP researchers:

- Generated the first long-term quantitative risk profiles for a full CO_2 storage system
- Developed predictive tools and conducted focused experimental studies to improve understanding of potential leakage pathway behavior
- Developed a comprehensive risk model for induced seismicity, as well as tools to forecast near-term seismic potential and estimate potential ground motion effects from induced seismicity
- Provided insights into the utility of select monitoring approaches and explored the potential for optimization of monitoring design
- Developed an integrated assessment model (IAM) coupling computationally efficient ROMs of various system components to describe whole-system CO_2 containment behavior and potential leakage risks and impacts

NRAP Phase I efforts have resulted in the generation of a set of ten risk assessment tools that have been openly distributed for testing and use by the international carbon capture and storage (CCS) community. Products from these efforts also include the publication of numerous peer-reviewed articles and technical reports detailing key findings from laboratory and computational studies, innovative reduced-order modeling approaches, new risk assessment and uncertainty quantification methodologies, and new insights into whole system risk performance and key storage security relationships and issues. Together, these accomplishments help to advance the state of understanding and provide a path forward for quantitative assessment of risks, risk management and uncertainty reduction.

The tools and improved science base developed by NRAP will help operators design and apply monitoring and mitigation strategies. They will help regulators and their agents quantify risks and perform cost-benefit analyses for specific CCS projects. Finally, financiers and regulators will be able to invest in, and approve, CCS projects with greater confidence because the costs of long-term liability can be estimated with less uncertainty. Armed with the ability to quantify risk and to estimate the cost of long-term liability, industry will gain the confidence necessary to invest in CCS projects and regulators, government agencies, and the public will gain confidence in predictions of CCS site performance.

"The NRAP toolkit provides users with the first complete suite of models to predict and diagnose the geological integrity of CO_2 geological storage sites. Previously this has been performed using discrete and independent models, so this is a significant accomplishment in providing assurance to stakeholders that CO_2 Capture and Storage (CCS) is safe and secure. Testing and comparison of results now is an important step to validate use, along with incorporation into risk management methodologies prior to deployment."

~ Nigel Jenvey, BP

2. PHASE I ACCOMPLISHMENTS BY WORKING GROUP

NRAP consists of multiple research organizations conducting integrated, collaborative research. NRAP Phase I is further broken down by technical WGs, comprised of researchers from technical teams from each NL. WGs are responsible for identifying key research needs to meet NRAP goals and for coordinating research across NLs. Throughout NRAP Phase I, six (6) WGs were structured around key technical elements associated with risk assessment at a potential storage site.

2.1 RESERVOIR PERFORMANCE WG ACCOMPLISHMENTS

The Reservoir Performance WG studies during Phase I focused on developing models, tools, and methods to quantify and assess pressure buildup and CO_2 plume behaviors in injection reservoirs. Extents of pressure buildup and CO_2 plume are important to describe area of review (AoR) for monitoring and assessment requirements based on the U.S. Environmental Protection Agency's (EPA) Class VI rule for CO_2 injection wells. The Reservoir Performance WG investigated and quantified the effects of both operational variables, such as injection rate and duration, and geological variables on the pressure buildup and CO_2 plume extents. The WG developed new mathematical models for more accurate prediction of post-injection CO_2 distribution and trapping. Significant effort was also given to develop computationally efficient algorithms for visualizing and analyzing reservoir simulation results and developing reservoir ROMs used in NRAP integrated assessment studies. Approaching the end of NRAP Phase I, the Reservoir Performance WG conducted other important transitional studies such as development of a methodology for risk–based description of AoR and development of adaptive management strategies for risk management. The Reservoir Performance WG accomplishments for NRAP Phase I are summarized under three categories: 1) Reservoir Modeling, 2) Tool Development, and 3) Method Development.

2.1.1 Assessment of Pressure and CO_2 Plume Behavior

Collaborative efforts between LANL, LBNL, and NETL produced numerical simulations under different reservoir conditions to assess maximum extents of critical pressure buildup and CO_2 plumes as function of injection rate and volume. Selected reservoir types and properties included 1) a generic sandstone formation (regional dip), homogeneous, and permeability variations; 2) multilayer, domal sandstone reservoir (based on Citronelle [Alabama] field data); 3) domal, sandstone, and limestone reservoir (based on Rock Springs Uplift in Wyoming) with heterogeneous properties and multiple injectors; and 4) Vedder formation, sandstone alternating with shale, Kimberlina, California. An NRAP Technical Report Series (TRS) document (Bromhal et al., 2014) reported the analyses of the reservoir simulation results in detail, with all the simulation results achieved. Some of these reservoir simulation results (e.g., the simulations in Vedder formation published in Wainwright et al., 2013) have been used to generate ROMs including look-up tables (LUTs) for NRAP integrated assessment studies. The results have been used across different NRAP groups for geo-mechanical damage and groundwater leakage risk assessments.

The simulation results in general, indicate that the pressure plume size increases rapidly during injection and decays at a relatively faster rate, depending on reservoir boundaries and properties. The CO_2 plume continues to grow slowly during post-injection time periods. Although the patterns of the plume sizes as a function of time look similar, the plumes sizes can be

significantly different for different sites. As shown by the global sensitivity analyses by Wainwright et al. (2013, 2014), the growth and decay of the pressure plume and extent of the CO_2 plume are very sensitive to different hydraulic and two-phase flow properties existing in different reservoirs. This indicates the importance of reservoir characterization for reliably estimating the plume sizes for actual CO_2 storage projects.

Extracting the data from different simulators and printing the risk metrics related to critical pressure buildup and CO_2 plume sizes required development of a Reservoir Evaluation & Visualization (REV) tool. Additionally, the REV tool has a graphical interface to visualize results from different models/simulators under the same platform.

