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Final Report
Carbon Sequestration Monitoring Activities

SUBMITTED BY

University of Wyoming
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SUBMITTED TO

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EXECUTIVE SUMMARY

In its “Carbon Sequestration Technology Roadmap and Program Plan 2007” the U.S. Department of Energy (DOE)’s Office of Fossil Energy National Energy Technology Laboratory (NETL) identified as a major objective extended field tests to fully characterize potential carbon dioxide (CO₂) storage sites and to demonstrate the long-term storage of sequestered carbon (p. 5). Among the challenges in this area are “improved understanding of CO₂ flow and trapping within the reservoir and the development and deployment of technologies such as simulation models and monitoring systems” (p. 20).

The University of Wyoming (UW), following consultations with the NETL, the Wyoming State Geological Survey, and the Governor’s office, identified potential for geologic sequestration of impure carbon dioxide (CO₂) in deep reservoirs of the Moxa Arch. The Moxa Arch is a 120-mile long north-south trending anticline plunging beneath the Wyoming Thrust Belt on the north and bounded on the south by the Uinta Mountains. Several oil and gas fields along the Moxa Arch contain accumulations of natural CO₂. The largest of these is the La Barge Platform, which encompasses approximately 800 square miles. Several formations may be suitable for storage of impure CO₂ gas, foremost among them the Madison Limestone, Bighorn Dolomite, and Nugget Sandstone.

This project responded to the challenges described above by preparing a geological site characterization study on the Moxa Arch. The project included four priority research areas: A) geological characterization of geologic structure of the Arch, the fault, and fracture patterns of the target formations and caprocks, B) experimental characterization of carbon dioxide-brine-rock reactions that may occur, C) optimization of geophysical and numerical models necessary for measurement, monitoring and verification (MMV), and D) a preliminary performance assessment. Research work to accomplish these goals was coordinated by one administrative task under the direction of Dr. Carol Frost, Professor of Geology and Geophysics (Task 1.0), and one task devoted to designing and creating an interdisciplinary, project-specific carbon cyberinfrastructure to support collaborative carbon dioxide sequestration research among University of Wyoming scientists and their collaborators, performed by Jeff Hammerlinck, Director of the Wyoming Geographic Information Science Center at the University of Wyoming (Task 1.5). The results of these tasks are presented in the Introduction and in Chapter 1, respectively.

Organization of Report

The overall objective for Priority Area A was the creation of a 3-D geological model of the potential injection site that includes thicknesses of target formations, locations and displacements of faults and fractures, the baseline geochemical and isotopic composition of the target aquifers, and locations and completion details of existing wells. Specific

products include: an electronic well database, geochemical and isotopic produced water database, a multiscale fault and fracture analysis, series of regional cross sections, and a three-dimensional subsurface structure model.

Five technical project tasks composed the research performed for Priority Area A:

Task 2.0—Geological characterization: Assembling and Validating a Well Database

PI: Dr. James D. Myers, Department of Geology and Geophysics

Task 3.0—Geological characterization: Geochemical Characterization of Produced Waters and Gases

PI: Dr. Shikha Sharma, Associate Director, UW Stable Isotope Facility

Co-PI: Dr. Carol Frost, Professor of Geology and Geophysics

Task 4.0—Geologic Characterization: Subsurface Structural Evaluation

PI: Dr. Erin Campbell-Stone, Department of Geology and Geophysics

Task 5.0—Geologic Characterization: Surface Structural Analysis

PI: Dr. Arthur W. Snoke, Department of Geology and Geophysics

The results of these tasks are presented in Chapters 2 through 5.

The overall objective for Priority Area B was to identify flow properties and fluid-rock reactions that will occur during carbon dioxide injection into the target aquifer. Specific products include description and computational models of major geochemical reactions, measurement of CO₂/brine relative permeabilities, and high-resolution 3-D images of reservoir rock and pore networks at the core scale.

Two technical project tasks composed the research performed for Priority Area B:

Task 6.0—Laboratory Experimental Activities: Mixed-phase (CO₂+H₂O) Fluid-Rock Reactions

PI: Dr. John Kaszuba, Department of Geology and Geophysics and School of Energy Resources

Task 7.0—Laboratory Experimental Activities: CO₂/Brine Relative Permeabilities

PI: Mohammad Piri, Department of Chemical and Petroleum Engineering

The results of these tasks are presented in Chapters 6 and 7.

The overall objective for Priority Area C was to determine the most appropriate seismic monitoring program and modeling strategies for monitoring this site, thereby preparing for a future carbon dioxide sequestration project. The specific objectives are to (1) evaluate the feasibility of geophysical modeling of CO₂ reservoirs using both active and passive seismic methods, (2) use modeling and numerical simulation to quantify the uncertainties associated with CO₂ sequestration in the deep geologic formations of the Moxa Arch, and (3) determine the optimal geological model complexity necessary.

Three technical project tasks composed the research performed for Priority Area C:

Task 8.0—Modeling Activities: Feasibility of Geophysical Modeling of CO₂-Reservoirs

PI: Dr Subhashis Mallick, Department of Geology and Geophysics and School of Energy Resources

Task 9.0—Modeling Activities: Multiscale Modeling and Numerical Simulation of CO₂ Injection

PIs: Dr. Felipe Pereira and Dr. Craig Douglas, Department of Mathematics and School of Energy Resources, Dr. Mohammad Piri, Department of Chemical and Petroleum Engineering, and Dr. Fred Furtado and Dr. Victor Ginting, Department of Mathematics

Task 10.0—Modeling activities: Determination of Optimal Geologic Model Complexity

PI: Dr. Ye Zhang, Department of Geology and Geophysics

The results of these tasks are presented in chapters 8 through 10.

The overall objective for Priority Area D was to create a model that will delineate the site in terms of suitable reservoirs for carbon storage, the capacity of target formations for carbon dioxide sequestration, projections of plume migration and brine displacement, and potential for leakage either along faults and fractures and/or existing wells. Successful completion of the performance assessment model is prerequisite to a future carbon dioxide injection demonstration project on the Moxa Arch.

The technical project task that accomplished the research for Priority Area D was performed by the Wyoming State Geological Survey:

Task 11.0—Performance Assessment

PIs: Wyoming State Geological Survey, Dr. Ronald C. Surdam, State Geologist, Rod DeBruin and John Jiao, Geologists

The results of this task are presented in Chapter 11.

Key Findings

Some of the most important conclusions drawn from the research in this project include the following (see individual chapters for additional key research conclusions):

- 95 wells lie within the footprint of the seismic survey on the Moxa Arch, which was used in Task 2 as the Moxa Arch Area of Review. Field checks revealed that 25 wells (27% of the total) were mislocated in the Wyoming Oil and Gas Conservation Commission website by an average of 565 feet. Task 2 demonstrated that standardized data mining and management procedures are necessary and that risk assessment must include errors in spatial locations of wells. A generalized workflow for compiling a well catalog based on a computationally defined Area of Review was developed for use at future geologic sequestration sites. (See Chapter 2 for more detail.)
- All available water quality data was compiled for four potential carbon dioxide receiving formations—Nugget Sandstone, Tensleep/Weber Sandstone, Madison Limestone, and Bighorn Dolomite—in the Greater Green River Basin, which encompasses both the Moxa Arch and the Rock Springs Uplift, two potential

carbon dioxide sequestration sites in southwestern Wyoming. The data suggest that except along the basin margins, the Tensleep/Weber, Madison, and Bighorn Formations are suitable targets under federal Class VI geologic sequestration regulations. However, low total dissolved solids in Nugget Sandstone groundwater in parts of the Rock Springs Uplift suggest the potential for local, fracture-assisted recharge in this area. For this reason the Nugget Sandstone is less suitable than the deeper formations for CO₂ storage in the Rock Springs Uplift. (See Chapter 3 for more detail.)

- The Bighorn Dolomite and Madison Limestone have distinctly different naturally occurring carbon dioxide volumes, with a CO₂ percentage of 84.7% within the Bighorn and 64.9% within the Madison. This information, along with independent pressure data confirms that these are two separate Paleozoic CO₂ reservoirs. The intervening Jefferson Formation isolates the two reservoirs. Fluid inclusion volatile analysis indicates that the confining system above the Madison Limestone is the Triassic Dinwoody Formation. (See Chapter 4 for more detail).
- The Moxa Arch is a gently dipping anticline (limbs dip 0–5 degrees). 3-D seismic interpretation reveals no faulting within the region in the resolution of the seismic data. Fracture intensity in the Madison Limestone and Bighorn Dolomite is related to rock composition. Most fractures are sub-vertical or parallel to bedding. Oriented core, which is not available at present, is required to create a complete fracture model. (See Chapter 5 for more detail.)
- The Madison Limestone contains natural accumulations of supercritical CO₂ and H₂S, SO₄²⁻ and S²⁻. Geochemical modeling and laboratory experiments identified the potential brine-rock-carbon sulfur reactions that take place during co-injection of supercritical CO₂ and SO₂ into a carbonate reservoir. Because the behavior of CO₂ in geological carbon storage will depend upon pore size, the range of pore sizes was assessed using SANS (small angle neutron scattering). The pore size measured in the Madison Limestone is too small to be accessible to CO₂ flow through capillary forces, but in small pores CO₂ may dissolve into the brine. (See Chapter 6 for more detail.)
- Unsteady-state drainage and imbibition full recirculation experiments in Berea and Nugget Sandstone used a medical CT scanner to measure in-situ saturations along the length of the samples during the flow experiments. The results indicate that relatively high fractions (about 50% to 75%) of the initial CO₂ saturation can be permanently trapped. (See Chapter 7 for more detail).
- Multicomponent seismic data are important for monitoring carbon dioxide in the subsurface, and seismic surveys should be conducted prior and following injection of carbon dioxide. Fluid substitution experiments showed that density is more sensitive to changes in CO₂ saturation than longitudinal (P) and transverse (S) wave velocities (V_P and V_S). Prestack waveform inversion techniques developed at UW produce more accurate models than traditional analysis of

amplitude variations versus offset, or angle of incidence (AVA/AVO) methods. Post-injection passive seismic monitoring may be a cost-effective strategy for locating fractures that may be associated with micro-seismic events related to above-normal pore pressure following sequestration. (See Chapter 8 for more detail.)

- Through our research we continued developing a multiscale parallel simulator for porous media flow problems. The combination of physically-based operator splitting for multiscale time discretization of nonlinear systems of partial differential equations arising in multiphase flows in porous media, domain decomposition for the parallel solution of elliptic and parabolic problems, and semi-discrete central finite volume schemes for hyperbolic systems have allowed us to produce very accurate simulations of multi-phase flow in porous media. (See Chapter 9 for more detail.)
- Geological and fluid flow simulation models for the Nugget Sandstone, the overlying Twin Creek Formation, and the underlying Ankareh Formation, allowed us to make two different estimates of gas storage, one using formation volumetrics, and the other using a porosity model. Petrophysical uncertainty was evaluated via a series of realizations; permeability hysteresis is the parameter that exerts the largest control on gas storage. The total predicted acid gas storage varies from 40% in a worst-case model to 94% in a best-case model. Future work is needed to expand the range of uncertainty by developing detailed facies models at the injection site. (See Chapter 10 for more detail.)
- Preliminary FEHM simulation and modeling work suggests that 1 Mt/year of CO₂ per injection well could be injected into the Bighorn Dolomite, the Madison Limestone, or the Weber Sandstone in the Moxa Arch area over 50 years at the Moxa Arch study site. Permeability is a major factor controlling the amount of CO₂ that can be injected into any of the target formations; lower relative permeabilities cause a rapid pressure buildup during the first years of injection. Geological heterogeneity of the storage domain is the greatest scientific uncertainty that must be addressed in order to produce more robust estimates of CO₂ capacity. (See Chapter 11 for more detail.)

INTRODUCTION: Geologic carbon sequestration in Wyoming

PI: Dr. Carol Frost, Department of Geology & Geophysics, University of Wyoming

Background

This introduction sets the stage for the project, giving a general background of carbon capture and sequestration (CCS) and then specifically outlining the regulatory situation and activities to advance geologic sequestration in Wyoming. It outlines the potential for carbon sequestration, the status of CCS technology, and the support and regulation of the technology that has occurred thus far in the U.S. and Wyoming. It then introduces the Moxa Arch project and explains how findings of the project have and will continue to inform a greater Department of Energy (DOE)-funded geologic carbon storage effort in Wyoming, or the Wyoming Carbon Underground Storage Project (WY-CUSP).

A project milestone for Task 1 (Task 1.6) was for the Principal Investigator to organize and edit a special issue of the peer-reviewed academic publication *Rocky Mountain Geology* that would showcase results and research undertaken through this DOE-funded project. This special issue was released in October 2010, and a number of the papers that appeared in this the special issue are included in this final report. The chapter that follows is part of this publication.

Geologic carbon sequestration in Wyoming: prospects and progress

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ABSTRACT

Coal supplies nearly 50 percent of electricity generation in the United States and 25 percent of the global energy supply; Wyoming produces approximately 40 percent of the coal consumed in the United States. It is likely that near-term energy strategies will include coal and other fossil energy sources in the fuel mix, therefore mitigating carbon dioxide emissions through geologic carbon capture and sequestration (CCS) is crucial. Here we discuss the current state of CCS technology across the globe and its future potential for development. We also outline the current regulatory structure for CCS in the United States, specifically Wyoming, and we introduce the study undertaken by University of Wyoming researchers and their collaborators to characterize Paleozoic deep saline aquifers on the Moxa Arch in southwestern Wyoming for long-term geologic carbon storage. The research presented in this special issue of *Rocky Mountain Geology* and future research that builds on these findings, such as the site characterization project underway on the Rock Springs Uplift in Wyoming, will be important steps to advance successful CCS technologies at a rate and scale that can make a meaningful impact on greenhouse gas emissions and to construct commercial geologic sequestration projects in the Rocky Mountain West.

KEYWORDS: geologic carbon dioxide sequestration, carbon sequestration regulation, deep saline formations, greenhouse gas emissions, Moxa Arch, Wyoming.

INTRODUCTION

Of the anthropogenic emissions of carbon dioxide (CO₂) to the atmosphere, more than 75 percent is contributed by combustion of fossil fuels for electrical power, industrial processes, and transportation (IPCC, 2007). A portfolio of technologies will be needed to help mitigate the impact of greenhouse gas emissions on climate, including energy efficiency, renewable fuels, and advanced transportation technologies. These pathways are part of the solution, but do not address pressing realities: coal supplies nearly 50 percent of electricity generation in the United States and 25 percent of the global energy supply (EIA, 2010a; Chu, 2009); and, the U.S., Russia, China, and India account for two-thirds of the world's known coal reserves, with the latter two countries accounting for 40 percent of the global population (CIA, 2009; Chu, 2009). As Secretary of Energy Steven Chu said in a recent editorial for *Science*, "... it is highly

unlikely that any of these countries (the U.S., India, and China) will turn their back on coal any time soon, and for this reason, the capture and storage of CO₂ emissions from fossil fuel power plants must be aggressively pursued." According to the International Energy Agency (2009), up to a fifth of mitigation in 2050 will need to come from capture and storage of CO₂ from the power and industrial sectors. And because the state of Wyoming produces some 40 percent of the coal consumed in the U.S., it has a particular interest in demonstrating safe and successful long-term storage of CO₂.

Carbon capture and geologic sequestration (CCS) is a promising technology among the portfolio of approaches needed to address climate change. In its most simplified form, it entails capturing CO₂ emissions from a point source, transporting them to a storage location, and compressing and injecting them underground into a geologic storage site where CO₂ will be stored for thousands of years. In practice, of course, the process is much more complicated, partic-

ularly with regards to characterizing and monitoring potential sequestration sites. If commercialized, however, CCS technology could be deployed in many locations across the globe (Dooley et al., 2006; IEA, 2009).

This special issue highlights some of the work undertaken by University of Wyoming (UW) researchers to characterize a deep saline formation located in southwestern Wyoming—the Moxa Arch—for long-term geologic CO₂ storage. UW researchers and their collaborators have determined through their preliminary characterizations that the Moxa Arch has the appropriate thickness, reservoir properties, overlying low-permeability lithofacies, formation fluid compositions, and structural integrity to be developed as a commercial storage site. In addition, data and processes developed from this project have played a key role in formation of a new characterization and possible demonstration project that will drill a stratigraphic test well in correlative formations on the Rock Springs Uplift in southwest Wyoming (Fig. 1). The research presented here and future research that builds on these findings will be important steps to construct successful commercial geologic sequestration sites in the Rocky Mountain West.

CARBON SEQUESTRATION POTENTIAL

CO₂ sequestration is a fundamental process of the Earth's chemical cycle. In the natural world, carbon sequestration occurs through processes such as photosynthesis, calcification of CO₂ by phytoplankton, and mineralization in root systems (Chu, 2009). In addition, natural underground geologic formations have stored CO₂ for millions of years (Haszeldine, 2009). A number of these CO₂ fields are located in the Rocky Mountain region, including in western Wyoming along the crest of the Moxa Arch and on the Rock Springs Uplift (Allis et al., 2001; Huang et al., 2007). These deep natural reservoirs of CO₂ can help us understand the movement, properties, and long-term effects of storing CO₂ underground (IPCC, 2005).

Global estimates of sequestration storage capacity range from 1700 to nearly 11,000 gigatons of carbon dioxide (GtCO₂) (Dooley et al., 2006; Orr, 2009). As a point of comparison, 30.4 GtCO₂ were emitted globally in 2008 (EIA, 2010b). It is unclear,

however, how much of this CO₂ storage capacity will be technically accessible (Brennan et al., 2010; Van Noorden, 2010). Currently, more than 60 percent of anthropogenic CO₂ emissions, or 8100 large point sources (primarily fossil-fuel electric generating plants), could potentially utilize CCS technologies. Of the 1715 of these large point sources that are located in the U.S., 95 percent of them are estimated to be within 50 miles of a potential geologic storage formation (Dooley et al., 2006).

Candidate geologic CO₂ storage formations include deep saline formations, depleted oil and natural gas reservoirs, deep unmineable coal seams, and deep saline-filled basalt formations. Of these formations, by far the largest potential and widespread storage source is deep saline formations, which are characterized by porous limestone or sandstone rocks that generally contain brine and may be capped by low-permeability formations that prevent vertical flows of CO₂. Global estimates of storage capacity in deep saline formations are ~9500 GtCO₂, with 3630 GtCO₂ of this residing in formations of the U.S. Injecting fluid waste into these deep saline formations is already a global practice (Dooley et al., 2006).

CURRENT STATUS OF CCS TECHNOLOGY

Carbon injection into underground geologic reservoirs has been in practice for over 30 years in the form of enhanced oil recovery (EOR). Currently, around 30 megatons of CO₂ (MtCO₂) are injected into oil reservoirs in western Texas every year, though most of this CO₂ is obtained from natural sources and only 3 MtCO₂ are captured from anthropogenic emissions (IPCC, 2005; Orr, 2009). Acid gas (a mixture containing hydrogen sulfide and carbon dioxide) injection is another common commercial practice that utilizes underground geologic storage to sequester unwanted gases. Despite the similarities between EOR, acid gas injection, and carbon sequestration, CCS injection projects would need to be at much larger volumes and scales than past projects to have meaningful impact.

Oil and gas well construction technologies may be adapted to the CO₂ injection wells through use of special cements and downhole materials selected to withstand acidic conditions that can result when CO₂ mixes with water (Myhre and Stone, 2009). Once the CO₂ is injected underground, the properties of its

Figure 1. The Moxa Arch and Rock Springs Uplift potential carbon sequestration sites in the Greater Green River Basin of southwestern Wyoming. The black rectangle on the axis of the Moxa Arch marks the location of the detailed site characterization of the structure; a second site characterization project has begun on the Rock Springs Uplift. Figure modified from Campbell-Stone et al. (2010).

subsurface flows are complex, involving multiphase fluid flow, CO_2 dissolution into groundwater, mineral precipitation and dissolution, and water-rock interactions (Schnaar and Cullen, 2009). Physical and chemical trapping of CO_2 occurs through structural trapping, residual or pore space trapping, and dissolution or solubility trapping (Myhre and

Stone, 2009). At depths below 2500 feet, supercritical CO_2 takes on a liquid-like density, which is an efficient storage form in the pores of sedimentary rocks (IPCC, 2005). Many research and development efforts are underway to model the location and behavior of underground CO_2 over time (Myhre and Stone, 2009).

Current cost estimates of the application of carbon sequestration technology to electricity production vary widely, and range as high as \$120–180/ton of CO₂ stored for first-of-a-kind plants and \$35–70/ton of CO₂ stored for subsequent, “nth-of-a-kind” plants (Al-Juaied and Whitmore, 2009). Carbon capture is the largest component of the cost of CCS, and research initiatives also are underway specifically to reduce the energy and cost component of this phase of the CCS process (IPCC, 2005). The increased energy requirements, which result in decreased net power plant output of 15–30 percent and doubled water requirements for post-combustion capture technology, are additional, significant concerns (Bauer, 2009).

While there are many current efforts to demonstrate CCS technology, no operational commercial-scale sequestration project associated with a major coal-fired power plant exists. There are, however, more than 20 experiments and pilot CCS projects operating throughout the world, though the largest captures one-tenth of the scale needed for a commercial power plant (Haszeldine, 2009). Of these 20 projects, four are fully integrated, commercial-scale plants (Sleipner, Snøhvit, In Salah, and Weyburn-Midale). Three of these projects inject CO₂ separated from natural gas production facilities, and the fourth captures emissions from a coal-based synfuels plant and injects them into an oil field for EOR purposes (IEA, 2009).

The Sleipner Project in the North Sea is a prime example of a large-scale CO₂ storage project in a saline formation. In this project, CO₂ separated from a gas field is re-injected approximately 1000 m below the floor of the North Sea into the Utsira saline formation (IEA, 2009). The Utsira Formation is a brine-saturated unconsolidated sandstone that has secondary thin shale layers that influence the movement of injected CO₂. Overlying the formation is a seal of thick shale, which secures the injected CO₂ in the formation (IPCC, 2005). The 1 million tons of carbon sequestered annually in this formation are equivalent to the emissions of a 150-megawatt (MW) coal-fired power plant (note that this is small compared to many coal-fired power generation facilities, which may be 1–2 gigawatt (GW) plants that emit on the order of 8 to 16 million tons of CO₂ annually). The CO₂ plume at the Sleipner site has been monitored over the past decade through seismic time-lapse surveys. These

show the footprint of the plume to encompass 8 km²; it is projected that over time the CO₂ will dissolve in the aquifer (IPCC, 2005). Injection of CO₂ since 1996 at the Sleipner site has demonstrated the safe and successful injection, storage, and monitoring of CO₂ in a deep saline formation.

U.S. AND WYOMING STATE GOVERNMENT SUPPORT AND REGULATION OF CCS

The United States federal government recognizes the importance of commercializing carbon capture and sequestration technology and is supporting CCS through a variety of initiatives. The 2009 American Reinvestment and Recovery Act invested \$3.4 billion in CCS research and development; this funding added to the regular Department of Energy (DOE) appropriations that support CCS activities (\$180 million in Fiscal Year (FY) 2010), including seven regional sequestration partnerships that are working to produce large-scale projects across the country. The International Energy Agency predicts that all nations with CCS targets will have to invest \$3.5 billion to \$4 billion in demonstration projects over the next decade to commercialize the technology by 2020 (Van Noorden, 2010); the Recovery Act funds combined with general appropriations mean that—at least for FY2010—the U.S. is thus far meeting this level of commitment.

Furthermore, in February 2010, the administration announced an Interagency Task Force on Carbon Capture and Storage, which was charged with seeking ways to overcome barriers to commercialization of CCS technologies. The Task Force, which was co-chaired by the Department of Energy and Environmental Protection Agency (EPA), submitted a plan to the president in August 2010 that identified barriers to CCS development and provided recommendations of how to overcome barriers and construct 5–10 commercial CCS projects by 2016 (Platts, 2010). In July 2010, the U.S. and 12 other countries also pledged to establish an international Carbon Capture Use and Storage Action Group that is charged with determining how best to enable deployment of carbon capture and storage technologies worldwide (Clean Energy Ministerial, 2010).

Geologic sequestration of carbon dioxide is unlikely to become widely adopted without a regulatory framework. Two items of most concern regard-

ing regulations for CCS projects include issues of who owns the pore space in the rock that will be used to store CO₂ and long-term liability issues of geologic storage. In the U.S., the EPA has the authority to monitor carbon sequestration activities through the Safe Water Drinking Act and its Underground Injection Control (UIC) program, which is in place to protect underground sources of drinking water (USDWs). In 2008 the EPA proposed a new class of regulation well, Class VI, and has outlined minimum technical requirements for geologic site characterization, well construction, operation, monitoring, and post-injection site care (EPA, 2008). The State of Wyoming has primary enforcement authority for the UIC program; in Wyoming permits for geological sequestration of CO₂ will be issued by the Wyoming Department of Environmental Quality according to its proposed Water Quality Rules and Regulations, Chapter 24 (2010).

In the Rocky Mountain West, Wyoming was the first state to pass legislation on carbon sequestration. House Bill Nos. 89 and 90, signed into law in March 2007 and put into effect in July 2008, design a legal framework for storing carbon underground. The legislation designates that pore space is owned by the surface owner; however, the legislation does not specify what entity is liable if sequestered carbon migrates beyond its intended reservoir (Nowakowski, 2007). Wyoming convened a working group to further investigate appropriate financial bond and long-term liability structures, which released its recommendations in September 2009 (see Wyoming Carbon Sequestration Working Group, 2009). Wyoming House Bill No. 17 passed in 2010 provides for carbon sequestration financial assurances and regulation and was based upon recommendations of the Carbon Sequestration Working Group report. Colorado, Utah, North Dakota, and Montana, amongst other Western states, also have pursued or are pursuing putting relevant CCS legislation or regulations in place.

Public acceptance of CCS technology and its safety is crucial to its success. Experts have largely concluded that in properly designed and managed CCS projects there is little to no chance of appreciable leakage from geologic formations (Dooley et al., 2006). Many existing activities, such as natural gas storage, enhanced oil recovery, and deep underground disposal of acid gas have similar risk pro-

files as CCS (IPCC, 2005). However, there remain concerns of contamination of groundwater, leakage of CO₂, or induced seismicity. To address public safety concerns and long-term liability issues, state governments must pass legislation and regulations that establish ownership, liability, and regulatory regimes. The public also will need to be educated about how the technology works and how developers will mitigate risks (DOE-NETL, 2009). Most importantly, the industry needs to build a track record of safety built on careful site selection, characterization, injection practices, and monitoring (IPCC, 2005).

UNIVERSITY OF WYOMING MOXA ARCH AND WY-CUSP PROJECT

Paleozoic deep saline aquifers in southwestern Wyoming are the most promising targets for geologic CO₂ sequestration in the state and are possibly the most promising sequestration sites in the Rocky Mountain region. One of the geologic structures containing these deep saline aquifers—the Moxa Arch—is a 200-km-long, north–south trending anticline that plunges beneath the Wyoming Thrust Belt on the north and is bounded on the south by the Uinta Mountains. Several oil and gas fields along the Moxa Arch contain large, natural accumulations of CO₂. The largest of these is the LaBarge Platform, which encompasses approximately 2000 square km² (Huang et al., 2007).

The University of Wyoming and its collaborators identified Moxa Arch as a promising site for commercial-scale sequestration for a number of reasons: (1) it is a geological structure that has stored over 100 trillion cubic feet (TCF) of CO₂ for many millions of years (Lynds et al., 2010a); (2) several formations appear to be suitable sequestration reservoirs (at pressures and temperatures for which CO₂ will be supercritical); and (3) CO₂ is presently being produced and sold for enhanced oil recovery, and more CO₂ is potentially available for this and other uses, including for a future sequestration demonstration. Several deep saline formations may be suitable for storage of CO₂, foremost among them the Madison Limestone, Bighorn Dolomite, and Nugget Sandstone. These storage units are overlain by a series of impermeable lithologies that serve as regional hydrocarbon, CO₂, and helium seals, ensuring fluid containment.

The Madison Limestone is a proven storage reservoir. ExxonMobil has been producing natural gas on the north end of the Moxa Arch on the LaBarge Platform from the Madison Limestone, which contains CO₂, methane, nitrogen, hydrogen sulfide (H₂S), and helium. Farther south, the Moxa Arch also already is used for sequestration purposes: ExxonMobil has been injecting CO₂ (up to 25 million cubic feet per day (MMCFD)) and H₂S (up to 65 MMCFD) into the Madison Limestone at its Shute Creek Gas Plant, located 65 km south of the producing field (Campbell-Stone et al., 2010).

The papers in this special issue present results from a University of Wyoming/Wyoming State Geological Survey/DOE-funded project that address some of the different aspects of characterizing the Moxa Arch structure in southwestern Wyoming. The overarching goal for the project was to improve the understanding of CO₂ flow and trapping within the targeted reservoir and develop simulation models to predict how much CO₂ could be stored in this potential site. The project characterized the geology, hydrogeology, geochemistry, and geophysical properties of the Moxa Arch and used these data and other laboratory experimental activities to construct appropriate monitoring and performance assessment regimes. This issue includes papers describing two of the major potential reservoirs, the Bighorn and Madison Formations (Lynds et al., 2010b; Thyne et al., 2010), the geochemistry of the groundwaters contained within the target formations in the Greater Green River Basin (Smith et al., 2010), and the development of a multiscale parallel simulator for porous media fluid flow that can provide accurate predictions of migration and trapping of injected carbon dioxide (Douglas et al., 2010). The cyberinfrastructure to support collaborative geologic sequestration research is explored by Hamerlinck et al. (2010), and the economics of fossil fuel and wind energy production under various carbon taxation scenarios are discussed by Geiger et al. (2010). Other publications forthcoming from these and other members of the Moxa Arch research group will complete the site characterization of that geological structure.

Building on results of this Moxa Arch project, the University of Wyoming has begun the Wyoming Carbon Underground Storage Project (WY-CUSP), a partnership of the University of Wyoming, the Wyoming State Geological Survey, Baker Hughes,

Inc., ExxonMobil, and Los Alamos National Laboratory. This project was funded by the U.S. Department of Energy and the State of Wyoming to assess the CO₂ storage potential of the Rock Springs Uplift, to develop a system for displaced fluid management, to plan monitoring and verification activities, and to design infrastructure in preparation for carbon sequestration. The target storage reservoirs on the Rock Springs Uplift are the Pennsylvanian Tensleep/Weber Sandstone and Mississippian Madison Limestone. These formations lie at depths of from 2 to 6 km below the surface, depending upon location on the anticline. The CO₂ accumulations and their extents appear to be controlled by faults with throws, and the project will work to understand the fault-dependent mechanisms that isolated the CO₂ traps on the Rock Springs Uplift to determine the feasibility of long-term storage at this site (Lynds et al., 2010a). An advantage of the Rock Springs Uplift study site is that it is adjacent to PacifiCorp's Jim Bridger power plant (a 2200 MW coal-fired power plant that emits 18 MtCO₂ per year), which is much larger than PacifiCorp's 700 MW Naughton power plant at Kemmerer on the Moxa Arch. Analysis has shown that CCS systems will be most economic when deployed with large baseload power plants and with reservoirs (most likely deep saline formations) that can ideally hold more than 50 years worth of the facility's CO₂ (Dooley et al., 2006).

The site characterization studies of the Moxa Arch and the Rock Springs Uplift site will provide critical scientific information needed for the University of Wyoming and its collaborators to select the best location to carry out a future geologic sequestration demonstration in southwestern Wyoming.

CONCLUSION

The Intergovernmental Panel for Climate Change has stated that for CCS to make significant cuts to global CO₂ emissions there must be thousands of large-scale geologic storage projects across the globe (IPCC, 2005). The International Energy Agency follows this up by saying that the cheapest way to provide 20 percent of the target to halve expected CO₂ emissions by 2050 is to employ CCS technologies; to meet this target, the volume of liquid CO₂ that would have been injected would be three

times the current amount of petroleum used globally each year. In other words, the CCS industry would have to scale up to the size of the oil industry, or even larger, by mid-century to have a significant impact (Van Noorden, 2010).

To safely and successfully operate the thousands of carbon sequestration projects that will be required, careful characterization of the subsurface, good design of the injection project, advanced monitoring, and state-of-the-art computational modeling techniques are needed (Orr, 2009; Schnaar and Cullen, 2009). The International Energy Agency (2009) calls for more experience to improve predictions of CO₂ behavior underground and tools to identify suitable storage sites, particularly for deep saline formations. The research being undertaken at the University of Wyoming—some of which is presented here—is therefore crucial to advance CCS technologies at a rate and scale that can make a meaningful impact on greenhouse gas emissions.

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REFERENCES CITED

- Al-Juaied, M., and Whitmore, A., 2009, Realistic costs of carbon capture: Belfer Center Discussion Paper, Belfer Center for Science and International Affairs, John F. Kennedy School of Government, Harvard University, http://belfercenter.ksg.harvard.edu/publication/19185/realistic_costs_of_carbon_capture.html?breadcrumb=%2Fproject%2F43%2Fenvironment_and_natural_resources.
- Allis, R., Chidsey, T., Gwynn, W., Morgan, C., White, S., Adams, M., and Moore, J., 2001, Natural CO₂ reservoirs on the Colorado Plateau and southern Rocky Mountains: candidates for CO₂ sequestration, *in* Proceedings, First National Conference on Carbon Sequestration, Washington, D.C., May 14–17, 2001: U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL), http://www.netl.doe.gov/publications/proceedings/01/carbon_seq/6a2.pdf.
- Bauer, C. O., 2009, Statement of Carl O. Bauer, Director, National Energy Technology Laboratory, U.S. Department of Energy, before the Energy and Natural Resources Committee, United States Senate, March 10, 2009, <http://www.netl.doe.gov/newsroom/testimony/3-10-09%20Final%20Testimony%20Bauer%20NETL.pdf>.
- Brennan, S. T., Burruss, R. C., Merrill, M. D., Freeman, P. A., and Ruppert, L. F., 2010, A probabilistic assessment methodology for the evaluation of geologic carbon dioxide storage: U.S. Geological Survey Open-File Report 2010-1127, 31 p.
- Campbell-Stone, E., Lynds, R., Frost, C., Becker, T. P., and Diem, B., 2010, The Wyoming carbon underground storage project: geologic characterization of the Moxa Arch and Rock Springs Uplift: Energy Procedia, in press.
- Chu, S., 2009, Carbon capture and sequestration: Science, v. 235, p. 1599.
- CIA (Central Intelligence Agency), 2009, The world factbook: country comparison – population, <https://www.cia.gov/library/publications/the-world-factbook/rankorder/2119rank.html>.

- Clean Energy Ministerial, 2010, Fact sheet: Carbon Capture Use and Storage Action Group, <http://www.energy.gov/news/documents/CCUS-Fact-Sheet.pdf>.
- DOE-NETL (U.S. Department of Energy National Energy Technology Laboratory), 2009, Best practices for public outreach and education for carbon storage projects, http://www.netl.doe.gov/technologies/carbon_seq/refshelf/BPM_PublicOutreach.pdf.
- Dooley, J. J., Dahowski, R. T., Davidson, C. L., Wise, M. A., Gupta, N., Kim, S. H., and Malone, E. L., 2006, Carbon dioxide capture and geologic storage: a core element of a global energy technology strategy to address climate change: College Park, Maryland, Global Energy Technology Strategy Program, Technology Report, 37 p.
- Douglas, C., Furtado, F., Ginting, V., Mendes, M., Pereira, F., and Piri, M., 2010, On the development of a high-performance tool for the simulation of CO₂ injection into deep saline aquifers: *Rocky Mountain Geology*, v. 45, p. 151–161.
- EIA (U.S. Department of Energy Energy Information Administration), 2010a, Electric power monthly April 2010, http://www.eia.doe.gov/cneaf/electricity/epm/epm_sum.html.
- , 2010b, International energy statistics: total carbon dioxide emissions from the consumption of energy, <http://tonto.eia.doe.gov/cfapps/ipdbproject/IEDIndex3.cfm?tid=90&pid=44&aid=8>.
- EPA (Environmental Protection Agency), 2008, EPA proposes new requirements for geologic sequestration of carbon dioxide, http://www.epa.gov/safewater/uic/pdfs/fs_uic_co2_proposedrule.pdf.
- Geiger, M., Coupal, R., and McLeod, D., 2010, Potential impacts of federal regulation of greenhouse gas emissions on Wyoming's energy-derived tax revenue: *Rocky Mountain Geology*, v. 45, p. 181–191.
- Hamerlinck, J. D., Wyckoff, T. B., Oakleaf, J. R., and Polzer, P. L., 2010, Cyberinfrastructure for collaborative geologic carbon sequestration research: a conceptual model: *Rocky Mountain Geology*, v. 45, p. 163–180.
- Haszeldine, R. S., 2009, Carbon capture and storage: how green can black be?: *Science*, v. 235, p. 1647–1652.
- Huang, N. S., Aho, G. E., Baker, B. H., Matthews, T. R., and Pottorf, R. J., 2007, Integrated reservoir modeling to maximize the value of a large sour-gas field with high concentrations of inerts: International Petroleum Technology Conference Paper 11202, presented at the IPTC conference in Dubai, UAE, 4–6 December 2007, 16 p.
- IEA (International Energy Agency), 2009, Carbon capture and storage: full-scale demonstration progress update: Paris, IEA/OECD, http://www.iea.org/G8/docs/ccs_g8july09.pdf.
- IPCC (Intergovernmental Panel for Climate Change), 2005, Carbon dioxide capture and storage, Metz, B., Davidson, O., de Coninck, H., Loos, M., and Meyer, L., eds.: Cambridge, Cambridge University Press, 431 p..
- , 2007, Couplings between changes in the climate system and biogeochemistry, in Solomon, S., Qin, D., Manning, M., Marquis, M., Averyt, K., Tignor, M.M.B., Miller, H.L., Jr., and Chen, Z., eds., *Climate Change 2007: The Physical Science Basis, Contribution of the Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change*: Cambridge, Cambridge University Press, 996 p.
- Lynds, R., Campbell-Stone, E., Becker, T. P., Frost, C., Liesch, A., Bentley, R., and Diem, B., 2010a, A sequestration systems approach to geologic characterization of CO₂ storage sites: examples from the Green River Basin, Wyoming: *Geological Society of America Abstracts with Programs*, v. 42, no. 5, p. 113.
- Lynds, R., Campbell-Stone, E., Becker, T. P., and Frost, C. D., 2010b, Stratigraphic evaluation of reservoir and seal in a natural CO₂ field: Lower Paleozoic, Moxa Arch, southwest Wyoming: *Rocky Mountain Geology*, v. 45, no. 2, p. 113–132.
- Myhre, R. J. and Stone, M., 2009, Opportunities for carbon capture and geologic storage, *Southwest Hydrology*, v. 8, p. 18–20.
- Nowakowski, S., 2007, State activities on carbon sequestration, prepared for the Montana State Legislature Interim Committee on Energy and Telecommunications, http://leg.mt.gov/content/committees/interim/2007_2008/energy_telecom/assigned_studies/co2page/ncslsupplement.pdf.
- Orr, F. M., Jr., 2009, Onshore geologic storage of CO₂: *Science*, v. 235, p. 1656–1658.
- Platts, 2010, White House task force on CCS launches web site with public postings, in *Global Power Report*, April 8, 2010, <http://www.platts.com/Products/globalpower-report/>.
- Schnaar, G., and Cullen, S. J., 2009, The hydrology of geologic sequestration: *Southwest Hydrology*, v. 8, p. 20–21.
- Smith, M. S., Sharma, S., Wyckoff, T. B., and Frost, C. D., 2010, Baseline geochemical characterization of potential receiving reservoirs for carbon dioxide in the Greater Green River Basin, Wyoming: *Rocky Mountain Geology*, v. 45, p. 95–114.
- Thyne, G. D., Tomasso, M., Bywater-Reyes, S. V., Budd, D. A., and Reyes, B. M., 2010, Characterization of porosity and permeability for CO₂ sequestration models in the Mississippian Madison Group, Moxa Arch-LaBarge Platform, southwestern Wyoming: *Rocky Mountain Geology*, v. 45, p. 133–150.

Van Noorden, R., 2010, Buried trouble: *Nature*, v. 463, p. 871–873.

Wyoming Carbon Sequestration Working Group, 2009, Report and recommendations of the Carbon Sequestration Working Group to the Joint Minerals, Business, and Economic Development Committee and the Joint Judicial Committee of the Wyoming State Legislature, September 2009, <http://deq.state.wy.us/out/downloads/1%20FinalReport081909.pdf>.

Wyoming Department of Environmental Quality, 2010, Water quality rules and regulations, Chapter 24, Draft for comment February 2010.

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CHAPTER 1: Cyberinfrastructure for Geologic Carbon Sequestration Research

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Background

Task 1.5 of the project sought to design and create the framework of an interdisciplinary, project-specific carbon cyberinfrastructure to support collaborative carbon dioxide sequestration research among University of Wyoming scientists and their collaborators. This work was intended to establish a custom science information infrastructure that integrated spatial data, non-spatial data, and research results to support: a) assessment of the best injection sites and gas resources; b) construction of sequestration performance models; and c) design of a measurement, monitoring, and verification (MMV) program for future sequestration activities in the state and region.

Results from the cyberinfrastructure sub-task were published in the special issue of *Rocky Mountain Geology*. Key findings, in the form of a peer-reviewed academic paper, follow.

Cyberinfrastructure for collaborative geologic carbon sequestration research: a conceptual model

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ABSTRACT

This paper describes the design and development of a conceptual framework for creating and implementing a cyberinfrastructure model to support interdisciplinary science associated with geologic carbon sequestration at the University of Wyoming. “Cyberinfrastructure” is a term increasingly used within the scientific community to represent information infrastructure networks connecting technology, data, and people to support research activities and the dissemination of its results. In this study, a cyberinfrastructure was designed for a multi-team, multi-task project case study centered on carbon sequestration research in the Moxa Arch, Wyoming. The design was based on a needs assessment conducted to identify information technology practices and requirements for each science team, resulting in a prototype carbon capture and storage knowledge-base workflow model. Major components of the workflow model include social networking functionality and geographic information system–based data management and visualization. The long-term goal of the effort is to build a cyberinfrastructure that fosters and enhances collaboration across research involved with geologic characterization, reservoir modeling, and long-term monitoring of geologic sequestration activities in Wyoming and throughout the Rocky Mountain Region.

KEYWORDS: carbon sequestration, computer-supported collaborative work, cyberinfrastructure, data management, design science, geographic information systems, information technology.

INTRODUCTION

Carbon capture and storage (CCS) refers to the long-term isolation of large-scale anthropogenic sources of carbon dioxide (CO₂) from the atmosphere. CCS encompasses a wide range of biological, chemical, and physical processes and a range of engineering technologies to support two distinct yet connected activities. The first, carbon capture, involves the separation, collection, and concentration of CO₂ from industrial power plant flue gas and other energy sources and the compression and transport of that CO₂ by pipeline to a storage location. The second, carbon storage, includes sequestration of CO₂ via numerous practices ranging from the injection of CO₂ into deep geologic formations or onto the deep ocean floor to no-till farming for soil carbon sequestration and terrestrial biomass sequestration through tree planting (IPCC, 2005).

Among storage options, geologic carbon sequestration is held by many to be the most viable for reduc-

ing greenhouse gas emissions over the next 30 years (Friedmann, 2007). Nevertheless, large-scale commercial deployment of geologic storage faces significant scientific, technical, economic, regulatory, and social challenges (Bachu, 2000; Benson et al., 2004; McFarland et al., 2004; IOGCC, 2005; Friedmann, 2006, 2007; DOE, 2007; Wilson et al., 2007; Gibbins and Chalmers, 2008; Grobe et al., 2010). Recently, attention has increasingly been given to a different type of CCS challenge associated with collecting, managing, and sharing data related to CCS and linking them with the information technologies necessary for supporting not only geologic sequestration science and management, but other aspects of the broader CCS process as well (Carr et al., 2007).

Building on the work of the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL) and the DOE Regional Carbon Sequestration Partnerships (DOE, 2007; Carr et al., 2009), we describe the development of a conceptual

framework for creating and implementing a cyberinfrastructure model to support interdisciplinary science at the University of Wyoming associated with geologic carbon sequestration. The cyberinfrastructure concept and its application in the geosciences are reviewed and the cyberinfrastructure needs for a multi-team, multi-task research project case study are assessed. A prototype CCS knowledge workflow model supporting a cyberinfrastructure is presented, which highlights the social networking and geographic information system-based data management and visualization components. The long-term goal of the effort is to build a cyberinfrastructure that fosters and enhances collaboration across research disciplines involved with geologic characterization, reservoir modeling, and long-term monitoring of geologic sequestration activities in Wyoming and throughout the Rocky Mountain Region.

CYBERINFRASTRUCTURE AND CYBERENVIRONMENTS FOR GEOSCIENCE RESEARCH

Cyberinfrastructure (CI) is a term increasingly used within the scientific community to describe information infrastructure networks connecting technology, data, and people to support research activities and the dissemination of its results. By more formal definition, a cyberinfrastructure:

...consists of computing systems, data storage systems, advanced instruments and data repositories, visualization environments, and people, all linked together by software and high performance networks to improve research productivity and enable [scientific] breakthroughs not otherwise possible (Pervasive Technology Institute, 2007).

Management of scientific data has long been a driving force behind the cyberinfrastructure concept, reflecting “the need for scientists to adapt to conducting research with data that come in rapidly increasing quantities, varieties, and modes of dissemination, frequently for purposes far more interdisciplinary than in the past” (NRC, 1997, p. 3).

Comprising ever-evolving information technologies, cyberinfrastructure implementations may be considered “both a continuous work-in-progress and a stable infrastructure driver for invention and innovation” (Berman, 2008, p. 20). This concept gained wide recognition following its promotion in a 2003 U.S. National Science Foundation (NSF) blue-ribbon committee report that addressed barriers to the evolution of and access to high performance computing (HPC) (Atkins et al., 2003). Since then, the NSF has made cyberinfrastructure a cornerstone in developing and delivering new technology environments to enable and enhance scientific discovery (NSF, 2007); prominent geosciences-related examples include the TeraGrid (www.teragrid.org) and the Open Science Grid (www.opensciencegrid.org).

Carr et al. (2007) outline the vision for a National Carbon Cyberinfrastructure (NCCI): “an integrated online computing environment that provides access to carbon science information, models, problem solving capabilities, and communication” (p. 138). The NCCI has initially been implemented as the NATional CARBOn Sequestration Database and Geographic Information System (NATCARB), supported by NETL and the DOE Regional Carbon Sequestration Partnerships (Carr et al., 2009). NATCARB is “an interactive relational database management system with spatial query capabilities to evaluate the geographic distribution, physical characteristics, and economic parameters of potential CO₂ sources and geologic sequestration sites” (NETL, 2007b, p. 33). The application supports information transfer to resource managers and decision makers through the Carbon Sequestration Atlas of the United States and Canada (NETL, 2007a), which provides a preliminary regional-scale assessment of carbon sources and storage sites for CO₂ sequestration projects over much of North America.

To date, the emphasis of most geosciences cyberinfrastructure efforts has been on the high performance computing aspects of information infrastructure creation (e.g., Gahegan et al., 2008). Recently, however, the potential of cyberinfrastructures to facilitate coordination of people and better address cross-disciplinary scientific inquiry has increasingly been considered. Acknowledging the human and organizational aspects

of cyberinfrastructures (Lee et al., 2006; Zimmerman and Nardi, 2006), Myers and Dunning (2006) propose the development of cyberenvironments—“the software infrastructure and [user] interfaces needed to realize this vision of CI as a systematic catalyst for transformative change in research practice and end-to-end productivity” (p. 1).

CASE STUDY: MOXA ARCH CARBON SEQUESTRATION PROJECT

Project initiation

In 2008, the University of Wyoming began a two-year research initiative focused on developing the background information and procedures necessary to prepare for geologic CO₂ sequestration in the Moxa Arch anticline of southwestern Wyoming. The initiative was developed in response to a desire by NETL to expand field tests that characterize potential CO₂ storage sites and to demonstrate the long-term storage of sequestered carbon. Among the challenges in conducting such demonstrations were “improved understanding of CO₂ flow and trapping within the reservoir and the development and deployment of technologies such as simulation models and monitoring systems” (NETL, 2007b, p. 20).

Study area

The Moxa Arch is a 200-km-long, north-south-trending anticline that plunges beneath the Wyoming thrust belt on the north and is bounded on the south by the Uinta Mountains (Fig. 1). The study area was chosen after being identified as having significant potential for geologic sequestration of impure CO₂ in a deep reservoir environment. Several formations were identified as potentially suitable for deep reservoir storage of impure CO₂ gas, foremost among them the Ordovician Bighorn Dolomite and the Mississippian Madison Limestone (for a more detailed description of the geologic characteristics and sequestration potential of the Moxa Arch anticline, see Lynds et al. (2010)). This site was also of interest for sequestration research activities due to a large abundance of natural CO₂ being produced as a byproduct of oil and gas development in the region and an already present CO₂ sequestration infrastructure and market to support enhanced oil recovery (EOR). These two factors provide both a potential

supply of CO₂ and future opportunities for CCS (Frost and Jakle, 2010).

Science objectives

The overall objective of the Moxa Arch project was to provide an improved analysis and understanding of the injectivity, capacity, and storativity of regionally significant formations that would be necessary for a future geologic carbon sequestration test on the Moxa Arch. The specific research activities pursued were related to four major areas of research aimed at improved knowledge and understanding of the Moxa Arch site and its suitability for CO₂ injection and storage: (1) geologic characterization of the arch structure, including fault and fracture patterns of the target formations and caprocks; (2) laboratory-based experimental characterization of carbon dioxide-brine-rock reactions; (3) optimization of geophysical and numerical models necessary for monitoring, verification, and assessment (MVA); and (4) construction of a preliminary performance assessment model for risk analysis of potential leakage rates and environmental impacts.

Opportunities and challenges for cyberinfrastructure-based collaboration

Table 1 outlines the individual tasks undertaken as part of the Moxa Arch project. In total, the project involved more than 35 individuals associated with 10 distinct research tasks and science teams (not including project management). The nature of the research activities associated with the tasks was diverse, involving heterogeneous data inputs, outputs, and procedures. Four tasks (Tasks 2–5) addressed various aspects of geologic characterization. Two tasks (Tasks 6 and 7) involved laboratory experimental activities. Four tasks (Tasks 8–11) centered on modeling activities. With the exception of Task 11, all of the tasks were led by science teams staffed by university personnel, including junior and senior faculty, post-doctoral research associates, and graduate and undergraduate students. Task 11—“Performance Assessment”—was staffed by research personnel from the Wyoming State Geological Survey (WSGS). As Task 11 was a risk assessment modeling activity, it was designed to incorporate data and results from Tasks 2 through 10.

In developing a project management plan (Task 1), both opportunities and challenges were identified for cross-task collaboration, making the overall proj-

Figure 1. Moxa Arch project study area. The Moxa Arch anticline is located in southwestern Wyoming to the east of the Wyoming thrust belt. The LaBarge area oil and gas fields are a major source of CO₂ and are served by a growing pipeline distribution system. Significant residual CO₂ injection is also currently taking place in the vicinity of the Shute Creek gas plant facility. Other CO₂ sources are present in the area, as evidenced by the location of numerous nearby refineries and power plants. Ongoing University of Wyoming CCS research activity is now focusing on the CO₂ storage potential associated with certain formations in the Rock Springs Uplift.

ect attractive for exploring cyberinfrastructure development. Having definable task deliverables and the involvement of only one academic institution and government partner, which are physically co-located on the same university campus, limited the complexity of designing a cyberinfrastructure. At the same time, the diversity of work to be performed and a relatively short project timeframe (12 to 24 months) for all deliverables provided two substantial challenges in implementing and testing the infrastructure's effectiveness. The remainder of this paper reviews the approach and results of that cyberinfrastructure design activity, and provides recommendations for potential future, full-scale implementation.

METHODOLOGY

Design-science theory in information systems research (Gregor, 2006) provided the context for development of the conceptual cyberinfrastructure model. As opposed to behavioral-science approaches to information systems research, which focus mostly on intentions of use, perceived usefulness, and impacts and benefits, design science attempts to create and evaluate information technology intended to serve human purposes and solve identifiable problems (March and Smith, 1995; Hevner et al., 2004).

In considering approaches to CI design, Zimmerman (2007) posits that cyberinfrastructure

Table 1. Moxa Arch project task summary.

Task	Title	Activity Type	Primary Objective	# of Primary Personnel
1	Project Management Planning	Oversight	Oversight, administration, and organization, with subtask 1.5 cyberinfrastructure design and initial development.	4
2	Assembling and Validating a Well Database	Geological Characterization	Development of a well database and spatial verification using GIS/GPS, procedures, and compilation of rules and regulations defined by U.S. EPA.	2
3	Geochemical Characterization of Produced Waters and Gases	Geological Characterization	Compile preliminary geochemical data on water/gas variation of target and overlying formations, analyze stable isotopic and major ion chemical compositions.	3
4	Subsurface Structural Evaluation	Geological Characterization	Analysis of seismic and well logs to create 3D subsurface model of shape, volume, lithology, fractures/faults, and thickness of reservoirs/seals.	2
5	Surface Structural Analysis	Geological Characterization	Multi-scale evaluation of the surface structural geology, identification of local and regional fracture and fault systems.	2
6	Mixed-phase (CO ₂ +H ₂ O) Fluid Rock Reactions	Laboratory Experimental Activities	Evaluation of mixed-phase fluid rock reactions and processes using rocking autoclaves and stirred reactors.	4
7	CO ₂ /Brine Relative Permeabilities	Laboratory Experimental Activities	Measurement of relative permeabilities, hysteresis, and capillary trapping of CO ₂ , and measurement of in-situ saturation using medical CT-scanner.	3
8	Feasibility of Geophysical Modeling of CO ₂ reservoirs	Modeling Activities	Model development for full waveform computation and inversion for elastic properties, micro-seismic sources for fracture characterization using existing geological data.	4
9	Multi-scale Modeling and Numerical Simulation of CO ₂ Injection	Modeling Activities	Simulation code development to predict migration and trapping of CO ₂ plume developed for high performance open source model computing environment.	4
10	Determination of Optimal Geologic Model Complexity	Modeling Activities	Build reservoir models to quantify volume/flow of mixed gases, storage, and leakage.	2
11	Performance Assessment	Modeling Activities	Incorporate data derived from Tasks 2–10 into a 3D EarthVision model.	4

design frameworks must be socio-technical in nature, as they involve interaction with people, as well as other technologies and infrastructures. “Socio-technical design” is defined in this context as concerning “advocacy of the direct participation of end-users in the information system design process...[including] the network of users, developers, information technology at hand, and the environments in which the system will be used and supported” (Scacchi, 2004, p. 655). Zimmerman (2007) presents six major elements to be accounted for when

conducting cyberinfrastructure design, all of which were incorporated into the design of the prototype CCS cyberinfrastructure framework. They include:

1. Maturity and complexity of the cyberinfrastructure
2. Users’ capabilities, expectations, and perceived need for cyberinfrastructure
3. Research problems and their relation to computing

4. Hardware, software, and associated technologies used by the cyberinfrastructure but produced and maintained by others
5. Role and influence of all key stakeholders
6. Mechanisms for coordination and feedback

Design principles

Overall design of the cyberinfrastructure conceptual framework was driven by the following overarching research question:

What types of cyberinfrastructure components are required to foster, support, and enhance collaborative research within the university's multidisciplinary carbon sequestration scientific community?

Five primary design principles guided the framework development process. They included the following:

- User-driven functionality
- Emphasis on improved communication
- Priority for information sharing, discovery, and access
- Inclusion of geospatially enabled content and methods
- Compatibility with DOE NATCARB infrastructure

Recognizing Zimmerman's (2007) advocacy for treating cyberinfrastructure design as an ongoing and long-term process, design considerations also incorporated the following criteria related to incremental implementation and sustainable fiscal investment:

- Stakeholder scalability—i.e., eventual support beyond scientists to managers and decision makers
- Geographic scalability—i.e., inclusion of both site-specific and regional characterizations

Needs assessment

Methods

The cyberinfrastructure design team conducted a series of semi-structured group interviews with the

principal investigators (PIs) and members of each of the task-specific science teams. The purpose of the interviews was to gain a better understanding of each task's use of information technology, including types and format of input data, application software employed, data standards, management practices, and information products generated. The team also sought to gain participants' perspectives on the potential value and benefits of cyberinfrastructures to collaborative science as well as their concerns with potential barriers to the implementation and long-term sustainability of such systems. The goal in collecting this information was threefold, and included: (1) identifying opportunities for data sharing and other interoperability actions among tasks; (2) determining requirements for implementing shared computing resources; and (3) proposing potential mechanisms for improving inter-task communication and coordination.

Appendix 1 details the overall structure of the interview inquiries. Prior to each interview, task PIs were asked to complete a spreadsheet containing more detailed questions regarding the technical nature of their task's software, hardware, data formats, and analysis methods. These details were reviewed during the interviews. Questions 8 and 9, pertaining to benefits and barriers of collaborative information infrastructures, were administered using the single-page questionnaire forms found in Appendices 2 and 3. These questions were based in part on previously published work by the Arctic Research Consortium of the United States (ARCUS) to develop a geographic information infrastructure to support collaborative Arctic research (Sorensen et al., 2001).

Results

The interview surveys provided a useful characterization of the science teams' technical needs (including differences and commonalities), their anticipated information products, and their individual and collective perceptions of the role of information infrastructures for collaborative science. Several key points related to data, software, hardware, and institutional context were identified through the initial qualitative assessment of the results.

Overall, data collection and management procedures varied widely across the tasks. Considerable heterogeneity existed not only in terms of data types,

but also relative to the various task-specific geographic extents (e.g., different geologic formations in different areas on the Moxa Arch) for which data were being collected. Data standards were most often employed where standards had been previously well established (e.g., well logs and seismic data), and less integrated in other situations (e.g., positional location specifications for Global Positioning System–based data collection). Issues also existed in some cases with restrictions on availability and use of proprietary data acquired from private sector sources.

Software use varied similarly among the tasks, ranging from commercial, off-the-shelf applications to highly customized open source solutions. Geographic information systems were prominent in several of the tasks but were not implemented using a consistent software platform due to varying familiarity and past experience, both across teams and among team members. At least three tasks made use of commercial, high-end modeling software, in this case, the Petrel® suite (Schlumberger Ltd, Houston, Texas) and EarthVision® (Dynamic Graphics, Inc., Alameda, California). Though both of these software packages are industry standards, these complex enterprise-scale solutions pose challenges for project-level implementations in terms of cost of licensing, training, and technical support. These challenges are compounded in situations such as this project where their use is not consistent across a multi-team project.

Relative to hardware, some tasks cited a need for additional system administration staff with necessary skills and experience to support research computing resources in a mixed environment (e.g., LINUX, UNIX versus Windows operating systems). Another concern for some was the possibility of reduced flexibility in maintaining individual computing clusters in the face of pending university-wide policies to consolidate high performance computing installations across campus (an action that could potentially alleviate the aforementioned system administration staffing issue).

Participants' impressions of the overall project structure identified the project's short duration as a hindrance to collaboration and cyberinfrastructure investment, with one task's PI noting that "groups needed to work independently before they could work collaboratively," a situation not well supported by the two-year timeline. In terms of perceived benefits (Appendix 1, question 8 and Appendix 2), the

science teams identified individual science projects and the broader scientific community as being the biggest beneficiaries of CI mechanisms, particularly in the areas of data sharing, communication and networking, better collaboration, and transparency. Relative to perceived barriers (Appendix 1, question 9 and Appendix 3), identified challenges were both technical and institutional in nature. Major technical barriers included interoperability concerns posed by the heterogeneity of data and the lack of specific scientist training in informatics principles. Institutional barriers included challenges posed by the shortness of the typical grant funding cycle and the "publish or perish" mentality common to the culture of academia, which fails to value or reward non-traditional research products like software code or databases. That same expectation to publish interpretations in a timely manner was also perceived as one roadblock for untenured faculty members to participate in collaborations with private partners, due to industry requirements for confidentiality agreements with extended internal review processes tied to publication or other dissemination of results.

CONCEPTUAL FRAMEWORK

Knowledge workflow model

Figure 2 provides a data flow and components diagram of the proposed cyberinfrastructure to support collaborative carbon management research at the University of Wyoming. Also termed a knowledge workflow model, this model specifies the elements necessary for developing, sharing, and accessing software applications, models, geospatial data, metadata, and other information products among academic, government, and industry contributors. Initially, project participants (contributors) interact with a collaborative interface application to populate and maintain information contained within the knowledgebase. This collaborative interface employs Web 2.0 social networking utilities to promote dynamic methods for contributor cooperation and organization of CCS data and information. Once information has been migrated into the knowledgebase, applications provide a variety of users with access to this information. Initially, focus is placed on supporting the research and education community, with additional phased development for regulatory and management agencies, industry, and policy and decision makers. Outreach functions could

also be extended to the general public. The final goal for the knowledge workflow model includes support of NATCARB and overall compatibility with the DOE vision for a national carbon cyberinfrastructure (Carr et al., 2007, 2009).

Figure 2. Carbon capture and storage knowledge workflow model. Graphic represents a conceptual cyberinfrastructure framework to support collaborative research among scientists working in the geologic carbon sequestration domain. Standardized collaboration interface, methods, and procedures facilitate contributions from, and interactions between, the scientific, regulatory/management, and industry communities. Supported end users include those same contributors, as well as policy and decision makers, the general public, and the National Carbon Sequestration Database and Geographic Information System.

Prototype implementation

The prototype implementation of the cyberinfrastructure was based on three key strategies. First, it was necessary to build on existing infrastructure components in order to take advantage of already established hardware, software, and database management applications. Second, given the centrality of geographic information to many of the tasks, all initial components needed to include geospatial visualization and query functionality. Finally, an emphasis had to be placed on fostering and supporting communication and coordination aspects of collaborative research. Implementation was realized by loosely coupling three distinct software applications: the Wyoming GeoLibrary, the WyGISC DataServer, and WyoSakai.

The Wyoming GeoLibrary (Fig. 3) is an Internet-based metadata registry that provides users the ability to easily and efficiently access and disseminate spatial data and information. For researchers associated with the Moxa Arch project, this application gave them an avenue by which to share or at least inform others about the spatial data and information being collected, used, and/or produced in their task. This allows researchers with similar data needs to use others' work without having to replicate data gathering or development and enhances the overall productivity of each task.

The WyGISC DataServer (Fig. 4) is an online mapping application that provides users with a rich environment for viewing, querying, mapping, and downloading spatial data. Data are organized into thematic topics and include transportation, hydrology, wildlife, energy and minerals, land management, geology, and aerial photography. This application initially gave researchers the ability to spatially relate to the project area and explore current conditions found at this location. Additionally, the

Wyoming GeoLibrary
Welcome. The GeoLibrary was developed by WYQSC and EUNER with funding from US Dept of Energy and Wyoming ELM.

Catalog Results Details

View: Summary | Showing: 1-4 | 10 results per page
Sort by: Title of Document

Aquifer Recharge Sensitivity Rating for Wyoming at 1:100,000 (Downloadable Data)
Updated: 2010-01-20 13:43:23
Location: set as Search Map
Data link: <http://pinkey.wyqsc.unwo.edu/d...>
Metadata: [XML](#) | [Full Document](#)

Aquifer Recharge Sensitivity Rating for Wyoming at 1:500,000 (Downloadable Data)
Updated: 2009-12-10 20:57:21
Location: set as Search Map
Data link: <http://pinkey.wyqsc.unwo.edu/d...>
Metadata: [XML](#) | [Full Document](#)

Aquifer Sensitivity of Wyoming at 1:100,000 (Downloadable Data)
Updated: 2010-01-20 13:41:46
Location: set as Search Map
Data link: <http://pinkey.wyqsc.unwo.edu/d...>
Metadata: [XML](#) | [Full Document](#)

Bedrock Geology for Wyoming at 1:500,000 (Downloadable Data)
Updated: 2009-12-10 20:54:16
Location: set as Search Map
Data link: <http://pinkey.wyqsc.unwo.edu/d...>
Metadata: [XML](#) | [Full Document](#)

Bedrock Geology of the Bridger Formation at 1:24,000 (Downloadable Data)
Updated: 2008-08-19 13:19:08
Location: set as Search Map
Data link: <http://pinkey.wyqsc.unwo.edu/p...>
Metadata: [XML](#) | [Full Document](#)

Clinker Regions in the Powder River Basin Wyoming at 1:24,000 (Downloadable Data)

Words:

Narrow search by:

Content Categories
GIS Data
Documents and Files
Other Geospatial Resources

Folders (show all)
Documents by WYQSC Projects
Wyoming State Census
Wyoming Travel and Tourism

Themes
Admin & Political Boundaries
Agriculture & Forestry
Atmosphere & Climate
Biology & Ecology
Cultural & Land Descriptions
Colonial & Society
Economics & Energy
Education & Derived Products
Environment
Facilities & Structures
Geologic & Geotechnical
Human Health & Disease
Infrastructure
Locations & Geospatial Networks
Military & Intelligence
Transportation Networks
Utility Networks
Water Resources

Figure 3. Wyoming GeoLibrary interface. This Web-based application serves as a metadata registry for sharing, discovery, and access of spatially related data for Wyoming, including information on geology, energy, and infrastructure. Records are organized and searchable by format and thematic category, as well as by specific project. Data documentation complies with the U.S. Federal Geographic Data Committee content standard for geospatial metadata. Examples of metadata summaries are composed of concise details for each record.

Figure 4. WyGISC DataServer interface. The WyGISC DataServer is an interactive, Web-based mapping application supporting overlay, display, and query of a variety of geospatial data themes as well as data download and map production. Standard query and display capabilities are augmented by a wide range of proximity-based functions, including theme-on-theme queries and buffer analysis. This figure depicts geologic formations of southwestern Wyoming and the overlying energy infrastructure.

DataServer provided a mechanism where researchers could again provide others access to view and possibly download their spatially derived information. Finally, the standards followed by the data supporting this mapping application provided a direct means by which data used and/or created in the Moxa Arch project could contribute to the National Carbon Atlas/Cyberinfrastructure.

WyoSakai is a customized version of Sakai software (Sakai Foundation, Ann Arbor, Michigan), which is an open source educational product designed to facilitate education and research collaboration (Fig. 5). WyoSakai fit the initial project need to create both an operable and proof-of-concept site for collaboration among the 11 tasks in the Moxa Arch CSS project. Functionality of WyoSakai includes: file upload and download, participant management, forums, wikis, and internal and external e-mail. All of these helped individual researchers stay informed about others' progress, concerns, ideas, and/or comments they had while working on their task. Additionally, it gave researchers the ability to quickly and efficiently share knowledge, which could assist others in their work.

SUMMARY AND FUTURE RESEARCH

Creation of a cyberinfrastructure conceptual framework for the Moxa Arch carbon sequestration project reflects the first stage design activities—"research, design, and initial development"—associated with Berman's cyberinfrastructure trajectory (subsequent stages include "engineering and prototyping" and "broad[-scale] use" (2008, p. 24)). The resulting workflow model and coupling of the WyoSakai collaboration interface, WyGISC DataServer, and Wyoming GeoLibrary was accomplished by following established guidelines for cyberinfrastructure design (Zimmerman, 2007) and incorporating recognized information system components critical to success, including a geo-enabled knowledgebase (Rich et al., 2007) and social networking components (Pierce et al., 2006). The design also integrated compatibility for interoperability with ongoing national carbon cyberinfrastructure efforts, specifically the NATCARB initiative (Carr et al., 2009).

Given the number and diversity of science teams involved in this project, initial infrastructure

implementation was likely overambitious. As previously noted, the project was hampered to a certain degree by the relatively short timeline and considerable uncertainty regarding project continuation. Nevertheless, both the needs assessment and the established framework should serve as valuable guidance for future cyberinfrastructure development for carbon management.

At the University of Wyoming, possible next steps in cyberinfrastructure could include a demonstration project establishing specific interoperability between two or more CCS research tasks and science teams, or the creation of common geographic information system-based analysis tools for long-term support of a specific research focus (e.g., geologic site characterization). Investment in cyberinfrastructure will become increasingly important as University of Wyoming CCS research expands into exploring the commercial-scale CO₂ sequestration potential of deep saline aquifers in the Rock Springs Uplift (Fig. 1) through the Wyoming Carbon Underground Storage Project (WY-CUSP). In this case, an increased level of cyberinfrastructure development would assist in addressing DOE monitoring, verification, and assessment requirements (NETL, 2009a) and recommendations for geographic information systems-supported and NATCARB-compliant outreach and education strategies (NETL, 2009b). Implementation of this next-generation CCS cyberinfrastructure would also benefit from WY-CUSP's longer project timeframe (allowing more time for protocol and standards development and training) and from the opportunity to better link with existing state and regional energy-related information transfer vehicles like the Wyoming Energy Resources Information Clearinghouse (www.weric.info).

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Figure 5, facing page. WyoSakai collaborative research environment. Examples of the WyoSakai collaborative research environment, including project description, task-specific document management, and embedded ArcServer 9.3-based energy and carbon storage mapping application. The WyoSakai open source programming environment is customizable to support unique, project-specific communication requirements.

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REFERENCES CITED

- Atkins, D. E., Droegemeier, K. K., Feldman, S. I., Garcia-Molina, H., Klien, M. L., Messerschmitt, D. G., Messina, P., Ostriker, J. P., and Wright, M. H., 2003, Revolutionizing science and engineering through cyberinfrastructure: report of the National Science Foundation Blue-Ribbon Advisory Panel on Cyberinfrastructure: Arlington, Virginia, Office of Cyberinfrastructure (OCI), The National Science Foundation, 84 p.
- Bachu, S., 2000, Sequestration of CO₂ in geological media: criteria and approach for site selection in response to climate change: *Energy Conversion and Management*, v. 41, p. 953–970.
- Benson, S. M., Hoversten, M., Gasperikova, E., and Haines, M., 2004, Monitoring protocols and life-cycle costs for geological storage of carbon dioxide, *in* Rubin, E. S., Keith, D. W., and Gilboy, C. F., eds., *Proceedings of 7th International Conference on Greenhouse Gas Control Technologies*, Vancouver: Elsevier, v. II, p. 1259–1265.
- Berman, F., 2008, Making research and education cyberinfrastructure real: *EDUCAUSE Review*, v. 43, p. 18–32.
- Carr, T. R., Rich, P. M., and Bartley, J. D., 2007, The NatCarb Geoportal: linking distributed data from the Carbon Sequestration Regional Partnerships: *Journal of Map & Geography Libraries*, v. 4, p. 131–147.
- Carr, T. R., Iqbal, A., Callaghan, N., Adkins-Heljeson, D., Look, K., Saving, S., and Nelson, K., 2009, A national look at carbon capture and storage – National Carbon Sequestration Database and Geographical Information System (NatCarb): *Energy Procedia*, v. 1, p. 7.
- Friedmann, S. J., 2006, The ICE Framework for CO₂ storage site characterization, *in* *Proceedings, Fifth Annual Conference on Carbon Capture and Sequestration*, Alexandria, Virginia, May 8–11, 2006: U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL), <http://www.netl.doe.gov/publications/proceedings/06/carbon-seq/Table%20of%20Contents.pdf>.
- _____, 2007, Carbon capture and sequestration technologies: status and future deployment: Livermore, California, Lawrence Livermore National Laboratory.
- Frost, C. D., and Jakle, A. C., 2010, Geologic carbon sequestration in Wyoming: prospects and progress: *Rocky Mountain Geology*, v. 45, p. 83–91.
- Gahegan, M., Luo, J., Weaver, S. D., Pike, W., and Banchuen, T., 2008, Connecting GEON: making sense of the myriad resources, researchers and concepts that comprise a geoscience cyberinfrastructure: *Computers & Geosciences*, v. 35, p. 836–854.
- Gibbins, J., and Chalmers, H., 2008, Carbon capture and storage: *Energy Policy*, v. 36, p. 4317–4322.
- Gregor, S., 2006, The nature of theory in information systems: *Management Information Systems Quarterly*, v. 30, p. 611–642.
- Grobe, M., Pashin, J. C., and Dodge R. L., eds., 2010, Carbon dioxide sequestration in geological media—state of the science: *American Association of Petroleum Geologists Studies in Geology* 59, 715 p.
- Hevner, A. R., March, S. T., Park, J., and Ram, S., 2004, Design science in information systems research: *MIS Quarterly*, v. 28, p. 75–105.
- IOGCC (Interstate Oil and Gas Compact Commission), 2005, Carbon capture and storage: a regulatory framework for states: Oklahoma City, Oklahoma, Interstate Oil and Gas Compact Commission.
- IPCC (Intergovernmental Panel for Climate Change), 2005, Carbon dioxide capture and storage, Metz, B., Davidson, O., de Coninck, H., Loos, M., and Meyer, L., eds.: Cambridge, Cambridge University Press, 431 p.
- Lee, C. P., Dourish, P., and Mark, G., 2006, The human infrastructure of cyberinfrastructure, *in* *Proceedings, 20th Anniversary Conference on Computer Supported Cooperative Work*, Banff, Alberta: New York, Association for Computing Machinery (ACM), p. 483–492.

