Global optimization of injection well placement toward higher safety of CO$_2$ geological storage

Takashi Goda$^{a, *}$, Kozo Sato$^b$

$^a$Dept. of Information & Communication Engineering, The University of Tokyo, 2-11-16 Yayoi, Bunkyo-ku, Tokyo 113-0032, Japan  
$^b$Frontier Research Center for Energy and Resources, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Abstract

Optimization of injection well placement deserves careful and thoughtful consideration to achieve the higher safety of CO$_2$ geological storage. In this study, a storage safety is quantified as a proportion of the immobile and dissolved CO$_2$ to the total injected amount. Here we revisit the definition of immobile CO$_2$ from a standpoint of long-term CO$_2$ migration. Owing to the irreversibility of relative permeability curves, a fraction of CO$_2$ which is displacing brine will eventually become trapped as residual CO$_2$ when the switchover from drainage to imbibition process takes place. From this observation, we propose a new definition for immobile CO$_2$, which is preferred as a measure of long-term storage safety. Using the above quantitative measure of storage safety as an optimality criterion, we attempt to optimize an injection well placement. We combine the popular numerical simulator TOUGH2/ECO2N with our recently-proposed derivative-free global optimization algorithm, and search an optimal well placement for a realistic heterogeneous reservoir model. Numerical examples confirm that our algorithm can find a promising optimal solution effectively within a practical number of simulation runs.

Keywords: CO$_2$ geological storage; storage safety; global optimization; well placement; residual trapping

1. Introduction

CO$_2$ geological storage is one of the most promising options to reduce the anthropogenic emissions of CO$_2$ into the atmosphere. Since over 3000 projects will be required by 2050 for a significant contribution to climate change mitigation [1], there is an urgent need to construct an integrated storage system toward a realization of a long-term secure storage. Here, secure storage means that the injected CO$_2$ will remain trapped within a target geological reservoir by effective physical and geochemical mechanisms. There are four well-known trapping mechanisms: structural, residual, solubility and mineral trappings. Structural
trapping plays a primary role in preventing the buoyant CO₂ from migrating upward. The secondary mechanisms, such as residual and solubility trappings, are crucial for CO₂ to be immobilized or to migrate downward within the reservoir. In general, storage safety of the secondary mechanisms is considered to be higher than that of the primary mechanism [2]. Thus, what we need to do for reliable implementations of CO₂ geological storage is to enhance the amount of immobile and dissolved CO₂. In this context, some researchers have discussed operational strategies [3, 4]. These studies, however, demonstrated their proposed strategies only through numerical simulations, and are still in the preliminary stages for practical applications.

In this study, we discuss optimization of injection well placement, which is one of the most practical strategies to enhance the amount of immobile and dissolved CO₂ [5, 6]. The objective is to maximize a proportion of the immobile and dissolved CO₂ to the total injected amount, or in other words, to minimize a proportion of the mobile CO₂. The parameters to be optimized consist of grid index and injection rate of each injection well. When the placement of multiple injection wells is to be optimized simultaneously, the number of parameters will grow linearly and the parameter space possibly contains a lot of local optima. For such a problem, local search algorithm yields different optimal solutions according to initial estimates and requires several independent runs until a reliable solution can be obtained, as in [5]. In order to avoid local optima, and yet to search a better solution, the population-based search algorithms have come under the spotlights as the versatile and practical means to cope with the global optimization problems. In the recent study, the authors proposed a new population-based search algorithm, iterative Latin hypercube samplings (ILHS), and demonstrated its applicability through comparison with other popular algorithms for many high-dimensional benchmark functions [7]. In this study, we apply ILHS to global optimization of injection well placement toward higher safety of CO₂ geological storage.

In this regard, however, a question arises as to at what point the objective function, a proportion of the immobile and dissolved CO₂, should be evaluated. In the previous studies [5, 6], the objective function is evaluated at a certain time \( t \), or time-averaged between \( t_1 < t < t_2 \). In these approaches, we cannot ensure a storage safety for a later period, that is, this optimality criterion is not suitable for measuring a long-term storage safety. To solve this problem, we revisit the definition of immobile CO₂ and propose a new definition which counts the potential amount of immobile CO₂ by taking into account the irreversibility of relative permeability curves. Using a new definition for immobile CO₂, we can ensure a storage safety for a later period. In Section 2, we review the relative permeability hysteresis and discuss how to define the immobile CO₂. In Section 3, we present the algorithm of ILHS and apply it to optimization of injection well placement for a realistic heterogeneous reservoir model. Section 4 concludes this study.

