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Numerical simulation and optimization of CO_2 sequestration in saline aquifers for enhanced storage capacity and secured sequestration

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Abstract
Saline aquifer geological carbon sequestration (SAGCS) is considered most attractive among other options for geological carbon sequestration (GCS) due to its huge sequestration capacity. However, in order to fully exploit its potential, efficient injection strategies need to be investigated for enhancing the storage efficiency and safety along with economic feasibility. In our previous work, we have developed a new hybrid code by integration of the multi-phase CFD simulator TOUGH2 with a genetic algorithm (GA) optimizer, designated as GA-TOUGH2. This paper presents the application of GA-TOUGH2 on two optimization problems: (a) design of an optimal water-alternating-gas (WAG) injection scheme for a vertical injector in a generic aquifer and (b) the design of an optimal injection pressure management scheme for a horizontal injector in a generic aquifer to optimize its storage efficiency. The optimization results for both applications are promising in achieving the desired objectives of enhancing the storage efficiency significantly while reducing the plume migration, brine movement and pressure impact. The results also demonstrate that the GA-TOUGH2 code holds a great promise in studying a host of other problems in CO_2 sequestration such as how to optimally accelerate the capillary trapping, accelerate the dissolution of CO_2 in water or brine, and immobilize the CO_2 plume.

Keywords: CO_2 sequestration; Computational fluid dynamics; Genetic algorithm; Injection pressure management; Water-alternating-gas (WAG) injection.

1. Introduction
In recent years, there has been significant emphasis on the development and implementation of safe and economical geological carbon sequestration (GCS) technologies due to heightened concerns on CO_2 emissions from pulverized-coal (PC) power plants. However, uncertainties about storage capacity as well as long-term storage permanence remain major areas of concern before proceeding with the actual deployment of CO_2 sequestration in large-scale aquifers with enormous investment. In addition, challenges remain in enhancing the storage efficiency and safety (by reducing the extent of plume migration, brine movement and pressure impact) as well as the energy efficiency and economic feasibility of GCS by improving the injection operations. Numerical simulations prior to actual sequestration can be employed to address some of these uncertainties. CFD solver Transportation of Unsaturated Groundwater and Heat (TOUGH2) has been widely used for this purpose [1, 2]. Due to the complexity of the mass/energy transport in GCS, injection strategies that may be beneficial in addressing

one aspect of the sequestration (e.g. reduction in plume migration) may not be as effective in addressing another important aspect of sequestration (e.g. reservoir pressure response and its management). In addition, the storage efficiency of an aquifer is also dependent on various injection strategies and parameters associated with them; the optimization of the storage efficiency of an aquifer is of great interest in GCS. Therefore, a simulation tool that has the capability of determining the optimal solutions by balancing various trade-offs among desired objectives in GCS is needed. As an effort to examine and address these issues, we have developed a genetic algorithm (GA) based optimization module for TOUGH2 which can optimally examine various injection strategies for increasing the storage efficiency as well as reducing the plume migration (Zhang and Agarwal, 2012). It is designated as GA-TOUGH2, and has been validated by conducting several benchmark studies [3, 4].

In this paper, we consider the optimization of two engineering techniques to increase the sequestration efficiency and safety of GCS in saline aquifers. In the first study, we employ a water-alternating-gas (WAG) injection technique to a generic saline aquifer to retard the vertical migration of in situ CO_2, i.e., to reduce the CO_2 plume size. In the second study, our goal is to seek a particular CO_2 injection scenario that will result in the management of injection pressure (with the constraint that it remains less than the aquifer's fracture pressure) so as to maximize the injection rate to increase the storage efficiency. In both the studies, we would like to determine the optimum strategy to achieve the desired objective. In the WAG injection scheme, the additional water injection results in greater pressure response and energy consumption which needs to be traded off with the goal of reduced CO_2 migration in an optimal manner. Optimization can help in determining the most efficient as well as effective WAG operation. For the injection pressure management study, the goal is to manage the injection pressure such that it optimizes the storage efficiency of the aquifer. The optimization results for both applications show great promise, by significantly reducing the CO_2 migration (up to 50% reduction in plume size compared to conventional CO_2 injection) and well regulated injection pressure (less than the formation's fracture pressure) to increase the storage efficiency.

2. Methodology

In previous research, we successfully developed an optimization module for TOUGH2 using a genetic algorithm (GA). GA belongs to a class of optimization techniques that are inspired by the biological evolution [5]. It can iteratively converge to the global optima without having detailed information about the design space. Implementation of GA-TOUGH2 is summarized in Figure 1. Details of this work can be found in our previous papers [4, 6].