- Lynds, R., Campbell-Stone, E., Becker, T. P., and Frost, C. D., 2010, Stratigraphic evaluation of reservoir and seal in a natural CO₂ field: Lower Paleozoic, Moxa Arch, southwest Wyoming: *Rocky Mountain Geology*, v. 45, no. 2, p. 113–132.
- March, S. T., and Smith, G. F., 1995, Design and natural science research on information technology: *Decision Support Systems*, v. 15, p. 251–266.
- McFarland, J. R., Reilly, J. M., and Herzog, H. J., 2004, Representing energy technologies in top-down economic models using bottom-up information: *in* Weyat, J. P., ed., EMF 19: Alternative Technology Strategies for Climate Policy: *Energy Economics*, v. 26, p. 685–707.
- Myers, J. D., and Dunning, T. H. J., 2006, Cyberenvironments and cyberinfrastructure: powering cyber-research in the 21st Century: Urbana, Illinois, National Center for Supercomputing Applications.
- NETL (National Energy Technology Laboratory), 2007a, Carbon sequestration atlas of the United States and Canada: Pittsburgh, Pennsylvania, U.S. Department of Energy, http://www.netl.doe.gov/technologies/carbon_seq/refshelf/atlas/index.html.
- _____, 2007b, Carbon sequestration technology roadmap and program plan: Pittsburgh, Pennsylvania, U.S. Department of Energy, http://www.netl.doe.gov/technologies/carbon_seq/refshelf/project%20portfolio/2007/2007roadmap.pdf.
- _____, 2009a, Best practices for monitoring, verification, and accounting of CO₂ stored in deep geologic formations: Pittsburgh, Pennsylvania, U.S. Department of Energy, http://www.netl.doe.gov/technologies/carbon_seq/refshelf/MVA_Document.pdf.
- _____, 2009b, Best practices for public outreach and education for carbon storage projects: Pittsburgh, Pennsylvania, U.S. Department of Energy, http://www.netl.doe.gov/technologies/carbon_seq/refshelf/BPM_PublicOutreach.pdf.
- NRC (National Research Council), 1997, Bits of power: issues in global access to scientific data, Committee on Issues in the Transborder Flow of Scientific Data: Washington, D.C., National Academies Press, 250 p.
- NSF (National Science Foundation), 2007, Cyberinfrastructure vision for 21st century discovery: Arlington, Virginia, National Science Foundation, NSF 07-28, <http://www.nsf.gov/pubs/2007/nsf0728/index.jsp>.
- Pervasive Technology Institute, 2007, University cyberinfrastructure news online newsletter (March): Bloomington, Indiana, University Information Technology Services, Indiana University, <http://pti.iu.edu/ci/cyberinfrastructure-news?d=200703>.
- Pierce, M. E., Fox, G., Yuan, H., and Deng, Y., 2006, Cyberinfrastructure and Web 2.0, *in* Proceedings, HPC2006, Cetraro, Italy, p. 1–18.
- Rich, P. M., Bollinger, J. S., Bhaduri, B., and Bleakly, D. R., 2007, Perspective on Department of Energy geospatial science: past, present, and future: *Journal of Map & Geography Libraries*, v. 4, p. 29–58.
- Scacchi, W., 2004, Socio-technical systems design, *in* Bainbridge, W. S., ed., *Berkshire Encyclopedia of human-computer interaction*: Great Barrington, Massachusetts, Berkshire Publishing Group, p. 655–659.
- Sorensen, M., Manley, W. F., Crain, R. D., and Warnick, W. K., 2001, Recommendations for a geographic information infrastructure to support Arctic research: outcomes of the Arctic GIS Workshop: Fairbanks, Alaska, Arctic Research Consortium of the United States.
- U.S. Department of Energy (DOE), 2007, Basic research needs for geosciences: Facilitating 21st Century energy systems: Bethesda, Maryland, U.S. Department of Energy.
- Wilson, E. J., Friedmann, S. J., and Pollak, M. F., 2007, Research for deployment: incorporating risk, regulation, and liability for carbon capture and sequestration: *Environmental Science and Technology*, v. 41, p. 5945–5952.
- Zimmerman, A., 2007, A socio-technical framework for cyberinfrastructure design, *in* Proceedings, e-Social Science Conference, Ann Arbor, Michigan, p. 1–10.
- Zimmerman, A., and Nardi, B. A., 2006, Whither or whether HCI: requirements analysis for multi-sited, multi-user cyberinfrastructures, *in* Proceedings, CHI 2006, Montreal.

MANUSCRIPT SUBMITTED MAY 21, 2010

REVISED MANUSCRIPT SUBMITTED AUGUST 18, 2010

MANUSCRIPT ACCEPTED AUGUST 30, 2010

Appendix 1. Needs assessment collaboration interview script.

UW-DOE Carbon Sequestration Research Cyberinfrastructure Needs Assessment Interview

Task: _____

PI / Co-PIs: _____

Interview Date: _____

Interview Participants: _____

Team Members Not Present: _____

Interviewees: _____

INTRODUCTIONS:

Thank you for taking the time to meet with us today. As you most likely know, in Task 1.5 we are developing a conceptual framework for creating a cyberinfrastructure to promote and support long-term collaborative interdisciplinary research among scientists at UW working on carbon capture and sequestration.

As part of this process, we are surveying the members of each task's science team to learn more about how they are using information technology, data, information, and supporting infrastructure in their task-specific research. We also seek to gain a better understanding of how teams and individuals view the relationship between their work and the other tasks, and to gain their insight on the potential benefits of and challenges with CI implementation and use.

In preparation for this interview, you all should have received an overview of this data gathering exercise. One of you should have also received an Excel spreadsheet to fill in and return prior to today. What we'd like to do now is ask the "team" a series of seven or eight open-ended questions. In the process, we'll also review with all of you the responses that one of your team members provided in the spreadsheet. Finally, we'll conclude by asking you to respond on paper to two or three specific survey questions on cyberinfrastructure benefits and implementation barriers. The entire session should take no more than 60 minutes, though we've budgeted for 90 minutes in case we go over time.

BACKGROUND

Q.1A: Briefly describe the primary objectives of your task:

Q.1B: How would you characterize the primary methodologies employed in this research? (e.g., fieldwork, laboratory experiments, simulation modeling, etc.)

Q.1C: What are the anticipated short- and long-term research products resulting from this work? (e.g., journal articles, bibliography, datasets, methods, software, etc.)

Q.2: Who do you consider to be the primary audience(s) for these products? (academics, resource managers, policy makers, etc.?)

THE NEXT FOUR QUESTIONS were forwarded to _____ a few days ago.

The purpose in asking for a response in the spreadsheet was to make sure that we accurately capture some of the

Appendix 1 (continued). Needs assessment collaboration interview script.

technical details associated with data and information inputs and outputs and the computational infrastructure required to support it.

DATA IN & OUT

Q.3: What types of "input" data are needed to support and carry out your work on this task?

Q.4: Please describe the types of digital data/information products (i.e., output) that will result from this task:

IT IMPLEMENTATION

Q.5: To what degree will your task utilize information technology?

Q.6A: What software are you using in your task?

Q.6B: Hardware / networking: briefly describe the hardware and networking capabilities required to support software use on the task.

THE FINAL SET OF QUESTIONS ADDRESS ISSUES OF COLLABORATION AND HOW THAT MIGHT BE ENABLED THROUGH INFORMATION INFRASTRUCTURE

Q.7: Describe the relationship of your research to the other 10 tasks...

- Degree of cooperation, coordination, collaboration – ideal v. actual
- Any dependencies (data, other?)
- What would you most like to see shared among the tasks? How would you like to see a CI environment designed to support future collaboration in the carbon sequestration research arena at UW?

FOR THE LAST TWO QUESTIONS, WE WOULD LIKE YOU TO RESPOND DIRECTLY ON PAPER AS INDIVIDUALS: [handouts – appendices 2 and 3]

Q.8: Benefits

Q.9: Barriers

WRAP-UP:

Q.10: Any other issues you'd like to see addressed with a project-wide cyberinfrastructure?

Appendix 2. Needs assessment collaboration benefits survey.

Benefits of implementing an interdisciplinary information infrastructure for collaborative research

Potential Benefits <i>Check all that apply for each user category</i>	Individual Scientists	Research Project	Broader Scientific Community	Educators and Students	Funding Agencies and Other Stakeholders	Policy Makers	Public
Better Institutional Collaboration	-	-	-	-	-	-	-
Better Science Collaboration	-	-	-	-	-	-	-
Communication and Networking	-	-	-	-	-	-	-
Cost Savings	-	-	-	-	-	-	-
Credibility	-	-	-	-	-	-	-
Data Management / Stewardship	-	-	-	-	-	-	-
Data Sharing – Discovery, Access, Use	-	-	-	-	-	-	-
Enriched Education	-	-	-	-	-	-	-
Guidance for PIs	-	-	-	-	-	-	-
Improved Productivity	-	-	-	-	-	-	-
Increased Efficiency	-	-	-	-	-	-	-
Information / Technology Transfer	-	-	-	-	-	-	-
Knowledge Synthesis	-	-	-	-	-	-	-
More Funding	-	-	-	-	-	-	-
New Analyses	-	-	-	-	-	-	-
Outreach	-	-	-	-	-	-	-
Project Management	-	-	-	-	-	-	-
Reduced Redundancy	-	-	-	-	-	-	-
Relevance	-	-	-	-	-	-	-
Serendipity	-	-	-	-	-	-	-
Transparency	-	-	-	-	-	-	-
Other:	-	-	-	-	-	-	-

Appendix 3. Needs assessment collaboration barriers survey.

In your opinion, what are the major barriers to implementing collaborative information infrastructures (technical/institutional)?

Potential Barriers	Minor	1	2	3	4	5	Major
Lack of integrated “commercial off the shelf” software	-	-	-	-	-	-	-
Emphasis of technical design over user dynamics	-	-	-	-	-	-	-
Heterogeneity of data	-	-	-	-	-	-	-
Human-computer interface issues	-	-	-	-	-	-	-
Scientists not explicitly educated in IT or informatics	-	-	-	-	-	-	-
“Publish or Perish” against the grain for data sharing	-	-	-	-	-	-	-
More time consuming	-	-	-	-	-	-	-
Lack of computational resources	-	-	-	-	-	-	-
Focus on grant funding cycle, short-term projects	-	-	-	-	-	-	-
More costly	-	-	-	-	-	-	-
Lack of system administrative support	-	-	-	-	-	-	-
Other:	-	-	-	-	-	-	-

CHAPTER 2: Assembling and Validating a Well Database

PI: Dr. James Myers, Department of Geology & Geophysics

Background

Large-scale sequestration of CO₂ in geologic reservoirs requires development of procedures and protocols to ensure that siting of injection and monitoring wells is accurate and that site risk assessment is robust. A sound pre-injection geologic model of the potential injection site requires data from pre-existing hydrocarbon wells. As part of characterization efforts, UW assembled and validated a database from the Wyoming Oil and Gas Conservation Commission that includes information about existing well locations in the study area of the Moxa Arch. This data is an essential part of site characterization because wells have the potential to act as conduits for leaks of CO₂ from the target reservoir. Results from the analysis are presented below.

Executive Summary

Since the beginning of the Industrial Revolution, atmospheric levels of carbon dioxide have steadily increased. Today carbon dioxide levels are around 380 ppm as compared to 250 ppm before the start of industrialization. Most of this increase has been linked to humankind's extensive use of fossil fuels. Yet our heavy reliance on fossil fuels (~85%) as a primary energy source means even if we wish to constrain carbon, we cannot quickly move away from this source of energy. Our reliance on fossil fuels is particularly evident for electricity generation where nearly 50% of all electricity is derived from the combustion of coal, the most carbon intense of all fossil fuels. Given our need to continue to rely on coal, many have suggested the geological sequestration (GS) of carbon dioxide may be a means of reducing anthropogenic carbon emissions from stationary sources and a bridge to the low-carbon energy sources of the future. To this end, DOE's NETL has been leading an effort to demonstrate the technical feasibility of GS, whereas the U.S. EPA has developed the regulatory framework to ensure that if expanded to an industrial scale, activities in this area will not impact human health, particularly in terms of the quality of underground sources of drinking water.

Although DOE's Regional Partnership Program has acquired much technical information about GS and how GS sites should be characterized as well as more limited operational experience, comparatively little information about the data management needs that the new regulatory framework for GS will require. In addition, there has been little investigation into how this data will be acquired, vetted and managed over the long-term (e.g., 50 to perhaps 100 years). This task, part of the larger Moxa Arch project at the University of Wyoming (UW), specifically investigated these issues. In particular, it developed a well catalog for the Moxa from publically available data sources and assessed, through field GPS work, the spatial reliability of the well locations recorded in these data sets.

EPA's GS regulation requires an Area of Review (AoR) for a project and specifies that it must be defined using computational modeling of the carbon dioxide injection plume and its associated pressure front. Because the investigation of the Moxa Arch did not reach this level of

detail, an alternative method was used to define a provisional Moxa Arch AoR for Task 2. Thus, the footprint of the seismic survey in the Moxa Arch was used to define a provisional Moxa Arch AoR. Within this area, we identified 95 mostly gas wells with either abandoned (34%) or actively producing (55%) the two largest well classes. None of these wells penetrate potential carbon reservoirs in the AoR or the overlying seals. An ArcGIS geodatabase with the associated information for these wells was created by the project team. To distribute this file electronically, it was converted to an ArcReader file and burned to a DVD. This disk also contains a copy of the ArcReader application as well as most of the figures and tables presented in this report. Information about systems requirements, installation and use is also included on the disk.

After compiling the well catalog, the spatial locations of the wells recorded in the Wyoming Oil and Gas Conservation Commission's (WOGCC's) database were checked for accuracy. An initial assessment of each well's location was performed by superimposing the well's location over satellite photos with 1 m resolution. Through inspection wells not plotting on a visible well pad were identified and flagged for field testing. Using GPS, the positions of 25 displaced wells were checked in the field. Except for one well with a displacement of 6,925 feet, these wells had an average displacement of 565 feet. Most were displaced due south from their recorded positions. Although Chevron had the most misplaced wells, eight other companies also owned wells that were mislocated in the WOGCC database. The 25 mislocated wells in the AoR represent 27% of the entire set of wells dataset.

In regards to moving GS from a research endeavor to commercial operations on a large industrial scale, this study notes two potential pitfalls. First, managing the well information necessary for site characterization, evaluation, and permitting will represent a complex, time-consuming, but vital process that will extend across decades. Our small-scale investigation quickly revealed the many problems associated with this endeavor. It should also be noted that this project concentrated on only a portion of the information that will be necessary for Class VI permitting. To prevent permitting from become too much of an economic burden for commercial operators, standardized data mining methodologies and management procedures should be worked out on an industry-wide basis. Second, the spatial locations of wells in state oil and gas or environmental agency databases may be characterized by significant error. These errors may have important consequences for constructing static 3-D geologic models of potential sequestration sites and assess the leakage, and hence risk, of individual wells. This possibility should be assessed by creating models and performing risk assessment that account for potential spatial errors in well location.

Despite being focused on a limited set of objectives with regard to well data management, this project has uncovered or highlighted several obstacles that will have to be addressed as sequestration projects migrate from the research to the commercial realm. It also suggests several fruitful avenues of future investigation (some of which are being pursued at UW as part of the NETL-funded WY-CUSP project). Specifically, future work should:

- Establish procedures to merge agency data updates with previously vetted and formatted data;
- Conduct additional field investigations to determine how well the spatial error of the Moxa Arch characterizes other regions of Wyoming;

- Investigate how the procedures developed in Wyoming to create a well catalog might or might not be portable to other states;
- Create procedures for incorporating well completion and formation data in the well catalog;
- Establish procedures for including data in the catalog from underground sources of drinking water (USDWs) in the AoR; and
- Investigate the methodologies needed to include wells outside the AoR that are needed to create a static 3-D geologic model.

Introduction

Geological carbon sequestration (GCS) has been proposed as a means of reducing anthropogenic atmospheric carbon emissions (IPCC, 2005; Praetorius and Schumacher, 2009). It involves capturing carbon dioxide at a source, compressing it to a supercritical fluid and transporting it to a storage site where it is injected underground and sequestered from the atmosphere for thousands of years. Initial efforts of carbon mitigation via GCS have focused primarily on large, stationary sources of carbon dioxide such as fossil fuel powered electrical generating stations (IPCC, 2005). Decades of enhanced oil recovery using carbon dioxide flooding have demonstrated that the technologies to compress and transport CO₂ are reliable and safe and that injection into oil and gas reservoirs can safely store some carbon dioxide.

Potential geologic formations for carbon storage include depleted oil and gas reservoirs, unmineable coal seams and saline formations (IPCC, 2005). Identifying, characterizing and validating geologic storage sites for carbon storage requires a large amount of geologic data. This information is necessary to determine the storage capacity of a reservoir, the integrity of its seal(s) and the potential risk for long-term leakage. An important source of the geologic data necessary to accomplish these tasks is boreholes, primarily oil and gas wells that penetrate potential reservoirs and their overlying seals. Boreholes provide a variety of indirect, i.e. logs, and direct, e.g. cuttings and cores, information about reservoir and seal rocks. Thus, one of the primary tasks of site characterization process is to compile a catalog of the boreholes in the area of interest as well as the information available from them.

Although boreholes provide valuable information necessary for characterizing a sequestration site, they also represent a potential pathway for CO₂ to leave the sequestration site. Thus, borehole characteristics and completion data are also important for assessing the potential risk associated with any particular storage site. It is not surprising, therefore, that EPA (2008) identifies well integrity as one of their main components for evaluating the vulnerability of a proposed sequestration site to leakage. EPA's well evaluation flowchart (Fig. 2-1) identifies three phases for establishing vulnerability: an initial well screening; assessment of well depth and/or connection to secondary conduits; and evaluation of individual well integrity. Unlike for site characterization, the information necessary for this evaluation is about the well itself, not the geological formations it penetrates. Information such as completion details and well integrity tests are critical for site evaluation.

Clearly, characterizing a potential geological sequestration site as well as evaluating it for potential risk requires acquiring and managing a variety of data about boreholes themselves and the geological formations they penetrate. The information obtained from even a single borehole can be quite extensive. Yet in areas favorable for GCS, well density can be very high (Nicot, 2008). Thus, assembling the borehole information necessary for site characterization, evaluating and permitting represents a significant exercise in data acquisition, vetting and management. At the same time, this information is spatially distributed and it is important to preserve this spatial component of the data. Presently, the mechanisms and procedures for assembling a borehole dataset vary from CGS project to project and have received only limited attention in the published literature (Ide et al., 2006). As sequestration moves from a research endeavor to a commercial operation, how borehole data is assembled and managed may have a significant impact on the economic viability of a particular sequestration project. In addition, it can dramatically impact how smoothly the permitting process proceeds.

This task of the Moxa project represents a first attempt at identifying the procedures and methods needed to assemble and vet a well catalog. It also examines some options available to manage these large datasets. To make the problem manageable, this first effort focused on borehole information necessary for site characterization. Subsequent work will build on this early effort by expanding the scope of the borehole catalog to include information necessary for evaluating the potential leakage risk associated with individual wells.

Project Tasks

Task 2 of the Moxa Project focused on assembling an electronic catalog of the wells in the area of interest. Specifically, it had two subtasks:

Subtask 2.1—Well Data Base Development: Using data from the Wyoming Oil and Gas Conservation Commission's website, an electronic catalog of wells was to be created using GIS conventions and standards. Information originally envisioned as being stored in the catalog included borehole location, depth, formations penetrated and completion details.

Subtask 2.2—Field verification of well database: The accuracy of WOGCC borehole spatial locations was to be field verified using GPS.

Task 2.1: Well Data Base Development

Overview: Oil and gas wells drilled in Wyoming are permitted by the WOGCC. In addition to permitting exploration and production wells, the WOGCC permits Class II oil and gas disposal wells under the EPA's Underground Injection Control (UIC) program. Information about these wells is made available to the general public through WOGCC's Web site (<http://wogcc.state.wy.us/>). This Web site provides a wealth of information on oil and gas wells. Some of the information maintained in the WOGCC's database includes well operator, location, status, and production history. Associated sundries also provide information about how the wells were completed, the logs run on them, and dates of any change in well status.

Data from the WOGCC's database can be accessed from their Web site in a number of different ways (Fig. 2-2). For assembling a well catalog, the Wells, Logs, Fields, and Sundries links are most useful. These links, however, do not produce downloadable files. These can be found by following the Down Load link in the left-most column on the page. From this page, well data can be downloaded according to a variety of criteria and in a variety of formats. The top two links produce either ArcView (left link) or Excel (right link) files. Both allow the user to choose wells by township and range, but the Excel format also permits well selection by section, township and range or field.

The last option (110810 Well Header DB5 (Zipped)) in the menu on the Down Load page, accesses a download-able file that contains information for all wells drilled or permitted to be drilled in Wyoming. (An important point to note is that this file doesn't contain information about wells that are confidential.) This file is updated at irregular intervals and is named [date]Wells.zip, where [date] represents the date the file was posted. This file is a zip package containing two files: 1) [date]PA.DBF which contains information on abandoned wells and [date]WH.DBF with information on active wells. Both files are in dbase format but can be imported directly into Excel or Access. The files contain 40 data fields or columns (see Appendix A) and each row corresponds to an individual well.

Data Compilation: The well header file from the WOGCC database was used to construct the final well data set for incorporation into the Moxa Arch well catalog. Although a variety of these files were downloaded over the course of the project, the final dataset was constructed from the download file dated 13-Jul-10 (i.e. 071310). These data were combined with GIS information from the Wyoming Geographic Information Science Center (WYGISC) to create the ArcReader file on the DVD that accompanies this final report. Details of how the final electronic catalog was constructed are provided in Appendix B.

Statewide Results: A data download from the WOGCC Web site on 13-Jul-10 identifies 112,505 oil and gas wells in Wyoming in various stages of production, drilling and permitting (Table 2-1). The wells, which are scattered across the state (Fig. 2-4), include oil, gas, oil-gas as well as coalbed methane (CBM) wells. Of these wells, 4,117 have been only permitted or represent active permits. The remainder of the wells (108,388) are actual wells that were drilled. The majority of these wells (59,361) are in various stages of abandonment or are shut-in (Fig. 2-5) with the remainder presently active (Fig. 2-6).

Moxa Results: According to EPA rules, all artificial penetrations in the AoR of a geological sequestration site are to be cataloged for permitting a Class VI carbon sequestration well. According to the EPA's recently finalized rule (22-Nov-10), the AoR is defined as "the region surrounding the geologic sequestration where USDWs may be endangered by the injection activity." Furthermore, the rule states the "AoR is delineated using computational modeling that accounts for the physical and chemical properties of all phases of the injected CO₂ stream and displaced fluids and is based on available site characterization, monitoring and operational data...". Because the Moxa project did not involve the type of computational modeling required to define an AoR and no particular part of the arch was designated as a potential injection site, determining an AoR for Task 2 was problematic and what was used as the definition changed several times during the course of the project.

Although the Moxa Arch is a well-defined geologic structure, defining its areal extent for use as a provisional AoR was difficult. One possibility uses the Moxa Arch Project Area defined by the BLM (Fig. 2-7). Because this footprint encompassed a large area on the flanks of the arch, the project team initially defined a different areal extent for the Moxa Arch (Fig. 2-8A). This footprint for the Moxa Arch more closely aligned with the axis of the Arch and omitted much of the flanks covered by the BLM definition. Within this footprint, a region of twelve sections centered on ExxonMobil's Shute Creek gas plant was identified as the provisional AoR for Task 2. The Wyoming well set from the WOGCC was clipped to these regions (Fig. 2-8B). A clipping of the WOGCC well dataset by WYGISC found 6,504 wells in the Moxa Arch footprint and 1,725 in the provisional AoR.

Subsequent to these efforts, UW acquired a seismic survey in the region of the Moxa Arch. In consultation with the project director, it was decided that this area (Fig. 2-7) would be the AoR for Task 2. Because the exact geographic outline of the seismic survey is unknown, a 500 m buffer was applied around the survey footprint for the purposes of well cataloging. Based on information from WOGCC's 071310WH.DB5 download, there are 95 wells in this AoR. These represent 17 operating companies (Table 2-2) with the majority of wells located on Federal land (Table 2-3). Most of these wells were permitted as gas wells (Fig. 2-9; Table 2-4). Thirty-two (34%) of the wells in the AoR are permanently abandoned whereas 56 (55%) are producing gas wells (Table 2-5). The majority of the wells in the area are completed in the Frontier formation (Table 2-6 and Fig. 2-10). None of the wells in the AoR penetrate any of the reservoirs being considered for carbon sequestration (Fig. 2-11).

Products Produced: Task 2 has produced two electronic products. First is the electronic well catalog. This file is ArcReader file and contains information for all 95 wells in the AoR. Layers in the well catalog include: distances (offset of WOGCC and actual well location); WOGCC wells; Wyoming Department of Transportation (WYDOT) roads; project area; project area buffer, Wyoming counties; PLSS (townships, ranges, sections and quarter-quarter layers); surface mineral (mineral ownership); NAIP (1 m resolution photos from National Agriculture Imagery Program). To distribute this catalog, Task 2 has also created a DVD. In addition to the well catalog, the DVD has the ArcReader application as well as instructions on how to install it and how to use the well catalog (Appendix C). Most of the tables and figures produced in this final report are also included on the DVD.

Task 2.2: Field verification of well database

Overview: Geologic modeling of a sequestration site is critically dependent upon data from boreholes. From this information, a static geologic model of the sequestration site is built (Jean et al., 2004; Sweetkind et al., 2010). Subsequent dynamic modeling of CO₂ injection is also critically dependent upon the well data since it is based initially on the site's static geologic model (Schnaar and Digiulio, 2009). Similarly, spatial location of a well is critical in evaluating its potential as a carbon dioxide leakage path. In this case, accurate spatial well location is necessary to determine the boreholes relation to indirect leakage paths such as faults. However, most site characterization and risk evaluation efforts to date apparently assume well location recorded in various databases is accurate. To evaluate this assumption and determine what types

of procedures might be necessary for vetting well spatial location, the accuracies of the spatial locations of wells in the AoR recorded in the WOGCC dataset was checked via a variety of mechanisms.

Procedures: An ArcGIS shapefile (using NAD 27 datum) was created from a spreadsheet that was downloaded from the Wyoming Oil and Gas Conservation Commission on July 13, 2010. After the shapefile was loaded into ArcGIS, WOGCC well locations were compared to 2009 true color, 1 meter resolution air photos from the National Agriculture Imagery Program to see if individual wells plotted on visible well pads. Of the 94 wells in the AoR, 25 or 27% did not plot on visible well pads. In all cases, there was a pad near the well. These wells were selected to check their field positions in light their discrepancies with the air photos.

Before commencing field work, five data fields were added to the WOGCC spreadsheet for collecting field data. The added fields included: measured field latitude, measured field longitude, comments (any observations in the field), collection date and photo. Locations for all wells that plotted off of their respective pad were converted using ArcMap to a mobile device format (ArcPad). This file was saved on a Trimble YUMA ruggedized tablet computer for subsequent field investigations. Base data (i.e. photos, and landowner layers) were added to the map in ArcPad. The tablet uses a Trimble GeoXT GPS receiver connected by a Bluetooth connection. The GPS receiver collects latitude and longitude positions that have an error less than 1 meter.

In the field, each well was driven to using GPS navigation. When at the well site a new GPS point was taken at the center of the well. The Field_Lat and Field_Lon were updated using the GPS location. Also, a digital picture was taken of the well stake or if there was no well stake, the well pad. The pictures were joined to the well point. In the office, field data was downloaded from the mobile device to a desktop computer for further analysis.

Results and Discussion: Of the 25 wells identified as displaced from their pads, one (Emigrant Springs UN - 28-22) is unusual in that it is offset 6,925 feet to the southeast. Aside from this well, the average well offset is 565 feet and varies from 123 to 799 feet (Table 2-6). All of these wells except two are displaced to the south (Fig. 2-11). The displaced wells were or are operated by nine companies with Chevron USA having the largest number of mislocated wells (Table 2-7). These well locations may be off because of a mix of NAD 27 vs NAD 83 datums. The shift could be as much as 150 meters depending on where they are in the state. There are also 17 wells in the AoR with erroneous latitudes or longitudes i.e. no negative signs, typos, missing decimal point, etc., and one well plots in Montana.

One well was identified in the field that did not show up in the WOGCC database. Upon visiting the well pad for Bridger 22-8 (API No: 49-023-21345) another well stake was present on the east side of the well pad with the name Slate Creek Federal #1, but a different API No. (49-023-20238). A subsequent search of the WOGCC website for Bridger 22-8 revealed an Application for Permit to Drill (APD) that showed the Slate Creek Federal #1 was, in fact, the same as Bridger 22-8. The APD stated “Marathon Oil Company requests approval to enter this plugged and abandoned well (Slate Creek Federal #1), drill out plugs, and clean out the existing well bore to 10,700’. The well will then be perforated ...” However, this operation was apparently never

done and the location of Bridger 22-8 well was moved 300 feet to the west and the well given a new API number.

Conclusion & Recommendations

Selecting, characterizing, evaluating and permitting a geological carbon sequestration site requires handling large amounts of diverse data derived from wells. These data are necessary to determine the storage capacity of the site as well as to evaluate the potential for leakage. A well provides three types or classes of information: 1) information about the borehole itself, e.g., location, construction, status, etc.; 2) data about the geologic formations intersected, i.e. rocks, mineralogy, porosity, etc.; and 3) information about subsurface formation fluids, e.g., oil, gas, water, brine. All of this information is needed either for the site characterizing process or site permitting. Since creating a geological sequestration site is a technological, social, economic and political process, the information characterizing a site must be available to a variety of individuals (e.g., regulators, risk assessors, MVA staff, investors) as well as institutions (e.g., state and federal agencies, commercial firms, non-governmental organizations, citizens groups). Clearly, the processes of data management used for sequestration research will not easily transfer to the commercial operations and the necessary scale that will be needed to mitigate significantly anthropogenic emissions of carbon dioxide (Pacala and Socolow, 2004).

Although demonstration projects in the U.S. have used such data in their characterization of sequestration sites, none have yet examined the issue of well data management in light of the regulatory framework that will oversee commercial sequestration operations. This project has focused on the processes that will be necessary by firms (operators) to obtaining Class IV permitting for future sequestration operations. For this project, we have focused only on the managing data on the wells themselves. Even with this limited focus, it is clear that managing well data in a manner that will satisfy site characterization and permitting as well as be relevant for the operational lifetime of a sequestration project, e.g., 40–50 years, will be difficult. It is also clear that the creation and use of a site well catalog must be an iterative process (Fig. 2-13). This is true from the earliest stages of planning through site operation and closure. The final EPA regulation for geologic sequestration sites will require a review of a project's AoR every five years. Thus, this on-going process will likely be carried out by different individuals over the course of a project's life time. Thus, institution or industry protocols will be needed to standardize and codify procedures for handling well data.

This project has been instrumental in testing some of the procedures necessary for moving geologic sequestration from a research endeavor to a commercial operation. In particular, it provides several important lessons in how a commercial company will need to manage well data to characterize adequately a potential geologic sequestration site and to move it through the regulatory process. First, the amount of data to be managed is large and varied in nature, including images of paper records, digital files, spatially distributed data as well as data with a significant temporal dimension. Similarly, data can be classed into two broad categories: information about wells themselves and information about formations (including their fluids) the wells penetrate. The latter data are marked by not only a spatial x-y component, i.e., well location, but also a vertical dimension, i.e. depth. Unfortunately, well data are scattered across many different governmental agencies, have different levels of public access, cataloged by a

variety of classification schemes and stored in a variety of different formats. In addition, there is little standardization of metadata between agencies. We have found that even within a single agency data downloads are often incomplete and not uniform in terms of information provided. This means several downloads followed by data consolidation is necessary. Despite these obstacles and barriers, this project has found that construction of an electronic well catalog will serve many purposes and, with further development, has the potential to address many of the data management issues future geological sequestration projects will face as they navigate the future sequestration regulatory framework.

The field component of this project has identified a potential significant problem in terms of site characterization that will have to be addressed as geological sequestration matures as a commercial and industrial process. Specifically, there appears to be significant error in well location for a sizeable fraction of wells in an AoR. Nearly 27% of the wells in the Moxa Arch provisional AoR are mislocated. Extrapolating these results to a site with 1,000 wells would mean that nearly 270 wells in the AoR would be incorrectly located. Checking the positions of this number of wells could represent a significant field effort. In light of these preliminary findings, individual risk assessments for wells should problem use a probabilistic approach with respect to well location rather than a deterministic approach. In this manner, field surveys of a subset of wells could be used to establish an average location error for wells in the AoR. This error could then be used in positioning wells and assessing the likelihood of communication with other leakage pathways. For the Moxa Arch, a preliminary location check was easy to perform since well pads from the 1960-70s are still visible on satellite images. In areas with different climates, this type of easy and quick location checking may not be available. This well location problems also suggest creation of static 3-D geologic models of sites should also consider the impact of spatial error in well location on the final geologic model.

Based on the result of this project, several steps are likely necessary to establish how to effectively deal with well data during the site characterization, permitting and operating phases of a geological sequestration project. These include:

- establishment of procedures to merge agency data updates with previously vetted and formatted data;
- additional field investigations to determine how well the spatial error of the Moxa Arch characterizes other regions of Wyoming;
- creation of procedures for incorporating well completion and formation data in the well catalog;
- establishment of procedures for including data in the catalog from USDWs in the AoR;
- investigation of the methodologies needed to include wells outside the AoR that are needed to create a static 3-D geologic model; and
- exploration of how the procedures developed in Wyoming to create a well catalog might or might not be portable to other states.

Figures

Figure 2-1: EPA’s flowchart for evaluating the level of vulnerability boreholes represent to a potential geological carbon sequestration site.

Figure 2-2: Screen capture of the Wyoming Oil and Gas Conservation Commission Web site's front page showing the various options for access data. Only the option Down Load provides electronically downloadable files about individual wells.

Figure 2-3: Screen capture of the Down Load page of the WOGCC’s Web site. Information about individual wells can be obtained following a variety of links on this Web page. Following the Well Data Excel format allows the user to create a downloadable file for wells by section, township and range, township and range or field. The last option in the menu box toward the bottom of the page (110810 Well Header DB5 (Zipped)) creates a zip file with information for all wells in the state.

Figure 2-4: The Wyoming Oil and Gas Conservation Commission lists 112,505 boreholes associated with energy production. Geographically, the boreholes are concentrated in the Powder River and Green River Basins. For the entire state, the average borehole density is 0.42 wells/km².

Figure 2-5: Permanently abandoned boreholes (43,621) comprised nearly 40% of all the wells drilled in Wyoming as of 13-July-10. Another 5,878 wells are in various stages of abandonment. There are also 9,862 shut-in wells in the state. These wells represent a potential leakage pathway for any carbon dioxide stored in the state.

Figure 2-6: As of 13-Jul-10, there were nearly 40,000 active oil, gas and CBM boreholes in Wyoming. This represents nearly 36% of the wells that have been drilled to date in Wyoming.

Figure 2-7: Moxa Arch footprint (purple outline) as defined by the BLM. The wells within this footprint are shown as dots. This footprint is unusually large and probably unrealistic for the area that would be affected by CO₂ injection. The area outlined in yellow represents the region of a seismic survey UW acquired for the Moxa project. This area was accepted as the final AoR for Task 2.

Figure 2-8: (A) Initial Moxa Arch (purple region) and AoR (gray region) definition for the purposes of Task 2. The AoR was originally defined as a twelve section footprint centered on ExxonMobil's Shute Creek gas plant. (B) A clipping of the WOGCC well dataset by WYGIS found 6,504 wells in the Moxa Arch footprint and 1,725 in the AoR.

Figure 2-9: Well by status in the Moxa Arch AoR. Most of the wells in the region are gas wells with one active injector.

Figure 2-10: Map showing wells by bottom formation. The most common formation in which wells are completed is the Frontier. None of the wells in the AoR penetrate likely carbon dioxide reservoirs or their seals.

Figure 2-11: Schematic cross-section of the Moxa Arch showing the number of wells penetrating each formation. None of the wells in the AoR penetrate formations likely to be used for carbon dioxide storage, i.e. Madison, Weber, or their seals. (Cross-section after Clarey et al., 2008).

Figure 2-12: Map showing wells checked in the field for spatial location. The green bar connects the WOGCC well locations with those determined by GPS in this study. Most wells are displaced to the south by an average of approximately 800 ft.

Figure 2-13: Generalized workflow for compiling a well catalog based on a computational defined Area of Review (AoR) for a particular geologic sequestration site.

Tables

Table 2-1: Energy production wells in Wyoming as of 13-Jul-10.

Producing Wells		
	Gas	29,367
	Oil	10,631
Abandoned Wells		
	Permanently	43,621
	Temporarily	1,389
	Subsequent Report of	2,732
	Notice of Intent to	1,757
	Shut In	9,862
Permit to Drill/Active Permit		
		4,117
Miscellaneous		
		9,029
Total		
		112,505

Table 2-2: Companies with boreholes in Moxa AoR (as of 13-Jul-10).

Company	# wells
BANNON ENERGY	1
BP AMERICA PRODUCTION COMPANY	18
CABOT OIL & GAS CORPORATION	1
CELSIUS ENERGY COMPANY	1
CHEVRON USA INC	18
DOMINION EXPLORATI ON & PRODUCTION INC	1
ENERGETIC S INC	1
EOG RESOURCES INC	26
KERR-MCGE E OIL & GAS ONSHORE LP	13
MARATHON OIL COMPANY	4
MERRION OIL & GAS CORPORATION	1
MIDGARD ENERGY COMPANY	1
PACIFIC TRANSMISSION SUPPLY	1
PETRAL EXPLORATION INC LLC	3
STONE ENERGY LLC	2
TEXACO EXPLORATI ON & PROD	1
TRUE OIL LLC	2
Total	95

Table 2-3: Number of wells by land types in Moxa AoR (as of 13-Jul-10).

Land Type	Code	# wells
Federal/Federal	11	84
Federal/Fee	13	-
Federal/State	14	-
Federal/Unknown	10	1
Fee	30	7
Fee/Federal	31	-
Fee/Fee	23	-
Fee/State	34	-
Fee/Tribal	36	-
Patented	20	-
State	40	3
State/Federal	41	-
State/Fee	43	-
State/Tribal	46	-
Tribal	60	-
Tribal/State	63	-
Total		95

Table 2-4: Number of wells by well class in the Moxa AoR (as of 13-Jul-10).

Classification	Code	# wells
active permit	AP	-
condensate	C	-
disposal	D	1
gas storage	GS	-
gas well	G	86
injector well	I	-
monitor well	MW	-
oil well	O	8
source well	S	-
strat test	ST	-
Total		95

Table 2-5: Number of wells by well status in Moxa AoR (as of 13-Jul-10).

<i>status</i>	<i>code</i>	<i>#</i>
active injector	AI	1
permit to drill	AP	1
dry hole	DH	-
dormant	DR	-
expired permit	EP	-
notice of intent to abandon	NI	1
no report	NR	-
permanently abandoned	PA	33
producing gas well	PG	56
producing oil well	PO	-
shut-in	SI	2
suspended operations	SO	-
well spudded	SP	-
subsequent report of abandonment	SR	1
temporarily abandoned	TA	-
unknown	UNK	-
waiting on approval	WP	-
Total		95

Table 2-6: Results of field verification of well location.

CAPINO	Offset (ft)	Offset Direction	Well Name	Field Name	WOGCC Longitude	Field Longitude	WOGCC Latitude	Field Latitude	Date Collected	Datum
49-023-21018	123	South	LAKE ALICE - 21-36	WC	-110.18883	-110.1889951	42.02460	42.02491552	9/8/2010	NAD 27
49-023-21150	741	South	BANNON USA - 30-4	EMIGRANT SPRINGS	-110.12872	-110.1285912	41.99728	41.99931259	9/9/2010	NAD 27
49-023-21162	799	South	SHUTE CREEK UNIT - 28	SHUTE CREEK	-110.15743	-110.1574096	41.96045	41.96264217	9/8/2010	NAD 27
49-023-21165	710	South	FONTENELLE DAM - 10-35	WC	-110.09496	-110.0951544	42.01968	42.02162326	9/8/2010	NAD 27
49-023-21208	731	South	RIDGE POINT - 22-18	SHUTE CREEK	-110.15996	-110.1600112	41.96437	41.96637752	9/8/2010	NAD 27
49-023-21251	705	South	BRIDGER - 21-8	EMIGRANT SPRINGS	-110.14904	-110.1490400	41.98092	41.98285529	9/9/2010	NAD 27
49-023-21254	780	South	TRAIL - 21-17	SHUTE CREEK	-110.15104	-110.1510154	41.96615	41.96829136	9/9/2010	NAD 27
49-023-21261	714	South	TRAIL - 11-17	SHUTE CREEK	-110.14958	-110.1495943	41.97531	41.97727113	9/9/2010	NAD 27
49-023-21262	699	South	SAGE - 22-7	EMIGRANT SPRINGS	-110.15679	-110.1568544	41.98012	41.98203749	9/9/2010	NAD 27
49-023-21264	696	South	CORRAL - 21-5	SHUTE CREEK	-110.14872	-110.1489677	41.99574	41.99764145	9/9/2010	NAD 27
49-023-21265	682	South	RIDGE POINT - 12-18	SHUTE CREEK	-110.15758	-110.1575859	41.97488	41.97675195	9/8/2010	NAD 27
49-023-21266	664	South	SAGE - 21-7R	EMIGRANT SPRINGS	-110.17149	-110.1717481	41.98062	41.98243370	9/8/2010	NAD 27
49-023-21267	712	South	PASCALI FEDERAL - 20-24	SHUTE CREEK	-110.17969	-110.1794791	41.96199	41.96393878	9/8/2010	NAD 27
49-023-21303	708	South	TRAIL - 12-17	SHUTE CREEK	-110.14074	-110.1408047	41.97486	41.97680330	9/9/2010	NAD 27
49-023-21304	683	South	RIDGE POINT - 11-18	SHUTE CREEK	-110.17025	-110.1702493	41.97501	41.97688609	9/8/2010	NAD 27
49-023-21319	625	South	RIMROCK - 12-13	SHUTE CREEK	-110.17931	-110.1796228	41.97681	41.97850848	9/8/2010	NAD 27
49-023-21414	694	South	COW HOLLOW UNIT - 83	COW HOLLOW	-110.09922	-110.0992903	41.93290	41.93480349	9/28/2010	NAD 27
49-023-21427	187	South	EWE - 22-12	SHUTE CREEK	-110.17944	-110.1794676	41.98527	41.98578162	9/28/2010	NAD 27
49-023-21456	408	West	SLATE CREEK BUTTE - 10-1	WC	-110.10778	-110.1063448	41.98750	41.98783028	9/9/2010	NAD 27
49-023-21627	221	South	COW HOLLOW UNIT - 102	COW HOLLOW	-110.10978	-110.1091459	41.92547	41.92585045	9/28/2010	NAD 27
49-023-21632	426	South	FONTENELLE DAM FED - 23-33	WC	-110.13055	-110.1300958	42.01416	42.01527907	9/8/2010	NAD 27
49-023-21655	387	South	RIM ROCK - 22-13	SHUTE CREEK	-110.18056	-110.1804490	41.97194	41.97299953	9/8/2010	NAD 27
49-023-21718	224	West	EMIGRANT SPRINGS - 24-15H	EMIGRANT SPRINGS	-110.10895	-110.1081327	41.96894	41.96902472	9/28/2010	NAD 27
49-023-21727	6925	Southeast	EMIGRANT SPRINGS UN - 28-22	EMIGRANT SPRINGS	-110.10820	-110.0990164	41.96900	41.95126885	9/28/2010	NAD 27
49-023-21964	234	South	SHUTE CREEK UNIT - 6-28E	SHUTE CREEK	-110.13226	-110.1314088	41.94212	41.94201831	9/9/2010	NAD 27

Table 2-7: Displaced wells group by operating company (as of 13-Jul-10).

<i>operating company</i>	<i>#</i>
Chevron USA Inc.	11
Petral Exploration Inc. LLC	3
EOG Resources Inc.	3
BP America Production Company	2
Kerr-McGee Oil & Gas Onshore LP	2
Bannon Energy Inc.	1
Cabot Oil & Gas Corporation	1
Celsius Energy Company	1
Stone Energy LLC	1
Total	25

References

- Environmental Protection Agency, 2008, Vulnerability evaluation framework for geologic sequestration of carbon dioxide: EPA430-R-08-009, 78 pp.
- Ide. T., S.J. Friedmann and H. Herzog, 2006, CO₂ leakage through existing wells: current technology and regulations: 8th International Conference on Greenhouse Gas Control Technologies, Trondheim, Norway, <http://sequestration.mit.edu/bibliography>. [accessed 4/14/08].
- Intergovernmental Panel on Climate Change, 2005, Carbon Dioxide Capture and Storage: B. Metz, O. Davidson, H. de Coninck, M. Loos and L. Meyer (eds), Cambridge University Press, 431 pp.
- Jean, G.A., J.M. Yarus, G.P. Flach, M.R. Millings, M.K. Harris, R.L. Chambers and F.H. Syms, 2004, Three-dimensional geologic model of southeastern Tertiary coastal-plains sediments, Savannah River Site, South Carolina: An applied geostatistical approach for environmental applications: *Environmental Geosciences*, vol. 11, pp. 205-220.
- Nicot, J.-P., 2008, A survey of oil and gas wells in the Texas Gulf Coast, USA, and implications for geological sequestration of CO₂: *Environmental Geology*, vol. 57, pp. 1625-1638.
- Pacala, S., and R. Socolow, 2004, Stabilization wedges: solving the climate problem for the next 50 years with current technologies: *Science*, vol. 305, pp. 968-972.
- Praetorius, B., and K. Schumacher, 2009, Greenhouse gas mitigation in a carbon constrained world: The role of carbon capture and storage: *Energy Policy*, Vol. 37, pp. 5081-5093.
- Schnaar, G., and D.C. Digiulio, 2009, Computational modeling of the geologic sequestration of carbon dioxide: *Vadose Zone*, vol. 8, pp. 389-403.
- Sweetkind, D.S., E.M. Taylor, C.A. McCabe, V.E. Langenheim and R.J. McLaughlin, 2010, Three dimensional geologic modeling of the Santa Rosa Plain, California: *Geosphere*, vol. 6, pp. 237-274.

Appendix I: WOGCC Download information

The download file from the WOGCC contains 40 columns with different types of information. This file is in DB5 format but can be imported directly into Excel. The Excel column, the column name displayed in the file and a description of the information in the column are summarized in the table below.

Column #	column	column name	description
1	A	APINO	unique identifier number assigned well by American Petroleum Institute (API)
2	B	COMPANY	company operating well
3	C	WN	well name
4	D	UNIT_LEASE	name of lease the well is located in
5	E	FIELD_NAME	name of oil/gas field well occurs in
6	F	HORIZ_DIR	
7	G	LAND_TYPE	indicates owner of mineral rights. Options: Federal/Federal; Federal/Fee; Federal/State; Federal/Unknown; Fee; Fee/Federal; Fee/Fee; Fee/State; Fee/Tribal; Patented; State; State/Federal; State/Fee; State/Tribal; Tribal; Tribal/State
8	H	SEC	Public Land Survey System (PLSS) section
9	I	TWP	Public Land Survey System (PLSS) township
10	J	T_DIR	Township direction
11	K	RGE	Public Land Survey System (PLSS) range
12	L	R_DIR	range direction
13	M	QTR1	Public Land Survey System (PLSS) quarter section
14	N	QTR2	Public Land Survey System (PLSS) quarter-quarter section
15	O	LON	well's longitude (assumed NAD 27)
16	P	LAT	well's latitude (assumed NAD 27)
17	Q	FOOT1	footage North-South in feet
18	R	FOOT2	footage East-West in feet
19	S	ELEV	ground elevation of well in feet
20	T	ELEVKB	elevation in feet from the rig's kelly bushing
21	U	BSEC	
22	V	BTWP	
23	W	BT_DIR	
24	X	BRGE	
25	Y	BR_DIR	
26	Z	BQTR1	
27	AA	BQTR2	
28	AB	BLON	
29	AC	BLAT	
30	AD	BOTFORM	the formation at the bottom of the well
31	AE	WELL_CLASS	well's class. options: active permit; condensate; disposal; gas storage; gas well; injector well; monitor well; oil well; source well; strat test

32	AF	TD	well's total depth
33	AG	PB	
34	AH	RN	
35	AI	COAL_BED	whether or not well is a coalbed methane well
36	AJ	STATUS	status of the well. options: active injector; permit to drill; dry hole; dormant; expired permit; notice of intent to abandon; no report; permanently abandoned; producing gas well; producing oil well; shut-in; suspended operations; well spudded; subsequent report of abandonment; temporarily abandoned; unknown; waiting on approval
37	AK	STATUSDATE	
38	AL	CAPINO	
39	AM	XSTSPUDDAT	
40	AN	XSTCMPLTDD	

Appendix II: Data Compilation Procedures

- 1.) The Quarter-Quarter (QQ) polygon layer was downloaded from the Wyoming Geographic Information Science Center (WYGISC). The following fields were added to the QQ layer:
 - a. QQ_NUM - Calculated by concatenating the QQ and converting the QQ into numbers by the following convention:
 - i. NE = 1
 - ii. NW = 2
 - iii. SW = 3
 - iv. SE = 4
 - v. QQ Example, NENE = 11
 - b. TRSQQ - Calculated by concatenating Township, Range, Section, and QQ_NUM
- 2.) Data from the WOGCC was downloaded and exported into a Geodatabase (GDB). The data was then prepped by adding the following fields:
 - a. Field_Lat (latitude NAD27 datum)
 - b. Field_Lon (longitude NAD27 datum)
 - c. Comments (any observations in the field)
 - d. Photo (Yes or No)
 - e. TRSQQ
 - f. TRSQQ_QQ
 - g. QQ_Check
- 3.) The TRSQQ was calculated for the WOGCC data by concatenating Township, Range, Section, and QQ. Then convert the QQ into numbers by the following:
 - a. NE = 1
 - b. NW = 2
 - c. SW = 3
 - d. SE = 4
 - e. QQ Example, NENE = 11
 - f. TRSQQ example, **231121311** (T23N, R112W, Section 13, NENE)
- 4.) Use the TRSQQ in each layer to join the two tables. Calculate the TRSQQ_QQ in the WOGCC well table from the joined QQ layer. Then unjoin the tables and calculate the QQ_Check using a true-false statement to see if TRSQQ equals the TRSQQ_QQ in the WOGCC layer. All of the false values mean that the well is plotting outside of its permitted legal location. These wells will need to be field verified.
- 5.) Next the data was checked using the 2009 True Color National Agriculture Imagery Program (NAIP) air photos. The well pad locations are visible on the 1 meter resolution imagery. A list of wells was compiled that did not plot on the well pads. The list of wells from the QQ check and the imagery check was then used to conduct the field verification.

Appendix III: Arc Reader Directions

Moxa Arch/La Barge ArcReader Map SOP

The base map was created using ArcGIS 10.0 and then exported to an ArcReader map using Arc Publisher. The map will provide information for the Moxa Arch Seismic Study area located in Lincoln County, Wyoming.

An ArcReader tutorial is located here:

<http://www.esri.com/software/arcgis/arcreader/index.html>

Data on the DVD includes:

ArcReader Software - DVD drive\\ ArcReader\\ArcReader10Windows**setup.exe**

Arc Reader map - DVD drive\\ ArcReader \\Moxa_Arch_La_Barge \\pmf\\ **La_Barge_Arc_Reader.pmf**

Figures - DVD drive\\ ArcReader \\Moxa_Arch_La_Barge \\Figures

1. Footprint_Companies.jpg
2. Footprint_Formations.jpg
3. Footprint_Well_Status.jpg
4. Moxa_Arch.jpg
5. Statewide_All_WOGCC_Wells.jpg
6. Statewide_Abandoned_WOGCC_Wells.jpg
7. Statewide_Active_WOGCC_Wells.jpg

Layers in the map:

- 1.) Distances – this layer represents the distance that the well was off compared to the WOGCC locations and the GPS field verified locations
- 2.) WOGCC – Wyoming Oil and Gas Conservation Commission (<http://wogcc.state.wy.us/>) downloaded as of 07/13/2010
 - a. Wells by Status – these are the reported statuses from the WOGCC
 - b. Wells by Operators
 - c. Wells by formation – these are the producing formation of the well
- 3.) WYDOT roads – Wyoming Department of Transportation
- 4.) Project Area – the seismic area footprint
- 5.) Project Area buffer – 500 meters around the footprint used to clip out wells from the WOGCC layer

- 6.) Wyoming counties – from the Wyoming Department of revenue
(http://cama.state.wy.us/DISTRICTS/MAPS_ONLINEDOCUMENTS/ShowMAPS_ONLINEDOCUMENTSTable.aspx)
- 7.) PLSS – Public Land Survey System comprised of Township, Range, Section, and Quarter-Quarter layers (Wyoming GeoLibrary – WyGIS - <http://wygl.wygisc.org/wygeolib/catalog/main/home.page>)
- 8.) Surface Mineral – BLM (<http://www.geocommunicator.gov/GeoComm/index.shtm>)
- 9.) NAIP – National Agriculture Imagery Program – data was downloaded from the USDA data gateway (<http://datagateway.nrcs.usda.gov/>) for each county for 2009. The image resolution is one meter.

Viewing a map

Starting ArcReader

1. Click Start on the Windows taskbar.
2. Click All Programs, point to ArcGIS, and click ArcReader.
3. ArcReader opens.

Opening an existing published map by navigating to DVD drive\\
ArcReader\Moxa_Arch_La_Barge\pmf\La_Barge_Arc_Reader.pmf

Note: The map will open in Data View format. There are two formats: Layout and Data View that can be toggled in the lower left hand of the map. The Layout View is for printing maps. Notice the page includes a title, legend, scale bars, North arrow, and some supporting text. In layout view, the Layout toolbar is displayed, which contains tools for navigating in layout view. Hover over each icon without clicking to see the name of each tool. The layout tools in the Layout toolbar are similar to the tools in the Data toolbar. They allow you to change the way the page is displayed. Notice that the data tools are still accessible for changing the view of the data within the data frame. The data view is for navigating in the map.

Querying a map

A map in ArcReader typically contains more information than you initially see. For example, a feature may hold attribute information that is not labeled or displayed on the map. With ArcReader, you can query that information

Identifying a location

You can use the Identify tool to obtain spatial and tabular information. You can see which features are at a specific location and also investigate the attributes of each feature.

Data Toolbar:

1.) **Identify** - Choose the Identify tool on the Data Toolbar and a Pop-Up window will appear. Select Wells by Operator from the drop down list in the upper right hand corner of the Identify window. Click on the well. The information for the well will appear in the Identify window.

Identify from: Wells by Operators

Wells by Operators

49-023-21264

Location: 570,565.987 4,649,649.264 Meters

Field	Value
COMPANY	PETRAL EXPLORATION INC LLC
WN	21-5
UNIT_LEASE	CORRAL
FIELD_NAME	SHUTE CREEK
LAND_TYPE	11
SEC	5
TWP	23
T_DIR	N
RGE	112
R_DIR	W
QTR1	SW
QTR2	SW
LON	-110.14872
LAT	41.99574
FOOT1	1120 FSL
FOOT2	1120 FWL
ELEV	6666.9
ELEVKB	0
WELL_CLASS	G
TD	11700
PB	0
RN	na
COAL_BED	N
STATUS	PA
STATUSDATE	19980701
CAPINO	49-023-21264
Field_LAT	41.997641
Field_LON	-110.148968
Date_Collected	9/9/2010 9:17:41 AM
WOGCC_Link	http://wogcc.state.wy.us/wellapi.cfm?wsdl=28&napino=2321264
Comments	no stake
Photo	<Raster>
Final_LAT	41.997641
Final_LON	-110.148968
Datum	NAD 27
Location_Source	Field GPS
Photo_	Yes

Identified 1 feature

Zoom in on Identify table

Click on the Hyperlink icon, and the WOGCC link for the well will open up in a Web-Browser. This page allows the User to access information about the well (i.e. APD's, well logs, and Sundries)

Apd File	Casing	Completions	Cores/Pressures/Reports
	Change of Operator	Display All Records	Geological Markers	Perforations	
	Production/Injection	Producing Intervals	Sales	Sundries	
	Tax Incentives	Treatments	Logs	Down Load Production/Injection	
	DownLoad All Records	Down Load Sales	Gas/Water Analysis	Well Site	

[Google Earth](#) | [AllTopo](#) | [BLM Master Title Plats](#) | [BLM Oil & Gas Plat](#) | [Cadastral Plats](#) | [NILS](#) | [Offset Wells](#)
[Codes](#) | [Images](#) | [Home](#) | [Disclaimer](#) | [About WOGCC](#)

<div>22</div>	Api Number 49-023-21727
	Well Name EMIGRANT SPRINGS UN 28-22
	Surface Location SE SE 22 TOWNSHIP 23 NORTH RANGE 112 WEST
	Spud 09/22/2002

Operator EOG RESOURCES INC	Lease No WYE024521A
Elevation GR 6542.7	Elevation KB 6558
Surface Location 50 FSL and 1200 FEL	Measured From SECTION LINE
Field EMIGRANT SPRINGS	Longitude -110.1082
Well Class GAS WELL	Latitude 41.969
Target Formation FRONTIER	Basin GREATER GREEN RIVER
Produced Formation FRONTIER-2	Status Date 08/2010
Group No FRONTIER-2 45720	Plug Back 10790
PA Case No. FRONTIER-2 π WYW 109503A	Unit Number π WYW109503X
Cum Production After 1978 20,171	Gas Mcf 1,613,379
Oil Bbls 20,171	Water Bbls 8,365
Gas Plant OPAL	
Commission Orders 155-94 (FRONTIER-DAKOTA)	Commission Orders 59-2005

10/19/10

Map On/Off ☐

Next, click on the Image icon, and the picture of the Monitor will open in the map. The picture can be resized, zoomed in to, and printed.

2.) **Go To XY**- Choose the Go To XY on the Data Toolbar and a Pop-Up window will appear. In the Units drop-down select Decimal Degrees and type in 41.969 for the Latitude and -110.1082 for the Longitude.

Then click drop point and a black dot will appear on the map at the coordinates. Then click on the add call-out.

3.) **Measure Tool**- Choose the Measure tool on the Data Toolbar and a Pop-Up window will appear.

4.) **Layout View** – The layout view will allow for printing of 8.5x11 pages. When a layer is turned on it will appear in the menu.

Well table metadata:

Columns	Data	Description
COMPANY	EOG RESOURCES INC	Comapany Name
WN	28-22	Well Name
UNIT_LEASE	EMIGRANT SPRINGS UN	Lease Name
FIELD_NAME	EMIGRANT SPRINGS	Oil/Gas Field
LAND_TYPE	11	FED/FEE/State
SEC	22	Section
TWP	23	Township
T_DIR	N	Township direction
RGE	112	Range
R_DIR	W	Range direction
QTR1	SE	Smallest Quarter-Quarter
QTR2	SE	Largest Quarter-Quarter
LON	-110.1082	WOGCC Longitude (assumed NAD 27)
LAT	41.969	WOGCC Latitude (assumed NAD 27)
FOOT1	50 FSL	Footage Nort-South in feet
FOOT2	1200 FEL	Footage East-West in feet
ELEV	6542.7	Ground elevation in feet (Above Mean Sea Level)
ELEVKB	6558	Elevation in feet from Kelly Bushing
WELL_CLASS	G	Well class (Gas/CBM/Oil etc.)
TD	10837	Total Depth in feet
PB	10790	Plug back depth in feet
RN	FRONTIER	Producing formation
COAL_BED	N	CBM well yes or no
STATUS	PG	Well status (Producing gas, abandoned etc.)
STATUSDATE	20021011	Well status date (YYYYMMDD)
CAPINO	49-023-21727	Well API
Field_LAT	41.951269	GPS'd latitude (NAD 27)
Field_LON	-110.099016	GPS'd longitude (NAD 27)
Date_Collected	9/28/2010	Date of GPS
WOGCC_Link	http://2321727	link to WOGCC
Comments	updated	Field comments
Photo	<Raster>	Photo link in map
Final_LAT	41.951269	Plotted location of latitude (NAD 27)
Final_LON	-110.099016	Plotted location of longitude (NAD 27)
Datum	NAD 27	Datum of plotted location
Location_Source	Field GPS	Location source WOGCC vs. GPS'd
Photo_	Yes	Photo taken Yes/No

CHAPTER 3: Geochemical Characterization of Produced Waters and Gases

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Background

For Task 3, researchers compiled and generated preliminary geochemical data on the natural geochemical variation in the water and gases of the Nugget Sandstone, the Madison Limestone, and overlying formations in the Moxa Arch formation. This work involved collecting a suite of produced water and gas samples from operational oil and gas wells established in the Nugget Sandstone and Madison Limestone and analyzing them for stable isotopic and major ion chemical compositions. Researchers also collected gas samples from the LaBarge platform and performed a gas compositional analysis.

Results of the chemical composition of produced waters were published in the special issue of *Rocky Mountain Geology*. Key findings, in the form of a peer-reviewed academic paper, follow. In addition, data from the gas compositional analysis performed on nine wells in the LaBarge gas field are included as an appendix.

Baseline geochemical characterization of potential receiving reservoirs for carbon dioxide in the Greater Green River Basin, Wyoming

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ABSTRACT

Geologic sequestration of anthropogenic carbon dioxide (CO₂) will be a necessary part of a carbon management strategy for reducing atmospheric CO₂ emissions so long as fossil fuels are a significant part of the energy mix. Proposed federal and state regulations for underground injection of CO₂ require that underground sources of drinking water be protected. Accordingly, proposed federal regulations require analysis of the suitability of different receiving formations for geologic sequestration.

This study compiles all available water quality data for four potential CO₂ receiving formations in the Greater Green River Basin of southwestern Wyoming. The Greater Green River Basin encompasses two large geologic structures, the Moxa Arch and Rock Springs Uplift, which potentially are capable of storing commercial quantities of CO₂ in a number of formations, including the Nugget Sandstone, Tensleep/Weber Sandstone, Madison Limestone, and Bighorn Dolomite. The data suggest that except along the basin margins, the Tensleep/Weber, Madison, and Bighorn Formations are suitable targets under proposed federal and state geologic sequestration regulations. However, low total dissolved solids in Nugget Sandstone groundwater in parts of the Rock Springs Uplift suggest the potential for local, fracture-assisted recharge in this area. For this reason the Nugget Sandstone is less suitable than the deeper formations for CO₂ storage in the Rock Springs Uplift.

KEYWORDS: Bighorn Dolomite, geologic sequestration, Madison Limestone, Moxa Arch, Nugget Sandstone, Rock Springs Uplift, Tensleep/Weber Sandstone, water quality.

INTRODUCTION

Geologic sequestration of anthropogenic CO₂ is one of a number of strategies for reducing CO₂ emissions to the atmosphere and thus for helping to mitigate anthropogenic climate change. It is part of the process of carbon capture and storage (CCS), in which CO₂ is captured from power plants or other anthropogenic sources, compressed to convert it to a relatively dense supercritical fluid, and delivered to the storage site. It is injected into a subsurface geologic receiving formation at sufficient depth (greater than ~2625 ft (800 m)) to maintain the CO₂ in a supercritical state. Natural subsurface accumulations of CO₂, including many in Wyoming, show that the gas can be trapped for millions of years (Huang et al., 2007; Lu et al., 2009).

Although in the long term it is anticipated that cleaner forms of energy will become competitive with energy from fossil fuels, in the near term geologic sequestration may be considered a bridging technology by which coal-rich nations such as the U.S., China, and India can continue to burn fossil fuels and limit CO₂ emissions to the atmosphere. According to the International Energy Agency (IEA), the least expensive approach to halve expected carbon emissions by 2050 would rely upon CCS to contribute almost 20 percent of the necessary cuts. As noted by Van Noorden (2010), in order to achieve this target, the CCS industry must develop quickly; by mid-century, the volume of supercritical CO₂ that must be injected underground each year would be three times the current amount of petroleum extracted every year. This requires that the regulatory

framework for CCS be established as soon as possible.

In 2008 the EPA proposed a new class of injection well, Class VI, under the authority of the Safe Drinking Water Act, that tailors existing Underground Injection Control (UIC) program standards for the geologic sequestration of CO₂ (40 CFR Part 144). The proposed rule outlines minimum technical requirements for geologic site characterization, well construction, operation, monitoring, and post-injection site care, among other criteria for Class VI. The purpose of both the proposed rule and the UIC program is to protect underground sources of drinking water (USDWs) from endangerment. USDWs are defined as an aquifer or a portion of an aquifer that currently supplies, or has sufficient capacity to supply, a public water system and contains less than 10,000 milligrams per liter (mg/L) total dissolved solids (TDS).

Under the EPA proposed geologic sequestration rule, the requirements for obtaining a Class VI injection permit include compiling information on the geochemistry of formation fluids of potential receiving formations within the three-dimensional region that may be impacted by injection activity (i.e., area of review). Pre-injection geochemical data can serve as a baseline against which data obtained throughout the injection phase may be compared. The State of Wyoming has primary enforcement authority (i.e., primacy) for the UIC program; in Wyoming, permits for geologic sequestration of CO₂ will be issued by the Wyoming Department of Environmental Quality (WDEQ) according to its proposed Water Quality Rules and Regulations, Chapter 24 (2010), once primacy for Class VI wells has been delegated to the state by EPA. Like the EPA rule, the WDEQ proposed regulations require baseline geochemical data on subsurface formations, including all USDWs in the area of review.

Demonstration of safe geologic sequestration of CO₂ is a priority for the State of Wyoming because of its dependence upon revenues from the mineral industry. As the producer of 40 percent of the nation's coal, Wyoming has a particular interest in minimizing CO₂ emissions, because coal-fired power plants emit 78 percent more CO₂ per unit of energy than natural gas-fueled plants. Paleozoic saline aquifers in southwestern Wyoming are promising targets for geologic sequestration. Two large geologic structures

that have the potential to store commercial amounts of CO₂ in these formations are the Rock Springs Uplift and Moxa Arch (Fig. 1). The Rock Springs Uplift is an intra-basinal, Laramide-age basement uplift within the Rocky Mountain foreland that is flanked to the south by the east–west-trending Uinta Mountains (Mederos et al., 2005). The Moxa Arch is a ~190-km-long, north–south-trending anticline, bounded on the south by the Uinta Mountains and over-ridden in the north by the leading edge of the Wyoming Thrust Belt (Kraig et al., 1987; Stillwell, 1989). Preliminary characterization of the Bighorn and Madison carbonate formations, as well as the Tensleep/Weber and Nugget Sandstone formations at the Rock Springs Uplift and Moxa Arch indicates that they lie at depths and pressures for which CO₂ will be supercritical, and they appear to have the appropriate thickness, reservoir properties, overlying low-permeability lithofacies, and structural integrity to be good candidates for CO₂ storage. The storage units are overlain by a series of shales and other sealing lithologies that are necessary to ensure CO₂ will be contained. These geologic sites are also adjacent to several significant point source emitters of anthropogenic CO₂, including PacifiCorp's Jim Bridger power plant at Point of Rocks on the Rock Springs Uplift and ExxonMobil's Shute Creek natural gas processing facility on the Moxa Arch.

The objective of this study is to compile pre-injection baseline geochemical data for water from four potential receiving formations in the Greater Green River Basin of southwestern Wyoming: the Ordovician Bighorn Dolomite, Mississippian Madison Limestone, Pennsylvanian Tensleep/Weber Sandstone, and Jurassic Nugget Sandstone. These data are used to identify the geochemical character of the water in these formations, the variability of water geochemistry within each formation across the study area, and whether or not these aquifers meet the criteria of USDWs. Data were collected from different sources available in the public domain, including the U.S. Geological Survey and the Wyoming Oil and Gas Conservation Commission.

GEOLOGIC BACKGROUND

The Moxa Arch and Rock Springs Uplift lie within the Greater Green River Basin located in southwestern Wyoming and northwestern Colorado

Figure 1. Map of the Wyoming portion of the Greater Green River Basin. Well locations for which water quality data are available are color coded according to the formation from which the geochemical data were collected. The axis of the Moxa Arch is shown by the black dashed line and the location of the cross-section shown in Figure 2 is indicated by line A-A'.

(Fig. 1). It encompasses an area of approximately 21,000 mi² (54,000 km²). The basin is bounded on the west by the western Wyoming Thrust Belt, on the south by the Uinta Mountains and the Axial Basin anticline, on the east by the Sierra Madre and Rawlins Uplift, and on the north and northeast by the Gros Ventre and Wind River Mountains.

The Moxa Arch is a south-plunging, intra-basin, asymmetrical buried anticline about 72 miles (116 km) long and 12 mi (19 km) wide (Figs. 1 and 2). It terminates against the Uinta Mountains of Utah to the south and continues north into the LaBarge Platform. Structural growth of the Moxa Arch began during Frontier Formation deposition and continued into late Campanian time. This movement was contemporaneous with deformation in the western

Overthrust Belt during the Sevier orogeny (Lehrer, 2006). Subsequent structural contraction during the late Laramide Orogeny reversed the original northward plunge of the arch and rotated it slightly to the east into its current structural position. This uplift resulted in the erosional truncation of over 3500 ft (1067 m) of Cretaceous Rock Springs and Hilliard Formations (Lehrer, 2006).