2. Definition of immobile CO₂ revisited

In this section, we revisit how to define the immobile CO₂. First we review the most popular model for relative permeability hysteresis developed by Land [8]. In the following, \( S \) denotes CO₂ saturation. Let us suppose that the switchover from drainage to imbibition takes place at CO₂ saturation of \( S_{hys}^g \). Then, the trapped CO₂ saturation \( S_{gr} \) is given by

\[
S_{gr} = \frac{S_{hys}^g}{1 + C \cdot S_{hys}^g},
\]

where the Land coefficient \( C \) is defined as

\[
C = \frac{1}{S_{gr,max}} - \frac{1}{1 - S_{g,max}}.
\]
Fig. 1. Definitions of immobile CO$_2$: (a) factual immobile CO$_2$; (b) potential immobile CO$_2$

Here, $S_{g.t,\text{max}}$ and $S_{g,\text{max}}$ are maximum trapped and maximum CO$_2$ saturation, respectively. We note that $S_{g.t}$ is a monotone function of $S_{g}^{\text{hys}}$ in Land model. The secondary drainage curve for $S_{g} < S_{g}^{\text{hys}}$ corresponds to the primary imbibition curve. Once $S_{g}$ becomes greater than $S_{g}^{\text{hys}}$ in the secondary drainage process, the primary drainage curve is followed. As shown in Fig 1(a), in the classical definition, there is no trapped saturation assigned for CO$_2$ both in the primary drainage process and in the secondary drainage process with $S_{g} > S_{g}^{\text{hys}}$. In order to distinguish from our new definition for immobile CO$_2$, we call the classical definition factual immobile CO$_2$, which can be usually written as follows.

**Definition 1 (Factual immobile CO$_2$)** Only the trapped CO$_2$ saturation in the imbibition process and in the secondary drainage process with $S_{g} \leq S_{g}^{\text{hys}}$ is counted as immobile CO$_2$.

$$S_{g,t}^{\text{fac}} (t) = \begin{cases} S_{g,t} \left( S_{g}^{\text{hys}} \right) & S_{g} (t) \leq S_{g}^{\text{hys}} \\ 0 & \text{otherwise} \end{cases}$$  \hspace{1cm} (3)

In this definition, when the switchover from the imbibition to the drainage takes place and $S_{g}$ becomes greater than $S_{g}^{\text{hys}}$, all the immobile CO$_2$ will turn into mobile. Although this might be the case if we focus on the state of a certain time $t$, it is quite confusing because ‘immobile’ can possibly become ‘mobile’. In order to avoid this confusion and to reflect the view of long-term CO$_2$ migration for a later period, we now propose a new definition for immobile CO$_2$, called potential immobile CO$_2$, as follows.

**Definition 2 (Potential immobile CO$_2$)** The trapped CO$_2$ saturations not only in the imbibition process but also in the drainage process are counted as immobile CO$_2$. For CO$_2$ in the primary drainage process and in the secondary drainage process with $S_{g} > S_{g}^{\text{hys}}$, the switchover saturation $S_{g}^{\text{hys}}$ is replaced by the current CO$_2$ saturation $S_{g}$.

$$S_{g,t}^{\text{pot}} (t) = S_{g,t} \left( S_{g}^{t} \right) \quad \text{where} \quad S_{g}^{t} = \sup_{t' \leq t} S_{g} (t')$$ \hspace{1cm} (4)

The schematic of the new definition is described in Fig 1(b). In the new definition, a fraction of CO$_2$ which is displacing brine is regarded as immobile because when the switchover from drainage to imbibition takes place in the future, at least $S_{g,t}^{\text{pot}} (t)$ will be trapped as residual CO$_2$. Even if the switchover from imbibition to drainage takes place, the irreversibility of relative permeability curve prevents CO$_2$ saturation from falling below $S_{g,t}^{\text{pot}} (t)$, from which we can claim that at least $S_{g,t}^{\text{pot}} (t)$ will be trapped eventually. Thus, the new definition gives us a lower bound of the possible amount of immobile CO$_2$ and is suitable for measuring a long-term storage safety.
Remark 1 Several researchers have developed sharp-interface models to study CO₂ migration in the geological reservoirs more analytically, such as [9, 10]. Our new definition for immobile CO₂ can also be applied to these models.

Remark 2 Non-monotone function for a trapping saturation was discussed in [11]. In that model, our new definition no longer gives a lower bound of the possible amount of immobile CO₂ and is not suitable for measuring a long-term storage safety. Hence, we need to generalize Definition 2 as follows.

\[ S_{gt}^{int}(t) = \min \left( S_{gt}(S_g)^{\gamma} \right) \inf_{s > S_g} S_{gt}(S_g), \]  

(5)

where the denotation \( S_g' \) is given in (4). For any monotone function, since the latter term in the right-hand side is always greater than the former term, we can reduce to the expression (4).

