Background and Induced Leakage Risk on Seismically Active Faults

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Cover Illustration: An example permeability field and the approximate locations of major zones (topo (the top soil layer), caprock, reservoir, and basement).


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Background and Induced Leakage Risk on Seismically Active Faults

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<thead>
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<th>Term</th>
<th>Description</th>
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<tbody>
<tr>
<td>°C</td>
<td>Degree(s) Centigrade</td>
</tr>
<tr>
<td>2-D</td>
<td>Two-dimensional</td>
</tr>
<tr>
<td>3-D</td>
<td>Three-dimensional</td>
</tr>
<tr>
<td>AIC</td>
<td>Akaike Information Criterion</td>
</tr>
<tr>
<td>BIP</td>
<td>Burn-in period</td>
</tr>
<tr>
<td>CO₂</td>
<td>Carbon dioxide</td>
</tr>
<tr>
<td>DOE</td>
<td>U.S. Department of Energy</td>
</tr>
<tr>
<td>GLM</td>
<td>Generalized linear model</td>
</tr>
<tr>
<td>LANL</td>
<td>Los Alamos National Laboratory</td>
</tr>
<tr>
<td>LBNL</td>
<td>Lawrence Berkeley National Laboratory</td>
</tr>
<tr>
<td>LLNL</td>
<td>Lawrence Livermore National Laboratory</td>
</tr>
<tr>
<td>m</td>
<td>Meter(s)</td>
</tr>
<tr>
<td>m²</td>
<td>Square meter(s)</td>
</tr>
<tr>
<td>Mt/yr</td>
<td>Megatonnes (million metric tonnes) per year</td>
</tr>
<tr>
<td>NETL</td>
<td>National Energy Technology Laboratory</td>
</tr>
<tr>
<td>NRAP</td>
<td>National Risk Assessment Partnership</td>
</tr>
<tr>
<td>PNNL</td>
<td>Pacific Northwest National Laboratory</td>
</tr>
<tr>
<td>ROM</td>
<td>Reduced-order model</td>
</tr>
<tr>
<td>STOMP</td>
<td>Subsurface Transport Over Multiple Phases</td>
</tr>
<tr>
<td>TSS</td>
<td>Total sum square</td>
</tr>
<tr>
<td>TOUGH2</td>
<td>Transport Of Unsaturated Groundwater and Heat, version 2</td>
</tr>
<tr>
<td>UTM</td>
<td>Universal Transverse Mercator</td>
</tr>
</tbody>
</table>
Acknowledgments

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The authors also acknowledge Hiroku Wainwright and Jens Birkholzer of Lawrence Berkeley National Laboratory (LBNL) for providing the TOUGH2 model of the Kimberlina site, as well as output from that model; and Susan Ennor of Pacific Northwest National Laboratory (PNNL) for editorial assistance.
EXECUTIVE SUMMARY

This report documents the National Risk Assessment Partnership (NRAP) third-generation fault leakage model. Reduced-order models (ROMs) were constructed for background leakage and for the increased leakage because of the increase in fault permeability that may be associated with induced seismic events. The simulations on which the ROMs are based are fully three-dimensional (3-D) and are roughly based on the Kimberlina site model in the southern San Joaquin Basin of California. Modeling results indicate that the impact of induced seismicity on brine leakage for the case studied is greater than that of carbon dioxide (CO₂) leakage because the main body of the CO₂ plume did not reach the vicinity of the fault during the simulation period. ROMs were developed and can be used for predicting CO₂/brine leakage given information about formation properties at similar sites.

The reservoir and fault permeability were found to be the dominant factors affecting both background and induced CO₂/brine leakage. The porosity for all zones appears to have secondary effects, and caprock properties are generally negligible. The results showed that increased resolution of the grids used in the finite difference model, especially near the faults, would provide a more physically realistic model of fault transport and leakage at the Kimberlina site. In addition, interpolation of output pressure results from finite element models to a finite difference grid often led to the development of non-physical artifacts in pressure distribution. The next steps needed to continue this work will be to increase the grid resolution, and to perform the simulation of injection through leakage within the finite difference model. The current plan is to use the revised models to update the ROMs for baseline and induced fault leakage.
1. **INTRODUCTION**

The U.S. Department of Energy’s (DOE’s) Office of Fossil Energy established the National Risk Assessment Partnership (NRAP) project to harness the breadth of capabilities across the DOE national laboratory system to develop a defensible, science-based quantitative methodology for determining risk profiles at carbon dioxide (CO2) storage sites. As part of this multi-year program, scientists from Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), Pacific Northwest National Laboratory (PNNL), and the National Energy Technology Laboratory (NETL) are developing models to evaluate the potential for induced seismicity associated with injection of CO2 into deep subsurface storage reservoirs, and the impact that induced seismicity might have on leakage of CO2 or brine from reservoirs along faults.

