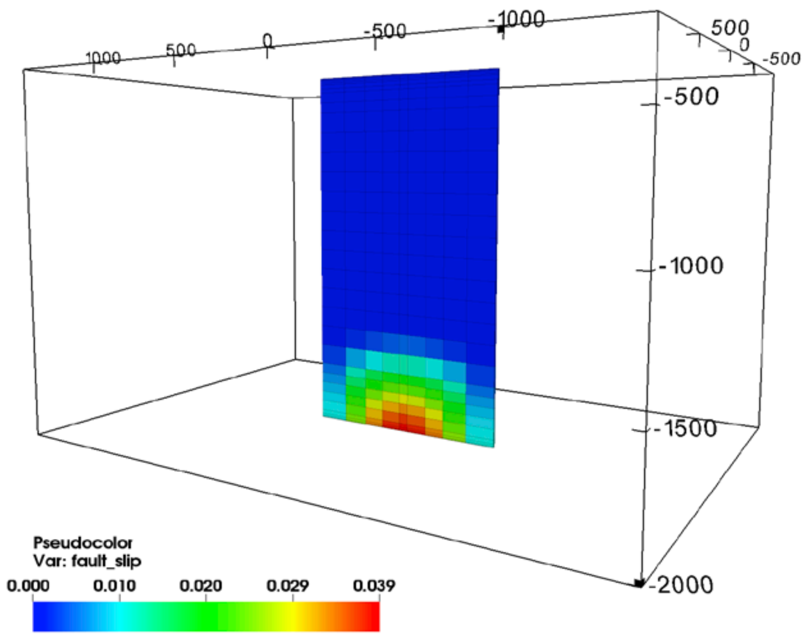
NRAP
National Risk Assessment Partnership



A Reduced-Order Model of Fault Leakage for Second-Generation Toolset

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Cover Illustration: Illustration of fault leakage study, showing the slip induced along fault due to reservoir pressurization.

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A Reduced-Order Model of Fault Leakage for Second-Generation Toolset

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Acronyms and Abbreviations

Term	Description
2-D	Two-dimensional
3-D	Three-dimensional
DOE	U.S. Department of Energy
LLNL	Lawrence Livermore National Laboratory
NETL	National Energy Technology Laboratory
NRAP	National Risk Assessment Partnership
NUFT	Nonisothermal Unsaturated-Saturated Flow and Transport model
ROM	Reduced-order model

Acknowledgments

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EXECUTIVE SUMMARY

This report describes the National Risk Assessment Partnership (NRAP) second-generation fault leakage model. The key features of the new model are:

- A three-dimensional (3-D) site model has been developed.
- Geomechanical changes in permeability due to fault slip are now included
- The Kimberlina reservoir model (Zhou and Birkholzer, 2011) is used as a reference to specify boundary conditions for pressure and saturation

This report briefly describes both the high-fidelity leakage simulations and their subsequent reduction to a response-surface model. This response-surface model constitutes a reduced-order model (ROM) that can be incorporated into a system model that predicts the potential for CO_2 or brine to be released from a storage reservoir to an overlying aquifer or the atmosphere (e.g., Pawar et al., 2013). This second-generation ROM builds on the first-generation ROM (Lu et al., 2016), which was two-dimensional (2-D) and did not incorporate geomechanical effects. Note that this ROM considered aseismic, quasi-static slip behavior. The third-generation ROM will look at leakage response due to seismic events.

1. LEAKAGE MODEL

1.1 GEOMETRY AND BOUNDARY CONDITIONS

The basic geometry under consideration is shown in Figure 1. A vertical fault extends from the reservoir interval at 2,000-m depth, through the caprock, to a shallow aquifer at 240-m depth. The overburden is considered homogeneous and isotropic in all cases, but the actual parameters vary as described below. The underburden is not explicitly included in the model. No vertical displacement is allowed at the lower surface, while the rock may freely deform laterally. The fault zone—i.e. the fault itself and neighboring gouge/brecciation—is 15-m wide and 1,000-m long. A discrete slip surface is not explicitly modeled, but rather the flow and geomechanical behavior was approximated in the fault zone through a continuum approximation. The fault zone behaves as a Darcy continuum, but the permeability in each fault block evolves with slip on the fault. For the geomechanical response, the fault zone is modeled using a non-associative Drucker-Prager elasto-plastic material. The surrounding caprock is assumed to behave elastically.

