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Targeted Pressure Management during CO_2 Sequestration: Optimization of Well Placement and Brine Extraction

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Abstract

Large-scale pressure increases resulting from carbon dioxide (CO_2) injection in the subsurface can potentially impact caprock integrity, induce reactivation of critically stressed faults, and drive CO_2 or brine through conductive features into shallow groundwater. Pressure management involving the extraction of native fluids from storage formations can be used to minimize pressure increases while maximizing CO_2 storage. However, brine extraction requires pumping, transportation, possibly treatment, and disposal of substantial volumes of extracted brackish or saline water, all of which can be technically challenging and expensive. This paper describes a constrained differential evolution (CDE) algorithm for optimal well placement and injection/ extraction control with the goal of minimizing brine extraction while achieving predefined pressure contraints. The CDE methodology was tested for a simple optimization problem whose solution can be partially obtained with a gradient-based optimization methodology. The CDE successfully estimated the true global optimum for both extraction well location and extraction rate, needed for the test problem. A more complex example application of the developed strategy was also presented for a hypothetical CO_2 storage scenario in a heterogeneous reservoir consisting of a critically stressed fault nearby an injection zone. Through the CDE optimization algorithm coupled to a numerical vertically-averaged reservoir model, we successfully estimated optimal rates and locations for CO_2 injection and brine extraction wells while simultaneously satisfying multiple pressure buildup constraints to avoid fault activation and caprock fracturing. The study shows that the CDE methodology is a very promising tool to solve also other optimization problems related to GCS, such as reducing 'Area of Review', monitoring design, reducing risk of leakage and increasing storage capacity and trapping.

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*Keywords:*carbon sequestration; pressure management;brine extraction; optimization; differential evolution algorithm

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1. Introduction

Large-scale pressure increases during geologic carbon sequestration (GCS) may impact caprock integrity, induce fault slippage, and cause leakage of brine and/or CO_2 into shallow fresh groundwater resources. Extraction of native brine during GCS operations is a pressure management approach for controlling pressure buildup to reduce risk of environmental impacts and increase storage capacity [1–4]. However, pumping, transportation, treatment and disposal of extracted brine can be challenging and costly [5, 6]. Therefore, minimizing the volume of extracted brine, while maximizing CO_2 storage and meeting other constraints needed for safe and efficient GCS operations, is an essential objective of pressure management with brine extraction schemes.

In earlier work [4], the concept of "impact-driven pressure management (IDPM)" was introduced with the goal of limiting pressure increases primarily where environmental impact is a concern, such as a critically-stressed faults and/or a leaky well field. To design and optimize "impact-driven" pressure management options, *Birkholzer et al.* [4] employed a gradient-based optimization methodology coupling the iTOUGH2 inverse-modeling framework [7, 8] and an analytical solution for single-phase flow in multilayered aquifer systems [9]. The optimization methodology was applied for brine extraction in response to a hypothetical injection scenario nearby a critically-stressed fault in a multilayered aquifer system. Time-dependent pumping rates from a series of extraction wells at fixed locations (either near to the injection zone or close to a fault) were computed to keep pressure buildup along the fault at/below a critical value for fault slippage, while minimizing the brine extraction ratio (Brine extraction ratio is defined as ratio of total volume of extracted brine divided by the total volume of injected fluid.). The results from this study suggest that optimization can allow for a significant reduction in the brine extraction volumes needed to keep pressure increase in the storage formation below a given critical value. However, placing of injection and extraction wells is not intuitive in real cases because of heterogeneity in reservoir properties and complex reservoir geometry. Optimization results without considering unknown well locations under such complex conditions will be likely suboptimal.

Efficient computerized algorithms combining reservoir models and optimization methods are needed to make proper decisions on well locations and control parameters. The irregularity of objective functions due to complex reservoir heterogeneity and geometry can easily cause gradient-based method solutions to be stuck in a local minimum. Derivative-free global optimization methods are more suitable for solving the coupled optimal well placement and rate control problems in application to GCS. However, global optimization methods such as commonly used evolutionary algorithms require a large number of forward model runs to reach a global optimum. Parallelization of the algorithms in a multi-processor computer or cluster environment is typically needed for solving larger reservoir problems in a computationally efficient manner [10, 11].