The NRAP Induced Seismicity Working Group has been developing an integrated assessment model for a synthetic CO2 storage site based on the geology and characterization data available for the Kimberlina site in the southern San Joaquin Basin of California. Kimberlina has been proposed as a potential storage site, but is not under active development. A significant quantity of characterization data is available for the site and the greater San Joaquin basin (Wagoner, 2009; Coblentz et al., 2017), which provides an opportunity to base the risk assessment techniques on a realistic storage scenario.

The fault leakage assessment described in this report is part of a larger, integrated modeling effort focused on several aspects of the induced seismicity risk. The components and their interconnections are presented graphically in Figure 1. The workflow consists of simulation-based assessments of the response of various system components—i.e., reservoir, seismically active faults, leakage pathways, protected aquifers—which are supported by underlying characterization studies. The workflow begins with a reservoir model that computes excess pressure and CO2 saturation in the reservoir. The reservoir model is then used to drive fault leakage simulations to assess the “background” risk of leakage along a major fault to the shallow aquifer. The computed pressures along the fault plane are used to drive simulations of fault reactivation and dynamic rupture. This computation provides seismic source events that can be used to estimate ground motions that are folded into a probabilistic seismic hazard assessment. In tandem, it is assumed that a given rupture on a fault may change the permeability of the fault and potentially increase the leakage potential. To capture this possibility, a modified permeability field is passed back to the fault leakage simulations, and an “induced” leakage hazard is computed and compared with the background potential. This assessment can then be used to drive aquifer simulations and a probabilistic assessment of groundwater contamination hazard.

Throughout this workflow, an attempt is made to propagate the inherent uncertainty in the underlying system through the analysis. A variety of strategies are used, but the general goal is to describe the likely range of responses that may be observed in practice. During an actual operation, this integrated assessment would be continually revised as new characterization and monitoring data are made available.

Following this workflow, the Induced Seismicity Working Group has developed reduced-order models (ROMs) that provide estimates of fault leakage under varying conditions based on statistical fits of detailed flow and transport model results. The first ROM is a baseline fault leakage model based on initial assumptions of fault permeability. The second ROM accounts for leakage after induced seismic events increased the permeability of the faults.
This report describes the detailed flow and transport models used for the fault leakage runs; the
geomechanical methods used to simulate the increase in fault permeability associated with a
seismic event of a given size, as well as the methods used to simulate the induced seismic events;
the statistical methods used to define the ROMs; and the results, discussion, and conclusions
regarding the fault leakage models and the ROMs.

Figure 1: Integrated seismicity and leakage risk assessment workflow for NRAP Induced Seismicity Working
Group (Bromhal and White, 2013).
2. METHODS
This section describes the characteristics of a specific site model and the methods used in modeling transport along the central faults, the methods used to modify the fault permeability after an assumed induced seismic event, and the methods used to develop the ROMs.

2.1 CHARACTERISTICS OF THE KIMBERLINA MODEL RECEIVED FROM LBNL
The “Kimberlina” model represents a hypothetical injection site that has been used for several studies of the sequestration of CO₂ in the subsurface (e.g., Birkholzer et al., 2011), and it has been adopted by various NRAP researchers as a model for future studies. The Kimberlina model is based on a geologic model of the southern San Joaquin Basin in California. It is a regional model covering approximately 83 km in the east-west direction by 113 km in the north-south direction (Wagoner, 2009). The model simulates storage of CO₂ in the Vedder Sand, with the Temblor-Freeman shale providing a barrier to flow.

The current study simulated CO₂ and brine leakage across a series of monitoring blocks along a monitoring plane near the top of the caprock, with 200 different realizations of permeability/porosity fields. The TOUGH2 (Transport Of Unsaturated Groundwater and Heat, version 2) modeling domain of the site used in prior analyses by LBNL is illustrated in Figure 2.

Note: The domain covers a region of 83 km in the eastern direction by 113 km in the northern direction. The figure is modified from Birkholzer et al. (2011).

Figure 2: TOUGH2 modeling domain for the three-dimensional (3-D) geological model and discretization model domain for CO₂ storage in the Southern San Joaquin Basin.
In the present simulations of CO2/brine leakage, a smaller domain of 79 x 79 km (i.e., inside the purple box in Figure 2) was considered. This smaller domain contained the injector and the two major fault systems (i.e., the Greeley, and the Pond-Poso) as illustrated in Figure 3. Another fault, the New Hope, is located further away from the injection location (see Figure A1). The smaller STOMP (Subsurface Transport Over Multiple Phases) domain has the same vertical extent as the original, larger TOUGH2 domain.

