PROBABILISTIC ASSESSMENT OF THE DEEP SEDIMENTARY GEOThermal SYSTEM WITH CO₂ INJECTION AT RESERVOIR DEPTH

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ABSTRACT

We have evaluated the potential effect of CO₂ as a working fluid for geothermal energy development in the deep sedimentary reservoirs. This study utilizes the response surface methodology for a probabilistic assessment of deep sedimentary geothermal system with CO₂ injection. Our approach includes the Box-Behnken design of numerical experiments, 3-D numerical simulations, stepwise regression, and Monte Carlo simulations at each time step. For the numerical experiments, a 5-spot well configuration is simulated within a simplified geological model consisting of a layered geological setting alternating with unfractured (low k) and fractured limestone (high k) to represent the deep sedimentary geology in the eastern Great Basin. Four independent variables or factors used for this study include pressure drop between injection and production wells, permeabilities of high- and low-k formation, and geothermal gradient. The permeabilities of unfractured and fractured limestone are assumed to be log-normally distributed. Uniform distribution is used for the remaining factors. We assess both the geothermal energy extraction and CO₂ storage potential given the range of input parameters. This study demonstrates that the response surface methodology associated with Monte Carlo simulation can be efficiently applied to the evaluation of a deep sedimentary geothermal system and accompanied CO₂ storage within the probabilistic framework.

INTRODUCTION

Deep sedimentary reservoirs with the high thermal gradients can be considered as a new type of geothermal power source (Allis et al., 2012; Porro et al., 2012). However, due to the scarcity of data for the deep subsurface environment, uncertainty in the input parameters should be incorporated into the assessment of system performance and environmental risk. In order to quantify the uncertainty, Monte Carlo-based methods are traditionally used to estimate a system’s output response (e.g., probability density function) from known or estimated statistical distributions of input parameters. While Monte Carlo simulation method is simple, it typically requires large number of probability-weighted samplings of inputs and subsequently high computational cost to yield a probability distribution of an output metric. Furthermore, complex multi-phase numerical simulation involves computationally intensive simulation efforts. Thus, new efficient and readily applicable methodology within the probabilistic framework is necessary for better compliance with the project goals and regulatory requirement in timely manner. Therefore, we introduced and utilized a response surface methodology integrated with Monte Carlo samplings for a probabilistic assessment of deep sedimentary geothermal system with CO₂ as a working fluid. Major goal of this study is to probabilistically delineate the system responses and performance due to the innovative application of CO₂ injection in the deep sedimentary geothermal system.

NUMERICAL PROBLEM SETUP

In this study, a 3-D conceptual model domain with a generic 5-spot pattern consisting of layers of fractured and unfractured limestone was chosen to be representative of a typical sedimentary basin in the eastern Great Basin. We elected to adopt a 5-spot well pattern because of its wide application in oil field and CO₂-geothermal systems (Pruess, 2006, 2008; Spycher and Pruess, 2010; Wan et al., 2011; Borgia et al., 2012; Randolph and Saar, 2011). The resulting 3-D model with its 5-spot well pattern is plotted in Figure 1. Due to the symmetry of the 5-spot well pattern, we employed a 1/8 symmetry domain (of the 5-spot pattern) for all simulations (Figure 1), but results are shown on a full-well basis (Pruess, 2006). Total thickness of the domain is 1,100 m. The 3-D domain in the vertical direction
was divided into three parts, a 500 m zone of unfractured limestone at the top, a 100 m thick zone consisting of 5 layers of alternating unfractured and fractured limestone, and a 500 m-thick section of limestone at the bottom (Figure 1). The grid cell size in the X and Y directions was kept uniform at 70.7 m. Vertical cell size of 12.5 m for unfractured limestone and 25 m for fractured limestone was used within the central section of the model, and 100 m thick cells in the top and bottom sections of the model.

Porosities were assigned as 2.5% and 10% for unfractured and fractured limestone, respectively based on representative measurements of limestones in the Great Basin carbonate system. The injection and production wells were placed at the bottom of the fractured limestone layer with a depth of 575 m from the top of domain. The system was initially at hydrostatic pressure with a conductive heat flow with the pressure of 300 bars and temperature of 200 °C at the depth of production well to represent a deep sedimentary reservoir at about 3 km depth in the eastern Great Basin.

The Dirichlet boundary condition with constant pressure was assigned to boundaries of injection and production, with a specified pressure drop between the injection and production wells. The pressure drop between the injection and production well was considered as an independent variable to represent the different injection rates in this study. The Neumann condition (no flow) was assigned on all other sides. Details of parameter settings are summarized in Table 1.

