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Development of a Hybrid Process and System Model for the Assessment of Wellbore Leakage at a Geologic CO_2 Sequestration Site

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Sequestration of CO_2 in geologic reservoirs is one of the promising technologies currently being explored to mitigate anthropogenic CO_2 emissions. Large-scale deployment of geologic sequestration will require seals with a cumulative area amounting to hundreds of square kilometers per year and will require a large number of sequestration sites. We are developing a system-level model, CO_2-PENS, that will predict the overall performance of sequestration systems while taking into account various processes associated with different parts of a sequestration operation, from the power plant to sequestration reservoirs to the accessible environment. The adaptability of CO_2-PENS promotes application to a wide variety of sites, and its level of complexity can be increased as detailed site information becomes available. The model CO_2-PENS utilizes a science-based-prediction approach by integrating information from process-level laboratory experiments, field experiments/observations, and process-level numerical modeling. The use of coupled process models in the system model of CO_2-PENS provides insights into the emergent behavior of aggregate processes that could not be obtained by using individual process models. We illustrate the utility of the concept by incorporating geologic and wellbore data into a synthetic, depleted oil reservoir. In this sequestration scenario, we assess the fate of CO_2 via wellbore release and resulting impacts of CO_2 to a shallow aquifer and release to the atmosphere.

1. Introduction

Anthropogenic emissions of greenhouse gases, such as CO_2 and methane, have been attributed to climate change (*1*). To mitigate climate change, a combination of strategies will need to be employed to reduce these emissions. Pacala and Socolow (*2*) describe a portfolio of existing options or "wedges" that can be used to limit atmospheric concentrations of CO_2. One of these options includes the capture and geologic sequestration of CO_2. Since fossil fuels are expected to make up a large component of the world's energy supply in the near future, geologic sequestration of CO_2 will likely need to play a role in reducing CO_2 emissions into the atmosphere (*2*). The technology for injecting CO_2 into deep geological formations already exists and has been applied for enhanced oil recovery and acid gas disposal (*3*). However, for geologic sequestration to become a viable option, sites must be assessed to determine if they can store much larger amounts of CO_2 over much greater periods of time.

Factors such as leakage need to be considered in any comprehensive study of a sequestration site. Because free-phase CO_2 is less dense than formation water, the potential for upward leakage in a geologic reservoir is enhanced due to CO_2 buoyancy (*3*). Leakage may occur through geological features, such as fractures and faults. Existing wells at sequestration sites also have the potential for leakage, since they often penetrate deep into the formation (*3*). Assessment of long-term viability of CO_2 storage is a complex function of CO_2–reservoir interactions, leakage pathways, and risks. It requires integrating theory, field observation, experiment, and simulation over a wide range of spatial and temporal scales, all of which involve substantial uncertainties. Existing risk and performance assessment models for geologic sequestration often rely on simplified analytical models for simulating processes and have been designed for a specific site (*1, 4*). A detailed model that incorporates all of the underlying physical, chemical, and geological processes is not computationally feasible. Instead, a methodology is required that abstracts these processes into a manageable, system-level model that is robust enough to apply to a wide variety of potential sequestration sites (*1*).

We are developing a system-level model, CO_2-PENS (predicting engineered natural systems) that links a high-level system model to models of physical and chemical processes of varying levels of complexity. The model CO_2-PENS has been designed to incorporate CO_2 injection and sequestration knowledge from the petroleum industry; principles of risk assessment, economics, and process-level experiments; and models for the physical and chemical interactions of CO_2 in a geologic reservoir (*5, 6*). When complete and fully validated, this system-level model is designed to assess the viability of sequestering CO_2 at specific sites as part of a formal, quantitative, site-specific risk assessment taking into account economic, environmental, health, and safety risks.

The use of coupled process models in the system model of CO_2-PENS provides insights into the emergent behavior of aggregate processes that could not be obtained by using individual models. In this manuscript, we illustrate the utility of the concept by assessing the fate of CO_2 via wellbore release to a shallow aquifer and the atmosphere.

2. CO_2-PENS Model

The model CO_2-PENS is a hybrid of system- and process-level models for simulating the following CO_2 pathways: (1) capture from a power plant, (2) transport to the injection site, (3) injection into geologic reservoirs, (4) potential leakage from the reservoir, and (5) migration of escaped CO_2 either to the resources (oil/gas reservoirs, freshwater aquifers, etc.) near the primary reservoir or into the atmosphere near the ground surface. The model is still being developed, and several of the modules are being constructed. Stauffer et al. (*5*) describes the injection module and provides a schematic

