Policy Analysis

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A System Model for Geologic Sequestration of Carbon Dioxide

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In this paper we describe CO_2—PENS, a comprehensive system-level computational model for performance assessment of geologic sequestration of CO_2. CO_2—PENS is designed to perform probabilistic simulations of CO_2 capture, transport, and injection in different geologic reservoirs. Additionally, the long-term fate of CO_2 injected in geologic formations, including possible migration out of the target reservoir, is simulated. The simulations sample from probability distributions for each uncertain parameter, leading to estimates of global uncertainty that accumulate through coupling of processes as the simulation time advances. Each underlying process in the system-level model is built as a module that can be modified as the simulation tool evolves toward more complex problems. This approach is essential in coupling processes that are governed by different sets of equations operating at different time-scales. We first explain the basic formulation of the system level model, briefly discuss the suite of process-level modules that are linked to the system level, and finally give an in-depth example that describes the system level coupling between an injection module and an economic module. The example shows how physics-based calculations of the number of wells required to inject a given amount of CO_2 and estimates of plume size can impact long-term sequestration costs.

Introduction

It is becoming abundantly clear that sharp increases in atmospheric CO_2 concentrations during the past 100 years are directly tied to human influences including the use of fossil fuels (*1, 2*). Recently the most comprehensive analyses using extensive data conclude that the current increases in average global temperature are likely a result of the increased concentrations of CO_2 and other greenhouse gases (*2*). One approach to mitigate excess anthropogenic CO_2 is to pump it into geologic formations, also known as geologic sequestration (*3, 4*). Geologic sequestration uses technology from the petroleum industry that has been effectively used to transport large quantities of naturally occurring subsurface CO_2 (e.g., as found in Colorado and New Mexico) through pipeline networks to oil fields where it is injected into reservoirs for enhanced oil recovery (EOR) (*5*). The EOR experience lends optimism to geologic sequestration, because much of the engineering experience necessary for transporting and injecting CO_2 at an industrial scale exists (*6*). Furthermore, CO_2-EOR projects have operated since the 1970s in or adjacent to population centers.

However, the issues involved with geologic sequestration are more complex than EOR operations. First, CO_2 storage in the context of EOR spans only a few decades whereas to be effective, sequestration requires CO_2 storage for hundreds to thousands of years (*3, 4*). Over such time frames, processes such as density-driven fingering and mineralization through water—rock—CO_2 interactions may become quite important (*7*). Second, the amount of CO_2 that will need to be sequestered is orders of magnitude larger than the amount currently being used in EOR projects. For example, US net emissions of CO_2 in 2003 were approximately 5841 Tg/yr (Mt/yr) whereas total integrated EOR operations in the US used only ~35 Tg/yr (*8*). Given a CO_2 injection density of approximately 600 kg/m^3 (*9*), each 5800 Tg of CO_2 would require a pore volume of approximately 7 km^3. Assuming an average porosity of 20%, no residual water saturation, and an average reservoir thickness of 50 m, the footprint required to sequester this volume of CO_2 would be 700 km^2, or an area 26 km × 26 km on the surface. Third, while EOR involves injection of CO_2 into a reservoir whose pressure has been depleted due to oil production, the largest capacity for geologic sequestration is in deep saline reservoirs for which pore pressures have not been reduced by fluid production. Finally, EOR is done in existing oil reservoirs that typically have been extensively characterized and have production histories. In contrast, geologic sequestration would likely involve sites other than oil/gas reservoirs for which characterization information may be limited.

These unique aspects of geologic CO_2 sequestration underscore the need for approaches and tools that allow the feasibility and safety of potential storage sites to be evaluated systematically prior to large-scale deployment of the technology. In other geologic waste repositories, long-term behavior is predicted using a numerical model of a given site that includes all relevant features, events, and processes. This modeling exercise is known as a performance assessment (PA). The PA should incorporate algorithms based on fundamental physics and chemistry over a large range of spatial and temporal scales and include uncertainties in parameters (*4, 10*). Although initial attempts at creating such comprehensive PA models for CO_2 sequestration have been made, none to date have included the necessary degree of process-level flexibility within a stochastic modeling framework on par with similar models developed for the geologic storage of dangerous waste (*11*).