2.1.2 Development and Testing of Improved Reservoir Models

Most of the existing reservoir simulators make the common assumption of constant residual saturation, neglecting the hysteresis effects. However, there is strong experimental evidence that residual saturation of the CO_2 depends on the history and the maximum value of CO_2 saturation experienced during the invasion of CO_2. This necessitated the Reservoir Performance WG to improve numerical reservoir models by considering hysteresis for accurate assessments and quantifications of post-injection reservoir processes. The Reservoir Performance WG developed new hysteretic two-phase flow models (Cihan et al., 2014a, b; 2016) and tested successfully against experimental data (Trevisan et al., 2014a, 2015). These studies indicated that both heterogeneity and hysteresis play significant roles for controlling migration and entrapment of supercritical CO_2 ($scCO_2$) during post-injection and also showed the limitations of the existing reservoir model predictions that neglect hysteresis effects.

2.1.3 Development of Reservoir ROMs

The Reservoir Performance WG developed and tested the applicability of different ROMs including LUTs, surrogate reservoir model (SRM) (Mohaghegh et al., 2012), and polynomial chaos expansion (PCE) (Pau et al., 2014; Shahkarami et al., 2014; Zhang and Sahinidis, 2013a, b). Some of these methods were reported to be applicable under certain reservoir conditions. The Reservoir Reduced-Order Model – Generator (RROM-Gen) tool, produced by the Reservoir Performance WG, interpolates the reservoir simulation results onto a workable grid using LUT for integrated assessment studies.

2.1.4 Upscaling Tool for Reservoir Modeling

The Reservoir Performance WG also developed an upscaling tool for computationally efficient calculations of reservoir pressure and CO_2 plume behavior using coarsened high-fidelity simulators. This tool generates coarser models from high-resolution reservoir models, including the effects of sub-grid scale heterogeneities.

2.1.5 Risk-Based Methodology for Area of Review

The Reservoir Performance WG developed a methodology to generate risk maps based on the potential impact to underground sources of drinking water (USDW) (Woodburn et al., 2016). Expanding a tiered-AoR description work by Birkholzer et al. (2013), the methodology can be used to provide risk-based descriptions of the AoR to inform site selection and monitoring during and post-injection. The demonstration studies assumed the two largest sources of uncertainty to be the location of the leaky well and the leaky well permeability. The results indicate that 1)

characterizing conductivity variations of abandoned wells in a storage site is critically important for reliable predictions of risks, and 2) presence of thief zones (i.e., high permeability non-USDW layers between the storage zone and USDW) can dramatically decrease risk of brine leakage into USDW through leaky wells.

2.1.6 Adaptive Management Approaches for "Conformance"

The Reservoir Performance WG developed adaptive management approaches and tested an initial computational algorithm under generic reservoir conditions. Under an actual CO_2 storage scenario, initial model predictions typically carry significant uncertainty due to incomplete knowledge, and model results can deviate significantly from actual observations. The Reservoir Performance WG studies demonstrate that conformity of long-term model results with the actual system behavior could only be approached reasonably closely, modeled within a reasonable variance by adaptively improving the model with the monitoring data. The adaptive strategies development initiated during NRAP Phase I will continue to be tested and expanded by adding "risk management" as part of the adaptive scheme during NRAP Phase II.

2.2 WELLBORE AND SEAL INTEGRITY WG ACCOMPLISHMENTS

Wells and seals represent the primary pathway through which leaking CO_2 and/or brine can leave the storage formation and impact groundwater or other resources. The focus of NRAP Phase I for wells and seals was on understanding fundamental behavior through laboratory experiments and detailed numerical simulations. This work was then used to develop predictive tools that enable the rapid estimation of leakage behavior at the field scale.

2.2.1 Laboratory Experiments

During NRAP Phase I, laboratory experiments conducted by the Wellbore and Seal Integrity WG were used to characterize the reactive transport processes that affect leakage along pathways in wells and seals. These resulted in critical observations that solidified the understanding of key chemical reactions and mechanical alterations that occur along leakage pathways (Carroll et al., 2016). While the cement used in wells is reactive with CO_2 and CO_2-saturated waters, the chemical reactions dissolve cement phases while leaving a silica-rich phase that resists flow and potentially precipitating calcium carbonates. This finding has been observed for a range of conditions, e.g., pressure, temperature, cement composition, presence of formation rock, and injected gas contaminants (Carey, 2013; Jung and Um, 2013; Newell and Carey, 2013; Zhang et al., 2014a, 2014b). Thus, under many conditions, a leak path involving well cement is not expected to become a self-enhancing leak path. However, there may be conditions when the system becomes self-sealing. Self-sealing was observed due to secondary mineral precipitation (Huerta et al., 2015; Um et al., 2014) and due to geomechanical closure of the pathway (Mason et al., 2013; Walsh et al., 2014). Less laboratory work has been performed on characterizing seal leakage due to the difficulty in obtaining representative samples and the inability for experimental apparatus to simulate the correct subsurface conditions, though several case studies were attempted (Crandall and Bromhal, 2013). Recent advances within NRAP now allow experimental studies of leakage processes in fractured caprock using direct shear devices (Carey et al., 2015). These studies reveal the important role of ductile deformation in limiting development of significant permeability in damaged caprock. These new tools can make use of more readily available samples (due to the shale drilling boom) to understand how leak-path permeability changes due to various subsurface phenomena. While there remains several areas

that need fundamental experimental observations (e.g., casing corrosion and more seal leakage work) NRAP's Phase I laboratory experiments have made significant contributions to understanding leakage risk in wells and seals.