The Rock Springs Uplift is a north-south-trending, anticlinal structure in southwest Wyoming that formed in the Late Cretaceous/early Tertiary. The uplift is approximately 60 mi (100 km) long by 40 mi (65 km) wide. The uplift lies in the middle of the Greater Green River Basin and separates the Green River sub-basin to the west from the Washakie and Sandwash sub-basins to the east (Mederos et al.,

Figure 2. Schematic east–west cross section through the Greater Green River Basin. Vertical exaggeration 8x. Modified from Clarey (2008).

2005). The uplift is characterized by its asymmetric, west-vergent, antiformal shape and doubly plunging geometry. Seismic data suggest that a high-angle, west-vergent reverse fault occurs under the steeper western flank of the anticline and that basement is involved in the uplift (Bradley, 1964; Garing and Tainter, 1985; Montgomery, 1996). The uplift displays 14,800 ft (~4.5 km) of structural relief relative to the surrounding basins (Fig. 2; Montgomery, 1996).

Four geologic formations appear to be the best candidates for CO₂ storage because they may have appropriate porosity, permeability, and capacity to hold large quantities of CO₂, they are overlain by thick shales and other sealing rock types, and they lie at sufficient depth to store CO₂ as a supercritical fluid. These are the Nugget Sandstone, Tensleep/Weber Sandstone, Madison Limestone, and Bighorn Dolomite (Fig. 3).

The Jurassic Nugget Sandstone is a major eolianite that, along with its probable equivalents such as the Navajo Sandstone, spans an area from northern Wyoming southward into Arizona and eastward into Colorado. In the Utah–Wyoming thrust belt, the Nugget is texturally heterogeneous with anisotropic reservoir properties inherited primarily from the eolian depositional environment (Lindquist, 1988). Nugget dune deposits primarily consist of grain-flow and wide-ripple cross-strata, the former of which have the better reservoir quality and the lesser heterogeneity in bedding texture. The thickness of the Nugget Sandstone in southwestern Wyoming varies from around 800 to 1000 ft (240 to 305 m), and porosity is

variable (Table 1; Johnson, 2005). Low-permeability, gouge-filled micro-faults compartmentalize the formation, whereas intermittently open fractures provide effective permeability paths locally (Lindquist, 1988).

The Pennsylvanian Tensleep/Weber Sandstone was deposited in a marginal-marine setting of low relief where coastal dunes, marine foreshores and shorefaces, and carbonate shoals shifted positions in response to minor changes in sea level and sediment supply; this fluctuation of environments resulted in a complex package of interfingering lithofacies (Johnson, 2005). The sandstone is called Tensleep throughout much of Wyoming, although it is referred to as the Weber at oil and gas fields on the east side of the Rock Springs Uplift and the Sand Wash Basin. The Weber is approximately equivalent stratigraphically to the Tensleep Sandstone, but the upper part of the Weber is younger than the Tensleep (Johnson, 2005). Numerous dolomite layers exist throughout the Tensleep/Weber Formation, some as much as 12 ft (4 m) thick. The intervening thick bodies of quartz sand exhibit prominent crossbedding, some sets more than 50 ft (15 m) thick, as well as distinctive intervals of large-scale contorted bedding (Boyd, 1993). The formation contains linear and barchan dunes as well as interdunal deposits. The thickness of the formation is highly variable and depends on specific location, but most geologists report an average of about 500–700 ft (150–215 m) (Table 1; e.g., Johnson, 2005).

The Mississippian Madison Limestone was deposited on a carbonate shelf along the western

Figure 3. Schematic Phanerozoic stratigraphic chart for southwestern Wyoming, including the Moxa Arch and Rock Springs Uplift. Simplified from Love et al. (1993).

rank as the Madison Limestone. Several of the equivalent strata, including Lodgepole Limestone, Mission Canyon Limestone, and Pahasapa Limestone, differ in ratio of dolomite to limestone, bedding type, texture, grain origin, and chert content (Boyd, 1993). The narrow seaway that extended into part of Wyoming in latest Devonian time was reestablished very early in Mississippian time after a brief absence. The limited areas drowned in these incursions received several tens of feet of conodont-bearing dark shale and silty dolomite now recognized as a basal member of the Madison sequence (Boyd, 1993). The Madison is the most productive gas reservoir in the Green River Basin, with an original in-place natural gas resource of 22 trillion standard cubic feet (TSCF; Huang et al., 2007). Production is mainly from the LaBarge Platform at the northern end of the Moxa Arch. The gas is on average composed of 66 percent CO_2 , 21 percent methane, 7 percent nitrogen, 5 percent hydrogen sulfide, and 0.6 percent helium. Some CO_2 is separated from natural gas and helium at ExxonMobil's Shute Creek processing facility and supplied for enhanced oil recovery operations within Wyoming and Colorado. The remaining CO_2 is vented or injected into down-dip acid gas injection wells (Huang et al., 2007). The Madison Limestone lies approximately 14,000 ft (4300 m) below ground level on the Moxa Arch near Shute

edge of the North American craton. Where exposed at the southern end of the Wind River Mountains, the Madison is at least 215 ft (66 m) thick (Table 1; Berry, 1960). Over most of the state of Wyoming, the Mississippian carbonate strata are given formation

Table 1. Number of wells with water quality data (Appendix 1) and reservoir properties of formations of interest (Johnson, 2005).

Formation	Number of Wells	Thickness (ft)			Porosity range (%)
		Mean	Max	Min	
Nugget	87	900	1050	800	11–18
Tensleep	87	640	840	500	4–12
Madison	41	250	410	215	10–13
Bighorn	7	450	500	200	2–8

Table 2. Average water quality by formation, in mg/L, for formations of interest. Data from Appendix 1.

Formation	Ca ²⁺	Mg ²⁺	Na ⁺	K ⁺	HCO ₃ ⁻	SO ₄ ⁻	Cl ⁻	TDS	pH
Nugget	960	161	14732	507	1460	1996	23015	42110	7.2
Tensleep	512	131	3431	104	1319	2541	4020	11570	7.6
Madison	613	135	4270	154	1014	2491	5814	14114	7.4
Bighorn	529	98	6037	339	1896	1750	8220	17974	8.1

Creek and 7500 ft (2300 m) below ground level at the crest of the Rock Springs Uplift.

The Bighorn Dolomite is an Upper Ordovician unit that is overlain by the Madison Limestone, Tensleep Sandstone, and the Nugget Sandstone, and like the other formations is also of sufficient thickness and adequate porosity to represent a potential target reservoir for geologic sequestration (Table 1). The Bighorn Dolomite shares stratigraphic, paleontologic, and petrologic similarities with correlative rocks from west Texas to east-central Montana (Zenger, 1996). Sweet (1979, p. 46) describes the lower part of the Upper Ordovician western midcontinent succession as characterized by "...thick-bedded to massive, burrow-mottled skeletal wackestone and packstone, which, in many parts of the area studied have been altered to microcrystalline dolomite with little indication of original limestone fabric." Water quality data from this unit in the Green River

Basin are sparse because relatively few wells penetrate this deepest formation.

GEOCHEMICAL DATA

The geochemical data used in this study were compiled from two online sources: the Wyoming Oil and Gas Conservation Commission (<http://wogcc.state.wy.us/>) and the United States Geological Survey (<http://energy.cr.usgs.gov/prov/prodwat/data.htm>). Average data for each formation is presented in Table 2; the complete data set are provided in Appendix 1.

Geochemical variation Piper diagrams were created with AqQaChem software (version 1.1.1) from RockWare from the compiled water quality data (Figs. 4–7; Appendix 1). Average water quality for each formation is presented in Table 2. Data for the Nugget, Tensleep/Weber, and Madison Formations are plotted spatially (Figs. 8–10) and contoured using kriging, an interpo-

lation method based on statistical models that use spatial autocorrelation. This method assumes that distance and direction between sample points reflects a spatial correlation that can be used to explain variation in the surface. Inspection of the maps reveals that the distribution of data points has a profound effect on the resulting surfaces. With well sample locations distributed sporadically and centering on certain fields, the results skew when a single input point influences the resulting prediction surface.

The waters in this study from the Nugget Sandstone are dominantly Na⁺-Cl⁻ plus a few samples of Ca²⁺-Cl⁻ type (Fig. 4). The TDS of Nugget Sandstone waters are highly variable, ranging from 100 to >100,000 TDS (Appendix 1). The waters from the Tensleep/Weber Sandstone are dominantly Na⁺-Cl⁻ to Ca²⁺-SO₄⁻ type, with TDS values >10,000 mg/L in the majority of the basin (Fig. 5; Appendix 1). The waters from the Madison Limestone are predominantly Na⁺-Cl⁻ type with a few samples trending to Ca²⁺-SO₄⁻ type (Fig. 6). In the majority of the basin, the TDS values are >10,000 mg/L (Appendix 1). On the basis of very limited data, the waters from the Bighorn Dolomite appear to be Na⁺-Cl⁻ type, and TDS values are variable, with three samples >18,000 mg/L and four samples <6000 mg/L (Fig. 7; Appendix 1).

DISCUSSION

The potential receiving formations in the Greater Green River Basin can be divided into two major types: the sandstone

Figure 4 (top). Piper diagram for the Nugget Sandstone showing chemical variation for water quality data from Nugget Sandstone groundwater. Black symbols represent samples with >10,000 mg/L TDS; gray symbols represent samples with <10,000 mg/L TDS.

Figure 5 (bottom). Piper diagram for the Tensleep Sandstone showing chemical variation for water quality data from Tensleep Sandstone groundwater. Black symbols represent samples with >10,000 mg/L TDS; gray symbols represent samples with <10,000 mg/L TDS.

aquifers comprising Nugget and Tensleep, and the carbonate aquifers comprising Madison and Bighorn. A great deal of research has focused on mineral trapping potential of sandstone aquifers. The findings indicate that reactions with Ca/Mg/Fe-bearing silicate minerals neutralize the acidic CO_2 and provide alkali metals that trap the CO_2 through the precipitation of carbonate (Gunter et al., 1997, 1999; Saylor et al., 2001; Hovorka et al., 2001). However, these chemical processes are very slow because of the low chemical reaction rates of the clay and feldspar minerals involved in the reactions. Injection of CO_2 into a sandstone reservoir like the Tensleep or Nugget Sandstone may initiate similar kinds of chemical reactions and utilize the buffering power of aluminosilicate reactions to take up the CO_2 through production of bicarbonates. However, the sandstone thickness, seal strata, grain size, permeability, porosity, and the mineralogy of these sandstones will be the prime determinants of their geologic sequestration potential. Mineralogy is important because the proportion of reactant CO_2 to the proportion

Figure 6 (top). Piper diagram for the Madison Limestone showing chemical variation for water quality data from Madison Limestone groundwater. Black symbols represent samples with >10,000 mg/L TDS; gray symbols represent samples with <10,000 mg/L TDS.

Figure 7 (bottom). Piper diagram for the Bighorn Dolomite showing chemical variation for water quality data from Bighorn Dolomite groundwater. Black symbols represent samples with >10,000 mg/L TDS; gray symbols represent samples with <10,000 mg/L TDS.

of reactant mineral in the rock will determine the amount of CO_2 stored as mineral precipitate. Moreover, the Nugget Sandstone, in which carbonate is the most prevalent cement, will have a different reactive potential than Tensleep Sandstone, which is cemented by quartz overgrowths as well as carbonate (Fox et al., 1975; Knapp, 1978). Much less is known about sequestration of CO_2 in carbonate-rich rocks like those of the Madison and Bighorn Formations. However, it is generally agreed the reactions between CO_2 and carbonate rocks involve dissolution of calcite and adsorption of dissolved calcium on clays and formation of bicarbonate ions neutralizing the dissolution of CO_2 and buffering carbonate dissolution (Gunter et al., 1993).

In both sandstone and carbonate reservoirs the reactions with minerals in the formation are hypothesized to be much slower than reactions with formation water. Therefore, the sequestration resulting from simple CO_2 –water interaction is more important on short time scales (Gilfillan et al., 2009). This is mainly because the dissolution of injected CO_2 into formation water produces

Figure 8. Geospatial map of the Green River Basin for the Nugget Sandstone showing the variation in TDS relative to well locations.

carbonic acid (H_2CO_3), which forms large sinks of CO_2 and initiates other water–rock reactions. The chemical composition of water is important because the solubility of injected CO_2 will be controlled by concentrations of Na^+ , K^+ , Ca^{2+} , Mg^{2+} , Cl^- , and SO_4^{2-} in the formation water (Duan and Sun, 2003; Chapoy et al., 2004; Duan et al., 2006).

Spatial variability of water quality data

The water quality data for the Nugget Sandstone show spatial variability, as displayed in the TDS geospatial map (Fig. 8). Areas of low TDS indicate potential recharge zones, both along basin margins and in the Rock Springs Uplift area in the central part of the basin. The inferred rock fracture permeability in the Nugget Formation is considered high in the Rock Springs Uplift region (Clarey, 2008),

and this could possibly account for the fresh water recharge in the central parts of the basin. It appears that the majority of Nugget wells in the Rock Springs Uplift are near surface faults (Fig. 1), which may provide conduits for fresh water recharge. If true, then the Nugget Sandstone may be a poor receiving formation for CO_2 storage in the Rock Springs Uplift because of the potential for leakage along these pathways.

Water quality data for the other formations studied suggest recharge is limited to the basin margins. The Tensleep/Weber waters with $<10,000$ mg/L TDS are present along the eastern edge of the basin and probably represent areas of fresh water recharge near the Rawlins and Sierra Madre-Park Uplift (Fig. 9). These waters also have low concentrations of Na^+ , Cl^- , and SO_4^{2-} . For the Madison Limestone, the low

Figure 9. Geospatial map of the Green River Basin for the Tensleep Sandstone showing the variation in TDS relative to well locations.

TDS waters characterize areas receiving fresh water recharge near the eastern and northwestern parts of the basin (Fig. 10). These recharge zones are present in parts of the basin where the Madison Limestone is exposed at or near the surface, such as areas surrounding the Rawlins Uplift in the northeastern part of the basin and the overthrust belt in the northwestern part of the basin. In both Tensleep/Weber Sandstone and Madison Limestone, the Na^+ , Cl^- , and SO_4^{2-} concentrations and TDS values tend to increase with increasing distance from recharge areas toward the basin margin. The presence of briny Na^+ , Cl^- , and SO_4^{2-} -rich waters in the deeper central part of the basin indicate that halite and gypsum/anhydrite dissolution was probably an important source of salinity in these formations in addition to, or instead of, evaporated seawater. Bighorn Dolomite

water quality data are limited to the western edge of the Green River Basin, where TDS values are variable. Because the data include some high TDS values even on the basin margins, then as was true for the overlying Madison and Tensleep aquifers, it is likely that TDS will exceed the definition of a USDW in the Bighorn Dolomite in the middle of the basin. Therefore the Bighorn Dolomite should be considered a viable target for geologic sequestration along with the other Paleozoic target formations.

The data compiled in this study indicate that the Tensleep/Weber Sandstone, Madison Limestone, and probably also the Bighorn Dolomite, contain water too saline to meet the definition of a USDW except near recharge zones along basin margins. The Nugget Sandstone also exceeds the definition of a USDW except along basin margins and on most of

Figure 10. Geospatial map of the Green River Basin for the Madison Limestone showing the variation in TDS relative to well locations.

the Rock Springs Uplift. The relatively high density of mapped surface faults and potential for fault and fracture permeability on the Rock Springs Uplift decreases the suitability of the Nugget Sandstone as a CO_2 storage formation.

CONCLUSION

To assess the long-term CO_2 storage potential of any geological formation it is important to develop a good understanding of these CO_2 -water-rock interactions. In order to develop accurate models it is necessary to have baseline chemistry information on the formation waters and rocks into which CO_2 is proposed to be injected. Field experiments are difficult to implement due to the long timescales of these reactions

and challenges associated with the sample accessibility. Laboratory experiments and numerical and geochemical models are commonly used for predicting the fate of these CO_2 -water-rock interactions. The preliminary geochemical data generated in this study can be used to characterize the chemical composition of formation waters and help to develop realistic geochemical models for these target formations.

Geologic sequestration should be considered in regions where TDS values of brines are greater than 10,000 mg/L and where baseline water quality data are available so that potential chemical reactions between CO_2 , the reservoir host-rock, and brines may be modeled and understood. Based on the available geochemical data in this study, the Madison Limestone and Tensleep/Weber Sandstone waters meet the EPA Class

VI requirements for injection in the majority of the Green River Basin. Although water quality data are sparse, the Bighorn Dolomite most likely also exceeds the EPA definition of a USDW. On the other hand, the water quality data for the Nugget Sandstone suggest that groundwater from this formation is below 10,000 mg/L TDS and meets the definition of a USDW on much of the Rock Springs Uplift. TDS on the uplift are variable; this variability may be related to proximity to faults, which may serve as conduits for recharge. The apparent higher fracture permeability for formations nearest the surface suggests caution is appropriate when considering younger units like the Nugget Sandstone for geologic sequestration.

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REFERENCES CITED

40 CFR Part 144, 2008, Federal requirements under the Underground Injection Control (UIC) Program for

Carbon Dioxide (CO₂) Geologic Sequestration (GS) Wells; Proposed Rule: Environmental Protection Agency, Federal Register, July 25, 2008.

Berry, D. W., 1960, Geology and groundwater resources of the Rawlins area, Carbon County, Wyoming: U.S. Geological Survey Water-Supply Paper 1458, 74 p.

Boyd, D. W., 1993, Paleozoic history of Wyoming, *in* Snoke, A. W., Steidtmann, J. R., and Roberts, S. M., eds., *Geology of Wyoming: Laramie, Wyoming*, Geological Survey of Wyoming Memoir No. 5, p. 164–187

Bradley, W. H., 1964, Geology of the Green River Formation and associated Eocene rocks in southwestern Wyoming and adjacent parts of Colorado and Utah: U.S. Geological Survey Professional Paper 496-A, 85 p.

Chapoy, A., Mohammadi, A. H., Chareton, A., Tohidi, B., and Richon, D., 2004, Measurement and modeling of gas solubility and literature review of the properties for the carbon dioxide–water system: *Industrial and Engineering Chemistry Research*, v. 43, p. 1794–1802.

Clarey, K. E., 2008, WWDC Green River Basin Plan II, groundwater study (Level I): Wyoming State Geological Survey, U.S. Geological Survey, Water Resources Data System Cooperative Water Study, http://74.125.155.132/search?q=cache:oIQN4VyVBckJ:waterplan.state.wy.us/BAG/green/briefbook/GRB_GWStudy_20081023.pdf+WWDC+Green+River+Plan+II&cd=1&hl=en&ct=clnk&gl=us&client=safari.

Duan, Z., and Sun, R., 2003, An improved model calculating CO₂ solubility in pure water and aqueous NaCl solutions from 273 to 533 K and from 0 to 2000 bar: *Chemical Geology*, v. 193, p. 257–271.

Duan, Z., Sun, R., Zhu, C., and Chou, I. M., 2006, An improved model for the calculation of CO₂ solubility in aqueous solutions containing Na⁺, K⁺, Ca²⁺, Mg²⁺, Cl⁻, and SO₄²⁻: *Marine Chemistry*, v. 98, p. 131–139.

Fox, J. E., Lambert, P. W., Mast, R. F., Nuss, N. W., and Rein, R. D., 1975, Porosity variation in the Tensleep and its equivalent the Weber Sandstone, western Wyoming—A log and petrographic analysis, *in* Bolyard, D. W., ed., *Deep drilling frontiers of the central Rocky Mountains: Denver, Colorado, Rocky Mountain Association of Geologists Guidebook*, p. 185–216.

Garing, J. D., and Tainter, P. A., 1985, Greater Green River Basin regional seismic line, *in* Gries, R. R., and Dyer, R. C., eds., *Seismic exploration of the Rocky Mountain region: Denver, Colorado, Rocky Mountain Association of Geologists and Denver Geophysical Society*, p. 233–238.

Gilfillan, S. M. V., and ten others, 2009, Solubility trapping in formation water as dominant CO₂ sink in natural gas fields: *Nature*, v. 458, p. 614–618.

- Gunter, W. D., Perkins, E. H., and McCann, T. J., 1993, Aquifer disposal of CO₂-rich gases: reaction design for added capacity: *Energy Conversion and Management*, v. 34, p. 941–948.
- Gunter, W. D., Wiwchar, B., and Perkins, E. H., 1997, Aquifer disposal of CO₂ rich greenhouse gases: Extension of the time scale of experiment for CO₂-sequestering reactions by geochemical modeling: *Mineralogy and Petrology*, v. 59, p. 121–140.
- Gunter, W. D., Perkins, E. H., and Hutcheon, I., 1999, Aquifer disposal of acid gases: Modeling of water rock reactions for trapping of acid wastes: *Applied Geochemistry*, v. 15, p. 1085–1095.
- Hovorka, S. D., Doughty, C., Knox, P. R., Green, C. T., and Benson, S. M., 2001, Evaluation of brine bearing sands of the Frio Formation upper Texas Gulf Coast for geological sequestration, *in* Proceedings, First National Conference of Carbon Dioxide Sequestration, Washington D.C., March 3–6, 2001: National Energy Technology Laboratory, http://www.netl.doe.gov/publications/proceedings/01/carbon_seq/carbon_seq01.html.
- Huang, N. S., Aho, G. E., Baker, B. H., Matthews, T. R., and Pottorf, R. J., 2007, Integrated reservoir modeling to maximize the value of a large sour-gas field with high concentrations of inerts: *International Petroleum Technology Conference* 11202, 16 p.
- Johnson, E. A., 2005, Geologic assessment of undiscovered oil and gas resources in the phosphoria total petroleum system, southwestern Wyoming province, Wyoming, Colorado, Utah, *in* Petroleum Systems and Geologic Assessment of Oil and Gas in the Southwestern Province, Wyoming, Colorado, and Utah, Chapter 4, http://pubs.usgs.gov/dds/dds-069/dds-069-d/REPORTS/69_D_CH_4.pdf.
- Knapp R. R., 1978, Depositional environments and diagenesis of the Nugget Sandstone: southcentral Wyoming, northeast Utah and northwest Colorado, *in* Boyd, R. G., Olson, G. M., and Boberg, W. W., eds., Resources of the Wind River Basin: Casper, Wyoming Geological Association 30th Annual Field Conference, Guidebook, p. 131–138.
- Kraig, D. H., Wiltshko, D. V., and Spang, J. H., 1987, Interaction of basement uplift and thin-skinned thrusting, Moxa Arch and the western Overthrust Belt, Wyoming: a hypothesis: *Geological Society of America Bulletin*, v. 99, p. 654–662.
- Lehrer, M. G., 2006, Revitalizing the Moxa Arch: exploiting resource play: *The Mountain Geologist*, v. 43, p. 201–205.
- Lindquist, S. J., 1988, Practical characterization of eolian reservoirs for development: Nugget Sandstone, Utah–Wyoming thrust belt: *Sedimentary Geology*, v. 56, p. 315–339.
- Love, J. D., Christiansen, A. C., and Ver Ploeg, A. J., 1993, Stratigraphic chart showing Phanerozoic nomenclature for the State of Wyoming: Wyoming State Geological Survey Map Series MS-41, 1 sheet., 1 p.
- Lu, J., Wilkinson, M., Haszeldine, R. S., and Fallick, A. E., 2009, Long-term performance of a mudrock seal in natural CO₂ storage: *Geology*, v. 37, p. 35–38.
- Mederos, S., Tikoff, B., and Bankey, V., 2005, Geometry, timing, and continuity of the Rock Springs Uplift, Wyoming, and Douglas Creek Arch, Colorado: Implications for uplift mechanisms in the Rocky Mountain foreland, U.S.A.: *Rocky Mountain Geology*, v. 40, p. 167–191.
- Montgomery, S. L., 1996, Brady Unit, Rock Springs Uplift, Wyoming: Migration and structural history: *American Association of Petroleum Geologists Bulletin*, v. 80, p. 1535–1546.
- Saylor, B., Matisoff, G., and Morrison, P., 2001, Geological and geochemical evaluation of the potential for CO₂ disposal in deep saline aquifers beneath Ohio: *in* Proceedings, First National Conference of Carbon Dioxide Sequestration, Washington D.C., March 3–6, 2001: National Energy Technology Laboratory, http://www.netl.doe.gov/publications/proceedings/01/carbon_seq/carbon_seq01.html.
- Stillwell, D. P., 1989, CO₂ resources of the Moxa Arch and the Madison Reservoir *in* Eisert, J. L., ed., Gas resources of Wyoming: Casper, Wyoming Geological Association 40th Field Conference, Guidebook, p. 105–115.
- Sweet, W. C., 1979, Late Ordovician conodonts and biostratigraphy of Western Midcontinent Province, *in* Sandburg, C. A., and Clark, D. L., eds., Conodont biostratigraphy of the Great Basin and Rocky Mountains: Brigham Young University Geology Studies, v. 26, p. 45–85.
- Van Noorden, R., 2010, Carbon sequestration: buried trouble: *Nature*, v. 463, 871–873.
- Wyoming Department of Environmental Quality, 2010, Class VI injection wells and facilities, underground injection control program, Chapter 24 (Draft for comment, February 2010), *in* Water quality rules and regulations: [http://deq.state.wy.us/wqd/events/public%20notices/UIC/Ch%2024%20Draft%20for%20WAB%20Sept%2025%2009%20\(1\).pdf](http://deq.state.wy.us/wqd/events/public%20notices/UIC/Ch%2024%20Draft%20for%20WAB%20Sept%2025%2009%20(1).pdf).
- Zenger, D. H., 1996, Dolomitization patterns in widespread ‘Bighorn Facies’ (Upper Ordovician), western craton, USA: *Carbonates and Evaporates*, v. 11, p. 219–225.

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Appendix 1. Water quality data used in this study. Cation, anion, and total dissolved solids (TDS) concentrations are in mg/L. Data sources: WOGCC = Wyoming Oil and Gas Conservation Commission (<http://wogcc.state.wy.us/>), USGS = United States Geological Survey (<http://energy.cr.usgs.gov/prov/prodwat/data.htm>); NA = not available; an entry of -3 = no data; and entry of -1 = trace quantity. Continued on pages 107–111.

Nugget Sandstone:

Well/API	LATITUDE	LONGITUDE	Ca	Mg	Na	HCO ₃	K	SO ₄	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
4904120184	41.386060	-110.841730	865	131	7650	244	232	3500	11200	23698	6.1	NA	NA	USGS
NA	41.4348	-110.8176	478	68	5316	244	157	3450	6700	16289	7.1	7492	7506	USGS
4904120080	41.45364	-110.81339	412	111	5006	195	150	4200	5700	15675	7.3	7956	7968	USGS
4904120113	41.448300	-110.812460	457	56	4801	256	-3	3150	5800	14779	NA	NA	NA	USGS
4904120080	41.453640	-110.807410	467	84	4705	268	-3	3145	5500	14539	NA	NA	NA	USGS
NA	41.4496	-110.7984	467	62	4657	281	130	3450	5600	14504	6.9	7459	7470	USGS
4904120236	41.5128	-110.78346	444	63	3297	154	-3	2800	3900	10658	6.8	8748	8818	USGS
NA	41.5682	-110.7792	356	44	2226	195	-3	3700	1350	7871	6.9	9551	9610	USGS
NA	42.472433	-110.666846	29	5.5	1.4	122	0.6	3690	1.2	168.1	8	NA	NA	USGS
4904105215	41.31693	-110.63675	1065	381	8245	559	-3	4398	12120	26498	7.6	2120	NA	WOGCC
4904105218	41.329300	-110.619010	1093	491	6013	48	-3	3884	9700	21268	7.8	NA	NA	USGS
4904105216	41.317780	-110.610400	929	374	7698	465	-3	4324	11400	25040	NA	NA	NA	USGS
4904105244	41.47508	-110.55462	1045	437	7307	550	-3	4304	10900	24264	7.9	1170	NA	USGS
4903520394	42.44045	-110.49079	330	44	6807	73	275	3280	9000	19772	7	11267	11294	USGS
NA	42.234661	-110.466280	51	11	4.3	210	0.9	2876	3.2	303.3	8	NA	NA	USGS
4903505776	42.41089	-110.45225	777	113	16400	380	-3	2416	25000	44893	7.4	11620	11646	USGS
4902360015	41.83405	-110.43624	568	275	4011	273	-3	5790	3540	14457	NA	2225	2230	USGS
NA	42.220217	-110.431279	50	745	3.6	0	-3	4576	2.5	79	NA	NA	NA	USGS
NA	42.022165	-110.418222	57	24	8.6	0	-3	1498	11	104	NA	NA	NA	USGS
4903520218	42.353210	-110.393010	1862	37	29931	342	-3	1300	50800	86139	NA	NA	NA	USGS
NA	42.5	-110.2622	2650	305	34471	451	2500	1029	60000	101177	6.2	9600	NA	USGS
4903520165	42.338690	-110.381540	1960	276	31269	342	-3	1251	53000	89865	NA	NA	NA	USGS
4903520198	42.33261	-110.37653	2107	239	31884	342	1800	1362	54000	91560	8	11008	11064	USGS
4903520345	42.33979	-110.37522	2167	172	32436	268	1800	1150	55000	92857	7.3	10974	10980	USGS
4903505833	42.433660	-110.349760	390	253	32767	635	-3	936	50000	85259	NA	NA	NA	USGS
4903520169	42.4374	-110.34886	3500	2135	31577	586	2200	1060	62000	102761	6.7	9796	9830	USGS
4903505819	42.42839	-110.34531	2573	214	35489	390	-3	1000	59000	98497	6.8	9770	9808	USGS
4903520058	42.42168	-110.34476	2812	135	31114	622	1860	934	54000	91161	6.8	9432	9464	USGS
4903505812	42.42476	-110.3428	3208	413	38527	236	-3	1145	65331	108740	6.5	9874	9891	USGS
NA	42.4234	-110.3415	2996	386	35973	220	-3	1069	61000	101532	6.5	9874	9891	USGS
4903505746	42.40369	-110.32238	2792	257	36526	403	-3	1078	61000	101851	6.2	10079	10101	USGS
4903505128	42.28565	-110.3215	1869	169	30019	415	1750	950	50800	85772	7.3	11020	11030	USGS
4903506320	42.28741	-110.31922	1674	230	29392	403	1720	400	50000	83614	7	10817	10840	USGS
4903505176	42.288550	-110.316180	1883	209	31412	378	317	1030	53000	89210	8.1	NA	NA	USGS
4903520035	42.28341	-110.31555	1090	109	18936	622	640	371	31400	52852	6.6	NA	NA	USGS

BASELINE GEOCHEMICAL CHARACTERIZATION FOR GEOLOGIC SEQUESTRATION

Well/API	LATITUDE	LONGITUDE	Ca	Mg	Na	HCO3	K	SO4	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
4903520062	42.276180	-110.310260	1961	123	32633	403	-3	848	55000	92629	NA	NA	NA	USGS
NA	42.2905	-110.2738	1850	305	31220	464	2300	868	53500	90272	6.2	10800	NA	USGS
NA	42.5	-110.2622	2650	305	34471	451	2500	1029	60000	101177	6.2	9600	NA	USGS
4903505450	42.3301	-110.23964	2288	320	35532	365	-3	785	59000	98105	6.8	10128	10178	USGS
4904105230	41.37155	-110.07275	1475	139	28645	990	-3	216	46500	77487	6.9	14526	14646	USGS
4904120019	41.25489	-110.06478	1078	239	27816	488	1000	184	46000	76557	7.7	14597	14643	USGS
NA	41.619131	-109.192070	78	37	2700	590	-3	210	3700	7511.1	NA	NA	NA	USGS
4903720754	41.01673	-109.15309	23	14	16781	3123	1127	1320	24200	45003	6.3	12040	12080	USGS
4903720396	41.36402	-109.12415	123	24	2596	2513	140	418	2650	7189	8	3619	3630	USGS
4903705644	41.63844	-109.12385	103	30	5703	6000	-3	918	4899	14004	7	4132	4700	USGS
4903705584	41.61675	-109.1187	80	37	4106	4600	-3	117	3823	10425	NA	4010	4078	USGS
4903705290	41.38876	-109.11855	100	44	2933	3550	203	-1	3000	8038	8.2	3826	3842	USGS
4903705353	41.51061	-109.11662	115	30	4616	4760	-3	59	4600	11764	8	4533	4554	USGS
4903705693	41.65449	-109.112	86	37	4088	4100	-3	-3	3900	10369	7.3	4064	4076	USGS
4903705757	41.67835	-109.11156	125	25	4066	4830	-3	78	3700	10372	7.9	4365	4375	USGS
4903705775	41.69287	-109.10299	39	41	4238	4150	-3	451	3980	10793	8	4577	4587	USGS
4903705660	41.64132	-109.1009	90	44	3936	4700	-3	11	3619	9011	NA	4290	4300	USGS
4903705641	41.63772	-109.10073	61	29	4049	4350	-3	-3	3908	10186	NA	4095	4135	USGS
4903705712	41.66199	-109.09769	48	-1	1613	1155	-3	1067	1115	4998	NA	4169	4223	USGS
4903705622	41.6314	-109.0973	34	37	3782	3375	-3	290	3564	9590	8.15	4015	4034	USGS
4903720156	41.84953	-109.09676	171	50	34887	5124	1550	14489	42000	95670	7.8	8115	8160	USGS
4903705630	41.635080	-109.092440	103	30	2909	2500	-3	443	2695	9111	7	NA	NA	USGS
4903705528	41.59123	-109.07643	106	51	3824	4490	-3	23	3380	9787	8.3	4377	4396	USGS
4903705377	41.53696	-109.06119	20	38	3899	4900	-3	60	3267	9677	NA	3333	3350	USGS
4903705440	41.56126	-109.0611	110	39	3459	3800	-3	9	3429	8916	NA	3542	NA	USGS
4903705658	41.64035	-109.00351	1087	398	26182	781	-3	1375	42000	71823	7.8	4680	4754	USGS
4903705196	41.21016	-108.98377	69	20	3392	3250	-3	34	3500	8617	7.5	7180	7207	USGS
4903720007	41.03787	-108.97443	729	176	21617	1952	1400	3634	32600	61117	7.4	14422	14465	USGS
4903705405	41.54574	-108.85859	207	34	9364	5480	-3	1658	10500	24462	7.4	6673	6683	USGS
4903705405	41.545740	-108.858590	229	27	9662	5620	-3	4850	10800	25276	7.3	NA	NA	USGS
4903705104	41.04986	-108.76042	279	17	6766	964	650	4850	7300	20518	8.6	13790	14253	USGS
4903705131	41.09511	-108.59389	56	8	14349	451	1385	340	23000	39360	6.7	14722	14940	USGS
4903720522	41.34927	-108.52861	25	6	3822	1635	39	57	5000	9754	7.2	NA	NA	USGS
4903706394	41.560680	-108.422340	112	51	5866	4002	285	95	4800	16498	8.6	NA	NA	USGS
4900705087	41.360930	-107.696760	1034	4	18532	476	-3	70	30000	51895	NA	NA	NA	USGS
NA	41.374000	-107.696600	837	26	16256	427	65	109	26600	45947	NA	4776	4816	USGS
NA	41.374000	-107.696600	949	58	19957	464	-3	105	32000	55165	NA	NA	NA	USGS
4900705095	41.370130	-107.693730	798	2	18941	476	24	81	28800	51289	NA	NA	NA	USGS
NA	41.368000	-107.691000	809	364	20483	488	45	106	32800	56427	7.6	3871	3913	USGS
4900705066	41.289980	-107.604120	46	7	1130	1175	-3	98	123	3292	NA	NA	NA	USGS
4900705062	41.259400	-107.601350	42	7	1725	1183	63	91	510	5143	8.1	2883	2918	USGS

Well API	LATITUDE	LONGITUDE	Ca	Mg	Na	HCO ₃	K	SO ₄	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
4903706001	42.238280	-107.563450	20	38	1521	2318	-3	90	990	3785	NA	NA	NA	WOGCC
NA	42.243200	-107.562300	11	2	1616	2562	-3	104	1080	4015	7.1	NA	NA	USGS
4903720134	42.242260	-107.549330	36	463	1724	2586	-3	1360	1280	4450	7.4	NA	NA	USGS
NA	42.250000	-107.510600	760	32	1826	622	-3	750	4800	8107	NA	3429	3475	USGS
4900720034	41.587190	-107.505120	95	84	3876	6954	26	1040	750	10316	NA	NA	NA	USGS
4900705219	41.098860	-107.423820	25	6	1997	2500	39	2428	630	5213	7.2	4240	4250	USGS
4900705816	42.161640	-107.412240	18	136	1271	1905	-3	1375	900	3132	NA	NA	NA	USGS
4900705816	42.161640	-107.412240	18	3	1275	1911	-3	1235	903	3141	7.6	NA	NA	USGS
4900705830	42.173010	-107.401310	10	74	1271	1320	-3	1500	880	3081	7.1	NA	NA	USGS
4900706984	41.095800	-107.389930	22	7	1716	2611	30	1750	780	4432	8.2	NA	NA	USGS
4900705722	42.081360	-107.173060	72	25	843	1074	-3	1720	316	2421	NA	NA	NA	USGS

Tensleep/Weber Sandstone:

Well API	LATITUDE	LONGITUDE	Ca	Mg	Na	K	HCO ₃	SO ₄	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
4904105094	41.22818	-110.65982	890	44	4549	-3	5200	4226	2432	15802	8.6	12877	12927	USGS
4904105215	41.31693	-110.63675	1086	105	5854	-3	3050	4172	5454	18979	7.4	12929	12997	USGS
4904105218	41.3293	-110.61901	820	34	4744	-3	3540	4021	5400	17297	8.2	13004	130092	USGS
4904105216	41.31778	-110.6104	526	140	3918	-3	1405	3876	4700	14013	8.2	6280	6305	USGS
4904105164	41.27724	-110.60089	945	75	3761	-3	4014	3647	3650	15619	7.4	6277	6300	USGS
4904105244	41.47508	-110.55462	962	87	4693	-3	1440	4326	6800	16764	7.9	6502	6527	USGS
4903505746	42.40369	-110.32238	43	44	3860	-3	1830	4852	1360	11192	8.6	12877	12927	USGS
4903705584	41.61675	-109.1187	528	-1	3812	-3	3060	697	4522	12619	NA	6502	6527	USGS
4903705655	41.64014	-109.10509	973	47	26637	-3	2013	1267	41000	72300	7.6	5515	5535	USGS
4903705660	41.64132	-109.1009	622	101	3732	-3	2100	1327	4952	12834	NA	6280	6305	USGS
4903705712	41.66199	-109.09769	1245	209	10606	-3	3550	1915	15694	33219	NA	6339	NA	USGS
4903705622	41.6314	-109.0973	921	296	15641	-3	0	1977	23760	42595	NA	6277	6300	USGS
4903705395	41.54499	-109.07796	289	65	5612	0	3050	2647	6831	15918	7.7	6217	6247	USGS
4903705377	41.53696	-109.06119	386	80	2347	-3	1740	3974	594	8237	NA	5339	NA	USGS
4903720724	41.198330	-108.827640	283	47	37646	-3	5514	3746	50000	101685	7.2	NA	NA	USGS
4903720384	41.372060	-108.757740	3410	68	4328	-3	1840	2398	11100	21871	NA	6543	6485	USGS
4903720385	41.398810	-108.738500	6860	35	5570	-3	-3	2765	20500	33003	NA	NA	NA	USGS
4900720209	41.36678	-107.65288	369	60	266	5	744	650	330	2046	6.7	10865	10913	USGS
4900705066	41.28998	-107.60412	98	99	8788	573	2093	2706	11219	25675	8.28	10224	10244	USGS
4903721115	42.25761	-107.58083	464	66	3183	138	793	3100	3300	10642	6.7	6624	6700	WOGCC
4903705994	42.23582	-107.5789	31	15	3919	-3	4404	3	3580	9717	7.6	5163	5575	USGS
NA	42.259	-107.5775	2975	1613	3204	180	281	1380	13900	23392	6.7	6204	6244	USGS
4903706285	42.2593	-107.57647	292	51	4571	210	1074	3400	4800	13858	8.1	7625	7807	USGS
4903706012	42.23924	-107.57218	332	75	3283	-3	1167	3903	2314	10481	7.4	6583	6633	USGS
4903706156	42.24645	-107.5718	362	34	7474	60	1183	3750	8900	21169	8.2	5635	6015	USGS
4903706108	42.24382	-107.57079	560	140	11636	795	878	3240	17200	34009	7.8	6106	6138	USGS
4903706018	42.23984	-107.56592	520	79	4884	450	952	2494	6700	15596	7.1	5420	5530	USGS
4903706281	42.25765	-107.56243	309	36	1968	146	493	1790	1785	6277	7.6	5205	5666	WOGCC

BASELINE GEOCHEMICAL CHARACTERIZATION FOR GEOLOGIC SEQUESTRATION

Well API	LATITUDE	LONGITUDE	Ca	Mg	Na	K	HCO3	SO4	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
4903706218	42.24999	-107.55919	447	99	4570	287	842	3185	5550	14553	7.6	5270	5585	USGS
4903705997	42.2374	-107.55742	507	105	3644	-3	813	2423	4565	11644	7	4500	NA	USGS
4903705968	42.23192	-107.55583	324	60	3295	-3	752	2818	3313	10179	7.2	NA	NA	USGS
4903705985	42.23404	-107.55514	503	22	1384	34	1318	1625	1160	5378	7.2	5445	5487	USGS
4903706087	42.24272	-107.55483	423	79	1644	-3	605	1828	1813	6392	NA	5262	6449	USGS
4903706146	42.24461	-107.55245	377	83	3114	275	1976	3150	2550	10534	6.8	6812	6916	USGS
NA	42.25	-107.5517	387	87	9404	760	2684	4981	10900	27841	7.9	NA	NA	USGS
4903705961	42.2246	-107.55002	608	61	1847	-3	560	3378	1285	7456	7.6	7081	7164	USGS
4903706273	42.25647	-107.54728	403	202	2731	240	1354	2380	3200	9825	7.3	7209	7270	USGS
4903706228	42.25027	-107.54411	1387	594	8962	805	2538	5850	13000	33146	7.2	7239	7291	USGS
4903706470	42.26008	-107.54	1620	836	1055	60	708	1240	5660	10820	6.4	7142	7176	USGS
4903706222	42.25007	-107.5389	948	431	8950	620	1769	3950	13400	29178	7	6904	7058	USGS
4903706238	42.25169	-107.52964	386	56	5433	-3	2390	5473	3800	16329	7	NA	NA	USGS
4903706214	42.24955	-107.52744	175	32	1908	-3	675	2568	1058	6416	NA	6130	NA	USGS
4903706245	42.25249	-107.52452	357	137	4433	258	1977	3892	4131	15112	7.07	6180	6280	USGS
4903706130	42.24441	-107.52314	410	126	4813	380	2147	4100	4600	15488	7.6	6270	6464	USGS
4900706007	42.25174	-107.52058	432	119	6348	-3	2850	4742	5746	20237		6000	6336	USGS
4900705990	42.24263	-107.51721	354	100	3623	-3	1905	3280	2980	11275	7.6	6022	6193	USGS
4900705985	42.24163	-107.51541	587	134	2441	-3	2087	2746	1956	8891	7.6	5869	5883	USGS
4900705987	42.24197	-107.51359	444	104	4000	-3	2380	3436	3340	12496	7.4	6043	6140	USGS
NA	42.2489	-107.5122	71	29	6767	-3	6686	101	6686	16946	7.8	NA	NA	USGS
4900705982	42.24115	-107.5103	24	11	4808	-3	6167	32	3882	11795	8.1	5754	6103	USGS
4900705978	42.23911	-107.5102	467	92	3404	-3	1995	3084	2909	10937	7.2	5757	6044	USGS
4900720034	41.58719	-107.50512	150	92	15617	1700	4453	3494	21000	44246	7.7	10505	10546	USGS
4900705950	42.21707	-107.46766	304	56	574	-3	241	1661	220	2932	7.2	6966	7320	USGS
4900705945	42.21548	-107.46491	335	58	347	9	156	1490	242	2558	7.6	NA	NA	WOGCC
4900705776	42.13147	-107.42624	411	78	381	-3	185	1551	289	2895	NA	4966	NA	USGS
4900705673	41.99278	-107.40684	344	44	1542	-3	260	1728	1690	5476	7.5	4776	NA	USGS
4900705746	42.09028	-107.38749	406	79	564	-3	100	1556	612	3317	NA	5047	NA	USGS
4900705671	41.99527	-107.38253	466	60	1581	-3	175	1675	2100	5968	7.3	3778	3796	USGS
4900705682	42.01304	-107.36344	421	39	1758	-1	317	2318	1697	6556	7.69	3857	3887	USGS
4900705680	42.00689	-107.35221	654	81	1505	-3	255	3217	1191	6773	NA	3404	NA	USGS
4900705860	42.18321	-107.34484	584	122	221	-3	420	1898	85	3330	NA	4408	4532	USGS
4900705860	42.18321	-107.34484	573	121	173	0	354	1757	132	2930	7.2	4410	4532	USGS
4900705861	42.18396	-107.34036	494	113	1164	-3	65	2567	1067	5470	NA	4293	4505	USGS
4900705867	42.18661	-107.34009	718	217	492	-3	420	2671	447	4965	NA	4346	4536	USGS
4900720385	42.18205	-107.33771	573	174	1129	150	342	2250	1285	5730	7.9	NA	NA	WOGCC
4900705866	42.18644	-107.33535	858	272	765	-3	150	2016	1915	5976	NA	4351	NA	USGS
4900705841	42.1796	-107.3349	556	125	761	-3	240	2270	708	4660	NA	4300	4445	USGS
4900705845	42.18046	-107.33224	494	129	245	-3	178	1833	172	2961	7.4	4324	4433	USGS
4900705280	41.64793	-107.27317	232	58	1808	-3	780	3123	608	6054	7.55	6122	6176	USGS
4900705311	41.6551	-107.27303	226	22	1771	-3	1110	1885	1160	5611	7.1	5750	5935	USGS
4900705338	41.6598	-107.27299	198	-1	2575	-3	1475	1646	2250	8144	7.3	5784	6072	USGS
4900705357	41.66259	-107.27299	78	36	4147	-3	1755	1771	4200	11192	8.4	5855	6084	USGS
4900705893	42.19006	-107.26478	303	66	389	-3	295	1530	29	2612	NA	4447	NA	USGS
4900705893	42.19006	-107.26478	341	70	330	0	250	1554	24	2442	NA	4302	NA	USGS
4900705333	41.65819	-107.26433	29	14	326	-3	334	332	156	1021	6.8	6332	6450	USGS

Well API	LATITUDE	LONGITUDE	Ca	Mg	Na	K	HCO ₃	SO ₄	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
4900705892	42.18991	-107.26178	530	105	47	-3	115	1680	10	2487	NA	4274	4316	USGS
4900705036	41.05145	-107.24339	130	17	381	19	146	950	100	1669	7.8	7642	7670	USGS
4900705036	41.05145	-107.24339	131	12	463	23	110	1150	90	1979	7.7	7642	7670	USGS
4900705414	41.67365	-107.23027	484	69	2053	-3	660	4123	800	7854	7.4	8176	8208	USGS
4900720110	41.59113	-107.21124	170	34	1203	17	329	2200	468	4421	7.7	5216	5287	USGS
4900705722	42.08136	-107.17306	524	97	1022	-3	307	2306	851	4999	8.6	6383	6454	USGS
4900705722	42.08136	-107.17306	772	139	1171	-3	476	3502	630	6399	8.2	6301	6316	USGS
4900705745	42.08972	-107.14401	433	85	1063	-3	367	2030	945	4737	7	6602	6648	USGS
4900706036	41.9638	-107.10584	593	86	1447	-3	842	2185	1430	6156	8.1	8871	8939	USGS
4900705753	42.09259	-107.09661	475	83	838	-3	236	1613	1048	4173	7.9	6891	7002	USGS
4900705572	41.82907	-107.08697	1035	55	2115	-3	3123	3794	640	9177	7.9	4808	4840	USGS
4900706031	41.76378	-107.01976	528	10	2440	-3	342	5514	460	9120	8.2	3885	3987	USGS

Madison Limestone:

Well API	LATITUDE	LONGITUDE	Ca	Mg	Na	K	HCO ₃	SO ₄	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
NA	41.351200	-110.956000	464	72	17092	-3	5185	3863	25100	47124	NA	NA	NA	USGS
4904120117	41.452941	-110.908270	3296	337	3021	-3	1232	2600	10100	21000	7.2	5778	5880	USGS
4902320446	42.121410	-110.718900	80	18	6864	517	1024	1926	1000	22003	8.5	NA	NA	WOGCC
4904105215	41.316930	-110.636750	816	337	6438	-3	2270	9929	8181	20751	7.2	5778	5880	USGS
4904120145	41.470000	-110.490000	536	626	8081	590	1170	1758	11200	23719	6.7	NA	NA	USGS
4903520090	42.312900	-110.477840	577	135	113	2	268	1750	14	2899	7.4	2877	2883	USGS
NA	42.272857	-110.340166	48	13	2.3	-3	190	7465	3.1	289	7.1	NA	NA	USGS
4903505746	42.403690	-110.322380	241	97	8674	-3	5100	2456	3800	25253	7.9	13718	14033	USGS
4903720754	41.016730	-109.153090	848	391	27188	1852	2635	1800	43400	76777	6.9	15840	16097	USGS
4903720948	41.571603	-108.412907	6335	845	11939	1755	378	1800	33400	54545	4.4	NA	NA	WOGCC
NA	42.252200	-107.587500	470	96	2508	-3	780	2180	2960	8483	6.8	NA	NA	USGS
NA	42.238700	-107.572900	569	64	4447	430	866	2495	6100	14450	6.9	7250	7630	USGS
NA	42.241000	-107.571900	385	93	3759	0	756	2432	4950	12218	7.6	NA	NA	USGS
4903706108	42.243820	-107.570790	1344	578	1514	130	549	1878	4820	10618	6.8	6471	6487	USGS
4903706232	42.251100	-107.567300	356	291	4114	0	667	2563	5504	13149	8.4	4794	5410	USGS
4903706232	42.251850	-107.566530	352	288	4073	0	660	2797	5450	13019	8.4	NA	NA	USGS
NA	42.248000	-107.566000	400	97	3510	-3	622	1700	4786	11115	7.65	4794	5410	USGS
4903706258	42.255750	-107.565570	304	60	2842	-3	488	2456	3240	8818	8.1	5570	5863	USGS
4903706281	42.257670	-107.562430	278	88	3871	-3	1305	7000	3800	11725	7.2	NA	NA	USGS
4903706045	42.240930	-107.562400	634	99	5493	271	587	1998	8465	17459	7.3	5814	5841	USGS
4903706011	42.239200	-107.562040	1330	143	6730	254	621	1998	13234	24142	7.4	NA	NA	USGS
4903706253	42.254020	-107.559700	790	17	5258	145	3404	1208	2400	17421	8.6	6047	6122	USGS
4903706084	42.242920	-107.557690	396	71	2816	-3	969	2526	3215	8973		6120	NA	USGS
4903705985	42.234040	-107.555140	396	71	2816	-3	969	2506	3215	9465	NA	NA	NA	USGS
NA	42.250000	-107.551700	666	101	7387	312	537	2534	10750	22937	7.7	4986	5412	USGS
4903706238	42.251690	-107.529640	309	53	997	-3	-3	2828	652	3823	7.7	7046	7102	USGS

BASELINE GEOCHEMICAL CHARACTERIZATION FOR GEOLOGIC SEQUESTRATION

Well API	LATITUDE	LONGITUDE	Ca	Mg	Na	K	HCO ₃	SO ₄	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
4903706262	42.255280	-107.528260	257	56	2173	-3	282	2445	2004	7074	7.2	5100	5600	USGS
4903706262	42.255280	-107.528260	275	68	2643	-3	1724	1812	1895	8255	7	NA	NA	USGS
4903706019	42.239590	-107.522570	112	36	1251	-3	575	3177	950	3888	8.3	7534	7599	USGS
4900706001	42.247650	-107.520670	399	9	3199	-3	848	2528	3301	10440	7.9	6975	7028	USGS
4900706000	42.246520	-107.519240	432	87	3804	-3	1556	1720	3971	12378	6	NA	NA	USGS
4900705990	42.242630	-107.517210	1251	134	1455	-3	549	2556	3260	8090	7	NA	NA	USGS
4900706003	42.249380	-107.516480	536	126	4884	-3	1730	1700	5500	15075	7.4	6670	7028	USGS
4900720380	42.247490	-107.515280	447	80	1610	138	720	1058	1960	6290	7.1	6838	6921	USGS
4900705993	42.243640	-107.514370	1278	131	4008	-3	1450	1058	6000	14820	8.2	6450	6577	USGS
NA	42.238500	-107.513200	437	88	3619	226	1573	2474	4015	12514	5.97	6750	6800	USGS
4900705945	42.215480	-107.464910	262	24	455	0	131	491	379	2242	NA	6604	6905	USGS
4900705934	42.205390	-107.412120	262	24	455	-3	-3	1300	379	2178	NA	6604	6905	USGS
4900706932	42.095610	-107.394300	191	39	1390	-3	172	647	1996	4467	7.8	5935	6015	USGS
4900705680	42.006890	-107.352210	300	79	1779	-3	195	1245	1568	6395	NA	4059	4444	USGS
4900705864	42.184780	-107.336800	54	21	302	-3	170	3423	162	1200	NA	5000	5259	USGS

Bighorn Dolomite:

Well API	LATITUDE	LONGITUDE	Ca	Mg	Na	K	HCO ₃	SO ₄	Cl	TDS	pH	Upper Depth (feet)	Lower Depth (feet)	Data source
4120282	41.47328	-110.9215	865	306	4712	2270	159	65	11053	18960	8.85	NA	NA	WOGCC
4902320423	42.25861	-110.1809	49	31	310	4	376	217	218	1046	8.4	NA	NA	WOGCC
4902320423	42.25861	-110.1809	45	29	616	6	323	276	636	1845	8.7	NA	NA	WOGCC
4902320423	42.25861	-110.1809	172	1	25157	92	1067	6900	32600	66198	9.6	NA	NA	WOGCC
NA	42.40369	-110.3224	386	35	145	0	1330	183	100	1504	6.6	15000	15025	USGS
NA	42.40369	-110.3224	1251	202	610	0	4270	1395	230	5791	7.3	15095	15125	USGS
NA	42.40369	-110.3224	938	81	10708	0	5750	3214	12700	30473	7.2	15266	15280	USGS

Appendix II: Results from Gas Compositional Analysis on LaBarge Field

Figure A3-1: Map showing the sampling locations and detailed flow line schematics of the manifolds

A gas compositional analysis for the produced gas samples collected from nine wells contributing to manifolds 9, 15, and 3 from the Fogarty Creek fields (Figure A3-1) was completed as part of Task 3. The gas compositional analysis (Table A3-1) shows that the percentage of methane in all gas samples ranges between 17–20%. Ethane is around .01% and propane and butane are below detection limit for all samples. The carbon isotope composition ($\delta^{13}\text{C}_{\text{CH}_4}$) and hydrogen isotope composition ($\delta\text{D}_{\text{CH}_4}$) of methane in the gas samples ranges between - 43.6 to - 44.2‰ V-PDB and -153 to -158 ‰ V-SMOW respectively. The percentage of CO_2 ranges between 64 to 71% for all samples and the carbon isotope composition ($\delta^{13}\text{C}_{\text{CO}_2}$) varies between -5 to -5.4 ‰ V-PDB (Table A3-1). The He, N, and Ar percent is also similar in all

samples and all samples have approximately 0.55% of He, 7.5% of N and .06% of Ar (Table A3-1).

We did not see any significant difference in the total gas composition and isotope values of gas samples collected from wells producing from different depth in Fogarty Creek Unit (wells contributing to manifolds 15 and 3) and Lake ridge Unit (manifold 9). One sample (FC 13-10) was collected directly from the sampling port at the well-head at Fogarty Creek. This sample was retrieved upstream of the corrosion inhibitor injection point to assess the effect of inhibitor injection and pipeline transport on the isotopic composition of the gas. We did not see any significant difference between the $\delta^{13}\text{C}_{\text{CO}_2}$ and $\delta^{13}\text{C}_{\text{CH}_4}$ composition of this sample or others collected from the manifold, indicating the inhibitor injection and pipeline transport are not significantly affecting the carbon isotope composition of methane and CO_2 component of the gas. However the hydrogen isotope composition of this sample is slightly higher, indicating that hydrogen isotope composition might have been affected. However, it is difficult to make any conclusions based on a single sample.

WELL	Location	Depth/ Zone	CH ₄	He	N	Ar	CO ₂	C ₂ H ₆	H ₂ S	$\delta^{13}\text{C}$ (CH ₄)	$\delta^{13}\text{C}$ (CO ₂)	δD (CH ₄)
Manifold 9												
LR 5-32	42°27' 33"N 110°27' 18"W	15372-16062 (Lake Ridge)	18.1	0.54	7.50	0.06	70.0	0.01	3.76	- 43.91	-5.15	-153
LR 6-14	42°24' 46"N 110°27' 35"W	15320-16120 (Lake Ridge)	21.3	0.55	7.61	0.06	64.3	0.01	6.08	- 44.17	-5.24	-156
Manifold 15												
FC 15-28	42°23' 14"N 110°25' 54"W	15234-16082 (Fogarty Creek)	19.2	0.60	7.73	0.07	67.3	0.01	4.95	- 43.89	-5.02	-153
FC 17-16	42°24' 32"N 110°23' 55"W	14503-15354 (Fogarty Creek)	21.5	0.53	7.53	0.06	63.8	0.01	6.48	- 43.97	-5.45	-154
FC 20-13	42°24' 35"N 110°26' 24"W	15178-16028 (Fogarty Creek)	20.7	0.56	7.64	0.06	65.2	0.01	5.76	- 43.67	-5.07	-154
Manifold 3												
FC 23-12	42°26' 31"N 110°22' 56"W	14130- 14878 (Fogarty Creek)	18.7	0.55	7.53	0.06	68.8	0.01	4.40	- 43.66	-5.27	-154
FC 21-03	42°25' 47"N 110°25' 43"W	14999-15670 (Fogarty Creek)	17.4	0.53	7.38	0.06	71.1	0.01	3.42	- 43.81	-5.16	-156
Well-head												
FC 13-10	42°25' 46"N 110°22' 56"W	14130-14878 (Fogarty Creek)	18.0	0.54	7.42	0.06	69.6	0.01	4.2	- 43.58	-5.05	-158

Table A3-1: Results of gas composition and isotope analysis of samples collected from LaBarge Field. Chemical compositions are normalized to 100%. Values reported in the table are Mol% and it is approximately equal to vol%. The $\delta^{13}\text{C}_{\text{CH}_4}$ and $\delta^{13}\text{C}_{\text{CO}_2}$ values are reported in permil (‰) w.r.t. to V-PDB and $\delta\text{D}_{\text{CH}_4}$ in permil (‰) w.r.t. to V-SMOW.

CHAPTER 4: Subsurface and Surface Structural Evaluation – Results 1, 2, and 3

PI: Dr. Erin Campbell-Stone, Department of Geology and Geophysics

Background

Tasks 4 and 5 focused on geological characterization of the surface and subsurface of the Moxa Arch. Researchers from these tasks analyzed seismic and well log data from the LaBarge Platform to provide the necessary foundation for the best possible reservoir characterization. Findings provide critical information about the shape and volume of potential targeted reservoirs, fault locations and offsets, and other information. The main results of Tasks 4 and 5 are 1) assessment of the Bighorn Dolomite as a potential storage zone, 2) characterization of overlying Devonian units as a confining zone, 3) identification of impermeable layers within the Triassic confining system through fluid inclusion volatile analysis, 4) subsurface structural interpretation through creation of east-west cross sections across the entire region and interpretation of 3-D seismic data from the central Moxa Arch, and 5) documentation of reservoir fractures from available data.

Results 1, 2, and 3 are summarized below. Two peer-reviewed academic papers follow that show methods, results, and conclusions of these three study areas in full detail. Results 4 and 5 are discussed in further detail in Chapter 5.

Executive Summary

The Moxa Arch is a geologic uplift that extends from northern Utah, north to the town of LaBarge, Wyoming, where it is covered by the eastern edge of the Wyoming fold-and-thrust belt. It is a gentle, asymmetrical anticline that formed during the late Cretaceous through early Eocene due to uplift along a basement-involved, west vergent thrust fault (Royse, 1993a; Becker et al., 2010). Possible storage zones in this uplift include the Mississippian Madison Limestone and the Ordovician Bighorn Dolomite. The confining zone between the Madison and Bighorn units is comprised of the Devonian units; the confining system that overlies both reservoirs and the entire Paleozoic section is comprised of key units within the Triassic section.

The Madison Limestone is a proven storage reservoir; for several years ExxonMobil has injected H₂S (as much as 65 MMCFD) and CO₂ (as much as 25 MMCFD) into the Madison Limestone at the Shute Creek Gas Plant. The Madison Limestone has been well-characterized by other researchers (e.g., Thyne et al., 2010).

Result 1

Our publication in *Rocky Mountain Geology* entitled “Stratigraphic evaluation of reservoir and seal in a natural CO₂ field: Lower Paleozoic, Moxa Arch, southwest Wyoming” (Lynds et al., 2010) summarizes the Ordovician Bighorn Dolomite CO₂ system overlain by the sealing Devonian Jefferson Formation. The Bighorn Dolomite is a thick (up to 120 m on the crest of the Moxa Arch) and laterally extensive dolostone found in all but southeastern Wyoming. The original depositional environment was a large carbonate ramp extending from southern Montana to northern Utah, and subsequent dolomitization occurred at least twice; soon after deposition and later after partial burial (Zenger, 1996). The dolomitization was selective resulting in patchy porosities and presumably permeabilities. Permeability data are not available for the Bighorn Dolomite on the Moxa Arch. Porosity values range from 0 to 15%.

Naturally occurring carbon dioxide volumes within the Bighorn Dolomite are distinctly different from the overlying Mississippian Madison Limestone storage system, with a CO₂ percentage of 84.7 within the Bighorn and 64.9 within the Madison (Stilwell, 1989). Independent pressure data helps to confirm our interpretation of two separate Paleozoic CO₂ reservoirs. Following this interpretation, the intervening Devonian Jefferson Formation must act to isolate the two reservoirs.

Result 2

The Jefferson Formation is composed of a series of interbedded siltstones, claystones, carbonates, and evaporites generally in the form of anhydrite. Wireline log correlations suggest the thinly bedded anhydrite zones are continuous enough to provide an adequate seal. ⁸⁷Sr/⁸⁶Sr isotopic analyses of anhydrite from several wells on the Moxa Arch provide the framework for interpreting the depositional environment. The Jefferson Formation appears to have been deposited as part of a large and very shallowly dipping continental shelf subject to high-frequency relative sea level fluctuations, resulting in evaporites deposited from a mixture of freshwater and seawater. This depositional model allows for the interpretation that the sealing facies within the Jefferson Formation are laterally continuous over tens to hundreds of kilometers.

Result 3

In cooperation with ExxonMobil we conducted a preliminary evaluation of the overall-confining system within the Greater Green River Basin, using a process of analyzing fluid inclusions. This technique, otherwise known as fluid inclusion volatile analysis, heats and crushes well cuttings in a vacuum. Gasses stored as fluid inclusions are released and recorded by a quadrupole mass spectrometer. This process assumes that all fluids (hydrocarbons or otherwise) that migrated through or were stored in the subsurface were captured as fluid inclusions. As published in our paper from the 2010 Greenhouse Gas Technology Conference, entitled “The Wyoming Carbon

Underground Storage Project: geologic characterization of the Moxa Arch and Rock Springs Uplift” (Campbell-Stone et. al., 2010), we have identified units above the Madison which show no indication of gas present now or in the past. Results indicate that the confining system operating above the Madison Limestone is the Triassic Dinwoody Formation. We are grateful for this collaborative effort with ExxonMobil, who provided the fluid inclusion analysis.

References

- Becker, T.P., McGroder, M.F., Rudolph, K., Hauge, T.A., and Fan, M., 2010, Paleogene influence of the Moxa arch on the architecture of the composite Darby-Hogsback-Prospect (DHP) thrust sheet near LaBarge, WY, U.S.A., American Association of Petroleum Geologists Annual Convention and Exhibition, New Orleans, LA, Abstracts, v. 19, p. 23.
- Campbell-Stone, E., Lynds, R. Frost, C., Becker, T.P., and Diem, B., 2010, The Wyoming carbon underground storage project: geologic characterization of the Moxa Arch and Rock Springs Uplift: Energy Procedia, in press.
- Lynds, R., Campbell-Stone, E., Becker, T., and Frost, C.D., 2010, Stratigraphic evaluation of reservoir and seal in a natural CO₂ field: Lower Paleozoic, Moxa Arch, southwest Wyoming, Rocky Mountain Geology, v. 45, no. 2, 113-132.
- Royse, F. Jr., 1993a, An overview of the geologic structure of the thrust belt in Wyoming, northern Utah, and eastern Idaho, Snoke, A.W., in Steidtmann, J.R., and Roberts, S.M., eds., Geology of Wyoming, The Geological Survey of Wyoming Memoir No. 5, v. 1: Laramie, Wyoming, Wyoming State Geological Survey, p. 273-311.
- Stilwell, D.P., 1989, CO₂ resources of the Moxa Arch and the Madison reservoir: Wyoming Geological Association Guidebook, 40th Annual Field Conference, Guidebook, p. 105-115.
- Thyne, G.D., Tomasso, M., Bywater-Reyes, S.V., Budd, D.A., and Reyes, B.M., 2010, characterization of porosity and permeability for CO₂ sequestration models on the Mississippian Madison Group, Moxa Arch-La Barge Platform, southwestern Wyoming, Rocky Mountain Geology, v. 45, n. 2, p. 133-150.
- Zenger, D.H., 1996, Dolomitization patterns in widespread “Bighorn Facies” (Upper Ordovician), Western Craton, USA: Carbonates and Evaporites, v. 11, p. 219-225.

Stratigraphic evaluation of reservoir and seal in a natural CO₂ field: Lower Paleozoic, Moxa Arch, southwest Wyoming

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ABSTRACT

The Moxa Arch in the Greater Green River Basin, southwestern Wyoming, hosts two potential reservoirs for CO₂ sequestration. The Bighorn Dolomite and Madison Limestone are interpreted to be independent reservoirs based on differing CO₂ compositions and production histories; the two reservoirs are separated by Devonian carbonates, siliciclastic rocks, and evaporites.

On the Moxa Arch, the Bighorn ranges in thickness from 67 to 120 m with porosities from 3 to 15 percent. The massive buff-colored Steamboat Point Member comprises the bulk of the subsurface Bighorn in southwest Wyoming. Mottled dolostone (light-colored patches with higher porosity and dark-colored patches with lower porosity) is very common and is presumably the result of preferential early dolomitization of bioturbation. Core study suggests that this factor affects gas saturation and storage in this extensive reservoir.

The Lower Member of the Jefferson Formation is the most probable seal within the Devonian stratigraphy. Strata of this member are interpreted to have been deposited in a shallow basin semi-isolated from the deeper marine environment to the west. ⁸⁷Sr/⁸⁶Sr isotopic analyses of anhydrite sampled from Moxa Arch well cuttings support the interpretation of a depositional environment exposed to a mixture of seawater and freshwater. High-frequency relative sea level fluctuations superimposed on a gently sloping shelf produced alternating layers of marine carbonates, peritidal siliciclastic rocks, and evaporites. The evaporites are interpreted to seal CO₂ in the Bighorn Dolomite from the overlying Madison Limestone. The Lower Paleozoic strata on the Moxa Arch provide an effective trap-reservoir-seal combination for naturally occurring CO₂ with potential applications to future studies at analogous locations in the central Rocky Mountain Region.

KEYWORDS: anhydrite, Bighorn Dolomite, Darby Formation, Devonian, Greater Green River Basin, Jefferson Formation, Moxa Arch, Ordovician, reservoir, seal, sequestration, strontium, Wyoming.

INTRODUCTION

All proposed sites for geologic sequestration of anthropogenic CO₂ should share three basic characteristics: (1) a geometric subsurface trap that contains the gas within a manageable area, (2) a reservoir with sufficient porosity and permeability, and (3) an effective and robust overlying seal that can sustain a buoyant gas column for an appropriate time period (i.e., greater than 10,000 years; Lindeberg, 2002). These characteristics also typify conventional hydrocarbon accumulations, which have been long-studied in the petroleum industry. Such accumulations are commonly in traps that have held buoyant columns of

gas, often for tens to hundreds of millions of years, demonstrating the feasibility of subsurface storage of carbon dioxide for geologically significant time periods.

Porosity and permeability are important factors for determining the storage capacity of the reservoir, its effectiveness as a reservoir, and the rate at which carbon dioxide can be put into the subsurface. Following Darcy's law, the permeability of the reservoir dictates the pressure required (and hence the energy required) to dispose of gas at a given rate. Capacity determination of a reservoir requires an understanding of variations in porosity and perme-

ability, which may compartmentalize a reservoir or create preferential pathways for flow. Depositional and post-depositional sedimentological features and structures need to be understood on a local and regional scale to properly determine the storage potential for CO₂.

The ability of the overlying, low-permeability sealing interval to hold a gas column is considered its sealing capacity (Downey, 1984). Assuming that the sealing interval is present over the entire extent of the trap, two independent factors determine capacity: mechanical strength and capillary entry pressure of the seal (e.g., Berg, 1975; Schowalter, 1979; Vavra et al., 1992; Gluyas and Swarbrick, 2004). The mechanical capacity of a seal is compromised when the buoyant pressure on the unit exceeds its opening mode tensile strength (Secor, 1965; Lorenz et al., 1991). Capillary seal capacity is related to the pore throat size of the grains that comprise the seal and the capillary entry pressure required to displace water in the pore throats (e.g., Li and Wardlaw, 1986). The pressure required to overcome the interfacial surface tension rises exponentially as the pore throat diameter decreases (Vavra et al., 1992). Evaporite deposits make extraordinarily good seals (in the absence of fractures), in large part because they effectively do not have any pore space, meaning that failure requires a column to exceed the mechanical strength of the evaporite.

This paper focuses on the characteristics of an Ordovician reservoir and the overlying Devonian seal in a subsurface structure that has acted as a natural reservoir for carbon dioxide. The purposes of this study are to document what little information is known about the Bighorn Dolomite and the Devonian strata on the Moxa Arch in southwestern Wyoming, to provide the background information for a modeling framework, and to encourage future research into analogous viable reservoirs for CO₂ sequestration.

GEOLOGIC SETTING

The Greater Green River Basin in southwestern Wyoming and northern Utah possesses several natural gas fields with high concentrations of carbon dioxide. The crest of the Moxa Arch, culminating at the LaBarge Platform near LaBarge, Wyoming (Fig. 1), supports many producing fields. At the LaBarge

Field over 100 trillion cubic feet of natural gas are stored, much of it in the Mississippian Madison Limestone and the Ordovician Bighorn Dolomite (Stilwell, 1989). Between these two reservoirs are Devonian deposits that are commonly called the “Darby Formation” in the hydrocarbon industry. Gas produced from the Bighorn Dolomite is composed of 84.7 percent CO₂, whereas gas from the Madison Limestone contains 64.9 percent CO₂ (Stilwell, 1989). Production histories combined with CO₂ gas composition indicates the Bighorn and Madison are likely separate reservoirs.