In this paper we describe the development of a comprehensive computational model that can be used to perform performance assessments of geologic CO_2 sequestration sites. The model, called CO_2—PENS (Predicting Engineered Natural Systems), is designed to link together many different processes (e.g., subsurface injection of CO_2, density fingering, and atmospheric mixing) required in analysis of long-term storage of CO_2 in geologic media (*4, 12*). Because the required processes operate using different sets of governing equations at different time-scales, such coupling is not easily done in standard physics-based simulators (*4*). Additionally, a powerful stochastic framework at the system-level allows CO_2—PENS to be used to explore complex interactions between large numbers of uncertain variables and can help to differentiate the likely performance of potential seques-

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tration sites. In the following sections, we provide an overview of the system model, briefly discuss the current set of process-level modules, and provide an example of the development of a reduced complexity injection and plume growth module that is coupled to an economic module which includes costs associated with drilling wells, installing field distribution pipelines, and long-term maintenance. In this example we calculate the number of injectors required and estimate the likely plume size for two potential sequestration reservoirs in the context of sequestration site selection. The economic module is then used to show how competing physically based requirements can affect overall costs and provide vital additional data to assist in site selection.

Model Description

System Level Model Description. CO_2−PENS is a system model that links together process-level modules that describe the entire CO_2 sequestration pathway, starting from capture at a power plant and following the CO_2 through pipelines to the injection site and into the storage reservoir. After injection, simulation of CO_2 migration continues through the subsurface where it may mineralize, dissolve into brine, or react with wellbore casing or grout. CO_2 that may escape from the storage reservoir is followed along pathways that lead back toward the surface, including leaking wellbores and faults.

The system level of the CO_2−PENS model manages global variables (e.g., CO_2 mass balance, CO_2 mass flow rate, and costs) and is being developed using GoldSim (*13*). GoldSim was chosen for several reasons. First, GoldSim is capable of passing variables into and out of modules including the reservoir simulators used to perform complex three-dimensional heat and mass transport calculations. Second, GoldSim contains libraries of probability distribution functions and has the capability to use correlated variables that can be used to perform multiple realization stochastic analyses in a Monte−Carlo approach. GoldSim also has the ability to store simulation data from large numbers of realizations and generate statistics on global probability distributions. In large system analysis it is vital to have easily reproducible simulations that can fulfill strict quality assurance requirements, and GoldSim permits each run to be saved in a single action, including all input data and results from Monte−Carlo analysis. Finally, GoldSim has built in GUI functions that allow the developer to quickly assemble interactive screens for user input.

Process-Level Description. The innovative approach that we are taking in building CO_2−PENS is to create all of the process-level modules outside of GoldSim, so that the modules can be created by collaborators in any programming language. For example, CO_2−PENS includes a wellbore leakage module created by the Princeton-CMI group (*14*). Modules can also be created from commercially available software called from within CO_2−PENS. Because of the large number of variables involved in system level calculations, some process-level calculations need to be abstracted or simplified to reduce simulation times and permit execution of multiple realizations necessary to gather statistical measures of overall system behavior. Both simple and complex process-level calculations are linked via dynamic link libraries (DLLs). These DLLs are used to perform such varied calculations as development of a three-dimensional CO_2 plume during injection, total flux through a leaking wellbore, fracture flow, mineral formation and dissolution, and atmospheric mixing. Finally, the modular design allows new process-level pathways to be incorporated in the system as our understanding advances. As development of CO_2−PENS continues, the library of modules for physical process models will grow, providing the users flexibility in creating diverse set of simulations. More detailed descriptions of the process modules currently available in CO_2−PENS can be found in Viswanathan et al. (*15*).

During site selection and preliminary performance assessment process, it is important to understand the following: (1) approximately how many wells will be needed to inject a given amount of CO_2, (2) the likely extent of the injected CO_2 plume in the target zone, and (3) the cost associated with distributing and injecting CO_2 at a given site. We next outline in detail the development and use of a process-level injection module that can be used in conjunction with our economic module to address these questions.

Process-Level Injection Module. This section describes the development of a reduced complexity model to calculate the number of wells required to inject a given mass of CO_2 into a target reservoir based on the temperature and pressure of the reservoir and the maximum safe injection pressure. In addition to calculating injection rate, the module uses another analytical solution to calculate the CO_2 plume extent and an estimate of the amount of CO_2 that may spill over the reservoir boundaries.

