CO2-PENS: A CO_2 SEQUESTRATION SYSTEM MODEL SUPPORTING RISK-BASED DECISIONS

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ABSTRACT

The injection of CO_2 into geologic repositories for engineered storage (i.e., sequestration) will require a robust science-based decision framework that can address issues of risk, cost, and technical feasibility at all stages of the sequestration process. We describe such a framework that is being used to guide the development of a system model called CO_2-PENS. CO_2-PENS is capable of performing stochastic simulations to address uncertainty in different geologic sequestration scenarios, including injection into poorly characterized target reservoirs such as brine aquifers. Results and observations from process level laboratory & field experiments, numerical simulations, economic data, and risk theory are being used to support the system level model that will be the basis for decision making. Despite its early state of development, the current version of CO_2-PENS is already proving to be useful in showing complex interactions between the different components of the framework. CO_2-PENS also provides a consistent platform to document decisions made during the site selection, implementation, closure and post-closure periods.

1. INTRODUCTION

Increases in atmospheric CO_2 concentrations during the past 100 years have been tied to human influences including the use of fossil fuels (Vitousek et al., 1997; Friedlingstein and Solomon, 2005). Additionally, global temperatures and CO_2 concentrations are highly correlated over the past 300 MA (Retallack, 2002). Rapid changes in CO_2 and temperature have been shown to cause potentially troubling changes to the earth's climate and oceanic flow patterns (Wagner et al., 2002). In order to minimize the potential risk of climate change, research suggests that the most prudent option may be to minimize human CO_2 emissions (Caldeira et al., 2003). Hence, researchers around the world are currently studying a variety of approaches to reduce the amount of CO_2 that enters the atmosphere (Gale and Kaya, 2002; Yamasaki, 2003).

One promising approach to mitigate excess anthropogenic CO_2 is to sequester CO_2 into geologic formations (Holloway, 2001). Geologic sequestration uses technology from the petroleum industry that has been effectively used to transport CO_2 from naturally occurring deposits through extensive pipeline networks to oil fields where the CO_2 is injected in geologic reservoirs for enhanced oil recovery (EOR) (Pearce et al., 1996; Stevens et al., 2001). The EOR experience lends optimism to geologic sequestration, inasmuch as many CO_2-EOR projects are at a scale commensurate with what may be anticipated for sequestration, so much of the engineering experience necessary for transporting and injecting CO_2 at an industrial scale exists. Furthermore, CO_2-EOR projects have existed since the 1970s in or adjacent to communities, demonstrating that injection of CO_2 into geologic reservoirs may be accomplished safely. However, there are several major differences between EOR and geologic sequestration. CO_2 storage in the context of EOR spans only a few decades whereas sequestration may require CO_2 storage for hundreds to thousands of years (Bachu, 2003). The amount of CO_2 that will need to be sequestered may be orders of magnitude above the amount currently used in total for EOR projects. For example, US net emissions of CO_2 in 2003 were approximately 5841 Tg whereas EOR operations in the US use only ~30 Tg (EPA, 2005; Allis et al., 2001) in total. Experience with CO_2-EOR has been limited to only a few types of geologic environments, whereas the scale of sequestration will likely require exploitation of numerous geologic settings. Furthermore, EOR involves injection of CO_2 into a reservoir whose pressure has been depleted due to oil production, yet sequestration may involve injection into saline reservoirs for which pore pressures have not been reduced by fluid production. Finally, EOR is done in reservoirs with extensive databases on both the geology of the site as well as production histories; however, sequestration may involve sites for which similarly detailed information is unavailable. These unique aspects of sequestration underscore the need for new tools that allow safety and feasibility of potential storage sites to be evaluated systematically prior to the development of an extensive infrastructure.

Storage of CO_2 over long periods of time will rely on three processes in the engineered geologic system: impermeable seals, dissolution of CO_2 into native fluids such as brines and/or oil, and mineralization through water-rock-CO_2 interactions. The first of these will likely be the primary mode for CO_2 containment in the short term, therefore predicting the flux through these seals is of critical importance. Large-scale implementation of geologic storage in the U.S. will require seals with a cumulative area amounting to hundreds of square kilometers per year and will require a large number of storage sites. At conditions found in proposed repositories, where CO_2 density is near 800 kg/m^2, each 5800 Tg of CO_2 would require a pore volume of approximately 10 km^3. Assuming an average porosity of 20% and an average reservoir thickness of 50 m, a subsurface area of around 1000 km^2 would be required to sequester this volume of CO_2. These factors highlight the need to develop a robust and reliable method for evaluating the suitability of specific sites to ensure that they will perform to required goals. This method must incorporate fundamental physics and chemistry over a large range in scale (length & time) and must address uncertainties both in process level phenomena and reservoir properties. In addition, the method must link the fundamental scientific inputs to site-specific decisions such as suitability, monitoring strategy, potential impacts of CO_2 release, and probability that CO_2 release will be within acceptable limits.

