Evaluating the Importance of Barometric Pumping for Subsurface Gas Transport Near an Underground Nuclear Test Site

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An underground nuclear explosion (UNE) generates and distributes radioactive gases that can be transported to the ground surface through preexisting and explosion-induced fractures over timescales of hours to months. If detected, the presence of short-lived radionuclides in gas is evidence of a recent UNE. Numerical modeling can provide estimates of surface arrival times that can help inform gas monitoring strategies at suspected foreign test sites. Efforts are underway at historic US UNE sites to better understand subsurface gas-transport processes following a UNE by geologic characterization of the near-field damage structures, field-scale tracer experiments, and subsurface air pressure monitoring. The development of numerical models using historical and experimental datasets from former UNE sites can improve predictions by testing conceptual models, highlighting key processes, and constraining parameter ranges. The models developed in this study represent the U20az site at the Nevada National Security Site where the Barnwell device was expended in December 1989. A two-phase (water and air), dual-permeability flow and transport model of the U20az site was built to investigate gas transport processes under recent experimental conditions and following the Barnwell nuclear event. Results indicate that the model can explain both the lack of arrival of radioactive gas tracers in a 2013 field experiment as well as the observed arrival of radioactive gases following the 1989 Barnwell event using barometric pressure records from the respective periods, even when additional advective processes associated with the Barnwell detonation are ignored. The results demonstrate that the character of the barometric records may be a key factor in explaining the differences in transport behavior.

Abbreviations: bgs, below ground surface; CCS, cavity–chimney system; FEHM, Finite Element Heat and Mass transfer code; GDKM, generalized dual permeability model; HFM, hydrostratigraphic framework model; HSU, hydrostratigraphic unit; MQ, Millington–Quirk; NGME, Noble Gas Migration Experiment; NNSS, Nevada National Security Site; SGZ, surface ground zero; UNE, underground nuclear explosion.

An underground nuclear explosion (UNE) produces and distributes radioactive gases around the working point of the detonation, and these gases migrate over short and long timescales away from the working point by advective and diffusive transport (Carrigan and Sun, 2014). Estimating the surface arrival time of radioactive gases is an important aspect for detection of clandestine nuclear tests. The arrival time depends on many variables, including rock matrix and fracture properties, detonation yield, depth of burial, water content, barometric pressure history, and gas transport properties (Carrigan et al., 1997, 2016; Jordan et al., 2014, 2015). Detection of certain ratios of radionuclide gases can provide clear evidence of a nuclear detonation in the subsurface (Kalinowski et al., 2010; Carrigan and Sun, 2014; Lowrey et al., 2013; Sun et al., 2015). These ratios evolve due to radioactive decay and subsurface fractionation processes during transport (Lowrey et al., 2013; Sun et al., 2015).

In addition to producing radionuclide gases, the detonation of an UNE will damage the subsurface around the working point, with damage potentially reaching the ground surface. This disturbance includes creation of a cavity and adjacent crush zones, a rubble chimney, and a network of explosion-induced fractures radiating from the working point (Fig. 1). Collapse of the chimney may cause collapse at the ground surface (crater...
Gas migration models have been developed to predict surface arrival times of gas following an UNE (Carrigan et al., 1996), and these have generally relied on simplified geometry, such as single-fracture, parallel-plate conceptual models, to estimate the effect of barometric pumping on gas migration (Sun and Carrigan, 2014). Carrigan et al. (2016) introduced two-dimensional models with simplified damage zonation representation including dual-permeability models, which include early-time UNE-related physics, such as thermal convection and phase changes due to the heat of detonation. Jordan et al. (2015) and Mourzenko et al. (2014) introduced further damage-zone complexity into the models with heterogeneous and anisotropic fracturing in radially symmetric two-dimensional models. However, until now, modeling of field-scale gas migration in a three-dimensional, two-phase system at an actual UNE site has not been undertaken. This study developed a three-dimensional representation of the geologic setting and damage structure around an UNE for the first time to analyze subsurface gas migration at the U20az site.

The U20az site is located on Pahute Mesa at the Nevada National Security Site (NNSS), where the Barnwell UNE was detonated in 1989. This joint US–UK UNE tested a device with an announced yield ranging between 18 and 136 kt (20–150 kilotons) buried at a depth of 600 m below ground surface (bgs) in tuff and rhyolitic lava flow deposits. The U20az site has been the subject of extensive pre- and post-test characterization and field experimentation. Pre-shot moisture and geologic conditions determined from cores taken from the emplacement shaft (Burkhard and Wagoner, 1989), as well as radioactive gas measurements at the ground surface following the Barnwell test (Hudson et al., 1990; Schoengold et al., 1996), were collected in 1989 and 1990. Radioactive gas leakage was observed at the ground surface approximately 10 d after the explosion, and continued to release for about 3 mo thereafter (Hudson et al., 1990; Schoengold et al., 1996). The initial release could have been facilitated several days after the detonation by post-test drilling of an angle-hole (U-20az PS1) to retrieve material to help diagnose device performance (Hudson et al., 1990). These historical data sets, in combination with subsurface pneumatic pressure and tracer data obtained in 2013 as part of the Noble Gas Migration Experiment (NGME) and core-scale permeability and porosity data and additional subsurface pneumatic pressure data measured in 2016 to 2017 for the Underground Nuclear Explosions Signature Experiment provide diverse datasets that allowed calibration and testing of the U20az site flow and transport model described here. This model uses a hydrostratigraphic model (HFM) of the Pahute Mesa area (Bechtel Nevada, 2002) in which stratigraphic units with roughly similar hydrologic and mechanical properties have been defined for pre-test conditions to support hydrologic modeling. The local hydrostratigraphy around U20az extracted from this larger scale model is augmented with idealized explosion-induced deformation zones to represent the post-detonation environment.