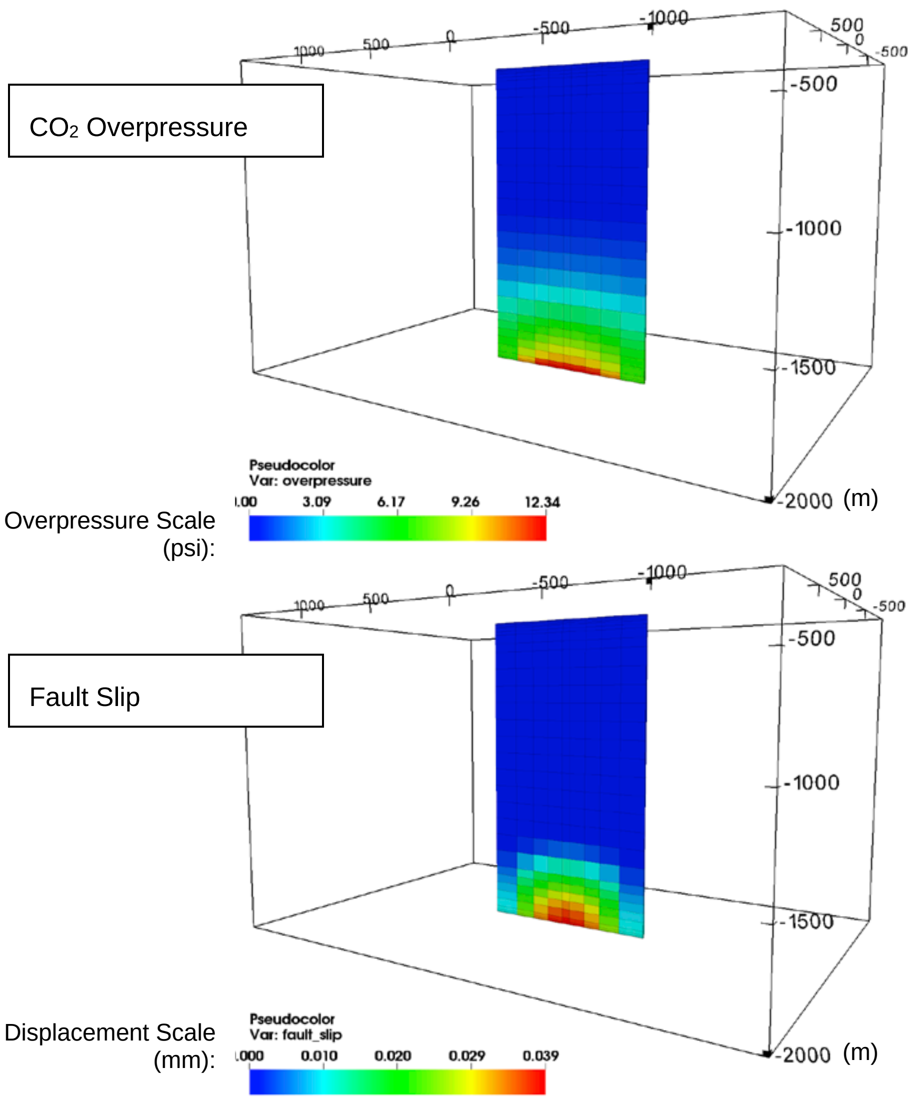

Figure 1: Analysis results: A typical realization of the fault plane of leakage model. (Surrounding caprock is hidden, so that only the fault plane is visible.)

1.2 MATERIAL RESPONSE

An in-situ stress state is given such that the fault experiences both normal and shear stresses, which vary linearly with depth. As the fault is pressurized, the reduction in effective mean stress in the fault zone can push the effective stress state to the yield surface and lead to plastic shear deformation. The shear strength of the fault is controlled by friction angle of the material, while the cohesion and dilation angle are assumed to be equal to zero. The friction angle remains constant after yielding, with no softening or hardening response.

The in-situ stress state is assumed to be a known quantity, increasing linearly with depth, and is not treated as an uncertain parameter. The shear stress is chosen such that the system is initially in limit equilibrium for a friction angle of 25 degrees. That is, any overpressure in this configuration will lead to slip. For larger friction angles the fault behaves elastically for some range of pressurization before slip is triggered. Thus, the uncertainty in the friction angle addresses the underlying uncertainty in how close the fault is to slip.