In this paper we describe the development of CO_2-PENS (Predicting Engineered Natural Systems). CO_2-PENS is a systems model designed to include existing knowledge from industry, risk assessment methodology, economic theory, as well as process models that describe the physical and chemical interactions of CO_2 in a sequestration environment. We are developing CO2-PENS as a science-based decision framework that links a high-level systems model, which can be used to make predictions, to detailed models of physical and chemical processes. Process level models use field data and laboratory experiment observations to represent fundamental scientific processes over a wide variety of scales. Because of the large number of variables involved in a system level risk analysis, process level calculations may be abstracted or simplified to reduce simulation times and permit execution of multiple realizations necessary to gather statistical measures of overall system behavior. Finally, CO_2-PENS is designed to be robust so that it can be used to assess the viability of sequestering CO_2 at a range of sites, both within the US and around the world. In the following discussion we provide an overview of the system model, present a brief description of a single processes level model that is part of the system, and finally present a discussion of the issues involved in efficient implementation of such a complex system model for risk assessment.

2. CO_2 PENS : OVERVIEW

CO_2-PENS is an integrated systems/process model for simulating the fate of CO_2 beginning from sources such as a power plant to emplacement in storage reservoirs and finally, through pathways that may lead to potential long-term impacts such as interaction with overlying aquifers and petroleum reservoirs or return to the atmosphere. The model considers the transport of CO_2 along the following pathways: 1) capture from a power plant, 2) transport to the injection site, 3) injection into the geologic repository, 4) potential release from the repository (either through well bores, caprock, or lateral releases), 5) transport from the primary storage reservoir to other geologic reservoirs such as the saturated zone and unsaturated zones above the caprock and 6) release into the atmosphere and dispersion of CO_2 near the ground surface. Economic considerations of capture, injection, and monitoring are also being built into the model. Finally, the system model is designed with the intent of performing probabilistic risk analysis and we are developing tools and flexibility for a robust treatment of risk.

2.1 System Level Description

The system level of CO_2-PENS is used to manage global variables such as time, CO_2 mass balance, CO_2 flux, total risk, well statistics, and costs. GoldSim, a commercially available system modeling tool developed to simulate complex scenarios, is used as the platform on which the system level of CO_2-PENS is built. GoldSim was chosen for three primary reasons. First, GoldSim is capable of passing variables into and out of subprograms including the reservoir simulators used to perform complex 3-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. Finally, our team has extensive experience using GoldSim in Performance Assessment studies related to waste remediation.

Use of a system modeling platform is necessary because the CO_2 sequestration problem requires calculation of CO_2 transport and fate across a wide range of environments that use different physical and chemical models that can not be efficiently coupled in typical physics based models. For example, flow in pipelines and during injection into a reservoir may require very different physical models than those used to describe porous flow or chemical interactions with geologic formations. In addition to the physical and chemical interactions, the system level approach can also be used to track costs and risk factors. Another benefit of the system platform is the ability to store simulation data from large numbers of realizations and generate statistics on global probability distributions.

2.2 Process Level Description

Although the GoldSim system level platform is robust and can be used to perform limited 1-dimensional finite difference type calculations, it is not the ideal platform on which to perform complex flow and transport calculations. Thus we rely on process level simulators, linked to GoldSim via dynamic link libraries (DLLs), to perform such varied calculations as development of a 3-dimensional CO_2 plume during injection, total flux through a leaking wellbore, fracture flow, mineral formation and dissolution, and atmospheric mixing. The DLLs for different processes such as atmospheric mixing or subsurface transport can be developed as independent subprograms. Variables can be passed into and out of the process level subprograms (e.g. atmospheric mixing module and subsurface module) which can be modified or replaced by anyone working on the systems model.

CO_2-PENS can quickly adapt to changes in our knowledge base as field data, laboratory experiments and process models are refined. The model is being developed so that it can be modified quickly to add new processes and interactions. Identification of additional processes and interactions can come through use of the system model itself, through expert elicitation, and/or through independent investigations undertaken to support the decision making process. Another benefit of the modular design is that collaborators from around the world can write DLLs that can be called from GoldSim. As development and applicability of CO_2-PENS continues, it will result in a library of modules for physical process models, providing the users flexibility in creating diverse set of simulations. For example, during final site selection, a user may require extensive 3-dimensional representation in a reservoir simulator, while during initial site selection simplified radial 2-dimensional or 1-dimensioanl models may be sufficient to quickly differentiate between acceptable and unacceptable sites.

3. EXAMPLE PROCESS LEVEL MODULE

This section briefly describes one of the analytical models used to calculate injection of CO_2 into the subsurface, a simplified approach for determining plume extent, and an estimate of the amount of the plume that has spilled over the edge of the reservoir. The 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 physics of 3-dimensional, multi-phase fluid flow with reservoir simulators. We end this section with a discussion of the ways in which the values calculated in the injection module affect the behavior of the overall storage system.