This study focused on calibration of field-scale gas flow and transport parameters for developing a three-dimensional model...
for U20az and the application of the model to evaluate the influence of barometric pumping on gas migration rates to the ground surface. Model calibration is done in multiple stages using different data sets that inform particular groups of parameters. These data sets can include historical data from the NNSS as well as current experimental results. For example, rock matrix properties are identified by calibration to core-scale moisture, porosity, and permeability measurements made in the laboratory and field-scale fracture and bulk permeability values are estimated from subsurface pneumatic pressure measurements. Field-scale gas-transport properties were then evaluated by comparison to field-scale tracer experiments. This approach made it possible to isolate and identify the parameters most strongly informed by the individual data sets. Using the calibrated model of Barnwell, two barometric pressure records were applied to the model to evaluate whether barometric pressure conditions alone can produce gas breakthrough at the ground surface following an UNE, which was observed at U20az following the Barnwell test.

**Experiment Description**

Experimental data available from the NGME, augmented with additional subsurface pneumatic pressure data from the Underground Nuclear Explosions Signature Experiment, are the primary data sets used to calibrate the field-scale pneumatic and gas transport properties of the U20az model. The National Center for Nuclear Security funded the NGME in 2012 to 2013 to study how fission-yielded and fission-activated noble gases would migrate from an UNE-induced chimney and cavity system to the surface and near-surface (Olsen et al., 2016). Atmospheric pressure and subsurface pneumatic pressure in the U20az post-shot hole were measured for about 15 mo beginning in 2012. One phase of this experiment involved the injection of gas-phase SF$_6$ and the radio-tracers $^{37}$Ar (half-life $t_{1/2} = 35.04$ d) and $^{127}$Xe ($t_{1/2} = 36.35$ d) in the post-shot hole (U20az PS1) adjacent to the collapsed chimney at a depth of 450 m bgs (Fig. 2). Surface sampling locations (see Fig. 3) were chosen for their distance to mapped fractures and surface ground zero (SGZ) to increase the likelihood of gas detection, either beneath tarps placed at the surface or buried in the soil (0.5–1.5 m deep) to reduce dilution by air and increase the chances for detection.

On 4 June 2013, 121 kg of SF$_6$, 44.8 GBq of $^{37}$Ar, and 92.1 GBq of $^{127}$Xe were injected into the post-shot hole during a 10-h period, diluted in air injected into the cavity at 7.59 m$^3$/min (Olsen et al., 2016). By 3 mo following tracer injection, no tracers had been detected at the surface sampling locations. To facilitate tracer recovery, the chimney was pressurized by injecting $6.3 \times 10^3$ m$^3$ of air into the post-shot hole during a 46-h period beginning 11 Sept. 2013. Radiotracers and SF$_6$ were detected at the surface gas samplers after pressurization, between 17 Sept. and 10 Oct. 2013. Simultaneous with the tracer experiments, barometric pressure at the ground surface and subsurface pneumatic pressure in the injection interval of the post-shot hole were monitored. These data allowed calibration of...
the subsurface pneumatic properties as well as gas transport properties during the experiment. Barometric pressure measurements from this data set are missing from 25 Sept. to 22 Oct. 2013, during the tracer gas experiment, so the barometric pressure measured at a weather station at nearby Mercury, NV, adjusted for altitude, was used to complete the barometric pressure record. Additional subsurface pressure data were collected at U20az between 10 and 31 Aug. 2017 in four angled boreholes (Fig. 3) reaching depths of 180 m and provide nine additional pressure measurement locations to calibrate permeability.

### Numerical Model

All simulations were performed using the Finite Element Heat and Mass transfer code (FEHM), a hydrologic multiphase flow and transport model developed at Los Alamos National Laboratory (Zyvoloski et al., 2012). The FEHM uses a finite volume method for solving the conservation of mass and momentum equations (Zyvoloski, 2007). Multiple studies have used FEHM for simulating gas flow and transport in the vadose zone (Stauffer et al., 2005; Kwicklis et al., 2006; Neeper and Stauffer, 2012; Jordan et al., 2014). A generalized dual permeability model (GDKM) is applied in the model to simulate flow and transport in both matrix and fracture nodes. The GDKM consists of two overlapping media at each computational node, one representing fractures and one representing porous media (Jordan et al., 2012). With the GDKM approach, gas can move quickly through fractures while still allowing Fickian diffusion of tracer gas into the matrix, which provides the bulk of the gas storage due to concentration gradients, with diffusion controlled by the fracture half-block spacing parameter \( \lambda_f \). The GDKM approach is consistent with the conceptual models of previous investigations that consider natural and explosion-induced fractures to be the dominant pathways for gas migration due to their high permeability and small gas-filled porosity (Carrigan et al., 1996, 2016; Jordan et al., 2014).

Isothermal conditions for the simulations were assumed because the experiments and data collection were performed either before or more than two decades after the UNE detonation, well after heat generated from the detonation had dissipated.

### Model Construction

The hydrostratigraphy of the model is based on an existing HFM of the Pahute Mesa area built by National Securities Technology (Bechtel Nevada, 2002; see Fig. 4). The three-dimensional HFM for the U20az site uses details from the larger-scale HFM to capture the local geology and topography, and adds the cavity and chimney damage structure. The software LAGRIT developed by Los Alamos National Laboratory (http://lagrit.lanl.gov, 2015) was used to generate a computational mesh. More details on the mesh generation approach can be found in Gable et al. (2007). The model domain is 1000 by 1400 m, extending from the water table at 1300-m elevation to the ground surface or about 700 m above the water table depending on surface topography. The 20- by 20- by 10-m grid spacing resulted in 256,311 matrix nodes, with a corresponding GDKM node at each location to represent the fracture continuum. All GDKM fracture nodes are connected. Thirteen hydrostratigraphic units (HSUs) and two faults are represented in the mesh. The HSUs in the HFM were grouped by rock type and mechanical properties into five categories, which included welded tuff, zeolitic tuff, vitric tuff, a vitrophyre, and rhyolitic lava, and were each assigned distinct properties. Hydraulic properties, including fracture and matrix permeability, within each of these rock categories are assumed to be homogeneous and isotropic; however, a large-scale anisotropy and heterogeneity is introduced by the layering itself and locally around the working point by the damage structure, as described below.