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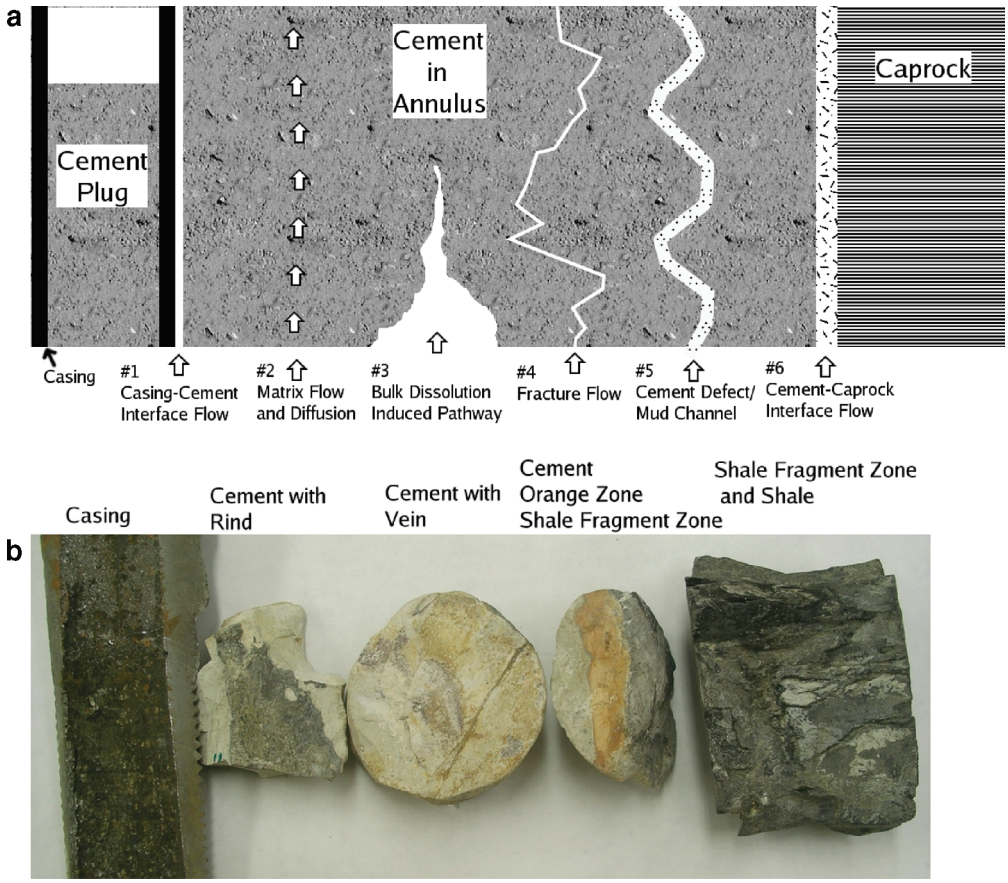

FIGURE 1. (a) Schematic of wellbore leakage processes and (b) samples from SACROC core.

of the overall structure of the CO_2-PENS model. The focus of the work in this manuscript is wellbore leakage and the impact of this leakage on a shallow aquifer and atmospheric CO_2 concentration near the site. We use a wellbore leak and an atmospheric dispersion process model to illustrate the utility of the hybrid system- and process-level model approach by incorporating geologic and wellbore details into a synthetic depleted oil reservoir and then perform calculations for a leakage scenario.

The model CO_2-PENS has been developed so that it can be quickly modified by adding new processes and interactions. A benefit of the modular design is that collaborators from around the world can write DLLs (dynamically linked libraries) that can be called from CO_2-PENS. For example, in this manuscript, the wellbore release model was developed by the Princeton-Carbon Mitigation Initiative (CMI) group. We have linked this model to the atmospheric model that was developed at Los Alamos National Laboratory. As CO_2-PENS becomes more widely used, there will be a library of modules available for each physical process model, allowing users to have flexibility in creating simulations.

We envision that CO_2-PENS will initially be used as a screening tool that can help to quickly decide the viability of sequestration sites. As site selection proceeds, CO_2-PENS can be adapted to a specific site, and its level of complexity can be increased as detailed site-specific information becomes available. For example, during final site selection, a user may require extensive 3-D representation in a numerical reservoir simulator, but during initial site selection, simplified analytical models may be sufficient to quickly differentiate between acceptable and unacceptable sites.

3. Wellbore Release and Groundwater Impact Modules

3.1. Processes that Contribute to Wellbore Failure. Wellbores represent one of the potential leakage pathways for CO_2 from the reservoir by the simple fact that they normally penetrate the caprock seal (*3*, *7*). Developing models for wellbore leakage is challenging because numerous parameters and uncertainties need to be assessed and because the processes and factors that determine wellbore integrity are not yet completely understood. A key parameter required to predict wellbore leakage is the effective wellbore cement permeability, which is difficult to estimate (*5*, *7*, *8*). A thorough characterization of the numerous wells that may exist at a site (which may number in the hundreds or thousands) is not feasible. Therefore, a leakage model must be stochastic and be based on probability distributions of possible failure mechanisms to include uncertainties associated with wellbore cement and other well completion parameters. We have used observations from a recent study of wellbore cements at Scurry Area Capital Reef Operations Committee (SACROC) (*9*) along with other general observations at SACROC to develop a first attempt at quantifying a probability distribution function (PDF) that can be used in a wellbore release model.