The Mississippian Madison Limestone has been the subject of extensive investigation (see Thyne et al., 2010), yet relatively little is known about the subsurface Bighorn Dolomite and the overlying Devonian strata on the Moxa Arch. This can be attributed in part to economics: the Madison Limestone is the only Paleozoic unit on the Moxa Arch from which natural gas has been produced. As a result, numerous wells have penetrated the Madison interval, but few extend below it.

The Lower Paleozoic history of western Wyoming is closely tied to eustatic sea level changes. The paleogeography during this extended time was generally a north–south-oriented shoreline separating source terrains to the east and depositional basins to the west. During early Cambrian time, subaerial erosion of Precambrian igneous and metamorphic rocks provided siliciclastic sediment to nearshore areas while thick successions of deep-water strata accumulated in what is now Utah and Idaho (Boyd, 1993). Middle to Upper Cambrian (and possibly Lower Ordovician; Tice et al., 2002) deposits accumulated during an overall cratonward transgression of facies, resulting in a vertical succession consisting of the siliciclastic coarse-grained Flathead Sandstone, overlain by shale with interbedded limestone of the Gros Ventre Formation, and the capping mud-rich Gallatin Limestone. A major unconformity separates these Cambrian to Lower Ordovician strata from the Upper Ordovician Bighorn Dolomite. The latter formation is part of the record of perhaps the largest transgression in the history of North America (Boyd, 1993). Intervals of subaerial exposure following deposition of the Bighorn Dolomite resulted in thinning and/or removal of that formation in southern and eastern Wyoming, and removal of all evidence of the Silurian from western Wyoming (i.e., the interval

Figure 1. Location map of study area showing Wyoming and surrounding states, with the Greater Green River Basin highlighted in gray. Insert shows location of Moxa Arch, eastern front of Sevier fold-and-thrust belt, and key wells, core, and mountain ranges mentioned in text. Abbreviations are as follows: Riley Ridge 8-24 (RR 8-24), Tip Top F14-13 (TT 14-13), Graphite 116 (G 116), Fontanelle II Unit 22-35 (FU 22-35), Keller Rubow 1 (KR 1), and Church Buttes Unit 19 (CB 19).

between the second-order Tippecanoe and Kaskaskia transgressions; Sloss, 1963).

Laterally discontinuous lenses of Lower Devonian calcareous dolostone and conglomerate record terrestrial and shallow marine deposition (Sandberg and Mapel, 1967). Subsequent Middle Devonian regression and erosion produced a surface capped by an Upper Devonian transgressive sequence of limestones, dolostones, siliciclastics, and evaporites (Jefferson Formation and Three Forks Formation;

Benson, 1966). The Late Devonian was a time of numerous and cyclical sea level fluctuations possibly controlled by Gondwanan glaciation (Isacson et al., 1999). The landscape was most likely a broad coastal area with a shallow sea, estuaries, lagoons, and a strong tidal influence. A major Mississippian transgression resulted in the greater than 300-m-thick Madison Limestone.

The Moxa Arch is a basement-involved anticline formed in the Late Cretaceous and Early Tertiary

during a two-phase growth process (Royse, 1993; Becker et al., 2010) that is generally associated with Sevier-Laramide orogenic deformation. This broad feature is 3.5 km high (Royse, 1993; Becker et al., 2010), with limbs dipping 0–5 degrees. It extends 200 km north-northwest from the Utah border to the eastern edge of the Wyoming fold-and-thrust belt (Fig. 1; Wach, 1977; Blackstone, 1990; Royse, 1993). Along much of its length, the Moxa Arch lacks emergent faults that displace any of the strata overlying the basement; the structure resembles a long, continuous, cylindrical, open fold (Wach, 1977; Royse, 1993). The LaBarge Platform represents the culmination of the Moxa Arch. The platform is located at its northern trace along its intersection with the thrust belt. The LaBarge Platform is characterized by a change in strike and the appearance of an emergent basement thrust fault along its southwestern edge (westward vergence) that displaces the overlying strata (Kraig et al., 1987; Royse, 1993).

BIGHORN DOLOMITE AS A CO₂ RESERVOIR

In subsurface reservoir characterization, an understanding of the degree of reservoir heterogeneity is directly proportional to the number of wells that penetrate the interval. Although there is a paucity of subsurface information about the Bighorn Dolomite on the Moxa Arch, the regional framework acquired from study of surrounding outcrops helps to constrain assumptions about the formation's age, extent, and stratal architecture.

Characteristics of the formation

The Bighorn Dolomite was deposited over a large portion of west-central North America as part of an extensive carbonate ramp (Wilson, 1975) that formed due to a major Late Ordovician (second-order Tippecanoe) transgression on the Laurentian cratonic shelf (Sloss, 1963; Boyd, 1993; Haq and Schutter, 2008). The Bighorn Dolomite crops out in southern Montana, far eastern Idaho, north-central Utah, and the northwestern half of Wyoming (Parker, 1950). The formation has a maximum thickness of 150 m (Teel, 1994) and is commonly divided into the basal Lander Sandstone Member, overlain by the Steamboat Point Member, the Leigh Member, and finally the Horseshoe Mountain Member, as defined by Goodwin (Fig. 2; 1964).

The Bighorn Dolomite is exposed throughout Wyoming as massive buff-colored cliffs. Although geologic study of this unit began as early as 1873, the first comprehensive investigation of the Bighorn Dolomite was by Darton (1906). Subsequent studies followed by Blackwelder (1913, 1918) and Tomlinson (1917). Many of these early papers, as well as several in the mid-1900s (e.g., Richards and Nieschmidt, 1957, 1961; Larimer, 1959), focused on the controversial age of the Bighorn Dolomite. Goodwin, in his 1964 summary of the literature, favored an age of Trenton-Maysville (late Middle Ordovician), but subsequent paleontological work (e.g., Sweet, 1979) has led to agreement on a Late Ordovician age for the formation. More recent work by

Zenger (1992) has concentrated on processes and controls on dolomitization of the formation.

According to Goodwin (1964), the basal Lander Sandstone Member ranges in thickness from 0 to 3 m, consists of medium- to coarse-grained sandstone with subrounded quartz grains, and can contain an abundance of shell fragments in isolated locations. This sandstone is primarily present in the Wind River Range near Lander, Wyoming, and grades into the overlying Steamboat Point Member. The Steamboat Point Member, 0 to 140 m thick, is a massive, mottled, buff-colored cliff-former (Fig. 3). It occurs from western to central Wyoming and

Figure 2. Generalized stratigraphic column showing members of the Ordovician Bighorn Dolomite in Wyoming, from Steamboat Point in the Bighorn Mountains. All lithologies are dolostone except for the Lander Sandstone. Modified from Zenger (1992).

throughout the eastern half of Montana and records a significant Late Ordovician transgression. The Leigh Member is 0 to 20 m thick, light to medium gray, very fine grained, “porcelaneous,” and breaks with sub-conchoidal fractures. The Leigh Member can be found from northern Wyoming into southern Montana but was erosionally removed in the southern Wind River and Bighorn Mountains (Goodwin, 1964). The capping Horseshoe Mountain Member is primarily massive mottled dolostone, interrupted by layers of thin-bedded dolostone; it crops out in northern Wyoming and southeastern Montana where it is up to 64 m thick in the northern Bighorn Mountains. Goodwin (1964) attributed the variation in distribution and thickness of the Horseshoe Mountain Member to pre-Devonian erosion.

These previous studies were based on detailed examination of outcrops primarily located in the Bighorn Mountains and the surrounding areas; the present work adds to the understanding of the Bighorn Dolomite through subsurface well log and core analysis.

Subsurface observations from the Moxa Arch and vicinity

Subsurface log data from the Moxa Arch show the Bighorn Dolomite thinning from greater than 120 m on the northern tip of the Moxa Arch to 67 m near the Wyoming–Utah border (Fig. 4). The thinning is believed to be the result of post-Ordovician erosion (Sloss, 1963; Goodwin, 1964). The Bighorn Dolomite is absent within the Uinta Uplift, located

in northern Utah and Colorado at the southern tip of the Moxa Arch (Rowley et al., 1985), where the Mississippian Madison Limestone lies disconformably on Cambrian strata. Log interpretations suggest the Steamboat Point Member comprises most of the Bighorn in the subsurface, however up to 21 m of an overlying less massive member may also be present (most likely the Leigh Member).

Cores are rare through the Lower Paleozoic section, yet one partial core of the Steamboat Point Member was available for viewing from the northern Moxa Arch (see Fig. 1 for location). This core, nearly 100 percent dolostone, shows three distinct textures. The most common texture, comprising as much as 85 percent of the available core, is the characteristic mottled dolostone (Fig. 5A). This texture has been described in outcrops by numerous authors, and Zenger (1996) most recently attributed it to preferential early dolomitization of *Thalassinoides*-like burrows. The mottled texture involves noticeable porosity contrasts (over several centimeters). Relatively coarse-grained light tan dolostone has vuggy porosity, whereas vugs are rare in the fine-grained dark tan to brown dolostone. The second texture is similarly mottled but on a smaller scale (mottles less than one centimeter long) and is most likely also the result of preferential dolomitization of pre-existing burrows (Fig. 5B). This texture comprises approximately 5 percent of the core and may result in less of a porosity contrast because the light and dark texture (porosity) variations occur on scales less than 1 cm and are often interconnected. The third texture is a dolomitic mudstone (Fig. 5C) that is medium brown to gray

Figure 3. Photograph of Steamboat Point Member of Bighorn Dolomite taken in Sinks Canyon, in the Wind River Range, near Lander, Wyoming, approximately 150 km northeast of the Moxa Arch. The Steamboat Point Member (black arrow) is 50 m thick.

Figure 4. Isopach map of the Bighorn Dolomite in Wyoming. Circles indicate thickness of Bighorn Dolomite as interpreted from well logs; the Greater Green River Basin is highlighted in gray; the front of the Sevier fold-and-thrust belt, Moxa Arch, and Rock Springs Uplift are represented with map symbols (see Fig. 1). Modified from Peterson (1989).

and comprises 10 percent of the core. It commonly includes thin wispy stylolites that are not well developed and are discontinuous laterally through the core. This dolomitic mudstone does not display visible porosity and very rarely contain vugs.

Reservoir characteristics

Although only visual inspection of the Bighorn Dolomite core was possible, it is clear that porosity and permeability, essential reservoir qualities, are affected by heterogeneities at a range of scales. In hand sample, there are centimeter-scale porosity variations probably resulting from the dolomitization process and subsequent deformation. Compaction produced a complex network of mutually cross-cutting stylolites, and deformation and change in stress resulted in the formation of fractures. Preferential fluid pathways and baffles and barriers to flow were formed by these permeability variations, suggesting reservoir heterogeneity at a multitude of scales.

Heterogeneities within the Bighorn Dolomite can be subdivided into three categories: structural, compaction-related, and lithologic. Structural het-

erogeneities are fractures and faults (Fig. 6A), which can enhance or hinder fluid migration within a reservoir, depending on the nature of the structural heterogeneity and the type of fill. In the core, fracture apertures ranged from less than 0.1 to 0.5 mm, and the fractures were variably unfilled or filled with calcite. Compaction resulted in the formation of stylolites, which are pressure-solution seams along which rock is dissolved, leaving an insoluble residue at the interface. The residue can be an impermeable barrier and, in the case of Figure 6B, creates a visible break between higher and lower porosity zones. Lithologic heterogeneities include variations in texture (Fig. 5) and in composition, such as the difference between a low-porosity dolomite mudstone and a higher-porosity mottled dolostone. Lithologic heterogeneities may be the result of stratigraphic variation over tens to thousands of meters, and encompass various facies and lithologies that are preserved during basin filling or subsequent diagenesis. As documented regionally, all four members of the Bighorn Dolomite display lithologic heterogeneities with varying amounts of dolomitization within and between members and locations. Structural, compaction, and lithologic heterogeneities combine to create internal baffles within the Bighorn Dolomite, complicating its evaluation as a reservoir.

JEFFERSON FORMATION AS A SEAL

More difficult than identification of a potential porous and permeable reservoir unit in the subsurface is assessment of the effectiveness of an overlying low permeability sealing unit. The seal must both hold a buoyant column and be laterally continuous across the trap.

Devonian stratigraphy in southwest Wyoming

Devonian strata in the subsurface of southwestern Wyoming have been the subject of unresolved discussion for several decades, most likely due to the scarcity of subsurface data. The Devonian section in the subsurface of the Greater Green River Basin is referred to as the "Darby Formation," as coined by Blackwelder (1918). The type locality of the Darby Formation is disputed (Love, 1969), and the naming scheme for Devonian formations/members in the subsurface is not clear. Original work by Peale (1893)

Figure 5. Textures observed in core (see Fig. 1 for location) from Steamboat Point Member of the Bighorn Dolomite. **A**, Mottled (bioturbated) dolostone. **B**, Small-scale mottled (bioturbated) dolostone. **C**, Dolomite mudstone.

subdivided the Devonian strata in southwestern Montana into the Jefferson Formation (lower) and the Three Forks Formation (upper). Subsequent studies proceeded to subdivide these formations into a variety of members based on studies at differing locations throughout Montana, Wyoming, Idaho, and Utah (e.g., Emmons and Calkins, 1913; Sandberg, 1962, 1965).

The most comprehensive study of the Devonian strata in western Wyoming was first published in a thesis by Benson (1965) and in his follow-up paper (Benson, 1966). Benson (1965, 1966) subdivided the Devonian section in western Wyoming into the Jefferson Formation and the overlying Three Forks Formation (Fig. 7). The Jefferson Formation

can further be subdivided into the unnamed Lower Member, which is a series of interbedded limestones, dolomites, evaporites, and clastics approximately 25 to 150 m thick, and the Birdbear Member, a distinctive massive and mottled buff-colored cliff-forming dolostone. Birdbear outcrops range in thickness from 18 to 35 m and are erosionally truncated along a north-south trend from the west side of the Big Horn Basin to the western Wind River Mountains and into the Green River Basin (Benson, 1966; Sandberg, 1965). Erosional truncation, evidence for subaerial exposure, and basal clastic beds in the Three Forks Formation (Benson, 1966) suggest sea level regression between deposition of the Jefferson Formation and the overlying Three Forks

Figure 6. Bighorn Dolomite core photograph showing structural and compaction heterogeneities. **A**, Small calcite-filled fracture with mm-scale offset (arrow). **B**, Well-developed stylolite near base of core with high porosity zone above stylolite and low porosity below stylolite.

Formation. There are few constraints on the age of the Jefferson Formation. Laird (1947) used faunal correlation from Montana to Nevada to New York

to propose a Late Devonian age. Benson (1966) suggested the Jefferson Formation is Frasnian (385.3 to 374.5 Ma), and Johnson et al. (1985) used conodont zonal sequences to place most Jefferson deposition during the Frasnian. More recent work by Grader and Dehler (1999) and Grader et al. (2009) correlated Frasnian strata in east-central Idaho with the Jefferson Formation in eastern Idaho and southwestern Montana (Fig. 7).

The Three Forks Formation, which extends from Montana to east-central Idaho and western Wyoming, comprises thick (up to 30 m) evaporites and solution breccias interbedded with carbonates (limestones and dolostones) and shales (Rau, 1962; Benson, 1966). Several members have been described within the Three Forks Formation at various locations (i.e., Logan Gulch Member, Trident Member, Sappington Member, etc.). For simplicity, and because these members were defined far from western Wyoming and are difficult to correlate to the subsurface record, we use the term “Three Forks Formation” without distinguishing members. The Three Forks is generally considered Famennian from detailed stratigraphic correlations and ammonite zones (Gutschick et al., 1962; Sandberg, 1963, 1965).

The Jefferson and Three Forks Formations are overlain in places by what Sandberg (1963) termed the dark shale unit. The dark shale unit is dark gray carbonaceous marine shale and mudstone, interbedded with light brown silty dolomite (Benson, 1966). The unit is up to 25 m thick in northwestern Wyoming and contains conodonts of latest Devonian age (Sandberg and Klapper, 1967). The dark shale unit is interpreted as lying above a regional unconformity and is associated with deposition of the overlying Mississippian Madison Limestone.

As noted above, the term “Darby Formation” is commonly applied to the entire Devonian section. Benson (1966) correlated the Darby Formation with the Lower Member of the Jefferson Formation and suggested using “Darby Formation” only when the Birdbear Member of the Jefferson Formation and the Three Forks Formation are absent. Following this reasoning, we will not use the term “Darby Formation” for the subsurface Devonian strata in western Wyoming, because we consider the Birdbear Member and the Three Forks Formation to be recognizable there.

Figure 7. Devonian and Lower Mississippian stratigraphic terminology, modified from Benson (1966) with additions from Grader and Dehler (1999). Ages (Ma, at left) from the International Stratigraphic Chart (2009).

Surface and subsurface observations

We created a measured section for the interval between the Bighorn Dolomite and the Madison Limestone to understand better the log signature of the Devonian strata in the Greater Green River Basin. The most complete accessible section is on the northeast side of Fred's Mountain near Grand Targhee Ski Resort, Wyoming (base at longitude -110.9097 W, latitude 43.7839 N; Fig. 8).

At this location, the entire Devonian section is 100 m thick (Fig. 8). The Lower Member of the Jefferson Formation forms a slope with thin ledges 30 cm to 3 m thick. The ledges are resistant dark to medium brown, sucrosic-textured, thin-bedded dolostone, or light brown to gray brecciated dolostone and limestone. The brecciated units are interpreted as the result of evaporite solution collapse and have also been documented in east-central Idaho (Grader et al., 2009). Minor chert

nodules and vugs are present, as are rare recognizable gastropods, echinoderm plates, and peloids. Interbedded with the dolostones and minor limestones are thin (30 cm or less) beds of non-resistant detrital siliclastic sandstone, siltstone, and claystone. These beds are primarily composed of very fine-grained to fine-grained, well-rounded and well-sorted, frosted quartz grains. The detrital beds are recessive and poorly exposed on the slope of the Lower Member. There is a 3.4-m-thick dolomitized bioturbated wackestone in the upper quarter of the Lower Member of the Jefferson Formation. Most of the Birdbear Member forms a covered slope, but the top 6 m is a resistant, massive, and heavily bioturbated cliff-forming dolostone. The Three Forks Formation is entirely covered at this location. The overlying 3-m-thick dark shale unit is recognizable by its dark gray color and distinctive *Zoophycos* trace fossils.

To complement the outcrop study, we were able to locate (at the United States Geological Survey (USGS) Core Research Center in Lakewood, Colorado) Devonian cuttings from four wells on the Moxa Arch and one complete Devonian core from the Rock Springs Uplift, 40 km east of the Moxa Arch. Analysis of the cuttings indicate that the primary lithologies include dolostone, limestone, sandstone, siltstone, claystone, and occasional coal fragments, micas, and pyrite. Textures are not apparent from the cuttings. The core is from the 4-UPRR-11-19-104 well (longitude -109.105 W, latitude 41.64011 N; Fig. 9), and the Devonian section in

Figure 8. Measured section through the Jefferson and Three Forks Formations, measured at outcrops in northwest Wyoming near Grand Targhee Ski Resort (base at longitude -110.9097 W, latitude 43.7839 N).

this core is 37 m thick (Fig. 9). The 4-UPRR-11-19-104 core is interesting because the primary lithology is sandstone with very fine-grained to medium-grained, well-rounded and well-sorted, frosted quartz grains that are distributed fairly evenly throughout the core. In addition, there are two brecciated intervals located midway and at the top of the core, suggesting possible surface exposure. The Devonian in this core has been called the Darby Formation, but as previously mentioned we will assign it to the Lower Member of the Jefferson Formation.

Correlating the Devonian strata in the subsurface is challenging. Only a few wells have been logged in the Devonian in the Greater Green River Basin, and there are no marker log signatures, because the detrital material, argillaceous mudstones, and carbonates of the Lower Jefferson Formation are interbedded over centimeters to meters. Furthermore, since detailed age control is not available in the subsurface, interpreting the Lower Jefferson Formation in a sequence stratigraphic context is nearly impossible.

Figure 10 is a north-south cross section along the crest of the Moxa Arch of the complete Devonian section. Lithologic correlation of the Lower Jefferson interval points to a recurring series of anhydrite beds, as evidenced by low gamma and high density

Figure 9. Lower Member of the Jefferson Formation core correlated with gamma ray log from the 4-UPRR-11-19-104 well, located on the Rock Springs Uplift (see inset map). Birdbear Member of Jefferson Formation and Three Forks were removed by pre-Mississippian erosion. A clastic horizontal scale was chosen for the core description because of the profusion of well-rounded quartz grains.

signatures. Although log correlation suggests some of these anhydrites may be continuous between wells, their minimal thickness (0.3 to 1.2 m) allows other interpretations. These anhydrite layers are significant because anhydrite may be the most common reservoir seal worldwide (Hangx et al., 2010).

Anhydrite Sr isotopic analysis

To determine if the anhydrite zones could be correlated from well to well, we identified several thin anhydrite beds from the logs and sampled anhydrite from Lower Jefferson Formation well cuttings (see Fig. 1 for geographic location of wells). Our intent was to use $^{87}\text{Sr}/^{86}\text{Sr}$ isotopic ratios as a possible correlation tool. If the anhydrite crystallized on broad and shallow tidal flats from the evaporation of seawater, then the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of anhydrite from equivalent stratigraphic levels should be identical. In addition, the Sr isotopic ratio should follow the Frasnian (385.3 to 374.5 Ma) seawater curve (e.g., Denison et al., 1997), which is not static throughout Frasnian time.

Laboratory methods

Anhydrite cuttings, averaged over a 10-ft (3-m) interval, were handpicked from cuttings stored at the USGS Core Research Center and dissolved in ultra-pure

Figure 10. Correlation of Devonian section in five wells from north to south on the Moxa Arch (see Fig. 1 for locations). Red indicates anhydrite layers, depths are measured in feet, and log values increase to the right. Note the datum is a lithostratigraphic correlation at the base of the Birdbear Member.

water. One ml of solute was dried and redissolved in dilute nitric acid. Strontium was isolated using Teflon columns filled with Eichrom® Sr-Spec resin. The strontium isotopic composition was determined by thermal ionization mass spectrometry at the University of Wyoming. All analyses were normalized to an $^{86}\text{Sr}/^{88}\text{Sr}$ ratio value of 0.1194. Analytical blanks are less than 0.2 ng Sr. Six analyses of NBS 987 strontium standard measured during the course of these analyses gave an average value of $^{87}\text{Sr}/^{86}\text{Sr} = 0.71026 \pm 0.00002$ (2 standard deviations), identical to a long-term average of 0.71026 ± 0.00002 (2 standard deviations) based upon 76 analyses of the standard. Values are reported relative to modern seawater, defined as:

$$\Delta_{\text{sw}} = (^{87}\text{Sr}/^{86}\text{Sr}_{\text{sample}} - ^{87}\text{Sr}/^{86}\text{Sr}_{\text{modern seawater}}) \times 10^5 \quad (1)$$

where the $^{87}\text{Sr}/^{86}\text{Sr}$ of modern seawater is taken to be 0.709173 (McArthur, 1995).

Sr isotopic results

Sr isotopic results for 29 samples of anhydrite are reported on Table 1. Twenty-seven samples were taken from the Graphite 116, Fontanelle II Unit 22-35, Keller Rubow 1, and Church Buttes 19 wells on the Moxa Arch (see Fig. 1 for location). Two additional samples, interpreted as secondary anhydrite that fills fractures, are from the 4-UPRR-11-19-104 core on the Rock Springs Uplift to the east (see Fig. 9 for location). Sr isotopic composition of most samples from the Moxa Arch wells are between $^{87}\text{Sr}/^{86}\text{Sr}$ of 0.70822 and 0.70905 ($\Delta_{\text{sw}} = -69.3$ to -12.3), but three are higher, ranging from 0.70931 to 0.71081 ($\Delta_{\text{sw}} = 13.4$ to 164.2). Both samples from the Rock Springs Uplift are among the most radiogenic: 0.70982 and 0.71083 ($\Delta_{\text{sw}} = 64.3$ and 165.3). All are higher than the estimates for contemporary Frasnian seawater (0.70795 to 0.70815; Denison et al., 1997; John et al., 2008).

Sr isotopic data discussion

All Sr isotopic ratios for our anhydrite samples are more radiogenic than Frasnian seawater values. This suggests that if the anhydrite is primary, it was not formed in an open marine environment, but instead was precipitated from a water body that was partially or totally isolated from the ocean. Denison et al. (1998) applied the term salina to such a body of water, which can be dominated by marine water, by continental runoff, or a combination of the two. If

Table 1. Sr isotopic data for anhydrite from well cuttings of Devonian rocks from the Moxa Arch and Rock Springs Uplift.

Top Depth (ft)	$^{87}\text{Sr}/^{86}\text{Sr}$	internal precision (% std. error)	Δ_{sw}
Keller Rubow 1			
17200	0.70848	0.0017	-69.27
17220	0.70845	0.0015	-72.03
17230	0.70877	0.0013	-39.87
17250	0.70823	0.0016	-94.61
17260	0.70861	0.0014	-56.57
17270	0.70879	0.0015	-38.44
17280	0.70931	0.0016	13.44
17290	0.71081	0.0014	164.18
17300	0.70882	0.0017	-35.52
Graphite 116			
17260	0.70868	0.0019	-49.32
17270	0.70855	0.0017	-61.85
17280	0.70905	0.0016	-12.3
17290	0.70863	0.0016	-54.69
Fontanelle II Unit 22-35			
15680	0.70874	0.0038	-43.01
15690	0.70815	0.0016	-102.54
15710	0.70856	0.0016	-61.47
15720	0.70943	0.0020	25.24
15730	0.70814	0.0014	-102.91
15740	0.70869	0.0016	-48.79
15760	0.70869	0.0026	-48.46
15770	0.70857	0.0017	-60.21
15780	0.71078	0.0014	160.85
15790	0.70839	0.0016	-78.55
15800	0.70852	0.0016	-65.23
15810	0.70841	0.0017	-76.24
15820	0.70880	0.0017	-37.65
Church Buttes 19			
19180	0.70868	0.0029	-49.79
4-UPRR-11-19-104			
7902	0.71083	0.0016	165.26
7921	0.70982	0.0013	64.27

Note: See Fig. 1 for Moxa Arch and Rock Springs Uplift locations. All depths are in measured depth.

the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio and Sr concentration of the seawater and the continental runoff are known, then the mass

balance of a mixture of marine and continental water may be determined. The Sr isotopic composition of seawater has been determined from analyses of marine carbonates and, as noted above, the Frasnian seawater values varied from 0.70795 (Δ_{sw} of -122) in Early Frasnian, to a high of 0.70815 (Δ_{sw} of -102) in Middle Frasnian. The concentration of Sr in seawater is approximately 8 ppm, much greater than in average river water (~60 ppb; Denison et al., 1998). Modern major river water has Δ_{sw} of 100 to 300 (Palmer and Edmond, 1992). However, the isotopic ratio and Sr concentration of individual rivers varies widely and are very much dependent upon the geology and geography of the drainage basin. Thus we do not know with any certainty the Sr isotopic composition and Sr concentration of the rivers that may have supplied a Devonian salina in present-day western Wyoming. A widespread unconformity at the base of the Paleozoic section in the Uinta Mountains, Wind River Range, and throughout the Laramide uplifts of Wyoming suggests that Precambrian rocks were a source for terrigenous input. Exposed Cambro-Ordovician carbonates are another potential source of non-marine Sr to the Late Devonian salinas. As a result, we can make only general estimates of the proportions of marine and meteoric water in the water body from which the anhydrite precipitated.

For the purpose of illustration we calculate the fraction of marine water in the salina using three different estimates of the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of the continental end member: one based upon modern rivers draining Paleozoic and older rocks on the margins of the Greater Green River Basin, a second estimate based upon modern average river Sr isotopic composition, and a third using the radiogenic $^{87}\text{Sr}/^{86}\text{Sr}$ ratios of the secondary anhydrite derived from the 4-UPRR-11-19-104 to approximate the continental end member. These three approaches give overlapping estimates of the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio for Devonian continental runoff in the vicinity of the present-day Green River Basin. First, modern water sampled in the Greater Green River Basin near the headwaters of the Green, Big Sandy, and Sweetwater Rivers where they have traversed mainly Archean and Paleozoic rocks have $^{87}\text{Sr}/^{86}\text{Sr}$ ratios of 0.7212 to 0.7157 (Fenner and Frost, unpublished data). Assuming these rocks also supplied Sr to meteoric water in Frasnian time and correcting for radiogenic ingrowth of ^{87}Sr by the decay of ^{87}Rb in the rocks since Frasnian time, the Δ_{sw} of Devonian mete-

oric water may have been around 100 to 400. Second, for modern rivers, mean Δ_{sw} is estimated at 100 to 300. Third, if the fluids from which the secondary anhydrite in the 4-UPRR-11-19-104 core (Rock Springs Uplift) precipitated represent an estimate of local continental meteoric water (Δ_{sw} of 64 to 165), then those Sr isotopic ratios may also be reasonable estimates of the continental end member. Accordingly, we performed mixing calculations using continental end members Δ_{sw} of 100, 300, and 400.

We used two different estimates of Sr concentration of continental runoff (60 ppb and 300 ppb) to represent the mean Sr concentrations of 60 ppb of modern rivers and a higher Sr content typical of arid river water (Denison et al., 1998). The results of the calculations are displayed in Table 2. The calculations were done using the two-component mixing model of Faure (1986). These calculations suggest that if the concentration of Sr in the continental water was 60 ppb, then the water body from which the anhydrite precipitated was dominated by the continental component; the fraction of marine water is less than 10 percent for all but the three anhydrites with the lowest Sr isotopic compositions, which are closest to contemporary seawater values. If the concentration of Sr in the continental end member was higher (300 ppb), then the proportion of marine water is higher, up to 36 percent for most samples and higher for the three anhydrite samples with the lowest Δ_{sw} (Fig. 11). If these anhydrites are secondary, then they precipitated from a different fluid than one that produced the higher ratio group.

The three samples from the Moxa Arch wells with higher Δ_{sw} and the two Rock Springs Uplift samples that are clearly secondary fracture fills precipitated from fluids with Sr isotopic characteristics expected of continental meteoric waters. It is possible that the three Moxa Arch samples are primary precipitates that formed when the salina was supplied entirely by continental runoff, or they could be secondary. In either case, the depositional environment was not entirely marine and exhibits a strong contribution of meteoric water, probably sourced from the adjacent continent.

Seal characteristics

Lithology alone indicates that depositional environments of the Jefferson Formation include marine (carbonates), marginal marine (carbonates, evapo-

Table 2. Mass balance calculations of proportions of seawater and continental runoff in Frasnian (Upper Devonian) salinas.

Top Depth (ft)	Anhydrite Δ_{sw}	fraction marine for various river Δ_{sw} , 60 ppb Sr			fraction marine for various river Δ_{sw} , 300 ppb Sr		
		$\Delta_{sw} =$	$\Delta_{sw} =$	$\Delta_{sw} =$	$\Delta_{sw} =$	$\Delta_{sw} =$	$\Delta_{sw} =$
		100	300	400	100	300	400
Keller Rubow 1							
17200	-69.3	0.03	0.06	0.08	0.13	0.25	0.30
17220	-72.0	0.03	0.07	0.09	0.15	0.27	0.32
17230	-39.9	0.01	0.04	0.04	0.07	0.15	0.19
17250	-94.6	0.09	0.16	0.19	0.32	0.49	0.55
17260	-56.6	0.02	0.05	0.06	0.10	0.20	0.24
17270	-38.4	0.01	0.03	0.04	0.07	0.15	0.19
17280	13.4	0.01	0.02	0.02	0.03	0.08	0.11
17290	164.2	0.00	0.00	0.01	-0.01	0.02	0.03
17300	-35.5	0.01	0.03	0.04	0.06	0.14	0.18
Graphite 116							
17260	-49.3	0.02	0.04	0.05	0.08	0.18	0.22
17270	-61.9	0.02	0.05	0.07	0.11	0.22	0.26
17280	-12.3	0.01	0.02	0.03	0.04	0.11	0.14
17290	-54.7	0.02	0.05	0.06	0.09	0.19	0.24
Fontanelle II Unit 22-35							
15680	-43.0	0.02	0.04	0.05	0.07	0.16	0.20
15690	-102.5	0.17	0.29	0.34	0.50	0.67	0.72
15710	-61.5	0.02	0.05	0.07	0.11	0.22	0.26
15720	25.2	0.00	0.02	0.02	0.02	0.07	0.09
15730	-102.9	0.18	0.30	0.35	0.52	0.68	0.73
15740	-48.8	0.02	0.04	0.05	0.08	0.18	0.22
15760	-48.5	0.02	0.04	0.05	0.08	0.18	0.21
15770	-60.2	0.02	0.05	0.06	0.11	0.21	0.26
15780	160.8	0.00	0.00	0.01	-0.01	0.02	0.03
15790	-78.6	0.04	0.08	0.10	0.18	0.31	0.36
15800	-65.2	0.03	0.06	0.07	0.12	0.23	0.28
15810	-76.2	0.04	0.08	0.10	0.16	0.29	0.35
15820	-37.7	0.01	0.03	0.04	0.07	0.15	0.18
Church Buttes 19							
19180	-49.8	0.02	0.04	0.05	0.09	0.18	0.12
4-UPRR-11-19-104							
7902	165.3	0.00	0.00	0.01	-0.01	0.02	0.12
7921	64.3	0.00	0.01	0.01	0.01	0.05	0.12

Note: For all calculations, the Δ_{sw} and Sr concentration of Frasnian seawater is assumed to be -110 and 8 ppm, respectively. All depths are in measured depth.

Figure 11. Number line plotting the Δ_{sw} of the end member seawater and three estimates of continental runoff used in binary mixing calculations (solid diamond symbols) and the Δ_{sw} of analyzed Frasnian anhydrite samples (open circle symbols). The maximum calculated percentage of the marine component, which is obtained using the most radiogenic Δ_{sw} of 400, is given for selected groups of anhydrite samples. The percentages in regular font are based on a continental Sr concentration of 60 ppb and the percentages in italics are based on a continental Sr concentration of 300 ppb. Because seawater has much higher Sr concentration than continental runoff, a small proportion of marine water in the salina yields mixtures with Δ_{sw} only slightly higher than the seawater value. Data from Table 2.

rites, clastics), and perhaps even periods of subaerial exposure (evaporites, breccias). The 4-UPRR-11-19-104 core from the Rock Springs Uplift (Fig. 9) is interpreted as a shallowing-upward sequence capped by a series of 14 peritidal coarsening-upward units. The abundance of cross-bedding with well-rounded and frosted quartz grains implies that this core represents parts of the Lower Jefferson Formation that were proximal to the source. Similar frosted grains are described in Upper Devonian sections as far away as east-central Idaho (Grader and Dehler, 1999) and southeast Idaho (Beus, 1968). If these grains were eolian in origin (marine quartz overgrowth is a second interpretation), then either large regional sandstorms carried sediment far into the basin, near-shore dunes migrated with the shoreline during sea level fluctuations, or eolian material was reworked by rivers and tides. The relatively rare occurrence of clastic units in our measured section and in Benson's (1966) description from outcrops farther west (Idaho and Montana) suggests that western Wyoming and eastern Idaho are more distal (west) to the source than the preserved 4-UPRR-11-19-104 core on the Rock Springs Uplift (east).

We know from limited well logs and well cuttings from the Moxa Arch that thin anhydrite layers of questionable continuity are present. The anhydrite is interbedded within a series of thin dolostones, mudstones, and siltstones. These most likely reflect intertidal to possibly supratidal depositional environments, occasionally interrupted by carbonate deposition during shallow flooding. Results from Sr isotopic analysis indicate that anhydrite precipitated

from a mixture of marine and continental waters, which leads us to conclude that the Lower Jefferson Formation in western Wyoming records the approximate position of the Frasnian shoreline. The coastal area was presumably broad with a very gentle slope toward the shelf and basin farther west.

The Sr isotopic ratios are not perfectly uniform either from well to well or vertically within wells. This suggests that the anhydrite layers did not form from a single, well-mixed water body. Perhaps there were several evaporative salinas that were spatially and temporally distinct. In this case, the waters in the salinas did not mix but contained water of similar Sr isotopic composition.

Alternatively, and perhaps more likely, the anhydrites at any one stratigraphic level may have been continuous. In this possibility, the salina would have received slightly varying amounts of meteoric water over time. We prefer this option because it is supported by well log interpretations. Logs from five wells on the Moxa Arch suggest a minimum of 130 km of correlatable dolostone and detrital units (Fig. 10). The anhydrites correlate over a maximum 60 km, as constrained by the few available well logs. This interpretation fits well with a broad shallow coastal area and high tidal influence (as noted in the 4-UPRR-11-19-104 core farther east).

We know independently from CO_2 concentrations on the Moxa Arch that the Jefferson and/or Three Forks Formations must seal the underlying Bighorn Dolomite reservoir from the overlying Madison Limestone. Our task, then, is to understand what makes the Devonian formations a successful seal.

Hangx et al. (2010) studied the mechanical behavior of anhydrite as a seal and found CO₂ penetration rates of approximately 3 m per 10,000 years. With this penetration rate, we must assume that the anhydrites in the Lower Jefferson Formation are far thicker than what can be determined from a gamma ray or neutron density log, and the combined effect of numerous thin but stacked anhydrite layers interbedded with lime mudstones and thin shales can seal a reservoir, or the evaporites in the overlying Three Forks Formation significantly contribute to the overall Devonian seal.

Based on one unpublished image log from the Jefferson Formation on the northern Moxa Arch and the amount of anhydrite recovered from cuttings where anhydrite was not interpreted from the density log signature, we believe there may be more and/or thicker anhydrite layers than originally noted. This stacked succession of laterally continuous (on the order of 50 to 100 km) evaporites may be the seal to the Bighorn Dolomite CO₂ reservoir.

CONCLUSIONS

Potential sites for long-term geologic storage of carbon dioxide should have a well-defined and well-understood trap, reservoir, and seal. The Lower Paleozoic rocks in the western Greater Green River Basin provide a natural CO₂ storage area because they possess all three attributes. The trap, the Moxa Arch, is a gently folded, doubly plunging anticline. The reservoir (Steamboat Point Member of the Upper Ordovician Bighorn Dolomite) has adequate porosity and permeability to hold large amounts of naturally occurring CO₂. The Lower Member of the Upper Devonian Jefferson Formation, perhaps in combination with the overlying Three Forks Formation, seals the CO₂ from the overlying Mississippian Madison Limestone.

Sr isotopic analyses of the anhydrite layers within the Jefferson Formation yield ⁸⁷Sr/⁸⁶Sr ratios mainly between 0.70822 and 0.70905, suggesting anhydrite formed in a salina environment and recorded a mixed seawater and meteoric water signature. This isotopic composition implies that, at least in the part of the section in which anhydrites are present, the Lower Jefferson Formation records the Frasnian paleo-shoreline. A few higher Sr isotopic ratios from wells on the Moxa Arch and from farther away on the Rock Springs Uplift most likely identify secondary fracture

fills precipitated from a more radiogenic fluid. Based on log interpretations and ⁸⁷Sr/⁸⁶Sr ratios, we interpret that the anhydrite layers noted in the few deep wells on the Moxa Arch are continuous on scales up to 100 km. These stacked and continuous anhydrite layers in the Lower Member of the Jefferson Formation probably form the CO₂ seal between the Bighorn Dolomite and Madison Limestone.

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REFERENCES CITED

- Becker, T. P., McGroder, M. F., Rudolph, K., Hauge, T. A., and Fan, M., 2010, Paleogene influence of the Moxa Arch

- on the architecture of the composite Darby-Hogsback Prospect (DHP) thrust sheet near LaBarge, WY, U.S.A.: American Association of Petroleum Geologists Annual Convention and Exhibition, New Orleans, Louisiana, Abstracts, v. 19, p. 23.
- Benson, A. L., 1965, The Devonian system in western Wyoming and adjacent areas [Ph.D. thesis]: Columbus, Ohio State University, 141 p.
- _____, 1966, Devonian stratigraphy of western Wyoming and adjacent areas: American Association of Petroleum Geologists Bulletin, v. 50, p. 2566–2603.
- Berg, R. R., 1975, Capillary pressure in stratigraphic traps: American Association of Petroleum Geologists Bulletin, v. 59, p. 939–956.
- Beus, S. S., 1968, Paleozoic stratigraphy of Samaria Mountain, Idaho-Utah: American Association of Petroleum Geologists Bulletin, v. 52, p. 782–808.
- Blackstone, D. L., Jr., 1990, Precambrian basement map of Wyoming: outcrop and structural configuration: Geological Survey of Wyoming Map Series 27 (revised version), scale 1:1,000,000, 1 sheet.
- Blackwelder, E., 1913, Origin of the Bighorn Dolomite of Wyoming: Geological Society of America Bulletin, v. 24, p. 607–624.
- Blackwelder, E., 1918, New geological formations in western Wyoming: Journal of the Washington Academy of Sciences, v. 13, p. 417–426.
- Boyd, D. W., 1993, Paleozoic history of Wyoming, in Snoke, A. W., Steidtmann, J. R., and Roberts, S. M., eds., Geology of Wyoming: Laramie, Wyoming, The Geological Survey of Wyoming Memoir No. 5, v. 1, p. 164–187.
- Darton, N. H., 1906, Geology of the Bighorn Mountains: U.S. Geological Survey Professional Paper, P0051, 129 p.
- Denison, R. E., Koepnick, R. B., Burke, W. H., Hetherington, E. A., and Fletcher, A., 1997, Construction of the Silurian and Devonian seawater $^{87}\text{Sr}/^{86}\text{Sr}$ curve: Chemical Geology, v. 140, p. 109–121.
- Denison, R. E., Kirkland, D. W., and Evans, R., 1998, Using strontium isotopes to determine the age and origin of gypsum and anhydrite beds: Journal of Geology, v. 106, p. 1–17.
- Downey, M. W., 1984, Evaluating seals for hydrocarbon accumulations: American Association of Petroleum Geologists Bulletin, v. 68, p. 1752–1763.
- Emmons, W. H., and Calkins, F. C., 1913, Geology and ore deposits of the Philipsburg Quadrangle, Montana: U.S. Geological Survey Professional Paper 78, 271 p.
- Faure, G., 1986, Principles of isotope geology, 2nd ed.: New York, Wiley, 589 p.
- Gluyas, J. G., and Swarbrick, R. E., 2004, Petroleum geoscience: London, Wiley-Blackwell, 376 p.
- Goodwin, P. W., 1964, Ordovician formations of Wyoming [Ph.D. thesis]: Iowa City, State University of Iowa, 201 p.
- Grader, G. W., and Dehler, C. M., 1999, Devonian stratigraphy in east-central Idaho: New perspectives from the Lemhi Range and Bayhorse area, in Hughes, S. S., and Thackray, G. D., eds., Guidebook to the Geology of Eastern Idaho: Pocatello, Idaho Museum of Natural History, p. 29–54.
- Grader, G., Pope, M., Doughty, P. T., and Isaacson, P., 2009, Devonian stratigraphic framework in western Montana and east-central Idaho: Paleogeographic highs and shared intra-shelf basin depositional patterns: American Association of Petroleum Geologists Annual Convention and Exhibition, Denver, Colorado, Abstract # 1010325.
- Gutschick, R. C., Suttner, L. J., and Switek, M. J., 1962, Biostratigraphy of transitional Devonian-Mississippian Sappington Formation of southwest Montana: Billings Geological Society Guidebook, 13th Annual Field Conference, p. 79–86.
- Hangx, S. J. T., Spiers, C. J., and Peach, C. J., 2010, Mechanical behavior of anhydrite caprock and implications for CO_2 sealing capacity: Journal of Geophysical Research, v. 115, p. B07402.
- Haq, B. U., and Schutter, S. R., 2008, A chronology of Paleozoic sea level changes: Science, v. 322, p. 64–68.
- International Stratigraphic Chart, 2009: International Commission on Stratigraphy, <http://www.stratigraphy.org/upload/ISChart2009.pdf>.
- Isaacson, P. E., Hladil, J., Shen, J. W., Kalvoda, J., and Grader, G., 1999, Late Devonian (Famennian) glaciation in South America and marine offlap on other continents, in Feist, R., Talent, J. A., and Daurer, A., eds., North Gondwana: Mid-Paleozoic terranes, stratigraphy and biota: Wien, Abhandlungen der Geologischen Bundesanstalt, v. 54, p. 239–257.
- John, E. H., Cliff, R., and Wignall, P. B., 2008, A positive trend in seawater $^{87}\text{Sr}/^{86}\text{Sr}$ values over the Early-Middle Frasnian boundary (Late Devonian) recorded in well-preserved conodont elements from the Holy Cross Mountains, Poland: Palaeogeography, Palaeoclimatology, Palaeoecology, v. 269, p. 166–175.
- Johnson, J. G., Klapper, G., and Sandbert, C. A., 1985, Devonian eustatic fluctuations in Euramerica: Geological Society of America Bulletin, v. 96, p. 567–587.
- Kraig, D. H., Wiltschko, D. V., and Spang, J. H., 1987, Interaction of basement uplift and thin-skinned thrusting, Moxa Arch and the Western Overthrust Belt, Wyoming: A hypothesis: Geological Society of America Bulletin, v. 99, p. 654–662.
- Laird, W. M., 1947, An Upper Devonian brachiopod fauna from northwestern Montana: Journal of Paleontology, v. 21, p. 453–459.
- Larimer, T. R., 1959, Paleogeography of the Pre-Mississippian surface, Bighorn Mountains, Wyoming [MS thesis]: Iowa City, State University of Iowa, 120 p.

- Li, Y., and Wardlaw, N. C., 1986, The influence of wettability and critical pore-throat size ratio on snap-off: *Journal of Colloid Interface Science*, v. 109, p. 461–472.
- Lindeberg, E., 2002, The quality of a CO₂ repository: What is the sufficient retention time of CO₂ stored underground?, *in* Gale, J., and Kaya, Y., eds., *Proceedings of the 6th Greenhouse Gas Control Technologies Conference: Kyoto, Japan*, Elsevier, p. 255–260.
- Lorenz, J. C., Teufel, L. W., and Warpinski, N. R., 1991, Regional fractures I: A mechanism for the formation of regional fractures at depth in flat-lying reservoirs: *American Association of Petroleum Geologists Bulletin*, v. 75, p. 1714–1737.
- Love, J. D., 1969, Type locality of Darby Formation, Western Wyoming: *American Association of Petroleum Geologists Bulletin*, v. 53, p. 167–170.
- McArthur, J. M., 1995, Recent trends in strontium isotope stratigraphy: *Terra Nova*, v. 6, p. 331–358.
- Palmer, M. R., and Edmond, J. M., 1992, Controls over the strontium isotope composition of river water: *Geochimica et Cosmochimica Acta*, v. 56, p. 2099–2111.
- Parker, H. B., 1950, The Bighorn Dolomite [M.S. thesis]: Oxford, Miami University, 71 p.
- Peale, A. C., 1893, Paleozoic section in the vicinity of Three Forks, Montana: *United States Geological Survey Bulletin*, v. 110, 56 p.
- Peterson, J. A., 1989, Future petroleum resource potential of Northern Rocky Mountain-Great Plains area, *in* Lorenz, J. C., and Lucas, S. G., eds., *Energy frontiers in the Rockies: Albuquerque, Albuquerque Geological Society*, p. 46–55.
- Rau, J. L., 1962, The stratigraphy of the Three Forks Formation: *Billings Geological Society Guidebook*, 13th Annual Field Conference, p. 51–65.
- Richards, P. W., and Nieschmidt, C. L., 1957, The Bighorn Dolomite in south-central Montana and northwestern Wyoming: *Billings Geological Society Guidebook*, 8th Annual Field Conference, p. 54–62.
- Richards, P. W., and Nieschmidt, C. L., 1961, The Bighorn Dolomite and correlative formations in southern Montana and northern Wyoming: *U.S. Geological Survey Oil and Gas Investigations Map OM-202*.
- Rowley, P. D., Hansen, W. R., Tweto, O., and Carrara, P. E., 1985, Geologic map of the Vernal 1°x2° quadrangle, Colorado, Utah, and Wyoming: *USGS Miscellaneous Investigations Series I:1526*, scale 1:250,000.
- Royse, F. Jr., 1993, An overview of the geologic structure of the thrust belt in Wyoming, northern Utah, and eastern Idaho, *in* Snoke, A. W., Steidtmann, J. R., and Roberts, S. M., eds., *Geology of Wyoming: Laramie, Wyoming, The Geological Survey of Wyoming Memoir No. 5*, p. 273–311.
- Sandberg, C. A., 1962, Stratigraphic section of type Three Forks and Jefferson Formations at Logan, Montana: *Billings Geological Society Guidebook*, 13th Annual Field Conference, p. 47–50.
- Sandberg, C. A., 1963, Dark shale unit of Devonian and Mississippian age in northern Wyoming and southern Montana: *U.S. Geological Survey Professional Paper 475-C*, p. C17–C20.
- _____, 1965, Nomenclature and correlation of lithologic subdivisions of the Jefferson and Three Forks Formations of southern Montana and northern Wyoming: *U.S. Geological Survey Bulletin 1194-N*, 18 p.
- Sandberg, C. A., and Klapper, G., 1967, Stratigraphy, age, and paleotectonic significance of the Cottonwood Canyon Member of the Madison Limestone in Wyoming and Montana: *U.S. Geological Survey Bulletin 1251-B*, 70 p.
- Sandberg, C. A., and Mapel, W. J., 1967, The northern Rocky Mountains and plains, *in* Oswald, D. H., ed., *International symposium of the Devonian system*, v. 1: Calgary, Alberta, Alberta Society of Petroleum Geologists, p. 843–877.
- Schowalter, T. T., 1979, Mechanics of secondary hydrocarbon migration and entrapment: *American Association of Petroleum Geologists Bulletin*, v. 63, p. 723–760.
- Secor, D. T., 1965, Role of fluid pressure in jointing: *American Journal of Science*, v. 263, p. 633–646.
- Sloss, L. L., 1963, Sequences in the cratonic interior of North America: *Geological Society of America Bulletin*, v. 74, p. 93–114.
- Stilwell, D. P., 1989, CO₂ Resources of the Moxa Arch and the Madison reservoir: *Wyoming Geological Association Guidebook*, 40th Annual Field Conference, Guidebook, p. 105–115.
- Sweet, W. C., 1979, Late Ordovician conodonts and biostratigraphy of the western Midcontinent Province, *in* Sandberg, C. A., and Clark, D. L., eds., *Conodont biostratigraphy of the Great Basin and Rocky Mountains: Geology Studies*, v. 26, Part 3, p. 45–86.
- Teel, S., 1994, Petrography and depositional environment of the Ordovician Bighorn Dolomite, south-central Montana and northern Wyoming [M.S. thesis]: Moscow, University of Idaho, 96 p.
- Thyne, G. D., Tomasso, M., Bywater-Reyes, S. V., Budd, D. A., and Reyes, B. M., 2010, Characterization of porosity and permeability for CO₂ sequestration models in the Mississippian Madison Group, Moxa Arch–LaBarge Platform, southwestern Wyoming: *Rocky Mountain Geology*, v. 45, p. 133–150.
- Tice, L. P., Myrow, P. M., Taylor, J. F., Ripperdan, R. L., and Ethington, R. L., 2002, Stratigraphy and sedimentology of the Cambrian and Ordovician Gallatin Formation, Wyoming and Montana: *Geological Society of America Abstracts with Programs*, v. 34, p. 138.

- Tomlinson, C. W., 1917, Middle Paleozoic stratigraphy of the central Rocky Mountain region: *Journal of Geology*, v. 25, p. 112–134, 244–257, 373–394.
- Vavra, C. L., Kaldi, J. G., and Sneider, R. M., 1992, Geological applications of capillary pressure: A review: *American Association of Petroleum Geologists Bulletin*, v. 76, p. 840–850.
- Wach, S., 1977, The Moxa Arch, an overthrust model?, *in* Heisey, E. L., Norwood, E. R., and Wach, P. H., eds., *Rocky Mountain thrust belt geology and resources: Casper, Wyoming Geological Association, 29th Annual Field Conference in conjunction with Montana Geological Society and Utah Geological Society*, p. 665–671.
- Wilson, J. L., 1975, *Carbonate facies in geologic history*: New York, New York, Springer-Verlag Publishers, 471 p.
- Zenger, D. H., 1992, Burrowing and dolomitization patterns in the Steamboat Point Member, Bighorn Dolomite (Upper Ordovician), northwest Wyoming: *Contributions to Geology*, v. 29, p. 133–142.
- , 1996, Dolomitization patterns in widespread “Bighorn Facies” (Upper Ordovician), Western Craton, USA: *Carbonates and Evaporites*, v. 11, p. 219–225.

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The Wyoming Carbon Underground Storage Project: geologic characterization of the Moxa Arch and Rock Springs Uplift

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Abstract

The state of Wyoming, in the northwestern United States, produces 40% of the nation's coal, most of which is transported out of the state. The remainder is used at power plants within Wyoming to generate approximately 7% of U.S. electricity. Carbon capture and storage from these power stations could significantly reduce U.S. carbon emissions. Wyoming statutes and rules proposed by the U.S. Environmental Protection Agency and Wyoming Department of Environmental Quality regarding subsurface carbon storage require that CO₂ injection must not affect established or potential drinking water aquifers, oil and gas fields, or other mineral estates. Wyoming has several potential large-scale geologic carbon storage reservoirs that meet these criteria, in the form of saline aquifers in regional basins and uplifts. The Wyoming Carbon Underground Storage Project has recently been funded by the U.S. Department of Energy and the state of Wyoming to 1) assess the CO₂ storage potential of two possible locations in southwestern Wyoming: the Moxa Arch and the Rock Springs Uplift, 2) develop a system for displaced fluid management, 3) plan monitoring and verification activities, and 4) design infrastructure in preparation for geologic carbon sequestration. The Wyoming Carbon Underground Storage Project represents collaboration between the University of Wyoming, the Wyoming State Geologic Survey, ExxonMobil Corporation, Los Alamos National Laboratory, and Baker Hughes Incorporated. The authors are involved primarily in the geologic stratigraphic and structural characterization of the Moxa Arch and Rock Springs Uplift.

The Moxa Arch is an anticline that trends from the Uinta Mountains, 200 km north-northwest to the eastern front of the Wyoming fold-and-thrust belt. Potential storage reservoirs on this large geologic structure include the Jurassic Nugget Sandstone, the Mississippian Madison Limestone, and the Ordovician Bighorn Dolomite. The Nugget Sandstone is a heterogeneous and anisotropic eolian deposit that has been extensively exploited for oil and gas at certain locations on the Moxa Arch, which complicates its usage as a repository for carbon dioxide. The Madison Limestone is a proven storage reservoir; ExxonMobil has been injecting CO₂ (up to 25 MMCFD) and H₂S (up to 65 MMCFD) into the Madison Limestone on the Moxa Arch for seven years at the Shute Creek Gas Plant. The Bighorn Dolomite is stratigraphically complex with large variations in porosity and

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permeability due to primary burrowing and repeated dolomitization and dedolomitization. Depending on location on the anticline, the Nugget Sandstone lies 3 to 6.5 km below the surface (-1 to -4.5 km subsea), and the Bighorn Dolomite and Madison Limestone range from 4.5 to 8 km below the surface (-2.5 to -6 km subsea).

The Moxa Arch is structurally uncomplicated; it is a basement-involved anticline formed by a west-vergent Late Cretaceous-age thrust fault, with gently-dipping limbs (0 to 5 degrees). Leakage risk is extremely low because impermeable evaporite (anhydrite) intervals overly the potential reservoirs, and preliminary interpretation of seismic data reveal that few faults exist other than the main thrust. The Naughton Power Plant, a 707 MW coal-fired power station emitting up to 6 Mt of CO₂ per year, lies 30 km west of the crest of the anticline.

The Rock Springs Uplift, 100 km east of the Moxa Arch, extends 80 km north from the Wyoming-Utah border. The target storage reservoirs are the Pennsylvanian Weber Sandstone (correlative to the Tensleep Sandstone) and the Mississippian Madison Limestone. The Weber Sandstone exhibits wide variations in reservoir properties (porosity and permeability) due to dune/interdune/intradune facies changes, and appears to have experienced local secondary diagenesis that further reduced porosity. The Madison Limestone is expected to have similar reservoir properties to its lithologic correlative on the Moxa Arch. The Weber Sandstone and Madison Limestone range in depth from 2 to 6 km below the surface (0.3 to -4.5 km subsea), depending on location on the anticline.

The Rock Springs Uplift offers challenges for structural analysis. Like the Moxa Arch, the Uplift was formed by a Late Cretaceous-age west-vergent basement-involved reverse fault, but the limbs of the fold are at steeper dips (approximately 15 degrees on the west limb, shallower on the east limb), and these limbs are cut at depth by additional reverse faults. In a hydrocarbon field on the southeastern flank of the uplift there is a possibility that condensate is migrating from the Weber Sandstone along one of these reverse faults, suggesting that the trap is breached. In addition, a series of east-west trending normal faults cut Cretaceous shales at the surface, possibly with throws that exceed the thickness of the uppermost regional seal. It is necessary to determine if these east-west faults also compromise the Triassic units that could provide a seal above the Weber Sandstone. The Jim Bridger Power Plant (coal-fired) is located on the east flank of the Rock Springs Uplift; it has 2200 MW capacity and emits up to 18 Mt of CO₂ per year.

Future U.S. energy demands will draw heavily on Wyoming's coal-fired power plants, and the state is taking steps to sequester the produced carbon. Wyoming hosts several large geologic traps that if properly risked and evaluated have promise as long-term, stable repositories for anthropogenic carbon dioxide. Based upon our preliminary assessment of the multiple clastic and carbonate receiving formations in the Moxa Arch and Rock Springs Uplift, and the experience of successful injection at ExxonMobil's Shute Creek Gas Plant, these geologic structures in southwestern Wyoming are among the most promising large CO₂ geologic storage sites in the United States.

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Keywords: Geologic carbon sequestration; Wyoming; Moxa Arch; Rock Springs Uplift

1. Introduction

The state of Wyoming possesses several geologically appropriate locations with great promise for underground storage of carbon dioxide in the United States due to an abundance of subsurface traps, reservoirs, and sealing intervals. In southwestern Wyoming, two geologic structures, the Moxa Arch and the Rock Springs Uplift (Figure 1), have been

studied to evaluate their potential for geologic sequestration of carbon dioxide. This paper discusses the general sequestration attributes of the two sites and highlights their similarities and differences.

2. Geologic Setting

2.1 Moxa Arch

The Moxa Arch is a gently-dipping, doubly plunging anticline that extends from beneath the Uinta Mountains at the Utah/Wyoming border, north to the town of La Barge, Wyoming, where it turns northwest and plunges beneath the western Wyoming fold-and-thrust belt (Figure 1). This structural history has been well-documented and indicates uplift along a basement-involved thrust fault beginning in the Late Cretaceous and continuing through the early Eocene (e.g., [1]). The limbs of the structure have a maximum dip of 5 degrees on the eastern limb, and 3D seismic and well data indicate major faulting is essentially limited to the basement-involved thrust along the southwestern edge of the structure.

Figure 1. Location map of the Moxa Arch and Rock Springs Uplift in southwestern Wyoming. The shaded area indicates the Greater Green River Basin. The Moxa Arch is a current injection site for CO₂ and H₂S; the Rock Springs Uplift is being evaluated as a potential CO₂ repository.

Significant accumulations of methane, CO₂, H₂S, and other gases are stored within the pore space of the early Carboniferous (Mississippian) Madison Limestone around the crest of the Moxa Arch. This gas is currently being produced by ExxonMobil, and the waste stream of naturally occurring carbon dioxide and hydrogen sulfide is being re-injected into the Madison below the gas-water contact at the Shute Creek Gas Plant at rates of ~60 MMCFD (~2650 tonnes/day). The ~240 meter-thick Madison Limestone has been affected by limited dolomitization, hydrothermal brecciation [2], stylolitization, karsting, and fracturing that has influenced the formation's porosity and permeability.

Porosity ranges from 0 – 35% and appears to be primarily related to stratigraphic trends and diagenesis [3]. Permeability has a generally positive correlation to porosity, but is also affected by fractures and microfractures; permeability values range from 0.001 to 100 md [3]. The Madison Limestone lies at depths of 4.5 to 8 km below the surface depending on location within the area of study, with multiple potential seals overlying the reservoir.

The 100-meter thick Mississippian to early Pennsylvanian Amsden Formation overlies the Madison Limestone (Figure 2), and consists of interbedded red clastic shales and sandstones, anhydrite, dolostone, and limestone, overlain by increasingly pure limestone [4]. This unit separates the Madison Limestone from the Pennsylvanian Weber/Tensleep Sandstone, which is a series of cross-bedded quartz-rich eolian dune facies interbedded with discontinuous interdune siltstones and claystones. Unlike the Madison, the Weber/Tensleep does not have a large gas accumulation within it, suggesting the Amsden is a potential seal between the two units. Although oil and gas is commonly produced from the Weber/Tensleep throughout Wyoming, at the Moxa Arch it was determined to have insufficient porosity and permeability for a suitable storage reservoir based on drill stem tests, core plug data, and wireline logs.

2.2. Rock Springs Uplift

The Rock Springs Uplift, located east of the Moxa Arch (Figure 1), is also a Late-Cretaceous to Early Eocene-age basement-involved anticlinal structure. However, the limbs of the Rock Springs Uplift are dipping at least twice as steeply as the Moxa Arch, and a series of east-west oriented normal faults are common across the structure. This structure is being evaluated by the Wyoming Carbon Underground Storage Project (WYCUSP) for suitability as a storage location for subsurface carbon dioxide. Because of its proximity to the large Jim Bridger Power Plant and its similarities to the proven storage reservoir on the Moxa Arch, the Rock Springs Uplift warrants thorough evaluation as a potential storage site. During fall of 2010, WYCUSP will drill a stratigraphic test well and will be collecting 3-D seismic data over a five-square mile area around a possible injection site near the power plant.

The Madison Limestone is also being considered as a potential storage reservoir on the Rock Springs Uplift site, because of its similarity to the Madison on the Moxa Arch from preliminary core examination. The Madison is approximately 4 km deep at the stratigraphic test well location.

The Pennsylvanian Weber Sandstone is a second potential reservoir. Although the Weber has been a prolific hydrocarbon producer on the southeast flank of the Rock Springs Uplift, it can exhibit extremely low porosity as a result of diagenetic destruction of porosity [5]. Therefore, WYCUSP will be testing core from the Weber extensively to evaluate its reservoir characteristics at the potential injection site on the northeast flank of the anticline.

The numerous normal faults that cut the Rock Springs Uplift could present a threat to the integrity of the trap. Logs indicate that these normal faults have up to 240 m of throw [7], but it is currently unclear if these faults cut down to the depth of the relevant reservoirs and seals. Although some of these normal faults may compartmentalize shallow Cretaceous reservoirs near the crest of the anticline [8], minor reverse faults on the southeast flank of the Rock Springs Uplift appear to have behaved as conduits rather than seals [5]. In all cases, 3-D seismic data will be crucial to assessing whether faults are present in the storage field and if they pose a risk.

Age		Moxa Arch	Rock Springs Uplift
JURASSIC	Upper	Stump Sandstone	Morrison Formation
		Preuss Formation	Entrada Sandstone
	Middle	Twin Creek Limestone	Carmel Formation
		Gypsum Springs Formation	
	Lower	Nugget Sandstone	
TRIASSIC		Ankareh Formation	
		Thaynes Limestone	Woodside Formation
		Dinwoody Formation	
PERMIAN		Phosphoria Formation	
PENNSYLVANIAN		Tensleep Sandstone	Weber Sandstone
		Amsden Formation	Morgan Formation
		Darwin Sandstone	
MISSISSIPPIAN		Madison Limestone	
DEVONIAN	Upper	Three Forks Formation	
		Jefferson Formation	Darby Formation
SILURIAN			
ORDOVICIAN		Bighorn Dolomite	
CAMBRIAN	Upper	Gallatin Limestone	
	Middle	Gros Ventre Formation	
	Lower	Flathead Sandstone	

Figure 2. Generalized stratigraphic column from Jurassic through the Cambrian units on the Moxa Arch and Rock Springs Uplift. Dashed lines denote erosional contacts and areas shaded gray represent missing time. Modified from Love et al. [6].

3. Seal Evaluation

Understanding the distribution and effectiveness of seals and sealing mechanisms for CO₂ storage is as important as defining the reservoir and mapping out the structural trap. Seal characteristics are frequently overlooked in the effort to identify adequate storage locations, making thorough seal analyses relatively rare (good examples include [9], [10] and [11]). The petroleum industry has carefully studied these parameters and their implications for holding large buoyant columns in the subsurface over geologically significant periods of time. Generally, seals need to have adequate mechanical strength and sufficiently low capillary entry pressure to ensure their effectiveness (e.g., [12], [13]), and these parameters are quantifiable through routine analyses. Feasibility studies of CO₂ storage could benefit from knowledge gained in the hydrocarbon industry, as well as an array of possible tests for seal assessment.

In petroliferous basins, hydrocarbons can serve as a potential leak test to determine if a proposed site is capable of holding a buoyant column in the subsurface. If a potential sequestration site is located within such a basin and contains a porous and permeable reservoir, the absence of a hydrocarbon column may be attributable to 1) the lack of any hydrocarbons within the trap fetch area, or 2) a compromised trap/seal. Analysis of fluid inclusion volatiles (FIV) can help distinguish between these two potential possibilities.

3.1 FIV Methodology

The conversion of smectite to illite, the maturation of organic matter to petroleum, and the formation of several different types of pore-occluding diagenetic cements occurs at coincident temperatures of ~100°C. The products of these reactions (hydrocarbons, water, and silica) migrate into available pore space. The silica precipitates as overgrowths and often traps the other fluid phases in the pore space as inclusions. Hydrocarbons, if present, can be detected by analyses of fluid inclusion volatiles. The technique works by crushing a small sample of cuttings twice, in a vacuum, and analyzing molecular weights of volatiles liberated from inclusions via a quadrupole mass spectrometer (e.g., [14]). Analyses of thousands of wells from around the world demonstrate that this technique is highly reliable in determining whether a trap has been charged with hydrocarbons, or is in a hydrocarbon “migration shadow”.

3.2 FIV results and conclusions

Cuttings were analyzed for fluid inclusion composition from the T62X-16S well on the northern Moxa Arch and the Amoco-Texas #1 on the western Rock Springs Uplift (Figure 1 and Figure 3). On the Moxa Arch, results show that hydrocarbons are present within the fluid inclusions in all of the Mississippian through Permian reservoirs. Distinctive reductions in the concentration of methane (C1), propane (C3), and other hydrocarbon constituents within the Amsden Formation and above the Phosphoria Formation suggest these are sealing intervals that prevented hydrocarbons from migrating upward. These interpretations are verified by what is known about the present day distribution of gas accumulations on the Moxa Arch. The Texas-Amoco #1 well on the Rock Springs Uplift, located over 100 km southeast from the T62X-16S, shows nearly identical results, indicating that hydrocarbons were present within the trap, although the exact amounts can only be speculated. However, the vertical segregation of the hydrocarbons in the inclusions by density suggests there was a stable column present. The present lack of a large hydrocarbon column in Mississippian through Permian reservoirs in the Texas-Amoco #1 hints that the trap was breached at this location. In this well very little gas is observed within the Weber Sandstone, yet all gases disappear above the Phosphoria Formation.

The FIV results indicate that the Amsden Formation is acting as a seal to the Madison Formation, and the Dinwoody and Woodside formations prove to be excellent seals, preventing essentially any buoyant phases from vertical migration above the Phosphoria formation. The 45-meter thick Triassic Dinwoody Formation consists primarily of interbedded siltstone, with minor limestone, dolostone, and rare thin beds of anhydrite [15]. The 90-meter thick Woodside Formation consists of laminated siltstone, dolostone, and impure halite. Both halite and anhydrite are known as excellent seals for CO₂ (e.g., [16][11]).

FIV analyses from two wells in two different locations within the Green River Basin (Figure 1) suggest that there are multiple seals within the Upper Paleozoic section, which are capped by lowermost Triassic rocks with excellent seal properties. This seal redundancy speaks to the great potential for carbon sequestration within Wyoming, and illustrates that understanding the distribution of sealing facies (e.g., halite and anhydrite – particularly the lower Triassic interval) and their breach points, is imperative for risking potential sites for CO₂ sequestration. The Rock Springs Uplift will require further study to document the effectiveness of the Triassic seal throughout the structure and to understand why the Weber Sandstone, in some locations, contains so little gas in the trap.

Figure 3. FIV analysis of well T62X-16S from the Moxa Arch and Amoco-Texas #1 from the Rock Springs Uplift. Both analyses indicate lower Triassic units have not hosted hydrocarbons in the past or present, and should act as seals above CO₂ storage reservoirs.

4. Conclusions

Because of the similarities between the Rock Springs Uplift, a potential CO₂ reservoir, and the Moxa Arch, a proven storage reservoir, the Rock Springs Uplift warrants further study as a repository for CO₂ to be recovered from the Jim Bridger Power Plant. FIV results demonstrate that the system has had an effective reservoir/seal combination. Although the reservoirs and seals on the two anticlines are similar, the Rock Springs Uplift has structural complexities which are being thoroughly studied to ensure secure trapping of the CO₂.

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6. References

- [1] Becker, TP, McGroder, M, Rudolph, KW, Hauge, TA, Fan, M. Paleogene influence of the Moxa Arch on the architecture of the composite Darby-Hogsback-Prospect (DHP) thrust sheet near La Barge, Wyoming, USA. AAPG Annual Meeting Abstract #90104; 2010.
- [2] Katz, DA, Eberli, GP, Swart, PK, and Langhorne, BS Jr. Tectonic-hydrothermal brecciation associated with calcite precipitation and permeability destruction in Mississippian carbonate reservoirs, Montana and Wyoming. AAPG Bulletin; 2006; 90(11):1803-41.
- [3] Hildegard, W, Eberli, GP, Smith, LB, Grammer, GM, and Kislak, J. Reservoir characterization of the Mississippian Madison Formations, Wind River basin, Wyoming. AAPG Bulletin; 2004; 88(4):405-32.
- [4] Boyd, DW. Paleozoic history of Wyoming. In: Snoke, AW, Steidtmann, JR, and Roberts, SM, editors. Geology of Wyoming: Geological Survey of Wyoming Memoir No. 5; 1993, p. 164-87.
- [5] Montgomery, SL. Brady Unit, Rock Springs Uplift, Wyoming: migration and structural history. AAPG Bulletin; 1996; 80(10):1535-46.
- [6] Love, JD, Christiansen, AC, and Ver Ploeg, AJ. Stratigraphic chart showing Phanerozoic nomenclature for the State of Wyoming. Geological Survey of Wyoming Map Series, report 41; 1993.
- [7] Van Horn, M. Stratigraphy of the Almond Formation, east-central flank of the Rock Springs Uplift, Sweetwater County, Wyoming. Master's Thesis, Colorado School of Mines; 1979.
- [8] Surdam, RC, and Jiao, Z., The Rock Springs Uplift: An Outstanding Geological CO₂ Sequestration Site in Southwest Wyoming (Challenges in Geological Development, 2). Laramie, WY: Wyoming State Geological Survey; 2007.
- [9] Lu, J, Wilkinson, M, Haszeldine, RS, and Fallick, AE. Long-term performance of a mudrock seal in natural CO₂ storage. Geology; 2009; 37(1):35-8.
- [10] Han, WS, McPherson, BJ, Lichtner, P, and Wang, Evaluation of trapping mechanisms in geologic CO₂ sequestration: case study of SACROC northern platform, a 35-year CO₂ injection site. American Journal of Science FP; 2010; 310:282-324.
- [11] Hangx, SJT, Spiers, CJ, and Peach, CJ. Mechanical behavior of anhydrite caprock and implications for CO₂ sealing capacity. Journal of Geophysical Research; 2010; 115:B07402.
- [12] Vavra, CL, Kaldi, JG, and Sneider, RM. Geological applications of capillary pressure; a review. AAPG Bulletin; 1992; 76(6):840-50.
- [13] Gluyas, JG, and Swarbrick, RE. Petroleum Geoscience: London, Wiley-Blackwell; 2004.
- [14] Pottorf, RJ, Hussenoeder, KL, Tseng, H, Petersen, K, Davis, CL, Richardson, et al. Downdip oil potential for an offshore Abu Dhabi petroleum system. Society of Petroleum Engineers; 2006; Paper 101676:395-403.