The extent of damage zones associated with the detonation were estimated from the maximum announced yield reported for the Barnwell test (18–136 kt or 20–150 kilotons; USDOE,
Using an equation relating cavity size to maximum yield, depth of burial, overburden pressure, and rock density (Pawloski, 1999; Boardman et al., 1964), a 62-m cavity radius was estimated. Damage zones are mapped onto the mesh as shown in Fig. 4, which include (i) the cavity–chimney system (CCS) extending one cavity radius ($R_c$) from the working point to an elevation of 1880 m; (ii) an outer cavity–chimney damage zone extending from $1R_c$ to $2R_c$; and (iii) two near-surface damage zones (from SGZ to $1R_c$ and from $1R_c$ to $2R_c$) extending from 1880-m elevation to the ground surface. Figure 2 shows a schematic of the CCS. The damage in the CCS ($1R_c$) applies to both the matrix and fracture nodes, and the fractures are assigned an 8% (v/v) fraction to represent a rubbled rock in the collapse chimney and cavity. This value is based on an average CCS bulk porosity determined from chimney pressurization and tracer tests conducted in the late 1970s at analog UNE sites on the NNS, where an average value of 8% chimney porosity was estimated for a series of post-detonation site characterization studies to evaluate chimney properties in tuff on Rainier Mesa (Peterson et al., 1977a, 1977b, 1978). All other damage zones assume that damage applies only to the fracture nodes where increased fracturing is expected; the matrix properties are assumed to remain at background values. The fractures in the outer and near-surface damage zones, and the background fractures, were assigned a 0.1% (v/v) fraction.

Boardman et al. (1964) and Boardman (1970) established general relationships between cavity size, explosive yield, and depth of burial for various rock types, including tuff. Additional relationships were developed between cavity size, chimney height, and the extent of permeability increase due to test-induced fracturing. Boardman (1970) reported that the extent of permeability enhancement from detonation-induced fractures is similar for different rock types and detonation yields, and extends about two to three $R_c$ laterally, 1.5 $R_c$ below, and six to eight $R_c$ overlying the working point. These general relationships were found to hold in tuff, granite, salt, and shale (Boardman et al., 1964; Boardman, 1970). These observations are the basis for the assumed geometry of the damage structure above and around the cavity at U20az shown in Fig. 2 and 4.

All surface nodes were assigned a transient barometric pressure boundary condition to mimic the measured atmospheric conditions and a constant infiltration flux to simulate a low rate of infiltration on Pahute Mesa (5 mm/yr). The infiltration rate is based on an estimate of the Pahute Mesa recharge rate of 7 mm/yr for elevations between 1800 and 2000 m, used for the USGS and Pahute Mesa Phase I Flow models (Cooper et al., 2013). The bottom has a fixed, fully saturated boundary to represent the water table, which provides a no-flow gas boundary.

Calibration Results

The calibration of the U20az model is informed by multiple data sets, each of which constrained different model parameters, during multiple iterative calibration stages (see Fig. 5). The first stage of the calibration relied on saturation ($S_w$) and porosity ($\theta$) profiles measured from a core from the U20az emplacement hole to determine initial estimates of fracture and matrix permeability ($k_f$ and $k_m$) and air-filled porosity ($\theta_a$) under predetonation or
background conditions. Following this step, the $k_m$ and $k_f$ values were calibrated against measured atmospheric and subsurface air pressure ($P_a$) for (i) a 60-d period (2013) and (ii) a 21-d period (2017). The calibration of the flow parameters is an iterative process: the results from the earlier calibration to the $S_w$ profile feed into the initial conditions for the pneumatic pressure calibration, and then the $S_w$ profile is refined again using fracture properties estimated from pneumatic properties, and so forth. Finally, a forward run simulating tracer-gas injection was performed to evaluate the gas transport properties by comparing model results to the measured surface breakthrough of SF$_6$, $^{37}$Ar, and $^{127}$Xe after the 2013 NGME injection.

### Saturation and Air-Filled Porosity

The degree of matrix $S_w$ at U20az controls the volume of air-filled porosity ($q_a$) available to buffer barometric pressure changes in the subsurface and to store tracers during gas transport. As mentioned above, calibration of the background $k_m$ values used the pre-shot, undamaged rock properties ($\theta$, $S_w$, and $q_a$), measured from a core taken during drilling of the emplacement hole (Burkhard and Wagoner, 1989), as the calibration targets. The calibration was further evaluated by comparing the calibrated $k_m$ values against laboratory measurements of $k_m$ and $\theta$ taken from the NG-4 core drilled in 2014 (Broome et al., 2016). The NG-4 core hole was drilled about 102 m northwest of the chimney boundary to a depth of 303 m. Cores were about 5 to 7 cm in length with a 5-cm diameter; thus these permeability measurements informed only the matrix permeability, not the fracture permeability that was expected to enhance field-scale permeability.

The steady infiltration rate of 5 mm/yr was applied to a pre-detonation model, which did not include the CCS and surrounding damage zones, to simulate long-term, steady-state moisture conditions in the pretest period. In this calibration step, pre-detonation $k_m$ and $k_f$ for each rock type were adjusted manually until the simulated $S_w$ and $\theta$ profiles matched the data from the emplacement hole. The comparison between the simulated and measured $\theta, S_w, \text{and } q_a$ profiles (Fig. 6a) shows that the major trends in the profiles were captured by the model. However, the field measurements show considerable variability relative to the simpler stratigraphic framework model, where homogeneity is assumed within each unit. The estimated $k_m$ determined from the calibration to the $\theta, S_w, \text{and } q_a$ profiles are compared with laboratory measurements of $k_m$ from the NG-4 core hole (Broome et al., 2016) in Fig. 6b. The laboratory measurements of $k_m$ reported by Broome et al. (2016) provided an additional check on the validity of the $k_m$ estimated by the calibration.