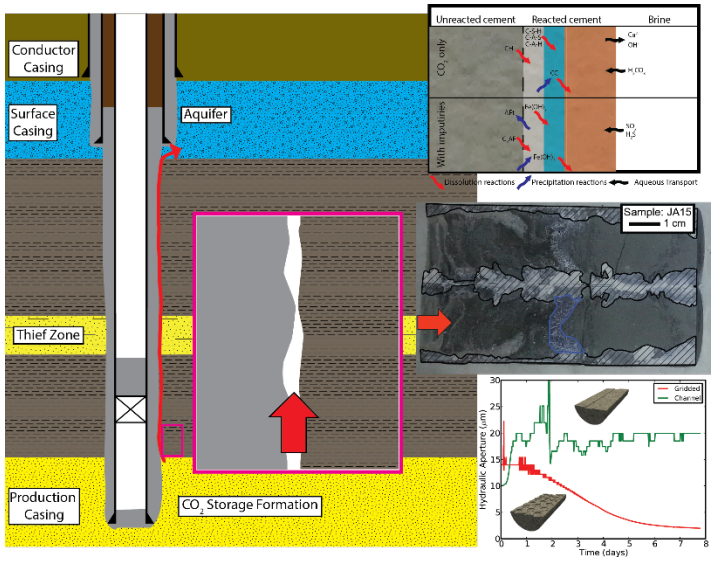

Figure 2: Well leakage research within Phase I focused on developing first-order models for well leakage at the field scale, while the fundamental processes for time-dependent leakage were studied using laboratory and numerical approaches. From this work, a deeper understanding was developed of the complex coupled reactive transport and geomechanical processes that can lead to self-sealing leakage behavior.

2.2.2 Numerical Simulations

Full physics simulations have been used to understand the effect of reservoir-scale phenomena on leakage and the time evolution of leakage that more recently incorporates findings from the laboratory experiments as a basis for the development of predictive tools. Numerical simulations for a leaky cemented well were conducted using the Finite Element Heat and Mass (FEHM) transfer code (Zyvoloski, 2007) to develop an understanding of the magnitude for leak flux. Input parameters considered were well permeability, well depth, reservoir pressure, and CO_2 saturation (Jordan et al., 2015). These results were instrumental in developing the ROMs discussed below. Additional simulations on more complex geometries, for example thief zones, provided insights to where the leaking brine and CO_2 may be transported. These observations are important for signal monitoring around wells (Harp et al., 2016). Parametric investigations of wellbore and thief zone permeabilities indicated that as long as wellbore permeabilities were less than 1×10^{-14} m^2, leakage remained extremely low, and that significant increases in leakage of brine or CO_2 only occurred when wellbore permeability was relatively high (1×10^{-12} m^2) and thief zone permeability was extremely low (1×10^{-18} m^2) (Harp et al., 2014). In order to simulate the worst case leakage scenario of an opened well, a drift-flux model was applied for transient two-phase non-isothermal flow of CO_2 and brine (Pan et al., 2011). These results were also used to develop the ROM for an open well. More advanced simulations were recently conducted to incorporate observations from the laboratory experiments of the geochemical effects (Brunet et al., 2016) and the combined geochemical and mechanical effects (Walsh et al., 2014a; Walsh et

al., 2014b). These results suggest that those effects significantly impact well response, and that a characteristic sealing behavior is observed at critical fluid residence times and as a function of several system parameters (e.g., gradient in potential, fracture aperture, leak length). Full-physics simulations provide not only field-scale understanding of how leakage evolves over time, but can also be used to develop more computationally efficient models that can, in turn, be used to create predictive tools for leakage risk assessment.

2.2.3 Predictive Tools

The Wellbore and Seal Integrity WG developed several user-friendly and computationally-efficient models for estimating leakage along compromised wells and seals. The Wellbore Leakage Analysis Tool (WLAT) is a collection of four models that captures various aspects of leakage along wells (Huerta and Vasylkivska, 2016). The NRAP Seal barrier Reduced-order model (NSealR) uses a stochastic approach to model the leakage of CO_2 and brine along relatively high permeability pathways (i.e., fractures) that traverse a low permeability sealing formation (Lindner, 2016). These tools can be used to get a rapid assessment of leakage flux and total leakage for different scenarios.

WLAT comprises models developed within NRAP and by external researchers. The first component model, the Cemented Wellbore Model, was developed by performing many full-physics simulations using LANL's FEHM code over a range of key parameters (Jordan et al., 2015; Harp et al., 2016). The results are constructed into ROMs to be sampled based on input conditions. These ROMs estimate the multiphase flow of CO_2 and brine along a cemented wellbore. The model can treat leakage to a thief zone, aquifer, or to the atmosphere. The second component model, the Multi-segmented Wellbore Model, is an adaptation of the models developed at Princeton University (Celia et al., 2011; Gasda et al., 2012; Nordbotten et al., 2009). Reduced-physics models were used to treat the leakage of CO_2 and brine along wells with multiple thief zones. This model provides a useful validation case for the Cemented Wellbore Model. The third component model, the Open Wellbore Model, is a reduced-physics model based on the drift-flux approach (Pan, 2011; Pan et al., 2011, 2009). This model treats the leakage of CO_2 up an open wellbore or up open (i.e., un-cemented) casing/tubing. The last model, the Brine Leakage Model, a reduced-physics model, was developed based on simple reactive transport theory and is tuned with experimental observations (Huerta et al., 2014). This model estimates the leakage of brine considering the effects that geochemical alteration (e.g., dissolution and precipitation) may have on the leak-path permeability.

The NSealR tool was developed at NETL to simulate the movement (leakage) of CO_2 over time through a thin, relatively impermeable layer of rock overlying a rock formation where CO_2 has been injected. The current theoretical base considers the one dimension (1D), two-phase flow of CO_2 through brine-saturated rock under CO_2 supercritical conditions.

2.3 GROUNDWATER PROTECTION WG ACCOMPLISHMENTS

The Groundwater Protection WG focuses on predicting potential impacts to groundwater systems that could occur as a result of CO_2 storage. A key element of this WG is to quantify potential changes over time to groundwater chemistry (related to groundwater quality) as a function of the introduction of fluids (CO_2 and/or brine).

2.3.1 Predictive Tools

The Aquifer Impact Model (AIM) consists of two ROMs that can be used to predict the impact potential in the event of a (out of zone migration) or leak that CO_2 and brine from a CO_2 storage reservoir might have on overlying aquifers. The models predict the size of "impact plumes" according to nine water quality metrics. The development of this computationally efficient tool, and the underlying reactive transport simulations it emulates, have been described in several publications (Bianchi et al., 2016; Carroll et al., 2014; Dai et al., 2014; Keating et al., 2016a, b; Keating et al., 2014). The AIM is well suited to applications that consider a large number of scenarios such as risk assessment, sensitivity analysis, and uncertainty analysis. In addition to the stand-alone AIM tool, the groundwater ROMs have also been incorporated into the NRAP-IAM-CS tool.