The CO2 injector in the TOUGH2 model is located approximately at 3932500N, 299500E, Zone 11S (Universal Transverse Mercator [UTM]). The origin of a local coordinate system for the STOMP simulations is defined (in meters) to be located at 3887000N, 260000E (UTM), and therefore, the injector in the local coordinate system is at 45500N, 39500E.

Two hundred realizations of input hydraulic property fields were generated by LBNL for this local domain by varying the permeability and porosity separately for the sand layers in the Vedder formation, the shale layers in the Vedder formation, as well as the overlying caprock—the Temblor-Freeman shale.

Boxplots of the 200 realizations of horizontal/vertical permeability (logarithmic) and porosity of the Vedder sand, Temblor-Freeman shale, and the fault, are shown in Figure 4 and Figure 5.
Figure 4: Horizontal and vertical permeability (geometric means) of the sand/shale/fault formations. The induced vertical permeability is the modified permeability after rupture occurs.

Figure 5: Average porosity of the sand/shale/fault formations.
2.2 TRANSLATION OF MODEL FROM TOUGH2 TO STOMP

The input hydraulic properties and output variables from the TOUGH2 finite element mesh were translated onto STOMP finite difference grids.

The input hydraulic properties include:

- Initial horizontal permeability (m²)
- Initial vertical permeability (m²)
- Initial porosity

The output variables from TOUGH2 that were translated as initial conditions for the STOMP simulations include:

- Temperature (°C)
- Gas saturation
- Aqueous/gas pressure
- Aqueous dissolved CO₂

Data on the 59,945 finite elements in the local domain used in TOUGH2 simulations were mapped onto a STOMP 3-D Cartesian grid with 35 x 37 x 31 = 40,145 cells. Examples of the spatial distribution of these heterogeneous fields are shown in Figure 6 and Figure 7. A 3-D fine mesh is shown as Figure A4 in the Appendix. The figures show the input properties translated from the TOUGH2 finite element mesh (Figure 2) to STOMP finite difference grids using the nearest-neighbor interpolation method.

Note: The section is at Y = 50000N.

Figure 6: An example permeability field and the approximate locations of major zones (topo [the top soil layer], caprock, reservoir, and basement [case #1]).
In the original LBNL reservoir simulation model CO\textsubscript{2} plume migration and pressure distribution were modeled with an injection rate of 1 Mt/yr for 50 years, and the model outputs were extracted at the following time steps:

**Table 1: Timesteps for which CO\textsubscript{2} saturation plume and pressure were extracted from the Kimberlina reservoir simulation model**

<table>
<thead>
<tr>
<th>Step</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>out1</td>
<td>1</td>
</tr>
<tr>
<td>out2</td>
<td>2</td>
</tr>
<tr>
<td>out3</td>
<td>5</td>
</tr>
<tr>
<td>out4</td>
<td>10</td>
</tr>
<tr>
<td>out5</td>
<td>15</td>
</tr>
<tr>
<td>out6</td>
<td>20</td>
</tr>
<tr>
<td>out7</td>
<td>25</td>
</tr>
<tr>
<td>out8</td>
<td>30</td>
</tr>
<tr>
<td>out9</td>
<td>35</td>
</tr>
<tr>
<td>out10</td>
<td>40</td>
</tr>
<tr>
<td>out11</td>
<td>45</td>
</tr>
<tr>
<td>out12</td>
<td>49</td>
</tr>
<tr>
<td>out13</td>
<td>50</td>
</tr>
</tbody>
</table>

Data for temperature, gas saturation, pressure, and aqueous CO\textsubscript{2} were used as initial and boundary conditions for STOMP background leakage simulations (Figure 8).
Various data interpolation approaches were compared for transforming the data and model outputs between the TOUGH2 and STOMP grids, including 3-D kriging, inverse-distance weighting, and nearest-neighbor interpolation methods. Because the grid aspect ratio of the domain was \( \frac{dx}{dz} = 10 \), vertical distances dominated the 3-D interpolation no matter which spatial interpolation methods were used. This caused translation issues, particularly for pressure interpolation. Given the generally horizontally layered structure (near-zero dipping angles), the interpolation of the properties was restricted based on the horizontal distances using the nearest-neighbor algorithm; the resulting fields were reasonable and helped with model convergence.