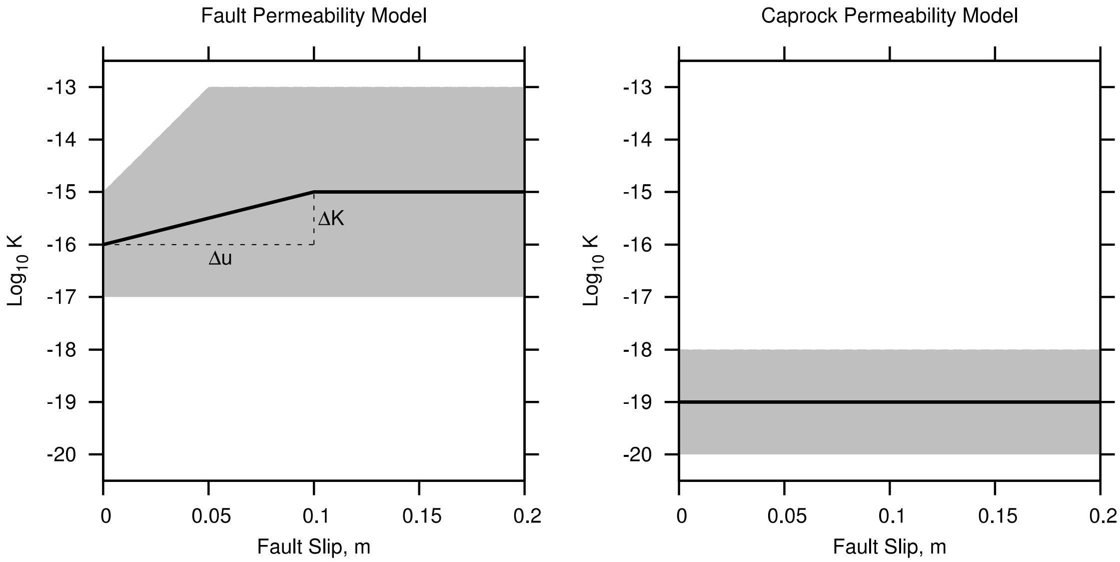

Figure 2: Fault and caprock permeability (K) models. Gray bars indicate explored uncertainty range.

Both the fault and caprock are assigned a homogeneous initial permeability. As plastic deformation occurs in the fault zone, however, the permeability in a fault grid block can grow (Figure 2). There is a critical slip distance, however, at which a maximum permeability increase is mobilized and subsequent slip does not lead to any further increase. Thus, the caprock permeability remains constant, while the fault permeability increases with fault slip up to a certain maximum value, after which it remains constant.

For the present study, the uncertain parameters under consideration are: 1) initial caprock permeability; 2) initial fault permeability; 3) the friction angle for the fault zone; 4) the critical slip distance, and 5) geomechanical permeability multiplier (the slope of the line $d(\log_{10}K)/du$ shown in Figure 2a), and their ranges are found in Table 1. The simulation model contains a variety of other parameters which are given fixed values.

Table 1: Uncertain model parameters and ranges

Parameter	Range	Units
Caprock Permeability	10^{-20}–10^{-18}	m^2
Initial Fault Permeability	10^{-17}–10^{-15}	m^2
Geomechanical Multiplier	0–10^2	---
Characteristic Slip	0.05–0.20	M
Friction Angle	25–40	(degrees)

The reservoir boundary conditions for pressure and saturation are taken from the Kimberlina reservoir model (Wainwright et al., 2012). The Kimberlina reservoir is un-compartmentalized, and pressure dissipates quickly as one moves away from the injector. To make the hypothetical leakage scenario interesting from a geomechanical point of view, the fault was positioned so that it passes right through the vertical injector, so that the fault experiences maximum pressurization. In reality, of course, it would be very unlikely that an operator would position an injector so close to a known fault. This leakage pathway is purely hypothetical, and does not correspond to a real fault at the Kimberlina site.

2. UNCERTAINTY QUANTIFICATION

2.1 MODEL BASIS

The Kimberlina reservoir model contains three uncertain parameters (storage reservoir porosity, storage reservoir permeability, and seal permeability), which were explored through 54 separate realizations of the reservoir model. Each of these 54 realizations contains a different history of pressure and saturation. To incorporate this uncertainty in the boundary conditions on the fault, an additional uncertain parameter for the fault leakage model is an integer index 1 to 54 denoting the boundary realization to employ, which were included in the NRAP-IAM-CS model (Stauffer et al., 2016).