Normally, wellbore completion involves the placement of cement (typically ordinary Portland cement) in the annular region between the steel casing and the surrounding rock to isolate the production (and injection) zone from overlying strata (Figure 1a). Once cured, hydrated Portland cement has a very low permeability ($\sim 10^{-9}$ Darcy), effectively eliminating fluid flow through the cement matrix. A good bond with the steel casing and the caprock would similarly ensure no flow of fluids from the reservoir along these interfaces. However, as noted by Gasda et al. (*10*), several broad factors might compromise the integrity of these wellbores. Figure 1a shows possible leakage pathways for CO_2 in the wellbore generated by a combination of mechanical (fracture formation, microannulus development) and chemical (CO_2-induced dissolution of cement) processes:

(1) flow at cement-casing interface, (2) flow through the cement matrix, (3) flow through pathways created by bulk chemical dissolution of the cement, (4) flow through fractures in the cement, (5) flow through an open annular region due to inadequate cement placement, and (6) flow at cement–caprock interface.

All of these leakage pathways can exist both outside the casing (as illustrated in Figure 1a) and inside the casing associated with cement plugs in abandoned wells. Some of these processes may be preexisting and could have occurred during drilling, completion, or abandonment.

CO_2 sequestration differs from typical oil-field scenarios because CO_2 (both supercritical CO_2 and CO_2-charged brine) can chemically react with Portland cement to corrode cement and to produce an assemblage of calcium carbonate and amorphous alumino–silica residue, potentially altering its hydrologic properties.

For any given well, a conceptual model of CO_2 leakage may be developed on the basis of a probability function for the significance of each of the above-mentioned processes. In the next section, we describe how many of the above-mentioned processes are considered in developing the cement permeability PDF.

3.2. Using Data from SACROC and Other Sites To Estimate PDFs. Determining the importance of individual processes requires a combination of experimental and theoretical information to identify key physical and chemical processes as well as validation of these phenomena with analogs from relevant field systems. Fortunately, there are two types of CO_2 sequestration analogs that have a multidecade history of CO_2 operations: natural CO_2 reservoirs and CO_2-enhanced oil recovery (CO_2-EOR) operations. Carey et al. (*9*) describe a core of cement extracted from a 55-year-old well with 30 years of CO_2 exposure during CO_2-EOR operation at the SACROC Unit in west Texas. A key finding from the study was that Portland cement can survive for 30 years in a CO_2-rich environment and can continue to maintain an adequate hydrologic barrier to fluid flow.

The SACROC cement samples did show evidence of CO_2 interactions along the cement–casing and cement–caprock interfaces. Figure 1b shows a cross section of samples, including the casing, cement, and shale–caprock, collected 3 m above the reservoir–caprock contact. A black deposit of calcium carbonate along the casing–cement interface appears to fill this microannular region (Figure 1b). The cement contains fractures filled with calcium carbonate. The samples also show extensive carbonation of the cement adjacent to the shale (orange region), resulting in the complete conversion of parts of the cement to an assemblage of calcium carbonate and amorphous alumino–silica residue. The CO_2 causing this reaction apparently migrated up the cement–caprock interface utilizing a pathway through a porous filter cake residue (*9*).

These observations indicate that at least for one well at SACROC, processes 2 and 3 (matrix flow and flow-through pathways created by bulk cement dissolution) were not important. Rather, the interfaces defined in processes 1, 4, and 6 are the most important flow pathways for CO_2 or CO_2-charged brine. Carey et al. (*9*) were not able to quantify the flux of CO_2 necessary to produce the carbonation features in the cement. However, they note that both the fractures within the cement and the annular region at the casing–cement interface appear to be filled with calcium carbonate, suggesting that at SACROC, precipitation of calcium carbonate may self-limit flow for these processes over time. The evidence at the cement–caprock interface was ambiguous as to whether porosity had increased or decreased as a result of CO_2 movement.