This study, built upon our earlier work in *Birkholzer et al*. [4], presents a global optimization methodology for pressure management during geologic CO_2 sequestration. A differential evolution (DE) algorithm is introduced for solving constrained global optimization problems involving well placement and brine extraction to control pressure increases during GCS. The constrained differential evolution methodology is described and tested by using a simple optimization problem whose optimal solution can be found with other optimization methods. Then, a more complex application of the global optimization methodology is presented for a hypothetical CO_2 injection scenario in a heterogeneous reservoir containing critically stressed faults. Optimal placements of wells and selection of injection and extraction rates are evaluated under the constraints that the maximum pressure buildup does not exceed critical pressure changes for fault activation and caprock fracturing, and that no CO_2 is to be pulled into extraction wells.

2. Problem Description

The focus in this paper is on optimization of brine extraction for controlling pressure locally in environmental impact zones (e.g., faults, caprock damage around injection wells). Let the total volume of injected CO_2 be denoted by V_{inj} and the total volume of extracted fluid by V_{ext}. The goal is to minimize the extraction ratio defined by V_{ext}/V_{inj}. The optimization problem involving the objective function and the constraints, respectively, can be formally expressed as

$$\text{Minimize} \qquad f(\boldsymbol{p}) = V_{ext}/V_{inj} \tag{1}$$

Subject to $g_1(\boldsymbol{p}) = V_{ext,CO_2} = 0$ (2a)

$$g_2(\boldsymbol{p}) = \max\left\{\Delta\boldsymbol{P}(\boldsymbol{x_{obs}}, \boldsymbol{y_{obs}}, t)\right\} - \Delta\boldsymbol{P_{crt}} < 0 \quad (2b)$$

where $\boldsymbol{p}$ is the parameter vector that may involve locations of injection wells (x_{inj}, y_{inj}) and extraction wells (x_{ext}, y_{ext}), and constant or time-dependent function parameters for controlling injection and extraction. Specific costs associated with the pumping per volume of injected or produced fluid and treatment of extracted brine are assumed to be proportional to the extraction ratio defined in Eq. (1). Other costs related to drilling of wells are not considered. The first constraint in Eq. (2) assures that no CO_2 breakthrough occurs at the extraction wells to keep the efficiency of the brine extraction scheme and secure for all the injected CO_2 to remain in the reservoir. The second constraint represents the pressure management goal of keeping reservoir pressure increases in defined impact zones below one (or more) critical pressure buildup values (ΔP_{crt}) (with respect to the pressure prior to the injection). We may assume that an environmental impact can be expected if the pressure buildup at any location in the impact zones exceeds ΔP_{crt}. Pressure buildup at impact zones is recorded through a vector of observation points (x_{obs}, y_{obs}) as many as required. The optimization problem may also involve additional constraints, such as parameter bounds, which are not included in Eq. (2).

3. Methodology

In this section, the basic strategies of the DE algorithm [12] and modifications to obtain a CDE (constrained differential evolution) algorithm for treatment of constraints are briefly described. DE is a parallel direct search method that was originally developed by *Storn and Price* [13] and has been proven to be a very powerful evolutionary algorithm [14] with good convergence properties, simplicity for using and understanding, and suitability for parallelization. Since the DE's first development, different variants have been proposed for accelerating its convergence rate [15], but the original method is in general applicable to unconstrained optimization problems. In this work, we have modified the DE algorithm based on *Deb* [16] to solve constrained global optimization problems relevant to GCS projects.