### 2.3 Fault Transport Modeling Approach

The STOMP-water-salt-CO2-energy code (module 33, July 2013 version) (White and Oostrom, 2006) was used to simulate the CO2 and brine migration processes. This code solves flow and transport problems for CO2 sequestration systems in aqueous saline formations. The modeling domain was discretized with structured orthogonal grids for spatial discretization and a fully implicit formulation for temporal discretization. The conservation equations were solved using a set of primary variables (macroscopic properties that fix the physical state of the system, such as aqueous/gas pressure). Secondary variables (e.g., phase saturation, phase relative permeability, porosity, tortuosity, viscosity, density, enthalpy, saturated vapor pressures, vapor mass fractions, and diffusion coefficients) were solved from the primary variables through the constitutive equations, which generally are nonlinear functions. Nonlinearities in the discretized governing equations and associated constitutive equations were solved using Newton–Raphson iteration.

The saturation-capillary pressure relations are described by the Brooks and Corey (1966) expression with Fayer and Simmons (1995) extension (Equation 1). With this function, the actual aqueous saturations are computed in terms of effective aqueous saturations according to Equation 2, in which the effective minimum aqueous saturation is computed as a function of aqueous-gas capillary pressure, as shown in Equation 3. The aqueous and gas relative permeability functions use the Burdine (1953) pore-size distribution model (Equations 4 and 5).
The saturation and relative permeability equations are as follows:

$$
\bar{s}_i = \left( \frac{P_g - P_l}{\bar{\rho}_l g} \right)^{-\lambda}
\begin{cases}
\text{for } (P_g - P_l) \geq \psi, \\
\text{for } (P_g - P_l) < \psi
\end{cases}
$$

$$
\bar{s}_i = 1
$$

$$
\bar{s}_i = \bar{s}_i(1 - \bar{s}_m) + \bar{s}_m,
$$

$$
\bar{s}_m = 1 - \ln\left( \frac{P_g - P_l}{\bar{\rho}_l g} \right) / \ln(h_{od})
$$

$$
k_{rl} = (\bar{s}_i)^{\lambda+2\lambda},
$$

$$
k_{rg} = (\bar{s}_g)^2 [1 - (\bar{s}_i)^{1+2/\lambda}],
$$

where

- $P_g$ = gas pressure
- $P_l$ = aqueous pressure
- $\bar{s}_i$ = the effective aqueous saturation
- $S_l$ = the actual aqueous saturation
- $\bar{\rho}_l$ = reference aqueous density
- $\psi$ = the Brooks and Corey air-entry head (m)
- $\bar{s}_m$ = the effective residual aqueous saturation
- $\lambda$ = the Brooks and Corey fitting parameter
- $\bar{s}_e$ = the effective aqueous saturation
- $h_{od}$ = the oven-dried gas-aqueous capillary head (m)
- $k_{rl}$ = aqueous relative permeability
- $k_{rg}$ = the gas relative permeability

Various boundary conditions (e.g., Dirichlet, zero flux, hydraulic gradient, initial conditions) were explored to check the convergence of the simulations, and to explore boundary conditions.
that were compatible with initial conditions. Zero flux boundaries were set at the top and bottom of the model, which helped with convergence and the stability of numerical solvers (e.g., PETSc), and avoided phase change issues that developed when pressure was too low at the top of the model. The CO₂ plume spread more horizontally than vertically, and in the current setup, the plume should remain in the supercritical state. Simulations were performed simultaneously at PNNL’s institutional supercomputing facility.

A monitoring plane was set near the top of the caprock, roughly 1,500 m below ground surface and 800 m above the injection point. A series of monitoring blocks were used to record the CO₂/brine leakage rates as a function of time. The leakage rates at selected times (e.g., t = 10, 15, 20 years after the stop of injection) were treated as output response variables for developing ROMs against input properties including permeability/porosity of sandstone/shale/fault formations.

### 2.4 EARTHQUAKE-INDUCED CHANGES TO FAULT PERMEABILITY

The simulated “background” pore pressure distribution is used to drive simulations of fault reactivation and seismicity, using the approach described by Foxall et al. (2013).

To capture the range of possible states of initial slip and stress on the faults in the Kimberlina model constrained by the allowable states, the fault is first “matured” (i.e., the simulation is run at a constant far-field stress state) until the statistics of seismicity reach stationarity. After this initial period, the “burn-in” period (BIP), the fault is assumed to have reached its long-term state, and the simulation is executed from this point until an appropriately long time, as determined by the convergence of the Gutenberg-Richter b-value over successive windowed periods. The events acquired over this period are used to determine the long-term seismicity statistics of the faults.