The results of analysis of SACROC samples can be used to develop a first attempt at a probability-based model for

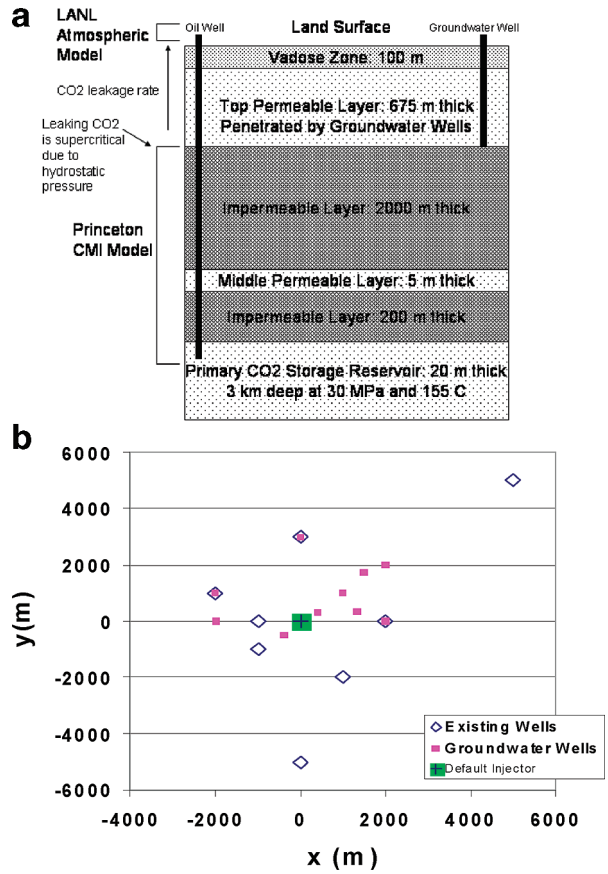

FIGURE 2. (a) Hypothetical reservoir cross section and (b) location of existing deep wellbores and shallow groundwater wells (top view).

CO_2 leakage. Information on details of well construction and completion (such as constituents of cement used) is very sparse, especially for the older wells. Most of the records are not available electronically. As a first step, therefore, we used the age of the well as a proxy for its integrity (or probability of wellbore failure), with the assumption that standard materials and techniques were used at various time intervals during the period of oil development in the Permian Basin (see Bachu and Watson (*11*) for other potential correlations between well attributes and performance). Next, we examined the relative importance of six leakage pathways (Figure 2a) and constructed a PDF for cement permeability using the knowledge gained from SACROC samples.

Pathway 1: A microannulus along the casing–cement interface is probable because of pressure and thermal stresses that occur during wellbore operations. The potential for CO_2 flow along the casing–cement interface is governed by the effective width of the interface. We assume that wells with a long history (e.g., > 5 years) of operation have a higher probability of having a microannulus at the casing–cement interface. However, exposure to CO_2 can lead to self-sealing of the microannulus through carbonate deposition for narrow, weakly transmissive widths (e.g., < 1 mm (*9*)). For larger widths, CO_2 flow could be significant. On the basis of the limited available data, we used transmissive widths of 5 mm as an approximate upper bound estimate for the effective cement permeability of these wells. A cubic law relationship between aperture (b) and effective permeability (k) for parallel fractures suggested by Snow (*12*) was used to calculate effective permeability

$$k = \frac{b^3}{12} \tag{1}$$

(A permeability distribution for cement permeability along the microannulus is used in CO_2-PENS.)

Pathway 2: Matrix flow is not significant in good quality cement, although diffusion and reaction of CO_2 could eventually modify cement permeability. The matrix permeability of cements in new wells is on the order of 10^{-9} Darcy, whereas at SACROC, it was found that in old wells, it is on the order of $\sim 10^{-4}$ Darcy (*9*). This greater value is still an effectively low matrix permeability, and with the extensive thickness of Portland cement in wellbore systems (1 to hundreds of meters), CO_2 flow through the matrix is not significant for timescales on the order of 1000 years. Preliminary studies indicate that cement permeability may not change significantly due to cement−CO_2 reactions (*9, 12*). Therefore, this process can be neglected. (No PDF required.)

Pathway 3: Formation of pathways by bulk chemical dissolution of the cement is also unlikely to be significant because of the extensive thickness of Portland cement in wellbore systems and based on the observations of Carey et al. (*9, 13*). Although situations creating a steady flux of acidic, CO_2-rich brine against the cement would dissolve cement rapidly (*14*), the thickness of the cement is sufficient to maintain seal integrity for timescales on the order of 1000 years. (No PDF required.)

Pathway 4: Fractures in the cement are probable because of cement exposure to pressure and thermal stress cycles in the wellbore environment. However, CO_2 flow through fractures in the cement may be self-limiting flow due to three-phase flow when CO_2 decompresses and, therefore, not significant (*15*). In the Carey et al. (*9*) study of SACROC, fractures through the cement matrix did occur but were filled with carbonate or calcium hydroxide, which indicates potential for some initial fluid flow but that carbonation ultimately limited the fluid flow. (No PDF required.)

Pathway 5: Inadequate cement placement depends on quality control used in completing and abandoning wells, with a probability that may be higher for very old wells. These problems can result in incomplete coverage of the annular region, incomplete displacement of drilling mud and formation of mud channels or sections of the wellbore without cement. The SACROC sample does not provide insight into this process. We propose a bimodal distribution that separates the wells into old wells that are assumed to be poorly completed and new wells that are properly completed. Research continues on the relationship between the age of a well and its probable completion and abandonment status (*11*). (For simplicity, we assume the wells in the simulation have been properly completed. No PDF required.)