Our reduced complexity injection calculations are predicated on the idea that the analytical solution contains the basic form of the solution for injection into a reservoir; however it cannot capture the details of the true multiphase solution with a relative permeability function. We show that for a given pressure, temperature, injection pressure, and relative permeability function, the regression of the analytical results to a full numerical solution is fairly linear over one standard deviation in reservoir properties of permeability and porosity. This allows use of the regression slope to tune the analytical solution to capture the general trend of the results from fully coupled numerical injection simulations. The major benefit of this approach is that the analytical solution can be solved orders of magnitude more rapidly than the numerical simulations.

The reduced complexity injection module is intended for use during the initial site selection calculations when preliminary estimates on quantities, such as reservoir capacity and number of wells required, etc., are made. For assessing performance of specific sites, this module can be replaced by a module that can perform complex calculations employing full multiphase physics in three-dimensional reservoir simulators.

The reduced complexity injection module uses an infinite radius reservoir solution with a defined pressure drop between the well and the far-field. The parameters passed from the GoldSim system model into the injection module are listed in Table 1. During a given time step, the fluid properties are assumed constant and the reservoir properties are assumed to be homogeneous and isotropic. The solution for the injection capacity (Q tons/day) of a well ((*16*); eq 2.33) is given by:

$$Q = \frac{(P_w - P_{\mathrm{inf}})4\pi kB}{[\ln(t_{\mathrm{d}}) + 0.80907]\mu_{\mathrm{c}}} \tag{1}$$

whereP_{w} is the pressure at the wellbore, P_{inf} is the far-field reservoir pressure, k is the average reservoir permeability, B is the thickness of the formation, and μ_{c} is the viscosity of the CO_2. Dimensionless time is given by:

$$t_{\mathrm{d}} = \frac{kt}{\varphi \mu_{\mathrm{c}} c r_{\mathrm{w}}^2} \tag{2}$$

where ϕ is porosity, r_{w} is the well bore radius, and t is time. The number of injection wells is calculated by dividing the amount of CO_2 needed to be sequestered by Q. During the initial time step, the total CO_2 from the power plant is divided evenly among the required injectors. Often, as injection continues, the injectivity of wells decreases due to changes

TABLE 1. Input and Output Parameters of the Injection Module

input parameters	output parameters
simulation time	number of wells affected
time step size	number of wells injecting
initial reservoir pressure	number of new wells
far-field reservoir pressure	number of wells shut off
reservoir thickness = B	number of existing wells used this time step
reservoir porosity = ϕ	number of new wells used this time step
available existing wells	total area of the injected CO_2
reservoir area	total volume of the injected CO_2
CO_2 viscosity	amount of CO_2 exceeding reservoir capacity at each time step
water viscosity	
CO_2 density	
vertical leakage + total reservoir CO_2 mineralization	
tuning parameter	

in the far-field pressure. In our injectivity module this decay is captured by a simple function that reduces the injectivity at each subsequent time step by a constant fraction. When the injectivity is reduced to below some nominal value (e.g., 10 tons per day), a well is shut off. The module keeps track of the total injectivity at any time step and determines whether additional wells are needed to inject given amount of CO_2. The injection module keeps track of the number of active and shut-off wells at any given time step and passes this information back to the system-level where it can be analyzed.

Plume Extent. To calculate the CO_2 plume thickness, b, as a function of radius and time (r and t) we use the analytical expression given by Nordbotten et al. (*17*):

$$b(r, t) = B\left(\frac{1}{\lambda_c - \lambda_w}\right)\left(\sqrt{\frac{\lambda_c \lambda_w V_t}{\varphi \pi B r^2}} - \lambda_w\right) \qquad (3)$$

where λ_c and λ_w are the CO_2 and water mobilities calculated as the ratio of phase relative permeability to phase viscosity, and V_t is the total available volume of CO_2. Equation 3 can be solved for the maximum plume radius, r, at a given time by setting the plume thickness, b, to zero as:

$$r = \sqrt{\frac{\lambda_c V_t}{\lambda_w \varphi \pi B}} \qquad (4)$$

In CO_2−PENS, the reservoir area is less than one would calculate for the entire amount of CO_2 injected at the site because V_t is reduced by the sum of leakage from the reservoir and includes contributions from caprock leakage, leakage through old boreholes, and mineralization within the reservoir. In the current injection module, the total volume injected in all wells is summed and this volume is used to calculate the plume extent. This is a very rough estimate of plume extent, because each injection well would have its own conical plume which may have a significantly different total extent than our assumption of putting all the injected CO_2 into a single borehole. However, this method gives an idea of relative differences in total subsurface area required for different sequestration sites.