- [15] Picard, MD. The early Mesozoic history of Wyoming. In: Snoke, AW, Steidtmann, JR, and Roberts, SM, editors. Geology of Wyoming, Geological Survey of Wyoming Memoir No. 5, Laramie, WY: Wyoming State Geological Survey; 1993, p. 210-48.
- [16] Peach, C, and Spiers, CJ. Influence of crystal plastic deformation on dilatancy and permeability development in synthetic salt rock. Tectonophysics; 1996; 256:101-28.

CHAPTER 5: Subsurface and Surface Structural Evaluation – Results 4 and 5

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Background

This chapter focuses on results of a multi-scale evaluation of the surface structural geology of the LaBarge Platform (also covered in Chapter 4). This research has provided critical information on regional and local fracture and fault systems through the preparation of serial cross-sections and outcrop-scale analysis of fracture arrays and populations of small-scale faults. Laboratory studies on fault rocks and mineralized fractures provide important information on deformation mechanisms and fluid composition that has affected the stratigraphic units targeted for carbon sequestration. Results 4 and 5 from Tasks 4 and 5 are presented in this chapter, which summarizes the subsurface structural interpretation through creation of east-west cross sections across the entire Moxa Arch region and interpretation of 3-D seismic data from the central Moxa Arch. The chapter also documents reservoir fractures from available data. A summary of results follows.

Executive Summary

The final results of Tasks 4 and 5 are 1) subsurface structural interpretation through creation of east-west cross sections across the study region and interpretation of 3-D seismic data from the central Moxa Arch, and 2) documentation of reservoir fractures from available data. For background on the study area (Figure 5-1), please see the executive summary of Chapter 4.

Result 4

The subsurface geology of the Moxa Arch can be interpreted from surface geology (where appropriate units are exposed at the surface), well data, and 3-D seismic data. A series of 2-D cross sections were created to predict the general subsurface structure across the entire Moxa Arch. 3-D seismic data were purchased over a small area on the crest of the Arch, and digital well logs across the Moxa Arch were donated by ExxonMobil. Subsurface interpretation of the seismic data corroborates the cross-section interpretation, which indicates that the Moxa Arch is a gently dipping anticline (limbs dip 0–5 degrees). There appears to be little structural complexity in terms of faulting within the reservoir. The Madison and Bighorn reservoirs lie at depths of 4.5 to 8 km below the surface (-2.5 to -6 km subsea) (Campbell-Stone et al., 2010).

Result 5

Fractures and stylolites were documented at the surface and in core in the Madison Limestone and Bighorn Dolomite. Fracture intensity is related to rock composition, and vertical fractures tend to terminate in stylolites. Most fractures are sub-vertical or parallel to bedding. Fractures range in fill from unfilled to 100% filled, and fill is predominantly calcite. Stylolites are generally horizontal

and can mark the boundary between zones of different porosity within the unit. Few cores were available on the Moxa Arch (none of which were oriented—a necessity for a complete fracture model), and no cores were available within the area of the 3-D seismic survey. Additional data would need to be acquired to create a fracture model for this field before injecting CO₂.

Report Details – Results and Discussion

Result 4: Subsurface interpretation from cross sections and 3-D seismic data

We have interpreted the subsurface of the Moxa Arch through the creation of cross sections and interpretation of 3-D seismic data from the crest of the structure. The two cross sections (Figure 5-2) were constructed in an east-west orientation across the Moxa Arch. This work was initiated by graduate student Lee Barnett, completed by Art Snoke, Ranie Lynds, and Erin Campbell-Stone, and drafted at the Wyoming State Geological Survey by Phyllis Ranz. The cross sections were created through compilation of published literature and previous MS-thesis and PhD-dissertation studies from Montpelier, Idaho, to La Barge, Wyoming. The cross sections are limited to the area outside the Wyoming fold-and-thrust belt, because the fold and thrust belt is extremely structurally complex and of a different structural style than the Laramide uplift (Figure 5-2).

Seismic data were purchased for a 22 square mile area on the crest of the Moxa Arch (see Figure 5-1 for location). Digital well logs were donated by ExxonMobil. The data were reprocessed by Geokinetics, and a velocity model was created by Amit Padhi and Subhashis Mallick (Chapter 8). Since no deep wells exist within the area of the seismic data, the velocity model and horizons were created by using data from nearby deep wells and published seismic interpretations (Garing and Tainter, 1985). The seismic data were interpreted using Petrel software (donated by Schlumberger) (Figures 5-3 and 5-4). The seismic data clearly show very shallow dips on the crest and nearby flanks of the anticline. The area is not faulted in this region within the resolution of the seismic data.

These two methods of subsurface interpretation show that, depending on location on the anticline, the Bighorn Dolomite and Madison Limestone lie at 4.5 to 8 km below the surface (-2.5 to -6 km subsea).

Result 5: Documentation of fractures

In order to understand reservoir properties, it is necessary to document the density, orientation, and fill of fractures. Full geomechanical analysis requires an understanding of paleo- and current reservoir stress. Our results encompass only the first phase of a geomechanical analysis: fracture documentation in terms of density and cross cutting relationships with other features. Fractures will enhance the reservoir permeability only if the fracture permeability is greater than the matrix permeability, so it is important to determine if the fracture fill will cause a fracture to act as a baffle, barrier, or conduit. Knowledge of the composition of the fill will also allow us to determine if the fill will react with injected CO₂ to enhance or degrade reservoir permeability.

Fracture intensity (or density) and orientation were visually documented on cores recovered from the Moxa Arch. Fracture intensity was classified as low, medium, high, and extreme. Because the cores are not oriented and the wells are subvertical, the orientation was documented in terms of

degrees from vertical (Figures 5-5 and 5-6; see Figure 5-1 for locations). Fractures were determined to have offsets ranging from 0 to a few mm (Figure 5-7). Moxa Arch core from the Madison Limestone and Bighorn Dolomite exhibited fracture intensities ranging from none to medium level. Cores from the fold-and-thrust belt showed zones of extremely high fracturing, but fracture density of that level is unlikely along the crest and eastern flank of the less-deformed Moxa Arch.

We were unable to sample Core 1 from the Moxa Arch, so thin section analysis and scanning electron microscopy analysis on fracture fill was conducted on a highly fractured core in the fold-and-thrust belt (Core 2; see Figure 5-1 for location). Microscopic analysis of fractures from the Madison Limestone indicates fractures are either open or filled with calcite. The host rock is consistently dolostone and fractures are calcite-filled according to analysis on the scanning electron microscope (Figure 5-8). Although fracture intensity from Core 2 (within the hanging wall of the overthrust belt) cannot be used to predict fracture intensity in the Moxa Arch, fracture fill may be similar between the two locations. Hand sample examination of Core 1 from the Moxa Arch indicates subsurface fractures on the Moxa Arch are predominantly filled with calcite.

A preliminary outcrop analog to better quantify subsurface fractures was located on the western edge of the Tetons, near Grand Targhee Ski Resort (western side of Fred's Mountain). Fractures were measured on pavement (top) surfaces of the Bighorn Dolomite and Cambrian Death Canyon Member of the Gros Ventre Formation. The results of these measurements are presented in Figures 5-9 and 5-10. The Teton Range has been subject to a complex series of folding and faulting to a degree not experienced by the Moxa Arch. In addition to being involved in the western Wyoming fold-and-thrust belt, the Tetons sit at the edge of the Basin and Range extensional province. Although the structural settings are vastly different and thus not analogous, we determined a surprising lithologic variation in fracture orientation. The Bighorn Dolomite, nearly 100% dolostone, consistently displayed two distinct orthogonal fracture sets. The Gros Ventre Member, primarily a limestone, showed a variable fracture pattern that requires further study and explanation. This preliminary outcrop fracture analysis demonstrates the need for a solid fracture characterization of any potential CO₂ injection location. The fracture analysis must account for lithology and not presume fracture orientations are consistent between formations or at different depths.

Conclusions

We believe the eastern flank and/or crest of the central Moxa Arch may have significant potential for long-term geosequestration of carbon dioxide within the Madison Limestone, and we recommend a more detailed subsurface structural study of this location. The western flank of the anticline is not recommended due to proximity to the fold-and-thrust belt and the structural uncertainty inherent in that position. The Madison Limestone should be encountered at depths of 4.5–8 km below the surface. The Bighorn Dolomite is another potential reservoir, but its high CO₂ content makes it more of a risk for storage because of the possibility that it is full. The Triassic Dinwoody Formation has been found to be the key confining layer within the Greater Green River Basin, and it is present across the Moxa Arch. Some structural uncertainty remains and needs to be addressed: fracture and stress data must be obtained for an injection site, and the data should be

interpreted in a geomechanical context to determine the maximum injection rate and to predict the influence of fractures on direction of plume migration.

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References

- Becker, T.P., McGroder, M.F., Rudolph, K., Hauge, T.A., and Fan, M., 2010, Paleogene influence of the Moxa arch on the architecture of the composite Darby-Hogsback-Prospect (DHP) thrust sheet near LaBarge, WY, U.S.A., American Association of Petroleum Geologists Annual Convention and Exhibition, New Orleans, LA, Abstracts, v. 19, p. 23.
- Blackstone, D.L., Jr., 1993, Precambrian basement map of Wyoming; outcrop and structural configuration, 1 sheet, scale 1:500,000, *In*: Schmidt, C.J., Chase, R.B., Erslev, E.A., eds., 1993, Laramide basement deformation in the Rocky Mountain Foreland of the Western United States: GSA Special Paper 280, Plate 2, Sheet 1.
- Campbell-Stone, E., Lynds, R. Frost, C., Becker, T.P., and Diem, B., 2010, The Wyoming carbon underground storage project: geologic characterization of the Moxa Arch and Rock Springs Uplift: Energy Procedia, in press.
- Coogan, James C., 1992, Thrust systems and displacement transfer in the Wyoming-Idaho-Utah thrust belt: University of Wyoming, Thesis (Ph.D.), maps, scale 1:24,000.
- Garing, J.D., and Tainter, P.A., 1985, Greater Green River Basin regional seismic line, *in* Gries, R. R. and Dyer, R.C., eds., Seismic Exploration of the Rocky Mountain Region, Rocky Mountain Association of Geologists and Denver Geophysical Society, Denver, CO, p. 233-238.
- Hollis, Steve, ed., 1980, Stratigraphy of Wyoming: Wyoming Geological Association 31st Annual Field Conference guidebook.
- Love, J. D. (compiler), Christiansen, Ann Coe (compiler), Geologic map of Wyoming, U.S. Geological Survey, State Geologic Map, 3 sheets, 1985.
- Lynds, R., Campbell-Stone, E., Becker, T., and Frost, C.D., 2010, Stratigraphic evaluation of reservoir and seal in a natural CO₂ field: Lower Paleozoic, Moxa Arch, southwest Wyoming, Rocky Mountain Geology, v. 45, no. 2, 113-132.
- Miller, W.R., ed., 1987, The thrust belt revisited: Wyoming Geological Association 38th Field Conference Guidebook.

- Oriel, Steven S., 1963, Geologic Map of the Fort Hill Quadrangle, Lincoln county, Wyoming: Oil and Gas Investigations, Map OM-212, I sheet, scale 1:48,000.
- Oriel, Steven S., 1969, Geology of the Fort Hill Quadrangle, Lincoln county, Wyoming: Department of the Interior, United States Geologic Survey, Geologic Survey Professional Paper 594-M, map in 2 sheets, scale 1:62,500.
- Oriel, Steven S., Platt, Lucian B., 1980 Geologic map of the Preston 1° x 2° quadrangle, Southeastern Idaho and Western Wyoming: Department of the Interior, United States Geologic Survey, Map I-1127, 1 sheet, scale 1:250,000.
- Royse, F. Jr., 1993a, An overview of the geologic structure of the thrust belt in Wyoming, northern Utah, and eastern Idaho, Snoke, A.W., *in* Steidtmann, J.R., and Roberts, S.M., eds., Geology of Wyoming, The Geological Survey of Wyoming Memoir No. 5, v. 1: Laramie, Wyoming, Wyoming State Geological Survey, p. 273-311.
- Royse, Frank, Jr., 1993b, Eight regional structural cross sections in the Wyoming-Utah-Idaho thrust belt, 2 sheets, *In*: Snoke, Arthur W; Steidtmann, James R; Roberts, Sheila M., eds., An overview of the geologic structure of the thrust belt in Wyoming, northern Utah, and eastern Idaho, Memoir: Geological Survey of Wyoming, vol.5, pp. 272-311.
- Rubey, W.W., Oriel, S.S., Tracey, J.I., Jr., 1980, Geologic map and structure sections of the Cokeville 30-minute quadrangle, Lincoln and Sublette counties, Wyoming: Department of the Interior, United States Geologic Survey, Map I-1129, 2 sheets, scale 1:62,500.
- Stilwell, D.P., 1989, CO₂ resources of the Moxa Arch and the Madison reservoir: Wyoming Geological Association Guidebook, 40th Annual Field Conference, Guidebook, p. 105-115.
- Thyne, G.D., Tomasso, M., Bywater-Reyes, S.V., Budd, D.A., and Reyes, B.M., 2010, characterization of porosity and permeability for CO₂ sequestration models on the Mississippian Madison Group, Moxa Arch-La Barge Platform, southwestern Wyoming, Rocky Mountain Geology, v. 45, n. 2, p. 133-150.
- Wyoming State Geological Survey, 2008, Geologic strip map of the Overthrust Belt and western Green River Basin, 2 sheets, scale 1:125,000.
- Zenger, D.H., 1996, Dolomitization patterns in widespread “Bighorn Facies” (Upper Ordovician), Western Craton, USA: Carbonates and Evaporites, v. 11, p. 219-225.

Moxa Arch Carbon Sequestration Characterization
Task 4 and 5
Subsurface and Surface Structural Evaluation

FIGURES

Figure 1. Map of study area along the northwest-trending Moxa Arch in southwest Wyoming.

A.

B.

C.

Figure 2. Cross sections over the Moxa Arch based on compilation of well data and existing maps and cross sections (Blackstone, 1993; Coogan, 1992; Hollis, 1980; Love and Christiansen, 1985; Miller, 1987; Oriel 1963, 1969, 1980; Royse, 1993b; and Rubey et al., 1980; Wyoming State Geological Survey, 2008). A. Location map showing position of the cross sections. B. Cross section X-X'. C. Cross section Y-Y'.

Figure 3. 2-D example of surface picks from cross-line 177 derived from the Moxa Arch 3-D seismic dataset. Y-axis is in milliseconds.

Figure 4. 3-D model (in depth) created from seismic data showing the structure at the crest of the Moxa Arch. No vertical exaggeration has been applied. Green arrow points north, reds indicate shallower depths (thus the northern red portion of the seismic area is shallower than the southern orange portion). Interpreted surfaces are from the Nugget Sandstone through the Bighorn Dolomite. From top to bottom: blue = Nugget, light blue = Ankareh, lime green = Thaynes and Morgan, orange = Dinwoody, pink = Phosphoria, purple = Tensleep, light blue = Amsden, mint green = Madison, yellow = Jefferson and Three Forks, light pink = Bighorn, fuchsia = upper to middle Cambrian.

Figure 5. Fractures documented in Core 1 on the northern Moxa Arch (location shown on Figure 1) showing cross sectional area and orientation of fractures in the Bighorn Dolomite. Cross sectional area was calculated from measured length and width of the fracture plane. Orientation was measured in degrees from vertical.

Figure 6. Fractures documented in Core 2 from the western Wyoming fold-and-thrust belt (location shown on Figure 1) showing fracture density and orientation in the Bighorn Dolomite. Sub-vertical fractures per centimeter were measured in a core-perpendicular line and sub-horizontal fractures per centimeter were measured in a core-parallel line. The core is not oriented. Extremely fractured zones exhibit primarily sub-vertical fractures while low to moderately fractured zones have a majority of sub-horizontal fractures. Over 90% of the fractures documented in this core are mineralized. A. Core photograph and thin section image of moderately-fractured dolostone. Fractures are focused around mechanically deformed argillaceous clasts. Sub-vertical fractures intersect and cross-cut stylolites (chemical dissolution features). Large, white fracture is filled with dolomite and darker, branching fractures are filled with argillaceous material, dolomite, and insolubles. B. Core and thin section photographs of extremely-fractured dolostone. Core photo shows well-developed tension gashes filled with dolomite and an unidentified black material; tension gashes terminate at a stylolite at the top of the core. Photomicrograph shows large fractures with crystalline dolomite fill cut by later, narrow fractures filled with fine-grained dolomite (white). C. Core photograph and photomicrograph of highly-fractured dolostone. White spots seen in core are calcite- and dolomite-filled fractures and calcite-filled burrows. Photomicrograph details 0.7 mm wide sub-vertical fracture filled with euhedral calcite (stained pink) at base and darker microcrystalline dolomite toward top. This fracture was subsequently offset by a partially-filled sub-horizontal fracture. D. Core photograph and photomicrograph of breccia zone in highly-fractured dolostone. Dolostone breccia is matrix-supported by dolomite gouge-like material. Fractures filled with calcite (stained pink) cut the breccia clasts, and are later cut by narrow, open fractures (assumed to be natural and not induced by coring).

Figure 7. Core photograph from Core 1 (location shown on Figure 1) showing 2 mm of offset along a fracture in the Bighorn Dolomite.

B.

Figure 8: SEM analysis of Bighorn dolostone, from Core 2 (location shown on Figure 1). A. Scanned polished thin section of Bighorn dolostone, from 15550.8' depth. Sample shows shale layering with stylolites propagating from a shale clast, and calcite-filled fractures cutting the sample. Site location is noted on thin section. B. Scanning electron microscope (SEM) elemental results from a stylolite/fracture (shown as arc from upper left to lower right). The SEM image of the site location (lower left) is rotated approximately 90° clockwise. The diagonal dashed black lines are camera artifacts. Note the clay lining along the stylolite/fracture walls and calcite fill in the fracture.

Figure 9. A. Fractured surface of Bighorn Dolomite showing at least 3 generations of fractures. B. Fractured surface of the Death Canyon Member of the Gros Ventre Formation, in nearly the same location as A. The photographs were not taken from the same view direction, but various distinct fracture sets are discernable in each photo.

Figure 10. Rose diagrams comparing fracture orientations in the two geologic units shown in Figure 9. A. Rose diagram showing the trend of the fractures from the Bighorn Dolomite (Figure 9A). Two distinct fracture sets are obvious from the data, trending at right angles. B. Rose diagram of fracture trends from the Death Canyon Member of the Gros Ventre Formation (Figure 9B). The fracture sets at this location and stratigraphic level show a wider range of orientations than in A.

CHAPTER 6: Laboratory Experimental Activities: Mixed-Phase (CO₂+H₂O) Fluid-Rock Reactions

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Background

Researchers from Task 6 experimentally evaluated mixed-phase fluid rock reactions and processes within the Nugget Sandstone and its caprock, the Twin Creek Limestone, using rocking autoclaves and stirred reactors. Supercritical CO₂ was introduced into ongoing reactions to evaluate CO₂ trapping mechanisms and interactions with actual aquifer rocks and caprocks while in-situ fluid/gas sampling gauged reaction progress. Results from these batch experiments will be used to constrain computational models and design future, more complicated dynamic core flood experiments that will account for hydrodynamic flow. Results from this task follow.

Executive Summary

This Chapter is divided into three parts, each discussing a component of Task 6 activities.

Part I. Supercritical CO₂ and sulfur in the Madison Limestone: a natural analogue in southwest Wyoming for geologic carbon-sulfur co-sequestration

Emissions from coal-fired power plants contain sulfur as well as CO₂, thus successful capture and storage of anthropogenic CO₂ requires an understanding of geologic carbon-sulfur co-sequestration. The Madison Limestone on the Moxa Arch, southwest Wyoming, contains large volumes (65–95%) of supercritical CO₂ that it has stored naturally for 50 million years, supercritical H₂S, aqueous complexes of sulfur (SO₄²⁻ and HS⁻), and sulfur-bearing minerals (anhydrite, pyrite, and native sulfur). The natural co-occurrence of SO₄²⁻, S²⁻, supercritical CO₂ and brine affords the opportunity to evaluate how a carbon-sulfur co-sequestration scenario may evolve. We do not suggest that SO₂ was naturally introduced into the Madison Limestone, but we observe that SO₄²⁻ and S²⁻, the products of SO₂ disproportionation, are naturally present in the Madison Limestone. A simple equilibrium geochemical model of the Madison Limestone was constructed using mineralogic data obtained from well core and validated against published aqueous data. The model simulates reactions among supercritical CO₂, sulfur-bearing and accessory aluminosilicate minerals, and resident brine and accurately predicts crystallization of analcime, feldspar, and illite. Dawsonite (NaAlCO₃(OH)₂), an important carbon sink in numerous sequestration modeling studies, does not occur in the Madison Limestone. CO₂-brine-rock reactions in the model Madison Limestone-fluid system decrease pH, from 6.4 to 4.0, as expected from dissolution of supercritical CO₂ and dissociation of carbonic acid. In addition, redox potential increased from -0.26 to -0.06 volts due to equilibrium among CO₂, anhydrite, and pyrite. Final Eh-pH conditions correctly predict coexisting H₂S, aqueous SO₄²⁻, anhydrite, pyrite,

and native sulfur observed in produced waters and core. The Madison Limestone serves as a natural example of the thermodynamic end point that similar fluid-rock systems will develop following emplacement of a supercritical CO₂-sulfur mixture and is a natural analogue for geologic carbon-sulfur co-sequestration.

Part II. Nanoporosity in limestones and dolomites of the Madison Limestone

The behavior of CO₂ in geological carbon storage will depend on the pore size. Here we estimate that pores < 20 microns will not be accessible to CO₂ flow through capillary forces. However, in small pores, CO₂ will dissolve into the brine. Thus, the main impact of CO₂ injection on small pores is dissolution and precipitation of minerals. By using small angle neutron scattering we have shown that like many other rock types, pores in the Madison Limestone are fractally distributed. Based on data collected for samples of Madison Limestone, the dolomitization of limestone appears to change the structure of nanopores but not the total volume. Thus, over long time periods, geochemical reactions in small pores may change the structure of the pore enough to allow capillary flow of CO₂. Quantification of pore network evolution using fractal dimensions may provide information useful for validating results from sophisticated lattice Boltzmann models of pore-scale processes.

Part III. Geologic carbon-sulfur co-sequestration: experimental investigation of sulfur in a natural analogue, Madison Limestone of the Moxa Arch in SW Wyoming

We performed laboratory experiments to understand potential brine-rock-carbon-sulfur reactions that take place during co-injection of supercritical CO₂ and SO₂ into a carbonate reservoir. Initial experiments (250 bars, 110°C) evaluated supercritical CO₂-brine-rock and brine-rock reactions in a Na-Ca-Cl brine (I=0.52 M, 80 mM SO₄²⁻) and two different synthetic rock types: 83% Do, 10% Cc, 6% Anh, 1% Py and 86% Do, 13% Cc, 1% Py. The synthetic rock is composed of 75% chips for textural analysis, 0.5–3.0 mm in size, and 25% powder (<45 µm) to enhance reaction rates. Fluid samples are collected in a time series throughout the experiment. On reaching steady state (~1080 hrs) supercritical CO₂ is injected into the ongoing reaction.

After injection, the dissolved CO₂ concentration in the brine of the Do-Cc-Anh-Py experiment increased from 1mM to 1.27 M (5.1% dissolved), and bench pH decreased from 7.4 to 6.4. In the Do-Cc-Py experiment, dissolved CO₂ increased from 0.78 mM to 1.22 M (5.1% dissolved) and bench pH decreased from 8.8 to 6.6. CO₂ injection mobilized Ba, Fe, Mn, Ni and Zn in both experiments. XRD and SEM data suggest calcite dissolved from the powders and re-precipitated as newly formed calcite. A decrease in Ca and SO₄²⁻ concentrations in both experiments suggests anhydrite precipitation. Calcite and anhydrite mineralization in the experiments is consistent with petrologic observations of the Madison Limestone. The injection of CO₂ drives the SO₄²⁻ concentrations down as the system is saturated with supercritical CO₂.

Part I. Supercritical CO₂ and sulfur in the Madison Limestone: a natural analogue in southwest Wyoming for geologic carbon-sulfur co-sequestration

Introduction

Geologic sequestration of CO₂ generated by coal-fired power plants is a critical component of Carbon Capture and Storage (CCS) (Pacala and Socolow, 2004). In addition to CO₂, coal combustion generates SO_x, NO_x, and other constituents (Thambimuthu et al., 2005). Purity requirements for CO₂ injected into a geologic reservoir are being debated worldwide and have yet to be established (Gale, 2009). Conventional CO₂ separation technologies (e.g., methyl ethanolamine absorption and stripping) that can be retrofitted to existing power plants yield CO₂ that is greater than 90% pure (Rao and Rubin, 2002). However, these technologies impose large parasitic energy costs of 30 to 40% of the net power plant output (Rao and Rubin, 2002). In addition, even just a few tenths of a percent of the common impurities (e.g., SO_x and NO_x) will influence the geochemistry of a water-rock system. Novel technologies such as oxy-fuel combustion and integrated gasification combined cycle (IGCC) power plants dramatically reduce parasitic energy costs but also produce higher levels of impurities in the combustion products (Apps, 2006). In either case, any industrial process is susceptible to off-normal occurrences and accidents that may inadvertently introduce impurities into the CO₂ that is injected into the geologic storage reservoir. Geologic sequestration of CO₂ that contains impurities is known as co-sequestration, a term first used with reference to co-injected CO₂ and H₂S (Williams, 2002). What are the geochemical effects of co-injected impurities on a geologic storage reservoir and its caprock? Can an understanding of the geochemical behavior of these impurities be integrated with separation strategies to optimize disposal of co-injected combustion gasses?

Natural accumulations of CO₂ in the crust provide analogues to geologic formations that will become artificially charged with anthropogenic CO₂ (Allis et al., 2001). These natural analogues have stored CO₂ for geologically significant time and provide a means of understanding and predicting how CO₂ will behave in a carbon repository. Initial studies of natural analogues focused on the Colorado Plateau and the Southern Rocky Mountains, including Bravo Dome in New Mexico, McElmo Dome and Sheep Mountain in Colorado, Farnham Dome in Utah, and the Springerville–St. Johns field in Arizona and New Mexico (Allis et al., 2001; Gilfillan et al., 2008; Gilfillan et al., 2009; Moore et al., 2005; Pearce et al., 1996; Stevens et al., 2001). Natural gas fields containing significant amounts of CO₂ (28 to 50 mol%) have also been studied as natural analogues (Lu et al., 2009; Wilkinson et al., 2009). To our knowledge, a suitable natural analogue for carbon-sulfur co-sequestration has not been described in the literature.

The Mississippian Madison Limestone on the Moxa Arch of southwest Wyoming is recognized as a natural analogue for geologic carbon sequestration (Allis et al., 2001). Several other Paleozoic formations on the Moxa Arch also contain natural accumulations of supercritical CO₂ (De Bruin, 1991), thus the Moxa Arch houses multiple natural analogues to geologic carbon sequestration. In addition to supercritical CO₂, the Madison Limestone contains sulfur in multiple oxidation states, including SO₄²⁻ in anhydrite and formation waters, S²⁻ in pyrite and as H₂S gas, and S⁰ in native sulfur. While SO₂ was not introduced into the Madison Limestone, these sulfur-bearing phases are known products of SO₂ reaction in other water-rock systems. The natural co-occurrence of aqueous and mineral SO₄²⁻, S²⁻, and S⁰ with supercritical CO₂ and brine

in the Madison Limestone affords the opportunity to evaluate how a carbon-sulfur co-sequestration scenario may evolve.

We present mineralogic data obtained from drill core and aqueous geochemical data from wells that penetrate the Madison Limestone on the Moxa Arch. We use these data to constrain geochemical reactions within the Madison Limestone supercritical CO₂-sulfur-brine-rock system, especially reactions among the sulfur-bearing and aluminosilicate accessory minerals that are present. Geochemical reactions among these accessory minerals and coexisting fluids serve to elucidate multiphase fluid (CO₂ + H₂O)-rock interactions in a carbonate-dominated system. We construct a geochemical model of this system based on the mineralogy and aqueous geochemistry, validate the model against published aqueous data, and illustrate modeling results using activity diagrams. The model suggests that the Madison Limestone fluid-rock system is at thermodynamic equilibrium and provides insight into the geochemical behavior of CO₂ and sulfur that naturally reside in the Madison Limestone on the Moxa Arch. Understanding this natural supercritical CO₂-sulfur-brine-rock system helps clarify potential long-term storage behavior of reactive CO₂ and sulfur in a carbonate reservoir and demonstrates the utility of the Madison Limestone as a natural analogue for carbon-sulfur co-sequestration. Our analysis also provides insight into fluid-rock interactions that take place during acid gas storage.

SO₂ Reactions in Water-Rock Systems

The essential problem facing geologic co-sequestration of a CO₂-SO₂ mixture is that SO₂, the most abundant constituent in SO_x, is very reactive in water-rock systems. Several reactions have been discussed in the literature, including hydrolysis of SO₂ to produce sulfurous acid, a weak acid (Ellis et al., 2010):

Reaction (1) can only proceed if no geochemical redox reactions involving SO₂ take place. Under strongly oxidizing conditions SO₂ reacts to produce sulfuric acid, a strong acid (Ellis et al., 2010):

SO₂ can also react with steam to produce sulfuric acid and hydrogen gas (Symonds et al., 2001):

but this reaction is limited to the gas phase. SO₂ reacts in water rock systems to form native sulfur and sulfuric acid by undergoing a disproportionation reaction (Holland, 1965):

Finally, SO₂ also reacts in water-rock systems to form sulfuric acid and hydrogen sulfide, a weak acid, by a different disproportionation reaction (Getahun et al., 1996; Holland, 1965; Symonds et al., 2001):

Disproportionation of SO_2 to form sulfuric acid and aqueous hydrogen sulfide is the predominant reaction in a variety of water-rock systems spanning a wide range of geochemical conditions (Getahun et al., 1996; Holland, 1965; Symonds et al., 2001), including the geochemical conditions of the Madison Limestone. SO_2 disproportionation to form sulfuric acid and hydrogen sulfide is also believed to be the predominant reaction for SO_2 in geologic carbon sequestration scenarios (Palandri and Kharaka, 2005; Palandri et al., 2005; Xu et al., 2007). Once formed, subsequent dissociation of sulfuric acid and aqueous hydrogen sulfide generates acidity. Significant changes to pH, the master variable of aqueous systems, perturb a wide range of water-rock reactions and processes and transform the manner in which the geochemistry of the system ultimately evolves.

Several types of fluid injection and disposal operations are somewhat comparable to large-scale CO_2 - SO_2 co-sequestration. For roughly 20 years, the oil and gas industry has disposed of H_2S by injection of CO_2 - H_2S mixtures into the subsurface (Bennion and Bachu, 2008; Chakma, 1997). An H_2S - CO_2 mixture, or acid gas, is the byproduct of “sweetening” hydrocarbons that contain H_2S , or sour hydrocarbons (Machel, 2005). Interest in CCS has spawned a new industrial paradigm coupling acid gas disposal to geologic carbon sequestration (Bennion and Bachu, 2008; Gunter et al., 2000; Machel, 2005). Within this paradigm, laboratory experiments have been performed to evaluate the effects of CO_2 - H_2S mixtures on the relative permeability of reservoir rocks (Bennion and Bachu, 2008) and the geochemistry of wellbore cements (Jacquemet et al., 2005; Jacquemet et al., 2008; Pironon et al., 2007). Experimental constraints restricted the latter to elevated temperatures and pressures (200°C and 50 MPa), from which the authors extrapolated to reservoir conditions. A recently completed field experiment injected 35,000 tons of a 70% CO_2 -30% H_2S mixture into a carbonate oil reservoir, the Zama oilfield, in Alberta, Canada (DOE Fossil Energy Techline, 2010).

The practice of deep well injection of acidic liquids into geologic formations is also well established. Acid injection in hydrocarbon production is a known technique to stimulate reservoir permeability (Hendrickson et al., 1992), and H_2SO_4 -bearing waste has been disposed by injection into subsurface carbonate formations (de Graaff, 1998). Finally, CO_2 - H_2S co-injection is planned for waste gas produced by the Hellisheidi geothermal power plant in southwest Iceland (Gislason et al., 2010).

The smattering of published research focused on CO_2 - SO_2 co-sequestration is largely computational. Most of these modeling studies predict that CO_2 - SO_2 co-sequestration will produce highly reactive water-rock systems (Gunter et al., 2000; Knauss et al., 2005; Palandri and Kharaka, 2005; Xu et al., 2007). Predicted outcomes include: 1) extreme acidity (to pH 1); 2) iron reduction and subsequent siderite precipitation; 3) precipitation of sulfate minerals as a sulfur trapping mechanism; 4) significant development of mineral alteration zones near points of injection; and 5) redistribution of porosity between mineral alteration zones and repository margins. In contrast, two modeling studies predict that CO_2 - SO_2 co-sequestration will not yield highly reactive water-rock systems because SO_2 will not readily diffuse out of the co-injected supercritical CO_2 and into coexisting brine (Crandell et al., 2010; Ellis et al., 2010).

Only two relevant experimental studies have been published. One evaluates the potential for SO_2 to reduce Fe^{3+} to Fe^{2+} and promote siderite precipitation (Palandri et al., 2005). The second

suggests that small amounts of SO₂ (<1 mol%) do not interfere with CO₂ sequestration, as compared to baseline CO₂ sequestration experiments without SO₂ (Nogueira and Mamora, 2008).

Our understanding of the geochemical behavior of SO₂ relative to geologic carbon sequestration is obviously limited. Assumptions and conflicting model predictions regarding SO₂ reactivity require testing and evaluation in natural as well as experimental systems, especially because multiphase fluid (CO₂-H₂O)-rock processes are exceedingly complex and often defy standard geochemical expectations (Kaszuba et al., 2003, 2005). For example, processes coupled to the reactivity and acidity of a multiphase fluid-rock system, such as mobilization and re-precipitation of silica, could armor and protect flow paths or plug them (Kaszuba and Janecky, 2009; Kaszuba et al., 2005).

Geologic Setting of Southwest Wyoming

The Moxa Arch is a 200-km-long, north-south trending Cretaceous uplift (Kraig et al., 1987) located in southwestern Wyoming (Figure 6-1). It is bound on the west by the Laramide Overthrust Belt and on the east by the Rock Springs Uplift. Paleozoic rocks, including the Mississippian Madison Limestone, contain CO₂ (between 65 and 95 vol%), CH₄ (up to 22%), N₂ (up to 7%), H₂S (up to 4.5%), and He (up to 0.5%) (De Bruin, 1991). Data from drill core within the gas cap show gas saturation values ranging from only a few percent to as high as 90% of the pore space (Wyoming Oil and Gas Conservation Commission, 2010). These rocks are at depths greater than 2000 meters, thus temperatures and pressures exceed the critical points of CO₂ (30.98°C, 7.38 MPa), CH₄ (-82.7°C, 4.596 MPa), and H₂S (100°C, 8.937 MPa) and these fluids occur in the supercritical state. The CO₂ was probably emplaced 50 million years ago in association with mantle-derived magmatic sources (Huang et al., 2007). The volume of CO₂ has been estimated at 114 trillion cubic feet (tcf) (3.23 x 10¹² cubic meters) in the Madison Limestone and 240 tcf (6.80 x 10¹² cubic meters) within the entire Paleozoic section (De Bruin, 1991).

Methods and Approach

A limited number of drill cores and water analyses exist for the Madison Limestone on the Moxa Arch. Nonetheless, enough of these data are available to constrain supercritical CO₂-sulfur-brine-rock interactions and to develop a geochemical model for these interactions. Samples of Madison Limestone from the Moxa Arch were collected from drill core available at the Core Research Center of the U.S. Geological Survey (USGS, 2010). Three wells defining a broad transect across the southern portion of the Moxa Arch were chosen for study. The Chevron Federal 1-29 and Union Pacific RR #4 are located on the western and eastern margins of the Arch, respectively, whereas the Church Buttes #31 is located on the crest of the Arch (Figure 6-1). Four samples from different depths within each of the three wells were evaluated (Figure 6-1, Table 6-1).

Mineralogy and petrology of the twelve samples were determined using X-ray diffraction (XRD), scanning electron microscopy (SEM), and standard petrographic thin section techniques. Samples for whole rock XRD analysis were ground and sieved to 325 mesh (less than 45 micron diameter) and analyzed from 2° to 70° 2θ using a SCINTAG XDS2000 powder diffractometer.

Once whole rock XRD analysis was completed the powdered samples were prepared for clay analysis. Each sample was suspended in a deflocculant (Calgon) by sonification and subsequently permitted to settle for approximately 2.5 hours. Clay fractions (less than 2 micron diameter) were separated from the rock powder by decanting the liquid. An oriented clay mount was prepared from the decanted material using vacuum filtration. Oriented clay samples were analyzed from 2° to 35° 2 θ using the SCINTAG XDS2000.

Available analyses of Madison Limestone formation waters were compiled from the USGS Produced Waters Database (Breit and Skinner, 2002) and the Wyoming Oil and Gas Conservation Commission website (WOGCC, 2010). The quality of these data was evaluated using charge and mass balance criteria. Samples exceeding $\pm 10\%$ charge or mass balance were excluded from consideration, resulting in a total of 14 acceptable water analyses (Table 6-2). In-situ temperature was calculated for each sample by comparing sample depth and regional geothermal gradient (22.4°C/km, 6.8°F/1000 feet). Potassium analyses were not reported for several samples. For these samples we estimated potassium concentrations based on Na:K ratios of the other samples. Water analyses were speciated using Geochemist's Workbench (GWB) version 8 (Bethke and Yeakel, 2009) to calculate ion activities for plotting on stability diagrams.

Our strategy is to constrain reactions within the supercritical CO₂-sulfur-brine-rock system by constructing a geochemical model using the actual mineralogy and aqueous geochemistry of the Madison Limestone. We validate and illustrate modeling results using activity diagrams that depict relationships for sulfur-bearing and aluminosilicate accessory minerals and provide insight into fluid-rock interactions in a carbonate-dominated system. For this investigation we use an equilibrium rather than kinetic model because of the elevated temperatures in the Madison Limestone (Table 6-2) and because fluid-rock reaction rates are fast relative to the long residence time of CO₂ (Huang et al., 2007) in the Madison Limestone. Our use of an equilibrium model also permits us to test whether the Madison Limestone is at equilibrium and to evaluate the efficacy of equilibrium models for evaluating long-term storage behavior of reactive carbon and sulfur. Simulations of sequestration injection scenarios will require kinetic models since the primary interest will be on short-term reactions and CO₂ mobility.

Numerical simulations were performed using GWB (Bethke and Yeakel, 2009), the database thermo.com.v8.r6+.dat and the B-dot ion association model. The partitioning constant of CO₂ into water that is resident in GWB was adjusted according to the equation of state of Duan et al. (2006). Since none of the brine analyses reported Si, Fe, or Al concentrations, values consistent with quartz equilibrium for Si, pyrite equilibrium for Fe and 10 parts per billion (ppb) total Al were assumed as initial values. Providing initial Si, Fe, and Al values are necessary to allow numeric stability during the reaction path calculation. The model is also constrained by specifying equilibrium with other minerals present in the Madison Limestone (anhydrite, dolomite, calcite, and illite, Table 6-1). Minerals not present in the Madison Limestone are suppressed from participating in reaction path calculations.

Results

Mineralogy and Petrography

The Madison Limestone on the Moxa Arch is a dolostone due to widespread early dolomitization (Budai et al., 1987). Euhedral dolomite (Figure 6-2) is the only carbonate mineral identified in seven of the samples and the predominant carbonate mineral, relative to calcite, in another four samples (Table 6-1). Calcite occurs mostly within pores and fractures in these four samples. Calcite is the only carbonate mineral identified in one sample from drill core, the Church Buttes #31 on the crest of the Arch at a depth of 5691 meters (Figure 6-1, Table 6-1). Interiors of dolomite grains in many samples are cloudy when viewed under plane polarized light whereas the edges are clear due to the presence or absence of fine-grained inclusions, respectively. Alternating bands of Fe-rich and Fe-poor dolomite are observed on grain margins, suggesting mineral recrystallization and a complicated fluid history.

In addition to dolomite and calcite, the Madison Limestone contains sulfur-bearing and aluminosilicate accessory minerals. Secondary anhydrite occurs in at least two samples from each of the drill cores (Table 6-1) as optically-continuous pore-filling precipitates and as secondary fracture fill (Figure 6-2). Gypsum casts filled with chert are observed in the Union Pacific RR #4 well at the 2391 meter interval, but gypsum was not identified optically or by XRD analysis. Recrystallized interstitial pyrite occurs in the Church Buttes #31 and Union Pacific RR #4 drill cores (Table 6-1, Figure 6-3). Native sulfur fills pores between euhedral dolomite crystals in one sample, the Union Pacific RR #4 at the 2368 meter interval (Figure 6-4).

Accessory quartz, feldspar, analcime, and illite are present in the Madison Limestone (Table 6-1). Interstitial quartz (Figure 6-2b) and chert cement occur in about half of the samples from each of the three drill cores. Small feldspar peaks are observed in XRD data for one sample of drill core, the Union Pacific RR #4 at the 2391 meter interval. Analcime was identified optically and by XRD analysis in one sample from each of the three drill cores (Table 6-1, Figure 6-2d). It occurs as euhedral grains interstitial to dolomite crystals in samples that contain no quartz. Illite is the only clay mineral identified by XRD analysis. It occurs in half of the samples from the Chevron Federal 1-29 and Union Pacific RR #4 drill cores.

Geochemical modeling

Our conceptual model assumes that the Madison Limestone outside the gas cap on the Moxa Arch represents burial diagenesis of this formation. Thus we choose as a starting fluid composition a representative water analysis from a well outside, but at a similar depth to, the gas cap (Champlin #549, Table 6-2). Since the timing of CO₂ emplacement is poorly constrained, we start the model at current burial conditions of 90°C and 35 MPa. On an Eh-pH diagram, the composition of the aqueous solution at these initial conditions plots on the phase boundary between the pyrite and anhydrite stability fields (Figure 6-5). CO₂ is subsequently injected into this ideal Madison Limestone-fluid system until final CO₂ values reach approximately 35 MPa.

Addition of CO₂ establishes a reaction path along the anhydrite-pyrite phase boundary such that pH decreases and Eh increases (Figure 6-5). pH decreases from 6.4 to 4.0 due to dissolution of CO₂ into the brine and the resulting dissociation of carbonic acid. An Eh increase of approximately 0.2 volts accompanies addition of CO₂ and the concomitant pH decrease. The

endpoint of this reaction path is near the junction of the stability fields of pyrite, anhydrite, native sulfur, and H₂S (Figure 6-5).

The simulation captures the fundamental changes expected in a Madison Limestone-brine system into which CO₂ is added. Total dissolved solids (TDS) increase with reaction progress to 75,000 mg kg⁻¹, mostly due to dissolution of calcite and an increase in dissolved bicarbonate. Simulating the production of fluid from 90°C and 35 MPa to surface temperature and pressure lowers dissolved CO₂, decreases dissolved bicarbonate and increases pH as a consequence of cooling and de-pressurization of the fluid, yielding water with a TDS value of 24,103 mg kg⁻¹. TDS values observed in formation water samples produced from the gas cap on the Moxa Arch (Tip Top Field, unit #22-19, Table 6-2) are 28,660 mg kg⁻¹, uncorrected for changes during production. Thus the composition of the final aqueous solution calculated by the model is both reasonable and very similar to water produced from the gas cap of the Moxa Arch.

The simulation also accurately predicts mineral assemblages that are observed in the Madison Limestone. Mineral stability diagrams that depict the activity of sodium versus silica and potassium versus silica are presented in Figures 6-6 and 6-7, respectively. Stability fields are plotted at both 90 and 110°C, temperatures bracketing those found in the Madison Limestone. Also plotted on Figures 6-6 and 6-7 are analyses of formation waters presented in Table 6-2. Formation waters in the CO₂ gas cap plot within the predicted stability fields for muscovite, albite, and microcline and within or adjacent to the predicted stability field for analcime. This assemblage compares well with the actual aluminosilicate mineral assemblage observed in drill core samples (Table 6-1). The presence of analcime in the Madison Limestone and in our geochemical models is also consistent with analcime crystallization in experiments emulating injection of supercritical CO₂ into a brine-rock system (Kaszuba et al., 2003, 2005). Finally, the endpoint of the reaction path in the Eh-pH diagram (Figure 6-5) predicts the same mineral assemblage (pyrite + anhydrite + native sulfur) that is observed in the drill cores (Table 6-1 and Figures 6-2, 6-3, and 6-4).

Carbon and Sulfur in the Madison Limestone

Supercritical CO₂ and multiple phases of sulfur (aqueous SO₄²⁻ and HS⁻, supercritical H₂S, anhydrite, pyrite, and native sulfur) are in thermodynamic equilibrium in the Madison Limestone on the Moxa Arch. The mineralogy and aqueous geochemistry of this brine-rock system offer endpoints in the likely reaction path of SO₂ disproportionation and provide insight for sulfur behavior during co-sequestration. The Madison Limestone thus serves as an analogue for long-term storage conditions for geologic co-sequestration of reactive carbon and sulfur.

Several modeling studies predict crystallization of dawsonite, NaAlCO₃(OH)₂, in carbon repositories (Johnson et al., 2001; Knauss et al., 2005; Xu et al., 2004; Xu et al., 2007; Zerai et al., 2006) and enhanced oil recovery projects (Cantucci et al., 2009). However, dawsonite is rarely observed in natural analogues (Klusman, 2003; Moore et al., 2005; Pearce et al., 1996; Wilkinson et al., 2009) and does not form in laboratory experiments that emulate a carbon repository (Hangx and Spiers, 2009; Kaszuba et al., 2003, 2005; Newell et al., 2008; Pearce et al., 1996). Consequently, the importance of dawsonite to CCS is the subject of ongoing debate (Bénézech et al., 2007; Hellevang et al., 2005; Wilkinson et al., 2009). XRD, SEM, and petrographic analysis revealed no dawsonite in the Madison Limestone, nor has any been

reported in previous studies of this formation (Budai et al., 1984; Budai et al., 1987; Meuzelaar et al., 2010). Instead, Al-bearing minerals in the Madison Limestone are analcime, feldspar, and illite whereas carbonate minerals are limited to dolomite and calcite. Our results suggest that dawsonite will not be an important carbon sink for long-term geologic carbon sequestration.

The geochemical model predicted the well-known pH decrease that accompanies addition of CO₂ to a water-rock system (Figure 6-5). The magnitude of the predicted decrease, roughly 2.5 pH units, is consistent with experimental (Kaszuba et al., 2003, 2005) and computational (Gunter et al., 2000) studies as well as with field studies of enhanced oil recovery (Bowker and Shuler, 1991) and pilot-scale sequestration projects (Kharaka et al., 2006) in siliciclastic reservoirs. In-situ pH data is not available for the Madison Limestone on the Moxa Arch. To our knowledge, in-situ pH has only been calculated, not measured, for carbonate reservoirs hosting enhanced oil recovery or pilot-scale sequestration projects. The Weyburn Oil Field, for example, is a carbonate reservoir that has been the site of both enhanced oil recovery and carbon sequestration. In-situ pH values of 6.8 to 6.9 and 5.1 to 5.3 are calculated for pre- and post-CO₂ emplacement, respectively (Cantucci et al., 2009). This calculated pH decrease (up to 1.8 pH units) compares favorably with values calculated in this study.

In the geochemical model, Eh increased as CO₂ was added. Final Eh-pH conditions place the solution at the junction of the stability fields of pyrite, anhydrite, native sulfur, and H₂S (Figure 6-5) suggesting that Eh may be controlled by equilibrium among the sulfur species. SO₂ disproportionation to sulfuric acid and hydrogen sulfide takes place in a variety of water-rock systems and is proposed as the predominant SO₂ reaction in geologic carbon sequestration scenarios (Palandri and Kharaka, 2005; Palandri et al., 2005; Xu et al., 2007). The natural co-occurrence of sulfur in multiple oxidation states, including SO₄²⁻ in anhydrite and formation waters, S²⁻ in pyrite and as H₂S gas, and S⁰ in native sulfur, together with supercritical CO₂ and brine affords the opportunity to evaluate how SO₂ reaction products may evolve in a carbon-sulfur co-sequestration scenario. This is not to suggest that SO₂ was naturally introduced into the Madison Limestone, only that both SO₄²⁻ and S²⁻, the products of SO₂ disproportionation, are naturally present in the Madison Limestone. Geochemical modeling of CO₂-SO₂ co-injection into a water-rock system predicts alunite, anhydrite, and pyrite precipitation (Xu et al., 2007). With the exception of alunite, these sulfur-bearing minerals are also present in the Madison Limestone.

To evaluate how a carbon-sulfur co-sequestration scenario might actually evolve in a carbonate reservoir we modified the geochemical model by adding 100 ppm SO₂ and repeated the calculations. In this revised calculation, SO₂ reacts according to equation (5) and produces a reaction path that coincides with the reaction path plotted in Figure 6-5. This revised model predicts SO₂ disproportionation leading to the same mineral assemblage and fluid chemistry as observed in the Madison Limestone on the Moxa Arch, reinforcing our conclusion that the Madison Limestone can serve as a natural analogue to geologic carbon-sulfur co-sequestration.

Identifying the source or sources for CO₂ and H₂S in the Madison Limestone on the Moxa Arch is beyond the scope of this study. CO₂ in fields on the Colorado Plateau and in the Southern Rocky Mountains, including Bravo Dome in New Mexico, McElmo Dome and Sheep Mountain in Colorado, Farnham Dome in Utah, and the Springerville–St. Johns field in Arizona and New

Mexico, is derived from mantle sources as determined by noble gas isotopes (Gilfillan et al., 2008). CO₂ on the Moxa Arch is also believed to be derived from mantle sources (Huang et al., 2007), although definitive geochemical data have yet to be published. H₂S is generated by a variety of natural processes that include thermogenic sulfate reduction and methane-anhydrite reactions (Cross et al., 2004; Machel et al., 1995). The intriguing possibility for the Madison Limestone is that supercritical CO₂ emplacement drove Eh-pH reactions and enhanced sulfate reduction to produce both methane and native sulfur.

Geochemical reactions among sulfur-bearing and aluminosilicate accessory minerals in the Madison Limestone on the Moxa Arch elucidate multiphase fluid (CO₂ + H₂O)-rock interactions and provide insight into the behavior of CO₂ and sulfur that naturally reside in a carbonate-dominated system. Understanding this supercritical CO₂-sulfur-brine-rock system provides insight into long-term storage behavior of reactive CO₂ and sulfur in a carbonate reservoir. Long-term storage behavior is the last of several stages in the life cycle of a carbon repository (Benson and Cook, 2005). Dynamic processes that accompany initial CO₂ injection, such as hydrodynamic flow and kinetic reactions, are beyond the scope of this paper but represent fruitful areas of future research. Identifying short term reactions in reservoirs and caprocks and determining the potential importance of metastable phases and intermediate reaction steps are critically important to understanding the short-term fate of sulfur introduced with CO₂, particularly for developing accurate risk assessments. Will SO₂ be mobile and reactive or will SO₂ persist within supercritical CO₂ because of limited diffusivity, as suggested by theoretical calculations (Crandell et al., 2010; Ellis et al., 2010)? Detailed petrographic and isotopic studies of the Madison Limestone and other formations on the Moxa Arch as well as relevant laboratory experiments are needed to address these questions.

Conclusions

A relatively simple equilibrium model of the Madison Limestone was constructed using mineralogic data and published water analyses to describe reactions among supercritical CO₂, Madison Limestone, and resident formation water. The model makes accurate predictions for crystallization of sulfur-bearing and accessory aluminosilicate minerals and captures the fundamental changes expected in a Madison Limestone-brine system into which CO₂ is added. The following are concluded:

- 1) The Madison Limestone-fluid system appears to be in thermodynamic equilibrium as determined by mineralogy and aqueous geochemistry of formation brines.
- 2) CO₂ was introduced into portions of the Madison Limestone and has been stored naturally for approximately 50 million years (Huang et al., 2007). Adding CO₂ to the model Madison Limestone-brine system decreases pH and increases both Eh and TDS. Final Eh-pH conditions predict the coexisting sulfur-bearing phases (pyrite, anhydrite, native sulfur, and H₂S) that are observed in core samples and produced waters. Eh may be controlled by equilibrium among CO₂ and the sulfur-bearing phases.
- 3) Multiple sulfur phases (aqueous SO₄²⁻ and HS⁻, supercritical H₂S, recrystallized anhydrite and pyrite, and native sulfur) predicted by the model and observed in the natural CO₂-brine-rock system offer thermodynamic endpoints in likely reaction paths and are a good indication of the fate of sulfur during carbon-sulfur co-sequestration.
- 4) Dolomite and calcite are the carbonate minerals in the Madison Limestone whereas the aluminum-bearing minerals are analcime, feldspar, and illite. No dawsonite, NaAlCO₃(OH)₂,

is observed. Although dawsonite is an important carbon sink in numerous sequestration modeling studies, the mineralogy of the Madison Limestone suggests that dawsonite will not be important to geologic carbon sequestration in carbonate reservoirs.

- 5) Geochemical reactions among sulfur-bearing and aluminosilicate accessory minerals in the Madison Limestone on the Moxa Arch elucidate multiphase fluid ($\text{CO}_2 + \text{H}_2\text{O}$)-rock interactions and provide insight into the behavior of CO_2 and sulfur that naturally reside in a carbonate-dominated reservoir. Thus the Madison Limestone on the Moxa Arch serves as a natural analogue for long-term geologic co-sequestration of reactive carbon and sulfur.

References

- Allis, R., Chidsey, T., Gwynn, W., Morgan, C., White, S., Adams, M., and Moore, J., 2001. Natural CO_2 reservoirs on the Colorado Plateau and Southern Rocky Mountains: Candidates for CO_2 sequestration. Proceedings of the First National Conference on Carbon Sequestration.
- Apps, J.A., 2006. A review of hazardous chemical species associated with CO_2 capture from coal-fired power plants and their potential fate in CO_2 geologic storage. Lawrence Berkeley National Lab.
http://esd.lbl.gov/FILES/research/programs/gcs/projects/storage_resources/report_2_EPA_Apps_LBNLReport57931.pdf. 59 p.
- Bénézech, P., Palmer, D.A., Anovitz, L.M., and Horita, J., 2007. Dawsonite synthesis and reevaluation of its thermodynamic properties from solubility measurements: Implications for mineral trapping of CO_2 . *Geochim. Cosmochim. Acta* 71, 4438-4455.
- Bennion, D.B., and Bachu, S., 2008. Drainage and imbibition relative permeability relationships for supercritical CO_2 /brine and H_2S /brine systems in intergranular sandstone, carbonate, shale, and anhydrite rocks, *Soc Petroleum Eng*, p. 487-496.
- Benson, S., and Cook, P., 2005. Underground geological storage, *in* Metz, B., Davidson, O., Coninck, H.d., Loos, M., and Meyer, L., eds., IPCC Special Report on CO_2 Capture and Storage, p. 195-276.
- Bethke, C.M., and Yeakel, S., 2009. The Geochemist's Workbench Release 8.0: Reaction Modeling Guide: Champaign, Illinois, University of Illinois, 84 p.
- Bowker, K.A., and Shuler, P.J., 1991. Carbon dioxide injection and resultant alteration of the Weber Sandstone, Rangely Field, Colorado. *AAPG Bull.* 75, 1489-1499.
- Breit, G.N., and Skinner, C., 2002. USGS Produced Waters Database.
<http://energy.cr.usgs.gov/prov/prodwat/index.htm>, last accessed September 18, 2010.
- Budai, J.M., Lohmann, K.C., and Owen, R.M., 1984. Burial dedolomite in the Mississippian Madison Limestone, Wyoming and Utah Thrust Belt. *Journal of Sedimentary Petrology* 54, 276-288.
- Budai, J.M., Lohmann, K.C., and Wilson, J.L., 1987. Dolomitization of the Madison Group, Wyoming and Utah Overthrust Belt. *AAPG Bull.* 71, 909-924.
- Cantucci, B., Montegrossi, G., Vaselli, O., Tassi, F., Quattrocchi, F., and Perkins, E.H., 2009. Geochemical modeling of CO_2 storage in deep reservoirs: The Weyburn Project (Canada) case study. *Chem. Geol.* 265, 181-197.
- Chakma, A., 1997. Acid gas re-injection - A practical way to eliminate CO_2 emissions from gas processing plants. *Energy Convers. Mgmt* 38, S205-S209.

- Crandell, L.E., Ellis, B.R., and Peters, C.A., 2010. Dissolution potential of SO₂ co-injected with CO₂ in geologic sequestration. *Environ. Sci. Technol.* 44, 349-355.
- Cross, M.M., Manning, D.A.C., Bottrell, S.H., and Worden, R.H., 2004. Thermochemical sulphate reduction (TSR): experimental determination of reaction kinetics and implications of the observed reaction rates for petroleum reservoirs. *Organic Geochemistry* 35, 393-404.
- De Bruin, R.H., 1991. Wyoming's carbon dioxide resources. Wyoming State Geological Survey. 20 p.
- de Graaff, J.W.P., 1998. Acidic waste disposal by underground injection. *J. Geochem. Exp.* 62, 325-329.
- DOE Fossil Energy Techline, 2010. Project successfully demonstrates important CCS components, including CO₂ storage, H₂S disposal, EOR. http://www.fossil.energy.gov/news/techlines/2010/10046-PCOR_Project_Demonstrates_Importan.html, last accessed October 16, 2010.
- Duan, Z.H., Sun, R., Zhu, C., and Chou, I., 2006. An improved model for calculation of CO₂ solubility in aqueous solutions containing Na⁺, K⁺, Ca²⁺, Mg²⁺, Cl⁻, and SO₄²⁻. *Marine Chem.* 98, 131-139.
- Ellis, B.R., Crandell, L.E., and Peters, C.A., 2010. Limitations for brine acidification due to SO₂ co-injection in geologic carbon sequestration. *Int. J. Greenhouse Gas Control* 4, 575-582.
- Gale, J., 2009. Impure thoughts. *Int. J. Greenhouse Gas Control* 3, 1-2.
- Getahun, A., Reed, M.H., and Symonds, R., 1996. Mount St Augustine volcano fumarole wall rock alteration: Mineralogy, zoning, composition and numerical models of its formation process. *J. Volcanol. Geotherm. Res.* 71, 73-107.
- Gilfillan, S.M., Ballentine, C.J., Holland, G., Blagburn, D., Lollar, B.S., Stevens, S., Schoell, M., and Cassidy, M., 2008. The noble gas geochemistry of natural CO₂ gas reservoirs from the Colorado Plateau and Rocky Mountain provinces, USA. *Geochim. Cosmochim. Acta* 72, 1174-1198.
- Gilfillan, S.M.V., Lollar, B.S., Holland, G., Blagburn, D., Stevens, S., Schoell, M., Cassidy, M., Ding, Z.J., Zhou, Z., Lacrampe-Couloume, G., and Ballentine, C.J., 2009. Solubility trapping in formation water as dominant CO₂ sink in natural gas fields. *Nature* 458, 614-618.
- Gislason, S.R., Wolff-Boenisch, D., Stefansson, A., Oelkers, E.H., Gunnlaugsson, E., Sigurdardottir, H., Sigfusson, B., Broecker, W.S., Matter, J.M., Stute, M., Axelsson, G., and Fridriksson, T., 2010. Mineral sequestration of carbon dioxide in basalt: A pre-injection overview of the CarbFix project. *Int. J. Greenhouse Gas Control* 4, 537-545.
- Gunter, W.D., Perkins, E.H., and Hutcheon, I., 2000. Aquifer disposal of acid gases: modelling of water-rock reactions for trapping of acid wastes. *Appl. Geochem.* 15, 1085-1095.
- Hangx, S.J.T., and Spiers, C.J., 2009. Reaction of plagioclase feldspars with CO₂ under hydrothermal conditions. *Chem. Geol.* 265, 88-98.
- Hellevang, H., Aagaard, P., Oelkers, E.H., and Kvamme, B., 2005. Can dawsonite permanently trap CO₂? *Environ. Sci. Technol.* 39, 8281-8287.
- Hendrickson, A.R., Thomas, R.L., and Economides, M.J., 1992. Stimulation of carbonate reservoirs, in Chilingarian, G.V., Mazzullo, S.J., and Rieke, H.H., eds., *Carbonate Reservoir Characterization: a Geologic-Engineering Analysis, Part I: Developments in Petroleum Science*: Amsterdam, Elsevier Science, p. 589-622.
- Holland, H.D., 1965. Some applications of thermochemical data to problems of ore deposits II. Mineral assemblages and the composition of ore forming fluids. *Economic Geology and the Bulletin of the Society of Economic Geologists* 60, 1101-1166.

- Huang, N.S., Aho, G.E., Baker, B.H., Matthews, T.R., and Pottorf, R.J., 2007. Integrated reservoir modeling to maximize the value of a large sour-gas field with high concentrations of inerts, International Petroleum Technology Conference: Dubai, U.A.E.
- Jacquemet, N., Pironon, J., and Caroli, E., 2005. A new experimental procedure for simulation of H_2S+CO_2 geological storage. *Oil & Gas Science and Technology-Revue De L Institut Francais Du Petrole* 60, 193-206.
- Jacquemet, N., Pironon, J., and Saint-Marc, J., 2008. Mineralogical changes of a well cement in various H_2S-CO_2 (-brine) fluids at high pressure and temperature. *Environ. Sci. Technol.* 42, 282-288.
- Johnson, J.W., Nitao, J.J., Steefel, C.I., and Knauss, K.G., 2001. Reactive transport modeling of geologic CO_2 sequestration in saline aquifers: The influence of intra-aquifer shales and the relative effectiveness of structural solubility and mineral trapping during prograde and retrograde sequestration, First Nat. Confer. on Carbon Seq.: Washington, D.C., NETL, US DOE.
- Kaszuba, J.P., and Janecky, D.R., 2009. Geochemical impacts of sequestering carbon dioxide in brine formations, *in* McPherson, B., and Sundquist, E., eds., *Carbon Sequestration and Its Role in the Global Carbon Cycle: American Geophysical Union Monograph*, AGU.
- Kaszuba, J.P., Janecky, D.R., and Snow, M.G., 2003. Carbon dioxide reaction processes in a model brine aquifer at 200°C and 200 bars: Implications for geologic sequestration of carbon. *Appl. Geochem.* 18, 1065-1080.
- Kaszuba, J.P., Janecky, D.R., and Snow, M.G., 2005. Experimental evaluation of mixed fluid reactions between supercritical carbon dioxide and NaCl brine: Relevance to the integrity of a geologic carbon repository. *Chem. Geol.* 217, 277-293.
- Kharaka, Y.K., Cole, D.R., Hovorka, S.D., Gunter, W.D., Knauss, K.G., and Freifeld, B.M., 2006. Gas-water-rock Interactions in Frio Formation following CO_2 injection: Implications for the storage of greenhouse gases in sedimentary basins. *Geology* 34, 577-580.
- Klusman, R.W., 2003. A geochemical perspective and assessment of leakage potential for a mature carbon dioxide-enhanced oil recovery project and as a prototype for carbon dioxide sequestration; Rangely field, Colorado. *AAPG Bull.* 87, 1485-1507.
- Knauss, K.G., Johnson, J.W., and Steefel, C.I., 2005. Evaluation of the impact of CO_2 , co-contaminant gas, aqueous fluid and reservoir rock interactions on the geologic sequestration of CO_2 . *Chem. Geol.* 217, 339-350.
- Kraig, D.H., Wiltschko, D.V., and Spang, J.H., 1987. Interaction of basement uplift and thin-skinned thrusting, Moxa arch and the Western Overthrust Belt, Wyoming - A hypothesis. *Geol. Soc. Am. Bull.* 99, 654-662.
- Lu, J.M., Wilkinson, M., Haszeldine, R.S., and Fallick, A.E., 2009. Long-term performance of a mudrock seal in natural CO_2 storage. *Geology* 37, 35-38.
- Machel, H.G., 2005. Geological and hydrogeological evaluation of the Nisku Q-Pool in Alberta, Canada, for H_2S and/or CO_2 storage. *Oil & Gas Science and Technology-Revue De L Institut Francais Du Petrole* 60, 51-65.
- Machel, H.G., Krouse, H.R., and Sassen, R., 1995. Products and distinguishing criteria of bacterial and thermochemical sulfate reduction. *Appl. Geochem.* 10, 373-389.
- Meuzelaar, T., Thyne, G., Alcott, A., and Budd, D., 2010. Reactive transport model parameterization via a CO_2 sequestration analogue. *Geol. Soc. Am., Abstr. with Prog.* 42, Abstract 183-10.

- Moore, J., Adams, M., Allis, R., Lutz, S., and Rauzi, S., 2005. Mineralogical and geochemical consequences of the long-term presence of CO₂ in natural reservoirs: An example from the Springerville-St. Johns Field, Arizona, and New Mexico, USA. *Chem. Geol.* 217, 365-385.
- Newell, D.L., Kaszuba, J.P., Viswanathan, H.S., Pawar, R.J., and Carpenter, T., 2008. Significance of carbonate buffers in natural waters reacting with supercritical CO₂ - Implications for monitoring, measuring and verification (MMV) of geologic carbon sequestration. *Geophys. Res. Lett.* 35, doi: 10.1029/2008GL035615.
- Nogueira, M., and Mamora, D.D., 2008. Effect of flue-gas impurities on the process of injection and storage of CO₂ in depleted gas reservoirs. *Journal of Energy Resources Technology-Transactions of the ASME* 130.
- Pacala, S., and Socolow, R., 2004. Stabilization wedges: Solving the climate problem for the next 50 years with current technologies. *Science* 305, 968-972.
- Palandri, J.L., and Kharaka, Y.K., 2005. Ferric iron-bearing sediments as a mineral trap for CO₂ sequestration: Iron reduction using sulfur-bearing waste gas. *Chem. Geol.* 217, 351-364.
- Palandri, J.L., Rosenbauer, R.J., and Kharaka, Y.K., 2005. Ferric iron in sediments as a novel CO₂ mineral trap: CO₂-SO₂ reaction with hematite. *Appl. Geochem.* 20, 2038-2048.
- Pearce, J.M., Holloway, S., Wacker, H., Nelis, M.K., Rochelle, C., and Bateman, K., 1996. Natural occurrences as analogues for the geological disposal of carbon dioxide. *Energy Convers. Mgmt* 37, 1123-1128.
- Pironon, J., Jacquemet, N., Lhomme, T., and Teinturier, S., 2007. Fluid inclusions as micro-samplers in batch experiments: A study of the system C-O-H-S-cement for the potential geological storage of industrial acid gas. *Chem. Geol.* 237, 264-273.
- Rao, A.B., and Rubin, E.S., 2002. A technical, economic, and environmental assessment of amine-based CO₂ capture technology for power plant greenhouse gas control. *Environ. Sci. Technol.* 36, 4467-75.
- Stevens, S.H., Pearce, J.M., and Rigg, A.A.J., 2001. Natural analogs for geologic storage of CO₂: An integrated global research program, *Proceedings of the First National Conference on Carbon Sequestration*: Washington, D.C., National Energy Technology Laboratory, US DOE.
- Symonds, R.B., Gerlach, T.M., and Reed, M.H., 2001. Magmatic gas scrubbing: implications for volcano monitoring. *J. Volcanol. Geotherm. Res.* 108, 303-341.
- Thambimuthu, K., Soltanieh, M., and Abanades, J.C., 2005. Capture of CO₂, in Metz, B., Davidson, O., Coninck, H.d., Loos, M., and Meyer, L., eds., *IPCC Special Report on Carbon Dioxide Capture and Storage*, p. 105-178.
- US Geological Survey, 2010. Core Research Center. <http://geology.cr.usgs.gov/crc/index.html>, October 16, 2010.
- Wilkinson, M., Haszeldine, R.S., Fallick, A.E., Odling, N., Stoker, S.J., and Gatliff, R.W., 2009. CO₂-mineral reaction in a natural analogue for CO₂ storage - implications for modeling. *J. Sediment. Res.* 79, 486-494.
- Williams, R.H., 2002. Major roles for fossil fuels in an environmentally constrained world, *Sustainability in Energy Production and Utilization in Brazil: The Next Twenty Years*: Universidade Estadual de Campinas (Unicamp), Campinas, Sao Paulo, Brazil.
- Wyoming Oil and Gas Conservation Commission, 2010. Database. <http://wogcc.state.wy.us/>, last accessed September 18, 2010.
- Xu, T.F., Apps, J.A., and Pruess, K., 2004. Numerical simulation of CO₂ disposal by mineral trapping in deep aquifers. *Appl. Geochem.* 19, 917-936.

- Xu, T.F., Apps, J.A., Pruess, K., and Yamamoto, H., 2007. Numerical modeling of injection and mineral trapping of CO₂ with H₂S and SO₂ in a sandstone formation. *Chem. Geol.* 242, 319-346.
- Zerai, B., Saylor, B.Z., and Matisoff, G., 2006. Computer simulation of CO₂ trapped through mineral precipitation in the Rose Run Sandstone, Ohio. *Appl. Geochem.* 21, 223-240.