3. Global optimization of well placement

Global minimization of a function \( f \) is a hard task due to the complicated interaction between the unknown parameters \( x \) and the lack of the prior information on \( f \). Even when we can compute the derivatives of \( f \) with respect to each parameter, it is quite challenging to find a global minimum because the derivatives give us only local information. Thus, the gradient-based optimization methods cannot be said to be robust, and the population-based search algorithms have come under spotlight as the versatile and practical means to cope with the global optimization problems. The fundamental idea is to generate a number of samples at once and to search a parameter space by changing their locations step by step without any information on the derivatives. These algorithms have two important capabilities in common: one is to search a better solution and the other is to avoid local minima. Another invaluable advantage from the viewpoint of the computational effort is that multiple simulation runs can be carried out in parallel at each step, reducing the effective computation time. The major disadvantage of these algorithms, on the other hand, arises in the slow rate of convergence.

As mentioned in Section 1, the authors recently proposed a new population-based search algorithm, iterative Latin hypercube samplings (ILHS) [7]. We confirmed the faster convergence rate of ILHS for a wide class of functions than other popular algorithms, such as particle swarm optimization and differential evolution. Further, the authors successfully applied ILHS to history matching for finding an optimal permeability distribution so as to reproduce the measurement data with a high degree of accuracy. Therefore, it is natural for us to apply ILHS to global optimization of injection well placement.

3.1. Iterative Latin hypercube samplings

Here, the rough sketch of our algorithm is described. See Fig 2 for the schematic of ILHS. In the following, \( s \) denotes the dimensionality of function that is determined by a particular problem.

**Algorithm**

1. Set \( n \), a population size at each iteration, and \( \gamma \), an exponent appearing in the process 3.
2. Generate a point set by Latin hypercube sampling with cumulative functions, \( F_j \) (j=1, ..., s). Note that the uniform distribution is used for each parameter at the first iteration. Considering the random permutation \( \{\pi_{ij}, ..., \pi_{in}\} \) of \( \{1, ..., n\} \) for each parameter. The \( i \)-th point for \( i=1, ..., n \) is given by

\[ x_{ij} = F_j^{-1} \left( \frac{\pi_{ij} - \varepsilon_{ij}}{n} \right), \]  

(6)
where $\omega_{ij}$ is an uniform variate $U[0,1]$.

3. Evaluate the function values at $n$ points, and project those values for each parameter axis.

4. Assign the weights for distinct $n$ intervals according to the rankings among them

\[
\omega_i = r_{ij}^{\gamma} / Z ,
\]

where $r_{ij}$ denotes the rank of the function value for the $i$-th interval among the entire $n$ values and $Z$ is the normalizing constant. Then, update the cumulative functions

\[
F_j(x_i) = \sum_{i=1}^{n} \omega_j \max \left[ 0, \min \left( \frac{x_i - x_{ij}^{-}}{x_{ij}^{+} - x_{ij}^{-}}, 1 \right) \right] ,
\]

where $x_{ij}^{-}$ and $x_{ij}^{+}$ denote the lower and upper bounds of the $i$-th interval.

5. If the stopping criterion is not satisfied, return to the process 2.

The authors empirically recommended to use $n \in [2\times5\times]$ and $\gamma$ such that its normalized entropy is in the range of $[0.7,0.99]$. Due to space limitation, we omit the detail explanations.

3.2. Problem setting

We constructed the geological structure using examples from Nagaoka pilot project whose reservoir model was enlarged so as to simulate a large-scale storage project. The reservoir size was $6400 \text{ m} \times 6400 \text{ m} \times 100 \text{ m}$ and was divided into $64 \times 64 \times 5$ grids of equal size. The permeability heterogeneity was randomly generated by the geostatistical method, sequential Gaussian simulation [12]. As for the relative permeability curves, the famous power-law model was used for the drainage process, and the Land model was applied to simulate the hysteresis of CO$_2$. We have modified the source code of TOUGH2/ECO2N for implementing these curves [13].
The injection rate and the injection period were set to 1 Mt/year and 20 years, respectively. The simulation period was set to 100 years, the injection period and its subsequent post-injection period of 80 years. The goal of optimization is to minimize a proportion of mobile CO₂ at the end of the simulation period. The objective function $f$ can be explicitly formulated as follows:

$$f = \frac{m_{\text{mobile}}}{m_{\text{total}}} = 1 - \frac{m_{\text{immobile}} + m_{\text{dissolved}}}{m_{\text{total}}}.$$  (9)

where $m_{\text{total}}$ is the total injected amount of 20 Mt, while $m_{\text{mobile}}$, $m_{\text{immobile}}$, and $m_{\text{dissolved}}$ are the amount of mobile, immobile and dissolved CO₂ at 100 years, respectively. The second equality is obtained because the sum of three individual amounts is equal to the total. In case that some CO₂ escapes from the model reservoir, the corresponding amount is counted as mobile in this example. As we discussed in Section 2, our new definition for immobile CO₂ is suitable for measuring a long-term storage safety and the objective function is less sensitive to the simulation period than the classical definition. Parameters to be optimized consisted of grid index and injection rate of each injection well. When only one injection well is considered, the grid index does matter. Each injection well was supposed to be vertical and be completed through all the layers, so that the horizontal placement is tunable.