Reservoir Capacity. To calculate reservoir capacity, at each time step the calculated plume extent is compared to the reservoir radius and any excess CO_2 is tracked as exceeded reservoir capacity. Exceeded reservoir capacity is approximated by calculating the difference between the plume volume at the maximum radius and the radius of the reservoir. The CO_2 in excess of reservoir capacity is returned to the system-level and used to calculate lateral release from the reservoir.

Interactions between the Injection Module and the System Model. Table 1 lists the variables that are passed from the injection module back into the CO_2−PENS system-level model. The injection module differentiates between the pre-existing wells which can be converted to injector (e.g., wells that may be available in depleted oil reservoirs) and new wells that will be drilled for a saline reservoir, because the costs of drilling a new well are calculated differently from the costs for refurbishing an existing well.

The calculated exceeded reservoir capacity becomes a source of CO_2 escaping from the reservoir. Any CO_2 that escapes the reservoir is then available for transport toward either (1) the atmosphere (as in the case of risk due to exposure to high levels of CO_2), (2) an overlying aquifer or oil reservoir (as in the case of economic risk to a resource), or (3) a separate section of a large, continuous reservoir that has been subdivided into storage parcels operated by different companies. Other pathways for leakage that are available in the model include leakage through the cap-rock, faults, or wellbores (*15*).

The area of the plume is used to estimate the number of existing wells that will be exposed to injected CO_2. These may be poorly completed and/or abandoned wells. The injection module keeps track of wellbore exposure time which can be used to estimate probability of wellbore failure. We are currently developing a method to determine the probability of failure of pre-existing boreholes based on how long cement has been exposed to CO_2 (*15, 18*).

Example Simulation

We present an example demonstrating how the reduced complexity injection module is used to compare two different target reservoirs based on the probability distributions for the number of injection wells needed to inject CO_2 from a 1 GW power plant. We also show how estimates of the total reservoir area occupied by the injected CO_2 plume are made. The results of the injection module are coupled to an economic module and are used to calculate the cost per ton to distribute and inject CO_2 for 50 years. The power plant is assumed to use coal with 74% carbon, with heat content 3.28e7 J/kg_{carbon}, and have an efficiency of 38%. Using these values and a CO_2 capture efficiency of 80%, the total amount of CO_2 that has to be sequestered is 20 kt/day. For the analysis presented below, the decay function for the wells is set to 1.0, so that the initial injection rate is maintained at a constant value.

The first case is a cold, shallow reservoir while the second case is a hot, deep reservoir, following the work of Nordbotten et al. (*17*) and consistent with analysis presented in Viswanathan et al. (*15*). The shallow reservoir is at 1 km depth and 35 °C while the deep reservoir is at 3 km depth and 155 °C. For both cases we assume that rock properties of the reservoirs are the same. The range of reservoir rock permeability and porosity used are based on reservoir measurements but are not meant to represent any specific reservoir. Rock permeability follows a log-normal distribution with a mean of 1×10^{-14} m^2 and a standard deviation of 5×10^{-15} m^2. Rock porosity also follows a log-normal distribution with a mean of 0.15 and a standard deviation of 0.02. As described in the Supporting Information, the maximum injection pressure before vertical hydrofracture occurs is equal to the minimum principle stress, leading to a maximum injection pressure of 15 MPa for the shallow case and 45 MPa for the deep case. The two cases are summarized in Table 2, which also includes the relevant fluid properties.

Preliminary analysis based on the fluid properties can give insight into which reservoir may have more injectivity

TABLE 2. Example Injectivity Simulations

	cold + shallow	hot + deep
depth	1	3 km
pressure	10	30 MPa
temperature	35	155 C
max injection pressure	15	45 MPa
water density	999	929 kg/m3
CO_2 density	714	479 kg/m3
water viscosity	7.2×10^{-4}	1.8×10^{-4} Pa s
CO_2 viscosity	5.8×10^{-5}	4.0×10^{-5} Pa s

for the given CO_2 amount. The conductivity of a rock to a given fluid is a function of the relative permeability (k_r), the viscosity, and density (ρ) of the fluid as

$$K = k_r \rho g / \pi \quad (5)$$

The properties of CO_2 vary significantly between these two cases, with the deeper case having 70% lower viscosity while the shallower fluid has 1.5 times higher density. Thus, as a first-order approximation, one would expect CO_2 at the deeper injection site to have nearly the same CO_2 mobility as at the shallower site. However, the situation is complicated by the fact that the injected CO_2 must displace water, whose properties also change with pressure and temperature (PT). The viscosity change in water is approximately a factor of 4 with very little change in density. Thus, more CO_2 should be able to be injected into the hot−deep case. Relative permeability functions that describe the ability of CO_2 and water to flow at partial saturation further complicate the analysis, and flow calculations involving these functions generally require numerical solution methods (*19*).