Tables and figures

TABLE 6-1. MINERALOGY OF MADISON LIMESTONE SAMPLES

Sample depth meters (feet)	Carbonate Minerals*	Silicate Minerals†	Sulfur-bearing Minerals§
<u>Chevron Federal 1-29</u>			
4511 (14801)	Do, Ca	N.O.	An
4514 (14810)	Do, Ca	Qz, It	N.O.
4735 (15534)	Do	Ac	N.O.
4740 (15552)	Do	Qz, It	An
<u>Church Buttes #31</u>			
5590 (18340)	Do, Ca	N.O.	An, Py#
5606 (18394)	Do	N.O.	Py
5691 (18670)	Ca	Qz	An#
5702 (18706)	Do	Ac	An, Py#
<u>Union Pacific RR #4</u>			
2288 (7505)	Do, Ca	Qz, It	Py#
2313 (7588)	Do	Ac	An#
2368 (7769)	Do	N.O.**	An, S, Py#
2391 (7843)	Do	Fs, Qz, It	An#, Py#

*Do = dolomite, Ca = calcite

†Qz = quartz, It = illite, Ac = analcime, Fs = feldspar

§Py = pyrite, An = anhydrite, S = native sulfur,

Mineral not identified by x-ray diffraction but observed in thin section

**N.O. = none observed

TABLE 6-2. MADISON FORMATION WATER CHEMISTRY FROM WELLS IN THE AREA OF THE MOXA ARCH

Well Name (API#)	Location	Date sampled	Depth meters (feet)	pH	T (°C) [†]	TDS (calc)	Na ⁺	K ⁺	Ca ²⁺	Mg ²⁺	HCO ₃ ⁻	Cl ⁻	SO ₄ ²⁻	Charge Balance (%)
Unit 17 M (4901305634)	T33N R96W S15	8/2/57	3400 (11155)	6.1	93	16203	585	53	3074	1522	256	10400	310	1.07
Unit 17M (4901305634)	T33N R96W S15	8/15/64	3354 (11002)	7.7	92	17329	802	10.3	3100	1630	314	10900	521	-0.27
Unit 32M (4901305652)	T33N R96W S10	8/15/64	3416 (11205)	7.3	93	22,098	512	11.3	4210	2270	251	14500	308	-0.13
34M (4901305702)	T33N R96W S10	9/28/55	3479 (11410)	7.0	94	31,507	8329	761	2508	601	245	18500	535	3.82
Unit No.1 (4902905822)	T53N R100W S27	6/22/49	3342 (10961)	7.4	91	17,284	3173	290	2249	231	3150	6360	1839	1.68
Unit No. 1 (4902905822)	T54N R100W S21	12/16/51	4739 (15545)	7.8	123	16,860	4676	427	939	91	1610	5800	3259	2.92
Teepee Mtn. Unit #1 (4903720754)	T12N R104W S17	6/6/72	4829 (15840)	6.9	125	79,486	27700	1890	864	398	2680	44200	1830	0.62
Unit 22-19 (4903505746)	T28N R113W S19	N.D.**	4182 (13718)	7.9	110	29,727	9000	823	250	101	5290	3940	10300	4.64
Champlin #549 (4904120145)	T17N R116W S3	3/21/74	2966 (9730)	7.5	83	24,904	8220	752	545	134	1190	11400	2650	4.94
ACG #2 (4904120117)	T17N R119W S18	8/6/74	4018 (13180)	6.7	107	22,465	3140	614	3430	651	1280	10500	2870	0.93
5 Amoco Chevron Gulf (4904120268)	T17N R119W S18	9/2/83	4073 (13360)	6.1	108	7,948	2720	248	180	18.9	205	4510	58.8	4.10
1-A Champlin 457 Amoco B (4904120265)	T18N R119W S31	5/21/8	3916 (12844)	6.5	104	156,821	42300	3860	10300	4000	1710	94000	719	4.32
Snow Hollow #1 (4902320226)	T24N R120W S35	8/18/73	3171 (10400)	8.2	88	12,228	3520	98.8	605	60.7	364	3810	3710	8.96
1 Champlin 323 Amoco B †† (04904120265)	T31N R119W S31	5/21/80	4396 (14420)	8.8	115	39,491	11800	1080	2290	666	200	22800	173	-0.74

All solutes in mg/kg. *Value at top of interval sample given in table. Average sample interval thickness is 148'.

†Temperatures calculated from depth and geothermal gradient (22.4°C/km, surf. T = 16.2°C).

** N.D. = no data

Figure 6-1. a) Generalized geologic map of southwestern Wyoming. Trace of the crest of the Moxa Arch and location of wells where Madison Limestone drill core was sampled are plotted. b) Stratigraphic correlation of major units within Madison Limestone as depicted in Katz et al. (2007). Correlation of Church Buttes#31 and Union Pacific RR #4 (UPRR #4) wells and locations of samples collected for this study (stars) are illustrated. Detailed stratigraphic information for the Chevron Federal 1-29 well (1-29 Federal) is not available.

Figure 6-2. Photomicrograph of Madison Limestone in Chevron Federal 1-29 well at depth of 4740 meters. a) Optically continuous, poikilitic secondary anhydrite (Anh) fills pores among euhedral dolomite (Do) rhombohedrons. Illite was identified by XRD analysis but is not pictured in this view. Quartz is present in this interval of drill core but is not pictured in this view. Scale bar is 600 μm . b) Optically continuous, poikilitic secondary anhydrite (Anh) fills pores among euhedral dolomite (Do) rhombohedrons. A small amount of interstitial quartz (Qtz) is also present in the pores. Illite was identified by XRD analysis but is not pictured in this view. Scale bar is 500 μm . c) Secondary anhydrite (Anh) fills a fracture that cuts a matrix of euhedral dolomite (Do) rhombohedrons. Scale bar is 2 mm. d) Photomicrograph of Madison Limestone in Church Buttes#31 well at depth of 5702 meters. Secondary anhydrite (Anh) fills pores among euhedral dolomite (Do) rhombohedrons. Euhedral analcime (Ac) crystals are also present within the pores. Pyrite is present in this interval of drill core but is not pictured in this view. Scale bar is 500 μm .

Figure 6-3. Images of pyrite in Madison Limestone from Church Buttes#31 well at depth of 5590 meters. a) SEM micrograph of recrystallized secondary pyrite (light grey) fills pores interstitial to euhedral dolomite (dark grey). Scale bar is 600 μm . b) Reflected light image of same view. Pyrite is bright colored, dolomite is grey in color, and pores are black.

Figure 6-4. Secondary electron SEM micrographs of native sulfur in Madison Limestone from the Union Pacific RR #4 well at a depth of 2368 m. Secondary native sulfur (lighter material labeled S) fills pores between surrounding euhedral dolomite (darker mineral labeled Do) rhombohedrons. This is the only sample in which native sulfur was identified. Scale bars are 200 μm .

Figure 6-5. Eh/pH diagram showing stability of sulfur species along a conceptual reaction path from seawater (black dot) through early burial and diagenesis (black line) with a model simulation reaction path (red line) of CO_2 addition to Madison Limestone. At the end point the system is in equilibrium with pyrite, native sulfur and anhydrite. All three minerals occur in Madison Limestone samples. Anhydrite occurs as primary and secondary minerals in most samples.

Figure 6-6. Log activity Na^+/H^+ versus log activity $\text{SiO}_2(\text{aq})$ diagram for endpoint of reaction path calculated by geochemical model of Madison Limestone-fluid system. Model starts with a fluid composition from a well outside, but at similar depth to, the gas cap (Champlin #549, Table 6-2) and current burial conditions of 90°C and 35 MPa. CO_2 is subsequently injected into this Madison Limestone-fluid system until final CO_2 values reach approximately 35 MPa. Stability fields for sodium silicate minerals that are potentially stable at the endpoint of this reaction path are depicted by solid lines. Also plotted are stability fields for sodium silicate minerals that would be stable at 110°C (dashed lines), temperatures observed in portions of the Madison Limestone. Brine analyses for Madison Limestone that are tabulated in Table 6-2 are also plotted (XX symbols for brines outside the gas cap and YY symbols for brines inside the gas cap). Brines sampled from within the gas cap plot inside the muscovite and albite stability fields and inside or adjacent to the analcime stability field. This predicted silicate mineral assemblage (phyllosilicate $\pm$ feldspar $\pm$ analcime) for the Madison Limestone-multiphase fluid ($\text{CO}_2 + \text{H}_2\text{O}$)-system

agrees well with the observed assemblage, indicating that formation brines are in equilibrium with the host formation.

Figure 6-7. Log activity K^+/H^+ versus log activity $SiO_2(aq)$ diagram for endpoint of reaction path calculated by geochemical model of Madison Limestone-fluid system. Stability fields for potassium silicate minerals that are potentially stable at the endpoint of this reaction path are depicted by solid lines. Also plotted are stability fields for potassium silicate minerals that would be stable at 110°C (dashed lines), temperatures observed in portions of the Madison Limestone. Brine analyses for Madison Limestone that are tabulated in Table 6-2 are also plotted (XX symbols for brines outside the gas cap and YY symbols for brines inside the gas cap). Brines sampled from within the gas cap plot inside the muscovite and microcline stability fields and inside or adjacent to the clinoptillite stability field. This predicted silicate mineral assemblage (phyllosilicate $\pm$ feldspar $\pm$ zeolite) for the Madison Limestone-multiphase fluid ($CO_2 + H_2O$)-system agrees well with the observed assemblage, indicating that formation brines are in equilibrium with the host formation.

Part II. Nanoporosity in limestones and dolomites of the Madison Limestone

Introduction

The capillary pressure curve of injected CO₂ controls the size of pores available for CO₂ transport within a reservoir. CO₂ will enter pore spaces by capillary drainage when the CO₂ capillary pressure is higher than that of the brine. In each reservoir there will be a population of pores too small for CO₂ to displace brine through capillary drainage. Given a model pore (cylindrical with smooth pore walls), realistic values of contact angle (~30°) between the CO₂ and brine, and hydrostatic pressure at 1 km depth it is likely that capillary pressures will not be high enough to displace brine in pores < ~100 nm (here termed nanopores). However, the influence of a changing pore network with reaction (surface roughness, volume and connectivity of nanoporosity) on the accessibility of small pores by CO₂ is currently unknown. Here we explore the potential size range of pores accessible to capillary flow of supercritical CO₂ in geologic formations using basic multiphase flow equations and interrogate the structure of nanopores in the Madison Limestone using small angle neutron scattering (SANS). The Madison Limestone is partially dolomitized and samples used in this study represent varying degrees of dolomitization. Approximately 80% of North America's carbonate oil and gas reservoirs are dolomite. Once depleted these dolomite reservoirs are good candidates for CO₂ storage. Therefore, understanding the pore structure of dolomite its evolution during dolomitization is important for predicting the behavior of supercritical CO₂ in mixed calcite-dolomite reservoirs.

Small-Angle Neutron Scattering (SANS)

When a beam of neutrons passes through a sample, the majority of the neutrons are simply transmitted, however, some effectively scatter off interfaces between phases of different chemistry and density (RADLINSKI, 2006). The intensity of scattered neutrons is proportional to the volume of scattering objects (ϕ pores) and the scattering contrast ($\Delta\rho$), i.e. the difference in scattering length density between pores and minerals.

$$I(q) = (\Delta\rho)^2 P(q) (\phi(1 - \phi)), \quad 1$$

where $P(q)$ is the form factor, assumed spherical objects for pores (RADLINSKI, 2006).

The coherent scattering length density of a single phase is given by equation 2

$$\rho = \sum_{i=1}^N b_i \frac{\rho_j N_A}{M_j}, \quad 2$$

where b_i is the bound coherent scattering length of atom i , N the total number of atoms and ρ_j the mass density, M_j is the molar mass, and $N_A = 6.023 \times 10^{23} \text{ mol}^{-1}$ the Avogadro constant. Common minerals have similar values of ρ making the two-phase approximation applicable (RADLINSKI, 2006). Here the value of ρ for each sample (Table 6-3) was calculated from the volume-weighted average of dolomite and calcite.

The intensity of scattered neutrons over a range of scattering vector (Q , a measure of the scattering angle) contains information about the internal microstructure of pores. The diameter of the scattering particle (d) is inversely proportional to the Q value ($d = 2\pi/Q$). For SANS, the Q -

range interrogated 3.8×10^{-3} to $2.45 \times 10^{-1} \text{ \AA}^{-1}$, thus providing information about pores with diameters from 2 to 165 nm.

Methods

Geologic Samples

Samples of Madison Limestone were taken from two wells on the Moxa Arch, Church Buttes #31 (4 samples) and Riley Ridge 33-24 (6 samples), at varying depths. These samples represent variable extent of dolomitization within the formation (Table 6-3). Madison Limestone in the Church Buttes 31 well is comprised mainly of dolomite and calcite with varying fractions of anhydrite, sulfides, quartz, feldspar, and in one sample, elemental sulfur. Mineralogy in the Riley Ridge 33-24 well is similar but with trace muscovite and no observed native sulfur.

Predicted CO₂ phase behavior in nanopores

The size range of pores accessible to supercritical CO₂ under capillary flow conditions (pore radius, r in mm) is a function of the interfacial tension (σ , mN/m), the contact angle between the wetting (water/brine) and non-wetting (supercritical CO₂) fluid phases (γ , radians), and the capillary pressure (P_c , mbar) (LAKE, 1989).

$$r = \frac{2\sigma \cos \gamma}{P_c} (10) \quad 3$$

P_c is a function of the relative saturation of brine and CO₂. The right side of equation 2 is multiplied by 10 for unit conversion purposes. Values for each of the parameters were determined from published studies.

Small Angle Neutron Scattering

Rock sections, 150 microns thick and glued to quartz slides with Krazy Glue™ (ANOVITZ et al., 2009), from the three wells (Table 6-3) were analyzed on the Low-Q Diffractometer (LQD) at the Los Alamos Neutron Science Center. The LQD is a time-of-flight instrument with a Q range of 3.8×10^{-3} to $2.45 \times 10^{-1} \text{ \AA}^{-1}$. Samples were placed in the neutron beam path with a cadmium collimator to reduce the size of the beam interacting with the sample to 4 mm diameter. Thus, the volume of sample interrogated was 1.88 mm^3 . Scattered neutrons were collected from each sample until a total count of 500k was reached or for 180 minutes, whichever was shorter. Transmission for all samples was >80%, indicating a low occurrence of multiple scattering (ANOVITZ et al., 2009). Scattering data were corrected for transmission from an empty beam and scattering from a blank quartz slide. The resulting data (differential cross section per unit area on an absolute scale) were divided by the sample thickness in cm (0.015 cm) to calculate the absolute scattering per unit volume (cm^{-1}).

Samples from the Church Buttes #31 well were also saturated with an H₂O-D₂O mixture with scattering length density similar to the rock ($5.3 \times 10^{-6} \text{ \AA}^{-2}$) effectively reducing the scattering contrast between minerals and connected pores to zero. Scattering data from these contrast-matched samples provides information about the unconnected pores and, by difference, the connected pores. Surface area was measured by gas adsorption techniques (BET) using nitrogen gas (N₂). Samples were degassed at 250°C overnight prior to analysis.

Results

Accessible pore sizes

All parameters in the pore radius calculation are dependent upon temperature and pressure. Data for interfacial tension and contact angle are generally not reported for very high pressures like those found in the Madison in the Moxa Arch (up to 1250 atm). Therefore, the accessible pore size is calculated for T and P just above the supercritical point of CO₂ (31°C and 75 atm). Interfacial tension measurements between brine and supercritical CO₂ near T = 30°C and P = 100 bars generally fall between 25 and 30 mN m⁻¹ (BACHU and BENNION, 2009; CHALBAUD et al., 2009; CHUN and WILKINSON, 1995). Contact angle between supercritical CO₂ and brine is highly dependent upon the mineral substrate. To our knowledge contact angle has not been measured on carbonate rocks. However, for muscovite and quartz at P = 100 bars measured contact angles are ~ 60° and 35° respectively (CHIQUET et al., 2007). Capillary pressure (P_c) is dependent upon the water saturation of the formation. As water saturation decreases P_c increases. For water saturations between 0.2 and 0.8 (80-20% of pore space filled with CO₂, respectively) predicted in the CO₂ plume (ZHANG et al., 2009) P_c ranges from ~6 to 11 mbar (PLUG and BRUINING, 2007). Given the above ranges in parameters, the radius of the smallest pore accessible to capillary CO₂ flow is 23 to 82 nm. As long as the difference between the injection pressure and the formation pressure is greater than the capillary pressure CO₂ will enter pores in the 10s of nm size range.

The size of pores analyzed by SANS ranges from 6 to 164 nm in diameter. From the basic calculation above, it does not appear that free-phase supercritical CO₂ will enter pores of this size. However, CO₂ will dissolve into and acidify brine in these pores. Thus, nanoporosity may be very important for geologically sequestering CO₂ in mineral form.

Nanoporosity

Scattering data were plotted on scattering diagrams, I(Q) vs. (Q) on log-log scale (Figure 6-8). Constant intensity data at high Q on this plot arises from incoherent scattering by hydrogen in the sample (Figure 6-8, inset). The high Q region was fit to equation G and the resulting incoherent scattering (parameter c, Table 6-3) was subtracted from scattering at all Q values,

$$I(Q) = bQ^m + c \quad 4$$

In some datasets, subtraction of incoherent scattering resulted in negative intensity at high Q. Thus, all data at Q values higher than the maximum Q with a negative intensity were removed from the data set. The incoherent corrected scattering data was used for all data fitting where values for *b* and *m* (slope of data) were determined from the scattering diagrams. Porod plots (I(Q)*Q⁴ vs. Q on log-log scale) were constructed to amplify changes in slope and identify any breaks in slope in the data (Figure 6-9a,b). Porosity was calculated from the incoherent corrected scattering data using the software program Prinsas (HINDE, 2004).

In the Madison Limestone samples, pores of diameter from 6 to 134 nm comprise < 1% of the total rock volume (0.3 to 0.4%) in all samples from both wells. The volume % nanoporosity calculated from SANS data is not correlated to extent of dolomitization of the sample. However, macro-porosity determined by point count analysis for the Riley Ridge 33-24 well increases with increasing dolomitization. Porosity calculated from the contrast-matched samples of the Church Buttes #31 well is lower than the total porosity for all but one sample indicating that a portion of

the nanoporosity is connected (50-75%). For sample 18670' from Church Buttes #31 the porosity calculated when saturated with contrast matched fluid is the same as the porosity calculated from the dry sample indicating that any connected nanoporosity in this sample is a very small fraction of the total nanoporosity.

Surface Area of Nanopores

Surface area was calculated from the Porod diagram (Figure 6-9a, RADLINSKI et al., 1996). The scattering intensity from a flattened low Q region on the Porod diagram is used to calculate the smooth surface area (S_0) of pores using equation 5

$$S_0 = \frac{a}{2\pi(\Delta\rho)^2} \quad 5$$

where a is the y-intercept of the flattened region on the Porod plot (Figure 6-9a) and $\Delta\rho$ is the difference in scattering length density between pores and minerals. Pores have a scattering length density of 0 and the scattering length density calculated for the rocks is the same as the $\Delta\rho$ (Table 6-3). The surface fractal dimension (D_s), determined from the scattering plot, is then used to estimate the rough surface area (S_r) with equation 6

$$S_r = S_0 \left(\frac{r}{\xi} \right)^{2-D_s} \quad 6$$

where r is the scale of the roughness (~ 5 nm) and ξ is the correlation length (~ 7.5 nm).

Pore-mineral interfacial area of the nanopores calculated from SANS data ranges from 0.3 to 1 $\text{m}^2 \text{g}^{-1}$ compared to 0.06 to 0.22 $\text{m}^2 \text{g}^{-1}$ from BET measurements. There is good agreement between the two methods (BET values are 2 to 4x the SANS surface area) for all samples except the Church Buttes well at 18670 feet. Determination of a flattening region on the Porod plot for 18670 feet was difficult and data fitting produced a negative y-intercept. Therefore, the SANS surface area is inconclusive and BET surface area is the most reliable for this sample.

Fractal Dimensions

Scattering data that follow a power law (equation 2) indicate a fractal distribution in the sample where the value of m is related to the fractal dimension. On scattering diagrams fractal distributions are expressed in linear portions of the data and therefore the slope is equivalent to the m value in equation 2. Scattering data for all the samples show fractal distributions with slopes between -2 and -4. The slope is indicative of either surface fractal behavior ($m = -2$ to -3) or mass fractal behavior ($m = -3$ to -4). In order to amplify changes in slope the data were plotted on Porod plots ($\log I(Q) \cdot Q^4$ vs. $\log Q$, Figure 6-9). Two samples, Church Buttes #31 at 18670' and Riley Ridge at 15925', are fit with a single slope (-3.5 for both) over the entire Q-range investigated. However, the rest of the carbonate samples exhibit a break in slope. Slopes in the low Q region range from -3.1 to -3.5 indicating surface fractal behavior while slopes in the high Q region range from -2.3 to -3.1 indicating mixed surface and mass fractal behavior. Both surface and mass fractal dimensions range from 2-3 and are calculated from the slope as $D_s = 6 + m$ and $D_m = -m$, respectively. Smooth surfaces produce $D_s = 2$ and as surface roughness increases D_s approaches 3. For mass fractals, $D_m = 3$ refers to space filling distributions, for example in rocks small pores fill in spaces between big pores. $D_m = 2$ refers to a sample, where the mass increases only with the square of the radius.

Discussion

Dolomite has a smaller molar volume than calcite and the process of dolomitization generally increases porosity (EHRENBERG et al., 2006 and references therein). Therefore, it is surprising that while there appears to be a change in pore structure with dolomitization, there is no systematic difference in volume or surface area of nanopores. This suggests that the dolomitization process that increases micro- and macro-scale porosity may be different than the nano-scale process.

While there are no changes in volume or surface area of nanopores, there are changes in the fractality of the nano-scale pore network. Fractal dimensions have been used to quantify scale-invariant distributions common in geologic systems. For example, fractals show the relative distribution of metals in a British Columbia mining area (CHENG, 1995). Additionally, fractals are very useful for extrapolating data beyond observed resolution or between data points in sparsely characterized systems (e.g. HERZFELD and OVERBECK, 1999). In this way fractals can be used to populate datasets for numerical models of large-scale field systems where parameters are not measured at regular or closely spaced intervals. The fractal dimensions obtained from neutron scattering of the Madison Limestone samples provides clues to how the nano-scale structure of the pore network changes with dolomitization.

Previous studies have demonstrated the fractal nature of pore networks in many different rock types using neutron scattering (KAHLE et al., 2004; RADLINSKI, 2006; RADLINSKI et al., 2004) and image analysis (DATHE et al., 2001; LEE et al., 2006; RISOVIC et al., 2008). However, only a handful of studies have shown changes to the fractal distribution of pore networks as a result of chemical or physical properties, such as oil generation (RADLINSKI et al., 2000a; RADLINSKI et al., 1996), metamorphism (ANOVITZ et al., 2009) and chemical weathering. The results from this study show that the process of dolomitization also changes the fractal distribution of pores and surface asperities in limestone (Figure 6-10). In samples where dolomitization is not extensive, indicated by a low percentage of dolomite, a single slope is fit to entire the Q range with a surface fractal dimension of 2.5. In contrast, samples that have experienced dolomitization show a break in slope. Interestingly, samples where ~50-60% of the carbonate is dolomite (moderate dolomitization) exhibit both mass and surface fractal behavior at high and low Q respectively, while samples with extensive dolomitization (>80%) exhibit only surface fractal behavior. For extensively dolomitized samples, the surface fractal dimension at high Q is 2.9 while surface fractal dimensions at low Q are similar to the surface fractal dimension observed in the samples where dolomitization is not extensive (2.3-2.5).

Since surface fractals indicate scattering from bumps on pore walls and mass fractals indicate scattering from discrete pores, the fractal dimensions determined from scattering data can provide clues to the nano-scale pore structure. In samples with a single surface fractal over the entire Q range investigated it can be inferred that one population of pores dominates the nano-scale pore structure. These pores have diameters larger than 125 nm, or the resolution of the SANS instrument, (i.e. no mass fractal) and < 6 to > 125 nm sized bumps on the pore surfaces.

From this initial pore structure, recrystallization creates a break in slope with mass fractal at high Q (very small pores) and a surface fractal at low Q (small bumps on pores larger than the SANS resolution) that can be interpreted as two distinct pore populations (Figure 6-10). The surface

fractal value at low Q is similar to the surface fractal value of undolomitized samples suggesting that the surface roughness of the larger pores does not change with dolomitization. This surface fractal value remains the same even for extensively dolomitized samples. Additionally, the high Q scattering, characterized by a mass fractal in moderately dolomitized samples, shows surface fractal behavior in extensively dolomitized samples. The surface fractal value is high, ~2.9, compared to the low Q surface fractal, ~2.2. Interpretation of this transformation is inconclusive without high-resolution images. The change in scattering pattern can be explained by either 1) growth of the very small population of pores inferred from moderately dolomitized scattering patterns to diameters larger than SANS resolution with no change in the surfaces of the second population of pores or 2) precipitation infilling the small pores and increased roughness at scales from 6 to 25 nm in the original larger population of pores.

Widespread dolomitization occurred early in the burial history of the Madison Limestone (BUDAI et al., 1984; BUDAI et al., 1987). In the area of the Moxa Arch CO₂ and other gasses were emplaced during the Cretaceous through Tertiary (ARMSTRONG and ORIEL, 1965). Currently the Riley Ridge well is located within the CO₂ gas cap on the Moxa Arch but the Church Buttes well is located outside this zone. While it is likely that rocks in both wells were exposed to CO₂ in the past, the rocks in the Riley Ridge 33-24 well may have been exposed to CO₂ for a much longer time period than those in the Church Buttes #31 well. Therefore, it is surprising that the scattering patterns from both the Riley Ridge and Church Buttes wells are similar indicating that the pore structure is the same in both wells at all stages of dolomitization (Figure 6-10). This suggests that either 1) no reaction has occurred at the nanopore scale since early dolomitization or 2) reaction after CO₂ emplacement had the same impact on the pore structure. In the second case the reactions would have been relatively fast and complete since the Madison in the area of the Riley Ridge 33-24 well has seen CO₂ for much longer time than in the area of the Church Buttes #31 well.

Conclusions

The behavior of CO₂ in geological carbon storage will depend on the pore size. Here we estimate that pores < 20 microns will not be accessible to CO₂ flow through capillary forces. However, in small pores, CO₂ will dissolve into the brine. Thus, the main impact of CO₂ injection on small pores is dissolution and precipitation of minerals. We have shown that like many other rock types (KAHLE et al., 2004; RADLINSKI, 2006; RADLINSKI et al., 2000b; SEN et al., 2002), pores in the Madison Limestone are fractally distributed. The fractal nature of rocks has been known for some time (AVNIR et al., 1984; KATZ and THOMPSON, 1985; WONG et al., 1986). However, changes in fractality with geochemical and physical processes have only been demonstrated a handful of times (RADLINSKI et al., 1996). Based on data collected for samples of Madison Limestone, the dolomitization of limestone appears to change the structure of nanopores but not the total volume. Thus, over long time periods, geochemical reactions in small pores may change the structure of the pore enough to allow capillary flow of CO₂. Quantification of pore network evolution using fractal dimensions may provide information useful for validating results from sophisticated lattice Boltzmann models of pore-scale processes.

References

- Armstrong, F.C., and Oriel, S.S., 1965. Tectonic development of Idaho-Wyoming thrust belt. *AAPG Bulletin* **49**, 1847-1866.
- Anovitz, L. M., Lynn, G. W., Cole, D. R., Rother, G., Allard, L. F., Hamilton, W. A., Porcar, L., and Kim, M. H., 2009. A new approach to quantification of metamorphism using ultra-small and small angle neutron scattering. *Geochim. Cosmochim. Acta* **73**, 7303-7324.
- Avnir, D., Farin, D., and Pfeifer, P., 1984. Molecular fractal surfaces. *Nature* **308**, 261-263.
- Bachu, S. and Bennion, D. B., 2009. Interfacial tension between CO₂, freshwater, and brine in the range of pressure from 2 to 27 MPa, temperature from 20 to 125°C, and water salinity from 0 to 334,000 mg/L. *Journal of Chemical and Engineering Data* **54**, 765-775.
- Budai, J.M., Lohmann, K.C., and Owen, R.M., 1984, Burial dedolomite in the Mississippian Madison Limestone, Wyoming and Utah Thrust Belt: *J. Sed. Pet.* **54**, 276-288.
- Budai, J.M., Lohmann, K.C., and Wilson, J.L., 1987, Dolomitization of the Madison Group, Wyoming and Utah Overthrust Belt: *AAPG Bulletin*, **71**, 909-924.
- Chalraud, C., Robin, M., Lombard, J. M., Martin, F., Egermann, P., and Bertin, H., 2009. Interfacial tension measurements and wettability evaluation for geological CO₂ storage. *Advances in Water Resources* **32**, 98-109.
- Cheng, Q., 1995. The perimeter-area fractal model and its application to geology. *Mathematical Geology* **27**, 69-82.
- Chiquet, P., Broseta, D., and Thibeau, S., 2007. Wettability alteration of caprock minerals by carbon dioxide. *Geofluids* **7**, 112-122.
- Chun, B.-S. and Wilkinson, G. T., 1995. Interfacial tension in high-pressure carbon dioxide mixtures. *Industrial & Engineering Chem. Res.* **34**, 4371-4377.
- Dathe, A., Eins, S., Niemeyer, J., and Gerold, G., 2001. The surface fractal dimension of the soil-pore interface as measured by image analysis. *Geoderma* **103**, 203-229.
- Ehrenberg, S. N., Eberli, G. P., Keramanti, M., and Moallemi, S. A., 2006. Porosity-permeability relationships in interlayered limestone-dolostone reservoirs. *AAPG Bulletin* **90**, 91-114.
- Herzfeld, U. C. and Overbeck, C., 1999. Analysis and simulation of scale-dependent fractal surfaces with application to seafloor morphology. *Computers & Geosciences* **25**, 979-1007.
- Hinde, A. L., 2004. PRINSAS - a Windows-based computer program for the processing and interpretation of small-angle scattering data tailored to the analysis of sedimentary rocks. *Journal of Applied Crystallography* **37**, 1020-1024.
- Kahle, A., Winkler, B., Radulescu, A., and Schreuer, J., 2004. Small-angle neutron scattering study of volcanic rocks. *European Journal of Mineralogy* **16**, 407-417.
- Kang, Q. J., Zhang, D. X., and Chen, S. Y., 2003. Simulation of dissolution and precipitation in porous media. *Journal of Geophysical Research* **108**, 2505-2515.
- Katz, A. J. and Thompson, A. H., 1985. Fractal sandstone pores - implications for conductivity and pore formation. *Physical Review Letters* **54**, 1325-1328.
- Lake, L. W., 1989. *Enhanced Oil Recovery*. Prentice Hall, Englewood Cliffs.
- Lee, G. J., Pyun, S. I., and Rhee, C. K., 2006. Characterisation of geometric and structural properties of pore surfaces of reactivated microporous carbons based upon image analysis and gas adsorption. *Microporous Mesoporous Mat.* **93**, 217-225.
- Plug, W. J. and Bruining, J., 2007. Capillary pressure for the sand-CO₂-water system under various pressure conditions. Application to CO₂ sequestration. *Advances in Water Resources* **30**, 2339-2353.

- Radlinski, A. P., 2006. Small-angle neutron scattering and the microstructure of rocks, *Neutron Scattering in Earth Sciences*.
- Radlinski, A. P., Boreham, C. J., Lindner, P., Randl, O., Wignall, G. D., Hinde, A., and Hope, J. M., 2000a. Small angle neutron scattering signature of oil generation in artificially and naturally matured hydrocarbon source rocks. *Organic Geochemistry* **31**, 1-14.
- Radlinski, A. P., Boreham, C. J., Wignall, G. D., and Jin, J.-S., 1996. Microstructural evolution of source rocks during hydrocarbon generation: A small-angle-scattering study. *Physical Review B* **53**, 14 153.
- Radlinski, A. P., Ioannidis, M. A., Hinde, A. L., Hainbuchner, M., Baron, M., Rauch, H., and Kline, S. R., 2004. Angstrom-to-millimeter characterization of sedimentary rock microstructure. *Journal of Colloid and Interface Science* **274**, 607-612.
- Radlinski, A. P., Radlinska, E. Z., Agamalian, M., Wignall, G. D., Lindner, P., and Randl, O. G., 2000b. The fractal microstructure of ancient sedimentary rocks. *J. Applied Crystallography* **33**, 860-862.
- Risovic, D., Poljacek, S. M., Furic, K., and Gojo, M., 2008. Inferring fractal dimension of rough/porous surfaces-A comparison of SEM image analysis and electrochemical impedance spectroscopy methods. *Appl. Surf. Sci.* **255**, 3063-3070.
- Sen, D., Mazumder, S., and Tarafdar, S., 2002. Pore morphology and pore surface roughening in rocks: a small-angle neutron scattering investigation. *J. Mater. Sci.* **37**, 941-947.
- Wong, P., Howard, J., and Lin, J., 1986. Surface roughening and the fractal nature of rocks. *Physical Review Letters* **57**, 637-640.
- Zhang, W., Li, Y., Xu, T., Cheng, H., Zheng, Y., and Xiong, P., 2009. Long-term variations of CO₂ trapped in different mechanisms in deep saline formations: A case study of the Songliao Basin, China. *International Journal of Greenhouse Gas Control* **3**, 161-180.

Tables and Figures

Table 6-3. Results from SANS experiments on Madison Limestone samples.

Depth (ft)	Location		API Number	Formation ¹	Porosity ²	Neutron Scattering Data				Fractal Dimensions ⁶			
	Township	Lat/Long				Scattering Length Density	Incoherent Scattering	Nano-porosity (connected)	Surface Area, m ² g ⁻¹	High Q ³	Low Q	Full Q range	BET surface area
Church Buttes #31	16N/112W/S21	41.35484/-110.04801	4937222680	Madison Lst									
18670				0	-	4.64x10 ⁻⁶	0.01	0.3 (0)	- ⁴			2.5	0.06
18706				100	-	5.40x10 ⁻⁶	0.017	0.4 (0.3)	0.31	2.9	2.1		0.15
18394				100	-	5.40x10 ⁻⁶	0.018	0.4 (0.2)	0.52	2.9	2.2		0.23
18340				50	-	5.06x10 ⁻⁶	0.01	0.3 (0.2)	0.46	2.5*	2.5		0.10
Riley Ridge #33-24	30N/114W/S33	42.53667/-110.42761	4903520673	Madison Lst									
15941.5				100	15	5.40x10 ⁻⁶	0.051	0.3	0.65	2.9	2.2		-
15953				66	15	5.13x10 ⁻⁶	0.065	0.3	0.30	2.5*	2.1		-
15933				100	30	5.40x10 ⁻⁶	0.081	0.4	0.71	2.9	2.2		-
15925				25	1	4.83x10 ⁻⁶	0.01	0.3	0.99			2.3	-
15532				83	40	5.23x10 ⁻⁶	0.022	0.4	1.10	2.9	2.3		-
15542				69	1	5.06x10 ⁻⁶	0.043	0.4	0.62	2.7*	2.2		-

¹For Madison Limestone the percent of carbonate that is dolomite is given as a measure of extent of dolomitization

²Determined by point counting thin section

³Values with * are mass fractal dimensions, all others are surface fractal dimensions

⁴Surface area from SANS data is inconclusive for these sample. No plateau in Q was observed on the Porod diagram.

⁶For samples where a break in slope was observed fractal dimensions are reported for two regions of the scattering curve, for samples where no break in slope was observed a single fractal dimension is reported for the entire scattering region.

Figure 6-8. Scattering diagram (intensity (IQ) vs. scattering vector (Q)) for the 18706' sample from Church Buttes #31 well. Inset graph shows intensity data before subtraction of incoherent scattering (shallower slope at high Q values) on the same scale as the main graph. These scattering data follow a power law indicating fractality of the sample. The slope on scattering plot is a measure of the fractal dimension. Here, there is a break in slope in the data that is difficult to see in the scattering diagram, as is the case for many samples. Therefore, porod plots (Figure 6-9) are used to determine the location of any changes in slope before slopes are fit to the scattering data.

Figure 6-9. a) Porod plot ($I(Q) * Q^4$ vs. Q) for sample 18706' in Church Buttes #31 well. A break in slope is observed at Q value $\sim 0.025 \text{ \AA}^{-1}$. Slopes are fit on the scattering diagram for data above and below this break point to determine the fractality of the sample. Line (need to add) shows flattened region used to calculate surface area. The value of parameter a in equation I is the y-intercept of this line. b) Porod diagram for both 18706' (closed squares) which has experienced dolomitization and 18670' (open squares) which has not. The slope and scattering intensity of the data at high Q is similar for the two samples. However, the slope at low Q is different and the intensity of scattering is higher for 18706' indicating a change in fractality and pore size distribution with dolomitization.

Figure 6-10. Porod plots from the Church Buttes 31 (top) and Riley Ridge 33-24 (bottom) wells showing changes in slope of scattering data with dolomitization. Scattering data for samples with no dolomite (left) are fit with a single surface fractal. Dolomitization induces a break in slope with a mass fractal at high Q and surface fractal at low Q (middle) or two surface fractal dimensions where dolomitization is extensive (right).

Part III. Geologic carbon-sulfur co-sequestration: experimental investigation of sulfur in a natural analogue, Madison Limestone of the Moxa Arch in SW Wyoming

Introduction

The purpose of this portion of the study is to investigate the added interaction that sulfur plays in the sequestration of CO₂ in a carbonate reservoir. We use the controlled conditions of geochemical laboratory experiments to test the conceptual model that was previously developed (Eh-pH diagram in Figure 6-5) for the Madison Limestone on the Moxa Arch.

Experimental Methods

Experiments were performed in the hydrothermal laboratory at the University of Wyoming using established experimental methods (Seyfried et al., 1987; Kaszuba et al., 2003, 2005). A model Madison Limestone was reacted with brine at 250 bars and 110°C to approach steady state with respect to major element concentrations (~1080 hrs). Carbon dioxide was then injected into the system and the experiment continued. At the conditions of the experiments, carbon dioxide is a separate supercritical fluid that is largely immiscible, but not totally insoluble, in brine and free to react with the Madison Limestone–brine system. To provide a basis of understanding for the effect of the two fluids in these experiments, separate brine–rock experiments were performed. Brine was periodically sampled and analyzed during all experiments. After the experiments were terminated, the solids and quenched brine were analyzed.

The rocks used in experiments are based on the mineralogy and petrology of the core samples from the Madison Limestone of the Moxa Arch (Section 5.1 and Table 1 of Part I). Two different rock types were evaluated. Rock type A was composed of 83 wt% dolomite (Do), 10 wt% calcite (Cc), 6 wt% anhydrite (Anh), and 1 wt% pyrite (Py) and rock type B was composed of 86 wt% Do, 13 wt% Cc, and 1wt% Py. Minerals of research grade quality were acquired from Wards Natural Science. For each experiment, 5 grams of minerals (75% mineral chips and 25% mineral powders) were reacted with approximately 150 ml of synthetic brine. Synthetic brine was formulated based on the brine chemistries summarized in Table 1, Part I. Nanopure water (18 Ω) was sparged with argon gas to remove any dissolved gases prior to mixing and storage of the brine.

Unreacted minerals and minerals recovered from the quenched experiments were analyzed by x-ray florescence (XRF) and inductively coupled plasma optical emissions spectroscopy (ICP-OES) following acid digestion for major, minor and trace element content. Scanning electron microscopy (SEM) was used for textural analysis and X-ray diffraction (XRD) for mineral identification.

Fluid samples were analyzed for dissolved cations and anions by ICP-OES, ICP-mass spectrometry (ICP-MS), and ion chromatography. Total inorganic carbon (as CO₂) and sulfur (S²⁻ and S⁴⁺) in the fluid was determined by coulometric titration (Huffmann, 1977). The pH of fluid samples cooled to 25°C was determined using a Ross micro electrode.

Results

The evolution of brine chemistry as a function of time is presented in Figures 6-11, 6-12, and 6-13. Each of the experiments reached approximate steady state conditions within the first 100 hours of the experiment. Upon the injection of supercritical CO₂, pH decreased to a calculated in-situ value of 4 and dissolved CO₂ increased by approximately 3 orders of magnitude. Aqueous calcium and magnesium both increase suggesting dissolution of dolomite. Aqueous sulfate and calcium subsequently decrease throughout the remainder of the supercritical CO₂-bearing portion of the experiments, suggesting precipitation of anhydrite. Dissolution of carbonate mineral and precipitation of anhydrite are verified by SEM and XRD analysis, respectively.

In Figure 6-14 the results of the experiments are plotted on the same Eh-pH diagram as the conceptual model that was previously developed (Eh-pH diagram in Figure 6-5) for the Madison Limestone on the Moxa Arch. Adding CO₂ to the experimental Madison Limestone-brine system decreases pH and increases Eh while crystallizing anhydrite and pyrite. Final Eh-pH conditions approach but do not exactly match predictions of the coexisting sulfur-bearing phases (pyrite, anhydrite, native sulfur, and H₂S) that are also observed in core samples and produced waters.

Conclusions

Injection of supercritical CO₂ into a carbonate-brine reservoir lowers pH and dissolves carbonate minerals. Calcium subsequently reacts with sulfate to precipitate anhydrite. These results suggest that disproportionation of SO₂ introduced during geologic carbon co-sequestration will lead to mineralization and storage of the sulfur as anhydrite.

References

- Bethke, C.M., and Yeakel, S., 2009, The Geochemist's Workbench Release 8.0: Reaction Modeling Guide: Champaign, Illinois, University of Illinois, 84 p.
- Huffmann, E., 1977, Performance of a new automatic carbon dioxide coulometer: Microchemical Journal, v. 22, p. 567-573.
- Kaszuba, J.P., Janecky, D.R., and Snow, M.G., 2003, Carbon dioxide reaction processes in a model brine aquifer at 200°C and 200 bars: Implications for geologic sequestration of carbon: Applied Geochemistry, v. 18, p. 1065-1080.
- , 2005, Experimental evaluation of mixed fluid reactions between supercritical carbon dioxide and NaCl brine: Relevance to the integrity of a geologic carbon repository: Chemical Geology, v. 217, p. 277-293.
- Seyfried, W.E., Jr., Janecky, D.R., and Berndt, M.E., 1987, Rocking autoclaves for hydrothermal experiments, II. The flexible reaction-cell system, *in* Ulmer, G.C., and Barnes, H.L., eds., Hydrothermal Experimental Techniques: New York, John Wiley & Sons, p. 216-239.

Figure 6-11. Brine chemistry as a function of time for brine–rock experiments. Symbols represent measured fluid composition and dashed lines are predictive geochemical calculations made with Geochemist’s Workbench (GWB) version 8 (Bethke and Yeakel, 2009) and the b-dot ion association model. Measured and predicted calcium and magnesium do not agree because GWB does not do well simulating solid solutions.

Figure 6-12. Brine chemistry as a function of time for supercritical CO₂-brine–rock experiments. Symbols represent measured fluid composition and dashed lines are predictive geochemical calculations made with GWB and the b-dot ion association model.

Figure 6-13. Interpretation of pH behavior in brine–rock and supercritical CO₂–brine–rock experiments. pH is measured at 25°C, 1 bar in samples from which CO₂ has degassed to atmospheric saturation (solid lines & symbols). Changes in the pH of the brine in response to increased temperature (110°C) and CO₂-saturation were calculated using GWB and the b-dot ion association model to determine an *in-situ* pH (dashed lines & open symbols).

Figure 6-14. Eh/pH diagram showing evolution of experimental fluids that have reacted with Madison Limestone and supercritical CO₂. Circle denotes composition of starting brine at 25°C and 1 bar and X denotes composition of brine once it reaches experimental conditions. Triangle and square denote final fluid compositions of brine–rock and supercritical CO₂–brine–rock experiments, respectively.

CHAPTER 7: Sequestration of CO₂ in Deep Saline Aquifers: Measurement of Drainage and Imbibition CO₂/Brine Relative Permeability, Hysteresis Cycles, and Permanent Capillary Trapping

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Background

In Task 7, researchers measured relative permeabilities, hysteresis, and capillary trapping of CO₂. Accurate, appropriately scaled relative permeabilities are important for determining the storage capacity and fate of sequestered CO₂. Research under this task employed a recently established state-of-the-art multiphase flow laboratory to carry out the experiments through aquifer core samples. The results discussed below are important to developing and validating models that are capable of predicting fluid flow behavior and properties. Utilizing the physically based flow properties can significantly reduce the uncertainties associated with estimations of storage capacity in geological formations and predictions of fate of CO₂. A summary of results follows.

Executive Summary

We present the results of an extensive experimental study on the effects of hysteresis and wetting on permanent capillary trapping and relative permeability of CO₂/brine systems. We performed 48 unsteady-state drainage and imbibition full-recirculation flow experiments in two different sandstone rock samples, i.e., Berea and Nugget. A state-of-the-art reservoir conditions core-flooding system was used to perform the tests. This system included nine cylinder Quizix pumping system that allowed full re-circulation of flow and a high-quality pressure control conditions leading to a superior equilibrium maintenance between CO₂ and brine. During the experiments the fluids were re-circulated to maintain equilibrium between the phases. Special core-flooding techniques had to be employed to minimize large variations in back pressure particularly at high CO₂ flow rates. This minimized the variations in the pressure of the system and consequently in the equilibrium between the phases. We utilized a medical CT scanner to measure in-situ saturations along the length of the samples during the flow experiments. The scanner was rotated to the horizontal orientation allowing flow tests through vertically-placed rock samples. The samples were about 3.8 cm in diameter and 15 cm long. The Berea and Nugget sandstone cores had about 20.1% and 14.3% porosities and 50 and 312 mD absolute brine permeabilities, respectively. Both supercritical CO₂/brine and gaseous CO₂/brine fluid systems were used. We used high purity CO₂ and brine with 10% NaI, 5.0% NaCl, and 0.5% CaCl₂ (all by weight) composition. The gaseous and supercritical CO₂/brine experiments were carried out at 502 and 1595.5 psig back pressures and 20 and 55 °C, respectively. Under the above-mentioned conditions, the gaseous and supercritical CO₂ have 0.081 and 0.393 gr/cm³ densities (Span and Wagner, 1996), respectively. The samples were first saturated with brine and

then flooded with CO₂ at different maximum flow rates. In each experiment, injection of CO₂ was continued until constant pressure drop and saturation distribution along the core were reached. The drainage process was then followed by a low flow rate (0.5 cm³/min) imbibition until residual CO₂ saturation was achieved. Wide flow rate ranges of 0.25 to 20 cm³/min for supercritical CO₂ and 0.125 to 120 cm³/min for gaseous CO₂ were used to investigate the variation of irreducible brine saturation (S_{wirr}) with maximum CO₂ flow rate and variation of trapped CO₂ saturation (S_{CO2r}) with S_{wirr} . For a given irreducible brine saturation, the trapped supercritical CO₂ saturation was less than that of gaseous CO₂ in the same sample. This was partly attributed to brine being less wetting in the presence of supercritical CO₂ than in the presence of gaseous CO₂. The ratio of S_{CO2r} to initial CO₂ saturation ($1 - S_{wirr}$) was found to be much higher for low initial CO₂ saturations. This means that greater fractions of injected CO₂ can be permanently trapped at higher initial brine saturations. The results indicate that very promising fractions (about 50 to 75%) of the initial CO₂ saturation can be permanently trapped. Maximum CO₂ and brine relative permeabilities at the end of drainage and imbibition and also variation of brine relative permeability due to post-imbibition CO₂ dissolution were also studied.

Experimental methods

In this section we present detailed information regarding the material, experimental setup, and procedure.

Rock Samples, Fluids, and Experimental Conditions

The flow experiments included series of unsteady-state CO₂ (drainage) and brine flooding (imbibition) tests in two different core samples, Berea and Nugget sandstones. Table 7-1 lists dimensions and some of the petrophysical properties of the cores. Both samples were outcrop cores and strongly water-wet. Nuggets sandstone core was obtained from SW Wyoming, while the Berea core was cut from a block obtained from a quarry in Ohio. In this work, two groups of experiments were carried out. In the first group, we used gaseous CO₂ and brine with 10 wt% NaI, 5 wt% NaCl, and 0.5 wt% CaCl₂ composition. The experiments were carried out at ambient temperature and 502 psig back pressure. These conditions fall within the gaseous region of the pressure-temperature diagram of CO₂, see Figure 7-1. In this group we performed nine drainage and nine imbibition experiments. Each experiment was started from brine saturated core ($S_w=1$). CO₂ was then injected (drainage) to establish an “irreducible” brine saturation. Each drainage experiment was carried out with a pre-specified maximum CO₂ flow rate. We increased the flow rate gradually until the pre-specified flow rate was reached. The “irreducible” brine saturation was then measured repeatedly. The measurements were considered final when the difference between two consecutive saturation profiles and pressure drop data were less than 2%. We used a wide range of maximum flow rates, i.e., 0.125–120 cm³/min, to create a broad range of irreducible brine saturations. All the flow rates used are listed in Table 7-2.

It is important to note that all the experiments presented in this work were carried out in a closed-loop system. This means that the fluids were fully re-circulated even at high flow rates, e.g., 120 cm³/min. Full re-circulation allows one to achieve and maintain equilibrium between the aqueous and CO₂-rich phases at the pressure and temperature of the experiment and hence minimize mass transfer between them inside the core sample. Performing full re-circulation flow experiments at various flow rates, and in the same time maintaining stable pressures in different parts of the experimental apparatus, e.g., core back pressure, core upstream pressure, and separator pressure,

is indeed a very difficult task, particularly in flow experiments in which variations in pressure can impact miscibility of fluids in each other as well as displacement mechanisms inside the core sample. We have successfully developed and implemented a full re-circulation flow system that is capable of performing experiments at flow rates as high as 180 cm³/min and still maintain stable pressures in different parts of the system, including core back pressure.

After obtaining “irreducible” brine saturation at the end of each drainage experiment, brine was injected into the core to displace and trap CO₂ (imbibition). The maximum brine flow rate in all the imbibition experiments was 0.5 cm³/min. The brine flow rate was first increased to 0.1 cm³/min and then gradually to a maximum of 0.5 in maximum 0.1 increments. It is critical to increase the flow rate gradually as sudden increase could lead to some dynamic effects and hence affect the trapping results. Our purpose in this work was to study trapping of CO₂ under capillary dominated conditions. When the variations in the saturation profile and pressure drop across the core were less than 5 % the experiment was considered complete.

In order to carry out a new set of drainage and imbibition flow experiments, an in-situ re-saturation technique was used to re-establish $S_w=1$. This allowed us to avoid disassembling and reassembling of the core-holder and the flow lines. During this step, brine was injected at relatively high flow rates, e.g., 10–14 cm³/min, to dissolve the trapped CO₂. As we will discuss shortly, due to small deviations from equilibrium, brine always has some small capacity left for dissolution of additional CO₂. This is regardless of the technique used to equilibrate the fluids. We take advantage of this in order to re-saturate the core with brine by dissolving the trapped CO₂. After the full re-saturation of the core is confirmed by a complete scan of the sample, a new drainage experiment with a new maximum CO₂ flow rate is started.

In the second group, we used higher pressures and temperatures, i.e., 55°C and 1595.5 psig back pressure, leading to a supercritical condition for CO₂, see Figure 7-1. Similar to the first group of the experiments, we performed drainage experiments followed by and brine floods. Due to higher viscosity and density of supercritical CO₂ compared to those of gaseous CO₂, see Table 7-3, the maximum CO₂ flow rate used during the drainage experiments was 20 cm³/min. A total of eight sets of drainage and imbibition experiments were performed in Berea core and a total of six sets in Nugget core, see Table 7-2 for the flow rates. We were able to establish comparable “irreducible” brine saturations with those of experiments with gaseous CO₂.

Experimental Setup

The experimental setup used in this work is a state-of-the-art multiphase core-flooding systems that includes various elements such as nine cylinder Quizix pumping system, three in-line viscometers, a compensation accumulator, an acoustic three-phase separator, pneumatic valves, differential and gauge pressure transducers, a Hassler type core holder, and mechanical convection ovens, see Figure 7-2 for a schematic flow diagram. All the wetted parts of the apparatus are made of Hastelloy and other corrosion resistant materials. The experimental setup is a closed-loop system that allows fluid to be injected/re-injected into the core at elevated temperatures and pressures.

We used high- and low-volume dual-cylinder Quizix pumps for injection of brine and CO₂, respectively. Each cylinder in the low-volume pump has about 9.3 cm³ capacity while this is 275

cm³ for each cylinder of the high-volume pump. Maximum possible flow rates for each of these pumps are 15 and 200 cm³/min, respectively. The core-flooding system maintains a constant back pressure, which allows us to achieve superior equilibrium even at very high flow rates. All of these pump cylinders were either located inside a large mechanical convection oven or heated by efficient heating tapes. Holes in the body of the oven allowed passage of the flow lines to the core holder.

The effluent of the core was sent to a large 3,500 cm³ acoustic three-phase separator, which was placed in another mechanical convection oven. The separator is made of Hastelloy and the level of fluids in it were monitored using acoustic transducers. As we mentioned earlier, we performed the experiments in a closed-loop full re-circulation apparatus. Therefore, the pumps that inject fluids to the core, retract their fluids from the separator. And hence it is critical to monitor fluids level in the separator to avoid retraction of wrong fluids to the injection pumps, particularly at high flow rates.

The overburden pressure was maintained using a single cylinder low-volume Quizix pump. Utilization of a Quizix pump allows automatic adjustment of overburden pressure with variations in the pore pressure. This is critical in experiments with rock samples that show significant sensitivity to variations in overburden pressure.

The setup also included a medical CT scanner tuned for petrophysical applications. The scanner was rotated to the horizontal orientation allowing us to carry out the experiments through vertically-placed rock samples, which reduced the gravity segregation effects. A vertical positioning system (VPS) was used to move the core holder vertically from bottom into the gantry. During an experiment with a core sample, the VPS was first synchronized with the horizontal patient table of the scanner. It is critically important to maintain this synchronization until the end of each group of experiments, i.e., until a new core sample is used.

The Quizix pumps and the VPS were supported by a full redundancy Liebert UPS. This was important as each group of experiments took about three weeks, and therefore utilization of a reliable emergency power system allowed us to not only protect the continuity of flow during an experiment but also the synchronization of the VPS with the scanner. Otherwise, a small interruption of power could lead to loss of experiments.

Experimental Procedure and Equilibrium

In this section, we explain the details of the experimental procedure used to perform the flow experiments with supercritical CO₂ (scCO₂). The procedure for the experiments with gaseous CO₂ was identical to those used in experiments with scCO₂.

Before the experiments, the core flood system was pressure calibrated and tested for possible leakages. To do this, the pumps were connected to atmospheric pressure to make sure their transducers measured zero gauge pressure. At this point, a highly accurate reference gauge pressure transducer was connected to the system. The core flood system was then saturated with water and pressurized using one of the pump cylinders until 9,500 psig pressure was read from the reference pressure transducer. At this point, all the pump transducers were set to read 9,500 psig. During this process, we also made sure that the system did not have any leakages and that

we could maintain the pressure at the set level for a day. This step is very important because one would need to be sure that all the pump transducers are calibrated and read pressures relative to a same reference.

For each set of experiments, a core was placed in a Hassler type core holder with a Viton sleeve. The core holder had spiral Hastelloy distribution end plugs with four holes with each connected to a 1/8" Hastelloy tubing. For the experiments with supercritical CO₂, the core was wrapped with several layers of Aluminum foil and Teflon tape to prevent CO₂ diffusing into the sleeve and ultimately into the overburden fluid. The core holder was then wrapped with high efficiency insulation material and located on the VPS system and moved into the CT scanner. The core holder assembly was then flushed with gaseous CO₂ from a pressurized bottle and then vacuumed. At this stage, the entire core was scanned with 1 mm slice thickness generating about 38-76 slices depending on the length of the core and slice spacing used. The samples were scanned at 130 kV and 100 mA.

The core flooding system was first saturated with brine and CO₂. The system was then pressurized (with additional CO₂) and heated to 1,600 psig and 55°C. A total approximate amount of 1,500 cm³ of brine was introduced into the separator. The remaining volume of this vessel was occupied by supercritical CO₂. At this point, brine pump (P1A and P1B) and CO₂ pump (P2A and P2B) were used to re-circulate brine and scCO₂ bypassing the core holder. Brine and CO₂ pumps were operated under paired constant flow rate mode allowing them to create continuous flow of these fluids. The fluids bypassing the core-holder ultimately arrived at the separator.

The above-mentioned full re-circulation of the fluids was continued (bypassing the core) for 12–24 hours under the pressure and temperature of the experiments. This technique was used to achieve equilibrium between the phases before the core flooding experiments were started. Also, the fluids were in continuous contact in the separator during their injection to the core.

At this point, the core was saturated with supercritical CO₂. The core-holder was heated at its two ends using two highly efficient heat bands and manual controllers. The level of heat was adjusted to obtain the desired temperature at the outlet of the core. The fluid temperature at the inlet was also monitored and controlled using heating tapes utilized on all the tubings outside the ovens. Temperature was monitored in other locations of the systems as well, e.g., inside the separator and inside both ovens. Flow of supercritical CO₂ through the core was continued for a few hours before it was scanned to acquire CO₂ saturated reference image of the core. During this period, CO₂ leaving the core was ultimately sent to the separator from which CO₂ was retracted again by P2.

After acquisition of CO₂-saturated image of the core, brine was injected into the core using P1, which again retracted it from the separator. As we mentioned earlier, brine and CO₂ always have slight deviations from “perfect” equilibrium at the pressure and temperature of the experiment and this proved to be very useful in our experiments. At the end of each imbibition, many pore volumes of brine was retracted from the separator and injected at relatively high flow rates into the core to dissolve the trapped CO₂. This process allowed us to perform in-situ re-saturation of the core with brine before a new drainage experiment was started. The re-saturation process,

however, was lengthy as brine was almost completely saturated with CO₂ in the separator. Brine injection was continued until subsequent scans did not show any “free” CO₂ in the core. Then the entire core was scanned to obtain a brine saturated image of the sample. At this point, the core was ready for the first drainage (CO₂ injection) experiment.

CO₂ was then injected into the brine saturated core. The effluent fluids were ultimately sent to the separator and re-circulated. For each drainage experiment, we used a maximum flow rate, see Table 7-2. The flow rate was gradually increased to reach the maximum and maintained at that point until the variations in pressure drop and saturation distribution along the length of the core were less than 2%. The brine saturation at that point was reported as “irreducible” saturation for the maximum CO₂ flow rate used.

The core at the end of drainage was then subjected to brine injection (imbibition). The maximum brine flow rate for all imbibition experiments was 0.5 cm³/min. The flow rate was increased gradually to reach this maximum and kept under this condition until all the CO₂ was either displaced or trapped. The core was then scanned to report the residual CO₂ saturation. As it was discussed earlier, the sample at this point was re-saturated with brine with extensive injection of brine retracted from the separator. This process was then followed by a new set of drainage and imbibition experiments.

All the experiments were carried out while the core holder was placed vertically inside the CT scanner. The fluids were injected from bottom and produced from top. The core-flooding system was a closed-loop apparatus and operated under full-recirculation condition.

Results and discussion

The experiments were divided into two groups: 1) injection of CO₂ into brine saturated core, and 2) injection of chase brine into a core at irreducible brine saturation. Below we present and the results and discussion for each category.

CO₂ injection

Figure 7-3 shows variation of maximum scCO₂ saturation reached versus scCO₂ injection flow rate. Each data point represent the steady state achieved at a given scCO₂ flow rate in an independent experiment and is averaged in the central 70% of the core. Maximum scCO₂ saturation increases sharply in lower flow rates and then gradually stabilizes at high flow rates. This is expected as it becomes more difficult to displace brine from smaller pores and crevices as brine saturation decreases. But the wide range of maximum scCO₂ flow rates allowed us to create a relatively wide range of initial brine saturations for the subsequent brine injection experiments. Maximum scCO₂ saturation ranged between 0.32 and 0.60 for flow rates between 0.25 and 20 cm³/min. Figure 7-4 presents the results for gaseous CO₂ and brine fluid system in the Berea sandstone core. To obtain a similar range of CO₂ saturation, we performed CO₂ injection experiments with flow rates as high as 120 cm³/min, which were much higher than those in scCO₂ experiments. This is mainly because scCO₂ is about three times more viscous than gaseous CO₂ (see Table 7-3) and therefore more effective in displacing brine at a given flow rate. Maximum gCO₂ saturation ranged between 0.33 and 0.65 for flow rates between 0.125 and 120 cm³/min. We performed experiments with gaseous CO₂ to allow us to study the effects of

wetting on trapping of CO₂ as we will discuss in the next section. As we mentioned earlier, all the experiments (regardless of flow rate) were performed under full re-circulation conditions and with equilibrated fluids.

Figure 7-5 depicts variation of scCO₂ saturation versus flow rate for scCO₂ injection experiments in Nugget sandstone core. For a given flow rate, displacement of brine in Nugget sandstone was more effective than in Berea core. We believe capillary elements in the Nugget core were larger with lower drainage threshold capillary pressure and therefore they get invaded by scCO₂ more easily. We were able to obtain an average of 67% scCO₂ saturation at 10 cm³/min scCO₂ flow rate in Nugget versus about 52% in Berea core for the same flow rate. Table 7-2 lists all the flow rates used in the experiments performed in Berea and Nugget sandstone cores.

Figures 7-6 and 7-7 include CT slices that show the variation of in-situ scCO₂ saturation in different locations of Berea and Nugget sandstone cores, respectively. CO₂ and brine were distributed more evenly in Berea than in Nugget as the former is more homogenous. Figures 7-8, 7-9, and 7-10 exhibit variations of $S_{CO_2}^{max}$ with porosity for experiments in Berea and Nugget sandstones. Expectedly $S_{CO_2}^{max}$ increases with increase in porosity in a given flow rate, which is consistent with the results presented by Perrin and Benson (2010).

At the end of each CO₂ injection experiment, the steady-state saturations and pressure drop along the length of the core were recorded when variation in two consecutive measurement was less than 2%. The pressure drop data was then used to calculate endpoint CO₂ permeability. Figures 7-11 and 7-12 show variation of endpoint scCO₂ relative permeability versus brine saturation for Berea and Nugget cores, respectively. Supercritical CO₂ exhibits particularly low relative permeability. This is consistent with the drainage relative permeability data presented by Perrin and Benson (2010).

Injection of chase brine

After reaching the steady state at the end of each CO₂ injection experiment, chase brine was injected at about 0.5 cm³/min. The brine was saturated with CO₂ under the conditions of the experiments before injection. The injection was continued until residual CO₂ saturation was reached. Multiple scans of the core during this process allowed us to determine the residual saturation point. We then recorded the in-situ saturation and pressure drop across the core. This process was done after every CO₂ injection experiment discussed in the previous section creating a wide range of residual saturations. Figures 7-13 and 7-14 present the end-point brine relative permeabilities at residual scCO₂ saturations. Figures 7-15 and 7-16 show variation of trapped CO₂ saturation with initial CO₂ saturation at the beginning of imbibition for experiments with scCO₂ and gCO₂, respectively, in Berea core. It is clear that for a given initial brine saturation, trapped gCO₂ saturation is greater than scCO₂ saturation in this sample. We think this may have been partly caused by brine being less wetting in the presence of scCO₂ than in the presence of gCO₂ in the same sample. These data indicate that residual scCO₂ saturation varies between 20% and 32% that is 50% to 70% of the initial CO₂ in place. This is a significant fraction of the CO₂ that was placed in the core. The remaining pore space is filled with brine saturated with CO₂, therefore the amount that is stored in the core permanently is the summation of trapped and dissolved CO₂. Figure 7-17 presents these quantities for experiments in Nugget core.

The residual scCO₂ saturation in Nugget is greater than those in Berea. We think this may have been caused by higher pore/throat aspect ratio in Nugget that directly affects the amount of trapping through various pore-level displacement mechanisms such as snap-off and pore-body filling.

Figures 7-18, 7-19, and 7-20 present the variation of per-slice trapped CO₂ saturation versus initial CO₂ saturation at the beginning of imbibition for experiments in Berea and Nugget core. The results are compared with those predicted by empirical trapping models of Land (1968) and Spiteri et al. (2005). Finally, Figure 7-21 presents variation of trapping efficiency ($R=S_{CO_2r}/S_{CO_2}^{max}$) with the initial CO₂ saturation at the beginning of imbibition for experiments with scCO₂ and gCO₂, respectively, in Berea core. These trapping efficiency for experiments in Nugget sandstone core are presented in Figure 7-22.

Table 7-1. Dimensions and petrophysical properties of the cores used in this study.

Sample	Diameter	Length	ϕ (X-ray)	K_{abs} (Brine)	Pore Volume
	cm	cm	%	mD	cm ³
Berea sandstone	3.81	15.0	20.08	50	34.34
Nugget sandstone	3.81	14.8	14.28	312	24.09

Table 7-2. Maximum CO₂ flow rates used in drainage (non-wetting phase injection) experiments. Gaseous CO₂ was used at 23°C temperature and 502 psig pressure, while supercritical CO₂ was at 55 °C and 1595.5 psig. The NWP stands for non-wetting phase and WP stands for wetting phase.

Sample	NWP	WP	0.125	0.25	0.5	1.0	2.5	5	10	15	20	30	60	100	120
			cm ³ /min												
Berea SS	scCO ₂	Brine		•	•	•	•	•	•	•	•				
Berea SS	gCO ₂	Brine	•	•	•		•		•			•	•	•	•
Nugget SS	scCO ₂	Brine		•	•	•	•	•	•						

Table 7-3. Properties of fluids used in this work (Span and Wagner, 1996; Michels et al. 1957; Bachua and Bennion, 2009). Salinity of the brine used in this work is 174,400 ppm.

Fluid	Pressure	Temperature	Viscosity	Density	CO ₂ /Brine IFT
	MPa	°C	cP	gr/cm ³	mN/m
Supercritical CO ₂	11.0	55	0.044	0.393	38.15
Gaseous CO ₂	3.46	20	0.016	0.081	51.24
Brine	3.46	20	1.57	1.125	—
Brine	11.0	55	0.91	1.126	—

Figure 7-1. Pressure-Temperature diagram of carbon dioxide, data from Span and Wagner (1996).

Figure 7-2. Schematic flow diagram of the experimental setup used in this work. The apparatus includes a medical CT scanner and a Vertical Positioning System, nine Quizix Hastelloy cylinders, a state-of-the-art Hastelloy three-phase acoustic separator, an Aluminum Hassler core-holder, differential and gauge pressure transducers, a back pressure maintenance module, and several temperature measurement devices. All the tubings used in the system are made of Hastelloy.

Figure 7-3. Variation of maximum scCO₂ saturation reached versus scCO₂ injection flow rate during scCO₂/brine drainage experiments in Berea sandstone.

Figure 7-4. Variation of maximum gCO₂ saturation reached versus gCO₂ injection flow rate during gCO₂/brine drainage experiments in Berea sandstone.

Figure 7-5. Variation of maximum scCO₂ saturation reached versus scCO₂ injection flow rate during scCO₂/brine drainage experiments in Nugget sandstone.

Berea Sandstone							
	84 mm from inlet		70 mm from inlet		40 mm from inlet		
Flow rate	$S_{CO_2}^{max}(1-S_{win})$	S_{CO_2r}	$S_{CO_2}^{max}(1-S_{win})$	S_{CO_2r}	$S_{CO_2}^{max}(1-S_{win})$	S_{CO_2r}	
$Q_{CO_2}^{max} = 0.25$ cc/min
Saturation	0.331	0.1994	0.3327	0.209	0.3944	0.272	
$Q_{CO_2}^{max} = 5.0$ cc/min
Saturation	0.4866	0.2604	0.4846	0.2776	0.5306	0.3326	
$Q_{CO_2}^{max} = 20$ cc/min
Saturation	0.6011	0.314	0.6112	0.3411	0.6568	0.356	

Figure 7-6. scCO₂ saturation distribution for Berea sandstone core at different flow rates and locations from inlet.

Nugget Sandstone							
	112 mm from inlet		88 mm from inlet		68 mm from inlet		
Flow rate	$S_{CO_2}^{max}$ (1- S_{witr})	S_{CO_2r}	$S_{CO_2}^{max}$ (1- S_{witr})	S_{CO_2r}	$S_{CO_2}^{max}$ (1- S_{witr})	S_{CO_2r}	
$Q_{CO_2}^{max} = 0.25$ cc/min
Saturation	0.2247	0.2158	0.19	0.1786	0.3664	0.3240	
$Q_{CO_2}^{max} = 2.5$ cc/min
Saturation	0.5424	0.3988	0.5667	0.409	0.65	0.4306	
$Q_{CO_2}^{max} = 10$ cc/min
Saturation	0.6484	0.52	0.6571	0.5167	0.66	0.4876	

Figure 7-7. scCO₂ saturation distribution for Nugget sandstone core at flow rates and locations from inlet.

Figure 7-8. scCO₂ saturation distribution versus porosity for Berea sandstone.

Figure 7-9. gCO₂ saturation distribution versus porosity for Berea sandstone.

Figure 7-10. scCO₂ saturation distribution versus porosity for Nugget sandstone.

Figure 7-11. Endpoint scCO₂ relative permeability for drainage in Berea sandstone core.

Figure 7-12. Endpoint scCO₂ relative permeability for drainage in Nugget sandstone core.

Figure 7-13. Endpoint brine relative permeability for imbibition in Berea sandstone core.

Figure 7-14. Endpoint brine relative permeability for imbibition in Nugget sandstone core.

Figure 7-15. Comparison between the experimental data and empirical trapping models available in the literature (Land, 1968; Spiteri et al., 2005) for $scCO_2$ /brine imbibition in Berea sandstone core.

Figure 7-16. Comparison between the experimental data and empirical trapping models available in the literature (Land, 1968; Spiteri et al., 2005) for gCO₂/brine imbibition in Berea sandstone core.

Figure 7-17. Comparison between the experimental data and empirical trapping models available in the literature (Land, 1968; Spiteri et al., 2005) for scCO₂/brine imbibition in Nugget sandstone core.

Figure 7-18. Variation of per-slice residual scCO₂ saturation with scCO₂ saturation at the end of drainage for Berea sandstone. The results are compared with those predicted by empirical trapping models available in the literature (Land, 1968; Spiteri et al., 2005).

Figure 7-19. Variation of per-slice residual gCO₂ saturation with gCO₂ saturation at the end of drainage for Berea sandstone. The results are compared with those predicted by empirical trapping models available in the literature (Land, 1968; Spiteri et al., 2005).

Figure 7-20. Variation of per-slice residual scCO₂ saturation with scCO₂ saturation at the end of drainage for Nugget sandstone. The results are compared with those predicted by empirical trapping models available in the literature (Land, 1968; Spiteri et al., 2005).

Figure 7-21. Trapping efficiency for experiments in Berea sandstones.

Figure 7-22. Trapping efficiency for experiments in Nugget sandstones.

Conclusions

The conclusions of this experimental study are summarized as:

- Developed a robust full-recirculation core-flooding system and procedure for CO₂/brine experiments with high quality back pressure regulation and separator pressure maintenance, which are crucial for maintaining equilibrium between the phases and hence generating meaningful results.
- Performed more than 46 drainage and imbibition CO₂/brine core-flood experiments in Nugget and Berea sandstone cores to investigate the effects of initial brine saturation and flow rate on the capillary trapping of CO₂
- In-situ re-saturation of the core samples allowed more sets of drainage and imbibition core-flooding test to be carried out in a given period of time and without a need to disassemble/reassemble the core holder.
- Lower initial water saturation lead to higher residual CO₂ saturations.
- Lower initial CO₂ saturation generated higher trapping efficiency ($R = S_{CO_2r} / S_{CO_2}^{max}$).
- Trapping efficiency was between 49 to 78%, i.e., the ratio of the residual CO₂ saturation to the initial CO₂ in place.