The flow/transport behavior is modeled using the Nonisothermal Unsaturated-Saturated Flow and Transport model *(*NUFT*)*, while the geomechanical response is modeled using Geocentric. A leap-frog scheme was used in which flow and geomechanics timesteps alternate, with pressures and updated permeabilities being passed back and forth. While the leap-frog scheme does not exactly satisfy the coupled mass and momentum balance equations at each time step, this loosely-coupled approach provides acceptable accuracy. The flow simulation models the behavior of supercritical CO_2 and brine below the supercritical depth, as well as the phase transition to gas as the CO_2 rises above the supercritical depth. To reduce computation time, however, the model is limited to isothermal conditions. Preliminary comparisons of an isothermal and fully-thermal leakage model produce comparable leakage rates, however, and so the additional expense of a fully thermal simulation was not deemed necessary. Higher-order corrections due to thermal behavior can easily be over-shadowed by the large uncertainty in fault permeability, for example.

2.2 SIMULATION APPROACH

The leakage model contains five uncertainty parameters. To study the range of uncertainty, 54 differing Kimberlina reservoir models were investigated. A Latin-Hypercube sampling design was used with 128 points to explore the uncertainty space for the five fault parameters, and repeated the same design for all 54 reservoir models. As a result, 54×128 = 6,912 realizations of the model were run. The maximum simulation time for all models is 200 years.

The decision to use the Kimberlina reservoir models was motivated by the difficulty of finding a simple parameterization of the reservoir boundary conditions. The fault plane intersects a 3-D pressure and saturation plume that evolves with time. It is quite difficult to reduce these time- and space-dependent conditions into a simple parameterization involving only a few variables. By simply using the Kimberlina reservoir results for input, this parameterization issue was avoided. Therefore, fidelity was maintained with respect to the true reservoir behavior, at the price of some increase in computational cost. As the fault leakage simulations are relatively cheap, however, this cost was deemed worthwhile.

The five uncertain parameters for the fault model itself are normalized to have unit range [0,1] for convenience. Within the simulation model the unit values (p_1, p_2, p_3, p_4, and p5) are then transformed into actual simulation parameters as:

$$log_{10}K_C = -20 + 2\,p_1$$

$$log_{10}K_F = -17 + 2\,p_2$$

$$log_{10}K_G = log_{10}K_F + 2\, p_3$$
$$\Delta u = 0.05 + 0.15 p_4$$
$$\phi = 25 + 15 p_5$$

where K_C is the caprock perm, K_F is the initial fault permeability, K_G is the maximum fault permeability due to geomechanical effects, Δu is the characteristic slip distance, and ϕ is the fault zone friction angle.

The CO_2 and brine mass flux through the top of the fault was then converted to a simplified parameterization described by three values: 1) the time until gas breakthrough at the surface (t_g, years); 2) the average brine mass flux before breakthrough (q_b, kg/m^2/year); and 3) the average gas mass flux after breakthrough (q_g, kg/m^2/year). In the simplified parameterization, it is assumed that only brine leaks (at a constant rate) prior to breakthrough, at which point brine flux drops to zero. After breakthrough, only gas leaks, again at a constant rate. This is an obvious simplification of the true flux behavior, but provides a simple approximation. Figure 3 shows results of the simulations for two Kimberlina boundary models, corresponding to the maximum and minimum pressurization in the reservoir. Since Kimberlina 37 has almost no overpressure, no geomechanical effects are evident. In contrast, the scatter in the Kimberlina 46 results are due to triggered fault slip that was evident in many realizations. Results using the other reservoir simulations fall between these two extremes.

For each set of 128 simulations, three response surfaces were then computed for each of the three output parameters. There are then 54 sets, for a total of 54×3 = 162 response surfaces. For a given choice of the six parameters, the approximate time history of leakage for brine and gas can be computed by sampling the appropriate surfaces.

