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SYSTEM-LEVEL MODELING FOR GEOLOGICAL STORAGE OF CO_2

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ABSTRACT

One way to reduce the effects of anthropogenic greenhouse gases on climate is to inject carbon dioxide (CO_2) from industrial sources into deep geological formations such as brine formations or depleted oil or gas reservoirs. Research has and is being conducted to improve understanding of factors affecting particular aspects of geological CO_2 storage, such as performance, capacity, and health, safety and environmental (HSE) issues, as well as to lower the cost of CO_2 capture and related processes. However, there has been less emphasis to date on system-level analyses of geological CO_2 storage that consider geological, economic, and environmental issues by linking detailed representations of engineering components and associated economic models. The objective of this study is to develop a system-level model for geological CO_2 storage, including CO_2 capture and separation, compression, pipeline transportation to the storage site, and CO_2 injection. Within our system model we are incorporating detailed reservoir simulations of CO_2 injection and potential leakage with associated HSE effects. The platform of the system-level modeling is *GoldSim* [*GoldSim*, 2006]. The application of the system model is focused on evaluating the feasibility of carbon sequestration with enhanced gas recovery (CSEGR) in the Rio Vista region of California. The reservoir simulations are performed using a special module of the *TOUGH2* simulator, EOS7C, for multicomponent gas mixtures of methane and CO_2 or methane and nitrogen. Using this approach, the economic benefits of enhanced gas recovery can be directly weighed against the costs, risks, and benefits of CO_2 injection.

INTRODUCTION

Over the past several hundred years, atmospheric CO_2 concentration has increased steadily and has already risen to over 370 ppm. Experts believe that in order to avoid significant disruption of the climate system and ecosystems, CO_2 concentrations must be stabilized within the next several decades [*Benson*, 2005]. One approach to address this challenge is CO_2 capture and storage (CCS), i.e., injecting CO_2 from industrial sources into deep geological formations such as brine formations or depleted oil or gas reservoirs. The combination of CO_2 sequestration with enhanced gas recovery (CSEGR) makes carbon sequestration more economically feasible and attractive. CCS is a four step process including capture, compression, pipeline transport and underground injection [*Benson*, 2005]. Related technologies and engineering designs, including capture, transportation, and injection technologies, have been developed and are still being developed to make carbon sequestration both economically practical and environmentally safe [*Thomas and Kerr*, 2005]. Research has and is being conducted to improve understanding of factors affecting particular aspects of CCS, such as storage security and integrity, storage optimization, monitoring and verification, risk assessment and mitigation, and cost reduction. Because CO_2 injection has not yet been undertaken widely, thus limiting real field data, researchers rely on numerical simulation to understand CO_2 injection and migration. The numerical simulator *TOUGH2* has been widely used for this purpose [e.g., *Doughty and Pruess*, 2005; *Oldenburg et al.*, 2001; *Oldenburg and Unger*, 2005; *Oldenburg et al.*, 2004b; *Xu et al.*, 2006; *Zhang et al.*, 2005].

Although system-level studies of CCS exist [*Singh*, 2004], the emphasis to date has not been on system-level analyses that consider geological, economic, and environmental issues by linking detailed process models to representations of engineering components and associated economic models. To improve the overall system performance and understanding, a system-level model is needed where relevant processes can be simulated simultaneously, and different components of the system can interplay with each other. The objective of this study is to develop such a system-level model to evaluate the economics, environmental impacts, and risks of geological CO_2 storage under uncertain conditions. We present an application of this integrated model to carbon sequestration with enhanced gas recovery (CSEGR) at the Rio Vista field in California. In this application, the environmental benefit from CO_2 storage is considered assuming the existence of carbon credits.