Because the periods over which the statistics can be considered stationary $O$ (1,000 yr) greatly exceed the duration of the pore pressure perturbation $O$ (10 yr), the possible states of the fault (both slip and stress states) contribute to the aleatoric uncertainty. To accommodate the variability associated with this and to enforce the constraint that the states be self-consistent, the state is sampled by running the simulation past the BIP for a duration sampled from a uniform distribution in the range of $[0, 1000 \text{ yr}]$. Currently, 10 such samples are drawn and simulated for each of the 200 pore pressure evolution cases evaluated by PNNL.

When combined with the contributions from all of the aleatoric and epistemic uncertainties, this should yield a more consistent evaluation of the hazard. However, as a first study to understand how different magnitude events may contribute to the risk, this study evaluated the expected permeability change based on five different (hypothetical) magnitude cases: 3.0, 3.5, 4.0, 4.5, and 5.0. The pore pressure realizations were sifted through to find one where at least one magnitude event close to each of the cases occurred after the pore pressure has been perturbed by the injection operation. Once a suitable pore pressure realization was identified, the first event occurring in any of the aleatoric realizations of slip and stress state resulting in the corresponding magnitude was selected. The time and the average rupture slip were recorded, and the surface was reconstructed for each such event.
The vertical permeability $\kappa$ for each cell, $i$, intersected by the fault rupture surface is then changed by the calculated permeability increase. $t$ and $t+1$ represent the time step right before and after the rupture respectively. This permeability increase relies on a linear shear-log(permeability) relationship to determine the increase in permeability across the surface of the fault:

$$k_i^{t+1} = k_i^t + \delta k_i$$

(6)

where

$$\delta k_i = \begin{cases} 0, & k_i > k_{\text{max}} \\ \frac{\delta}{\delta_{\text{max}}}, & \text{otherwise} \end{cases}$$

$$k_{\text{max}} = 10^{\alpha_{\text{max}}},$$

$$\delta = \begin{cases} 10^{i(\delta + c_i)}, & \delta < \delta_{\text{max}} \\ 10^{-c_i}, & \text{otherwise} \end{cases}$$

and

$$k = \frac{\alpha_1 - \alpha_0}{\delta_{\text{max}}}.$$  

Here the values are arbitrarily:

$$\delta_{\text{max}} = 0.2 m$$

$$\alpha_0 = 18$$

$$\alpha_{\text{max}} = 17$$

$$\alpha_1 = 15$$

The change in permeability due to slip is shown in Figure 9.
2.5 APPROACH FOR DEVELOPMENT OF ROMS (BASELINE AND QUAKE-MODIFIED)

The CO₂/brine leakage rates at different monitoring locations were recorded as a function of time. ROMs were developed for the leakage vs. input hydraulic properties of different geological formations (sandstone/shale/fault). The generalized linear model (GLM) analysis (McCullagh and Nelder, 1989) was adopted for developing the ROMs. The GLM analysis starts with the following model:

\[
Y_i = \theta_0 + \sum_j \theta_j p_{i,j} + \sum_{jk} \theta_{jk} p_{i,j,k} + \sum_j \gamma_j p_{i,j}^2 + \varepsilon_i, \quad i = 1, \ldots, n
\]

where \( p_{i,j} \) and \( p_{i,k} \) = the \( i \)th realization of the \( j \)th and \( k \)th parameters, respectively

\( \theta_0 \) = the intercept term

\( \theta_j, \theta_{jk}, \) and \( \gamma_j \) = coefficients of the linear, interaction, and quadratic terms, respectively

\( Y_i \) = the \( i \)th realization of the response variable (e.g., CO₂/brine leakage rates)

\( \varepsilon_i \) = the corresponding fitted residual

This model assumes that the model-fitting residuals \( \varepsilon \) follow independent normal distributions with zero mean and unit variance. The significance of the terms in the GLM model can be evaluated with different measures. One approach is to employ the \( p \)-value of the null hypothesis that no statistical significance exists in a set of given observations (i.e., the coefficient \( \theta_j \) is zero). A parameter passes the significance test only if the corresponding \( P \)-value is smaller than the chosen significance level of the test (e.g., 0.05 or 0.1) (McCullagh and Nelder, 1989; Venables and Ripley, 2002). Another measure is the coefficient of determination \( (R^2) \) of model fitness, which directly shows the contribution of the factors to the total sum square (TSS). The relative contribution (fitted sum square) of each factor can also be calculated, and then used to rank the relative contributions of the input parameters.
3. RESULTS/OBSERVATIONS
This section describes the fault transport modeling results and the ROMs developed from the modeling results.