Although the calibration is most sensitive to the matrix porosity and permeability assumed for the different HSUs, some sensitivity to fracture permeability also occurs because, if the $k_f$ is too high, there is less water available to flow into the matrix, which then becomes too dry relative to observed conditions. With $k_m$ constrained to honor the measured values, the maximum background $k_f$ is estimated to be $3 \times 10^{-10}$ m$^2$, giving a background bulk $k$ of $3 \times 10^{-12}$ m$^2$ if weighted by the 0.1% fracture volume. This result provided a pretest,
steady-state initial condition to perform subsequent calibration steps, including the post-detonation damage structure.

Post-Detonation Flow Properties

With the background initial conditions and permeability structure established, the model was further developed to include the CCS (see Fig. 4) and other damage zones discussed above to represent the post-detonation conditions at U20az. The post-shot damage structure was superimposed on the background stratigraphy, and $k$ values were further optimized based on pneumatic pressure changes. The use of subsurface pneumatic pressure responses to barometric pressure changes to estimate field-scale permeability is documented in many previous studies (Ahlers et al., 1978; Stallman, 1967). The approach makes use of the fact that the attenuation and phase lag of the atmospheric pressure signal in the subsurface is controlled by the pneumatic diffusivity of the medium, which reflects the ratio of gas conductivity to gas storage:

$$\alpha = \frac{k \rho_a}{\mu_a \theta_a}$$  \hspace{1cm} [1]

where $\alpha$ is the pneumatic diffusivity ($m^2/s$), $k_c$ is the effective air permeability ($m^2$) under the prevailing moisture conditions, $p_o$ is the average gas pressure (Pa), $\mu_a$ is the dynamic viscosity of air (Pa s), and $\theta_a$ is the air-filled porosity (dimensionless). The calibration of $k_c$ values from the subsurface pneumatic pressure response assumes that the values of $\theta_a$ are known from the preceding calibration step and that $k_c$ values constitute the only unknowns to be calibrated during this stage. Model results for average $\theta_a$ and $k_c$ define the pneumatic diffusivity for the HSUs and damage zones, and are listed in Table 1.

The flow properties at U20az were calibrated using the response of subsurface pneumatic pressure data to the barometric pressure signal, collected during two time periods: (i) between 4 June and 3 Aug. 2013 and (ii) from 11 to 31 Aug. 2017. The 2013 subsurface pressure data were collected in the open interval of the post-shot hole near the chimney boundary at a vertical depth of approximately 450 m bgs, while the 2017 data were collected from four angled boreholes drilled around the chimney to a depth of up to 180 m. The PEST code (Parameter ESTimation software; Doherty, 2010; Doherty and Hunt, 2010) was used to optimize the fracture parameters using the responses of pneumatic pressure at depth to both the 2013 and 2017 barometric pressure records. Parameters estimated include $k_f$ and fracture half-spacing ($\lambda_f$) for all damaged zones and undisturbed rock. The value of $\lambda_f$ is equal to half of the width of the block between two fractures. A large $\lambda_f$ limits gas exchange between the fracture and matrix, whereas a small $\lambda_f$ promotes gas exchange between the fracture and matrix. Constraints to the calibration, in the form of prior information, were provided by the laboratory-measured $k_m$ (Broome et al., 2016; see Table 1). As indicated in Fig. 6b, $k_m$ values tend to be small compared with the estimated background fracture permeability. The prior information limits PEST to search only for parameter combinations that honor the measured matrix properties for individual formations, while also providing a good fit between the observed and simulated subsurface pneumatic pressures. Results of the calibration show a good match of the measured and modeled subsurface pneumatic pressure (Fig. 7), with matrix parameters consistent with laboratory measurements. The calibration results (Table 1) indicate that a high $k_f$ and moderately large $\lambda_f$ (to limit fracture–matrix interactions) are necessary for surface barometric pressure changes to reach a depth of 450 m with the observed amplitude change and phase lag.

<table>
<thead>
<tr>
<th>Material</th>
<th>$k$ ($m^2$)</th>
<th>Sensitivity to $k$</th>
<th>Avg. $\theta_a$</th>
<th>$\alpha$</th>
<th>$\lambda_f$</th>
<th>Sensitivity to $\lambda_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Matrix</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rhyolitic lava†</td>
<td>$1.05 \times 10^{-16}$</td>
<td>–</td>
<td>0.015</td>
<td>$3.87 \times 10^{-6}$</td>
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<td>–</td>
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<tr>
<td>Vitric tuff†</td>
<td>$1.44 \times 10^{-13}$</td>
<td>–</td>
<td>0.13</td>
<td>$6.12 \times 10^{-4}$</td>
<td>–</td>
<td>–</td>
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<tr>
<td>Welded tuff†</td>
<td>$4.14 \times 10^{-15}$</td>
<td>–</td>
<td>0.004</td>
<td>$2.49 \times 10^{-6}$</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Zeolitic tuff†</td>
<td>$1.80 \times 10^{-17}$</td>
<td>–</td>
<td>0.95</td>
<td>$5.82 \times 10^{-8}$</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Chimney material</td>
<td>$1.00 \times 10^{-16}$</td>
<td>–</td>
<td>0.95</td>
<td>$5.82 \times 10^{-8}$</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td><strong>Fracture</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Background</td>
<td>$3.07 \times 10^{-12}$</td>
<td>0.599</td>
<td>$8.62 \times 10^{-4}$</td>
<td>1.94</td>
<td>1.48</td>
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<td>$2.14 \times 10^{-11}$</td>
<td>0.077</td>
<td>$7.88 \times 10^{-2}$</td>
<td>0.22</td>
<td>0.31</td>
<td>0.268</td>
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<td>Chimney–cavity $2R_e$</td>
<td>$3.77 \times 10^{-12}$</td>
<td>1.000</td>
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<td>1.11</td>
<td>1.19</td>
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<td>$1.9 \times 10^{-6}$</td>
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<td>1.10</td>
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<td>–</td>
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<tr>
<td>Damage zone $2R_e$</td>
<td>$6.84 \times 10^{-12}$</td>
<td>0.437</td>
<td>$9.80 \times 10^{-4}$</td>
<td>1.04</td>
<td>1.48</td>
<td>–</td>
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</table>