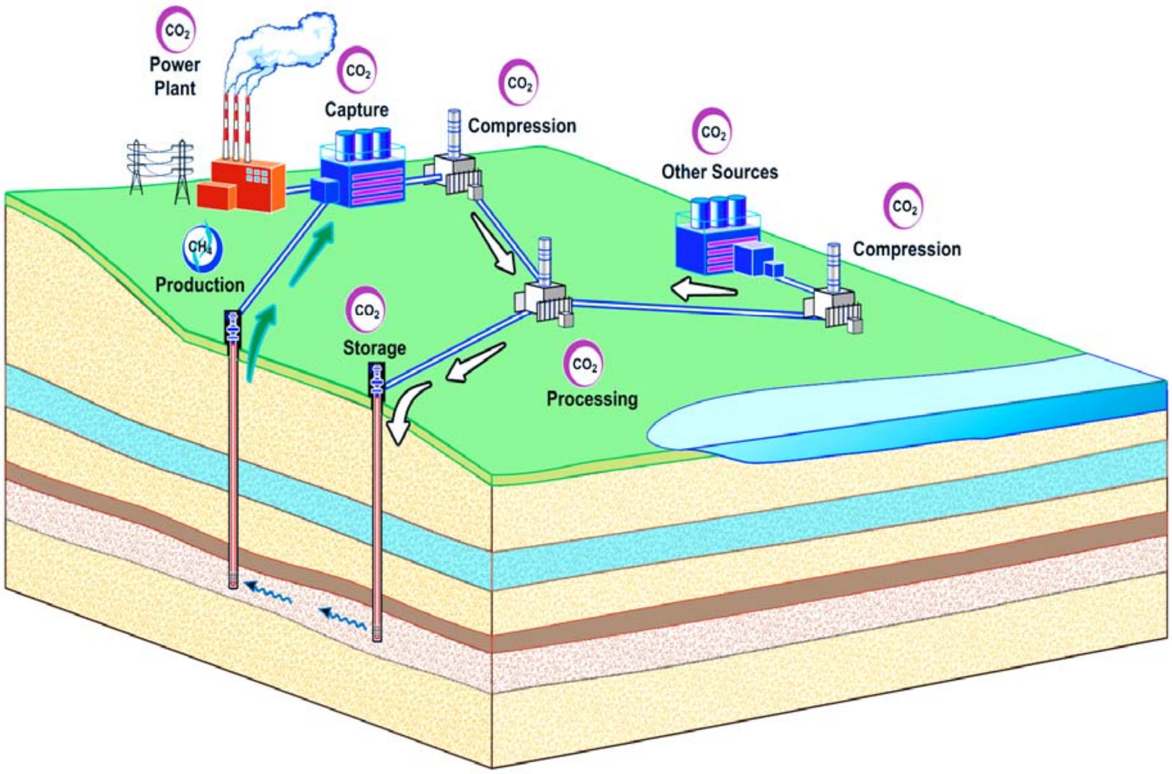

Figure 1. Schematic of a CO_2 capture and storage (CCS) system.

APPROACH

A schematic of the studied system is shown in Figure 1. In the system we consider the following components: CO_2 injection into a natural gas (methane, CH_4) reservoir, a natural gas power plant that burns CH_4, CO_2 capture and compression processes, and the transportation of captured CO_2 to the injection site. This system is complex and highly uncertain. Describing the various components of the system requires multidisciplinary expertise. A comprehensive feasibility study of such a system requires evaluations of economics and environmental risks. The economic feasibility of the system is affected by three uncertain factors: 1) economic factors including the capital costs and maintenance costs of the infrastructure, current and future prices for natural gas and electricity, interest rates, inflation rates, and CO_2 credits, etc., 2) uncertain decision factors, including the number of injection wells, monitoring wells, injection rates, etc., and 3) the so-called FEPs (Features, Events and Processes) [*Wildenborg et al.*, 2005]. Examples of FEPs are geological features (aquifer, existing leakage pathways, etc.), opening of abandoned wells due to corrosion, escape of CO_2 through faults or fractures caused by high injection pressure, and incidents (e.g., pipeline break). The failure of the CCS system insofar as health and safety are concerned is associated with the FEPs. One challenge of system modeling is to assess and quantify the subsequent health, safety and environmental (HSE) impact.