A DE algorithm has four main steps consisting of initialization, mutation, crossover and selection [12]. The initialization step involves generation of D-dimensional parameter vectors. The dimension D is equal to the number of unknown parameters, and each parameter vector represents one member of a NP-sized population. The number of members, NP, stays fixed during optimization process. Parameters of the vectors at the initial generation can be selected randomly from the entire parameter space based on user-defined parameter bounds and/or prior knowledge if available. Let the NP D-dimensional parameter vectors be denoted as $\boldsymbol{p}_i^G; i = 1, 2, \ldots, \mathrm{NP}$, where G is the generation (or iteration) number, and G is equal to 0 at the initial generation step. At each new generation step G+1, DE produces an intermediary population containing mutant vectors for each member of $\boldsymbol{p}_i$ (referred to as target vector). The basic DE strategy constructs new parameter vectors (mutant vectors) by adding weighted differences of two population vectors to a third vector. This step is called mutation. Since the first development of the basic strategy, many different mutation strategies have been devised and used for different types of optimization problems [15]. In this study, a variant of the basic mutation strategy based on linear combination of the best member ($\boldsymbol{p}_{best}^G$, the vector giving the best objective function value) and current members of the population at G has been selected because of its higher computational efficiency for the problems tested in this manuscript. For each target vector $\boldsymbol{p}_i$ (i=1,...,NP), a mutant vector $\boldsymbol{v}_i$ is produced by adding contributions of the differential variations $F_c(\boldsymbol{p}_{best}^G - \boldsymbol{p}_i^G)$ and $F_m(\boldsymbol{p}_{r1}^G - \boldsymbol{p}_{r2}^G)$, where F_c is a random combined factor $\in$[0,1], F_m is the mutation scaling factor $\in$[-1,1], and r_1 and r_2 are random mutually different integers $\in$ {1,2,...,NP}, selected to be different from the index *i*. Then, parameters of the mutant vectors ($v_{i,j}^{G+1}$, j=1,...,D) are combined with the parameters of the target vector ($p_{i,j}^G$, j=1,...,D). This is called crossover operation, and the resultant vectors are trial vectors, $\boldsymbol{u}_i^{G+1} = (u_{i,1}^{G+1}, u_{i,2}^{G+1}, \ldots, u_{i,D}^{G+1})$, whose parameters are selected from the mutant vectors if randomly generated numbers for each $j \in$[0,1] is greater than a user-specified crossover probability $\in$[0,1], or else they are equal to the target vectors . The last step in the DE algorithm is the selection process for the surviving members of the population. In this step, the objective function values of the trial vector, obtained by evaluating running forward model for each population member, are compared to those of the target vector. The trial vectors giving smaller objective functions are replaced with the corresponding target vectors, and otherwise the old values are kept. If the tolerances specified (and other possible termination options) are met, then the algorithm terminates, or else it returns to the mutation step for the next iteration. *Price et al*. [15] discussed several termination options that can be selected based on the specific nature of an optimization problem. In this work, termination occurs if the difference between the best and the worst value of the population becomes less than a predetermined tolerance at the end of an iteration, which was set to 10^{-5}.

In this work, the selection process of the DE algorithm specifically comparing the trial vectors with the target vectors is modified to take into account constraints. We refer to this modified algorithm as constrained differential algorithm, or CDE. *Deb* [16] proposed a general constraint handling methodology for evolutionary algorithms. A penalty term is added to the objective function to penalize infeasible solutions (violating constraints), but different from conventional penalty function methods, no penalty terms are needed for constraints. *Deb* [16] proposed a tournament selection operator based on the following criteria: 1) Any feasible solution is preferred to any infeasible solution, 2) among two feasible solutions, the one having the smaller objective function value is preferred, and 3) among two infeasible solutions, the one with the smaller constraint violation is preferred. Compared to DE, CDE requires evaluations at each new generation and storage of not only the objective functions but also of the constraints by running the forward model for NP parameter vectors. We implemented the CDE algorithm described above by modifying an existing FORTRAN90 code for DE algorithm developed by Dr. Feng-Sheng Wang and his students (http://www1.icsi.berkeley.edu/~storn/code.html#f90c). The modified code was parallelized for running multiple forward model simulations simultaneously in multi-processor computing environments.

4. Verification and Application

4.1. Testing of the optimization algorithm for a simple pressure management problem

The performance of the CDE algorithm is tested for a simple optimization problem involving placement of a brine extraction well and optimization of the extraction rate. The test problem is defined such that the optimal extraction location is in fact known and that a gradient-based optimization method can be used to determine the extraction rate. An injection well placed into origin injects fluids at a constant rate of 1.67×10^{4} m^3/d for 50 yr into a 60m-thick aquifer overlaid by a 100m-thick aquitard. The aquifer has a permeability of 3.0×10^{-13} m^2, fluid density of 1095.62 kg/m^3 and a specific storativity of 1.69×10^{-6} m^{-1}. The aquitard has a permeability of 10^{-18} m^2, fluid density of 1078.41 kg/m^3 and a specific storativity of 1.98×10^{-6} m^{-1}. Two abandoned wells exist (red colored) at 20 km east and south of the injection well (Fig. 1), and they are assumed to have potential to leak and transmit poor-quality water into a freshwater aquifer above the aquitard. The critical pressure buildup (ΔP_{crt}) for brine leakage to occur into the freshwater aquifer through the potentially leaky abandoned wells is assumed to be 0.2 MPa.