Pathway 6: The existence of a porous interface between caprock and cement is probable because of the difficulty in forming a tight bond between cement and caprock either because of problems with the mechanical integrity of the caprock (e.g., swelling shale) or because of failure to adequately clear the drilling mud and rock debris (wall cake) during placement of the cement. CO_2 flow along the casing−caprock interface is governed by the effective width of the interface and is also related to permeability using a cubic law (Equation 1). As with the casing−cement microannulus, we assume that this pathway is more probable for older wells (>5 years). Cement bonds against shale are more likely to have wider interfaces. Exposure to CO_2 can lead to self-sealing of the interface if the flux of CO_2 is moderate. (A permeability distribution for cement permeability along the caprock−cement interface is used in CO_2-PENS.)

Pathways 1 and 6 need to be considered when constructing a PDF for wellbore permeability. As stated under pathway 1, exposure to CO_2 can lead to self-sealing for narrow, weakly transmissive widths (e.g., < 1 mm (*9*)). However, for larger widths, CO_2 flow could be significant. On the basis of the limited available data, we used transmissive widths of 5 mm as an approximate upper bound estimate for the effective cement permeability of these wells, which is a conservative estimate. To estimate the well permeability distribution, we assume that the effective aperture is 3 mm with a standard deviation of 2 mm.

We assume that in a block of well cement, we have parallel flow through one or more pathways up the block, and the flow rate is controlled by the pathway with the highest permeability. However, across the block with linear one-dimensional flow, the leakage rate is controlled by the lowest permeabilities in the distribution, resulting in harmonic averaging. The Princeton model requires the permeability along the leaky well to calculate flow from the well to the permeable layers. For the assumed aperture distribution, the mean effective permeability of 3×10^{-15} m^2 is calculated with a standard deviation of 1×10^{-15} m^2 for fractured cement. The permeability distribution is calculated using the cubic law (eq 1) and using harmonic averaging of the permeabilities. We assume a log-normal distribution for the wellbore permeability.

3.3. CO_2-PENS Wellbore Release Module. The effective permeability of wellbores (specifically, of wellbore cements), which were estimated as mentioned above, are used to predict the release of CO_2 through wellbores. The model CO_2-PENS has multiple options to estimate this process:

(1) The user can specify a distribution of leakage rates, assuming it is estimated by the user through means other than CO_2-PENS. The estimation method could include field observations, numerical simulation results, etc.

(2) The user can specify calculation of leakage rate through CO_2-PENS using the embedded continuum-scale, numerical simulator Finite Element Heat and Mass-Transfer (FEHM) (*16*). The model FEHM is a multiphase, multidimensional reservoir simulator. This option lets the user estimate the wellbore leakage rates by performing detailed numerical simulation of CO_2 leakage while taking into account critical processes, such as CO_2 phase change. These simulations are complex and require significant computational time. However, if other leakage pathways in addition to leakage associated with cement are required in the simulation, the FEHM option is required. For example, FEHM can simulate the "open hole" scenario as well as large fractures and cracks in the cement seal.

(3) Finally, the user can also specify calculation of leakage rate through a semianalytical model. We have embedded the wellbore release model developed by Princeton University (*3, 8*) in CO_2-PENS. The Princeton model can be used to simulate migration of CO_2 in a reservoir during the injection phase while taking into account potential release due to CO_2 release through any preexisting plugged wells. The model allows simulation of multiple stacked aquifers, which could be connected by plugged wellbores (single or multiple) intersecting them. The model assumes constant CO_2 density and is isothermal. It is not capable of incorporating complex processes, such as CO_2 phase change, but provides reasonable estimates of CO_2 release when such processes are not critical. It also does not currently simulate migration of CO_2 after injection is stopped. The biggest advantage of the semianalytical model is significant reduction of computational time while providing reasonable estimates of CO_2 leakage through wellbores. For system-level analyses, an efficient simulator is critical due to the large number of realizations required by the Monte Carlo approach.

Both FEHM and the Princeton model are embedded in CO_2-PENS as external DLLs, demonstrating the flexibility of CO_2-PENS to incorporate various external numerical simulators and process models. Notwithstanding the limitations

stated above, in the forthcoming case study, we have used the Princeton model to calculate wellbore leakage to illustrate CO_2-PENS.

4. Atmospheric Dispersion Model

We have developed a process level model to calculate changes in atmospheric CO_2 concentration using a mixed layer approximation for the atmospheric boundary layer. The model assumes diffuse, aereally uniform leaks and relatively flat topography. These assumptions are valid for many potential sequestration sites, provided that CO_2 does not propagate from the reservoir to the surface along discrete, localized paths, such as faults and wellbore blowouts. For many scenarios, localized wellbore and caprock leaks will be dispersed by the interceding stratigraphic layers between the CO_2 reservoir and the surface. However, it is assumed that leaks from fast pathways can be easily identified and remedied, but the diffuse leaks will be difficult to identify. The assumption of diffuse leaks will be relaxed in future versions once point source leaks are incorporated.