3.1 FAULT TRANSPORT MODELING RESULTS
An example of the spatial distribution of the CO2 plume is shown in Figure 10.

![Figure 10: Simulated CO2 mass fraction distribution at 10 years after injection stops.](image)

Note: The section is at Y = 50,000 m

Figure 11 shows that earthquake-induced CO2 leakage is slightly higher than the background CO2 leakages, while the induced brine leakage is several percent higher than the brine leakage for the baseline simulations. This is reasonable, because the main body of the CO2 plume has not arrived at the fault zone during the simulation period. Therefore, although the pressure evolution has reached the fault zone and increased the fault permeability due to rupturing, such an increase in permeability has little impact on the CO2 leakage near the fault zone. But the increase in vertical permeability immediately affects brine leakage because brine already exists in the fault zone.

Figure 12 and Figure 13 show the background CO2/brine background leakage rates (across the top of the caprock near the fault at 10 years after injection stops) as a function of sandstone/shale/fault properties.

Reservoir (sandstone) permeability has a weak positive relationship with background CO2 leakage, and has a strong positive relationship with background brine leakage. The effect of sandstone porosity is generally secondary. Caprock (shale) properties, including both permeability and porosity, have weaker effects on leakage as no clear positive or negative impacts can be identified. Fault properties, on the other hand, have effects comparable to reservoir properties.

The above findings are physically reasonable and indicate the permeable zones dominate the leakage of either CO2 or brine through the monitoring planes. The statistical significance of the
parameters/factors is evaluated in the following section about ROMs. The similarity of fault parameter leakage patterns to the reservoir parameter leakage patterns (e.g., Figure 13) is partially due to the rather coarse grid resolution in the current model settings and the use of the nearest-neighbor interpolation approach for translating the formation properties, which reduces the contrast between the reservoir and faults.

Note: leakage is at 10 years after injection stops across the top of the caprock near the fault

Figure 11: Probability density distribution of the CO₂/brine leakage rates
Note: Leakage is at 10 years after injection stops across the top the caprock near the fault kh, kv, and por refer to horizontal permeability, vertical permeability, and porosity, and are considered for storage interval (sandstone), sealing layer (shale), and fault. Permeabilities are log10 transformed.

Figure 12: CO2 background leakage rate versus formation properties.
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Note: leakage is at 10 years after injection stops across the top the caprock near the fault. kh, kv, and por refer to horizontal permeability, vertical permeability, and porosity, and are considered for storage interval (sandstone), sealing layer (shale), and fault.

Figure 13: Brine background leakage rate versus formation properties.

Fault rupture causes modifications of the fault properties such as permeability, based on the relationships shown in Figure 9. The simulated rupture results for several cases are shown in the Appendix. Figure 14 and Figure 15 show the induced CO2/brine background leakage rates (across the top of the caprock near the fault at 10 years after injection stops) as a function of sandstone/shale/fault properties, where the permeability has been updated due to rupturing.
In general, porosity of all formations has weak or negligible effects on induced CO₂ and brine leakage. Caprock (shale) properties still have negligible effects. Fault and reservoir permeability seem to have relationships with the induced leakage rates that are similar to those for background leakage. But as shown in Figure 11, the induced leakage, especially the brine leakage, has been clearly increased. Section 3.2 explores how the relationships (ROMs) vary for the background and induced cases.

Note: Leakage is at 10 years after injection stops across the top the caprock near the fault. kh, kv, and por refer to horizontal permeability, vertical permeability, and porosity, and are considered for storage interval (sandstone), sealing layer (shale), and fault.

**Figure 14: CO₂ induced leakage rate versus formation properties - due to fault rupture.**
Background and Induced Leakage Risk on Seismically Active Faults

Note: Leakage is at 10 years after injection stops across the top the caprock near the fault. $kh$, $kv$, and $por$ refer to horizontal permeability, vertical permeability, and porosity, and are considered for storage interval (sandstone), sealing layer (shale), and fault.

**Figure 15:** Brine induced leakage rate versus formation properties - due to fault rupture.

### 3.2 REDUCED-ORDER MODELS

The CO$_2$ leakage rate has weak positive relationships with the permeabilities of the sandstone, shale, and fault; and has negligible relationships with porosity. The brine leakage rate, on the other hand, has a more obvious correspondence to the formation properties, even with the current coarse grid resolution that tends to smear the corresponding relationships.
As a result, better ROMs for the brine leakage rate can be obtained than for the CO₂ leakage rate. Figure 16 shows the fitted background CO₂/brine leakage rates across the top of the caprock near the fault (at 10 years after injection stops) using a quadratic model of sandstone, shale, and fault properties. Figure 17 shows the model fits for the induced CO₂/brine leakage rates.