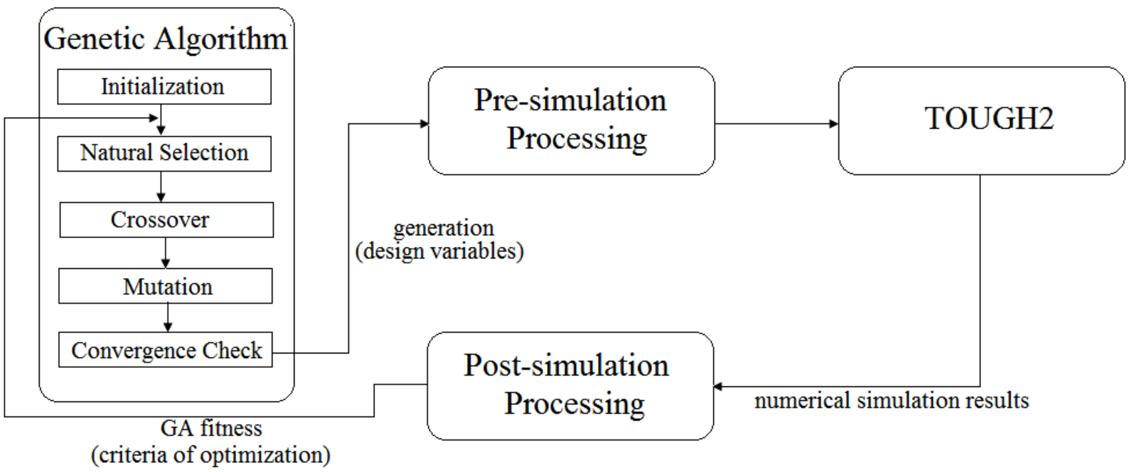


Figure 1. Dataflow schematic of GA-TOUGH2 numerical simulator

3. Optimization of WAG technique for reducing the plume migration

The storage efficiency of saline aquifer geological carbon sequestration (SAGCS), based on the aquifer's pore space, is usually very low. This is due to the inherent nature that injected CO_2 is less dense than brine, with which the aquifer is filled. Consequently, CO_2 tends to rise up to the ceiling (caprock) of the aquifer and forms a large spreading plume, decreasing both the storage capacity, safety and economic feasibility of SAGCS considerably. To address this problem, we examined the potential benefits of a reservoir engineering technique called water-alternating-gas (WAG) injection for carbon sequestration compared to the constant-gas-injection (CGI) technique for its effect on both the storage capacity and the plume migration. We employed GA-TOUGH2 to determine the most efficient injection pattern. As shown later in this section, our calculations indicate that the adoption of WAG operation to SAGCS can lead to significant gain in sequestration efficiency. One of the key parameters that determine the migration of the in situ CO_2 is the mobility ratio M, defined as:

$$M = \frac{m_n}{m_w} = \frac{\mu_w \cdot k_{rn}}{\mu_n \cdot k_{rw}} \tag{1}$$

where m_n, μ_n, and k_{rn} are the mobility, viscosity, and relative permeability of the non-wetting phase (CO_2) respectively and m_w, μ_w, and k_{rw} are the mobility, viscosity, and relative permeability of the wetting phase (brine) respectively. Typically a mobility ratio of 10~20 is expected for SAGCS with CGI operation. Under the scenario of WAG operation, the alternating CO_2-water slugs can be treated as quasi-mixture entering the aquifer, leading to mobility ratio lower than that for pure CO_2 injection. The success of WAG technique for SAGCS operations is supported by the following reasons: (1) lower M results in more stable displacement of the reservoir fluid, (2) lower M reduces the upward migration of CO_2 [7], and (3) injection of brine into the aquifer with or after CO_2 injection can accelerate the dissolution of CO_2 and enhance its residual trapping by the enhanced convective mixing [8-11]. More details of the benefits of WAG operation can found in the Appendix.

In the study of WAG operation, target CO_2 sequestration amount is set to be 0.5 million metric tons per year, which is roughly half of the emission from a typical medium-sized PC power plant. For demonstration purpose a WAG enabled SAGCS operation is assumed to last for 600 days before it is shut down, although a typical lifespan of a PC power plant is around 30 years. Thus, a total of 0.822 million metric tons of CO_2 will be sequestered. During the 600 days of injection, 20 cycles of alternating CO_2-water slugs (each known as a single WAG cycle) will take place, as schematically shown in Figure 2. Four independent variables determine a unique WAG injection pattern: CO_2 injection rate, water injection rate, WAG ratio (the injected CO_2 mass to injected water mass per cycle), and cycle duration. Fitness function for optimization is defined as the CO_2 plume migration reduction (compared to the migration under constant gas injection (CGI) operation) normalized by the total amount of water injection, as given by Equation (2). The fitness function serves as the criteria for evaluating how efficient a certain WAG operation would be. This choice of the optimization fitness function takes into consideration both the performance and economic aspects of adapting the WAG operation, since the water injection consumes extra energy for transportation and pumping. WAG injection pattern with the largest fitness function value is most desirable. We define

$$fitness = \frac{R_{CGI} - R_{WAG}}{m_{water}} \tag{2}$$

where R_{CGI} and R_{WAG} are the CO_2 plume radius under CGI operation and WAG operation respectively. m_{water} is the total mass of injected water during WAG operation. R_{CGI} and R_{WAG} are measured at the top of the reservoir due to the buoyancy of CO_2. For simplicity, the following two assumptions are made: (a) each WAG cycle has duration of 30 days and (b) all WAG cycles are identical to each other. The 30-day cycle duration is chosen based on the authors' judgment, following Nasir and Chong's conclusion that for oil recovery purpose, different WAG cycle durations do not lead to significant difference in recovery efficiency [12]. With these assumptions, the number of independent variables reduces to two. The injection rates of CO_2 and the injection rates of water are chosen as the final optimization design variables.

Optimization of WAG operation for a generic cylindrical aquifer with a vertical injector was investigated. The principle of determining the size of the computational domain is that it should be able to capture the CO_2 footprint until the end of simulation, and it should be sufficiently large so that the boundary conditions have no significant effect on CO_2 migration. Following this principle, a hypothetical cylindrical saline formation with radius of 3,000 m was modeled, while the radius-thickness ratio was set to be 300. The injection well was located at the center of the domain above the bottom 20 m. Due to symmetry, only a radial slice of the domain was considered in the modeling. The computational domain is shown in Figure 3 (a) in blue color (not to scale).