We selected 4 independent variables to be considered key engineering or geologic factors, including pressure drop between injection and production wells, permeabilities of unfractured limestone (low k) and fractured limestone (high k), and the geothermal gradient. Their range and statistical distribution are given and discussed in the Response Surface Method section.

Table 1: Hydrologic parameters, initial, and production/injection conditions.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fractured limestone porosity</td>
<td>10%</td>
</tr>
<tr>
<td>Unfractured limestone porosity</td>
<td>2.5%</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>2.51 W/m°C</td>
</tr>
<tr>
<td>Rock specific heat</td>
<td>1,000 J/kg °C</td>
</tr>
<tr>
<td>Rock grain density</td>
<td>2,650 kg/m³</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Initial Condition</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir fluid</td>
<td>all water</td>
</tr>
<tr>
<td>Initial temperature</td>
<td>200°C at the layer of production well depth</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>Hydrostatic with 300 bar at the layer of production well depth</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Production/Injection condition</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Well distance</td>
<td>707 m</td>
</tr>
<tr>
<td>Injection temperature</td>
<td>50°C</td>
</tr>
</tbody>
</table>

Simulation Tool

The fluid property module of TOUGH2 code, ECO2H, was employed to simulate the mass flow and heat extraction rates for CO₂ as a working fluid in deep sedimentary reservoirs. The ECO2H equation-of-state (EOS) algorithm was designed for applications to geological sequestration of CO₂ in saline aquifers at high temperature and pressure (Spycher and Pruess 2011). This EOS is purposed to provide an accurate and comprehensive description of thermodynamics and thermophysical properties of water-brine-CO₂ mixtures under the conditions of temperature up to 243 °C and pressure up to 676 bar (Borgia et al., 2012).

RESPONSE SURFACE METHOD

Figure 2 summarizes the workflow for the response surface method combined with Monte Carlo simulation we followed in this study. We first determined independent variables/factors to construct the design of experiment based on a Box–Behnken design (BBD) followed by the numerical experiments defined in the previous section. Then, the system responses due to CO₂ injection was delineated by constructing the response surface (or proxy) model for each different time. We utilized stepwise regression technique to eliminate insignificant factors from the regression equation. Lastly, Monte Carlo samplings of mutually independent input parameters
through the obtained response surface models for each time generated temporal evolution in the cumulative distribution functions (CDFs) of output responses from the given input distributions.

Minimum and maximum geothermal gradient is 30 and 50°C/km, respectively. The geothermal gradient determines the variations in the formation temperature profile in the model from 200 °C at the production well depth. The pressure drop between injection and production wells ranges from 20 to 30 bars for the minimum and maximum values. Since constant pressure conditions were set at the injection and production wells, the pressures at the two wells were assigned to initial pressure plus/minus a half of the specific pressure drop, respectively in order to keep the specified pressure drop.

Table 2 summarizes the three levels for each factor. Variations of each factor given in Table 2 are scaled to -1 and 1 for minimum and maximum of the range, respectively for the BBD. Total 25 runs specified by BBD (Meyers and Montgomery, 2009) provide the corresponding output variables from the numerical experiments.

<table>
<thead>
<tr>
<th>Independent variables assigned in the design of experiment.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Independent variables (Xi)</td>
</tr>
<tr>
<td>X1 Pressure drop (bar)</td>
</tr>
<tr>
<td>X2 High-k permeability</td>
</tr>
<tr>
<td>X3 Low-k permeability</td>
</tr>
<tr>
<td>X4 Geothermal gradient</td>
</tr>
</tbody>
</table>

Given the design of experiment specified with the BBD, the 5-spot well configuration defined in the previous section was simulated for the numerical experiments within a simplified geologic model consisting of a layered geological setting alternating with unfractured and fractured limestone to represent the carbonate system of the eastern Great Basin. Total 25 simulation runs were accomplished to represent the carbonate system of the eastern Great Basin. 25 simulation runs were accomplished to represent the carbonate system of the eastern Great Basin.

We conducted the flow and heat simulations for 100 years with CO₂ as working fluids using the ECO2H module of TOUGH2 code for each simulation run. Then, we post-processed the numerical results and selected 6 dependent variables or responses for the

**Figure 2: Workflow for the response surface methodology combined with Monte Carlo simulation.**
regression modeling; net energy extraction rate, cumulative total CO₂ mass in the layer of injection and production wells, total CO₂ mass at overlying aquifer, CO₂ leakage ratio, CO₂ mass fraction at the production well, and temperature drawdown relative to initial temperature. The net heat extraction rate is defined as follows:

\[
\text{net heat extraction rate} = \Sigma a(\rho_{a,\text{out}}q_{a,\text{out}}H_{a,\text{out}} - \rho_{a,\text{in}}q_{a,\text{in}}H_{a,\text{in}}) \quad (1)
\]

where \( q_{a,\text{out}} \) and \( q_{a,\text{in}} \) are volumetric flow rates, \( \rho_{a,\text{out}} \) and \( \rho_{a,\text{in}} \) are density, and \( H_{a,\text{out}} \) and \( H_{a,\text{in}} \) are enthalpies of the \( a \)-th phase at the production and injection wells, respectively (Pruess, 2008).