† Values are based on measurements from core-scale analyses by Broome et al. (2016).
Initial calibration attempts showed that higher $k_m$ and smaller values of $k_f$ and $l_f$ could also reproduce the observed $S_w$ profile and pneumatic pressure record reasonably well, demonstrating the non-uniqueness of the calibration when only field observations were used. Thus, a key step in the calibration process was to bring in $k_m$ measurements from the laboratory as prior information and ensure that the calibration results are consistent with the conceptual model, which assumes that $k_f$ is much greater than $k_m$.

**Tracer Transport during the Noble Gas Migration Experiment**

With flow properties established through an iterative calibration process, the model was used to evaluate gas transport properties by applying the conditions that prevailed during the NGME, including the tracer- and air-injection rates, barometric pressure, and chimney pressurization, as described by Olsen et al. (2016). The gas transport properties, including matrix and fracture tortuosity factors that influence tracer flow and diffusivity, and Henry’s Law partitioning, were evaluated by comparing the observed breakthroughs of SF$_6$, $^{37}$Ar, and $^{127}$Xe at the surface with simulated surface arrival times and concentrations. Gas half-life and transport parameters are shown in Table 2. The locations of the tracer concentration measurements around SGZ are shown in map view in Fig. 3 along with the areal extent of each damage zone.

Preliminary simulations of the NGME showed that radiotracer breakthrough is very sensitive to tortuosity, which adjusts...
the free-air diffusion for the tracer gases. Tortuosity is a measure of how complicated a flow path is and thus relies on having a good estimate of porosity and saturation to reduce diffusion rates. To account for this, an option was invoked in FEHM to use the Millington–Quirk (MQ) relationship (Millington and Quirk 1961; Baehr, 1987) to estimate a tortuosity factor ($t$) for both the matrix and fractures:

$$
\tau = \frac{q_t}{\theta^2}
$$

where $\tau$ is the tortuosity factor (dimensionless), $q_t$ is the air-filled porosity, and $\theta$ is the total porosity. This tortuosity factor, which is different for the fractures and matrix, is then used to adjust the free-air diffusion coefficient for each tracer gas according to

$$
D^* = \tau D_{fa}
$$

where $D^*$ is the effective diffusivity ($m^2/s$) and $D_{fa}$ is the free-air diffusion coefficient ($m^2/s$). The MQ function is sometimes presented with an exponent of 10/3; however, in many porous media simulators, including FEHM, the factor is reduced to 7/3 because an air content term ($\theta_a$) is embedded in the numerical transport equations (Stauffer et al., 2009).

A highly tortuous path, represented by a small value of $\tau$, results in a longer path for gas transport and effectively decreases the diffusivity of the tracer gases. Using the $\tau$ values determined by the MQ function, the $D_{fa}$ for each tracer gas is modified at each fracture and matrix node. For the small air-filled porosities simulated for the matrix nodes in the model, values of $\tau$ can be on the order of $10^{-3}$, which greatly limits the loss of tracer gas into the rock matrix by diffusion. Conversely, the low simulated $S_w$ and large $\theta_a$ (nearly equal to 1.0) of the fracture continuum result in much larger values of $\tau$ in the fracture nodes (between 0.47 and 0.95) and values of $D^*$ close to the free-air diffusion coefficient, facilitating migration through the fracture network. This result highlights the need to have good estimates of porosity and saturation to calculate tortuosity.

All tracers were simulated to test how well the model could reproduce flow and transport properties at U20az. All tracers broke through to the ground surface only after chimney pressurization was necessary to drive gases to the ground surface under the experimental conditions. The experimental results show enrichment of SF$_6$ relative to the radiotracers $^{37}$Ar and $^{127}$Xe (see Fig. 8), and the simulations reproduced the observed difference in dilution of the chemical and radiotracers. Olsen et al. (2016) attributed the SF$_6$ enrichment to the relatively low Henry’s Law partitioning factor of SF$_6$ relative to both $^{37}$Ar and $^{127}$Xe (see Table 2). Additionally, the ratio of $^{127}$Xe to $^{37}$Ar remained constant for the samples measured at the ground surface during the NGME (see Fig. 9), suggesting that the pressurization changed the experimental conditions of the NGME to an advection-driven experiment, reducing the impacts of differing gas diffusivity and solubility on breakthrough. The simulations reproduced the breakthrough ratio of radiotracer gases at a roughly constant activity ratio of about 2, which is approximately the activity ratio of $^{127}$Xe to $^{37}$Ar in the gas injected at the start of the experiment (2.06). However, Olsen et al. (2016) did note that the injection rate for each tracer was not constant throughout the injection period, which may have influenced the tracer concentration and mixing in the chimney. Thus, it may be difficult to explain the variable tracer breakthrough based on Henry's Law partitioning alone if initial concentrations were not uniform.

Details of the observed and simulated $^{127}$Xe concentrations for the tracer experiment are compared in Fig. 10 for each of the surface sampling locations. The other tracers are not shown at constant for the samples measured at the ground surface during the NGME (see Fig. 9), suggesting that the pressurization changed the experimental conditions of the NGME to an advection-driven experiment, reducing the impacts of differing gas diffusivity and solubility on breakthrough. The simulations reproduced the breakthrough ratio of radiotracer gases at a roughly constant activity ratio of about 2, which is approximately the activity ratio of $^{127}$Xe to $^{37}$Ar in the gas injected at the start of the experiment (2.06). However, Olsen et al. (2016) did note that the injection rate for each tracer was not constant throughout the injection period, which may have influenced the tracer concentration and mixing in the chimney. Thus, it may be difficult to explain the variable tracer breakthrough based on Henry’s Law partitioning alone if initial concentrations were not uniform.