2-D Radial Calculations. The Los Alamos multiphase porous flow simulator, FEHM (*20*), has recently been updated to perform simulation of CO_2 injection and migration in saline reservoirs. We use FEHM to generate 2-D radial solutions for injection into the two reservoirs described in this example.

The domain used for the 2-D calculations is composed of a radial grid that is 5 km long and 30 m thick. The radial node spacing increases from 1.0 m at the interior to more than 400 m at 5 km, while vertical node spacing is constant at 3 m. Because of the radial symmetry, the borehole radius is 0.5 m and is given a high permeability to allow injection along the entire 30 m of the reservoir. The 2-D radial calculations use a simple linear relative permeability curve with residual water and CO_2 set to 0.1. Relative permeability must be defined in the regions on either side of the residual saturation values because dissolution of one phase into the other can lead to saturations below residual, analogous to evaporation drying a water wet rock below the laboratory measured value for residual water saturation. The far-field boundary at 5 km is held at a constant pressure, equal to the initial reservoir pressure. Therefore, the simulations effectively mimic a classic nine-spot injector−producer system where the producing wells are used to lower the reservoir pressure and allow continued fluid injection. Without the drain on the system, injection of CO_2 causes the total reservoir pressure to quickly exceed the minimum principle stress. The results from the 2-D radial simulations are then used to tune the reduced complexity analytical solution (eq 1). More details on the numerical/analytical tuning are available in Supporting Information.

Economic Module. Coupled to the injection module is an economic module that has been designed to show differences in the costs associated with the two cases. Because the two cases were designed explicitly to show differences in a small subset of a total CO_2 sequestration system directly related to previous published material (*17*), we also confine

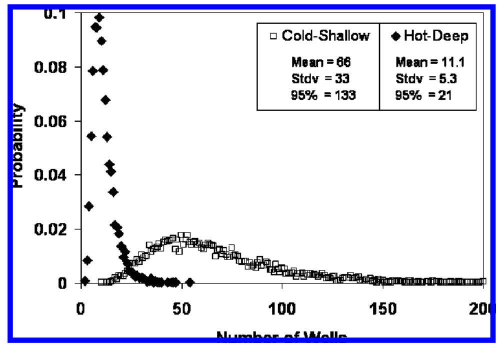

FIGURE 1. Results for the two test cases showing the number of boreholes required to inject the CO_2 from a 1000 MW power plant. In each case 5000 realizations were run with values of permeability and porosity randomly chosen from the input parameter distributions.

the scope of the economic analysis to details that are pertinent to differentiating between these two cases. The obvious first difference in the cases is the depth of drilling, where the cold−shallow and hot−deep cases require 1 km and 3 km drilling depths, respectively. Limited data exist on drilling wells specifically designed for injection of CO_2, and we assume that drilling costs will be comparable to those of oil wells drilled on-shore in the United States. We use published data on well completion costs from the Joint Association Survey (JAS) of the American Petroleum Institute to generate a polynomial function that is used to calculate drilling completion costs per meter based on the total depth of drilling (*21*). Second, because the two cases result in significantly different numbers of wells required to inject the same mass of CO_2 as a function of time, we include an analysis of the costs associated with the pipelines required to distribute the CO_2 around a given field site. We also include estimated maintenance costs associated with both the injection boreholes and the field distribution pipelines. In this analysis, we assume that for both cases, the initial capital costs (e.g., drilling wells and buying pipeline) will be amortized over a 10-year period. However, maintenance costs must be included for the lifetime of the injection scenario (50 years). Thus, each year the two different cases will have different combined costs. To allow a consistent basis for cost comparison, we use a present value (PV) integration that returns all future costs to their present day dollar equivalents before summing to calculate total costs. We further assume that the sites have no pre-existing wells so that all wells must be newly drilled. More details of the economic analysis, including equations, figures, and additional references, can be found as Supporting Information.