**Regression Modeling**

The response surface method (RSM) or regression modeling consists of mathematical and statistical techniques to develop a functional relationship between a response or dependent variable \( y \) of interest and associated independent variables or factors \( (x_1, x_2, ..., x_k) \). The response surface method is typically a polynomial approximation to the responses \( y \) obtained with a linear regression given the input/design variables \( X_i \) in a chosen design of experiment. A full second-degree response surface model for \( k \) independent variables is

\[
y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1,j=2}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \varepsilon \quad (2)
\]

where \( \beta_0, \beta_i, \) and \( \beta_{ij} \) represent regression coefficients and \( \varepsilon \) is random error assumed to have a zero mean. \( k \) is four in this study. Unlike the laboratory experiment, the random error due to the non-repeatability does not exist in a deterministic numerical experiment and is ignored in this study. Eqn. (2) contains linear, two-way interactions, as well as quadratic terms. We used a least square method to determine the coefficients of the polynomial/response surface model at each time. The least squares estimator of beta is

\[
\hat{\beta} = (X^T X)^{-1} X^T y \quad (3)
\]

Only significant variables and interaction terms (at the 95% significance level) were included in the response surface model after application of stepwise regression procedure. The stepwise procedure is a multi-linear regression of the response values with iterative stepping based on their statistical significance in a regression (Draper and Smith, 1998). That is, it is repeatedly altering the model at the previous step by adding or removing a predictor variable in accordance with the entry and removal criteria, respectively until the stepping or altering is no longer possible given the stepping criteria or the maximum number of steps is reached.

After regression modeling with a stepwise method, a series of response surface models for the dependent variable at each time step were identified. Given the statistical input parameter distributions, then we performed Monte Carlo samplings (10,000) associated with the response surface model for each time and combined all of the Monte Carlo results to construct the cumulative distribution functions (CDFs) of each dependent variables. CDF shows the probability level associated with the dependent variable greater than or less than a certain level.

**RESULTS**

As a base case, we first conducted the flow and heat simulation to evaluate the energy extraction for CO₂ as a working fluid in a deep sedimentary reservoir based on the determined variables with their values at midpoint (\( \mu \)). We also conducted the base case simulation with water as a working fluid for comparative purpose only. Then, we proceeded to the remaining 24 runs to probabilistically assess the geothermal energy extraction and potential CO₂ leakage within the response surface method framework.

**Flow and Heat Simulation Results**

Figure 3 shows the net heat extraction rate, mass flow rate, temperature, and gas saturation at the grid block next to the injection and production wells for CO₂ as a working fluid over a period of 30 years. Water only is produced at a rate of around 50 kg/s in the initial stage of simulation. After 0.5 years, the produced water flow rate sharply decreases as CO₂ reaches the production well. With continuous CO₂ injection and increasing gas saturation at the production well, the produced CO₂ flow rate significantly increases. The oscillation in mass flows and heat extraction rates at the early stage of simulation (Figure 3) is an artifact of its location being immediately next to the injection and production wells. The oscillation is a necessary numerical response to maintain constant pressure at the wellbores.

The net heat extraction rate is around 30 MW in the initial stage of simulation and decreases to 20 MW after 0.5 years. This trend is similar to the trend of the produced water flow rate. With increases in the produced CO₂ flow rates, the net heat extraction increases its maximum of 34 MW after 15-year CO₂ injection. With the continuous increase of CO₂ gas saturation at the production well, the net heat
extraction rate decreases to 30 MW after 30 years of CO₂ injection. This is due to more rapid thermal depletion of CO₂ compared to water. This can be observed from the rapid decrease of simulated temperature (Figure 3b).

After 2 years of CO₂ injection, the areas adjacent to the injection well are fully saturated. The CO₂ breaks through to the production well after 0.5 years of injection and the gas saturation keeps increasing to 1.0 after 30-year CO₂ injection. The temperature next to the injection well gently decreases from the initial temperature of 200 °C to the injection temperature of 50 °C.

The simulated corresponding results for water as a working fluid are also plotted in Figure 3. The net heat extraction rate for water is almost constant at 20 MW for year one but decreases to 12 MW after 30 years of injection. Compared to the results for CO₂ as a working fluid, the net heat extraction rate for water is much smaller. However, the differences in the net heat extraction between these two cases decrease with time after 15 years. This is explained by the more rapid thermal depletion when CO₂ is used, a conclusion consistent with the larger drop of temperature for CO₂ when compared to water (Figure 3b).