Details of the observed and simulated $^{127}$Xe concentrations for the tracer experiment are compared in Fig. 10 for each of the surface sampling locations. The other tracers are not shown at

## Table 2. Transport parameters used in simulations for the 2013 Noble Gas Migration Experiment tracer gases.

<table>
<thead>
<tr>
<th>Transport parameter</th>
<th>SF$_6$</th>
<th>$^{127}$Xe</th>
<th>$^{37}$Ar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Half-life, d</td>
<td>–</td>
<td>36.4</td>
<td>35.04</td>
</tr>
<tr>
<td>Henry’s Law coefficient ($K_{H1}^{(n)}$, mol kg$^{-1}$ MPa$^{-1}$)</td>
<td>0.0024</td>
<td>0.043</td>
<td>0.014</td>
</tr>
<tr>
<td>Molecular diffusion coefficient in air ($D_{fa}$), m$^2$ s$^{-1}$</td>
<td>$9.10 \times 10^{-6}$</td>
<td>$1.24 \times 10^{-5}$</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>Molecular diffusion coefficient in water ($D_{fa}$), m$^2$ s$^{-1}$</td>
<td>$1.2 \times 10^{-7}$</td>
<td>$1.5 \times 10^{-7}$</td>
<td>$2.3 \times 10^{-8}$</td>
</tr>
</tbody>
</table>

† From Sander (2018).
‡ From Carrigan et al. (1997).
§ From King and Saltzman (1995).
¶ From Jähne et al. (1987).
# From Wise and Houghton (1966).
the same detail, but the breakthrough results show similar trends. Simulated tracer concentrations did not exceed the detection limit at any of the sampling stations for the first 99 d of the experiment, consistent with observations. After chimney pressurization on Day 99, $^{127}$Xe quickly broke through at the surface above the detection limit ($9.99 \times 10^{-7}$ Bq/L) for both the measured and simulated results. However, the simulated relative timing and magnitude of $^{127}$Xe breakthrough at individual sampling stations did not always match the observations. This is probably because local fractures influenced breakthrough at the individual monitoring locations and these fractures were not represented in the simulations.

**Discussion**

**Flow Model Calibration**

The multistep calibration process provided estimates of the flow and transport properties that matched the calibration targets well and were also consistent with the conceptual model for rock damage zonation around the working point at U20az. Calibration results were most sensitive to the parameterization of fracture flow properties. This is consistent with the existence of multiple fracture sets at the U20az site (Prothro, 2016). Fracture sets include cooling-related fractures from when the tuffs and lavas were deposited, fractures related to regional faulting (Drellack and Mercadante, 2014), and possibly UNE-related fractures.

The pneumatic pressure signal at depth responded to the surface barometric pressure variation, showing a strong connection with the ground surface (Fig. 7). The high amplitude and short phase lag of the pneumatic signal, even at a significant depth of 450 m bgs, suggests a highly breathable and well-connected fracture network around the CCS that extends to the ground surface. The high $k_f$ and meter-scale $\lambda_f$ values (Table 1) were calibrated with 10 pneumatic pressure records, nine of which were measured in the upper 120 m bgs in the uppermost welded tuff HSU. The nearly instantaneous response of these records to the barometric pressure changes suggests that the PEST-determined permeability values for the inner and outer surface fracture zones in Table 1 may represent minimum values, since even higher permeability values would result in nearly no phase lag or amplitude decrease at the shallow monitoring stations. The value of $k_f$ weighted by the fracture volume, or bulk $k$, ranges from $3.07 \times 10^{-12}$ m$^2$ in the undamaged zones to $2.14 \times 10^{-11}$ m$^2$ for the $1R_c$ CCS. The permeability values for the background, $2R_c$ CCS, and $2R_c$ surface damage zone given in Table 1 are in agreement with the single bulk $k$ value of $4.13 \times 10^{-12}$ m$^2$ at U20az obtained by Carrigan et al. (2016) based on inversion of barometric pressure data from 2013. The current model estimates that the permeability of the $1R_c$ CCS and $1R_c$ surface damage zone are an order of magnitude higher than the corresponding outer zones, but the calibration is relatively insensitive to the permeability of these zones. However, the best-fit $k_f$ based on the pre-test saturation profile is $3.12 \times 10^{-13}$ m$^2$, which is about an order of magnitude lower than the estimate based on the pneumatic pressure in the post-shot environment. The difference in calibrated $k_f$ may suggest that UNE-related damage does, in fact, increase fracturing beyond $2R_c$ from the working point; the simplified zonation of rock damage used in the model may not allow estimation of low-level damage beyond the $2R_c$ spatial extent of the outer damage zone. The high sensitivity of the calibration to the background fracture properties, as well as the relatively high value of $k_f$ determined using the three-dimensional model, suggests that portions of the model extending beyond $2R_c$ from SGZ that should be treated as damaged are being lumped with the background, undamaged zones. Additional subsurface pressure monitoring locations located two to three $R_c$ from SGZ would be necessary to confirm this speculation.
A notable result is the low sensitivity of the model to the pneumatic properties of the fractures in the 1Rc CCS, where the greatest damage and permeability alteration are expected. This is attributed to two factors: (i) the lack of pneumatic pressure measurements in the 1Rc CCS, and (ii) the low value of pneumatic diffusivity (\(\alpha\)) of 0.22 compared with values >1.0 for all other fracture zones (Table 2). The small \(\alpha\) value of the CCS indicates that a pressure signal will undergo greater attenuation and phase lag in the 1Rc CCS than in the adjacent fractured rock. Although the permeability is highest in the CCS, the 8% fracture porosity and high permeability create high \(q\) conditions that reduce the value of \(\alpha\) and limit barometric pumping effects in the CCS. The limited barometric pumping in the CCS thus reduces the sensitivity of the calibration to the \(k_f\) of the CCS.