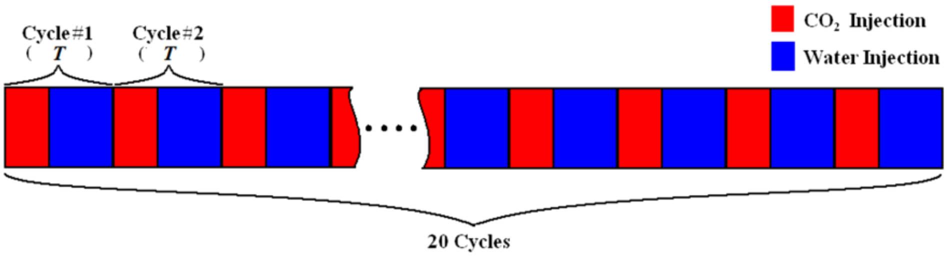


Figure 2. Schematic of the considered WAG operation

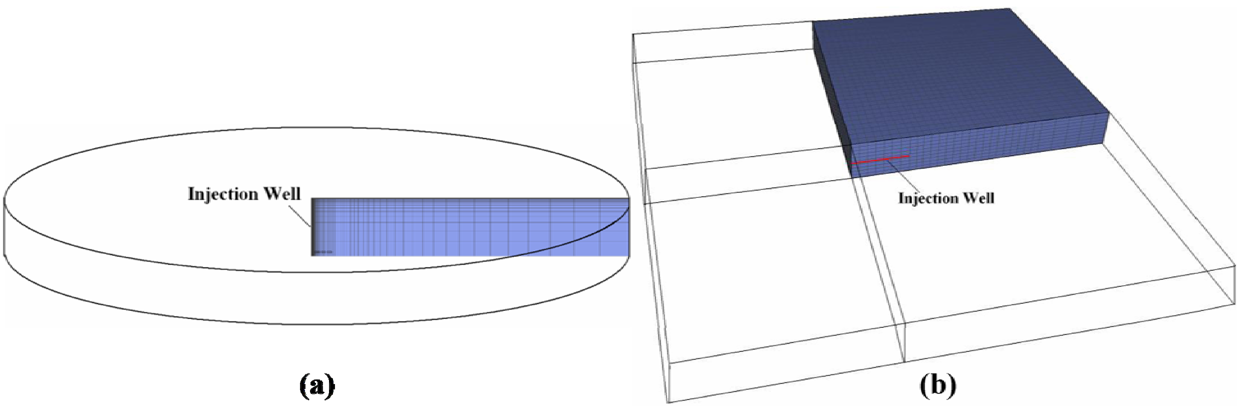


Figure 3. Computational domains for optimization of (a) WAG operation and (b) pressure management

Typical hydrogeological properties of a semi-heterogeneous saline aquifer with depth of 1,300m were assigned to the simulation domain. No mass flow boundary condition was maintained at the ceiling and the floor of the domain to simulate non-permeable cap-rock. Fixed-state boundary condition was applied at the outer lateral boundaries of the domain, allowing the mass and energy to flow freely in and out of the domain through the outer lateral boundaries as necessary. The fixed-state boundary condition essentially represents an open system. Brine pumping was not modeled in the simulation domain by assuming that the saline aquifer is sufficiently large and that the brine production is sufficiently far away from the storage site; therefore, the induced CO_2 directional flow due to the presence of brine production well is negligible. Steady-state simulations were conducted prior to the simulations of interest to establish equilibrium condition throughout the domain. The equilibrium conditions were then used as the initial conditions for the simulations of interest. Table A1 in the Appendix summarizes the details of the domain properties.

Since it is inevitable that CO_2 will eventually rise and concentrate near the ceiling (caprock) of the aquifer, the saturation of gaseous phase (SG) near the top-most layer of the simulation domain is examined to estimate the CO_2 migration. In the plan-view of the top most layers, the final shape of the CO_2 plume is expected to be circular due to the assumption that the formation properties of the aquifer are homogenous. Table 1 gives details of the optimal WAG operation for each WAG cycle.

Table 1. Optimal WAG operation (per cycle)

I_{CO2}(kg/s)	Injection duration (day)	I_{water} (kg/s)	Injection duration (day)	WAG ratio	Optimization fitness (m/1000 tons of water)
36.13	13	33.35	17	0.847	0.1438

The lateral extent of the CO_2 plume is determined by examining the gaseous phase distribution at the ceiling of the aquifer. The intersection of the SG curve with the *x*-axis indicates the tip of the CO_2 plume, i.e., the extent of CO_2 migration. Beyond this point, the aquifer is free from CO_2 contamination, so the area up to this point is the CO_2 impact area. Any CO_2 leakage/contamination will occur only in the impact area. Figure 4 shows the SG curve in the top-most layer of the simulation domain for optimized WAG scheme and its comparison with SG curves obtained by three other non-optimized injection schemes. The three other schemes are constant-gas-injection with low injection rate (low-CGI), constant-gas-injection with high injection rate (high-CGI), and cyclic CO_2 injection. For the low-CGI case, CO_2 is injected with a constant mass flow rate of 15.85 kg/s for 600 days; for the high-CGI case, CO_2 is injected with a constant mass flow rate of 31.71 kg/s for 300 days; the cyclic CO_2 injection is the same as the optimized WAG operation but without water injection. All cases have identical amount of sequestered CO_2 as 0.822 million metric ton during the 600 days of operation.

Figure 5 shows the SG contours for the optimized WAG and non-optimized injection operations after 600 days of injection at the radial cross-section of the modeled formation.

Table 2 provides a detailed comparison among the optimized WAG and other three non-optimized injection operations. The improvement (i.e., reduction) in plume migration is prominent.

The results presented above clearly show the benefits of the WAG operation for CO_2 sequestration. However, we need to address the tradeoff of these benefits – i.e., the effect on other sequestration variables, particularly the pressure, for ensuring the safety of sequestration. Pressure plays a crucial role in ensuring the efficiency and safety of sequestration. According to the present investigation, adopting the optimized WAG injection will cause the injection pressure to oscillate as the CO_2 injection and water injection alternates. Considering the peak pressure under the optimized WAG injection, an 8% increase of reservoir pressure from its pre-injection hydrostatic condition is found near the injection well. Compared to this increase, a maximum of 2% increase in reservoir pressure is likely to be induced by the three non-optimized injection scenarios. Although injection condition under WAG injection is harsher due to increased injection pressure, it is not a cause of concern since the increase in injection pressure due to WAG is small. However, it should be noted that the reservoir pressure response to the injection of CO_2 and water is very sensitive to the hydrogeological properties of the saline formation, such as porosity and permeability. Thus pressure analysis of WAG injection for different saline formations should be made on a case-to-case basis. Figure 6 illustrates the injection pressure response for the four injection scenarios studied.