![Figure 16: Fitted model responses using quadratic models - background leakages.](image1)

Note: Leakage is at 10 years after injection stops across the top the caprock near the fault. The x-axes are the fitted values of background leakages of CO₂ and brine, respectively.

![Figure 17: Fitted model responses using quadratic models - induced leakages.](image2)

Note: Leakage is at 10 years after injection stops across the top the caprock near the fault. The x-axes are the fitted values of induced leakages of CO₂ and brine, respectively.

To rank the significance of the parameters and their interactions, the GLM analysis was adopted to perform statistical tests of the linear (the first-order terms), interaction (cross-products), and quadratic terms (the second-order terms) of the input parameters. This analysis starts with a quadratic GLM regression model that takes the form as given in Equation 7. The model is fit using n sets of response and explanatory variables. Then the unnecessary terms are dropped one by one using a stepwise backward removal approach based on the Akaike Information Criterion (AIC) (Akaike, 1974).
The fitted and finalized GLM models for background/induced CO₂/brine leakages at the selected monitoring location near the fault are given in Tables 2, 3, 4, and 5.

Table 2: Fitted coefficients and their t/P-values for the finalized quadratic GLM model for CO₂ background leakage rate

| Parameter                                                                 | Coefficient | Std. Error | t-value | P(>|t|) |
|---------------------------------------------------------------------------|-------------|------------|---------|---------|
| Vertical permeability of the storage interval (kv.sandstone)              | 588.4       | 296.3      | 1.986   | 0.0484  |
| Porosity of the storage interval (por.sandstone)                         | -25,468.9   | 12,978.8   | -1.962  | 0.0512  |
| Vertical permeability of the fault (kv.fault)                            | -516.2      | 317.8      | -1.624  | 0.1060  |
| Porosity of the fault (por.fault)                                       | 40,879.7    | 25,587.0   | 1.598   | 0.1118  |
| Interaction between vertical permeability and porosity of the storage interval (kv.sandstone:por.sandstone) | -1,958.5    | 996.9      | -1.965  | 0.0509  |
| Interaction between vertical permeability and porosity of the fault (kv.fault:por.fault) | 2,562.2     | 1,601.7    | 1.600   | 0.1113  |

Table 3: Fitted coefficients and their t/P-values for the finalized quadratic GLM model for brine background leakage rate

| Parameter                                                                 | Coefficient | Std. Error | t-value | P(>|t|) |
|---------------------------------------------------------------------------|-------------|------------|---------|---------|
| Vertical permeability of the storage interval (kv.sandstone)              | -73.5183    | 35.1340    | -2.093  | 0.0377  |
| Vertical permeability of the fault (kv.fault)                            | 164.4497    | 70.8696    | 2.320   | 0.0214  |
| Squared vertical permeability of the storage interval kv2.sandstone       | -2.8461     | 1.3488     | -2.110  | 0.0361  |
| Squared vertical permeability of the fault kv2.fault                      | 5.1621      | 2.2180     | 2.327   | 0.0210  |
| Squared porosity of the fault por2.fault                                  | 1.2189      | 0.6954     | 1.753   | 0.0812  |
Overall, caprock properties have negligible effects on either background or induced CO₂/brine leakage and were eliminated from the models using the stepwise backward removal approach.

Based on the AIC, the relevant factors affecting background CO₂ leakage rate include sandstone permeability, sandstone porosity, fault permeability, and fault porosity. The interactions between permeability and porosity also passed the significance tests (Table 2). Among these four factors, sandstone porosity is unimportant for background brine leakage rate. Sandstone permeability, fault permeability, and fault porosity all have nonlinear impacts (i.e., second-order effects) on background brine leakage (Table 3).

The dominant factors affecting induced CO₂ leakage rate include sandstone permeability, sandstone porosity, and fault permeability, as well as the interaction between sandstone
properties (Table 4). Regarding induced brine leakage, only the sandstone and fault permeability are important and they both have nonlinear impacts on induced brine leakage (Table 5).