3.1 Injection Module

The injection module uses an infinite radius reservoir solution with a defined pressure drop between the well screen 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 thickness of the reservoir is fixed, the physical properties of the injected fluid are assumed constant, and the reservoir properties are homogenous and isotropic. The injection capacity (Q tons/day) of a single well is calculated using an analytical solution to a radial boundary problem (e.g. Matthews and Russel, 1967). The number of wells necessary to inject the total amount of CO_2 coming from the power plant is then calculated by dividing the required total injection rate by the rate per well (Q). During the initial time step, the total mass of CO_2 from the power plant is divided evenly among the required injectors. The wells are given a simple decay function that reduces their capacity at each subsequent time step, requiring additional wells to be brought online. When capacity is reduced to below 10 tons per day, a well is shut off, potentially requiring a new well to be brought on line.

3.1.1 Plume extent

Reservoir plume extent (r) at a given time (t) is calculated by solving Equation 8 of Nordbotten et al. (2005) for plume thickness (b) = 0:

$$b(r,t) = B(\frac{1}{\lambda_c - \lambda_w})(\sqrt{\frac{\lambda_c \lambda_w V_t}{\phi \pi B r^2}} - \lambda_w) \qquad \text{eq. (1)}$$

where λ_c and λ_w are the CO_2 and water mobilities calculated as functions of viscosity and relative permeability, and V_t is the total available volume of CO_2. V_t is affected by the sum of vertical 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. The modular nature of the system model allows the injector subroutine to be easily modified and we plan to test model sensitivity to a more detailed analysis that includes individual areas associated with each injection well.

3.1.2 Reservoir capacity

At each time step the 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 GoldSim and used in calculations of release from the reservoir.

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	

3.1.3 Interactions between the Injection Module and the System Model

Table 1 lists the variables that are passed from the injector module back into the Goldsim system model. Existing wells, such as those that may be found in depleted oil reservoirs and new wells that must be drilled are differentiated because the costs of drilling a new well are calculated differently from the costs for refurbishing an existing well. Elsewhere in the system model, the user can base the well cost on parameters such as the depth of the well, the permeability of the formation, and rock types through which drilling will occur. Additionally, these costs can be based on distributions that incorporate the typical uncertainty associated with drilling. The value of exceeded reservoir capacity also affects the system model in that it provides a source of CO_2 escaping from the reservoir. Any CO_2 that escapes the reservoir is then available for transport through the subsurface toward the accessible environment. The accessible environment may include the atmosphere (as in the case of risk due to exposure to high levels of CO_2), or an overlying aquifer or oil reservoir (as in the case of economic risk to a resource). The area of the plume is very important for estimating the number of existing wells (including some that may be very poorly completed and abandoned) that are exposed to CO_2. We are currently developing a method to determine the probability of failure of preexisting boreholes based on exposure history. Another module that is under construction is the wellbore leakage module that will implement the analytical expressions of Nordbotten et al., (2004) into CO_2-PENS to calculate the amount of CO_2 that leaks upward from the reservoir through failed wellbores.

4. RISK ANALYSIS: CONCERNS AND DISCUSSION

This section provides a discussion of the technical hurdles that need to be overcome to create a useful risk analysis tool using the system model described above. Existing risk analysis techniques used for various industries cannot be easily modified to encompass the complexity of the CO_2 sequestration problem. The investigation of complex systems described by hundreds of parameters represents a significant computational effort even given today's available computational resources. For example, Ghosh (2006) has estimated the computational demands needed to sample the entire distribution of each uncertain parameter and using every combination of these parameters at a 1% interval would require in excess of 100^{330} runs. Given that computational times per run can range anywhere from minutes to hours, such an interrogation is largely impractical. Previous attempts to reduce the computational difficulty have led to the use of techniques such as Latin Hypercube sampling (LHS) (Helton, 1997). Although LHS ensures that the full range of each parameter will be sampled and propagated, it does not ensure that all combinations are tested. To improve the sampling and further explore the parameter space to gain additional insight we plan to utilize statistical techniques such as step wise regression analysis, K-S test, response surface methodology, Fourier amplitude sensitivity test, and differential analysis (Helton, 2003). Furthermore, an assessment of the correlations among input parameters should also assist in reducing the available combinations of parameters. The use of the Generalized Sensitivity Analysis Technique should also prove useful in reducing the number of computations required to achieve an acceptable analysis (Hornberger, 1981). This technique and other sensitivity analysis techniques may allow for a potential reduction in the dimensionality of the system and hence computational savings in estimating the probability of exceeding a given performance metric. Finally, the application of modified Kriging techniques in conjunction with LHS could also offer a potentially attractive means to address the computational challenges (Kleijnen, 2005).

5. CONCLUSIONS

CO_2-PENS is being developed as a platform that can be applied consistently at diverse sites as well as at different times with varying complexity at a single site. It can be initially used as a screening tool that can help to quickly decide on the suitability of sequestration sites. As site selection proceeds, CO_2-PENS can be modified for individual sites as detailed site specific information becomes available. It is very important to have a consistent platform for calculations of performance and risk at different sites to provide meaningful comparisons. Natural systems are inherently heterogeneous and complex, which necessitates incorporation of parameter uncertainty into our models using probability distributions for model inputs and outputs, as well as sampling the distributions in an efficient and effective manner that ensures that critical areas of the solution space are not overlooked.

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