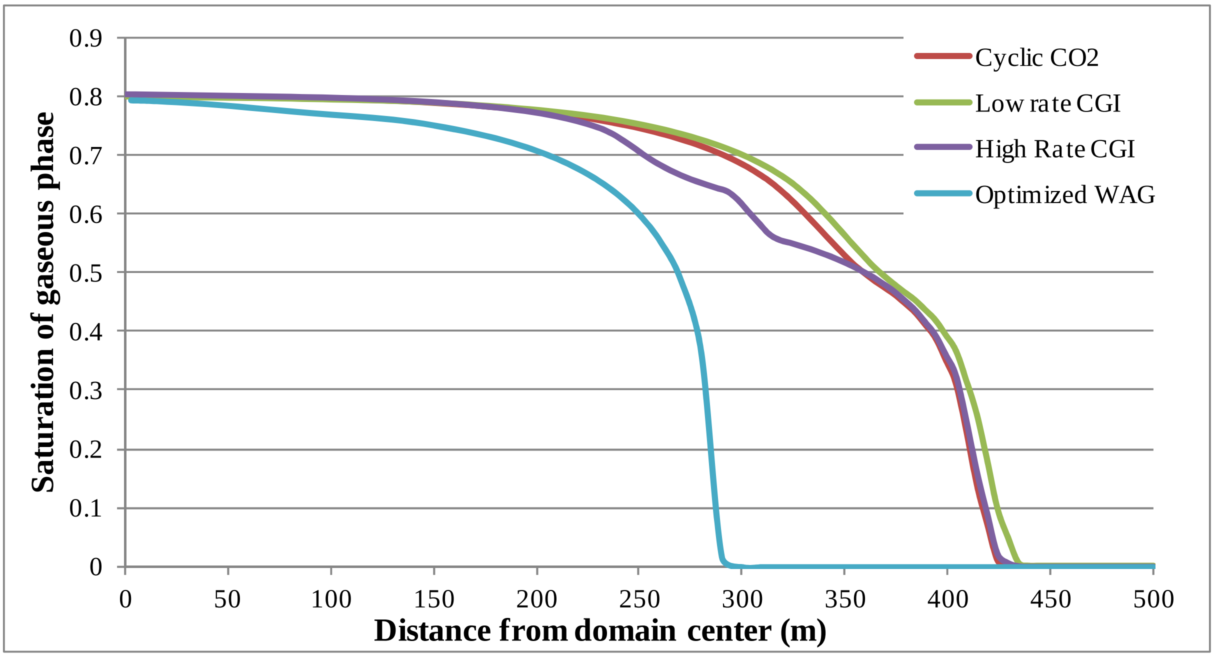


Figure 4. SG underneath the caprock, optimal WAG and non-optimized injection operations

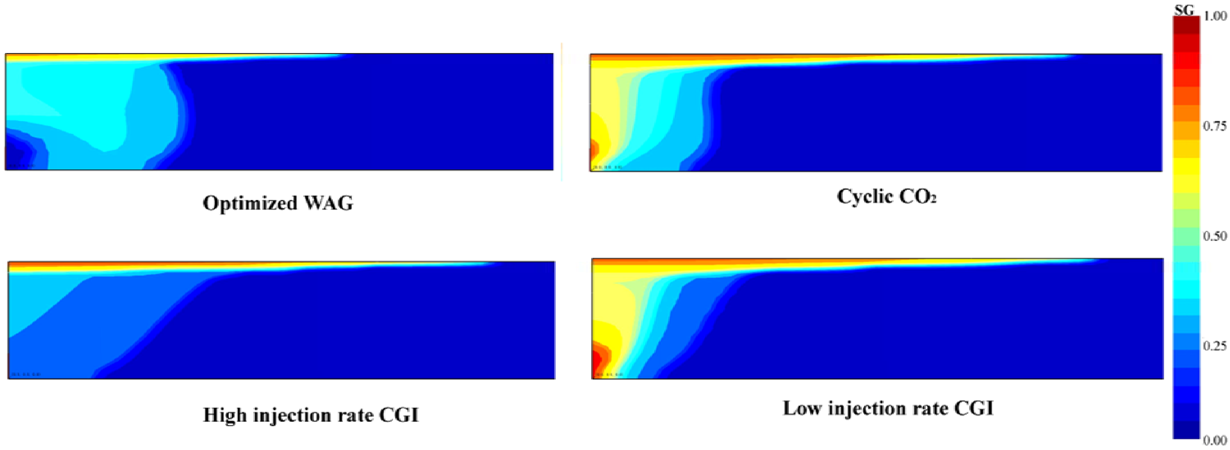


Figure 5. Radial gas saturation for optimized WAG and other non-optimized injection techniques

Table 2. CO_2 migration comparison of optimized WAG and other non-optimized injection schemes

Relative to WAG	Optimized WAG	Cyclic CO_2 injection	High injection rate CGI (15.7 kg/s)	Low injection rate CGI (31.4 kg/s)
CO_2 plume migration	290 m	420 m	420 m	430 m
Additional migration	-	130 m	130 m	140 m
Increased plume radius	-	44.83 %	44.83 %	48.28 %
Increased footprint area	-	109.75 %	109.75 %	119.86 %