The complexity and interdependent nature of the studied system requires an integrated tool that is capable of coupling processes in different disciplines. A system-level model is a powerful tool to address these issues. With system-level modeling, the relevant discrete and continuous processes can be simulated simultaneously, and the system responses to different FEPs can be modeled correspondingly. The subsystems can interact with each other, either continuously or triggered at the time of a specific incident. It is thus possible to account for the uncertain factors in the different subsystems and to assess risks and evaluate the impact on the entire system. Finally, we can better understand the trade-offs between the economic benefits and the costs and risks of a particular venture such as CSEGR.

In system modeling, a hierarchical model is built using a top-down method. First, for CSEGR subsystems are identified and they are connected in order to track CO_2 and CH_4 flows. Then, components are identified and grouped into subsystems. Finally, potential FEPs are identified and corresponding feedbacks are incorporated in the system. The level of detail increases at lower levels of the system hierarchy. The advantage of this top-down method over a bottom-up method is that processes in different sectors can be well coupled, connected and feedbacks considered.

The system-level tool we use is *GoldSim* [2006], a flexible platform for visualizing and dynamically simulating different kinds of physical, financial or organizational systems. The reservoir simulation is performed using *TOUGH2* [*Pruess et al.*, 1999], a numerical simulator for non-isothermal flows of multicomponent, multiphase fluids in porous and fractured media. The linking of the system-level model to the physically based process model is a unique aspect of this study.

SYSTEM COMPONENTS

Figure 2 shows the highest level of subsystems of the model. The white arrows represent CO_2 flow. The green arrow represents methane production (profit). The grey arrow represents the flue gas (including CO_2), and the black arrows are information flows. Components considered in each of the subsystems are:

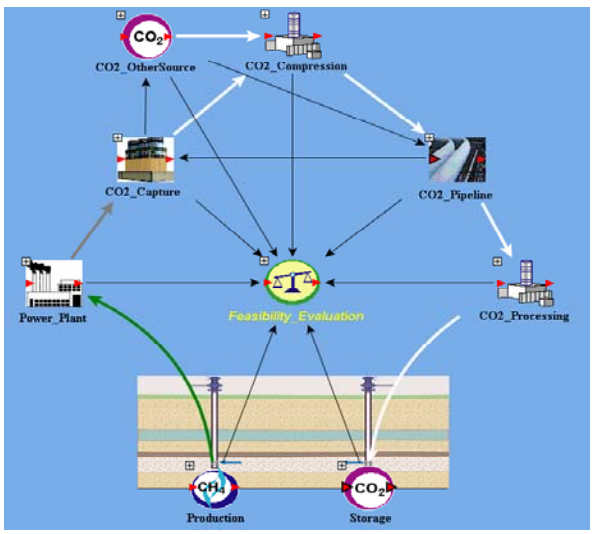

Figure 2. Top level of the system model.

- CO_2 Storage and Methane Production: *TOUGH2* simulation of CO_2 injection, inputs to *TOUGH2* and output for calculation of CH_4 production, possible CO_2 breakthrough and leakage, possible FEPs (fractures, corrosion) and their feedback to the system, and costs incurred in the subsystem.
- Power_Plant: the amount of CH_4 needed (either produced on-site or purchased from other suppliers), CH_4 heating value, power plant capacity and efficiency, flue gas produced, electricity generated, and related costs.
- CO_2_Capture: the amount of CO_2 captured from the power plant flue gas, the amount of CO_2 emitted to the atmosphere, and related costs.
- CO_2_OtherSource: the amount of CO_2 needed from other sources to meet the injection goal, and related costs.
- CO_2_Compression: compression of CO_2 to pipeline pressure, and related costs.
- CO_2_Pipeline: pipeline capacity, number of pipelines, probability of pipeline break, and related costs.
- CO_2_Processing: processing of CO_2 to injection pressure, and related costs.
- Feasibility_Evaluation: a financial model that processes all costs and profits from previous components, and environmental impact calculation.