The goal is to use an extraction well, operating with a minimum extraction ratio (V_{ext}/V_{inj}), to keep the pressure buildup below the critical pressure buildup at the abandoned well locations for preventing any possible leakage. In this example, a single-phase analytical model [9] is selected as the forward model to simulate pressure buildup in the layered aquifer system in response to injection and extraction. As single-phase flow conditions are assumed, the minimization problem contains only the second constraint in Eq. (2) (i.e. pressure buildup constraint), excluding constraints on parameter bounds.

In this simple example, the optimal extraction well location is known to be at (x=10km, y=-10km), but the optimal rate is not known and can vary as a function of time. We tested an extraction scenario in which the extraction rate is assumed to be constant during the duration of the injection. Since the location of the extraction well is known, a gradient-based algorithm can easily be implemented to find optimal extraction rates. Additionally, the CDE algorithm is applied to estimate both optimal extraction rate(s) and optimal well location, in this case assuming the location is unknown. Then, the results of the CDE algorithm are compared against the known well location, and against the extraction rate results obtained from the gradient-based optimization method, using a sequential quadratic programing (SQP) algorithm built into the Fortran IMSL library. We use the SQP algorithm that was developed by *Spellucci* [17] for nonlinear optimization problems with equality and inequality constraints to estimate optimal extraction rate(s) with known well locations.

The number of unknown parameters for the CDE is equal to 3 (D=3). As shown in Table 1, the CDE search finds the optimum well location, and the extraction rates obtained by CDE agree very well with those calculated by the

SQP method. NP was selected as 10×D. The dimension or number of unknowns for the problem solved by the SQP is two parameters less than the CDE because the SQP method does not solve for the extraction well location. The table also compares the number of function evolutions during optimization by the CDE and the SQP algorithms. Although the larger number of forward models required for the CDE may seem to be an issue for very large numerical forward models, the CDE algorithm is easily parallelizable, which allows for very fast computation in a multi-processor computer or cluster environment.

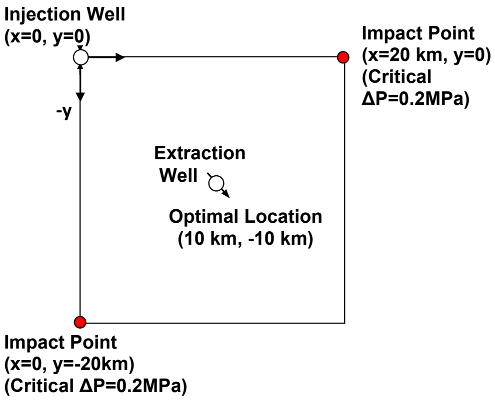

Fig. 1. Example problem for testing the CDE optimization method

Table 1. Optimization results for the simple test problem

	CDE D=3	SQP D=1
x (km)	10.07	-
y (km)	-10.07	-
Q (m^3/d)	-1.049×10^4	-1.049×10^4
Optimal Ext. Ratio	0.774	0.774
Number of Obj. Func. Evaluations	1620	12

4.2. Application to a hypothetical scenario of CO_2 injection and brine extraction in a heterogeneous reservoir

In this section, we demonstrate the applicability of the CDE algorithm for a CO_2 injection scenario in a large-scale geological setting. In the hypothetical application scenario below, injection of CO_2 is planned from a limited number of injection wells at an unknown constant optimum rate over 30 years. To simplify the problem, we assume that the heterogeneous reservoir involves only one fault and four different facies with varying hydraulic properties (Fig 2a). The injected reservoir is 60m thick and bounded at the top and bottom by impermeable formations. We assumed that the pressure buildup along the fault must be below 0.55 MPa to prevent possible fault activations. The threshold pressure increase for fracturing of the caprock overlying the storage reservoir is assumed to be 8 MPa. Prior numerical simulations without optimization indicate that when an industrial-scale CO_2 injection occurs from a single well at a rate of 1.5 million tons per year over 30 years, as shown in Figure 2b, the fault would experience pressure buildup significantly higher than the threshold value for the activation. Thus, pressure management via targeted brine extraction is particularly suitable because the pressure control needs to be along the fault. On the other hand, well locations and pumping rates need to be carefully designed to minimize extraction volumes and to avoid pulling CO_2 into the extraction wells and even near the faults. The initial results also indicate that caprock damage may occur if injection occurs at rates higher than 1.5 million tons per year. In this example, we also seek to estimate maximum possible CO_2 injection mass with multiple injection wells without violating the pressure buildup constraint of 8 MPa for the caprock integrity.