References

- Bachua, S., D. B. Bennion (2009), Dependence of CO₂ -brine interfacial tension on aquifer pressure, temperature and water salinity, *Energy Procedia*, 1 (1), 3157-3164.
- Land, C. S. (1968), Calculation of Imbibition Relative Permeability for Two- and Three-Phase Flow From Rock Properties. *SPEJ*, Trans. AIME, 243, 149–156.
- Michels, A., A. Botzen and W. Schuurman (1957), The viscosity of carbon dioxide between 0°C and 75°C and at pressures up to 2000 atmospheres, *Physica*, 23 (1-5), 95-102.
- Perrin, J. C., and S. Benson (2010), An Experimental Study on the Influence of Sub-Core Scale Heterogeneities on CO₂ Distribution in Reservoir rocks, *Transport Porous Media*, 82, 93-109.
- Span, R., and W. Wagner (1996), A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100 K at pressure up to 800 MPa, *Journal of Physical and Chemical Reference Data*, 25 (6), 1509-1596.
- Spiteri, E. J., R. Juanes, M.J. Blunt, and F.M. Orr Jr., (2005), Relative Permeability Hysteresis: Trapping Models and Application to Geological CO₂ Sequestration, SPE 96448, presented at SPE Annual Tech. Conf., Dallas, October 9–12.

CHAPTER 8: Monitoring of carbon-sequestered aquifers – a feasibility study

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Background

Researchers in Task 8 conducted a detailed study on full waveform synthetic computation and inversion for elastic properties and micro-seismic sources for fracture characterization for the purpose of CO₂ sequestration and monitoring in the Moxa Arch. The study used known physical properties from relevant Wyoming aquifers to fluid substitute aquifer water with different concentrations of CO₂ and compute full waveform synthetic seismograms. Inverting these synthetics for elastic properties allowed for compiling the sensitivity of the inversion to various levels of CO₂ saturation and volume. The work was also able to simulate the micro-seismic responses from simulated injection rates by inverting the computed waveforms for source signatures to characterize the space-time fracture evolution. Results from this task follow in the chapter below.

Executive Summary

Monitoring of carbon sequestered brine reservoirs requires (1) detailed characterization of the reservoirs for their respective acoustic and fluid properties, and (2) detection of possible fracture zones within and above the sequestered formations that could be potential leakage pathways so that mitigation steps could be taken beforehand to stop such leakage-risk conditions. Since seismic method is the most effective tool at the depths of our interest (10,000 feet or higher), we have investigated the usage of both active- and passive source seismic data for our analysis.

To characterize reservoir acoustic and fluid properties, we used a real well-log data from the Moxa-Arch, Wyoming, and conducted fluid substitution experiments within various brine reservoir formations. In our fluid substitutions, we replaced the brine with different saturations of carbon dioxide (CO₂) and observed the changes in the acoustic properties within the formations caused by these replacements. When in-situ brine is replaced by CO₂, our observations indicated that the although longitudinal (P) and transverse (S) wave velocities are sensitive to such replacement by a change of P-to-S velocity ratio (V_P/V_S) or Poisson's ratio, it is the formation density that is affected the most. For an effective monitoring, it is therefore necessary to use a methodology that can measure the changes in density in the subsurface reservoirs.

Following the fluid substitution experiments, we computed theoretical seismic responses for the original (brine saturated) and CO₂ sequestered models. Using a waveform inversion methodology, we demonstrated that the density cannot be accurately estimated from such an inversion when we use only the vertical component seismic data. Vertical component seismic data are sensitive to the changes in P-wave reflection amplitudes at various separation distances between the seismic source and the receivers (source-to-receiver offsets). These P-wave reflection amplitudes, in turn, are

primarily sensitive to the subsurface variations of V_P and Poisson's ratio and not so much to the variations of density. Consequently, when we used only the vertical component, we could accurately predict the subsurface V_P and Poisson's ratio, but not the density. However, in addition to the vertical component, if we use the radial component of the seismic response in a multicomponent waveform inversion scheme, we find that the density can be accurately predicted from such inversion. Radial component of seismic response is sensitive to the variations of the mode-converted (P-S) reflection amplitudes at different source-to-receiver offsets. These reflection amplitudes are sensitive not only to Poisson's ratio but also to the density, and therefore the multicomponent waveform inversion allowed an accurate prediction of subsurface density variations.

To characterize fractures, we introduced micro-earthquakes with various fault (fracture) plane geometries in the layer just above the sequestered formation, and computed theoretical seismic responses at the surface from these micro-earthquakes. Comparing both vertical and radial components of these computed responses, we demonstrated that they are sensitive to the fault-plane geometry. Therefore, if passive seismic sensors are deployed, microseismic responses can predict fractures and the potential leakage pathways after sequestration.

Although multicomponent seismic data are needed to predict subsurface density, acquiring multicomponent seismic data for both baseline survey and for subsequent monitoring could be prohibitively expensive. However, if passive seismic sensors are deployed; in addition to predicting fractures, they could also be used for monitoring and could turn out to be very cost-effective.

In conclusion, we think that for a cost effective monitoring of CO_2 sequestered brine reservoirs, the following steps are necessary,

- (1) Acquire multicomponent seismic data for baseline survey.
- (2) Invert the multicomponent seismic data and predict the subsurface acoustic and fluid property model before sequestration.
- (3) Deploy permanent passive seismic sensors and record microseismic responses during and after sequestration.
- (4) Use the recorded microseismic responses to predict fractures and to monitor the sequestered formation.

Experimental Methods

Monitoring is an integral component of carbon sequestration study as it is necessary to ensure (1) the sequestered gas is in place, (2) above-normal pore pressure due to sequestration does not fracture surrounding rock formations generating potential pathways for CO_2 leakage, and (3) geological integrity of the entire region is maintained during and after sequestration.

According to the recent studies (Juanes et al. 2006; van der Meer and Wees, 2006), brine reservoirs could provide permanent storage of large volumes of CO_2 underground. In this investigation, we therefore limited ourselves to effective usage of geophysical data in monitoring carbon sequestered brine reservoirs. Our experimental methods were primarily focused on three objectives (1) change

in the physical properties expected in the subsurface when a brine saturated reservoir is replaced with CO₂, (2) suitable geophysical methodology that can effectively measure the changes in the physical properties in the formation when the brine is replaced by CO₂, and (3) if the formations above the sequestered reservoir are fractured due to above-normal pore pressure, whether or not the passive seismic responses generated from these fractures could be effectively utilized for fracture detection and monitoring.

During the first stage of our experiment, we focused on the objective 1 to find out the physical properties that are likely to change in a formation when the in-situ brine is replaced by CO₂. Using Gassman fluid substitution equations (Mavko et al., 1998), we replaced different brine-saturated formations in real well-log data from Moxa-Arch with different concentrations of CO₂ and analyzed what physical properties that are mostly affected from these replacements. Our substitution experiments demonstrated it is the formation density that is affected the most when the in-situ brine is replaced by CO₂.

Next, we concentrated on the objective 2. To avoid migration of the sequestered CO₂ into fresh groundwater, all future sequestration projects will take place in saline aquifers existing at depths in excess of 12,000–13,000 feet (3700–4000 meters). Since seismic is the only accepted geophysical methodology that can effectively be used to analyze subsurface formations to these or even greater depths, we concentrated on the usage of seismic method in predicting the changes in the physical properties expected from carbon sequestration. We used the original (brine saturated) and CO₂ saturated models and computed theoretical seismic responses from each model using a wave-equation based modeling methodology. Using prestack seismic waveform inversion, we then demonstrated that the changes in the formation density due to carbon sequestration could be predicted from these computed seismic responses.

Finally, to fulfill objective 3, we introduced micro-earthquakes with different fault (fracture) plane geometries and computed theoretical passive seismic responses at the surface generated from each micro-earthquake. Our results indicated that the computed passive seismic responses are in fact sensitive to the fault plane geometry. Therefore, deploying permanent passive seismic sensors during and after sequestration could be a useful tool for detecting fractures, predicting possible conduits for CO₂ leakage, and for monitoring of the post sequestration CO₂ movements within the reservoirs.

Results and Discussion

Figure 8-1 is a real well-log from the Moxa-Arch, Western Wyoming. Gassman fluid substitution relation (Mavko et al., 1998; also see Appendix-A) was used to replace 100% brine saturated reservoir, immediately below 5.1 km in depth with a homogeneous mixture of 50% CO₂ and 50% brine. The original log curves are shown in black and the CO₂ substituted log curves are shown in red.

Figure 8-1: Well-log data from the Moxa-Arch. A brine reservoir between 5100–5200m is sequestered with 50% CO₂. The original logs are in black while the CO₂ sequestered logs are in red.

Notice that replacing in-situ brine with CO₂ results in a small decrease in the P-wave velocity (V_P), a small increase in the S-wave velocity (V_S) and a large drop in density. While these small changes in V_P and V_S result in a change in the P-to-S-wave velocity ratio (V_P/V_S) or the Poisson's ratio, our fluid substitution experiments with different CO₂ saturations at reservoirs at various depths indicate that it is the density that is affected the most by these substitutions. Figure 8-2 shows the Poisson's ratio and density from another fluid substitution experiment on a different well-log where a brine-saturated formation between the depth interval of 4520 and 4560 meters were replaced by different concentrations of CO₂. Notice from Figure 8-2 that the formation Poisson's ratio is drops drastically when the in-situ brine is replaced with as little as 20% CO₂ and stays nearly constant when the CO₂ concentration is increased further. Formation density, on the other hand shows a gradual drop when the CO₂ saturation is increased from 20 to 80%. To effectively monitor the post-injection CO₂ movements, the available geophysical method must therefore be able to accurately predict the subsurface density changes.

Figure 8-2: Poisson's ratio and density when a brine saturated Nugget sandstone formation between 4520 and 4560m is replaced with different concentrations of CO₂.

Figures 8-3 and 8-4 are the synthetic seismic responses computed using the original 100% brine saturated and the 50% CO₂ and 50% brine saturated models shown in Figure 8-1. From now on, we will refer these two models as the original (un-sequestered) and the sequestered models respectively. The synthetic seismic responses were computed using an exact wave equation methodology (Mallick and Frazer, 1987, 1988, 1990, 1991). They are therefore complete seismic responses including all wave-modes as will be expected from real seismic data. In Appendix-B below, we provide a brief background theory used for computing these synthetic responses. Both vertical and horizontal (radial) components of the response are shown in Figures 8-3 and 8-4.

To investigate the potential of seismic data in estimating subsurface properties so that they could be used for monitoring carbon sequestered formations, we first invert the vertical component of the computed responses using a full waveform P-wave inversion methodology (Mallick, 1999). For these inversions, we first velocity analyze (Yilmaz, 1990) the original (un-sequestered) vertical component synthetic data to obtain the initial P-wave velocity model. We then extract the overall V_P - V_S and V_P -density relations from the well data and use these relations to estimate initial V_S and density models from the initial V_P model extracted from the velocity analysis. We then use this initial model of V_P , V_S , and density to invert the un-sequestered vertical component synthetic seismic data. Finally, we use the inverted model from the un-sequestered synthetic data as the

initial model for inverting the sequestered vertical component synthetics. Figures 8-5 and 8-6 are the results from these inversions.

Figure 8-3: Vertical and horizontal (radial) components of response for the original (un-sequestered) model of Figure 8-1.

Figure 8-4: Vertical and horizontal (radial) components of response for the sequestered model of Figure 8-1.

Figure 8-5: P-wave (vertical component) waveform inversion result of the un-sequestered synthetics of Figure 8-3.

Figure 8-6: P-wave (vertical component) waveform inversion result of the sequestered synthetics of Figure 8-4. The initial model used for this inversion was the inverted model (red curves) of Figure 8-5.

Figures 8-5 and 8-6 clearly demonstrate that while V_P and V_S estimates from inversion are quite good, the density estimates are rather poor. We could, in fact constrain the density heavily to the initial models and get a good density estimate as it is typically done for a 3-term amplitude-variation-with-offset (AVO) inversions (for details, see Mallick 2007). However, our primary objective here is to look for a robust methodology for estimating density from seismic data so that it could be effectively used in carbon sequestration monitoring. Considering the volume of CO_2 that must be captured and sequestered in the near future, many sequestration experiments are likely occur in areas where 3-D seismic data will be available, but well control may be sparse. Obtaining a good initial density model and constraining density heavily is not therefore feasible in most of these situations.

Inversion results of Figures 8-5 and 8-6 are for the vertical component of seismic response. Vertical component responses are dominated by primary (P-wave) reflections. Notice that in the vertical component responses in Figures 8-3 and 8-4 the primary reflections (between 1.5 and 1.9s zero offset time) are strong while the mode-converted reflections (between 2.0 and 2.5s zero offset time) are rather weak. Since P-wave reflections are not very sensitive to density, it is not surprising that these inversions do not give a very reliable density estimate.

Instead of the vertical components, if we draw our attention to the radial components in Figures 8-3 and 8-4, notice that they show strong mode-converted reflections. In addition, the P-wave reflections are also strong in the radial components with increasing offsets. Mode-converted reflection coefficients are sensitive to density. This follows directly from the Bortfeld approximations to reflection coefficients (Bortfeld, 1961; Aki and Richards, 1980). Using both vertical and radial components in a multicomponent waveform inversion should therefore give a better estimate of density compared to what could be obtained from vertical component inversion results of Figures 8-5 and 8-6.

We developed a nonlinear multicomponent waveform inversion methodology using Genetic Algorithm (GA) in which both vertical and radial components of the responses are simultaneously inverted. Exact procedure for GA inversion can be found in Goldberg (1989) and its application to seismic inversion problem can be found in Stoffa and Sen (1991) and Mallick (1995, 1999). For completeness, here we give a brief description of the method in Appendix-C. For multicomponent inversion, we used exactly the same initial models that were used for the vertical component inversion. Figure 8-7 shows the density estimates from both un-sequestered and sequestered synthetics from multicomponent inversion. Estimates of V_P and V_S are similar to the ones in Figures 8-5 and 8-6 and are therefore not shown. Notice from Figure 8-7 that the multicomponent inversion could correctly predict the density changes within the sequestered reservoir formation.

Considering that the density is likely to be the key player and multicomponent waveform inversion can estimate density much more reliably than the P-wave only inversion, we believe that the multicomponent seismic data are necessary for an effective monitoring of carbon sequestered reservoirs. Acquisition and processing of multicomponent seismic data is however much more

expensive than conventional P-wave data. Acquiring multicomponent seismic data as pre-sequestration baseline survey and subsequent acquisitions during and after sequestration for monitoring may not therefore be very cost effective, and we must look for some alternative methods. It is likely that the above normal pore pressure due to CO₂ sequestration will fracture the surrounding rock formations. If we deploy passive seismic sensors, microseismic events from these fractures could then be recorded. Assuming that we have a baseline pre-sequestration multicomponent data and obtain a reliably good subsurface model, these microseismic data could then be potentially used for subsequent monitoring. In addition, as these fractures are the potential conduits for CO₂ leakage, detecting and characterizing them will have an added advantage of mitigating such leakage-risk conditions.

Figure 8-7: Density estimates from multicomponent waveform inversion. As for the vertical component inversion, the initial model for sequestered synthetics is the inverted model from the un-sequestered synthetics.

To investigate the possibility of using passive seismic data for monitoring, we induce microseismic events with different focal mechanisms slightly above the sequestered formation at 5100 m in Figure 8-1. We compute a point double-couple moment tensor solution for a given microseismic event caused by a fracture from the fracture strike, dip, and rake following the procedures given in Aki and Richards (1980). We then incorporate this moment tensor source into the modeling algorithm and compute the passive seismic responses at the surface for each microseismic event. Keeping the strike and rake fixed, Figures 8-8 and 8-9 show the vertical and radial components of the response from fractures with different dip angles.

Figure 8-8: Vertical component of passive seismic response caused by fractures with different dips induced immediately above the sequestered formation in Figure 8-1.

Figures 8-8 and 8-9 demonstrate that the observed passive seismic responses clearly depend upon the dip of the fracture planes inducing the micro-seismicity. Also notice that the responses from 30° and 150° fracture dips are identical. Similarly the responses from 60° and 120° dips are also identical. These identical responses from different fracture dips belong to the classical problem of fault-plane ambiguity in earthquake focal mechanism solutions (for details, see Aki and Richards, 1980). For carbon sequestrations, we will be mostly interested in the fractures above the sequestered formation through which CO_2 may leak out. Because these fractures are likely to be caused by the above normal pore pressure in the sequestered formation underneath, they are more likely to be near vertical and reverse-fault solutions than normal fault solutions. Based on this argument, we should then be able to resolve the fault plane ambiguity from recorded passive seismic data. Assuming that the initial subsurface model is known from the baseline multicomponent data, we can therefore invert the passive seismic data for fracture characterization and micro-seismic event location. Once the focal mechanism from each micro-seismic event is obtained, we can then invert the same data for changes in the properties of the carbon sequestered reservoirs. This should in turn, provide a cost effective way to monitor carbon sequestered brine reservoirs combining multicomponent active source seismic data as baseline survey and successive passive seismic recordings for monitoring. This strategy will not only allow us monitoring the sequestered formations, but it can also detect fractures during and after sequestration that could potentially be the pathways for possible leakage.

Figure 8-9: Radial component of passive seismic response caused by fractures with different dips induced immediately above the sequestered formation in Figure 8-1.

Conclusion

Sequestering CO₂ in different saturations and computing the equivalent fluid-substituted properties indicate that the density is more sensitive to the change in CO₂ saturation than V_P and V_S . To effectively monitor carbon sequestered reservoirs, the available geophysical tools must therefore be able to predict density to a reasonable accuracy. Because multicomponent seismic data can accurately predict density, it is necessary to use multicomponent seismic data for monitoring CO₂ sequestered reservoirs. Since acquisition and processing of multicomponent seismic data is expensive, acquiring such data for pre-sequestration baseline survey and for monitoring surveys during and after sequestration is expensive. Above normal pore pressure due to sequestration is likely to cause fractures, and computing micro-seismic events caused by such fractures we find that the passive seismic data could potentially be used to characterize and locate these fractures and monitor the carbon sequestered formations. We therefore believe that using multicomponent seismic data as a baseline survey prior to sequestration and combining it with passive seismic data for subsequent monitoring during and after sequestration is a cost-effective strategy. This will allow us (1)

monitor the movement of CO₂ during and after sequestration and (2) detect fractures that could potentially be the conduits for CO₂ leakage.

References

Aki K., and Richards, P.G., 1980, Quantitative Seismology, **1**: W.H. Freeman.

Batzle, M., and Wang, Z., 1992, Seismic properties of pore fluids: Geophysics, **57**, 1396-1408.

Bortfeld, R., 1961, Approximation to the reflection and transmission coefficients of plane longitudinal and transverse waves: Geophys. Prosp., **9**, 485-502.

Fryer, G.J., and Frazer, L.N., 1984, Seismic waves in stratified anisotropic media: Geophys. J. Int., **78**, 691-710.

Kennett, B. L. N., 1983, Seismic wave propagation in stratified media: Cambridge University Press.

Goldberg, D.E., 1989, Genetic Algorithms in Search, Optimization, and Machine Learning: Addison-Wesley Publishing Company.

Juanes, R., Spiteri, E.J., Orr, F.M., and Blunt, M., 2006, Impact of relative permeability hysteresis on geological CO₂ storage: Water. Resour. Res., **42**, W12418, doi: 10.1029/2005WR004806.

Mallick, S., 1995, Model-based inversion of Amplitude-variation-with-offset data using a Genetic Algorithm, Geophysics, **60**, 939-954.

Mallick, S., 1999, Some practical aspects of prestack waveform inversion using a genetic algorithm: an example from the east Texas Woodbine gas sand: Geophysics, **64**, 326-336.

Mallick, S., 2007, Amplitude-variation-with-offset, elastic impedance, and wave-equation synthetics- a modeling study: Geophysics, **72**, C1-C7.

Mallick, S., and Frazer, L.N., 1987, Practical aspects of reflectivity modeling: Geophysics, **52**, 1355-1364.

Mallick, S., and Frazer, L.N., 1988, Rapid computation of multi offset vertical seismic profile synthetic seismograms for layered elastic media: Geophysics, **53**, 479-491.

Mallick, S., and Frazer, L.N., 1990, Computation of synthetic seismograms for stratified azimuthally anisotropic media: J. Geophys. Res., **95**, 8513-8526.

Mallick, S., and Frazer, L.N., 1991, Reflection/transmission coefficients and azimuthal anisotropy in marine seismic studies: Geophys. J. Int., **105**, 241-252.

Mavko, G., Mukerji, T., and Dvorkin, J., 1998, The Rock Physics Handbook, tools for seismic analysis in porous media, Cambridge University Press.

Press, F., 1968, Earth models obtained by Monte-Carlo inversions: J. Geophys. Res., **73**, 5223-5234.

Stoffa, P.L., and Sen, M.K., 1991, Nonlinear multiparameter optimization using genetic algorithms: Inversion of plane-wave seismograms: Geophysics, 56, 1794-1810.

van der Meer, L.G.H., and Wees, J.D., 2006, Effects of CO₂ solubility on the long-term fate of CO₂ sequestered in a saline aquifer: The Leading Edge, **25**, 10, 1276-1280.

Yilmaz, O., 1987, Seismic data processing, – Investigations in Geophysics, **2**: Society of Exploration Geophysicists.

Appendix I: Gassman Fluid Substitution

Fluid substitution involves two fundamental steps: (1) computation of the physical properties (acoustic velocity and density) of fluids, and (2) fluid substitution.

Computation of physical properties of gases and fluids: For computing physical properties of gases and fluids, we use the brine and gas (CO₂) properties using the empirical relations summarized in Batzle and Wang (1992) and described in detail by Mavko et al. (1998), p. 214–220. The steps involved in computing the fluid properties are explained very clearly in this reference, and therefore are not repeated here.

Fluid Substitution: For fluid substitution, we use Gassman relationship given as (see Mavko et al., 1998, p168-170).

$$\frac{K_{sat}}{K_0 - K_{sat}} = \frac{K_{dry}}{K_0 - K_{dry}} + \frac{K_{fluid}}{\phi(K_0 - K_{fluid})}, \quad (A-1)$$

$$\mu_{sat} = \mu_{dry}. \quad (A-2)$$

Where

- K_{dry} = Effective bulk modulus of the dry rock,
- K_{sat} = Effective bulk modulus of the rock with pore fluid,
- K_0 = Frame bulk modulus,
- K_{fluid} = Effective bulk modulus of the pore fluid,
- ϕ = Porosity,
- μ_{dry} = Effective shear modulus of the dry rock,
- μ_{sat} = Effective shear modulus of the rock with pore fluid.

In addition, the effective density ρ_{sat} of the fluid saturated rock can be expressed in terms of the density of the rock grain ρ_{grain} , effective fluid density ρ_{fluid} , and porosity ϕ as

$$\rho_{sat} = \phi \rho_{fluid} + (1 - \phi) \rho_{grain} \quad (A-3)$$

To replace one given pore fluid by another we use the above equations as follows:

- (1) Obtain the physical properties of the original and replacing fluids, either from direct user input, or by calculating their physical properties from the parameters as described by Mavko et al. (1998), p 214-220.
- (2) Use equation (A-3) to compute grain density from the density of the saturated rock, porosity, and the density of the original fluid.
- (3) Use the grain density obtained from step 2 above, porosity, and the density of the replacing fluid in equation (A-3) to compute the effective density of the rock, saturated with the replacing fluid.
- (4) Use equation (A-1) to compute the effective bulk modulus of the dry rock (K_{dry}) from effective bulk modulus of the rock saturated with the original fluid (K_{sat1}), porosity ϕ , Bulk modulus of the original fluid (K_{fluid1}), and Frame bulk modulus (K_0).

- (5) Use the K_{dry} from step (4) and the effective bulk modulus of fluid 2 (K_{fluid2}) in equation (A-1) to compute the effective bulk modulus K_{sat2} of the rock, saturated with the replacing fluid. Note that according to equation (A-2), effective shear modulus does not change from fluid substitution.
- (6) Compute P-wave velocity from effective density computed from step (3) and the effective bulk modulus, computed from step (5).
- (7) Compute S-wave velocity from the effective density computed from step (3) and the effective shear modulus.

Appendix II: Background Theory for Computing Synthetic Seismic Responses

Consider the propagation of a seismic wavefield in a depth-dependent anisotropic elastic medium. In the frequency-slowness domain, it can be shown that the displacement-stress vector field $\mathbf{b}$ satisfies the following equation (Fryer and Frazer, 1984)

$$\partial_z \mathbf{b} = i\omega \mathbf{A} \mathbf{b} + \mathbf{F}, \quad (\text{B-1})$$

where

$$\mathbf{b} = [u_x, u_z, \tau_{xz}, \tau_{xx}, u_y, \tau_{yz}]^T, \quad (\text{B-2})$$

is the vector containing the x-, y-, and z- components of the displacement vector $\mathbf{u}$ and the vertical component of the stress tensor $\boldsymbol{\tau}$. The matrix $\mathbf{A}$ in equation (D-1) is the 6X6 elastic system matrix whose components are functions of the elastic stiffness coefficients (c_{ij}), density (ρ), and x- and y components of the slowness p_x and p_y . Finally, $\mathbf{F}$ in equation (1) is the source term. Now, let the eigenvectors of the elastic system matrix $\mathbf{A}$ be given by the matrix $\mathbf{D}$, i.e.,

$$\mathbf{A} = \mathbf{D}^{-1} \boldsymbol{\Lambda} \mathbf{D}, \quad (\text{B-3})$$

so that $\boldsymbol{\Lambda}$ is the diagonal matrix of the eigenvalues. We also define a new vector $\mathbf{v}$, given as $\mathbf{b} = \mathbf{D} \mathbf{v}$. From equations (D-1) and (D-3), we can see that in a source-free region, the vector $\mathbf{v}$ satisfies the wave equation, and the individual components of $\mathbf{v}$ represent the up- and downgoing quasi-P (qP), quasi-S₁ (qS₁), and quasi-S₂ (qS₂) wavefield amplitudes, propagating with their respective vertical slowness values given by the eigenvalues in the diagonal elements of $\boldsymbol{\Lambda}$. The vector $\mathbf{v}$ is, therefore, called the wave vector. It can also be seen that for isotropic or transversely isotropic medium with vertical symmetry axis (VTI medium), the properties are azimuthally independent, i.e., instead of x- and y- components of the slowness p_x and p_y , the medium is dependent the total horizontal slowness p given as

$$p = \sqrt{p_x^2 + p_y^2}, \quad (\text{B-4})$$

the six-by-six system given by equations (B-1) and (B-2) decouples into a four-by-four P-SV system and a two-by-two SH system.

In our methodology, we solve for the reflection and transmission matrix for the entire medium by successively adding a layer and a half space to the existing stack of layers. The details can be found

in Kennett (1983). Once the reflection and transmission matrices for the entire stack of layers are computed, the particle displacement and/or the pressure response is computed in the frequency-wavenumber domain. Finally the response in time-offset domain is computed using a Fourier-Hankel transform (Aki and Richards, 1980).

Appendix III: Application of Genetic Algorithm in Seismic Inversion

Figure 8C-1: Implementation of Genetic Algorithm in seismic inversion problem.

Genetic Algorithm (GA) belongs to class of Monte-Carlo optimization (Press, 1968). Figure 8C-1 is a brief outline of GA implementation to solve seismic inversion problem. As shown in Figure 8C-1, given a prior distribution of model parameters, a random population of models is initially generated within a specified search window. Using the wave equation modeling approach, outlined above (Appendix-B), synthetic seismic responses for each random model are then computed. These synthetic seismic responses are then matched with the observed seismic data to obtain an objective fitness for each model. The models are then modified using the GA operations of reproduction, crossover, mutation, and update (see Mallick, 1995 for details) to produce a new generation of models. Synthetic responses for this new generation of models are again computed and matched with observation and then modified to create another new generation. This process is continued until a satisfactory match between the synthetic and observed data is obtained. Objective fitness, computed for each model, generated for the entire course of the run are stored in the model space and at the end, they are normalized to obtain the a-posteriori probability density distribution (PPD). Finally, the inverted model is then estimated from the computed PPD.

CHAPTER 9: Multiscale Modeling and Numerical Simulation of CO₂ Injection

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Background

Task 9 of the project focused on the development of an open-source, noncommercial computer model to quantify the uncertainties associated with CO₂ sequestration in the deep geologic formations of the Moxa Arch. The simulation code developed is designed to aid the assessment and monitoring of CO₂ sequestration by providing accurate predictions of the migration and trapping of the CO₂ plume. The simulator built has unique capabilities to handle the strongly nonlinear physics and chemistry of the CO₂/brine flow and its interaction with multi-scale geological heterogeneities.

Results of the modeling were published in the special issue of *Rocky Mountain Geology*. Key findings, in the form of a peer-reviewed academic paper, follow.

On the development of a high-performance tool for the simulation of CO₂ injection into deep saline aquifers

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ABSTRACT

We report on the development of a multiscale parallel simulator for porous media flow problems. We combine state-of-the-art numerical techniques in a new object-oriented, high-performance simulation tool. The new multiscale parallel software will adapt itself to the type and number of available processing cores. The combination of:

- physically based operator splitting for multiscale time discretization of nonlinear systems of partial differential equations arising in multiphase flows in porous media,
- domain decomposition for the parallel solution of elliptic and parabolic problems, and
- semi-discrete central finite volume schemes for hyperbolic systems

allows us to produce new very accurate simulations of multiphase flow in porous media problems that are of interest in many areas of science and technology, such as petroleum reservoir and environmental engineering. The new simulation code may aid the assessment and monitoring of CO₂ sequestration projects by providing accurate predictions of the migration and trapping of injected CO₂ plumes.

KEYWORDS: CO₂ injection, CPU/GPU clusters, high-performance computing, operator splitting, saline aquifers.

INTRODUCTION

Scientifically correct models based on first principles and accurate numerical simulators are of utmost importance in producing reliable predictions of multiphase flows in the subsurface. Traditional simulations of multiphase flows rely on ad hoc up-scaling techniques along with coarse grid simulations of the up-scaled models. The models for multiphase flows are defined at the lab (or Darcy) scale (a few centimeters) while simulations of interest to important problems (such as the migration, trapping, and possible leakage of CO₂ plumes in the subsurface; enhanced oil recovery; or production of gas from unconventional resources) have to be performed in the field scale (a few kilome-

ters). Figure 1 indicates the length scales that are of importance for the modeling of flows through porous media. Depending on the spatial scales involved, there are well-established theories to perform the upscaling from a finer to a coarser scale. For example, in going from the atomic to the pore scale one could use Statistical Mechanics. However, in going from the lab to the field scale, ad hoc up-scaling techniques frequently developed and tested for some flow regimes for single- or two-phase problems may produce serious errors when applied to more complex compositional flows. There are not rigorous theories to perform this up-scaling: difficulties in deriving up-scaled models arise both from the highly nonlinear fluid-fluid interactions in the flow of multiphase fluids and from the

Figure 1. Important length scales for the modeling of flows through porous media along with theories that allow up-scaling from a shorter to a longer length scale. Depending on the scales involved there are well-established theories to up-scale between scales. We are concerned with models defined at the Darcy scale for making predictions in the field scale. There are no rigorous theories to perform this up-scaling. The authors believe that the field-scale behavior should be determined by a combination of fine-grid simulations along with stochastic models for the underlying heterogeneity.

complex interactions between heterogeneities and nonlinearities (see Furtado and Pereira, 2003).

Although up-scaled solutions may be important in some areas, e.g., in identifying trends of flow

patterns in oil reservoir simulation, there are important practical problems where the fine-scale details of the numerical simulations should be numerically captured. We mention, for example, the simulation of injected CO_2 leakage from saline aquifers: the fine-scale preferential paths for flow that may lead to leakage cannot be captured by coarse grid, up-scaled simulations. We use state-of-the-art numerical techniques aiming at solving large-scale multiphase flows directly in fine computational grids that properly resolve the underlying physical heterogeneities. Here we report on the development of software for a Linux cluster. This is the first step toward the use of hybrid central processing unit/graphics processing unit (CPU/GPU) machines, which are becoming common in computational science environments. Within each processing unit of such systems, memory and computing power vary: while most of the memory of such devices is connected to the CPUs, most of the actual computations take place in the GPUs. GPUs have less memory but are much faster by up to one or two orders of magnitude. Such state-of-the-art hybrid machines are useful in studies aimed at quantifying the underlying uncertainty of field-scale, realistic models for multiphase flows. In such studies thousands of simulations have to be performed to produce reliable predictions in a statistical, Bayesian-type framework (Glimm and Sharp, 1999; Efendiev et al., 2005; Douglas et al., 2006).

To put the work to be described here in perspective, we remark that there is a difference in the algorithms we use based on the

number of cores or processors available. There are three distinct ranges of cores that are important:

- Range 1: 1–16 cores, suitable for desktops or laptops based on multicore processors (CMPs).
- Range 2: 64–256 cores, suitable for small clusters or large shared memory multiprocessors (SMPs).
- Range 3: 10,000+ cores, suitable for use on large clusters that could be petascale in performance.

Most commercial software that is widely used for field-scale simulations of porous media flow problems is in range 1. This is by far the most common computing platform in use at corporations that purchase products instead of developing in-house software. Eclipse is a good example for this range. As clusters become commonplace in engineering labs, many research groups have pursued range 2. The computational tool described in this paper fits within this range. We are in the process of developing new optimized kernels for range 3. Most numerical methods currently in use for porous media flow problems do not scale well in this range of cores. It is far more common to run multiple problems in parallel as an ensemble with some sort of statistical filtering method that merges the parallel predictions into a common analytic prediction during a time step. Making the code switch automatically among the three ranges of cores will provide a multiscale parallel code that will be useful on all three ranges of cores. Our research group at the University of Wyoming (UW) has recently installed a new 8 CPU/64 GPU cluster that has 15,360 GPU cores that will be useful for testing different levels of parallel scaling. We note that recent scaling results on machines like Texas Advanced Computing Center's (TACC's) Ranger system show that codes that scale well at 10,000–20,000 cores seem to scale well with 60,000 cores with little or no changes. A vital understanding of the code at 10,000 cores seems to indicate that the parallelism is understood to a point that the code should work well at the order of 100,000 cores unless there is a radical change of architecture in the near future, which is distinctly possible with all of the recent accelerator (GPU and field-programmable gate array (FPGA)) announcements for enhancing traditional computers inexpensively (Exascale, 2010).

We refer the reader to Schnaar and Digiulio (2009) for a recent review of the simulation tools that have been applied in the study of CO₂ sequestration. Most of them are designed for ranges 1 or 2 indicated above. None of these codes can make effective use of all three ranges of cores. Moreover they cannot make effective use of the new, state-of-the-science hybrid CPU/GPU systems.

In the UW-team simulator to be described here, we combine state-of-the-art numerical techniques in a new object-oriented, high-performance simulation tool. Our new computational tool is based upon: (1) physically based operator splitting for multiscale time discretization of nonlinear systems of partial differential equations arising in multiphase flows in porous media; (2) domain decomposition for the numerical solution of elliptic and parabolic problems; and (3) semi-discrete central finite volume schemes for hyperbolic systems. The new simulator allows us to produce new and accurate simulations of multiphase flows in multiscale heterogeneous porous media.

The new simulation code may aid the assessment and monitoring of CO₂ sequestration projects by providing accurate predictions of the migration and trapping of injected CO₂ plumes.

The impetus of this study was our participation in a geological site characterization of the Moxa Arch in southwestern Wyoming. This interdisciplinary project, funded by the U.S. Department of Energy's National Energy Technology Laboratory, recognizes the potential for geologic sequestration of impure carbon dioxide in deep reservoirs of the Moxa Arch in Wyoming. The Moxa Arch is a 120-mile-long (~120 km) north–south-trending anticline plunging beneath the Wyoming thrust belt on the north and bounded on the south by the Uinta Mountains. Several oil and gas fields along the Moxa Arch contain natural accumulations of CO₂. The largest of these is the La Barge Platform, which encompasses approximately 800 mi². Several formations may be suitable for storage of impure CO₂ gas, foremost among them the Madison Limestone and Nugget Sandstone. The simulator presented here will provide an accurate computational tool to monitor plume migration if CO₂ is injected into aquifers, whether in Wyoming or elsewhere.

This paper is organized as follows. In the next section we define the model that we use. Then, we review operator-splitting methods that are applied to our model. Central schemes for solving hyperbolic

systems of conservation laws are discussed and the object-oriented software design we use is described. In the last section we provide numerical evidence that our methodology works.

MODELING

We use the model proposed in Obi and Blunt (2006) to perform numerical simulations of the injection of CO₂ in saline aquifers. Our focus is on the primary physical processes that affect the transport of two components, CO₂ and water, in a two-phase system encountered during the injection of supercritical CO₂ into deep saline aquifers. Most of the injected CO₂ will initially reside in its own phase, which will contact and displace the resident fluid (brine). The displacement of the resident brine is controlled by the relative permeability functions, viscosities, and densities of the CO₂ and aqueous (brine) phases, as well as by the spatial structure of the permeability and porosity fields. Some CO₂ will dissolve into the aqueous phase, and the extent of dissolution is controlled by pressure and temperature alone; we neglect the effect of salinity in dissolution. We also ignore evaporation of water from the aqueous phase to the CO₂ phase.

Our focus is on the relatively short-term period of injection, so we emphasize convective processes. Slower flow processes, such as diffusion and buoyancy effects of dissolved species, are not included. Chemical reactions between acidic brine and supercritical CO₂ with rock minerals and non-isothermal effects are also ignored.

We assume incompressible two-phase flow and neglect capillary pressure and dispersive effects. Supercritical CO₂ is relatively incompressible in the high-pressure (well above the critical pressure) conditions of deep aquifers that we intend to simulate. Moreover, most deep consolidated rocks also have low compressibility, so we ignore mechanical stress effects.

The governing equation for transport of CO₂ in its own phase (indicated by a subscript *c*) is then given by the following (volume) balance equation:

$$\phi \frac{\partial S_c}{\partial t} + \nabla \cdot \left(u F_c - k \frac{\lambda_c \lambda_a}{\lambda} (\rho_a - \rho_c) g \nabla d \right) = -T_d + q_c, \quad (1)$$

where ϕ is porosity, k is absolute permeability, S_c is the saturation of the CO₂ phase, u is the total Darcy velocity, T_d represents the transfer of CO₂ to the aqueous phase due to dissolution, and q_c denotes sinks and

sources. ρ_α denotes the density of phase α (*c* for CO₂ and *a* for aqueous), the parameter d represents depth, and g is the acceleration of gravity. The total mobility $\lambda = \lambda_c + \lambda_a$ is the sum of the phase mobilities, the latter defined in terms of the phase relative permeabilities k_α and the phase viscosities μ_α as follows: $\lambda_\alpha = k_\alpha / \mu_\alpha$.

Moreover, the fractional flow functions are given by $F_\alpha = \lambda_\alpha / \lambda$.

The transport equation for the CO₂ dissolved in the aqueous phase is:

$$\phi \frac{\partial (1 - S_c) C}{\partial t} + \nabla \cdot \left(u (1 - F_c) + k \frac{\lambda_c \lambda_a}{\lambda} (\rho_a - \rho_c) g \nabla d \right) = m_c T_d. \quad (2)$$

Here C is the concentration of CO₂ in the aqueous phase, measured in moles per unit volume, and m_c is the molar density of CO₂.

The two equations above can be combined with the transport equation for the aqueous phase to yield an equation that expresses the incompressibility of the two-phase system:

$$\nabla \cdot u = q_c. \quad (3)$$

This last equation can be viewed as a “pressure equation” once the total velocity u is related to the pressure p by a multiphase version of Darcy’s law:

$$u = -k \left(\lambda \nabla p - (\rho_c \lambda_c + \rho_a \lambda_a) g \nabla d \right). \quad (4)$$

The specification of appropriate initial and boundary conditions completes the description of our physical model. Sample boundary conditions are contained later in this paper in the Numerical Experiments section.

OPERATOR SPLITTING

Operator-splitting schemes have recently been developed for the approximation of multiphase flows in porous media (Abreu et al., 2006). These schemes are aimed at decomposing the underlying physical processes and treating each such component appropriately. Thus, instead of solving the governing system of differential equations in the form which results directly from the basic conservation laws supplemented by constitutive relations (or other fundamental equations), the equations are rewritten in such a way as to exhibit clearly each physical process. Then they are solved by appropriate numerical techniques that furnish effective and efficient schemes designed

to resolve the sharp gradients and dynamics evolving at vastly different rates that are the hallmarks of multiphase flows in porous media.

In addition to the ability to vary the numerical schemes with the physics, operator splitting enables the use of multiscale time step discretizations: different time steps are used for the different physical processes. These properly chosen time steps lead to a significant reduction in overall computing times. This set of ideas has been successfully applied to several multiphase flow problems: multicomponent gas flow (Douglas et al., 2003), two-phase flows in unfractured and fractured porous formations (Douglas, 1997a; Douglas, 1997b; Douglas et al., 2000), and three-phase flows (Abreu et al., 2006; Abreu et al., 2008; Abreu et al., 2009).

For the simulation of the injection of CO₂ into saline aquifers, we employ an operator-splitting technique based on separating the underlying physical processes and treating each such process appropriately to define the mathematical model that was investigated in this project. The obvious primary physics-based splitting is the separation of the pressure-velocity calculations from the saturation-concentration calculation. Since only the total Darcy velocity u is needed in the transport equations, a natural choice of a numerical method for the pressure equation is a mixed finite element method, well known for producing accurate velocity fields in the presence of rapidly varying coefficients (e.g., Douglas, 1997a) so that u is approximated directly.

The secondary splitting is to separate the convective transport from the dissolution process. For the numerical solution of the nonlinear system of conservation laws that is associated with convective transport, we employ higher-order, conservative, central finite difference schemes to capture the sharp fronts that typically develop in this problem. We shall discuss the recent development of these schemes later in the paper. Finally, the dissolution of CO₂ into the aqueous phase is accounted for using Henry's law (Smith et al., 2005) and assuming ideal mixing.

CENTRAL DIFFERENCE SCHEMES FOR MULTIPHASE FLOWS

Recently, high-resolution, semi-discrete central difference schemes have been used for the solution

of systems of hyperbolic conservation laws arising in the simulation of multiphase flows in multidimensional heterogeneous porous media. These schemes have some desirable properties for the approximation of porous media flow, which we shall discuss below.

The Lax-Friedrichs (LxF) scheme (Lax, 1954) is the canonical first-order central scheme, which is the forerunner of all central differencing schemes. It is based on piecewise constant approximate solutions. It also enjoys simplicity, that is, it does not employ Riemann solvers and characteristic decomposition. Unfortunately, the excessive numerical dissipation in the LxF scheme (of order $O(\Delta X^2/\Delta t)$) yields poor resolution, which seems to have delayed the development of high-resolution central schemes when compared with the earlier developments of the high-resolution upwind methods. Only in 1990 did Nessyahu and Tadmor (NT) introduce a second-order generalization to the LxF scheme (Nessyahu and Tadmor, 1990). They used a staggered form of the LxF scheme and replaced the first-order piecewise constant solution with a van Leer's Monotone Upstream-centered Schemes for Conservation Laws (MUSCL)-type piecewise linear second-order approximation (Leer, 1979). The numerical dissipation in this new central scheme has an amplitude of order $O(\Delta X^4/\Delta t)$. When applying these methods to multiphase flows in highly heterogeneous aquifers we need to use decreasing time steps as the heterogeneity increases, yielding greater numerical diffusion. Kurganov and Tadmor (KT; Kurganov and Tadmor, 2000) combined ideas from the construction of the NT scheme with Rusanov's method (Rusanov, 1961) to obtain the first second-order central scheme that admits a semi-discrete formulation, which is then solved with an appropriate ordinary differential equation (ODE) solver. The resulting scheme exhibits a much smaller numerical diffusion than the NT scheme. In fact, due to the semi-discrete formulation, this numerical diffusion is independent of the time step used to evolve the ordinary differential equation. This property guarantees that no extra numerical diffusion will be added if the time step is forced to decrease. The KT scheme for multidimensional problems is based on a dimensional splitting scheme. Some of the authors and their collaborators have recently derived a multidimensional version of the KT scheme that retains the advantages of the earlier semi-implicit procedures while avoiding dimensional splitting (see also Kurganov and Petrova, 2001 and Balbas

and Qian, 2009 for related efforts). In the numerical simulations reported here, we will use the original KT schemes, because some preliminary results indicate that the dimension-by-dimension approach leads to a much better speed up of the numerical solution produced in a hybrid CPU/GPU system (Pereira and Rahunanthan, 2010).

SOFTWARE DESIGN

To explain the framework of the software developed, we first discuss the main features that simulation software must have for reliable computational modeling of multiphase flows in porous media. These were the main principles that guided us during the software design phase.

One of the main characteristics about this type of simulation software is that some of its requirements change often. This happens because the computational modeling of physical systems is an iterative procedure. We begin by describing the physical phenomena with simple equations that model the most fundamental processes in the problem with trivial constitutive laws. This original system is incremented in subsequent iterations by increasing the complexity of the mathematical model. This has a great impact on the software requirements, because numerical methods must be added or extended in the code to solve the new system of equations.

Another interesting aspect of the software design is that the same set of equations can be solved by many numerical methods with different degrees of programming labor, computational efficiency, and precision. In fact, we often implement many methods to solve the same set of equations. By reproducing verified results available in the referenced literature we can investigate which method is better suited for the class of problems of interest.

Due to frequent additional requirements for our simulation software, we must be able to add new numerical methods written by different collaborators while preserving the correctness of the code. Although efficiency is a desirable feature of any scientific software, we also have to carefully consider the relative cost of efficiency and code maintenance.

The considerations presented above motivated the UW team to build a simulator in modules that can be chosen by the user in a configuration file. Each module corresponds to a specific numerical method used to solve a specific set of equations. This

framework is easily implemented in the context of C++ template-based object-oriented programming.

In the simulator developed for CO₂ sequestration, the governing system of partial differential equations was decomposed through an operator-splitting procedure in three sets of equations (this is our mathematical model described above):

- *Transport system*: It is composed of the transport equations of the fluid phases, for example, the supercritical CO₂, the brine, and the water vapor. It is generally formulated in terms of the phase saturations.
- *Poro-mechanics system*: It defines the tension interaction between the fluids and the porous media. The main variables are the pressure of the fluids and the solid displacement in the case of deformable media. In the current stage of the project we have worked only with rigid porous media.
- *Thermodynamics system*: It defines the equilibrium flash calculations used to define the chemical interactions among the components in the phases (solid, brine, and supercritical CO₂).

For each subsystem there is a family of modules. To solve the transport system, for instance, there are three modules corresponding to four numerical schemes: Lax-Friedrichs, Upwind, Russanov, and Kurganov-Tadmor (KT). For the poro-mechanics we implemented the mixed and the mixed-hybrid finite element methods that can be combined with three linear solvers: algebraic multigrid (AMG), a direct frontal solver, the unsymmetric multifrontal sparse LU factorization package (UMFPACK), and conjugate gradient with a symmetric successive overrelaxation method (SSOR) preconditioner. We also used the message passing interface library (MPI) to implement an iterative domain decomposition scheme (Douglas et al., 1997a) for the parallel implementation of the mixed hybrid finite element method in Linux clusters. The thermodynamics system has just two modules: a null module (trivial thermodynamic equilibrium without dissolution) and another one based on Henry's Law (Obi and Blunt, 2006).

The subsystems are coupled among themselves since the primary variables in one subsystem can be the input parameters for other modules in a dataflow

programming style. Once a module is chosen for each subsystem, the set of modules needs to evolve through the simulation time in a consistent manner using a staggered algorithm that exchanges module solutions every time step. We have implemented two algorithms: one that simply evolves the subsystems without checking for convergence between them and another based on the search for a fixed point. These algorithms receive as parameters the three modules, one for each subsystem. The unified modeling language (UML) diagram (Fig. 2) illustrates the framework. The base classes *FlashBase*, *DynamicBase*, and *TransportBase* define the interface among the modules that implement, respectively, the three subsystems: thermodynamics, poromechanics, and transport. This design favors encapsulation and teamwork. For example, to add a new transport method a collaborator just creates a new class inherited from *TransportBase* and overrides its four methods. Constant parameters (in time) like the permeability field, initial conditions, and time-independent boundary conditions are passed to the classes on instantiation.

The UML diagram shows some of the methods already implemented:

- For transport methods we have the classes *LaxFriedrichsMethod*, *UpwindMethod*, *RusanovMethod*, and the *KTMethod*. Each one corresponds to a specific finite volume method.

- For the poromechanics modules we have *HybridModule*, *HybridModuleCG*, and *HybridModuleAGM*. All of them discretize the poromechanics subsystem using the hybridized mixed finite element method. They differ only by the type of linear solver they employ. We also have implemented a domain decomposition version of each one of the poromechanics modules (not shown in the UML diagram).

When the program runs, it instantiates one of the modules for each type of subsystem and calls a procedure of the sequencer class while passing the instantiated classes as parameters. The UML diagram shows the code of one of the sequencer's methods called *Staggered*. This method simply advances the modules in time and exchanges their solutions each time step. For the modules based on finite element methods, we use the deal.II C++ library (Differential Equations Analysis Library) that implements a wide range of finite element methods for 3D quadrilateral non-structured meshes. It is bundled with a large collection of iterative linear solvers that we use extensively. We also used the UMFPACK (Davis et al., 2010) for debugging purposes. For data output we used a data input/output system, HDF5, which is designed specifically for scientific data (HDF, 2010); it is a versatile data model that

Figure 2. UML class diagram for the software architecture.

can represent very complex data objects and a wide variety of metadata commonly used on high-performance computing systems. It supports a large variety of data types and is designed for flexible and efficient input/output and for large volumes of complex data.

NUMERICAL EXPERIMENTS

We first present the result of a grid refinement study for the numerical simulation of the injection of supercritical CO₂ in a three-dimensional aquifer having 128 meter (m) versus 64 m versus 64 m. The CO₂ is injected through two horizontal wells located at 32 m from the bottom of the aquifer. Dirichlet conditions are imposed for the pressure on the lateral (left and right) boundaries and no-flow conditions are imposed on the other boundaries. Due to the effect of gravity the plume is displaced upwards. In the simulations, the reservoir initially contains 100 percent brine. CO₂ is injected into the aquifer at a constant rate of 93 m³ per day for 3.3 years. We consider a scalar, heterogeneous absolute permeability field with six horizontal layers. The constant-by-parts absolute permeability field is defined on a 64 versus 32 versus 32 uniform grid. Each layer is taken to be (the log of) a realization of a (Gaussian) random fractal field (see Glimm et al., 1992, 1993) with moderately large heterogeneity strength where the mean permeability value is prescribed as 100 millidarcy. The data below are held fixed in all flow studies:

- Viscosity: $5 \cdot 10^{-4}$ Pas (aqueous); $6 \cdot 10^{-5}$ Pas (CO₂)
- Porosity: 0.3
- Residual saturations: $s_{ra} = 0$; $s_{rc} = 0$
- Relative permeability functions: $k_{ra}(S_c) = (1 - (1 - s_{ra})^{-1} S_c)^2$; $k_{rc}(S_c) = (1 - s_{rc})^{-2} (S_c - s_{rc})^2$

We use the same parameters for Henry's Law as those values given in Obi and Blunt (2006). Figure 3 displays the result of a grid refinement study where the dissolution was not taken into account. The grids used are finer in going from top to bottom, and have 64 versus 32 versus 32 (top), and 128 versus 64 versus 64 (bottom) elements. CO₂ saturation surface plots are shown after 1200 days of simulation. The numerical results indicate that the coarse and fine grid results are quite similar; this is an indication that an adequate

level of numerical convergence has been achieved in the coarser grid simulation. The numerical results for both grids used show perfect mass conservation.

The coarse grid simulation depicted on Figure 4 takes dissolution into account. In Figure 4 the plume on the top was simulated without dissolution, and the plume on the bottom was simulated with dissolution. As expected, the volume of the plume simulated with dissolution is smaller.

CONCLUSIONS

We remark that details of the implementation of the software in both multiple CPU and multiple hybrid CPU/GPU computer systems will appear elsewhere. The authors and their collaborators intend to continue the development of the software described here. We intend to add a geomechanics module and investigate the robustness of our splitting procedure in the approximation of extremely difficult problems involving strong couplings, e.g., porosity and permeability dependence on CO₂ acidity, that can imply wormhole formation processes.

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Figure 3. CO₂ injection in a heterogeneous, 3D brine aquifer. The pictures show the saturation of the injected CO₂ in a mesh refinement study. The picture on the top refers to a coarser computational grid; the picture on the bottom refers to a finer computational grid. As the computational grid is refined one can observe finer-scale details of the injected CO₂ plume.

Figure 4. Simulated plumes without dissolution (top picture) and with dissolution (bottom picture). As expected, the volume of the plume in the bottom picture is smaller because a fraction of the injected CO_2 is dissolved in the resident brine phase.

REFERENCES CITED

- Abreu, E., Douglas, J., Jr., Furtado, F., and Pereira, F., 2008, Operator splitting based on physics for flow in porous media: *International Journal of Computational Science*, v. 2, p. 315–335.
- _____, 2009, Operator splitting for three-phase flow in heterogeneous porous media: *Communications in Computational Physics*, v. 6, p. 72–84.
- Abreu, E., Douglas, J., Jr., Furtado, F., Marchesin, D., and Pereira, F., 2006, Three-phase immiscible displacement in heterogeneous petroleum reservoirs: *Mathematics and Computers in Simulation*, v. 73, p. 2–20.
- Balbas, J., and Qian, X., 2009, Non-oscillatory central schemes for 3D hyperbolic conservation laws: *Hyperbolic Partial Differential Equations, Theory, Numerics and Applications*, in *Proceedings of the 12th International Symposia in Applied Mathematics*, College Park, University of Maryland.
- Davis, T., Duff, I., Amestoy, P., Larimore, S., Gilbert, J., Ng, E., and Hadfield, S., 2010, UMFPACK, <http://www.cise.ufl.edu/research/sparse/umfpack>.
- Douglas, C., Efendiev, Y., Ewing, R., Ginting, V., and Lazarov, R., 2006, Dynamic data driven simulations in stochastic environments: *Computing*, v. 77, p. 321–333.
- Douglas, J., Furtado, F., and Pereira, F., 1997a, On the numerical simulation of waterflooding of heterogeneous petroleum reservoirs: *Computational Geosciences*, v. 1, p. 155–190.
- Douglas, J., Pereira, F., and Yeh, L. M., 1997b, A parallelizable method for two-phase flows in naturally fractured reservoirs: *Computational Geosciences*, v. 1, p. 333–368.
- _____, 2000, A locally conservative Eulerian-Lagrangian numerical method and its application to nonlinear transport in porous media: *Computational Geosciences*, v. 4, p. 1–40.
- Douglas, J., Frias, D., Henderson, N., and Pereira, F., 2003, Simulation of single-phase multicomponent flow problems in gas reservoirs by Eulerian-Lagrangian techniques: *Transport in Porous Media*, v. 50, p. 307–342.
- Efendiev, Y., Datta-Gupta, A., Ginting, V., Ma, X., and Mallick, B., 2005, An efficient two-stage Markov chain Monte Carlo method for dynamic data integration: *Water Resources Research*, v. 41, W12423.
- Exascale, 2010, International Exascale software project, White paper, <http://www.exascale.org>.
- Furtado, F., and Pereira, F., 2003, Crossover from nonlinearity controlled to heterogeneity controlled mixing in two-phase porous media flows: *Computational Geosciences*, v. 7, p. 115–135.
- Glimm, J., and Sharp, D., 1999, Prediction and the quantification of uncertainty: *Physica D*, v. 133, p. 152–170.
- Glimm, J., Lindquist, W. B., Peierls, R., and Pereira, F., 1992, The fractal hypothesis and anomalous diffusion: *Computational and Applied Mathematics*, v. 11, p. 75–93.
- Glimm, J., Lindquist, W. B., Pereira, F., and Zhang, Q., 1993, A theory of macrodispersion for the scale-up problem: *Transport in Porous Media*, v. 13, p. 97–122.
- HDF, 2010, The HDF group, <http://www.hdfgroup.org/HDF5>.
- Kurganov, A., and Petrova, G., 2001, A third-order semi-discrete genuinely multidimensional central scheme for hyperbolic conservation laws and related problems: *Numerische Mathematik*, v. 88, p. 683–729.
- Kurganov, A., and Tadmor, E., 2000, New high-resolution semi-discrete central schemes for Hamilton-Jacobi equations: *Journal of Computational Physics*, v. 160, p. 720–742.
- Lax, P., 1954, Weak solutions of non-linear hyperbolic equations and their numerical computation: *Communications on Pure and Applied Mathematics*, v. 7, p. 159–193.
- Leer, B., 1979, Toward the ultimate conservative difference scheme V: A second-order sequel to Godunov's method: *Journal of Computational Physics*, v. 32, p. 101–136.
- Nessyahu, H., and Tadmor, E., 1990, Non-oscillatory central differencing for hyperbolic conservation laws: *Journal of Computational Physics*, v. 87, p. 408–463.
- Obi, E., and Blunt, M., 2006, Streamline-based simulation of carbon dioxide storage in a North Sea aquifer: *Water Resources Research*, v. 42, W03414.
- Pereira, F., and Rahunanthan, A., 2010, Numerical simulation of two-phase flows on a GPU, in *Proceedings, High Performance Computing for Computational Science, 9th international meeting (VECPAR 2010)*, Berkeley, California.
- Rusanov, V., 1961, The calculation of the interaction of non-stationary shock waves with barriers: *Journal of Computational Mathematics and Mathematical Physics USSR*, v. 1, p. 267–279.
- Schnaar, G., and Digiulio, D., 2009, Computational modeling of the geologic sequestration of carbon dioxide: *Vadose Zone Journal*, v. 8, p. 389–403.
- Smith, J., Van Ness, H., and Abbott, M., 2005, *Introduction to chemical engineering thermodynamics*: New York, McGraw-Hill, 7th edition, 817 p.

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CHAPTER 10: Determination of Optimal Geological Model Complexity in CO₂ Sequestration Simulation: a Pre- Injection Scoping Analysis at Moxa Arch, Wyoming

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Background

Task 10 of the project generated geological and fluid flow simulation models for the Nugget Sandstone, its overlying formation (Twin Creek Formation), and its underlying formation (Ankareh Formation), together referred to as the Nugget Storage Suite (NSS). Using conditional geostatistical simulations, data were integrated at the regional-scale to create a geological fine-grid model. Based on this model, two different estimates of acid gas storage were made: one using formation volumetrics, the other using the porosity model. This data could then be used to discern the total predicted acid gas storage of a specific injection site.

This work has been accepted for publication in the journals *AAPG Bulletin* and *Water Resources Research*. A summary of results follows.

Executive Summary

In this study, geological and fluid flow simulation models were built for the Nugget Sandstone, its overlying formation (Twin Creek Formation), and its underlying formation (Ankareh Formation), or together, the Nugget Storage Suite (NSS). At the regional scale, geological and engineering data were assembled for the NSS, screened for accuracy, and digitized, covering an average formation thickness ~1700 feet. The data include ~900 wireline logs, 780 ft core measurements, 4 cross sections, and 3 isopach maps. Data were interpreted and correlated for geological formations and facies, the later categorized using Gaussian Hierarchical Clustering and Neural Network algorithms. Well log porosities were calibrated with core measurements. Well log permeabilities were estimated using porosity-permeability transforms. Using conditional geostatistical simulations (first indicator simulation of facies, then Sequential Gaussian Simulation of porosity), data were integrated at the regional-scale to create a geological fine-grid model. Based on this model, two different estimates of acid gas storage were made: one using formation volumetrics, the other using the porosity model. Results suggest a variation of 56% in the capacity estimate, with the later model providing the higher estimate.

From the regional model, a local model surrounding the injection site was extracted. To evaluate petrophysical uncertainty, 200 porosity realizations were generated in this model from which P10, P50, and P90 models were selected for flow simulations. These models capture the range of pore volume uncertainty given the currently available site data and modeling assumptions. For computation efficiency, all models were upscaled to a coarsened flow simulation grid with which multiphase compositional simulations were conducted to model acid gas injection at the Shute Creek Gas Plant. A simulation time of 2000 years was used with the first 50 years the injection phase. With

the P50 model, sensitivity of geological and engineering variables on acid gas predictions is first explored. Results suggest that at the simulation time scale, low TDS, large relative permeability hysteresis, and small k_v/k_H all contribute to enhanced acid gas storage in both residual and dissolved forms. Parameter that exerts the largest control on gas storage is relative permeability hysteresis. Given the uncertainty ranges of the model parameters, total predicted acid gas storage varies significantly, ranging from 40% from a worst-case scenario model to 94% from a best-case scenario model. The range of prediction uncertainty further increases in the order of dissolved gas, trapped gas, and mobile gas. In comparison, petrophysical uncertainty as represented by the P10-P50-P90 models has limited impact on prediction, thus the P50 model is considered representative for the reservoir system, although future work is needed to expand the range of uncertainty by developing detailed facies models at the injection site.

Overview

The Moxa Arch anticline is a northwest-trending, basement-cored uplift in western Wyoming that formed during the Late Cretaceous period (Fig. 10-1). Natural gas is produced from the deeply buried Madison Limestone, located at the crest of the anticline. The produced gases contain carbon dioxide (CO_2), methane (CH_4), nitrogen (N_2), hydrogen sulfide (H_2S), and helium (He). In 2005, a portion of the produced CO_2 and all of the H_2S was injected into the Madison Limestone below a depth of 18,000 feet, at the Shute Creek gas plant which lies 40 miles south of the producing field (La Barge platform). Since that time, over 2 million tons of mixed gas has been sequestered in this formation. Since this gas contains H_2S , the deep injection qualifies as acid gas injection.

In this project, potential for expanded waste gas storage in the deep geological formations of the Moxa Arch region is evaluated. Candidate geological formations include Nugget Sandstone, Tensleep Sandstone, and Bighorn Dolomite, all saline aquifers lying at depths exceeding 13,000 ft and containing brine with greater than 10,000 ppm total dissolved solids (TDS). Within the 12 townships surrounding the gas plant, only 31 wells penetrate these deep formations, minimizing potential leakage via wellbores. The existence of abundant natural CO_2 in the Paleozoic Tensleep, Madison, and Bighorn formations further suggests that adequate seals and hydrogeological isolation exist at depths. As part of the larger goal of determining the suitability of each formation for storing the waste gas, this study conducts a numerical scoping analysis by building reservoir models and conducting acid gas flow simulations in the Nugget Sandstone, its overlying Twin Creek Formation, and its underlying Ankareh Formation, or together, the Nugget Storage Suite (NSS). The Twin Creek and Ankareh formations are included in the storage model since low-permeability units exist above Twin Creek and within the lower intervals of Ankareh. Gas injected into the Nugget will migrate into these formations before encountering any significant flow barrier.

In the Moxa Arch, the NSS is a deep saline aquifer for which the available characterization data are limited. Thus, multiple sources of uncertainty exist in both geological model building and fluid flow simulation. This study identifies several sources of uncertainty that can be constrained or delimited by the existing data and evaluates their impact on acid gas predictions. Specifically, a regional estimate of acid gas storage in the NSS is made first using volumetric principles with different approaches. Acid gas injection at Shute Creek is then modeled to provide a more detailed assessment of gas migration and storage. In particular, the simulation integrates several sources of geological and engineering uncertainties by conducting a parameter sensitivity study and identifying their relative impact on predictions. In the simulations, gas dissolution in brine is considered as well as its

partitioning among mobile and trapped gas (herein “gas” refers to a combination of gas-phase acid gas components, thus mobile or trapped gas refers to, respectively, the combined components as well). Since mobile gas can migrate away from the injection site due to its buoyancy compared to formation brine, gas storage is defined as the total trapped gas plus the total dissolved gas. A simulation run predicting a higher percentage of gas in trapped and dissolved forms is considered to have higher storage security.

In the remainder of the report, data used to build the reservoir models are first described. Procedure for building the models is presented, which leads to the creation of a fine-grid geostatistical model. Multiple porosity realizations are created from which 3 models corresponding to P10, P50, and P90 total pore volumes are selected for the simulation study. An upscaling analysis is then conducted using multiple grid sizes until a coarsened flow simulation grid is obtained with reasonable accuracy to represent the fine-grid. Using the flow grid, acid gas injection into the Nugget Sandstone is simulated with all models. Results of the simulations are presented within the framework of a sensitivity analysis. Results are discussed before conclusions are presented. The symbols and units of this report is shown (Table 10-1).

Methods

Data & Interpretations

For the NSS, a regional-scale geological model was built using public-domain geological characterization data, consisting of (1) wireline logs from 165 wells that penetrate the Nugget Sandstone (WOGCC; Table 10-2), (2) 784 feet (239 m) of core measurements (porosity and permeability), (3) four geological cross sections (Lamerson, 1982; Royse, 1982) (Fig. 10-1), and (4) three regional-scale isopach maps, one for each formation of the NSS (Maclachlan, 1972; Peterson, 1972; Fraley, 1998). Two of these cross sections are shown in Fig. 10-2 (their locations are marked in Fig. 10-1). All cross sections were used to determine the subsurface extent of the Moxa Arch structure within the NSS.

The well logs provide the majority of the characterization data. The 165 wells include 14 located in the Moxa Arch region (Fig. 10-1) and 151 in the Overthrust Belt (location not shown). For the 165 wells, a total of more than 900 logs were digitized. The logs were first screened for accuracy – those with inconsistent depth or incorrect datum information were removed and not used in geological modeling. Subsets of the logs were then used in various interpretation tasks. The 14 wells that penetrate the Moxa Arch structure were used in interpreting the regional-scale structure of the NSS, i.e., major formation contacts. An example structure interpretation from correlating well log formation picks is shown (Fig. 10-3). In this chart, log signatures at each well are plotted against the Sub-Sea True Vertical Depth (SSTVD). The columns are Sonic log (DT), Gamma Ray (GR), calculated Clay Volume of the formation (V_c), and a discrete petrofacies log (details on how petrofacies are generated will be introduced). Along the transect through which the correlation chart was built (Fig. 10-1), the Nugget top rises slightly towards north, while the thickness of the Nugget does not change significantly. For these same 14 wells, logs were also interpreted to obtain estimates, at each well, of formation fluid type and saturation content. For the Nugget Sandstone, data such as spontaneous potential, resistivity, and production records indicate that in most of the Moxa Arch, formation fluid is dominantly by NaCl-type brines. For some wells, temperature measurements also

exist. These data were used to provide estimates of average formation temperature and vertical temperature gradient which were used to assign an initial temperature field to the simulation model. Further, due to a lack of relevant data in the Moxa Arch, well logs in the Overthrust Belt are used to provide facies and petrophysical information for modeling the Moxa Arch NSS facies and porosity.

Core measurements provide direct information on petrophysical properties. For the Nugget Sandstone, for example, well-log-derived porosity was calibrated against core measurements at the same well to obtain a linear transform. This function was used to calibrate the well-log-derived porosity in locations where no core measurements exist. Further, a semi-log transform between porosity and horizontal (N-S) permeability was obtained for the Nugget. Such a transform was later used to populate a horizontal permeability from the geostatistically generated porosity models. From the available core data, Nugget permeability is nearly isotropic in the horizontal plane, but exhibits a range of anisotropy in the vertical direction. This uncertainty will be evaluated in the acid gas simulation study. For the Twin Creek and Ankareh Formations, public-domain core measurements of significant length intervals do not exist. The porosity models for these formations were populated using well-log-derived porosity which thus cannot be calibrated. The permeability models for these formations were obtained by borrowing the porosity-permeability transform developed for the Nugget Sandstone.

Building the Reservoir Model

Well logs, geological cross sections, and isopach maps were integrated at the regional scale to create formation horizons for the NSS in the Moxa Arch. Four horizons were interpreted, each representing a major contact between formations: Twin Creek Top, Nugget Top, Ankareh Top, and Ankareh Bottom (Fig. 10-4). Using this structure model, an acid gas storage capacity can be estimated using the volumetric principle:

$$SC = V \times \phi \times E \times \rho$$

where SC is acid gas mass storage capacity, V is bulk volume of NSS, ϕ is mean effective porosity of the formations (obtained by volume-weighting mean porosity of each formation), ρ is mean gas density under in-situ condition, E is the storage factor describing pore-filling efficiency due to the combined effects of gravity segregation, formation heterogeneity. A range of E is given from CO_2 storage studies, ranging from 0.03 to 0.35 (DOE, 2008). Using the parameters and volume of the structural model, the total acid gas storage capacity in the NSS was estimated to range from 0.96 Gt to 11.25 Gt, the uncertainty in the storage factor introducing one order of magnitude variation to this estimate.

Petrophysical properties typically vary by facies (Bahar and Mohan, 1997, 2004), thus facies modeling is essential for the determination of reservoir versus non-reservoir quality units within a geological formation. In this study, a distinction is made between lithofacies, which is linked to sediment physical characteristics (e.g., grain size, sorting, primary and/or secondary structures), and petrofacies, which is linked to sediment properties influencing fluid flow (e.g., porosity and permeability). Though many lithofacies can be distinguished within a reservoir unit, different lithofacies can have overlapping petrophysical properties (Melick and Gardner, 2009). Thus, for porosity and permeability modeling, petrofacies is the most relevant. In the NSS, petrofacies are

modeled using geostatistical techniques based on well log data which indicate the existence of distinct petrofacies types within the formations (Fig. 10-3). The overall approach is described below (in the rest of the report, “facies” is used to represent petrofacies).

Within the structure framework, distinct facies types were obtained using Gaussian Hierarchical Clustering (GHC), a computationally efficient categorization algorithm (Fraley, 1998). At each well, GHC integrates and converts multiple continuous log signals to discrete facies types. For the Twin Creek, 3 facies were identified (ID=0—2), using well logs within this formation only. For the Nugget, based on the computed V_c , an upper sand-rich zone was manually divided from a lower clay-rich zone. Then, using logs specific to a zone, facies was categorized. Three facies each were identified for the upper Nugget (ID=3—5) and lower Nugget (ID=6—8). However, Ankareh has poorer reservoir quality and fewer associated logs, preventing the direct application of GHC. No facies types can be automatically identified. However, from V_c of the few wells that logged this interval (Fig. 10-3), a lower shale-rich region is observed. Ankareh is thus divided manually into a lower interval (ID=11) and two upper intervals of equal thickness (ID=9—10). The above facies category (i.e., for Nugget and Twin Creek) were corroborated by conducting an independent Neural Network Analysis using the same well data. Since facies information only exists at wells, a geostatistical approach is needed to populate facies spatially, with the requirement that facies be conditioned by well data and their global proportions be honored within the facies modeling group. For each group (i.e., Twin Creek, Upper Nugget, Lower Nugget), this is accomplished with two steps: (a) experimental facies variograms were constructed in the horizontal and vertical directions. Since no significant trends were observed in the variograms, stationary spherical models were fitted. To model horizontal anisotropy, N40E was selected to be the major azimuth angle, reflecting the mean angle of deposition; (b) based on the variogram models and estimated facies proportions, Sequential Indicator Simulation (SIS) was conducted to populate facies within the group, conditioned to the well data and honoring the prescribed facies proportions (obtained at wells after the previous facies categorization analysis) (Deutsch and Journel, 1998). All realizations capture the same facies proportions. Though SIS can generate multiple realizations, only one is selected for subsequent modeling. This realization is considered equally likely as the next realization, since all have the same expected pore volume (i.e., mean porosity of each facies is known from well logs). Finally, using this facies realization, a 12-unit NSS model is created at the regional scale (i.e., 9 Nugget and Twin Creek facies and 3 Ankareh intervals), represented by a high-density grid with 35,385,840 grid cells (Fig. 10-5).