PROCESS MODEL – TOUGH2 SIMULATION

TOUGH2 is compiled as a DLL (dynamic link library) application and linked to *GoldSim*. We use module EOS7C – the *TOUGH2* module for multicomponent gas mixtures in the systems methane-carbon dioxide (CH_4-CO_2) or methane-nitrogen (CH_4-N_2) with or without an aqueous phase and H_2O vapor [*Oldenburg et al.*, 2004]. Five or six components are considered: water, brine, non-condensible gas (CO_2 or N_2), gas tracer, methane, and optional heat. EOS7C does not model the transition to liquid or solid CO_2 conditions. The real gas properties module has options for Peng-Robinson, Redlich-Kwong, or Soave-Redlich-Kwong equations of state to calculate gas mixture density, enthalpy departure, and viscosity.

Table 1. Rock Properties in TOUGH2 Simulation

	CH_4 reservoir	Cap rock	Overburden	Aquifer	Fracture or abandoned well
Porosity	0.35	0.01	0.1	0.30	0.30
Permeability_X direction (m^2)	1.e-12	1.e-18	1.e-12	1.e-11	1e-11
Permeability_Z direction (m^2)	1.e-14	1.e-18	1.e-12	1.e-11	1e-11
Van Genuchten [1980] α (P_a^{-1})	8.4e-4	3.2e-7	5.1e-6	5.1e-5	5.1e-5
Van Genuchten [1980] *m*	0.2	0.457	0.457	0.457	0.457
Residual liquid saturation	0.25	0.3	0.3	0.3	0.05

Our reservoir simulation model is based on CSEGR at the Rio Vista field in California [*Oldenburg et al.*, 2001a]. The methane gas reservoir, with a thickness of 50 m, is located at a depth of 1450 m to 1500 m below ground surface. The cap rock above the gas reservoir is about 20 m thick. We assume there is an aquifer at a depth of about 700 m. There are 25 injection wells and 25 production wells in the field. The system is modeled using a simplified 2D vertical slice. The model domain has a size of 800 m × 1 m × 1500 m, representing 1/25 of the field. The main rock properties used are listed in Table 1.

We model the following four FEPs in the system, three of which invoke feedbacks between the system model and the *TOUGH2* model:

(1) Potential creation of a fracture due to high injection pressure. Pressure at the injection point is obtained from the *TOUGH2* simulation and monitored in the system model. When this pressure is above the lithostatic pressure, we assume a fracture is created at that location; the resulting leakage of CO_2 is simulated by *TOUGH2*. The properties for this potential fracture are listed in Table 1;

(2) Potential leakage pathway through an abandoned well. We assume there is an abandoned well at x = 400 m. The CO_2 concentration at the interface of the abandoned well and the gas reservoir is calculated by *TOUGH2* and compared with a CO_2 concentration threshold value in the system model, above which we assume there will be CO_2 corrosion of well cement, resulting in the development of high-permeability channels (from cap rock to ground surface) and CO_2 leakage to the land surface, which is simulated by the *TOUGH2* model. The properties for the opened abandoned well are listed in Table 1;

(3) Potential pipeline break. In the CO2_Pipeline subsystem, we assume the probability for a pipeline to break is a function of time and pipeline length. If a pipeline breaks in its lifetime, we simply assume CO_2 capture from the flue gas is halted. Whatever is in the pipeline will be emitted to the atmosphere, and the injection of CO_2 into the gas reservoir will be stopped;

(4) The CO_2 concentration in the aquifer above the gas reservoir at 750 m depth. If there is CO_2 leakage, it might contaminate this aquifer. The maximum CO_2 concentration is observed during the simulation.

For our case, the *GoldSim* model runs for 10 time steps to a total simulation time of 50 years, i.e., there is an output every five years. *GoldSim* calls *TOUGH2* every five years. Each time when *TOUGH2* finishes the previous 5-year simulation, it saves its results to a file SAVE, which will be copied as the initial condition file INCON for the next five-year calculation. Within the five years, *TOUGH2* controls its own time-step size.

BASE CASE SIMULATION

In our base-case simulation, the total CO_2 injection rate for 25 wells is 9 x 10^6 MMt/yr, i.e., 1.7 x 10^8 Mcf/yr. The economic parameters and prices (current value) used are listed in Table 2. Injected CO_2 is accounted for as credit. The lifetime of all the utilities considered in the study is assumed to be 50 years.