More specifically, the NRAP AIM predicts the size of "impact plumes" in shallow aquifers caused by point-source CO_2 and/or brine leaks introduced at the base of the aquifer. The input variables are 1) the location and number of point-source leaks, 2) flow rate of CO_2 and brine at each point source, and 3) hydrogeologic and geochemical characteristics of the aquifer. The output variables are above threshold plume sizes for each of nine water quality metrics and the flux of CO_2 across the water table. If the user is interested in predicting impacts due to time-varying sequences of flow rates, the AIM will be called at each time in the sequence. For each point in time, the AIM inputs will be the instantaneous CO_2 and brine mass flow rate and the cumulative mass of CO_2 and brine leaked since the start of the leakage scenario. Although the AIM tool was developed using site-specific data from two aquifers (Edwards and High Plains), the models accept aquifer characteristics as variable inputs and therefore, may have more broad applicability.

2.3.2 Full-Physics Simulations

The AIM ROMs were derived from thousands of full-physics simulations of reactive CO_2 and brine plumes in shallow aquifers. These simulations have been archived and can be accessed for future analyses. Potential applications include monitoring network design (DREAM or other similar tools) and risk assessment. If new water quality thresholds or metrics are developed in the future, new versions of the AIM tool could be derived from the archived simulations.

2.3.3 Laboratory Experiments

A series of batch and column experiments and solid phase characterization studies (quantitative X-ray diffraction and wet chemical extractions with a concentrated acid) (Lawter et al., 2016) and associated modeling work (Zheng et al., 2016) were conducted with representative rocks and sediments from an unconfined, oxidizing carbonate aquifer, i.e., the Edwards Aquifer in Texas, and an unconsolidated sand and gravel aquifer, i.e., the High Plains Aquifer in Kansas. These materials were exposed to a CO_2 gas stream to simulate CO_2 gas leakage scenarios, and changes in aqueous phase pH and chemical composition were measured in liquid samples (batch experiments) and effluent samples (column experiments) collected at pre-determined experimental times.

Laboratory experiments (Varadharajan et al., 2013) and field tests (Trautz et al., 2013) funded by other agencies, but leveraged with NRAP funding, were also carried out for an aquifer in Mississippi and simulated with reactive transport models (Zheng et al., 2015). These experiments

and models significantly enhanced the understanding of which elements could potentially be released in response to the leakage of CO_2, to what extent could they be released, and what are the controlling processes and key parameters of these events.

Results from these experimental efforts provided valuable insights for the development of groundwater impact ROMs, including characterization of release mechanisms for trace metals from aquifer rock. The results from these investigations provided useful information to support site selection, risk assessment, and public education efforts associated with geologic, deep subsurface CO_2 storage and sequestration (Harvey et al., 2013; Harvey et al., 2016; Lawter et al., 2015; Lawter et al., 2016; Qafoku et al., 2014; Shao et al., 2015).

2.3.4 No-Impact Thresholds

In order to develop the aquifer impact ROMs, it was necessary to establish baseline datasets and statistical protocols for determining statistically significant changes between background concentrations and predicted concentrations that would be used to quantify and define a contamination plume (Last et al., 2016).

The initial effort examined selected portions of two aquifer systems: the urban shallow-unconfined aquifer system of the Edwards-Trinity Aquifer System (being used to develop the ROM for carbon-rock aquifers), and a portion of the High Plains Aquifer (an unconsolidated and semi-consolidated sand and gravel aquifer being used to develop the ROM for sandstone aquifers). No-impact threshold values were determined for cadmium, lead, arsenic, pH, and total dissolved solids (TDS) that can be used to identify potential areas of contamination predicted by numerical models of carbon sequestration storage reservoirs. No-impact threshold values were later determined for chromium and barium specifically to support the ROM being developed by LLNL for the High Plains Aquifer. These threshold values are based on an interwell approach for determining background groundwater concentrations as recommended in the U.S. EPA Unified Guidance for Statistical Analysis of Groundwater Monitoring Data at Resource Conservation and Recovery Act (RCRA) Facilities.

The resulting no-impact threshold values can be used to inform a “no change” scenario with respect to groundwater impacts, rather than using a maximum concentration limit or secondary drinking water standard that in some cases could be significantly higher than existing concentrations in the aquifer. These no-impact threshold values are intended for use in helping to predict areas of potential impact and are not intended for use as alternate regulatory limits.

2.4 SYSTEM (RISK) MODELING WG ACCOMPLISHMENTS

2.4.1 Quantification of Environmental Risk Profiles

Through the first phase of research, the NRAP System (Risk) Modeling WG developed and demonstrated a new approach to quantify environmental risks through time at GCS sites. Even though the concept of environmental risk profiles has been used effectively to communicate risks since its introduction in 2007 by Benson, examples have largely been “qualitative.” The NRAP quantification approach brings together the concepts of science based predictions and systems modeling. An example risk profile for probability of CO_2 leakage to the atmosphere in excess of selected hypothetical cutoff values is shown below in Figure 3. The approach is embodied in NRAP’s flagship simulation tool for quantification of potential leakage risk: NRAP-IAM-CS.