Fracture half spacing \(l_f\) was also calibrated for some of the damage zones (the inner and outer surface damage zones were lumped with the background value in the calibration). The 1Rc CCS has the smallest \(l_f\) (0.31 m), where the greatest degree of damage and rubblization is expected, and is in agreement with measurements of rubble particle size for three other UNE chimneys reported by Boardman (1970). For the background rocks, a larger \(l_f\) of 1.48 m was estimated, and the sensitivity is moderately high (0.408 m). The relatively high sensitivity of background \(l_f\) in this case could be due to lumping the surface damage zone 2Rc with the background \(l_f\) since nine pressure records from this zone were used in the calibration. The calibration is highly sensitive to the \(l_f\) of the 2Rc CCS (1.19 m), the zone where the subsurface pressure in the post-shot hole was monitored.

**Gas Transport Simulations**

With confidence in the calibrated pneumatic properties, gas transport properties were evaluated by comparing the tracer breakthrough for SF\(_6\), 37Ar, and 127Xe for the NGME tracer gas injection. Multiple preliminary simulations were performed, and breakthrough concentrations at the surface prior to chimney pressurization were highly sensitive to tortuosity in the model. Ultimately, the MQ formulation was used to estimate a correction to the free-air diffusivity, and using this empirically based relationship, the model reproduced the absence of measurable concentrations of 127Xe and 37Ar prior to pressurization as well as the measured breakthrough concentrations at the ground surface following pressurization (Fig. 10). Without the MQ relationship to determine the tortuosity factors, simulated tracer breakthrough at the ground surface occurred earlier than observed. These results highlight the need for defensible simulated values of \(\theta\) and \(\theta_a\) in both the fractures and matrix that can be used to calculate gas-phase tortuosity values that allow prediction of tracer arrival at the ground surface.

Variable ground surface breakthrough concentrations simulated around SGZ are probably due to the subsurface heterogeneities built into the three-dimensional model, such as the damage structure and non-uniform HSUs. For example, both the P7P and P2P monitoring locations are approximately equidistant from the surface projection of the injection point, yet both the...
Influence of Barometric Pressure

The relative importance of early-time gas convection driven by post-UNE thermal and pressure gradients compared with the longer term effects of barometric pumping has been discussed by Sun et al. (2014) and Carrigan et al. (2016). Citing Nilson et al. (1991a), they discussed the possibility that pushing gases outward from the cavity during the early-time high-pressure stage may promote lateral rather than vertical gas transport, especially in anisotropic environments in which there is higher horizontal than vertical permeability because of layering. There is evidence that chimney collapse occurs only after significant reductions in initially high cavity pressures have occurred (Hudson and Stubbs, 1991), so that a significant vertical pathway from the cavity to the surface is absent at early times when pressures are highest (typically several megapascals). Moreover, pressure dissipation and chimney collapse occur at timescales of less than a day, limiting the opportunity for upward migration due to elevated pressure. Conversely, vertical transport of gases to the ground surface is more effectively achieved by pulling them upward through barometric pumping and by thermal convection once the chimney has collapsed, which is supported by the conclusions of Nilson et al. (1991a) that barometric pumping, while a much slower and more passive effect, is the primary control on vertical gas migration.

Modeling of the NGME, done as part of the present study, demonstrated that gas overpressures resulting from air injection were clearly responsible for the surface arrival of tracers during the NGME. In addition, modeling the gas migration following the 1989 Barnwell test was also undertaken to assess whether barometric pumping alone can reproduce the radioactive seepage observed post-detonation, without the UNE-related effects of temperature and pressure in the simulations. Four scenarios were simulated for comparison using the two barometric pressure records and two tracer gas source terms from the 1989 Barnwell test and the 2013 NGME. The Barnwell source term was calculated from estimates of radio-isotope production per kiloton yield listed in England and Rider (1994) using the maximum of the announced yield range (18–136 kilotones or 20–150 kilotons) to estimate the total isotope mass following the Barnwell UNE. Following an UNE, most of the Xe isotopes in the subsurface result from the radioactive decay of iodine precursors rather than fission products from the detonation (Sun et al., 2015). Simplified decay chains for both 133Xe and 133Xe were simulated following the Barnwell UNE, starting with their immediate parents 131I and 131I, which are themselves derived from isotopes of Sn, Sb, and Te. The mass of short-lived parents of iodine from these two decay chains were added to the initial 131I and 133I masses estimated for the Barnwell detonation, resulting in an initial cavity concentration of 1.16 × 10^7 Bq/L for 131I and 2.38 × 10^6 Bq/L for 133I. The rest of the decay chains for 131Xe and 133Xe followed the paths outlined by Sun and Carrigan (2014).

The estimated radioactive source terms for the Barnwell detonation for 131I and 133I were distributed in the fracture nodes in the cavity, exceeding the 127Xe concentration of 2.02 × 10^4 Bq/L from tracer injection into the chimney during the NGME by three to four orders of magnitude. The NGME tracer injection is described above. No UNE-related heat or over-pressurization was applied in the Barnwell simulations to observe the influence of pure barometric pumping. The two barometric pressure boundary conditions are shown in Fig. 11, including the comparison of tracer breakthrough at SGZ for the four scenarios shown beneath their respective pressure records. The four scenarios include: (i) the 1989 Barnwell source term and barometric pressure record (Fig. 11b-1); (ii) the Barnwell source term with the NGME barometric pressure record (Fig. 11b-2); (iii) the NGME source term with the 1989 barometric pressure record (Fig. 11c-1); and (iv) the 2013 NGME source term and NGME barometric pressure record (Fig. 11c-2).