We conducted an optimization of CO_2 injection and brine extraction (well locations and rates) to minimize the brine extraction ratio without violating the pressure threshold values along the faults and the injection zone, with the additional goal of not pulling any CO_2 into the extraction wells. The locations of the injection wells are constrained to be inside a rectangular zone as shown in (Fig 3a). The automated optimization algorithms require many forward runs of the numerical model to achieve the optimum solution. Thus, an efficient forward model is needed. We employed a numerical vertically-averaged two-phase flow model, recently developed at LBNL, for representing CO_2/brine flow in the reservoir. The numerical discretization for this model is based on the Finite Volume Method. Nonlinear systems of equations are linearized by using the Newton-Raphson (NR) method. The system of linear equations for each NR iteration value is solved using an iterative solution method (preconditioned restarted GMRES algorithm). Discretization of the numerical model domains was done in a manner that minimizes computational costs while maintaining sufficient accuracy. In this application, we generally discretized the model domains with seven to ten thousand finite volume grid blocks. The grid sizes used in the numerical model vary from few meters to few kilometers, and typically finer grid sizes were selected around the injection and extraction wells. The lateral boundaries of the numerical model domain are set as fixed pressure boundary conditions.

Fig 3 shows the estimated well locations and resulting CO_2 distribution (contour flood filled with color) and pressure buildup (contour lines). The CDE successfully estimated the locations of both injection and extraction wells. Figure 4 shows how the developed methodology simultaneously satisfies the pressure buildup constraints along the fault and the injection zone (Fig 4a) and estimates optimal injection and extraction rates (Fig 4b). The optimization results show that for this hypothetical scenario, about 3.5 million tons supercritical CO_2 per year can be injected from four injection wells without causing fracturing of the caprock, and that fault activation can be prevented by using two extraction wells nearby the fault operating with an extraction ratio of about 22%.

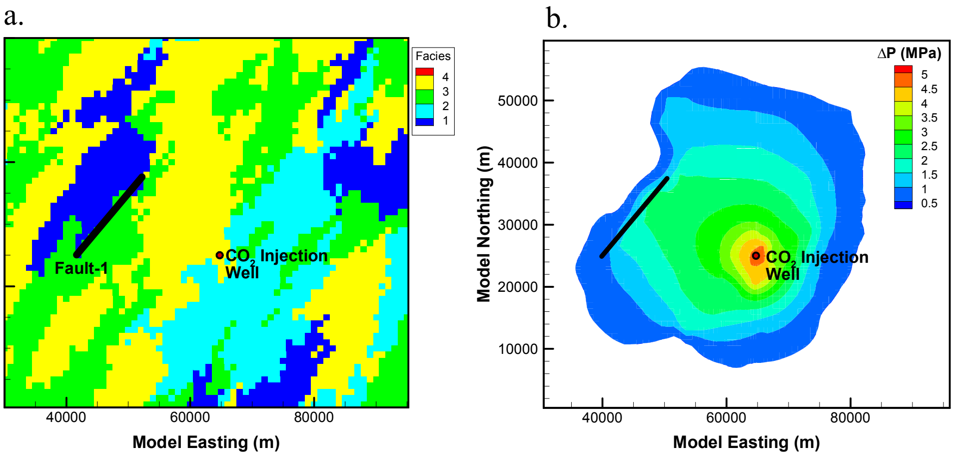

Fig 2. (a) A hypothetical heterogeneous reservoir for CO_2 injection through a vertical well nearby a critically-stressed fault; (b) Pressure buildup distribution at the end of the injection (30 yr) of 1.5 million tons per year from a single well without optimization through brine extraction.