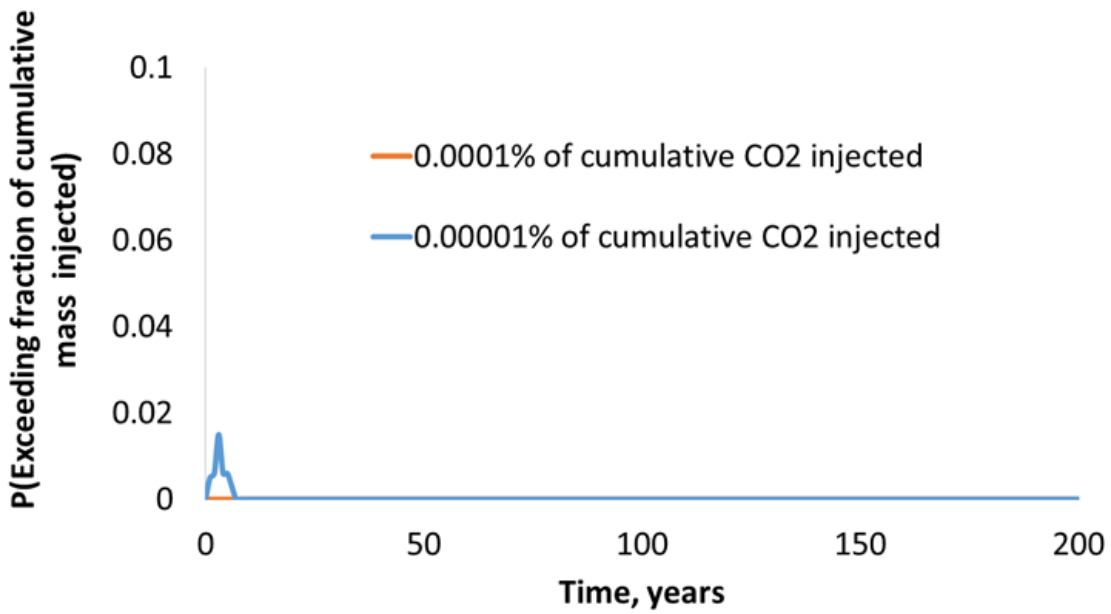

Figure 3: Risk Profile of CO_2 Leakage.

2.4.2 Integrated Assessment Model (NRAP-IAM-CS)

NRAP-IAM-CS is a first of its kind integrated model that can be used to perform stochastic simulations of long-term storage performance (hundreds to thousands of years) of GCS sites while exploring a wide range of system uncertainties. NRAP-IAM-CS is a system model that links ROMs for critical system components, including the primary storage reservoir, wellbore, groundwater and atmosphere, to simulate the total system behavior. The model can be used to estimate whether CO_2 injection induced pressure and saturation changes in storage reservoirs can lead to CO_2 and brine leakage and, if so, to estimate possible impacts due to those leaks in groundwater aquifers as well as potential changes in CO_2 concentration in the atmosphere above GCS sites.

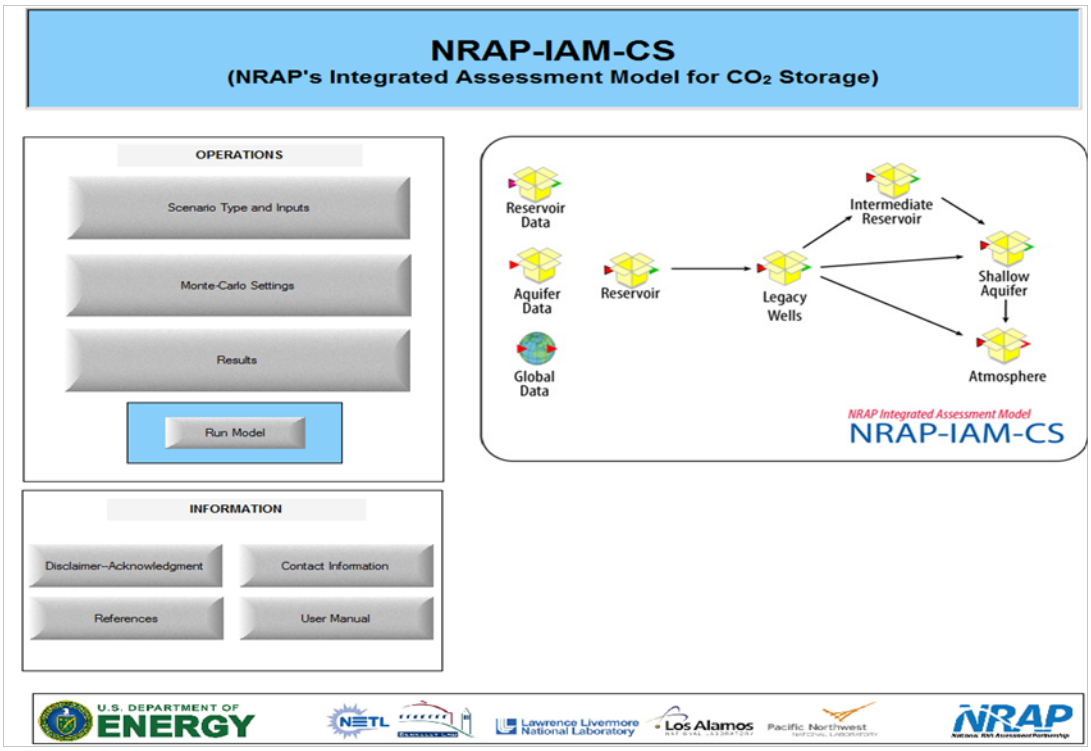

Figure 4: NRAP-IAM-CS Home Screen.

The NRAP approach to develop NRAP-IAM-CS is described in Figure 1 in the Executive Summary; Figure 4 shows an image of the NRAP-IAM-CS front page.

The ROMs utilized in NRAP-IAM-CS make it extremely computationally efficient, where stochastic simulations with thousands of realizations, each one simulating long-term storage site performance, can be performed in a matter of hours. During the stochastic simulations with NRAP-IAM-CS multiple, uncertain key parameters in all system components can be sampled to assess impact of parameter uncertainties over system performance and predicted leakage risks.

2.4.3 Informing Decision Making with Uncertainties

In order to effectively manage risks at GCS sites it is necessary to inform decision making related to site operations and risk management on how uncertainties in site characteristics affect overall risks. The System (Risk) Modeling WG demonstrated through the application of NRAP-IAM-CS the effect of site specific uncertainties and site operational parameters on CO_2 and brine leak rates as well as impacts of leakage on groundwater aquifers (Pawar et al., 2016).

Figure 5 demonstrates the importance of uncertain parameters in various parts of a CO_2 storage system on the change in TDS concentration in a groundwater aquifer at a hypothetical GCS site due to CO_2 and brine leakage.