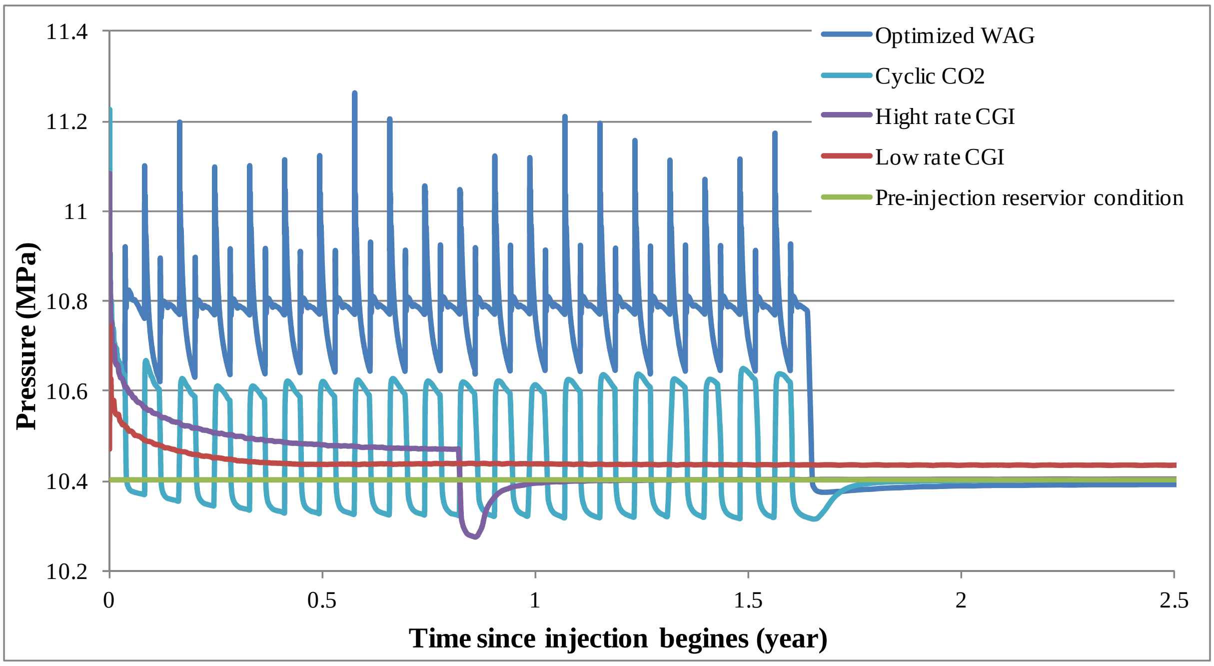


Figure 6. Injection pressure of optimized WAG and other non-optimized injection scenarios

4. Optimal management of injection pressure to increase the storage efficiency

Another key issue associated with GCS is the pressure response of the target storage site due to the presence of the sequestered CO_2. Because of the very limited compressibility of water, supercritical CO_2, and formation matrix, the pressure disturbance due to the injection may travel orders of magnitude faster than the mass transportation. However, such pressure disturbance is not desirable. It compromises the energy efficiency of GCS by increasing the required injection pressure to maintain well injectivity, and most importantly, it can potentially jeopardize the integrity of the formation matrix. Therefore, it becomes crucial to manage the pressure response optimally to ensure the efficiency as well as the safety of GCS operation. Two issues make the injection pressure one of the most important operation parameter for SAGCS. One is the well injectivity and the other is the fracture pressure of the formation matrix. The well injectivity is defined in Eq. (3); it serves as an indicator of the ability of an injection well to deliver supercritical CO_2 to the reservoir.

$$injectivity = \frac{Q_{CO2}}{p_{injection} - p_{reservior}} \tag{3}$$

where Q_{CO2} is the injection mass rate (kg/s), $p_{injection}$ is the injection pressure (Pa), and $p_{injection}$ is the mean reservoir pressure (Pa).

Following Darcy's law, the achievable CO_2 injection mass rate (Q_{CO2}) is proportional to the product of relative permeability of CO_2 ($k_{r,g}$) and pressure gradient near the injection well (Δp). Recall that for two-phase flow of supercritical CO_2 and brine, $k_{r,g}$ is a function inversely proportional to the saturation of brine (S_b). At the early stage of the CO_2 injection, the pore space near the injection well is primarily occupied by brine, i.e., by high S_b at the adjacent area of the injection well. Consequently, $k_{r,g}$ is relatively low and this results in considerable difficulty to inject a given amount of CO_2. A direct indicator of such difficulty is the significant elevation in injection pressure, or in other words, extremely low injectivity. The injectivity of CO_2 will not stay constant. As CO_2 injection continues, more brine will be pushed out of the pore space adjacent to the injection well, thus lowering the S_b. Simultaneously, $k_{r,g}$ will increase in a semi-exponential fashion. Therefore, during intermediate and late stage of CO_2 injection, it is expected that CO_2 injectivity should greatly improve, resulting in low injection pressure if the injection mass rate remains unchanged. Therefore, one can obtain the schematic of the above discussion as shown in Figure 7. It is intuitive to inject CO_2 at high injection rate, as higher injection rate leads to greater amount of CO_2 to be sequestered for a given period, resulting in a time-efficient injection. However, it is also true that higher injection rate requires greater injection pressure. Like any other solid structure, geologic formation can only bear limited stress to maintain its integrity. Exerted with excessive stress, it may fracture or collapse.