Table 2. Material properties as input for vertically integrated models

Properties	Facies 1	Facies 2	Facies 3	Facies 4
Porosity	0.2	0.2	0.2	0.2
Permeability (m^2)	10^{-15}	10^{-14}	10^{-13}	3×10^{-13}
$*\alpha$ (m^{-1})	8.31×10^{-3}	2.81×10^{-2}	6.29×10^{-2}	9.91×10^{-2}
S_{rw}	0.2	0.2	0.2	0.2
$*n$	2.42	2.00	2.59	2.94
$*L_w$	0.01	0.01	0.01	0.01
$*L_n$	1.4	1.26	1.17	1.25

* α, n : van Genuchten model parameters [18]

* L_w, L_n: Modified van-Genucten-Mualem relative permeability model parameters
* Effective parameters obtained by fitting vertically averaged capillary pressure-saturation-relative permeability functions to van-Genuchten and Mualem models.

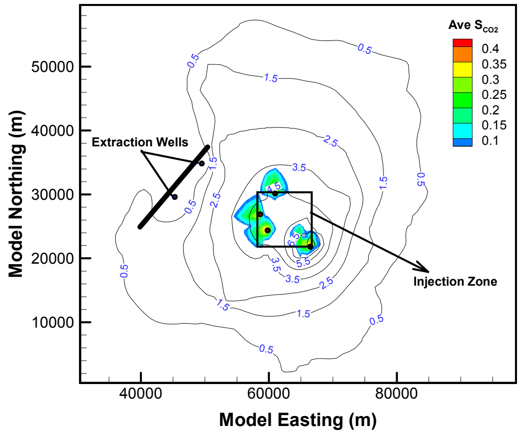

Fig 3. The optimized pressure buildup (in MPa) and average CO_2 saturation distribution at the end of 30 years. This scenario involves two extraction and four injection wells, the latter injecting about 3.5 million tons supercritical CO_2 per year.

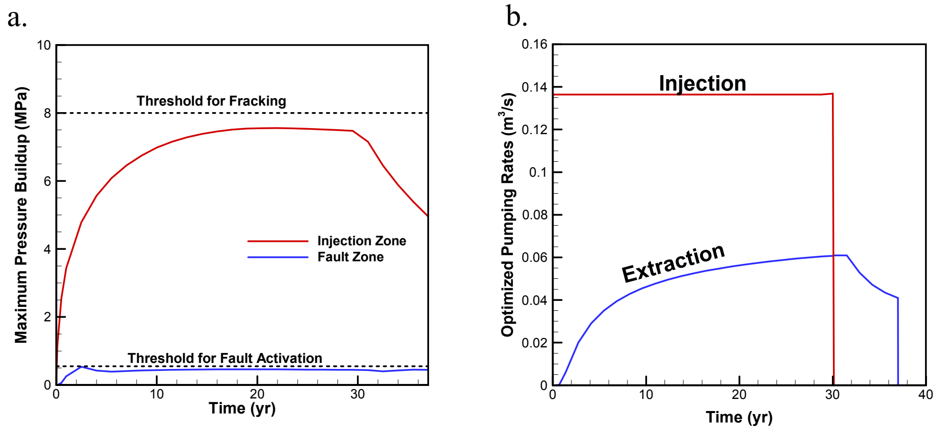

Fig. 4. (a) Maximum pressure buildup along the fault zone and in the injection zone; (b) estimated optimal total injection/extraction rates.

5. Conclusion

This study demonstrated applications of a constrained differential evolution (CDE) algorithm for solving global optimization problems involving well placement and injection/extraction control. The CDE methodology was tested for a simple optimization problem whose solution can be partially obtained with a gradient-based optimization methodology (SQP). The CDE successfully estimated the true global optimum for both extraction well location and extraction rate. A more complex example application of the developed strategy was also presented for a hypothetical CO_2 storage scenario in a heterogeneous reservoir consisting of a critically stressed fault nearby an injection zone. Through the CDE optimization algorithm coupled to a recently developed numerical vertically-averaged reservoir model, we successfully estimated optimal rates and locations for CO_2 injection and brine extraction wells while simultaneously satisfying multiple pressure buildup constraints for the fault activation and the caprock fracturing.

The CDE methodology is general enough to solve other optimization problems related to GCS, such as reducing 'Area of Review', monitoring design, reducing risk of leakage and increasing storage capacity and trapping. Our future work includes real-time applications of the optimization methodology for realistic CO_2 storage studies in actual reservoir systems. Geological uncertainty in reservoir properties needs to be taken into account in real applications. We will continue to apply and determine appropriate optimization strategies and range of parameter sets to deal with geological uncertainty in the CDE algorithm for efficiently and accurately solving specific optimization problems mentioned above.

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