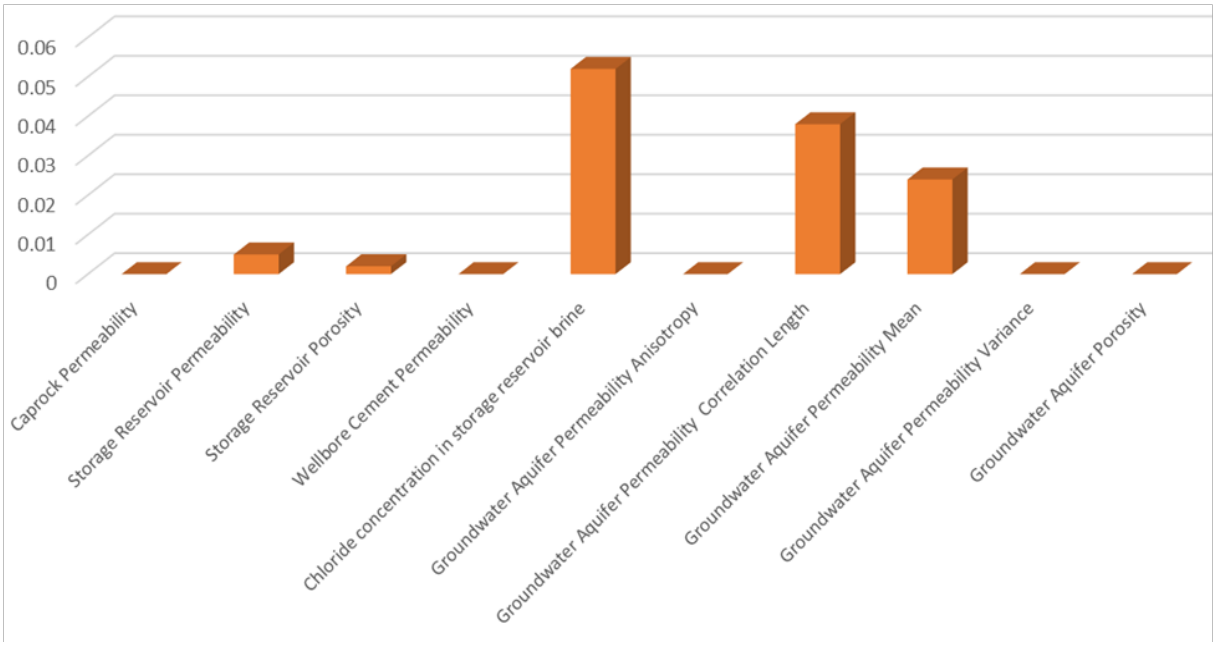

Figure 5: Predicted importance of various uncertain parameters on change in TDS due to leakage under a hypothetical scenario at a hypothetical GCS site.

2.4.4 Key Findings

In all cemented well scenarios evaluated with application of NRAP-IAM-CS, cumulative leakage is predicted to remain well below the Intergovernmental Panel on Climate Change (IPCC) storage permanence goal (99% retention after 1000 years), even in scenarios with very high cemented well density (10 wells per km^2).

Accounting for residual saturation improves storage reservoir performance, resulting in leakage profiles that decline following the period of active injection.

In the scenarios evaluated for impact of leakage on groundwater, results showed that extremely low volumes of groundwater were impacted due to leakage. Additionally, the results also showed that the groundwater volume with pH change due to leakage was different than that with change in TDS which has implications on deployment of monitoring technologies.

Overall, the multi-variate and sensitivity analysis for CO_2 leakage to atmosphere shows that the wellbore cement permeability is the most important uncertain variable.

On the other hand, the analysis for shallow aquifer impacts showed that, for low leak rates, the importance of wellbore cement permeability was lower than the groundwater aquifer uncertain parameters.

2.5 STRATEGIC MONITORING WG ACCOMPLISHMENTS

Monitoring approaches for GCS depend on objectives, subsurface reservoir/site dimensions, and the stage of a CO_2 storage site. Different monitoring techniques should be selected for site characterization before CO_2 injection starts, for monitoring while injecting CO_2, or for a post-

injection stage. Phase I Strategic Monitoring WG efforts focused on the demonstration of geophysical monitoring approaches and capabilities at existing test sites as well as the development of approaches using synthetic models/datasets. The former was done in cooperation with regional partnerships that were undertaking these field demonstrations; the latter was based on internally developed synthetic models, both having an overall goal of developing tools and approaches that can be integrated into risk assessment models/tools. The integration of monitoring with quantitative risk assessment requires an understanding of limitations and detection capabilities of each monitoring method as those translate into the field-scale uncertainties.

Initially, the NRAP Strategic Monitoring WG focused on underlying science issues related to monitoring CO_2 storage. The goals driving this early work included: 1) assess and improve the resolution of individual monitoring technologies; 2) quantify and improve the temporal and spatial uncertainty of monitoring data; and 3) develop comprehensive joint/combined inversion of monitoring data. A focus of NRAP's Strategic Monitoring WG was the development of a journal publication (Harbert et al., 2016). Field scale monitoring gaps were identified and priority, risk-driven, monitoring needs were evaluated.

2.5.1 Monitoring Technologies at Field Sites

An example of NRAP work addressing these goals was the collaborative work with the Southeast Carbon Sequestration Partnership (SECARB) on monitoring at the Cranfield, Mississippi detailed area study (DAS) injection site. NRAP extended planned vertical seismic profile (VSP) monitoring to include investigations of 3D-VSP resolution, VSP uncertainty and joint inversion of hydrologic, seismic, and electrical monitoring data (e.g., Ajo-Franklin et al., 2013; Carrigan et al., 2013; Commer et al., 2016; Daley et al., 2015b; Doetsch et al., 2013). The 3D-VSP processing addressed the improvement of subsurface seismic image quality and evaluation of monitoring with expensive 3D surface seismic versus less expensive, higher frequency, borehole-based 3D-VSP surveys at the Cranfield site. This work was later supplemented with an acoustic anisotropic analysis of two sonic dipole geophysical logs from the DAS site. As part of the Cranfield VSP work, the Strategic Monitoring WG developed a novel least-squares reverse-time migration method to enhance image resolution and enlarge the imaging region. Other NRAP work focused on electrical resistance monitoring at Cranfield- both the electrical resistance tomography (ERT) and uncertainty quantification and as part of joint inversion (Yang et al., 2014; Yang et al., 2015). For the ERT method, for example, the maximum standard deviation of CO_2 saturation was found to be around 6% with a corresponding maximum saturation of 30% for a dataset collected 100 days after injection began. There was no apparent spatial correlation between the mean and standard deviation of CO_2 saturation but the standard deviation values increased with time as the saturation increased.