**Probabilistic Assessment**

For CO₂ as a working fluid, Figures 4 – 9 showed the temporal evolution of net energy extraction, cumulative total CO₂ mass, total CO₂ mass at overlying aquifer, leakage ratio, CO₂ mass fraction at the production well, and temperature drawdown with the CDFs.

Given the range/distributions of input variables and simulation settings, net energy extraction tends to undergo four different stages (Figure 4). During the initial time period (0 – 2 years), 95 percentile (P₉₅) of predicted net energy extraction showed negative values. The second stage until about 12 years showed an increase of net energy extraction (positive values), but variation reduced significantly. Then the net energy extraction tends to slightly decrease again for the third and final stage. However, the variation among the outcomes peaked at about year 20 (third stage) and decreased after that.

![Figure 3: Simulated heat extraction rate, mass flow rate, temperature, and gas saturation next to the production and injection wells for CO₂ (solid line) and water (dashed line) as working fluids, respectively.](image3)

![Figure 4: CDFs contour map of the net energy extraction.](image4)
The arrival of CO₂ and mass fraction out of total fluids at the production well are also presented in Figure 8. The CO₂ mass fraction tends increases rapidly for the first 5 years as CO₂ plumes arrive at the pumping well. The 50th percentile of the predicted CO₂ mass fraction is approximately 0.87 and 0.95 at year 10 and 60, respectively. Note that after about 35 years, the 95th percentile values of the results are greater than the possible maximum ratio (=1), which is caused due to the regression.

Figure 5: CDFs contour map of the cumulative CO₂ mass in the model domain.

Figure 6: CDFs contour map of the cumulative CO₂ mass only at overlying aquifer.

Temperature drawdown next to the production well is gradually increasing over 100 years in the mean sense (P₅₀). The probability that temperature drawdown falls below about 25 °C drawdown after 100 years (Figure 9) is 0.75. However, it is noted that the range of the temperature drawdown between P₇₅ and P₉₅ of the results is dramatically increasing.

Figure 7: CDFs contour map of the CO₂ leakage ratio.

Figure 8: CDFs contour map of the CO₂ mass fraction at the production well.
SUMMARY AND DISCUSSION

The general purpose of this study is to assess the innovative application of using CO$_2$ as a working fluid and to investigate its effects on energy extraction and risk assessment in deep sedimentary reservoirs. We designed a 3-D conceptual model utilizing a generic 5-spot well pattern to evaluate the performance of several attributes of the geothermal system in deep sedimentary reservoirs, including energy extraction and risk of CO$_2$ leakage in deep sedimentary geothermal options. We compared the results for CO$_2$ as a working fluid with the ones for water as a working fluid.

We presented the probabilistic evaluation of system responses due to the CO$_2$ injection in the deep sedimentary geothermal system. Our work includes the development of response surface model (RSM) associated with the Box-Behnken design (BBD), corresponding numerical modeling experiments, and Monte Carlo simulations. Our approach accounted for the probability distributions to characterize variability or uncertainty in prediction estimates for the probabilistic evaluation of deep sedimentary geothermal system with CO$_2$ injection.

The following implication can be drawn based on our simulation results:

1. The large energy extraction rate could last the whole period of 30-year simulation time, demonstrating that the designed conceptual model with 5-spot well pattern is suitable for the operation using CO$_2$ as a working fluid in deep sedimentary geothermal reservoirs;

2. The net heat extraction and mass flow production rate for CO$_2$ as a working fluid were much larger compared to water as a working fluid, indicating CO$_2$ as a working fluid could enhance heat extraction;

3. Predicted net energy extraction during the initial time period (0 – 2 years) is likely negative. Then, the net energy extraction tends to be positive and peak at about year 12;

4. CO$_2$ tends to keep accumulating both in the target formation and overlying aquifer at reservoir depth. Under the simulation settings and uncertainties of input parameters specified in this study, P$_{50}$ of the leakage ratio reaches about 0.43 after 100 years.

5. Predicted CO$_2$ mass fraction at the production well shows that it takes about 5 years for CO$_2$ to become major fraction in the extracted fluids.

6. Temperature drawdown next to the production well is gradually increasing and the probability that temperature drawdown falls below about 25 °C drawdown after 100 years is 0.75.

7. Our results demonstrate that the response surface method associated with Monte Carlo simulation can be efficiently applied to the evaluation of a deep sedimentary geothermal system and accompanied CO$_2$ storage within the probabilistic framework.

ACKNOWLEDGEMENTS

This study was funded by the Department of Energy (Award # DE-EE0005128).

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