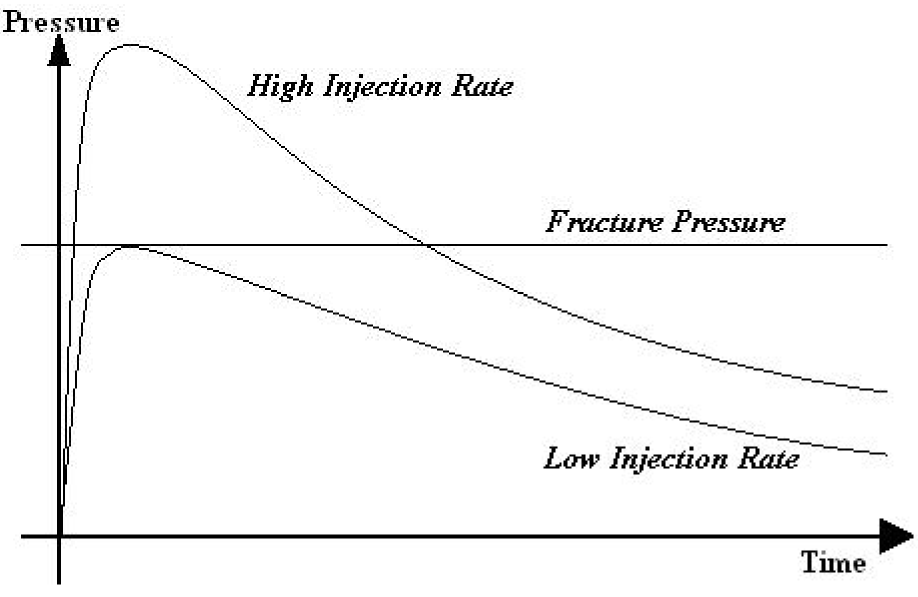


Figure 7. Schematic of injection pressure response under constant rate injection

The injection induced fracture will serve as passages for the mobile CO_2 to migrate to shallower aquifers or even to the ground surface, endangering the ecosystem at the storage site. Therefore, every effort should be made to ensure that under no circumstance the injection pressure shall exceed the fracture pressure of the formation. Since the fracture pressure is an intrinsic property of the formation, it is likely to remain constant during the injection, shown as horizontal line in Figure 7. Figure 7 illustrates a crucial issue that must be addressed. If CO_2 is pumped into the aquifer with a relatively high injection rate (following the “High Injection Rate” curve in Figure 7), the excessive pressure response at the early stage of injection can easily jeopardize the integrity of the formation; in contrast, if CO_2 is pumped with a relatively low injection rate to ensure formation's integrity, the injection will be time-inefficient at the intermediate and late stage (following the “Low Injection Rate” curve in Figure 7). If the injection rate can be adjusted such that the injection pressure levels off, as it approaches the fracture pressure, the overall time-efficiency of the sequestration will be greatly improved without compromising the sequestration safety. Because the injection pressure is almost constant in such a scenario, we call it the constant-pressure-injection (CPI). To achieve CPI, the injection rate must be adjusted with time than being uniformly maintained. With injection rate as the design variable and threshold pressure (the pressure limit chosen based on the formation's fracture pressure) as the constraint, optimization can be carried out by maximizing the fitness function defined as:

$$fitness\ function = modified\ injectivity = \frac{Q_{CO2}}{\left| p_{threshold} - p_{injection} \right|} \tag{4}$$

With fitness function approaching infinite (large value), CPI is obtained and the corresponding injection scenario can be determined. The optimization designs with CPI were carried out using GA-TOUGH2. Unlike the optimization design of WAG, it raised a challenge of how to describe the CO_2 injection rate as a time-dependent continuous function, with limited discrete data points contained by the GA individuals. The concept of Bézier curve was introduced to address this challenge. A Bézier curve is a parametric curve frequently used in computer graphics and related fields [13]. It is defined by a set of control points, and uses them as coefficients of a certain polynomial to describe continuous curves (refer to Appendix for details). In this work, each CO_2 injection scenario is described by a cubic Bezier curve. An example of cubic Bezier curve, using four control points defined as P_1, P_2, P_3, and P_4, is illustrated in Figure 8.

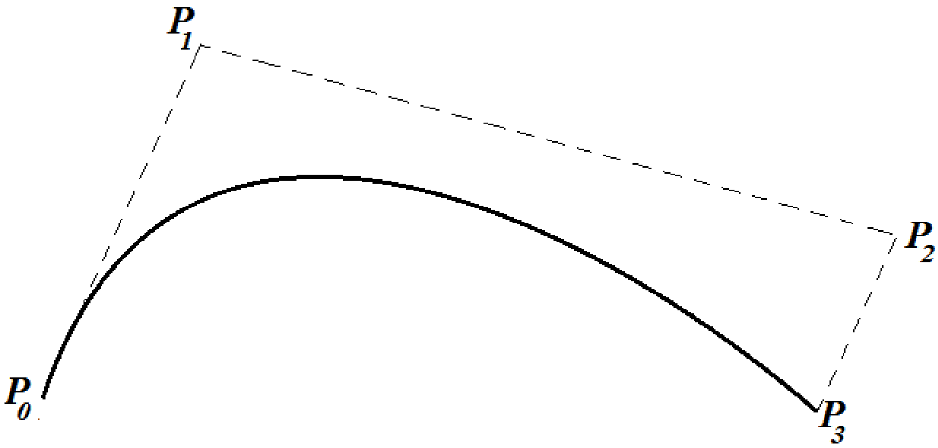


Figure 8. Schematic of a cubic (3rd order) Bezier curve

The CO_2 injection scenario is essentially a time dependent function of mass flow rate. Although being smooth and continuous, discretization of the injection scenario with respect to time is needed to make the problem tractable to numerical simulation. With such discretization, CO_2 injection rates become step functions for each time interval, and ultimately approximate to the smooth injection scenario as time interval becomes small enough. Injection rate for each discrete time interval is described at the midpoint of the interval, called the sample point. Since both the information of time (x-axis) and flow rate (y-axis) is needed to describe a certain injection scenario in GA-TOUGH2, an alternative expression of Bezier curve in Cartesian coordinate system was derived. Assuming that the four control points are $P_0(x_0, y_0)$, $P_1(x_1, y_1)$, $P_2(x_2, y_2)$, and $P_3(x_3, y_3)$, then any point $P(x(t), y(t))$ on the Bezier curve can be expressed as:

Time: $x(t) = A_x t^3 + B_x t^2 + C_x t^1 + x_0$ Injection rate: $y(t) = A_y t^3 + B_y t^2 + C_y t^1 + y_0$ (5)

where the coefficients are defined as:

$$\begin{aligned} C_x &= 3(x_1 - x_0) & C_y &= 3(y_1 - y_0) \\ B_x &= 3(x_2 - x_1) - C_x & B_y &= 3(y_2 - y_1) - C_y \\ A_x &= x_3 - x_0 - C_x - B_x & A_y &= y_3 - y_0 - C_y - B_y \end{aligned} \tag{6}$$

Because the injection time must start from zero, the first control point is anchored to the *y*-axis by setting $x_0 = 0$, i.e., $P_0(x_0, y_0) = P_0(0, y_0)$. Other than that, the control points' coordinates are arbitrarily generated for each GA individual. With this formulation, an arbitrary CO_2 injection scenario beginning at $t = 0$ is obtained by letting the parameter t increase from 0 to 1.

The simulation domain for the CPI study was a generic aquifer with a horizontal injection well. A thin aquifer with the dimension of 8,000 m×8,000 m×100 m was modeled for the optimization study of CPI operation. In the middle of the thickness direction sits an 800 m horizontal well. It is claimed by Jikich and Sams [14] that significantly increased well injectivity could be achieved by using a horizontal well. Due to symmetry, only a quarter of the domain is modeled, schematic of which is shown in Figure 3 (b) in blue. Hydrogeological properties, initial conditions and boundary conditions applied to this computational domain of Figure 3 (b) were identical to those for the WAG optimization. A threshold pressure of 180 bar (50% increase from the initial pressure) was chosen to be the maximum allowable injection pressure. The choice of the threshold pressure should result from a collaborative consideration of various aspects, such as the fracture pressure and the safety factor. In the design, injection rate could vary freely between 0 kg/s and 150 kg/s. Injection duration was 5 years.

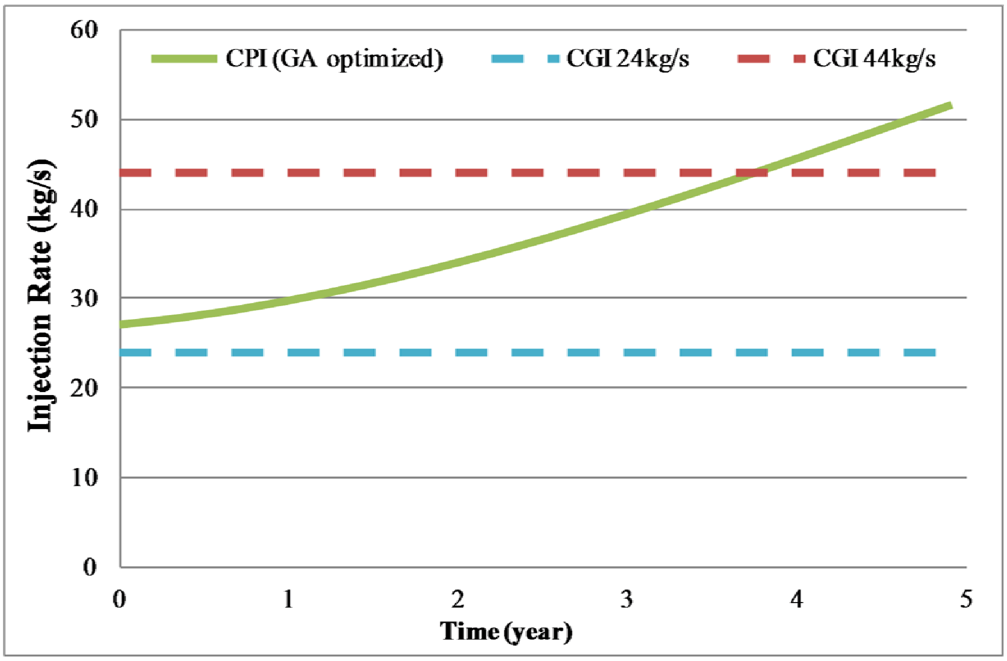
Injection scenario obtained by the CPI design and the corresponding injection pressure is given in Figure 9. Two CGI cases, one with high injection rate (44 kg/s) and one with low injection rate (24 kg/s), are also included in this figure for comparison. It can be clearly seen that GA-TOUGH2 successfully found the optimized injection scenario, which keeps the injection pressure less than 1bar close to the designated threshold pressure.

The advantage of CPI operation can be clearly seen comparing it to two CGI operations. It can be seen that for the high rate CGI the injection pressure reaches 220 bar, a 40 bar overshoot from the threshold pressure, and such an overshoot lasts for over 3.5 years before the injection pressure falls below 180 bar. Such an intense and prolonged pressure overshoot can lead to catastrophic consequence to formation's integrity. On the other hand, it can also be seen that for the low rate CGI the injection pressure diverted from the threshold pressure at early stage after it peaked. Although the integrity of the formation is not threatened, storage capacity is severely compromised. Only the CPI operation with five-year-averaged injection rate of 38 kg/s ensures both storage efficiency and security.