2.5.2 Monitoring Approaches using Synthetic Datasets

In the late stages of NRAP Phase I, and in preparation for the integration of strategic monitoring into the NRAP-IAM-CS, the Strategic Monitoring WG began work on an integrated synthetic dataset based on the Kimberlina site. Kimberlina was a proposed storage site in the southern San Joaquin Basin in California that could be used to test the NRAP-developed ROMs and to test the risk-driven monitoring designs. One Kimberlina ROM dataset, based on the High Plains Aquifer, simulates CO_2 and brine leaked into the overlying aquifer with variable heterogeneity.

A second synthetic dataset involves leakage from a compartmentalized aquifer along a well into the overburden containing multiple permeable and impermeable strata. The output models from these ROMs become the input to monitoring models. During this process, it was learned that the ROMs may not have the parameters necessary for geophysical simulations unless the parameters are specified in the design criteria. Further, before using ROMs to demonstrate monitoring tools and their capabilities, it is necessary to establish the capabilities and limitations of geophysical techniques (EM, seismic, InSAR [Interferometric Synthetic Aperture Radar], gravity, etc.) using full-resolution models.

Previously, monitoring strategies have been selected using site specific information and expert judgment. However, quantitative risk assessments need more rigorous tools. One approach investigated within NRAP was a value of information (VOI) approach (Trainor-Guitton et al., 2013). This approach was demonstrated for a post-injection stage, a scenario in which CO_2 and accompanying brine would leak from a deep reservoir into a shallow aquifer via an abandoned wellbore. Geochemical reactions of CO_2 and brine would cause an increase in groundwater salinity or TDS. Since this groundwater would be used to irrigate corn crops, high saline concentrations would result in economic losses. VOI uncertainty quantification evaluation was done using TDS and a range of possible economic outcomes from an agricultural decision, and showed that any information would be relevant only when plumes would exceed 2,000 ppm TDS. Remote sensing geophysical methods, e.g., electrical and EMs, can detect these TDS plumes as electrical resistivity is sensitive to TDS changes. The value of the crop resources can then be compared to the cost of monitoring and decisions made based on those results.

2.5.3 Monitoring Tools

During Phase I, the NRAP Strategic Monitoring WG produced software tools to improve monitoring. The Designs for Risk Evaluation and Management (DREAM) tool is used to develop risk-based monitoring strategies by designing and evaluating monitoring networks (Yonkofski et al., 2016b). DREAM is an optimization tool that reads ensembles of CO_2 leakage simulations generated by common multiphase flow simulators. DREAM then generates monitoring configurations based on user-specified technologies, budgetary constraints, and spatial constraints. A simulated annealing algorithm optimizes over the ensemble evaluating the generated configurations in order to minimize time to CO_2 leakage detection (Yonkofski et al., 2016a).

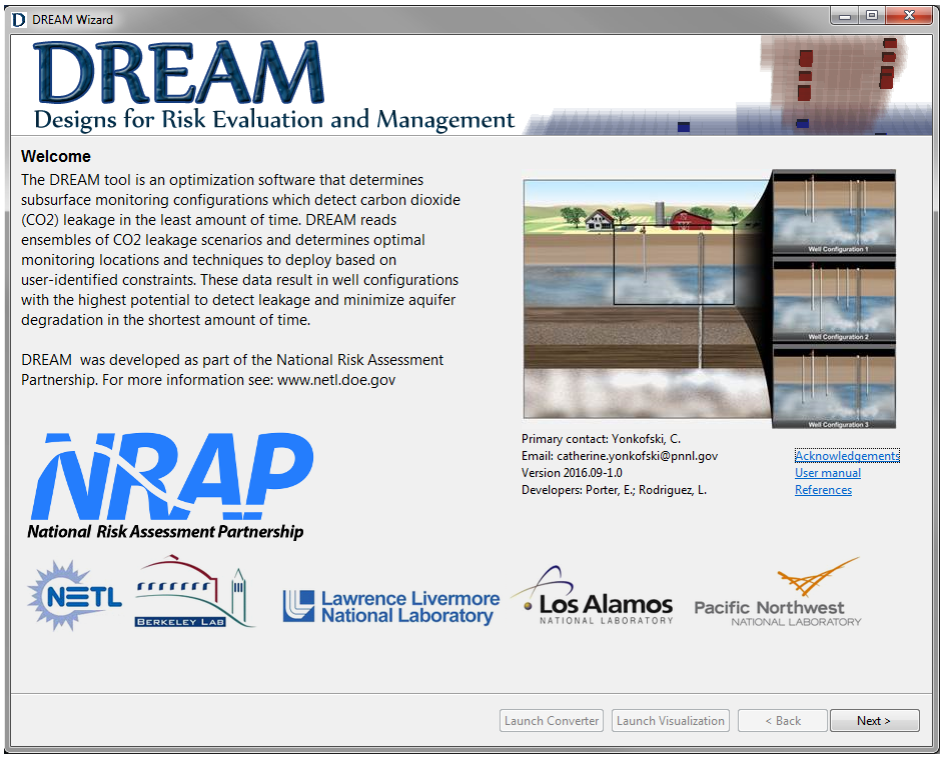

Figure 6: DREAM Welcome Window.