Results and Discussion

CO_2−PENS is run using the tuned analytical injection solution for 5000 realizations for the cold−shallow and hot−deep cases. Because we want to show very clearly the interactions of a few select parts of the system model, we do not include any leakage in these cases. For each of these simulations the porosity, permeability, and reservoir thickness were sampled from the distributions discussed above using an efficient Latin hypercube sampling approach. The stochastic sampling leads to a distribution of results for each case, shown in Figure 1. Note that the hot−deep case requires approximately 1/6 the number of injection wells as the cold−shallow case. This result is mainly caused by the hot−deep case having lower water viscosity and a higher injection pressure gradient.

The primary reason for using the reduced complexity model in this example is to reduce simulation times and to allow more of the parameter space to be sampled. The reduced complexity approach reduces the time required for

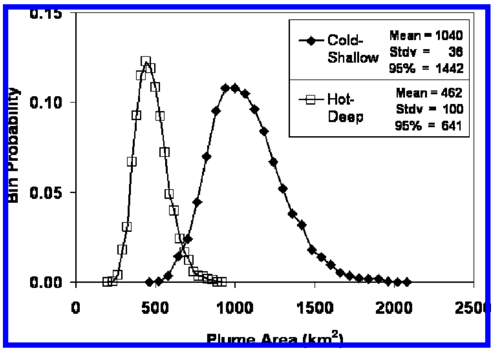

FIGURE 2. Results for the two test cases showing the area of the CO_2 plume after 50 years of injection. In each case 5000 realizations were run with values of permeability, porosity, and reservoir thickness randomly chosen from the input parameter distributions. Bin probability is the percent of the 5000 realizations found in a given bin used to create the histogram. The bin sizes are different for the two cases to allow the data to be plotted on the same figure.

5000 realizations from more than 4400 min when using FEHM to less than 40 min using CO_2–PENS. Such reductions in computing time for a given process-level model will become much more important when multiple number of processes will need to be coupled in a full performance assessment or risk analysis.

We next present differences in plume area required to contain the volume of injected CO_2 for the two cases. The plume area is calculated from eq 4. Figure 2 shows histograms for 5000 realizations split into 10 km^2 bins. An initial guess would generally lead one to assume that the hot–deep reservoir would require a larger area to contain the plume because the density of CO_2 is lower at the higher temperatures in the deeper system. However, eq 4 also includes the square root of the ratio of the CO_2 mobility ratio to the water mobility ratio, both of which are inverse functions of viscosity. Therefore, the maximum plume radius is directly proportional to the square root of the ratio of water viscosity to CO_2 viscosity. The quantity of interest, evaluated at the injection temperature and pressure, becomes:

$$r \propto \sqrt{\frac{u_w}{u_c \rho_c}} \tag{6}$$

For the hot–deep case, this value is 0.073, while for the cold–shallow case this value is 0.109, meaning that the cold–shallow case should have a larger plume area by a factor of approximately $(1.5)^2 = 2.25$. The numerical analysis confirms that the mean area of the cold–shallow plume is larger than the mean area of the hot–deep plume, and the ratio of the means is indeed equal to 2.25, confirming the validity of the reduced complexity stochastic approach.

The results presented in Figures 1 and 2, as noted in Nordbotten et al. (*17*), are both of great importance to the analysis of sequestration sites. The number of wells needed as well as their distribution can both be important variables in the decision making process for CO_2 sequestration site selection. Similarly, the size of a plume after 50 years of injection will also help to differentiate injection sites. In the cases presented, the fact that the cold–shallow injection site requires more than twice the areal footprint to contain the plume could easily be a decisive factor in siting a sequestration project. For example, operators may be given a limited areal extent of a larger permeable horizon in which to inject, and spillover from this area could result in fines or payments to owners of adjacent parcels. In the example presented, an operator would require a mean footprint with a radius of approximately 18 km for the cold–shallow case versus a footprint with a radius of only about 12 km for the hot–deep case. Understanding the probability distribution of reservoir areas that could be impacted by an injection operation will therefore be vital to calculations of risk for any sequestration sites. Additionally, the area calculations impact other leakage estimates for any site because as the plume grows, there is higher probability that leaking boreholes, faults, or gaps in the caprock may be encountered. Leakage from existing boreholes would be more of a concern in the cold–shallow case because the there are many more existing wells in the depth range of 1 km.