The tables above show the significant factors for CO2 and brine leakage near the fault, and indicate how the relationships (i.e., coefficients) vary for background and induced leakage. These coefficients, however, are approximate due to the coarse grid and are expected to change once simulations are performed with refined grids near the fault and across the domain.
4. DISCUSSION

The geomechanical model used for this study assumed that rupture causes increases in vertical permeability, which facilitates both CO2 and brine leakage through the caprock. It is certainly possible that faults in a shale unit would show no substantial permeability change. The assumption that rupture increases fault permeability is a conservative assumption with regard to CO2 release, and the uncertainty quantification is attempting to bound the range of possible behavior that might be seen in practice. From the current analyses, the effect of the increased permeability due to rupture is more significant for brine leakage than for CO2 leakage. Caprock, sandstone, and fault permeabilities have weak positive relationships with CO2 leakage rates, and stronger positive relationships with brine leakage rates. One reason that the parameters have stronger impacts on brine leakage than on CO2 leakage is that the main body of the CO2 plume has not arrived at the fault zone during the simulation period. Therefore, although the pressure evolution affected a large area and increased the fault permeability due to rupturing, there is little impact of that permeability increase on the CO2 leakage near the fault zone. On the other hand, the increase in vertical permeability affects brine leakage because brine was already present in the fault zone.

Permeability generally was found to have stronger impacts than porosity, which agrees with previous studies (e.g., Hou et al., 2012). Porosity is more of a storage parameter and does not necessarily facilitate or slow down migration of CO2/brine.

These findings and the ROMs developed for CO2/brine leakage rates are possibly subject to change if a finer grid is used instead of the current coarse mesh. The use of the coarse mesh, in addition to insufficient resolution of the location and properties of the faults, also introduces artifacts in vertical pressure gradients when translating data from TOUGH2 mesh to STOMP grids. To avoid such artifacts, one option is to refine the numerical grid to be able to capture the actual locations of and better represent the Greeley and Pond-Poso faults. Fault properties would then be assigned to the corresponding grid cells associated with the faults. The increase in spatial resolution near the faults is necessary for the results to be more physically realistic.

In future studies, it would be helpful to adopt the multiple realizations of intrinsic properties provided by the LBNL team (e.g., sandstone/caprock/fault permeability/porosity), but not the state variables (pressure/saturation) that were produced using TOUGH2. Instead, it is more credible for the analysis to use STOMP to simulate the CO2 migration and CO2/brine leakage from the beginning of injection. This approach should avoid the pressure distribution artifacts caused by interpolation of output pressures from finite elements to finite difference grids. Updated ROMs will then be developed for CO2/brine leakages for baseline conditions and after fault rupture.
5. **CONCLUSIONS**

This study identified the dominant parameters/factors affecting background and rupture-induced CO₂ and brine leakage near the fault zones for the Kimberlina site data set in the San Joaquin Basin of California. ROMs were developed and can be used for predicting CO₂/brine leakage given information about formation properties at similar sites.

The reservoir and fault permeability were found to be the dominant factors affecting both background and induced CO₂/brine leakage. The porosity for all zones appears to have secondary effects, and caprock properties are generally not important. Overall, the parameters have stronger impacts on brine leakage than on CO₂ leakage because the CO₂ plume had not reached the fault zone during the simulation period while brine already existed in the same zones.

The results showed that increased resolution of the grids used in the finite difference model, especially near the faults, will be necessary to provide a more physically realistic model of fault transport and leakage at the Kimberlina site. In addition, interpolation of output pressure results from finite element models to a finite difference grid often led to the development of non-physical artifacts in pressure distribution. The next steps needed to continue this work will be to increase the grid resolution, and to perform the simulation of injection through leakage within the STOMP finite difference model. The revised models will then be used to update the ROMs for baseline and induced fault leakage.
6. REFERENCES


Bromhal, G. S.; White, J. Quantitative risk assessment approaches for induced seismicity. NRC Committee on Earth Resources Induced Seismicity and Energy Tech, Washington, DC. November 2013.


APPENDIX

The rupturing simulation results are shown in Figures A1 through A3.

Figure A1: The evolution of fault slip at 400, 800, and 1,000 years from an unstressed state for the Kimberlina faults (Greeley, Pond-Poso, and New-Hope structures).
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Figure A2: A visualization of the distribution of slip at 1,100 years with the hypo centers of events with a magnitude greater than 4.

Figure A3: A visualization of the change in stress on the fault surface with the vector field indicating the rake direction (normal faulting is consistent with Kimberlina).
Figure A4: A 3-D mesh with an example of initial porosity distribution.
NRAP is an initiative within DOE’s Office of Fossil Energy and is led by the National Energy Technology Laboratory (NETL). It is a multi-national-lab effort that leverages broad technical capabilities across the DOE complex to develop an integrated science base that can be applied to risk assessment for long-term storage of carbon dioxide (CO2). NRAP involves five DOE national laboratories: NETL, Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Pacific Northwest National Laboratory (PNNL).

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