### 3.3. Numerical results for one to three wells

For one injection well, we have two parameters; $x$- and $y$-grid indices of the well. We gave the population size of 6 and the normalized entropy of 0.9. The maximum iteration was set to 30. Thus, the number of simulation runs was 180 for one trial. We repeated four independent trials with the same parameter setting and obtained four different but close solutions as follows:

(48, 21), (45, 23), (46, 23), and (48, 29)
The corresponding values of $f$ are 0.0438, 0.0534, 0.0471, and 0.0558, respectively. Therefore, every optimal solution shows that about 95% of the injected CO$_2$ can be trapped by the secondary mechanisms in 100 years. As a population-based search algorithm, ILHS could avoid local minima effectively, and find a similar solution for every trial.

When the placement of two injection wells is to be optimized at the same time, we have five parameters: two pairs of $x$- and $y$-grid indices of each well, and a proportion of injection rate of one well to the total rate, $p$. This means that the injection rate of one well is $p$ Mt/year and that of the other well is $(1-p)$ Mt/year. We gave the population size of 10 and the normalized entropy of 0.9. The maximum iteration was set to 30. Two independent trials were repeated with the same parameter setting. The optimal solutions became as follows:

$$\{(47, 19), (52, 34), 0.727\}, \{(48, 20), (51, 32), 0.573\}$$

Well locations of two solutions are similar to each other, and the former well lies in the vicinity of the optimal solutions for one-well case. The injection rates of former are larger than that of the latter for both the trials. The corresponding values of $f$ are 0.0338 and 0.0276, respectively, and both are smaller than all the four trials for one-well case.

Finally, we attempted three-well case for global optimization. In this case, we have eight parameters: three pairs of $x$- and $y$-grid indices of each well and the proportion of injection rate of the first well, $p$, and the proportion of the remaining injection rate of the second well, $q$. This means that the injection rates of the first, second and last well are $p$, $(1-p)q$ and $(1-p)(1-q)$ Mt/year, respectively. We gave the population size of 20 and the normalized entropy of 0.9. The maximum iteration was set to 30. The optimal solution for one trial is as follows:

$$\{(27, 27), (48, 18), (51, 32), 0.157, 0.548\}$$

The location of the latter two wells is quite close to the two-well cases. As for the injection rate, the first well has the smallest value, while the remaining two wells have relatively similar values to each other. The corresponding value of $f$ is 0.0212, smaller than the two-well cases.

3.4. Discussion

As can be seen from the minimized values of $f$, storage security could be enhanced by increasing the number of injection wells and optimizing those locations. We note, however, that we have found many solution candidates for two- and three-well placement, whose function values are larger than the optimal one-well case during the ILHS iterations. It stresses that we need to design well placement carefully, and that global optimization plays a key role in finding a promising solution.

In the above examples, the number of simulation runs for one trial is 180, 300 and 600 for each case. These numbers are quite small as compared to the number of the possible candidates for well location, $64^2 (=4096)$, $64^3 (\approx 1.7 \times 10^5)$ and $64^6 (\approx 6.9 \times 10^{10})$. Further, if multiple simulation runs can be executed in parallel, the time required for each iteration step is reduced at most to that required for one simulation run. The reduction rate, of course, depends on how many runs can be executed in parallel.

In general, if we attempt to optimize $m$ well placement, $2m$ and $(m-1)$ parameters are required for grid indices and injection rates, respectively. Thus, as the number of injection wells increases, the number of parameters to be optimized also increases linearly. When a population size $n\in[2s,5s]$ is too large to be executed in practical time constraint, we need to discuss how to reduce the dimensionality of optimization problems. One feasible approach is to optimize the placement well by well. As shown in this subsection, the optimal well location for three-well case includes those for two-well cases, which includes those for one-well cases. From this observation, a well-by-well optimization approach deserves thoughtful consideration for further study. So far, we have only the empirical evidence though our reservoir model and it might be possible for this approach to fall into trivial local optimum for other problem settings.
4. Conclusions

In this study, we propose a new definition for immobile CO₂ which takes the irreducibility of relative permeability curves into account and explain why we claim that our new definition is more suitable than the classical one for measuring a long-term storage safety. Using this definition for an optimality criterion, we attempted to find an optimal well placement which maximizes the proportion of the immobile and dissolved CO₂ to the total injected amount. Our recently-proposed global optimization algorithm named iterative Latin hypercube samplings can search a parameter space effectively and yield a promising solution within a practical number of simulation runs.

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