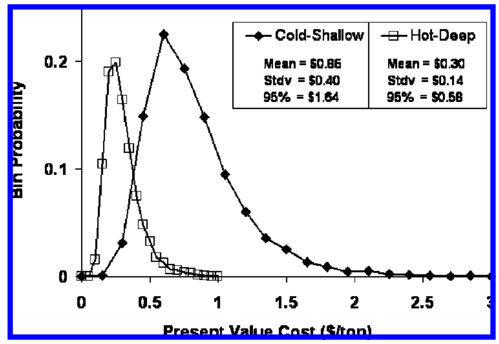

FIGURE 3. Present value cost per ton associated with wells and local pipelines. Bin probability is the percent of the 5000 realizations found in a given bin used to create the histogram. The bin sizes are different for the two cases to allow the data to be plotted on the same figure.

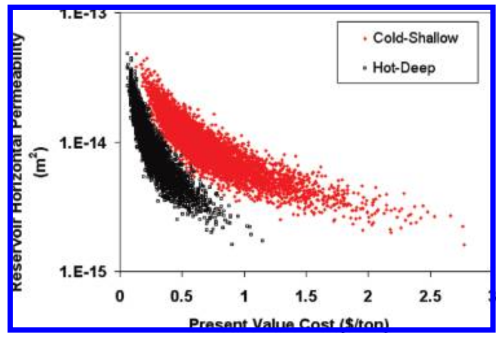

FIGURE 4. Multivariate correlation plot showing correlation between PV cost per ton and the reservoir horizontal permeability.

The results from the coupled economic module are summarized in Figure 3 which presents the cost per ton, in present value dollars, to drill the wells, install pipeline to connect the wells, and maintain the system for 50 years. This figure shows that the hot–deep scenario leads to a much lower total cost than the cold–shallow case. Although both cases have a mean well below a likely current acceptable field injection costs of \$1.31 per ton CO_2 (*22*) (not including any capture or long-range transportation costs), the system level approach allows delineation of confidence intervals for different costs. The full economic analysis shows that there is a 7% probability that costs for the cold–shallow case could be above the acceptable cost, while the hot–deep case has less than a 0.1% risk of exceeding this value. Thus, by tying the economic module to the injection module through the system approach we have gained important insight into the coupled system.

Finally we present model results that highlight the power of system level approach to explore the underlying correlations between disparate variables from different modules. The correlation between the present value cost per ton and the reservoir horizontal permeability for the two cases is shown in Figure 4. Each realization for each case is plotted separately, showing the range of values spanned by the combined 10 000 realizations. In both cases, cost per ton is negatively correlated to reservoir horizontal permeability, with a correlation coefficient of −0.744 for both cases. Correlation statistics are a powerful tool in deciding which variables are of greater importance in a complex, multivariable simulation, and can be used to guide data collection to better constrain output from system level models such as CO_2−PENS.

Acknowledgments

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Supporting Information Available

Detailed description of the economic module that we used to perform the present value analysis. This material also contains additional references, equations, and figures that can be used to gain a more complete understanding of our approach. This material is available free of charge via the Internet at http://pubs.acs.org.

Literature Cited

(1) Friedlingstein, P; Solomon, S. Contributions of past and present human generations to committed warming caused by carbon dioxide. *Proc. Natl. Acad. Sci. U.S.A.* **2005**, *102*, 10832–10836.

(2) IPCC. *Climate change 2007: The physical sciences basis*; contribution of Working Group I to the fourth assessment report of the Intergovernmental Panel on Climate Change; approved at the 10th Session of Working Group I of the IPCC, Paris, 2007.

(3) Bachu, S. Sequestration of CO_2 in geological media: criteria and approach for site selection in response to climate change. *Energy Convers. Manage.* **2000**, *41*, 953–970.

(4) Metz, B.; Davidson, O.; de Coninck, H. C.; Loos, M.; Meyer, L. A. IPCC. *IPCC special report on carbon dioxide capture and storage*; prepared by Working Group III of the Intergovernmental Panel on Climate Change; Cambridge University, 2005.

(5) Pearce, J. M.; Holloway, S.; Wacker, H.; Nelis, M. K.; Rochelle, C.; Bateman, K. Natural occurrences as analogues for the geological disposal of carbon dioxide. *Energy Convers. Manage.* **1996**, *37*, 1123–1128.