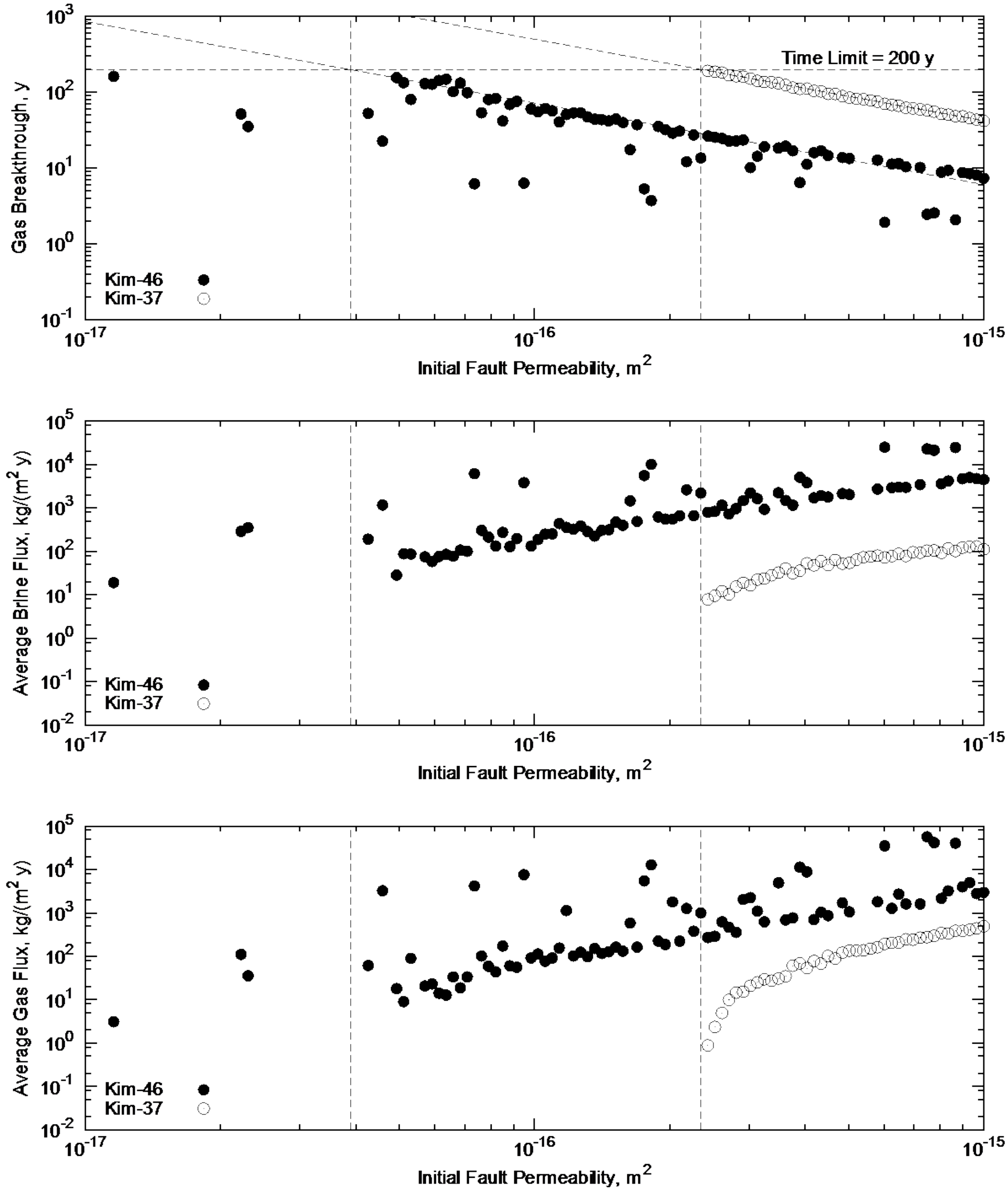

Figure 3: Fault leakage model results for two Kimberlina boundary models. Kimberlina 46 has the highest pressure distribution, while Kimberlina 37 has the lowest pressure distribution.

3. APPLICABILITY AND LIMITATIONS

This ROM was developed to simulate the flux of CO_2 and brine from a deep reservoir to a shallow groundwater aquifer. It should be emphasized that the ROM predictions are site specific, and critically depend on the assumed geometry and reservoir boundary conditions. The proposed ROM generation method, however, is quite general. To examine a new site, the geometry and reservoir boundary conditions can be modified, and the high-fidelity simulations re-run. A new site-specific ROM can then be constructed from these results.

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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 (CO_2). 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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