Other modeling options exist for evaluating the impact of leaks from a pollution standpoint; for example, plume dispersion models (*17*). These models are generally used for nondiffuse sources and make assumptions about certain atmospheric parameters; for example, wind velocity profiles and eddy diffusivities. Additionally, these parameters are often held constant in time, which overlooks the large diurnal and seasonal variability of atmospheric boundary layer mixing. It is also more difficult in the dispersion framework to include natural CO_2 sources that are key in characterizing background CO_2 variability, which in turn is important in monitoring and verification of sequestration integrity. For this reason, we have chosen a different approach.

For generality and computational efficiency, the surface impact process model is driven with archived data from the NASA Goddard Space Flight Center Global Modeling and Assimilation Office GEOS-1 model. The model GEOS-1 is a comprehensive atmospheric general circulation model (*18, 19*) with 2.0° latitude by 2.5° longitude horizontal spatial resolution. GEOS-1 is constrained using atmospheric data from rawinsonde reports; satellite retrievals; cloud-motion-derived winds; and aircraft, ship and rocketsonde reports. The GEOS-1 boundary layer data are available for the years 1985 to 1993 in 3 h intervals.

The GEOS-1 data allow us to abstract the complex and computationally costly boundary layer mixing calculation incorporating the effects of surface properties, including vegetation type, topography, and surface roughness, without having to directly link a complex numerical model for atmospheric mixing into CO_2-PENS. We use a lookup table of boundary layer heights that depends only on location and time of year based on the GEOS-1 data, making it extremely useful for quick estimates of the leak impact. The coarse resolution limits application of GEOS-1 data to areas with relatively flat topography.

5. Case Study

We demonstrate CO_2-PENS with a synthetic model simulating CO_2 injection in a depleted oil reservoir. Our hypothetical scenario consists of simulating the transport of CO_2 in a sequestration reservoir and migration out of the sequestration reservoir through plugged wellbores. In this example, we simulate migration of escaped CO_2 to an overlying aquifer as well as to the atmosphere. We do not calculate the ultimate impact on the aquifer, such as changes in water quality, but demonstrate how CO_2-PENS can be used to determine which groundwater wells will be impacted by escaped CO_2. We also calculate the change in local atmospheric changes in CO_2 concentrations, those immediately above the site. Standards for leakage from a sequestration site have not yet been established. In this example, we evaluate the site on the basis of an example regulatory limit. Specifically, we propose a limit in which no more than 0.01% of the total CO_2 is allowed to leave the primary sequestration reservoir.

TABLE 1. Key Parameters for CO_2-PENS Example

depth to bottom of sequestration reservoir	3 km
pressure in sequestration reservoir	30 MPa
temperature in sequestration reservoir	155 °C
max injection pressure	45 MPa
injection duration	50 years
injection rate	50 kg/s
simulation duration	50 years
number of Monte Carlo realizations	1000
mean of permeable layers porosity (normal distribution)	0.14
standard deviation of permeable layers porosity (normal distribution)	0.03
mean of effective aperture in cement (normal distribution)	3 mm
standard deviation of effective aperture in cement (normal distribution)	2 mm

The example consists of a sequestration target reservoir, impermeable and permeable layers in the saturated zone, a vadose zone, and the land surface (Figure 2a). CO_2 is injected through one injection well. We assume that the migration of CO_2 out of the sequestration reservoir takes place through eight plugged and abandoned wells in the primary target reservoir. We also assume that there are 10 shallow wells in the vicinity that penetrate only the topmost permeable layer (aquifer) and do not extend all the way to the sequestration target reservoir. Figure 2b provides locations of all the wells in the example. Note that a few groundwater wells are quite close to the injection wells. The key parameters used in the example are shown in Table 1. In the preceding sections, we described how these parameters were determined for use in the model.

To be a useful screening tool, CO_2-PENS must be able to quickly evaluate numerous scenarios at multiple sites. The underlying process models used by CO_2-PENS require numerous data inputs to accurately model a site, and these data may reside on a wide variety of databases. Tools specifically designed to interface with CO_2-PENS provide the means for data selection, abstraction, and preprocessing for use at the system level.