The Strategic Monitoring WG also developed a tool (currently in internal testing) for optimal design of passive seismic monitoring using surface and/or borehole geophones (Shang and Huang, 2012). This method provides the optimal number of geophones needed for a given tolerable error in event locations and target monitoring regions such as the reservoir or fault zones.

2.6 INDUCED SEISMICITY WG ACCOMPLISHMENTS

The central objective of the NRAP Induced Seismicity WG is to develop practical tools to support the management of induced seismicity at carbon storage operations. The goal is to identify site characteristics and operational approaches that can lower seismic risk. The Induced Seismicity WG is also developing new techniques to quickly identify hazardous situations and address problematic seismicity, should hazardous situations appear.

2.6.1 Short-Term Seismic Forecasting Tool

A central control on seismic risk is the rate and magnitude-distribution of earthquakes in the vicinity of a project. Unfortunately, the seismicity rate and its connection to subsurface injection are site-specific and difficult to accurately predict prior to injection. As a result, operators must use continuous microseismic monitoring of their site to properly assess the ongoing seismic hazard and react quickly to problematic situations as they arise (White and Foxall, 2014). To support this monitoring and management feedback loop, the Induced Seismicity WG developed the Short-Term Seismic Forecasting (STSF) tool (Bachmann et al., 2016). The tool uses a statistical analysis of observed seismicity, injection rate, and injection pressure to automatically calibrate a site-specific empirical model for seismicity rate and its relationship to injection activities (Bachmann et al., 2011; Mena et al., 2013). The tool then uses the planned injection

schedule to forecast an expected seismicity rate within a forecast window, usually looking ahead a few days to weeks. As new microseismic and injection data is recorded, the underlying data model and forecast are continuously updated. The impact of alternative injection scenarios on future seismicity can also be explored. In Phase I, an initial version of this forecast model was deployed and tested against a number of available induced seismicity datasets. In Phase II, model development will continue by improving the physical fidelity of the underlying statistical models and further testing the approach against recently acquired datasets.

2.6.2 Ground Motion Prediction Tool

A second key control on seismic risk is the severity of ground motion caused by induced earthquakes. This ground motion can be a nuisance to nearby populations or cause structural damage. Ground motion is both site- and earthquake-specific, and is strongly influenced by a number of geologic factors. To help operators appropriately identify nearby structures and communities at risk from induced events, the Induced Seismicity WG developed the Ground Motion Prediction applications to potential Induced Seismicity (GMPIS) tool (Coblentz et al., 2016). This tool, based on empirical Ground Motion Prediction Equations (GMPEs), was developed using shallow, small-magnitude (<M4) earthquake data (Douglas et al., 2013). The tool also includes a model for site-specific ground motion amplification effects due to near-surface geology (Abrahamson and Silva, 2008; Boore and Atkinson, 2008). Storage operators can use this tool to compute shakemaps for the local region under different earthquake scenarios to help improve seismic risk management plans.

2.6.3 Probabilistic Seismic Risk Assessment Tool

A logical approach for quantifying induced seismicity risk is to adapt the standard Probabilistic Seismic Risk Assessment (PSRA) technique widely used to estimate the risk of structural damage from naturally occurring (tectonic) earthquakes. As certain regions of the world are now dealing with both natural and induced events, a unified framework can also provide a common language for risk communication. PSRA couples the probability of earthquake occurrence with its societal consequences, which in the case of induced seismicity includes nuisance from felt ground motion as well as structural damage. While the general PSRA framework remains useful for induced seismicity, a number of substantial modifications are necessary to address important nuances associated with the underlying physical process (White and Foxall, 2016a; Pawar et al., 2015). Therefore, the Induced Seismicity WG created a new code framework (RiskCat) to support seismic risk assessment at carbon storage projects. RiskCat takes input regarding earthquake occurrence, ground motion potential, and community vulnerability and generates an output of a probabilistic estimate of project risk. The resulting risk profile can be used to guide project design and can be continuously updated as new site characterization and monitoring data becomes available.

2.6.4 Hydromechanical Simulators

During Phase I, the Induced Seismicity WG developed a number of improved hydromechanical simulation capabilities for modeling static and dynamic fault slip and the potential for fluid leakage along faults. In particular, the WG helped support the development and application of RSQSim, a quasi-dynamic earthquake simulator originally developed at the University of California, Riverside for modeling natural earthquakes sequences (Richards-Dinger and Dieterich, 2012; Dieterich et al., 2015). RSQSim has been coupled to a number of reservoir

simulators to study the impact of different injection scenarios on the statistical distributions of induced events that may be observed. The WG also performed detailed studies on different aspects of fault reactivation and fluid leakage using various hydromechanical simulation packages developed at DOE laboratories—e.g. (Cappa and Rutqvist, 2011, 2012; Lu et al., 2012; Rinaldi et al., 2014; Nguyen et al., 2016).

3. SUMMARY

The NRAP project has completed Phase I activities (2011–2016) focused on developing approaches to quantitatively assess site-scale risk performance. Phase I included efforts to build a critical science base to constrain key uncertainties in the behavior of important system components, develop methodologies and predictive tools for rapid estimation of system risk performance and related uncertainties, and communicate the functionality and utility of those products to key GCS stakeholders. These efforts resulted in the development of insights on key storage-security relationships, methodologies for quantitative assessment of risk performance in CO_2 storage systems, and a novel set of tools that have been made freely available to the international GCS research, development, and deployment community.

NRAP is now entering a second phase of collaborative research in which predictive capabilities, methodologies, and insights developed through Phase I will be applied and extended to consider the active management and mitigation of risk associated with large-scale CO_2 storage, and reduction of associated uncertainties through strategic monitoring. NRAP Phase II activities will include:

- Development of methodologies and tools to assure effective containment of CO_2 and evaluation of select mitigation alternatives
- Advancement of seismic risk assessment and management strategies
- Development of strategic monitoring for conformance assessment and uncertainty reduction
- Field demonstration, application, and validation of NRAP tools and methodologies

These efforts will be focused toward addressing critical questions related to assessment and management of environmental risk at CO_2 storage sites.

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4. PHASE I PUBLICATIONS PRODUCED

Reservoir Performance WG

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