Table 2. Economic Base-Case Parameters

CO_2 credit (\$/t CO_2)	35
Electricity price (\$/kWh)	0.07
CH_4 selling price (\$/MMBtu)	10
CH_4 buying price (\$/MMBtu)	10
CO2 buying price (\$/t CO_2)	20
Inflation rate	0.05
Inflation-free interest rate	0.10
Tax rate	0.3

In the base case, the purchasing and selling prices for methane are assumed to be the same. There is an option for them to be different due to seasonal price fluctuations.

To see the impact of pipeline break on the system, we set the probability for a pipeline longer than 1 km to break after 40 years to 0.8 in our simulation.

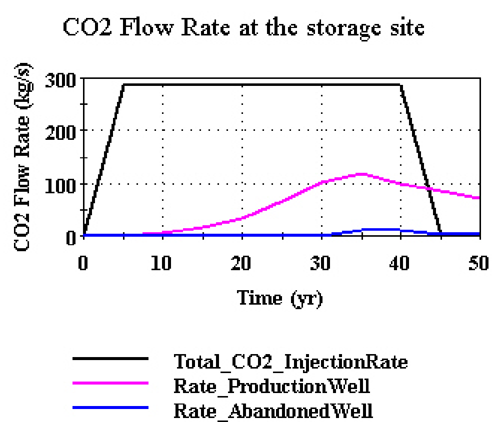

Figure 3. CO_2 flow rates in the gas reservoir.

Figure 3 shows the CO_2 flow rates at the storage site calculated by *GoldSim*. The black line shows the total injection rate for 25 wells. The pink line is the CO_2 breakthrough at the production well, which starts after about 10 years of injection. This early breakthrough is due to the high injection rate. The blue line shows the CO_2 leakage rate from the abandoned well. The CO_2 mass fraction in the gas phase at this abandoned well reaches 0.5 around year 30, a concentration at which it is assumed that corrosion and escape of CO_2 will occur The CO_2

breakthrough rate gets smaller when CO_2 starts to leak from the abandoned well. The black line drops to zero at year 45 due to the pipeline break sometime between year 40-45, after which the CO_2 capture and injection are stopped.

During the 50-years simulation, the injection pressure never reaches levels sufficient to create a fracture. The maximum mass fraction of CO_2 in the liquid phase in the aquifer is 0.0074.

Figure 4 shows the CH_4 production rate at the production wells. During the first 20 years the production rate of CH_4 is relatively high, which accounts for a large amount of income for that period (the corresponding income in current value is shown on the right-hand axis). The production rate is reduced after CO_2 breakthrough. For the last 20 years the production is much lower due to the leakage from the abandoned well, and later after the injection was halted due to the pipeline break. Even if no abandoned well is present, CO_2 breakthrough will also reduce CH_4 production.

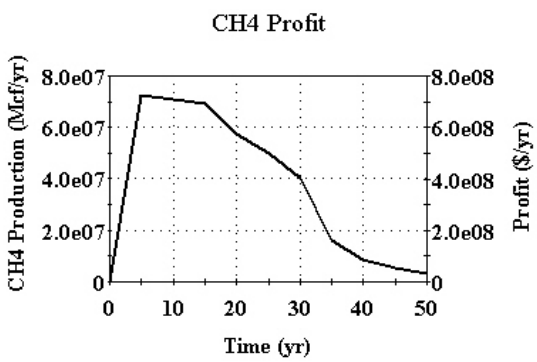

Figure 4. Methane production rate and profit.

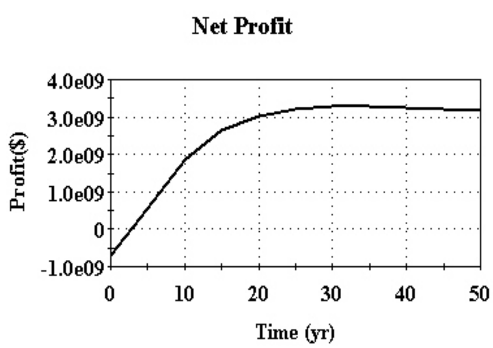

Figure 5. Net present value of the system.