To obtain reasonable parameters and to showcase the GIS tools linked to CO_2-PENS, we assume that the reservoir permeability and porosity are similar to that of the SACROC Unit in the Permian basin in west Texas. The SACROC site is the second oldest continuously operated, CO_2-flood-enhanced oil recovery (EOR) operation in the world (*9, 20*). The GIS tools in CO_2-PENS were used to extract parameters from this oil reservoir. The first step was to create a spatial database for the geographical area of interest by combining multiple sources of information about the site. For example, the reservoir model was based on a detailed reservoir model of the site developed by Kinder Morgan CO_2 Company, LP's reservoir model of the SACROC Unit (*20*). Reservoir data characterizing the SACROC Unit, including rock properties such as porosity, permeability and thickness of reservoir formations and caprock were obtained from the SACROC reservoir database. In the absence of direct measurements, permeability was derived from porosity by using an empirical relationship appropriate for SACROC. For nonvuggy carbonates such as the SACROC unit, a simple power-law relationship maps variations in porosity (ϕ) to the appropriate permeability (k) in units of meters squared (*6*):

$$k = 10^{(3.77\varphi - 2.4)} \times 10^{-15}\ \mathrm{m}^2 \qquad (2)$$

From the area of interest, the individual measurements of formation porosity were generalized to represent the entire formation by developing a mean value and standard deviation weighted by the thicknesses of the individual formations. Using eq 2, the permeability was estimated, resulting in a mean of 1×10^{-16} m^2 and a standard deviation of 5×10^{-16} m^2. In the model, we assume a normal distribution for porosity and a log-normal distribution for permeability (Table 1).

The key input parameters for the Princeton wellbore release model are spatial extent, thickness, and permeability and porosity of the aquifer layers, as well as spatial locations of the injection and plugged wells and effective cement permeabilities for plugged wells (see Table 1 and Figure 2). For this case study, the mean of the formation permeability is slightly lower than the mean of the wellbore permeability. This is since we are assuming fairly large fracture apertures in the cement to be conservative. In addition, since we are using the Monte Carlo method, there is significant spread in both the wellbore and formation permeabilities for each realization. Therefore, for some realizations, the formation permeability is higher than the wellbore permeability. The model assumes homogeneous aquifer properties. In addition, the current version allows simulation of injection only through a single injector. For the example problem, the permeability and porosity of the aquifer layers were generated using the GIS tools as described above.

Once the statistics are developed for the input parameters, multiple Monte Carlo model realizations can be run by sampling the distributions of input parameter values within CO_2-PENS. To simulate migration of CO_2 through plugged wellbores, parameters such as wellbore cement permeability are needed. We determined the wellbore cement permeability values on the basis of field observations and laboratory experiment results as described in the wellbore model (Section 3.2).

We performed 1000 Monte Carlo simulations of CO_2 injection and wellbore leakage over a 50 year injection period. To ensure enough realizations we performed, we confirmed that the mean and standard deviations of the calculated CO_2 leakage did not change significantly after 100 realizations. The time-dependent amount of CO_2 in the different aquifers is shown in Figure 3. As expected, the topmost layer accumulates significantly less CO_2 than the underlying aquifer layer. This is because the flow of CO_2 to the overlying aquifer is moderated by the intervening layers (*5, 9*). The mean of the total amount of CO_2 that escapes the reservoir approaches 6×10^4 kg over 50 years, which is a small fraction ($\ll$0.01%/yr) of the injected CO_2 (8×10^{10} kg). Thus, in these calculations, CO_2-PENS predicts that CO_2 leakage from wellbores is much smaller than our proposed limit for the site (0.01%/yr).

The flow of CO_2 is further moderated by top permeable layer and the unsaturated zone before it reaches the surface. We assume an unsaturated zone of 100 m in this example. A comprehensive model for the unsaturated zone is still under development. To demonstrate the coupling between the wellbore release module and the atmospheric module, we assume that a fraction of the CO_2 that reaches the top layer reaches the surface. We discuss the implications of this assumption later in this section. A fraction of the leakage rate is output to the system model at each model time step and is then passed into the atmospheric model. The atmospheric model then takes higher resolution timesteps to simulate diurnal variations in the surface CO_2 concentrations.

One of the important elements of risk associated with CO_2 leakage through wellbores is to determine the ultimate impact of leaked CO_2. The predictions of time-dependent CO_2 mass accumulated in each aquifer in the model due to wellbore leakage are used to calculate the time-dependent CO_2 plume extent. This information is subsequently used by CO_2-PENS to calculate whether the leaked CO_2 plumes intersect any groundwater wells in the groundwater aquifer. Results of our example calculation show that of the 10 shallow wells, up to 3 wells will be impacted after 50 years of injection for the 1000 realizations. The radius of the leakage plumes ranged from 1 to 20 m. This information can be used to calculate the ultimate impact, such as change in groundwater chemistry due to the leaked CO_2 plume. Although it is not used in this example due to data limitations, we have recently linked the geochemical code PHREEQC (*21*) to CO_2-PENS. In future calculations, PHREEQC could be used to quantify the potential changes in groundwater chemistry due to leaked CO_2.