From the regional facies model of the NSS, a local-scale model surrounding the injection site is extracted for gas simulation (Fig. 10-6). This model contains 3,725,568 grid blocks and is the basis for porosity (ϕ) modeling using a geostatistical approach. The data used are well-log-derived ϕ after applying the core-based correction (only for Nugget; raw well-log-derived ϕ is used for Twin Creek and Ankareh). Due to data limitation, porosity data were first pooled into five groups for which stable variograms could be obtained: Twin Creek Group, Upper Nugget Group, Lower Nugget Group, Upper Ankareh Group, Lower Ankareh interval. Within each porosity group, based on the well data, experimental ϕ variograms were computed in the horizontal and vertical directions. Directional spherical models were fitted from which ϕ correlation ranges are obtained. On the horizontal plane, the selection of the major and minor statistical axes of correlation was based on the same angles chosen for facies modeling. Again, stationary functions were selected to model the ϕ variograms, since a priori trend analysis on the data did not identify significant trends. (2) Based on the variogram model and ϕ histogram, ϕ was populated in the model using Sequential Gaussian Simulation (SGS)

(Deutsch and Journal, 1998). This population was conducted one facies unit at a time, for all 12 NSS units. For example, the single set of ϕ variogram and histogram obtained for the Twin Creek Group was used in populating ϕ in each of the Twin Creek facies (ID=0—2). Though these facies share the same univariate and bivariate statistics, ϕ distribution was delimited by facies distribution and was locally conditioned by facies-specific well data (i.e., well ϕ were separated into the NSS units). (3) The above step was repeated using different random seeds to create 200 ϕ realizations in the model. A total pore volume (TPV) was computed for each realization, and to reduce the number of input to flow simulations, three final ϕ realizations were selected whose TPVs are ranked at P10, P50, and P90 among the TPVs of the realizations. The P50 ϕ realization is shown for the local model in Fig. 10-6 (Lower Left).

Based on the ϕ - k_H transform obtained from core measurements, 3 k_H fields were populated in the model, corresponding to the 3 porosity models (the P50 permeability model is shown in Fig. 10-6, Lower Right). Note that the realization with higher TPV will have a porosity distribution that is shifted towards higher values, which then translates to a higher permeability distribution via the transform. As discussed previously, the transform was developed for the Nugget Sandstone but was used in populating all formations, thus for Twin Creek and Ankareh, porosity modeled by SGS (based on the respective well-log data) exerts a primary control on the magnitude of their permeabilities. Due to the same limitation, a single k_v/k_H ratio was assigned to all formations, although this ratio is varied in the sensitivity study to evaluate the influence of fractures on simulation outcomes.

Using the same volumetric principles, the P50 porosity model is used to estimate a gas storage capacity, which ranges from 0.15 Gt to 1.75 Gt in the local model. Given that the volume of the local model is approximately 10.0% of the volume of the regional model and assuming stationarity of the porosity field (formation depth does not vary significantly), this range can be extrapolated to the regional scale to be 1.50 Gt ~17.5 Gt, 1.56 times that estimated by the structure model. Since the porosity model incorporates formation-specific information as well as porosity spatial correlation, the above capacity estimates are considered more accurate.

Upscaling

In gas disposal studies, a long simulation time is desired to understand gas migration and trapping in the storage formation (Korre et al., 2009). Due to the large computation cost of modeling compositional flow with multiple gas species in three-dimensions over a long time, petrophysical properties of the fine-grid local model (i.e., P10, P50, P90 models; Fig. 10-6) were spatially averaged or upscaled to a coarse flow simulation grid (or, a “flow grid”). To determine the appropriate cell spacings for the flow grid, a grid resolution study was conducted using permeability upscaling (Wen and Gomez-Hernandez, 1996; Renard and de Marsily, 1997). In this analysis, the P50 model was used and k_v/k_H was assigned 1.0. The results are expected to be similar for the other models with different k_v/k_H . Based on the fine-grid model (horizontal and vertical cell spacing of ~200 ft and ~25 ft, respectively), increasingly coarsened grids were built which honor the formation contacts. These grids have a horizontal spacing of ~300, 400, 500, 600, and 700 ft, respectively, and a vertical spacing of ~50 ft (15 m). For each coarse grid, a cell permeability tensor was computed with flow-based upscaling by conducting single-phase (water) steady-state flow simulations in the fine-grid. Since heterogeneity in the fine-grid is dominated by lateral stratification, a diagonal tensor upscaling technique was used. Thus, along every two opposing cell faces, no-flow and linear-potential-drop

boundary conditions were assigned for the computation of the three principal permeability components. To enhance the accuracy of permeability upscaling, a local method with three skins was used (Wen et al., 2003). Since porosity is additive, arithmetic volume-weighted average was used to obtain porosity for the coarse grid cells.

To determine which coarse grid was sufficient to capture fine-grid flow, single-phase steady-state flow was simulated with all grids to determine a bulk flow rate across the outflow boundary. By comparing to the flow rate of the fine-grid, a coarse grid with a horizontal spacing of 600 ft was selected which gave a relative error in flow rate around 10%. Note that although finer grids predicted better results (e.g., 400-ft grid gave a relative error of 3%), numerical experimentations with acid gas modeling took an unreasonable amount of time (e.g., up to three weeks for a single simulation run). Further, since higher accuracy is desired near the injection well where gas plume emanates, the 600-ft grid is modified by local grid refinement (LGR) near the injector (total grid cells in this model is 275,028). LGR is a common simulation technique which can enhance the accuracy of modeling in the refined region (here, the near-well region that matters the most). As shown by later simulations, most of the plume travels through this region, which also traps and dissolves most of the gas. Thus, in the 600-ft grid, near-well LGR will offset the global flow error in the coarsened cells elsewhere. Numerical experimentations were also carried out comparing a suite of 5 end-member simulations (defined in Results), with and without LGR. The average enhancement in flow rate prediction due to LGR is 4.70%.

Acid Gas Simulations

Using the flow grid, acid gas simulations were conducted with GASWAT of Eclipse 300 (Schlumberger, 2009), a multiphase, multispecies compositional simulator. GASWAT is applicable to modeling geological storage of CO₂ in aquifers and depleted gas reservoirs. Gas composition, however, is not restricted to CO₂. Other gases and their solubilities in water can be modeled assuming phase equilibrium. GASWAT solves the pressure and molar density of each component in the fluid system. The mole fractions of components in gas (or vapor phase) and aqueous phase are computed through a flash process. Both phase saturations as well as aqueous concentrations of dissolved gas components can be determined. In this study, acid gas injected into the Nugget Sandstone consists of five components: CO₂ (75%), N₂ (7%), H₂S (5%), CH₄ (10%) and C₂H₆ (3%), reflecting an average composition of the waste gas stream in the Moxa Arch. Formation water is the sixth component. All components' parameters relevant to compositional simulation were obtained using a fluid property package developed by Schlumberger, Inc. Since significant salinity is observed in the Nugget formation waters, solubility correction was made to reflect the effects of salinity on reducing aqueous solubilities of the gas components. With GASWAT, temperature of the reservoir can vary with depth, which can affect gas solubility, density, and viscosity. Thus an initial temperature field was assigned to the model by interpolating temperature data from well logs.

Due to the importance of relative permeability on gas flow, mobility, and residual trapping, gas-phase relative permeability is of significant interest in acid gas modeling. In saline aquifers, gas relative permeability hysteresis was found to significantly contribute to residual CO₂ trapping (e.g., Ide et al., 2007; Qi et al., 2009). However, experimental data for CO₂-brine systems conducted under in-situ conditions in different lithologies suggest that gas relative permeability may not exhibit significant hysteresis, depending on host rock mineralogy, pore size distribution, and dissolution effects (Bennion and Bachu, 2005, 2006a, 2006b; Horne, 2008). Uncertainty in gas relative permeability will

be evaluated using end-member values observed in experiments. The brine phase is assumed non-hysteretic; its relative permeability end-point saturations were selected from those obtained for the Viking Sandstone (Bennion and Bachu, 2006a, 2006b). Though capillary pressure can affect gas storage locally, it is assumed 0.0 in the simulations. A single fluid pressure is computed, an assumption often invoked in field-scale modeling (e.g., Kumar et al., 2004; Nordbotten et al., 2005; Juanes et al., 2006; Obi and Blunt, 2006). During injection, gas flow is controlled by competition between viscous force, gravity, formation heterogeneity, and fluid mobility. Since gas has a lower density than formation brine, post-injection gas migration tends to be dominated by gravity. The effect of adding capillarity will predict a more smoothed plume front, while ignoring capillarity will give a more conservative estimate for gas storage since capillarity enhances residual trapping.

Initial pressure in the simulation model is specified as hydrostatic. Reference pressure is set as 5,701 psi at a vertical depth of 12,901 ft, assuming a brine column with a density of 63.68 lb/ft³. At the initial time, the model is equilibrated with a single brine phase. During simulation, boundary condition is represented by a Carter Tracy Analytical Aquifer of large radius and thickness. This ensures an open-flow boundary that allows the injected gas to flow out of the model. The choice of the side boundary, in effect, reflects the regional extent of the NSS reaching far beyond the model. Model top is open since the overlying Stump-Pruess cannot be assumed sealing at Shute Creek. The bottom of Ankareh is also open, since it sits above the Triassic Thaynes Formation, which locally contains sandstone facies (Picard et al., 1969). However, Stump-Pruess and Thaynes are not part of the NSS since virtually no well log or core data exist for them in the Moxa Arch.

During acid gas simulation, one injection well at Shute Creek is used (API: 2321674), perforated in Nugget only. A fixed injection rate of 75,000 Mscf/day is used. To prevent geomechanical damage to the storage formations, the injection rate was chosen so that the maximum formation fluid pressure will not exceed 1.8 times hydrostatic pressure, a threshold typically used in reservoir modeling. The injector bottomhole pressure (BHP) constraint is thus set at 10,260 psi. The injection phase lasts 50 years and the reservoir is monitored for 1950 years, for a total simulation time of 2,000 years. This time scale is consistent with the typical injection and monitoring phases modeled in gas storage studies.

Results & Discussion

Overview

In this scoping study of acid gas storage in the NSS, we aim to understand the influence of parameter uncertainty on prediction uncertainty. For each of the P10, P50, and P90 models (upscaled from the appropriate fine-grid parameter fields), a sensitivity analysis was conducted for which several parameters were varied from those of a base case simulation. Parameters of the base case have the average, or the expected values, for the storage formations. Parameters varied in the sensitivity analysis are those that can be constrained by the existing data and include (Table 10-2): (1) TDS of formation brine, (2) k_V/k_H of the fine-grid block cells (its impact on gas simulation will be reflected by the upscaled permeability tensors computed for the flow grid), (3) relative permeability hysteresis, and (4) scanning curve interpolation method (Carlson, Killough, and Jargon). In Table 10-2, run 31 is the base case. To understand the sensitivity of prediction to parameter uncertainty, four outcomes are defined at the end of simulation: dissolved gas, mobile gas, trapped gas, and a gas storage ratio. The storage ratio is fraction of the total immobile gas (dissolved plus trapped) in the NSS versus the total

injected gas (TIG). Due to the open boundary condition, a small fraction of the TIG (generally less than 0.8% among the sensitivity runs) has flowed out of the model through the top boundary.

In the Results section, simulation results pertaining to the P50 model are presented first, before relevant results are compared to those of the P10 and P90 models. For accuracy, numerical stability was checked for all sensitivity runs. In each run, simulation progress was monitored by checking the time profile plots of various prediction outcomes (e.g., mass, pressure, flow rate) over time. Convergence issues, if they occurred, were identified earlier on and solver parameters were fine-tuned whenever appropriate. A few sensitivity runs were re-run after convergence issues developed in later phases were identified and addressed. All results reported below were obtained from numerically stable solution of the compositional model.

Base Case Simulation (P50 Model)

In the base case, at the end of simulation, 48.06% of TIG is stored in the form of dissolved and trapped gas and 51.09% remains mobile. Gas plume is visualized (Fig. 10-7). Total gas saturation, including both mobile and trapped gas, is plotted along a N-S cross section, at the end of the injection and monitoring periods. During injection (top left), gas flow is dominated by viscous driving force and gravity, i.e., both lateral and vertical migration is observed. Post-injection (top right), gas flow is dominated by gravity. At the end of simulation, a gas cap has formed beneath the Twin Creek Top, where a slight updip migration is also observed. Due to the open boundary condition, some mobile gas has migrated upward out of the NSS (not shown). Since around half of the TIG is still mobile at this time, buoyancy-driven flow will impact long-term gas migration. Thus, if the base case parameters reflect the expected condition in the NSS, sealing capability of the overlying formations need to be investigated in detail.

By the end of simulation, around 1/3 of the TIG becomes trapped, which is shown as a plume with lower saturations surrounding the injector (top right). Over longer periods of time (not simulated), this trapped gas will slowly dissolve into the formation brine, transferring mass into the dissolved phase. By the end of simulation, around 17% of the TIG is dissolved, with a plume shape closely tracking the gas-phase plume. Over longer time periods, increasing fractions of the TIG will become trapped and dissolved, eventually immobilizing all the mobile gas components in both NSS and overlying formations.

Time profile plots suggest that during injection, mobile, trapped, and dissolved gases all increase in the NSS. After injection ceases, total mobile gas decreases, while the other two increase, as expected. As gas migrates away from the injector, it is trapped within cells when its saturations are beneath critical gas saturation (i.e., below this, gas relative permeability is zero). Although this trapping mechanism differs from the imbibition induced residual trapping, a significant amount of gas can still be immobilized. This is similarly observed in the other sensitivity runs when relative permeability hysteresis was not modeled. Further, formation fluid pressure reaches a maximum at the end of injection, before declining due to the stoppage (Fig. 10-7). The pressure never exceeded the BHP constraint, and as a result, the injection rate was maintained at a constant value (e.g., the simulator will adjust the rate down if the computed fluid pressure exceeds the constraint). This behavior is observed in all the sensitivity runs, thus the same total amount of gas is injected into the NSS (Table 10-2), facilitating comparison among simulations.

Sensitivity Analysis (P50 Model)

For the sensitivity runs, prediction outcomes are tabulated in Table 10- 2. Runs of particular interest are discussed here. Run 45 predicts the least amount of the trapped gas. Run 59 predicts the most amount of the dissolved gas. Run 19 predicts the most amount of the trapped gas. Run 61 predicts the highest gas storage ratio (best-case scenario). Run 3 predicts the most amount of the mobile gas, thus the least amount of the immobile gas and the lowest gas storage ratio (worst-case scenario). Run 4 predicts the least amount of the dissolved gas. To quantify results of the sensitivity study and to compare the importance of each parameter to an outcome against the other parameters, a Tornado Diagram is constructed where an absolute sensitivity measure is computed for each parameter (Fig. 10-8). Results suggest that for the chosen ranges of the parameters varied, the effect of hysteresis (i.e., sensitivity averaged over all the scanning curve options, not shown) has the largest impact on nearly all the predicted gas forms, followed by k_v/k_H and TDS. This parameter, by exerting the strongest control on mobile gas (which is equivalent to the total immobile gas since the TIG is the same in all runs), also exerts the strongest control on the gas storage ratio. Interestingly, when a particular scanning curve option (Jargon) is used by the hysteric model, trapped gas becomes more sensitive to hysteresis than when the other scanning curve options are chosen. This suggests that the exact scanning curve option needs to be understood if residual trapping prediction is of interest.

Prediction Range and Uncertainty (P10, P50, P90 Models)

With the P50 model, if the gas storage ratio (GSR) at the end of simulation is used as a measure of storage security, among all simulation cases, the worse-case scenario is Run 3 which has the lowest GSR (40%). The best-case scenario is Run 61, which has the highest GSR (94%). By comparison, GSR is 48% in the base case, which is closer to Run 3. Run 3 (worst case) has the highest TDS, no relative permeability hysteresis, and the highest k_v/k_H . Gas saturation and profile plots for this run are shown in Fig. 10-9, where a significant gas cap is observed at the end of simulation. Run 61 (best case) has the lowest TDS, the largest hysteresis, and the lowest k_v/k_H . Fig. 10-10 shows gas saturation and profile plots for this run. Compared to Run 3, gas cap is much smaller while significantly more trapped gas is predicted. Comparing gas saturation at the end of simulation time (Upper right versus Middle right), gas plume almost entirely consists of the trapped gas. This plume will no longer migrate and is effectively immobilized in the storage formations. Finally, for all runs with high GSR (above 90%), common characteristics of their parameters is large hysteresis (Killough option), medium to small k_v/k_H (0.2 and 0.02), while all TDS levels are observed. This confirms the sensitivity analysis result (Fig. 10-8).

The effect of petrophysical uncertainty on prediction uncertainty is evaluated by comparing outcomes from the P10, P50, and P90 models. Since the same sensitivity study is conducted, the outcomes are displayed as cumulative distribution function (CDF) of the dissolved, mobile, and trapped gas at the end of simulation (Fig. 10-11). Results suggest that given the current modeling assumptions, porosity and associated permeability uncertainty exerts very minor influence on gas predictions. The P50 model, which predicts an average pore volume in the NSS, can be reasonably representative of the other petrophysical models. This result is not surprising, since prediction uncertainty arising from a stochastic property model based on a fixed set of geostatistical parameters is usually smaller than that due to the uncertainty of the parameters and uncertainty in the modeling choice (e.g., alternative facie models). However, given the computation challenge of simulating acid gas over a long time and limitation in the current site data to delimit and provide bounds for these additional uncertainties, they are not evaluated. Future work will aim to better understand these uncertainties by incorporating

detailed site data including dynamic well-test behaviors, thus improving the prediction uncertainty estimated in this study.

Using the P50 model, prediction range of the three gas forms can be computed. Difference between the maximum and minimum predicted trapped gas is 109%, while differences in the dissolved gas and mobile gas are 77% and 162 %, respectively. Clearly, given the uncertainty ranges of the parameters, range of uncertainty increases in the prediction of dissolved gas, trapped gas, and mobile gas. This suggests that a large variation in the prediction outcomes is possible. In particular, prediction of the mobile gas is the most variable and thus any individual prediction becomes the least reliable. Mobile gas is also the most sensitive to the parameters varied, while dissolved gas is the least sensitive (thus any individual prediction of this outcome becomes the most reliable). The reliability in predicting trapped gas lies in the middle.

Conclusions

In this study, geological and fluid flow simulation models were built for the Nugget Sandstone, its overlying formation (Twin Creek Formation), and its underlying formation (Ankareh Formation), or together, the Nugget Storage Suite. At the regional scale, geological and engineering data were assembled for the NSS, screened for accuracy, and digitized, covering an average formation thickness ~1,700 feet. The data include ~900 wireline logs, 780 ft core measurements, 4 cross sections, and 3 isopach maps. Data were interpreted and correlated for geological formations and facies, the later categorized using Gaussian Hierarchical Clustering and Neural Network algorithms. Well log porosities were calibrated with core measurements. Well log permeabilities were estimated using porosity-permeability transforms. Using conditional geostatistical simulations (first indicator simulation of facies, then Sequential Gaussian Simulation of porosity), data were integrated at the regional-scale to create a geological fine-grid model. Based on this model, two different estimates of acid gas storage were made: one using formation volumetrics, the other using the porosity model. Results suggest a variation of 56% in the capacity estimate, with the later model providing the higher estimate.

From the regional model, a local model surrounding the injection site was extracted. To evaluate petrophysical uncertainty, 200 porosity realizations were generated in this model from which P10, P50, and P90 models were selected for flow simulations. These models capture the range of pore volume uncertainty given the currently available site data and modeling assumptions. For computation efficiency, all models were upscaled to a coarsened flow simulation grid with which multiphase compositional simulations were conducted to model acid gas injection at the Shute Creek Gas Plant. A simulation time of 2000 years was used with the first 50 years the injection phase. With the P50 model, sensitivity of geological and engineering variables on acid gas predictions is first explored. Results suggest that at the simulation time scale, low TDS, large relative permeability hysteresis, and small k_V/k_H all contribute to enhanced acid gas storage in both residual and dissolved forms. Parameter that exerts the largest control on gas storage is relative permeability hysteresis. Given the uncertainty ranges of the model parameters, total predicted acid gas storage varies significantly, ranging from 40% from a worst-case scenario model to 94% from a best-case scenario model. The range of prediction uncertainty further increases in the order of dissolved gas, trapped gas, and mobile gas. In comparison, petrophysical uncertainty as represented by the P10-P50-P90 models has limited impact on prediction, thus the P50 model is considered representative for the

reservoir system, although future work is needed to expand the range of uncertainty by developing detailed facies models at the injection site.

Future work will also consider modeling reactions of acid gas components with formation minerals and brines. Additional uncertainty parameters (e.g., reaction paths, mineral surface area, and kinetic rate constants) under in-situ temperature and pressure condition will be constrained by laboratory experiments. Finally, when field injection test takes place at the gas plant, the model developed in this study will be calibrated against observed pressure and saturation data to further reduce its uncertainty.

References

Bahar, A. and K. Mohan, 1997, Integrated lithofacies and petrophysical properties simulation. SPE 38261, Society of Petroleum Engineers, Long Beach, California.

Bahar, A. and K. Mohan, 2004, Seismic integration for better modeling of rock type based reservoir characterization: a field case example. SPE 88793, Society of Petroleum Engineers, Dhobi, U.A.E.

Bennion, B. and S. Bachu, 2005, Relative permeability characteristics for supercritical CO₂ displacing water in a variety of potential sequestration zones in the Western Canada Sedimentary Basin. SPE 95547, Society of Petroleum Engineers, Dallas, Texas.

Bennion, B. and S. Bachu, 2006a, The impact of interfacial tension and pore-size distribution/capillary pressure character on CO₂ relative permeability at reservoir conditions in CO₂-brine systems. SPE 99325, Society of Petroleum Engineers of Europe/EAGE, Vienna, Austria.

Bennion, B. and S. Bachu, 2006b, Supercritical CO₂ and H₂S-brine drainage and imbibitions relative permeability relationships for intergranular sandstone and carbonate formations. SPE 99326, Society of Petroleum Engineers of Europe/EAGE, Vienna, Austria.

Deutsch, C.V. and A.G. Journel, 1998, GSLIB: Geostatistical software library and user's guide, second edition. Oxford University Press, Inc. 369 p.

Dischinger, J.D. and S. Mitra, 2006, Three-dimensional structural model of the painter and east painter reservoir structures, Wyoming fold and thrust belt. AAPG Bulletin, v. 90, p. 1171-1185.

DOE, 2008, Methodology for development of geologic storage estimates for carbon dioxide. Technical report, http://www.netl.doe.gov/technologies/carbon_seq/refshelf/refshelf.html

Horne, R.N., 2008, Physical modeling of CO₂ sequestration, final project report, prepared for California Energy Commission. Technical Report CEC-500-2007-113, Stanford University.

Ide, S.T., K. Jessen, and F.M. Jr. Orr, 2007, Storage of CO₂ in saline aquifers: effects of gravity, viscous, and capillary forces on amount and timing of trapping. International Journal of Greenhouse Gas Control, v. 1, p. 481-491.

- Juanes, R., E.J. Spiteri, F.M. Jr. Orr, and M.J. Blunt, 2006, Impact of relative permeability hysteresis on geological CO₂ storage. *Water Resources Research*, v. 42.
- Korre, A., Shi J.Q., C. Imrie, and S. Durucan, 2009, Modeling the uncertainty and risks associated with the design and life cycle of CO₂ storage in coalbed reservoir. *Energy Procedia*, v.1, p. 2525-2532.
- Kumar, A., M. Noh, G. A. Pope, K. Sepehrnoori, S. Bryant, and L. W. Lake, 2004, Reservoir simulation of CO₂ storage in deep saline aquifers. SPE 89343, Society of Petroleum Engineers, Tulsa, Oklahoma.
- Lamerson, P.R., 1982, The fossil basin and its relationship to the Absaroka thrust system, Wyoming and Utah. In Powers, R.B., editor, *Geological Studies of the Cordilleran Thrust Belt*, v. 1, p. 279-340.
- Maclachlan, M.E., 1972, Triassic system, geological atlas of the Rocky Mountain Region. Rocky Mountain Association of Geologists, p. 166-176.
- Melick, J. J. and M. H. Gardner, 2009, Incorporating geologic heterogeneity in 3-D basin-scale models for CO₂ sequestration: Examples from the Powder River Basin, NE Wyoming and SE Montana. SPE 126443, Society of Petroleum Engineers, San Diego, California.
- Nordbotten, J. M., M. A. Celia, and S. Bachu, 2005, Injection and storage of CO₂ in deep saline aquifers: Analytical solution for CO₂ plume evolution during injection. *Transport in Porous Media*, v. 58.
- Obi, E. and M. J. Blunt, 2006, Streamline-based simulation of carbon dioxide storage in a North Sea aquifer. *Water Resources Research*, v. 42.
- Peterson, J.A., 1972, Triassic system, geological atlas of the Rocky Mountain Region. Rocky Mountain Association of Geologists, p. 177-189.
- Picard, M. D., R. Aadland, and R. Lee, 1969, Correlation and stratigraphy of Triassic Red Peak and Thaynes formations, Western Wyoming and adjacent Idaho. *AAPG Bulletin*, v. 53, 2274-2289.
- Qi, R., T.C. LaForce, and M.J. Blunt, 2009, Design of carbon dioxide storage in aquifers. *International Journal of Greenhouse Gas Control*, v. 3, p. 195-205.
- Fraley, C., 1998, Algorithms for model-based Gaussian hierarchical clustering. *SIAM Journal of Scientific Computing*, v. 20, p. 270-281.
- Renard, P. and G. de Marsily, 1997, Calculating equivalent permeability: a review. *Advances in Water Resources*, v. 20, p. 253-278.
- Royse, F., 1982, An overview of the geological structure of the thrust belt in Wyoming, northern Utah and eastern Idaho. *Geology of Wyoming*, p. 273-311.
- Schlumberger, 2009, Eclipse technical description manual. Technical report, Schlumberger Inc.

Wen, X.-H. and J. Gomez-Hernandez, 1996, Upscaling hydraulic conductivities in heterogeneous media: an overview. *Journal of Hydrology*, v. 183, p. ix-xxxii.

Wen, X.-H., L. Durlofsky, and M. Edwards, 2003, Use of border regions for improved permeability upscaling. *Mathematical Geology*, v. 35, p. 521-547.

Generalized Stratigraphic Column of Moxa Arch

AGE	FORMATION	
	CENOZOIC	TERTIARY
MESOZOIC	CRETACEOUS	GREEN RIVER (clay/mudstone)
		WASATCH (mudstone)
		EVANSTON (siltstone)
		ADAVILLE (fine sandstone)
MESOZOIC	CRETACEOUS	HILLIARD (shale)
		FRONTIER (sandstone)
		ASPEN (mudstone/sandstone)
		BEAR RIVER (mudstone/sandstone)
MESOZOIC	CRETACEOUS	GANNETT (sandstone)
		STUMP-PREUSS (shale/salt)
		TWIN CREEK (limestone)
		NUGGET (sandstone)
TRIASSIC	JURASSIC	ANKAREH (shale, muddy sand)
		THAYNES (limestone)

Modified after Royce (1993)
and Dischinger (2006)

Modified after Lamerson (1982)

Modified after Royce (1993)

Parameter	Unit	Symbol
Porosity	fraction	ϕ
N-S principal horizontal permeability	mD	k_{H0}
E-W principal horizontal permeability	mD	k_{H90}
Vertical permeability	mD	k_V
Pressure	Psia	P
Temperature	°F	T
Saturation of free phase species i	fraction	S_i
Concentration of species i in brine	ppm	C_i
Residual water saturation	fraction	S_w^{res}
Critical gas saturation	fraction	S_g^c
Residual gas saturation	fraction	S_g^{res}
Water endpoint relative permeability	fraction	k_{rw}^{end}
Gas endpoint relative permeability	fraction	k_{rg}^{end}
Injection rate	Mscf/d	r_i
Pore volume	cf	V_p
Component mass	LB-M	-
Phase Density	lb/ft ³	ρ
Phase Viscosity	cP	μ

Runs	TDS (ppm)	k_V/k_H	Hyster- esis	Scanning Curve Interpo- lation	Dissolved Acid Gas LB-M (10^8)	Mobile Acid Gas LB-M (10^9)	Trapped Acid Gas LB-M (10^9)	Total Injected Acid Gas LB-M (10^9)	Immobile Acid Gas ratio %	Mobile Acid gas ratio %
0	100,000	2.0	small	Carlson	3.58	1.03	1.98	3.39	69.97	30.35
1	100,000	2.0	small	Killough	3.68	0.99	2.01	3.39	70.07	29.18
2	100,000	2.0	small	Jargon	3.91	1.22	1.76	3.39	63.37	35.86
3	100,000	2.0	no		4.30	2.00	0.94	3.39	40.44	58.82
4	100,000	2.0	large	Carlson	2.99	0.60	2.47	3.39	81.44	17.68
5	100,000	2.0	large	Killough	3.23	0.43	2.61	3.39	86.47	12.67
6	100,000	2.0	large	Jargon	3.47	0.60	2.42	3.39	81.58	17.74
7	100,000	0.2	small	Carlson	3.77	0.86	2.14	3.39	74.24	25.34
8	100,000	0.2	small	Killough	3.83	0.83	2.17	3.39	75.17	24.40
9	100,000	0.2	small	Jargon	4.24	1.09	1.86	3.39	67.34	32.23
10	100,000	0.2	no		4.71	1.80	1.10	3.39	46.41	52.95
11	100,000	0.2	large	Carlson	3.00	0.49	2.58	3.39	84.94	14.55
12	100,000	0.2	large	Killough	3.28	0.32	2.73	3.39	90.69	9.31
13	100,000	0.2	large	Jargon	3.68	0.51	2.50	3.39	84.60	14.91
14	100,000	0.02	small	Carlson	4.11	0.76	2.22	3.40	77.50	22.40
15	100,000	0.02	small	Killough	4.17	0.72	2.25	3.40	78.46	21.31
16	100,000	0.02	small	Jargon	4.59	1.00	1.92	3.40	70.03	29.52
17	100,000	0.02	no		5.00	1.69	1.19	3.40	49.83	49.75
18	100,000	0.02	large	Carlson	3.24	0.43	2.64	3.40	87.12	12.66
19	100,000	0.02	large	Killough	3.37	0.22	2.84	3.40	93.39	6.33
20	100,000	0.02	large	Jargon	4.02	0.47	2.52	3.40	85.85	13.92
21	50,000	2.0	small	Carlson	4.45	1.01	1.90	3.39	69.00	29.88
22	50,000	2.0	small	Killough	4.56	0.98	1.92	3.39	70.04	28.94
23	50,000	2.0	small	Jargon	4.84	1.21	1.67	3.39	63.45	35.54
24	50,000	2.0	no		5.28	1.93	0.90	3.39	41.97	57.00
25	50,000	2.0	large	Carlson	3.73	0.59	2.39	3.39	81.41	17.42
26	50,000	2.0	large	Killough	4.02	0.43	2.54	3.39	86.57	12.53
27	50,000	2.0	large	Jargon	4.32	0.61	2.32	3.39	81.11	17.89
28	50,000	0.2	small	Carlson	4.63	0.84	2.07	3.39	74.55	24.78
29	50,000	0.2	small	Killough	4.71	0.81	2.10	3.39	75.61	23.78
30	50,000	0.2	small	Jargon	5.20	1.08	1.78	3.39	67.68	31.67
31	50,000	0.2	no		5.75	1.73	1.06	3.39	48.06	51.09
32	50,000	0.2	large	Carlson	3.69	0.49	2.51	3.39	84.78	12.53
33	50,000	0.2	large	Killough	4.04	0.31	2.66	3.39	90.13	9.16
34	50,000	0.2	large	Jargon	4.54	0.51	2.40	3.39	84.14	15.08
35	50,000	0.02	small	Carlson	5.05	0.73	2.15	3.40	78.19	21.37
36	50,000	0.02	small	Killough	5.09	0.70	2.18	3.40	79.07	20.55
37	50,000	0.02	small	Jargon	5.62	0.99	1.83	3.40	70.46	28.99
38	50,000	0.02	no		6.07	1.63	1.15	3.40	51.56	47.89
39	50,000	0.02	large	Carlson	3.97	0.42	2.57	3.40	87.45	12.27
40	50,000	0.02	large	Killough	4.37	0.21	2.73	3.40	93.34	6.27
41	50,000	0.02	large	Jargon	4.97	0.47	2.42	3.40	85.75	13.89
42	10,000	2.0	small	Carlson	4.97	1.01	1.84	3.39	68.99	29.80
43	10,000	2.0	small	Killough	5.09	0.98	1.87	3.39	70.08	28.74
44	10,000	2.0	small	Jargon	5.39	1.20	1.62	3.39	63.54	35.28
45	10,000	2.0	no		5.87	1.90	0.87	3.39	42.88	55.85
46	10,000	2.0	large	Carlson	4.18	0.58	2.36	3.39	81.86	17.06
47	10,000	2.0	large	Killough	4.49	0.42	2.48	3.39	86.44	12.26
48	10,000	2.0	large	Jargon	4.82	0.61	2.27	3.39	81.02	17.92
49	10,000	0.2	small	Carlson	5.13	0.83	2.03	3.39	74.81	24.52
50	10,000	0.2	small	Killough	5.24	0.80	2.04	3.39	75.59	23.51
51	10,000	0.2	small	Jargon	5.75	1.07	1.72	3.39	67.72	31.41
52	10,000	0.2	no		6.36	1.71	1.03	3.39	49.02	50.27
53	10,000	0.2	large	Carlson	4.12	0.49	2.47	3.39	84.87	14.38
54	10,000	0.2	large	Killough	4.48	0.31	2.61	3.39	90.18	9.13
55	10,000	0.2	large	Jargon	5.03	0.51	2.36	3.39	84.39	14.88
56	10,000	0.02	small	Carlson	5.58	0.72	2.11	3.40	78.50	21.11
57	10,000	0.02	small	Killough	5.64	0.68	2.14	3.40	79.46	20.13
58	10,000	0.02	small	Jargon	6.22	0.97	1.79	3.40	71.07	28.55
59	10,000	0.02	no		6.70	1.60	1.12	3.40	52.59	47.04
60	10,000	0.02	large	Carlson	4.44	0.41	2.53	3.40	87.64	12.07
61	10,000	0.02	large	Killough	4.85	0.21	2.69	3.40	93.55	6.27
62	10,000	0.02	large	Jargon	5.52	0.47	2.36	3.40	85.83	13.75

CHAPTER 11: Carbon Sequestration Monitoring Activities

PIs: Wyoming State Geological Survey, Dr. Ronald C. Surdam, Former State Geologist, Rod DeBruin and John Jiao, Geologists

Background

The Wyoming State Geological Survey (WSGS) was tasked with incorporating the geological, geophysical, and petrophysical data derived in Tasks 2–10 into a 3-D Earthvision model (i.e., Dynamic Graphics Spatial Modeling software) of an area with a 10 mile radius of the proposed CO₂ injection site. Initially from this model 1-D well profiles and 2-D cross sections were extracted to approximate CO₂ injection and flow in the subsurface. Next, a probability based performance assessment model utilizing the 1 and 2 dimensional grids extracted from the hydrostratigraphic/flow models was developed within the GoldSim, FEHM, and CO₂ – PENS software packages. The performance assessment model of subsurface CO₂ flow provides first approximations of probabilities of leakage rates, likely storage capacity, and impacts on accessible environments.

Executive summary

Task 11 of the Moxa Arch Project, the responsibility of the Wyoming State Geological Survey, focused on the performance assessment of the Paleozoic Bighorn/Madison/Weber stratigraphic section as a commercial CO₂ storage site. Results of Task 11 suggest that in the study area (950 km²), with appropriate management, the Paleozoic section on the Moxa Arch could accommodate up to 900 Mt of CO₂ over a 50-year period. This conclusion is based on 1) construction of a 3-D geological model of the study area using EarthVision® software; 2) generation of a 3-D computational mesh; 3) input of well log data from deep wells in the area; and 4) numerical simulation of a diverse set of CO₂ injection scenarios for each of the targeted formations using Los Alamos National Laboratory's FEHM simulator. Numerical simulations of single injector wells demonstrate that an injection rate of 1 Mt of CO₂ per year could be used in any of the targeted CO₂ storage reservoirs (the Bighorn, Madison, and Weber Formations). Permeability is the most critical parameter in the injection scenarios, and appears to control pressure build-up in all injection scenarios.

The greatest scientific uncertainty in numerical simulations of CO₂ injection/storage scenarios on the Moxa Arch is the characterization of geological heterogeneity in three dimensions. As in most potential commercial CO₂ injection/storage projects, displaced fluids must be managed to control pressure spikes and pressure excursions. The results of Task 11 demonstrate that the Paleozoic stratigraphic section on the Moxa Arch is a viable candidate site for commercial CO₂ storage. We know that the Madison Limestone is a viable candidate because ExxonMobil has injected more than one million tons/year of waste gas consisting of hydrogen sulfide and carbon dioxide into the Madison Limestone since 2005. The Weber and the Bighorn appear to have good injection zone characteristics conducive to injection, but uncertainty is greater because these two formations have no injection history.

Introduction

The Wyoming State Geological Survey completed Task 11 of the Moxa Arch project—the performance assessment of the geological CO₂ storage capacity for potential CO₂ storage injection zones. This report deals with an area on the Moxa Arch in southwestern Wyoming covering 950 km² within Townships 21 to 24 North and Ranges 111 to 113 West (Figure 11-1). A smaller simulation area (10 km × 10 km) was selected within the study area, and includes a potential CO₂ injection well site in the center of the area, with the ExxonMobil Shute Creek gas processing plant located approximately 10 kilometers southeast of the injection well site (Figure 11-1).

Task 11 focuses on assessing the potential impacts of injecting CO₂ into the three different subsurface injection zones on the Moxa Arch: the Ordovician Bighorn Dolomite, the Mississippian Madison Limestone, and the Pennsylvanian Weber Sandstone (Figure 11-2). These assessments can be separated into two major categories: risk assessment and performance assessment. The risk assessment evaluates the potential for leakage of stored CO₂ through confining system layers, existing faults or induced faults, and existing wells, along with the impacts of such leakage on health, safety, and the environment. The performance assessment evaluates injection rates, storage capacity, injection zone pressure evolution and distribution, CO₂ plume migration and saturation, and displaced fluid management under different geological injection zone conditions and different CO₂ injection scenarios.

Results of this study suggest that with appropriate management, injected CO₂ could remain trapped for extremely long time periods in the target injection zones. However, stored CO₂ could be accidentally released via one of the following mechanisms: (1) upward leakage of fluid through the confining system layers due to either catastrophic confining system failure or gradual failure; (2) release through existing fractures or induced faults due to the increased injection zone pressure resulting from CO₂ injection; (3) lateral or vertical leakage into adjacent aquifers from an unknown structural or stratigraphic fluid migration connection with the targeted injection zone; and/or (4) upward leakage of fluid through inadequately constructed wells, abandoned wells, or undocumented wells (IPCC, 2005). No faults were reported within the 10 km by 10 km modeling domain by investigators from Task 4 (Geological characterization subsurface structural evaluation) or Task 5 (Geological characterization surface structural analysis). Therefore, the leakage risk related to faults is not covered in this report. A total of 1,040 completed wells are located in the large regional modeling area comprising all or parts of Townships 21 N–24 N, Ranges 111 W–113 W. Most of these wells have total depths (TDs) that are within Cretaceous formations (Figure 11-2) and less than 12,000 ft. Only 138 wells have TDs of more than 12,000 ft, and only 30 wells have TDs of 12,500 ft or more; only one well (one of ExxonMobil's acid gas injection [AGI] wells) penetrates the targeted Bighorn Dolomite, and four wells penetrate the targeted Weber Sandstone and Madison Limestone. Except for these wells, no abandoned wells or undocumented wells were reported from Task 2 (Geological characterization assembling and validating a well database). Because most wells in the modeling area have TDs far above the targeted storage formations, the probability of leakage through a well borehole is considered very low.

This report focuses on performance assessment, which includes (1) constructing the three-dimensional geological structural model as a framework for the numerical CO₂ injection

simulations; (2) performing a series of numerical CO₂ injection simulations using various injection rates, porosities, and permeabilities for targeted injection zones—the Weber Sandstone, Madison Limestone, and Bighorn Dolomite; and (3) determining likely storage capacity, injection zone pressure evolution, CO₂ plume migration, and displaced fluid flow based on the numerical simulations using different geological injection zone conditions.

Geological structural modeling

A 3-D geological model was constructed for this project based on the 30 geophysical from the deeper wells, a 2-D seismic line (GRB 200 located on Figure 11-1) interpreted by the Wyoming State Geological Survey, and geological data assembled by the Wyoming State Geological Survey. The model covers a 25 km by 38 km area that includes all or parts of Townships 21 N to 24 N and Ranges 111 W to 113 W. The model was built using EarthVison[®], a commercial 3-D geospatial modeling software package. Most well TDs are within Cretaceous-age formations, and only four of the wells penetrate the Weber Sandstone and Madison Limestone (ExxonMobil's AGI 3-14 and AGI 2-18, both TD in the Darby Formation; the Whiskey Butte No. 1 TDs in the Madison Limestone; and the Keller Rubow No.1 TDs in the Bighorn Dolomite). The formation tops below the Cretaceous are mainly extrapolated from interpreted 2-D seismic reflections and from well logs for the four deep wells that penetrate the targeted formations. Based on the results from Tasks 4 and 5, no faults are included in this geological structural model. The gridding sizes for the x, y, and z axes are 21 by 21 by 41, or 1,250 m by 1,900 m by 160 m, respectively. 2-D and 3-D minimum tension gridding was used to construct this model. Figure 11-3 shows the incline view to the north of the geological structural model for the study area.

Generation of the 3-D computational mesh

Following the logic and methodology outlined in Miller et al. (2007), the WSGS used a geologic framework model to create a numerical mesh that maintains sharp material interfaces between the units of interest. In this computational mesh, the simulation cells or nodes are aligned to follow the curvature of the unit interfaces and do not stair-step in the manner of a traditional finite element grid. This type of gridding allows for a more accurate calculation of CO₂ moving along the caprock in the up-dip direction. The numerical mesh used in this paper consists of a block that is 10 km by 10 km in map view in the middle of the 25 km by 38 km geological structural modeling area (Figure 11-1), and extends from 6,000 ft above sea level to 14,000 ft below sea level. Grid spacing is 250 m in the x and y directions, and variable in the vertical direction. The total mesh consists of 19,965 nodes with 120,000 volume elements.

Carbon dioxide injection simulation scenarios

Simulations of CO₂ injection were run on the Los Alamos National Laboratory multiphase porous numerical flow simulator (Finite Element Heat and Mass Transfer, or FEHM). FEHM has been used successfully for many multiphase applications, including isotopic fractionation in the vadose zone, methane hydrate dissolution and transport, geothermal energy analysis, and simulations of CO₂ injection into saline aquifers (Kwicklis et al., 2006; Stauffer et al., 2009a, 2009b). The CO₂ equations of state are built into a lookup table that can capture the transition from supercritical fluid to liquid/gas across the region of discontinuous derivatives. Solubility of CO₂ in brine is determined according to the model of Duan and Sun (2003) and Stauffer et al. (2009b).

Initial conditions for the modeling domain include a geothermal gradient of 25.5°C/km with a temperature of 155°C at the bottom of the storage domain (Weber Sandstone, Madison Limestone, and Bighorn Dolomite) and a temperature of 93°C at the top of the storage domain, and a hydrostatic pressure gradient ranging from 47.8 MPa at the top of the domain (6,000 ft below sea level) to 59.7 MPa at the bottom of the domain (14,000 ft below sea level). Further simplifying assumptions for the 3-D injection calculations are that thermal conductivity of the rocks is constant at 0.5 W/(m K), rock density is constant at 2,650 kg/m³, and heat capacity is constant at 1,000 J/(kg K). Relative permeability for all rocks is assigned residual saturation of 10% for both brine and CO₂, using a linear relationship. Capillary pressure effects are ignored; brine total dissolved solids (TDS) are constant at 20,000 ppm for all formations, and water viscosity is calculated independent of brine content or dissolved CO₂. The WSGS set initial dissolved CO₂ concentration to zero as a bounding calculation. During CO₂ injection, the simulator allows for the possibility of CO₂ dissolution in water. For all simulations, the down-dip sides (east and south sides) of the domain are closed, whereas the up-dip sides (north and west sides) are open for the reservoir fluids to flow freely out of the simulation area.

A thickness of 400 ft (392 ft in the model based on equally spaced injection points within the formation) was used for the Bighorn Dolomite, based on an isopach map of the formation (Figure 11-4). More accurate thicknesses derived from well logs are unavailable for this area. Well logs in two nearby injection wells showed thicknesses for the Madison Limestone and the Weber Sandstone in the range of 800 feet each; however, we chose to use 400 ft for the Madison Limestone based on equally spaced injection points within the formation, and 400 ft for the Weber Sandstone. A proprietary seismic line (Line GRB 200) near the simulation area (Figure 11-5) and all available well logs were used to construct a 3-D geological structural model (geological modeling area, 25 km × 38 km) in EarthVision[®] of the Shute Creek area that includes the 100 km² study area (Figure 11-3).

A series of FEHM CO₂ injection simulations was performed using various injection rates, porosities, and permeabilities for the Bighorn Dolomite, Madison Limestone, and Weber Sandstone in order to evaluate potential variation in the impacts of injection rate, porosity, and permeability on storage capacity, injection zone pressure evolution, CO₂ plume migration trends, and displaced fluid volumes.

Bighorn Dolomite simulations and results

An important consideration in the CO₂ injection simulation results from FEHM is the buildup of pressure during injection. A limiting value of 65% of overburden pressure was selected for our simulations to ensure the Bighorn Dolomite was not fractured during injection. This limiting value was also used for the Madison Limestone and the Weber Sandstone. Throughout the remainder of this paper, 65% of lithostatic pressure will be designated as the fracture constraint pressure. An average porosity of 8% and a relative permeability of 5 md for the Bighorn Dolomite were considered the most typical values for preliminary simulation runs, since they were derived from well data of the upper part of the Bighorn Dolomite in two wells. These parameters were used in several of the FEHM CO₂ injection simulations; however, a number of combinations of different porosities and relative permeabilities were also tried in order to evaluate outcomes under different conditions.

A series of FEHM CO₂ injection simulations were used to evaluate the CO₂ storage characteristics of the Bighorn Dolomite (injection rates 0.6 Mt/year, 1.0 Mt/year, and 1.5 Mt/year; porosities of 5% and 8%; permeabilities of 1 and 5 md; and a formation thickness of 392 ft). Two simulations were run with an injection rate of 0.6 Mt/year over a 50-year period, one with 5% porosity and 1md of relative permeability and one with 8% porosity and 5md of relative permeability (Figure 11-6 and Figure 11-7). In both cases, the injection of CO₂ resulted in pressures well below hydro-fracture pressure, and 32 and 33 Mt of formation fluids were displaced over a 50-year period.

Two simulations were run with an injection rate of 1.0 Mt/year over a 50-year period, one with 5% porosity, and 1 md of permeability and the other with 8% porosity and 5md of relative permeability (Figure 11-8 and Figure 11-9). These combinations resulted in initial pressures that approached hydro-fracture pressure, and 52.6 Mt and 53.9Mt of formation fluids were displaced over a 50-year period. When another simulation was run with an injection rate of 1.5 Mt/year, 5% porosity, and 1md of relative permeability, pressure exceeded hydro-fracture pressure during the first 9 years, and 87.0 Mt of formation fluids were displaced over a 50-year period (Figure 11-10).

Map views of the injected CO₂ plume on the top of the targeted Bighorn Dolomite after 10 years and 50 years of injection of 1Mt/year, 8% porosity, and 5 md of relative permeability show that the size of the plume increases from about 1 mile in diameter to about 1.5 miles in diameter (Figure 11-11 and Figure 11-12) of injection. The plume is still only about 1.5 miles in diameter 50 years after injection stops (Figure 11-13).

An incline view of the injected CO₂ plume for the targeted Bighorn Dolomite after 50 years of injection of 1 Mt/year, porosity of 8%, and relative permeability of 5 md shows that the main body of the plume is contained within the targeted Bighorn Dolomite (Figure 11-14).

Madison Limestone simulations and results

Two injection simulations were performed to evaluate the storage potential of the Madison Limestone (injection rates of 0.6 Mt/year and 1.0 Mt/year using 5% porosity and 1 md permeability with a formation thickness of 400 ft). The simulations with injection rates of 0.6 and 1.0 Mt/year remained well below the hydro-fracture pressure over the 50-year injection period, with total formation fluid displacements of 33 Mt and 52.8 Mt respectively (Figure 11-15 and Figure 11-16). When the injection rate was 0.6 and 1.0 Mt/year with 10% porosity and 5 md of relative permeability with a formation thickness of 400 ft, the pressure remained well below the hydro-fracture pressure over the 50-year injection period (Figure 11-17 and Figure 11-18). Fluids displaced over the 50-year injection period in these two examples were 33 Mt and 53.7 Mt respectively.

Map views of the injected CO₂ plume on the top of the targeted Madison Limestone after 10 years and 50 years of injection of 1Mt/year, 5% porosity, and 1md of relative permeability show that the size of the plume increases from about 1 mile in diameter to about 1.2 miles in diameter

(Figure 11-19 and Figure 11-20). The plume is still only about 1.5 miles in diameter 50 years after injection stops (Figure 11-21).

An incline view of the injected CO₂ plume for the targeted Madison Limestone after 50 years of injection of 1 Mt/year, porosity of 5%, and relative permeability of 1md shows that the main body of the plume is contained within the targeted Madison Limestone (Figure 11-22).

Weber Sandstone simulations and results

A series of injection simulations for the Weber Sandstone were performed (injection rates over a 50-year period of 0.6 Mt/year and 1 Mt/year; porosities of 5% and 10%; permeabilities of 1 md and 5 md; and a formation thickness of 400 ft). The simulation for 0.6 Mt/year, 5% porosity, and 1 md relative permeability had pressures that remained well below hydro-fracture pressure and leveled off after the first two years of injection; 30 Mt of pore fluids were displaced over the 50-year injection period (Figure 11-23). The same injection rate with 10% porosity and 5 md relative permeability showed the same pressure behavior at a slightly lower level; 28 Mt of pore fluids were displaced (Figure 11-24). A simulation with an injection rate of 1.0 Mt/year, 5% porosity, and 1 md of relative permeability again had pressures that remained well below hydro-fracture pressure and leveled off after the first two years of injection; 51 Mt of pore fluids were displaced (Figure 11-25). The same injection rate with 10% porosity and 5 md relative permeability showed the same pressure behavior at a slightly lower level; 49 Mt of pore fluids were displaced (Figure 11-26).

Map views of the injected CO₂ plume on the top of the targeted Weber Sandstone after 10 years and 50 years of injection of 1Mt/year, 10% porosity, and 5 md of relative permeability show that the size of the plume increases from about 1 mile in diameter to about 1.5 miles in diameter (Figure 11-27 and Figure 11-28). The plume is still only about 1.5 miles in diameter 50 years after injection stops (Figure 11-29).

An incline view of the injected CO₂ plume for the targeted Weber Sandstone after 50 years of injection of 1 Mt/year, porosity of 5%, and relative permeability of 1md shows that the main body of the plume is contained within the targeted Madison Limestone (Figure 11-30).

Conclusions

The FEHM simulations showed that permeability was the main factor, besides thickness of the target formation, controlling the amount of CO₂ that could be injected into any of the target formations; lower relative permeabilities caused a rapid pressure buildup during the first years of injection, whereas higher relative permeabilities led to smaller pressure buildups. Varying the porosity had little effect on pressure, but higher porosities slightly increased the amount of pore fluids that were available for displacement. As would be expected, faster injection rates with constant porosities and permeabilities caused higher initial pressures and increased the volume of pore fluids displaced.

The simulation and modeling work resulting from this task shows that at least 1.0 Mt/year of CO₂ per injection well could be injected into the Bighorn Dolomite, the Madison Limestone, or the Weber Sandstone in the Moxa Arch area over a 50-year period at the proposed injection site. In fact, since 2005, ExxonMobil has used two deep acid gas injection wells to dispose of more

than 1.0 Mt/year of waste gas (Wyoming Oil and Gas Conservation Commission, 2010), consisting of carbon dioxide (30%) and hydrogen sulfide, into the Madison Limestone.

The greatest scientific uncertainty in numerically simulating CO₂ storage processes in the Moxa Arch area is characterizing the geological heterogeneity of the storage domain in three dimensions. More characterization of the prospective reservoirs— including degree of compartmentalization of the rock/fluid system, lithology, porosity and permeability variations within injectable thicknesses of each of the storage formations, and potential injectivity properties—must be evaluated in three dimensions before initiation of CO₂ storage. More accurate values of injectable thicknesses, average porosities, and average relative permeabilities would greatly assist in refining the FEHM simulations and the three-dimensional CO₂ distribution models, and would give a more accurate picture of how much CO₂ could be stored in the targeted formations.

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References

Duan, Z. and R. Sun, 2003, An improved model calculating CO₂ solubility in pure water and aqueous NaCl solutions from 273 to 533 K and from 0 to 2000 bar. *Chemical Geology*, 193, p. 257-271.

Foster, N.H., 1972, Ordovician System, in W.W. Mallory, ed., *Geologic Atlas of the Rocky Mountain Region*, U.S.A.; RMAG, Denver, Colorado, p. 76-85.

Intergovernmental Panel on Climate Change (IPCC), 2005, Carbon dioxide capture and storage, Intergovernmental Panel on Climate Change Special Report: Cambridge University Press, New York.

Kwicklis, E.M., Wolfsberg, A.V., Stauffer, P.H., Walvroord, M.A., and Sully, M.J., 2006, Multiphase multicomponent parameter estimation for liquid and vapor fluxes in deep arid systems using hydrologic data and natural environmental traces, *Vadose Zone Journal*, v. 5: 934–950.

Miller, T.A., Vessilinov, V.V., Stauffer, P.H., Birdsell, K.H., and Gable, C.W., 2007, Integration of geologic frameworks in meshing and setup of computational hydrogeologic models, Pajarito Plateau, New Mexico. New Mexico Geological Society Guide Book, 58th Field Conference, Geology of the Jemez Mountains Region III.

Stauffer, P.H., Surdam, R.C., Jiao, Z., and Miller, T.A., 2009a, Combining geologic data and numerical modeling to improve estimates of the CO₂ sequestration potential of the Rock Springs Uplift, Wyoming, *Energy Procedia*: 1(1), p. 2717–2724.

Stauffer, P.H., Viswanathan, H.S., Pawar, R.J., and Guthrie, G.D., 2009b, A system model for geologic sequestration of carbon dioxide, *Environmental Science and Technology*: 43(3), p. 565–570.

Wyoming Oil and Gas Conservation Commission, 2010, (website), <http://wogcc.state.wy.us>.

Age		Moxa Arch	Rock Springs Uplift
Tertiary	Eocene	Wasatch Formation.	
	Paleocene	Ft. Union Formation	
Cretaceous		Mesaverde Group	
		Baxter Shale	
		Frontier Formation	
		Mowry Shale	
		Muddy Sandstone	
		Thermopolis Shale	
		Cloverly Formation	
Jurassic		Morrison Formation	
		Sundance Formation	
		Twin Creek Ls/Gypsum Spring Fm.	
		Nugget Sandstone	
Triassic		Chugwater Formation	
		Dinwoody Formation	
Permian		Phosphoria Formation	
Pennsylvanian		Tensleep/Weber Sandstone	
		Amsden Formation	
Mississippian		Madison Limestone	
Devonian		Darby Fm	
Silurian			
Ordovician		Bighorn Dolomite	
Cambrian		Gallatin Limestone	
		Gros Ventre Formation	
		Flathead Sandstone	

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CO2 Injection Simulation Results from FEHM for the Bighorn Dolomite
Injection Interval 392 ft, Porosity 5%, Relative Permeability 1 md,
Injection Rate 19kg/s, 0.6MT/year

CO2 Injection Simulation Results from FEHM for the Bighorn Dolomite
Injection Interval 392 ft, Porosity 8% , Relative Permeability 5 md,
Injection Rate 19kg/s, 0.6MT/year

CO2 Injection Simulation Results from FEHM for the Bighorn Dolomite.
Injection Interval 392 ft, Porosity 5% , Relative Permeability 1 md,
Injection Rate 31.68kg/s, 1 MT/year

CO2 Injection Simulation Results from FEHM for the Bighorn Dolomite
Injection Interval 392 ft, Porosity 8% , Relative Permeability 5 md,
Injection Rate 31.68kg/s, 1 MT/year

CO2 Injection Results from FEHM for the Bighorn Dolomite, Shute Creek

Injection Rate 32 kg/s, Phi 8%, K 5 md, after 10 Year Injection

Property color key

P Units: Unknown

XY units: meters

Z units: feet

Z exag: 3.28084

CO2 Injection Results from FEHM for the Bighorn Dolomite, Shute Creek

Injection Rate 32 kg/s, Phi 8%, K 5 md, after 50 Year Injection

Property color key

P Units: Unknown

XY units: meters

Z units: feet

Z exag: 3.28084

CO2 Injection Results from FEHM for the Bighorn Dolomite, Shute Creek

Injection Rate 32 kg/s, Phi 8%, K 5 md, 50 Years Post -Injection

Property color key

P Units: Unknown

XY units: meters

Z units: feet

Z exag: 3.28084

CO2 Injection Results from FEHM for the Bighorn Dolomite, Shute Creek

Injection Rate 32 kg/s, Phi 8%, K 5 md, after 50 Year Injection

Property color key

P Units: Unknown

XY units: meters
Z units: feet
Z exag: 1.67979

CO2 Injection Simulation Results from FEHM for the Bighorn Dolomite, La Barge Platform
Injection Interval 392 ft, Porosity 5% , Relative Permeability 1 md,
Injection Rate 47 kg/s, 1.5 MT/year

CO2 Injection Simulation Results from FEHM for the Madison Limestone
Injection Interval 400 ft, Porosity 5%, Relative Permeability 1 md,
Injection Rate 19 kg/s, 0.6 MT/year

CO2 Injection Simulation Results from FEHM for the Madison Limestone
Injection Interval 400 ft, Porosity 5%, Relative Permeability 1 md,
Injection Rate 31.7 kg/s, 1 MT/year

CO₂ Injection Simulation Results from FEHM for the Madison Limestone
Injection Interval 400 ft, Porosity 10%, Relative Permeability 5 md,
Injection Rate 19 kg/s, 0.6 MT/year

CO₂ Injection Simulation Results from FEHM for the Madison Limestone
Injection Interval 400 ft, Porosity 10%, Relative Permeability 5 md,
Injection Rate 31.7 kg/s, 1 MT/year

CO2 Injection Results from FEHM for the Madison Limestone, Shute Creek

Injection Rate 32 kg/s, Phi 5%, K 1 md, after 10 Year Injection

Property color key

P Units: Unknown

XY units: meters

Z units: feet

Z exag: 3.28084

CO2 Injection Results from FEHM for the Madison Limestone, Shute Creek

Injection Rate 32 kg/s, Phi 5%, K 1 md, after 50 Year Injection

Property color key

P Units: Unknown

XY units: meters

Z units: feet

Z exag: 3.28084

CO2 Injection Results from FEHM for the Madison Limestone, Shute Creek

Injection Rate 32 kg/s, Phi 5%, K 1 md, 50 Years Post-Injection

Property color key

P Units: Unknown

XY units: meters

Z units: feet

Z exag: 3.28084

CO2 Injection Results from FEHM for the Madison Limestone, Shute Creek

Injection Rate 32 kg/s, Phi 5%, K 1 md, after 50 Year Injection

Property color key

P Units: Unknown

XY units: meters
Z units: feet
Z exag: 1.34383

C02 Injection Simulation Results from FEHM for the Weber Sandstone
Injection Interval 400 ft, Porosity 5% , Relative Permeability 1 md,
Injection Rate 19 kg/s, 0.6 MT/year

CO2 Injection Simulation Results from FEHM for the Weber Sandstone
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Injection Rate 19 kg/s, 0.6 MT/year

CO2 Injection Simulation Results from FEHM for the Weber Sandstone
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Injection Rate 31.7 kg/s, 1 MT/year

C02 Injection Simulation Results from FEHM for the Weber Sandstone
Injection Interval 400 ft, Porosity 10% , R relative Permeability 5 md,
Injection Rate 31.7 kg/s, 1 MT/year

CO2 Injection Results from FEHM for the Weber Sandstone, Shute Creek

Injection Rate 32 kg/s, Phi 10%, K 5 md, After 10 Year Injection

CO2 Injection Results from FEHM for the Weber Sandstone, Shute Creek
Injection Rate 32 kg/s, Phi 10%, K 5 md, After 50 Year Injection

CO2 Injection Results from FEHM for the Weber Sandstone, Shute Creek
Injection Rate 32 kg/s, Phi 10%, K 5 md, 50 Years Post-Injectionw

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BIBLIOGRAPHY

The following is a list of publications, abstracts, and presentations resulting from this funding. Please see the supplemental submission to this final report for copies of publications, where available.

Task 1:

Frost, C. D., and Jakle, A. C., 2010, Geologic carbon sequestration in Wyoming: prospects and progress: *Rocky Mountain Geology*, v. 45, p. 83–91.

Hamerlinck, J. D., Wyckoff, T. B., Oakleaf, J. R., and Polzer, P. L., 2010, Cyberinfrastructure for collaborative geologic carbon sequestration research: a conceptual model: *Rocky Mountain Geology*, v. 45, p. 163–180.

Hamerlinck, J., 2009, “Wyoming Energy Resources Information Clearinghouse,” online demonstration at the Western States Energy and Environment Symposium, Jackson, WY, 25 October, 2009.

Hamerlinck, J.D., Oakleaf, J.R., Polzer, P.L., and T.B. Wyckoff, 2009, Developing a Geospatially Enabled Cyberinfrastructure for Collaborative Carbon Sequestration Research, Poster presentation at 2009 ESRI International GIS Users Conference: July 13, San Diego, CA.

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Buss, A.R., J.D. Myers and D.K. Myers, 2009, The Site Well Catalog I: A Means for Managing Borehole Data for Sequestration Site Characterization, Selection and Permitting: Geological Society of America Annual Meeting, http://gsa.confex.com/gsa/2009AM/finalprogram/abstract_166278.htm.

Myers, J.D., A.R. Buss, and D.K. Myers, 2009, The Site Well Catalog II: Identifying requirements and Establishing Design Criteria, Geological Society of America Annual Meeting, http://gsa.confex.com/gsa/2009AM/finalprogram/abstract_166318.htm.

Task 3:

Frost, C., DeBruin, R., Jiao, J., Bentley, R., Li, S., Zhang, Y., 2009, Geologic CO₂ sequestration at the Moxa Arch, Wyoming, USA. Oral presentation, Eighth Annual Conference on Carbon Capture and Sequestration, May 4-7, 2009, Pittsburgh, PA.

Smith, M. S., Sharma, S., Wyckoff, T. B., and Frost, C. D., 2010, Baseline geochemical

characterization of potential receiving reservoirs for carbon dioxide in the Greater Green River Basin, Wyoming: *Rocky Mountain Geology*, v. 45, p. 95–114.

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Tasks 4 and 5:

Campbell-Stone, E., Lynds, R., Frost, C., Becker, T. P., and Diem, B., 2010, The Wyoming carbon underground storage project: geologic characterization of the Moxa Arch and Rock Springs Uplift: *Energy Procedia*, in press.

Lynds, R., Campbell-Stone, E., Becker, T. P., and Frost, C. D., A geologic deconstruction of one of the world's largest natural accumulations of CO₂: the stratigraphy, structure, and hydraulic connectivity within the Paleozoic of the Moxa Arch, southwestern Wyoming, U.S.A., in preparation.

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Kaszuba, J.P., A. Navarre-Sitchler, G. Thyne, and C. Chopping, “Supercritical CO₂ and sulfur in the Madison Limestone: A natural analogue in southwest Wyoming for geologic carbon-sulfur co-sequestration,” *Earth and Planetary Science Letters* (submitted).

Kaszuba, J.P., Navarre-Sitchler, A., Thyne, G., and C. Chopping, 2010, A natural analogue in southwest Wyoming for geologic carbon-sulfur co-sequestration: *Geochimica et Cosmochimica Acta*, v. 74, no. 11, p. A498.

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Navarre-Sitchler, A., J.P. Kaszuba, G. Thyne, T. Meuzelaar, and C. Chopping, The Madison Limestone as a natural analogue for long-term CO₂ storage in a carbonate reservoir, The manuscript is scheduled to be submitted to a journal in February 2011.

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Akbarabadi, M. and M. Piri, 2010, The effects of hysteresis and wetting on permanent geologic storage of CO₂: An experimental study of capillary trapping and relative permeability, Gordon Research Conference, Bates College, Lewiston, Maine, USA, July 11-16.

Akbarabadi, M. and M. Piri, 2010, The effects of hysteresis and wetting on permanent geologic storage of carbon dioxide: An experimental study of capillary trapping and relative permeability, International Advanced Coal Technologies Conference, Laramie, WY, USA, June 24.

Akbarabadi, M. and M. Piri, 2009, The Impact of Hysteresis on Permanent Storage of CO₂ in Deep Saline Aquifers, Wyoming Mining Association Convention, Laramie, WY, USA, June.

Akbarabadi, M. and M. Piri, 2009, The Impact of Hysteresis on Permanent Storage of CO₂ in Deep Saline Aquifers, UW-DOE-ExxonMobil CO₂ Sequestration Project Meeting, Laramie, WY, USA, March.

Piri, M. and M. Akbarabadi, 2010, Geologic sequestration of supercritical carbon dioxide: An experimental study of capillary trapping and relative permeability, AGU Fall Meeting, San Francisco, CA, USA, December 13-17.

Piri, M., 2010, Three-Phase Flow in Porous Media and Computed Tomography Research Laboratory, Enhanced Oil Recovery Institute, University of Wyoming, Laramie, WY, USA, June.

Piri, M., 2009 & 2010, Three-Phase Flow in Porous Media and Computed Tomography Research Laboratory, SPE Student Chapter, University of Wyoming, Laramie, WY, USA, September.

Task 8:

Mallick, S., Mukhopadhyay, P., Alvarado, V., 2009, Geophysical monitoring of carbon sequestered aquifers—a feasibility study. Poster presentation, Eighth Annual Conference on Carbon Capture & Sequestration, May 4-7, Pittsburgh, PA.

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Douglas, C., Furtado, F., Ginting, V., Mendes, M., Pereira, F., and Piri, M., 2010, On the development of a high-performance tool for the simulation of CO₂ injection into deep saline aquifers: *Rocky Mountain Geology*, v. 45, p. 151–161.

Ginting, V., A. Malqvist, M. Presho, 2010, A Novel Method for Solving Multiscale Elliptic Problems with Randomly Perturbed Data, *SIAM Multiscale Modeling and Simulation*, vol. 8, no. 3, pp. 977–996.

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Pereira, F., and Rahunathan, A., 2010, Numerical Simulation of Two-phase Flows on a GPU, In: Proceedings of 9th International Meeting, High Performance Computing for Computational Science (VECPAR 2010). Berkeley, CA.

Pereira, F., 2009, Multiphase Flows in Multiscale Porous Media. Event: Workshop in Computational Modeling, Federal University of Juiz de Fora, Juiz de Fora, Brazil, August 17-18, 2009 (invited).

Pereira, F., 2009, Computational Modeling of the Injection of CO₂ in Brine Aquifers. Event: Brazilian Applied Mathematics Meeting (CNMAC), Cuiabá, Brazil, September 8-11, 2009 (invited plenary presentation).

Presho, M., A. Malqvist, and V. Ginting, 2010, Density Estimation of Two-phase Flow with Multiscale and Randomly Perturbed Data, *Advances in Water Resources*, 33(9): 1130–1141.

Task 10:

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Zhang, L. and S. Li, "Local-scale acid gas simulation," Poster presentation, AGU annual meeting, December 2009.

Task 11:

Stauffer, P., Miller, T., Deng, H., Gable, C., Dai, Z., Jiao, Z., Surdam, R., Bentley, R., 2009, Numerical modeling of CO₂ sequestration in the Rock Springs Uplift, Wyoming. Poster presentation, Eighth Annual Conference on Carbon Capture & Sequestration, May 4-7, Pittsburgh, PA.

ABBREVIATIONS AND ACRONYMS

AGI	acid gas injection
AMG	algebraic multigrid
AoR	area of review
APD	Application for Permit to Drill
ARCUS	Arctic Research Consortium of the United States
AVO	amplitude-variation-with-offset
BHP	bottomhole pressure
CBM	coalbed methane
CCS	carbon capture and sequestration
CDF	cumulative distribution function
CI	cyberinfrastructure
CMP	multicore processor
CPU	central processing unit
DT	Sonic log
EOR	enhanced oil recovery
FEHM	Finite Element Heat and Mass Transfer
FIV	fluid inclusion volatiles
FPGA	field-programmable gate array
FY	fiscal year
GA	Genetic Algorithm
GCS	geological carbon sequestration
GHC	Gaussian Hierarchical Clustering
GPU	graphics processing unit
GR	Gamma Ray
GS	global sequestration
GSR	gas storage ratio
GtCO ₂	gigatons of carbon dioxide
GW	gigawatt
GWB	Geochemist's Workbench
HPC	high-performance computing
IEA	International Energy Agency
IGCC	integrated gasification combined cycle
LGR	local grid refinement
LQD	Low-Q Diffractometer
MMCFD	million cubic feet per day
MMV	measurement, monitoring, and verification
MtCO ₂	megatons of carbon dioxide
MPI	message passing interface library
MUSCL	Monotone Upstream-centered Schemes for Conservation Laws
MW	megawatt

NATCARB	National Carbon Sequestration Database and Geographic Information System
NSF	National Science Foundation
NSS	Nugget Storage Suite
ODE	ordinary differential equation
PI	principal investigator
SANS	using small angle neutron scattering
scCO ₂	supercritical carbon dioxide
SEM	scanning electron microscope
SMP	shared memory multiprocessor
SSOR	symmetric successive overrelaxation method
SSTVD	Sub-Sea True Vertical Depth
TACC	Texas Advanced Computing Center
TCF	trillion cubic feet
TDs	total depths
TDS	total dissolved solids
TIG	total injected gas
TPV	total pore volume
UIC	Underground Injection Control
UMFPACK	unsymmetric multifrontal sparse LU factorization package
UML	unified modeling language
USDW	underground source of drinking water
USGS	United States Geological Survey
UW	University of Wyoming
V _c	Clay Volume
VPS	vertical positioning system
WDEQ	Wyoming Department of Environmental Quality
WOGCC	Wyoming Oil and Gas Conservation Commission
WSGS	Wyoming State Geological Survey
WY-CUSP	Wyoming Carbon Underground Storage Project
WYDOT	Wyoming Department of Transportation
WYGISC	WYGISC
XRD	X-ray diffraction

PUBLISHED WORKS

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