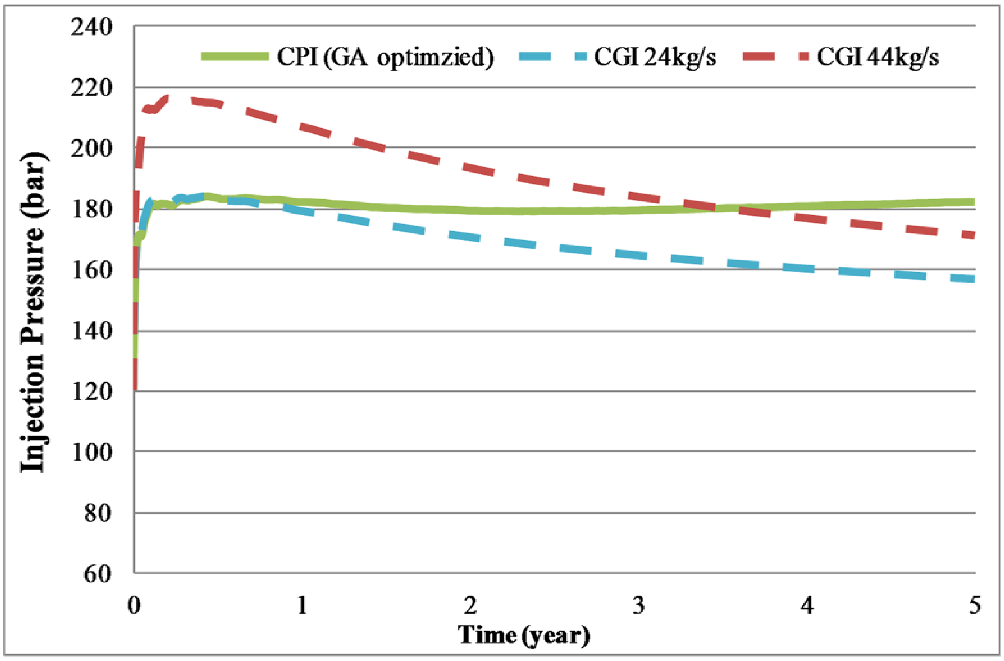
5. Conclusions

The feasibility of adopting the water-alternating-gas (WAG) technique for CO_2 sequestration in saline aquifers has been investigated with the objective of determining its sequestration efficiency compared to the standard constant-gas injection (CGI) operation and its relative environmental risk (namely the extent of plume migration). Using the GA-TOUGH2, optimization studies were conducted to determine the most efficient WAG operations. For the generic aquifers considered, it was shown that CO_2 footprint under the optimized WAG operation could be as small as half of the size compared to other non-optimized injection operations. In addition, the additional water injection in WAG also brings down the average gas saturation. The accelerated CO_2 dissolution is always desirable; since once dissolved, CO_2 becomes immobilized and is no longer considered as potential leakage risk.

GA-TOUGH2 was also successfully employed for optimizing the constant-pressure-injection (CPI) design. In the optimized injection design it was ensured that the injection pressure never exceeded the designated threshold pressure (the fracture pressure of the aquifer). The optimized injection pressure design resulted in improved injectivity and thus in higher storage capacity. Both the reservoir engineering techniques presented in this paper hold great promise towards increasing the carbon sequestration efficiency and safety. These studies also demonstrate that GA-TOUGH2 is a computationally accurate and efficient code to address various optimization problems in GCS.



(a)



(b)

Figure 9. Injection scenarios and corresponding pressure response, CPI and two CGI injection cases

Appendix

A.1 Numerical Simulation domain and GA Setup

Typical hydrogeological properties of a semi-heterogeneous saline aquifer with depth of 1,300 m were assigned to the simulation domain. No mass flow boundary condition was maintained at the ceiling and floor of the domain to simulate non-permeable cap-rock. Fixed-state boundary condition was applied at the outer lateral boundaries of the domain, allowing the mass and energy to flow freely in and out of the domain through the outer lateral boundaries as necessary. The fixed-state boundary condition essentially represents an open system. It should be noted that brine pumping well was not modeled in the simulation domain. This is valid by assuming that the saline aquifer is sufficiently large and that the brine production is sufficiently far away from the storage site; therefore, the induced CO_2 directional flow due to the presence of brine production well is negligible. Steady-state simulations were carried out prior to the simulations of interest to establish gravity-capillary equilibrium condition throughout the domain. The equilibrium conditions were then put back into the domain as the final initial conditions for the simulations of interest. Table A1 summarizes details of the domain properties. It should be noticed that there is a factor of 10 between the horizontal permeability and vertical permeability, making it easier for CO_2 to travel in the lateral direction than upward. Geological characterizations of various saline aquifers have shown that in the actual aquifers the horizontal permeability to vertical permeability ratio (or equivalent directional permeability ratio) could be up to the order of hundred to thousand. For example, the ratio is approximately 18 for the Utsira formation based on the layered model obtained from the core sample.

Table A1. Geological properties, initial conditions and boundary conditions of the domain

Permeability (anisotropic)	$k_H = 1.0 \times 10^{-12}$ m^2, $k_V = 1.0 \times 10^{-13}$ m^2
Porosity	0.12
Residual brine saturation	0.2
Residual CO_2 saturation	0.05
Relative permeability	Van Genuchten - Mualem
Capillary pressure	Van Genuchten - Mualem
Thermal condition	Isothermal
Boundary conditions	Fixed-state on circumference of lateral boundary; no mass flux on ceiling and floor
Initial condition	P = 120 MPa, T = 45 ^{o}C for equilibrium simulation
Initial CO_2 mass fraction	$X_{CO2} = 0$
Initial salt mass fraction	$X_{sm} = 0.15$

A.2 Bézier curve

A Bézier curve is a parametric curve frequently used in computer graphics and related fields. It is defined by a set of control points, and uses them as coefficients of a certain polynomial to describe continuous curves [13]. The control points of a Bézier curve can be denoted as P_0 through P_n, with (n -1) being the order of the Bézier curve. The order determines the complexity of the Bézier curve. A generalized mathematical expression of an nth order Bézier curve can be formulated explicitly as follows.

$$B(t) = \sum_{i=0}^{n} \binom{n}{i} (1-t)^{n-i} t^i P_i \tag{A1}$$

where (n, i) is the binomial coefficient, P_i is the i^{th} control point defined prior to the generation of Bezier curve, and t is a variable defined on [0,1]. An example of cubic Bezier curves, using four control points defined as P_1, P_2, P_3, and P_4, is illustrated in Figure 8.

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