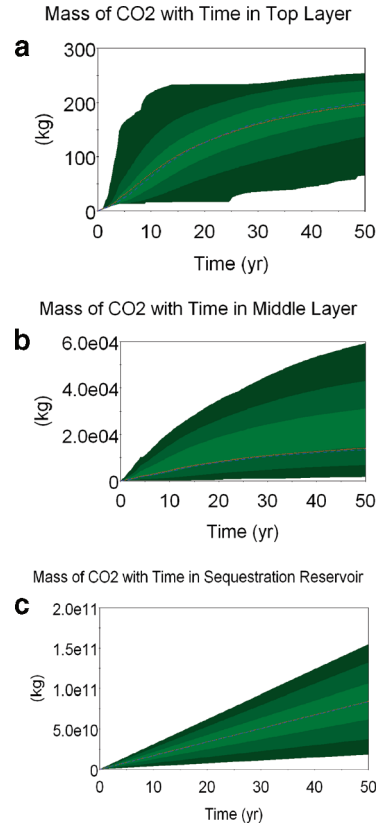

FIGURE 3. The average (dotted line), 1 standard deviation (light green), 2 standard deviation (darker green), and 3 standard deviation (dark green) CO_2 accumulations calculated for 1000 simulations of a 50 year injection period. (a) Amount of CO_2 accumulating in the top permeable layer due to wellbore leakage, (b) amount of CO_2 accumulating in the middle permeable layer due to wellbore leakage, and (c) amount of CO_2 accumulating in the sequestration reservoir (the sum of quantity injected minus amount released through wellbores).

The atmospheric mixing module is used to calculate changes in atmospheric CO_2 concentration produced by leakage estimated by the wellbore release model. One limitation of the Princeton analytical model is that it can not be used to predict migration of CO_2 to shallow regions, such as the vadose zone, where CO_2 will change phase from supercritical fluid to gas. In the example problem, we assume that 10% of the CO_2 leakage rate into the topmost permeable layer (as predicted by the Princeton model) is subsequently released to the atmosphere. Specifically, at each time step in the system model, the wellbore leakage model is queried and the leakage rate to the topmost permeable layer is predicted. This leakage rate is passed back to the system model, which then passes the leakage rate multiplied by the 10% attenuation factor to the atmospheric model. The atmospheric model subsequently takes the higher fidelity time steps required to capture diurnal variations of CO_2 concentration near the surface. We assume a 10% attenuation factor, since the unsaturated zone is expected to significantly

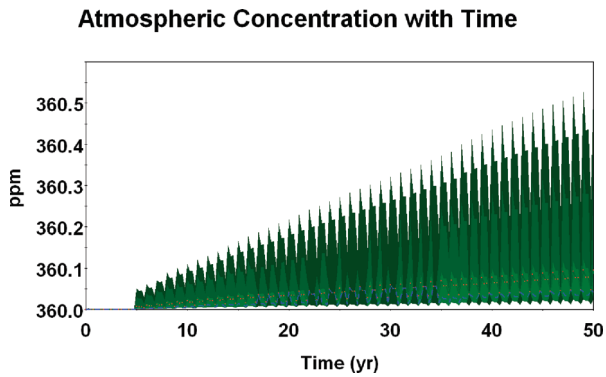

FIGURE 4. The average (dashed line), 1 standard deviation (light green), and 2 standard deviation (dark green) increase in predicted atmospheric CO_2 concentration due to wellbore leakage obtained from 100 Monte Carlo simulations. CO_2 concentrations include contributions both from biosphere and from a diffuse leak.

diminish the leakage rate of CO_2. Scoping calculations using FEHM have indicated significant attenuation. In the future, the attenuation factor will be quantitatively determined by coupling an unsaturated zone model to CO_2-PENS.

The model assumes a background CO_2 concentration of 360 ppm and a semiarid terrain. Figure 4a shows the seasonal variation in CO_2 concentrations. As can be seen from the figure, very little change in the atmospheric CO_2 concentration is predicted for the parameters used in this study. This is expected, since in this hypothetical scenario, in which <0.01% of the total mass of CO_2 injected is released, the atmospheric effects are minimal and presumably below detection. More data and a fully developed unsaturated zone model will be required to truly predict the performance of the site.

6. Discussion

The case study demonstrated the utility of linking the two embedded process modules, which have significantly different physics, and determining their interaction. For the hypothetical example used for this study, the predicted leakage resulted in small discrete plumes in close proximity to leaking wells as well as very small changes in local atmospheric CO_2 concentrations.

The modular structure of CO_2-PENS permits individual, interacting process models to contain detailed physics yet remain computationally efficient. The goal is to use CO_2-PENS as a screening tool that can help to quickly decide the suitability of sequestration sites as well as to use it as an assessment tool for determining performance of individual sites as detailed site-specific information becomes available. CO_2-PENS also provides a consistent platform for predicting the overall performance of different sites for comparing and evaluating multiple sites.

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