The net present value (NPV) including CO_2 credit over time is shown in Figure 5. For the scenario considered, the CO_2 credit is able to keep the net profit positive. Income from sale of CH_4 is high at the beginning, but drops considerably when leakage and CO_2 breakthrough start. The main cost comes from purchasing additional CO_2, capturing CO_2 from flue gas, and separation of CH_4 and CO_2 at the production site. The uncertainty of the net profit curve results mainly from the uncertainty in CH_4 and CO_2 prices relative to the CO_2 credit, the total injection rate, and inflation and interest rates.

Figure 6 shows CO_2 mole fraction in the gas phase at the end of 50 years. The abandoned well is located at X = 400 m. The large CO_2 concentration at that location indicates the leaked CO_2 escapes the reservoir through the abandoned well. The anomaly at 700 m depth is due to the high permeability of the aquifer.

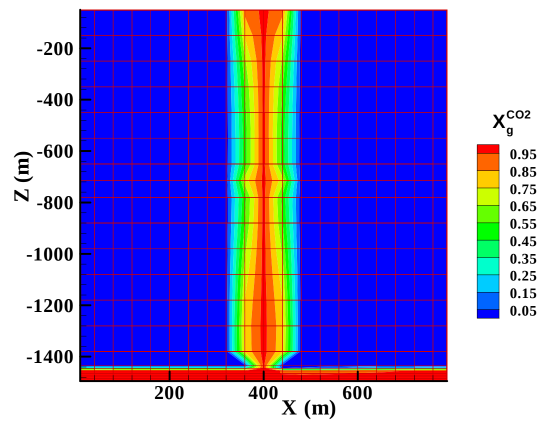

Figure 6. CO_2 mass fraction in the gas phase at the end of simulation.

OPTIMIZATION

The system model can also be used to maximize the profit of the system over 50 years. In this problem, we assume that in addition to the CO_2 produced from the natural gas power plant, there are two other sources CO_2 to supplement the total CO_2 injection rate. The first 5 MMt supplementary CO_2 comes from a power plant close by, with a CO_2 price at $20/tonne. The extra amount needed comes from another source with a much higher price, $50/tonne.

Obviously, there is a trade-off between net profit of the system and the total CO_2 injection rate. Although a higher injection rate means more profit from CO_2 credit, and CH_4 production at early stage, it may also cause early CO_2 breakthrough, which reduces CH_4 production and CO_2 credit (although in reality reduction in CO_2 caused by breakthrough may be ignored). A higher injection rate also means a much higher cost for supplementary CO_2 and pipeline cost.

The objective is to find an optimal injection rate to maximize the net profit of the system, assuming all the other settings are the same as in the base case. This is done using the optimization algorithm in *GoldSim*. The algorithm is based on box's complex method [*GoldSim*, 2006]. The method begins by developing an initial complex, which is a set of solutions that meet all the requirements specified by the user. The algorithm searches the solution space iteratively until the solution converges or *GoldSim* determines optimal solution cannot be achieved.

The optimal solution is achieved when the CO_2 injection rate is 23.9 MMt/yr, 1/8 of which is captured from the flue gas of the natural gas power plant in the system. When the injection rate is above this threshold, the net profit drops quickly.

CONCLUSIONS

We have developed a system-level model for analyzing geological storage of CO_2. Within our system model we are incorporating detailed reservoir simulations of CO_2 injection and potential leakage with associated HSE effects. This is done through the system-level modeling tool *GoldSim*. The application of the system model is focused on evaluating the feasibility of carbon sequestration with enhanced gas recovery (CSEGR) in the Rio Vista region of California. The reservoir simulations are performed using a special module of the *TOUGH2* simulator, EOS7C, for multicomponent gas mixtures. Using this approach, the economic benefits of CO_2 sequestration and enhanced gas recovery can be directly weighed against the costs and risks of CO_2 injection. The current model is highly simplified, but nevertheless models key processes and interactions while simultaneously demonstrating the power and potential value of system-level modeling of CCS.

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