(6) Stevens, S. H.; Fox, C. E.; Melzer, L. S. McElmo Dome and St. Johns natural CO2 deposits: Analogs for geologic sequestration. In *Greenhouse Gas Control Technologies*; Smith, A. Y., McMullan, P., Paulson, C. A. J., Eds.; CSIRO: Australia, 2001.

(7) Hellevang, H.; Aagaard, P.; Oelkers, E. H.; Kvamme, B. Can Dawsonite permanently trap CO_2? *Environ. Sci. Technol.* **2005**, *39*, 8281–8287.

(8) EPA. *Inventory of US Greenhouse Gas Emissions and Sinks: 1990–2005*; US EPA: Washington D.C., April 15, 2007.

(9) Brennan, S. T.; Burruss, R. C. Specific storage volumes: A useful tool for CO2 storage capacity assessment. *Nat. Resour. Res.* **2006**, *15* (3), 165–182.

(10) Robinson, B. A.; Li, C.; Ho, C. K. Performance assessment model development and analysis of radionuclide transport in the unsaturated zone, Yucca Mountain. *J. Contam. Hydrol.* **2003**, *62*−*63*, 249–268.

(11) LeNeveu, D. M. CQUESTRA, a risk and performance assessment code for geological sequestration of carbon dioxide. *Energy Convers. Manage.* **2008**, *49*, 32–46.

(12) Stauffer P. H.; Viswanathan H. S.; Pawar R. J.; Klasky M. L.; Guthrie G. D. CO_2−PENS a CO_2 sequestration system model supporting risk-based decisions. In Proceedings of the 16th International Conference on Computational Methods in Water Resources; Copenhagen, Denmark, June 19−22, 2006.

(13) *Goldsim User's Guide*; Goldsim Technology Group: Issaquah, WA, 2006.

(14) Nordbotten, J. M.; Kavetski, D.; Celia, M. A.; Bachu, S. A model for CO_2 leakage including multiple geological layers and multiple leaky wells. *Envrion. Sci. Technol.* **2009**, *43*, 743–749.

(15) Viswanathan, H. S.; Pawar, R. J.; Stauffer, P. H.; Kaszuba, J. P.; Carey, J. W.; Olsen, S. C.; Keating, G. N.; Kavestski, D.; Guthrie, G. D. Development of a hybrid process and system model for the assessment of wellbore leakage at a geologic CO_2 sequestration site. *Environ. Sci. Technol.* **2008**, *42*, 7280–7286.

(16) Matthews, C. S.; Russel D. G. Pressure buildup and flow tests in wells. *Monographs of the Society of Petroleum Engineers*; Society of Petroleum Engineers: New York, 1967; Vol. 1.

(17) Nordbotten, J. M.; Celia, M. A.; Bachu, S. Injection and storage of CO2 in deep saline aquifers: Analytical solution for CO_2 plume evolution during injection. *Transport Porous Med.* **2005**, *58*, 339–360.

(18) Carey, J. W.; Lichtner, P. C. Calcium silicate hydrate (C-S-H) solid solution model applied to cement degradation using the continuum reactive transport model FLOTRAN. In *Transport properties and concrete quality: materials science of concrete, special volume*; Mobasher, B., Skalny, J.; Eds.; American Ceramic Society, John Wiley & Sons, 2007; pp 73−106.

(19) Bennion, B.; Bachu, S. Relative permeability characteristics for supercritical CO_2 displacing waters in a variety of potential sequestration zones in the Western Canada Sedimentary Basin. Presented at the Annual Technical Conference and Exhibition, Dallas, TX,Oct 9−12, 2005.

(20) Zyvoloski, G. A.; Robinson, B. A.; Dash, Z. V.; Trease, L. L. *Summary of the models and methods for the FEHM application-A finite-element heat- and mass-transfer code*; Los Alamos National Laboratory Report, LA-13307-MS; 1997.

(21) American Petroleum Institute (API). *2004 Joint Association Survey (JAS) on drilling costs*; Washington D.C., 2006.

(22) Lucier, A.; Zobak, M. Assessing the economic feasibility of regional deep saline aquifer CO2 injection and storage: A geomechanics-based workflow applied to the Rose Run sandstone in Eastern Ohio, USA. *Int. J. Greenhouse Gas Control* **2008**, *2*, 230–247.

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