The results show that Xe breakthrough at the surface relied strongly on the barometric pressure record and much less so on the concentration and initial distribution of the source term. The model accurately predicted tracer breakthrough timing for the two real scenarios: (i) 133Xe broke through at SGZ following the Barnwell test within 10 d (Fig. 11b-1), and (ii) the NGME had no gas breakthrough at SGZ during the 80-d period (Fig. 11c-2). Other Xe isotopes (e.g., 133Xe, 131mXe, and 133mXe) demonstrated breakthrough behavior similar to 127Xe. The relatively quiet barometric pressure signal in the summer of 2013 during NGME did not drive tracer breakthrough to the surface even with the larger 131I and 133I source terms from the Barnwell detonation (Fig. 11b-2). However, both source terms produced tracer breakthrough at SGZ within 10 d using the barometric pressure record associated with the Barnwell UNE (Fig. 11b-1 and 9c-1). The pressure record from the winter of 1989 to 1990 has greater variability, with a particularly large swing from high to low pressure at 5 d following the test, and this pressure drop was sufficient to drive gas to the surface from both initial source terms. Figure 12 shows a detailed comparison of the measured dose at a point 134 m north of SGZ in the first 5 wk following the Barnwell test with the simulated breakthrough of Xe isotopes at SGZ for 80 d. It is apparent from both the measured dose and modeled 133Xe concentration that barometric pressure dominates the signal, with elevated concentrations and dose coinciding with barometric pressure lows. These modeling and measured results support the hypothesis that barometric pumping is, in fact, capable of causing vertical gas migration to the ground surface if the barometric pressure conditions are...
Fig. 11. Results of the four-scenario comparison: the barometric pressure boundary conditions (a-1) for the 1989 Barnwell post-test period and (a-2) following the 2013 Noble Gas Migration Experiment (NGME) tracer injection; simulated tracer gas breakthrough (b-1) using the Barnwell source term and (b-2) the post-Barnwell and post-NGME injection barometric conditions; and the results for (c-1) the NGME injection concentrations and (c-2) the post-Barnwell and post-NGME injection barometric conditions.
strong enough, and it cannot be ruled out as a primary driver of early-time gas flow following an UNE during periods of stormy conditions with significant low-pressure swings. It should be noted, however, that the original interpretation of the observed surface seepage (Hudson, unpublished data, 1990) speculated that part of the transport path may have been through the slanted post-shot hole, since the observed seepage north of SGZ was aligned with the orientation of this hole.

The $^{133}$Xe concentration in the subsurface for simulated results at 10.3 d following the 1989 Barnwell test (Fig. 13) shows how the inclusion of local geology at U20az introduces subsurface heterogeneity into the model, influencing where the gas concentration may be expected to be highest. The gas preferentially flows toward a canyon to the northwest of SGZ. This region not only has lower elevation, so the barometric pressure boundary is effectively applied lower in the domain, but is also the location of a fault. The fault has not been parameterized with different flow properties; only the offset of the HSUs is represented in the model. This offset allows a faster pathway for gases to reach the surface, in particular because a gap in the high-porosity vitric tuff unit is caused by offset across the fault. The vitric tuff has a high air-filled porosity, and similar to the chimney, limits the effects of barometric pumping and provides storage for radioactive gases. The fault and other heterogeneities in the geometry of the HSUs may provide a faster path to the ground surface toward the canyon relative to vertical flow toward SGZ through the vitric tuff. There is no measured data to verify if gas migration during the Barnwell test or NGME actually had greater gas concentrations in the canyons than around SGZ. However, a two-dimensional model that assumes radially symmetric geometry would not have predicted this result, showing that, for certain applications, a three-dimensional model may be valuable for predicting the locations of gas breakthrough at the ground surface.

**Application to Foreign Sites**

Although the pneumatic pressure data set and surface tracer gas seepage observations from the NGME were not sufficient to fully calibrate all the detonation-induced damage features in the model, the analysis supports the use of a generalized conceptual model of damage around the working point. The damage features involve a cavity, a chimney, a zone of enhanced permeability due to fractures extending out to $2R_c$ from the working point, and the near-surface damage zones above and adjacent to the chimney that provide the flexibility to parameterize the model consistently with the observational data. The model calibration to the 2013 NGME pressure and tracer data was sufficient to predict the observed seepage of $^{133}$Xe following the Barnwell detonation in 1989 using only the surface barometric pressure data collected immediately before
and after the detonation. Although it was not necessary to invoke elevated temperatures and pressures following the Barnwell event as an important driving force for post-test seepage, additional studies may indicate that these are important drivers of post-test seepage at other sites, as suggested by recent experimental and numerical studies (Sun et al., 2014; Carrigan et al., 2016). The successful match of the model to the post-Barnwell gas seepage data indicates that, when calibrated with site-specific data, the simplified representation of the damage zones and near-field permeability structure is adequate for the subsurface transport of radioisotopes following an UNE.

The NGME gas seepage data and model for the U20az site have demonstrated that knowledge of subsurface conditions and detailed maps of fractures and faults may be necessary to predict the exact locations of gas seepage. The result does suggest that subsurface heterogeneities may be important to consider for determining sampling strategies for future experiments or at other sites. However, for remote gas sampling, where knowledge of the exact locations of seepage is unnecessary, the idealized damage-zone structures used in this study appear to be adequate for estimating the approximate surface arrival time of subsurface radioisotopes if the barometric pressure conditions and approximate yield and depth of burial can be estimated from other information.

Although additional air permeability and subsurface pneumatic pressure data are needed to fully constrain the model, the relative magnitudes of the porosity and permeability changes in the damage zones associated with the detonation and chimney collapse may be relevant to suspected foreign test sites conducted in porous rock such as tuff and sandstone. The applicability of these relationships to non-porous rocks such as granite and schist is more uncertain.

Conclusions and Future Work

Although U20az is a relatively well studied and characterized UNE site, many subsurface parameters remain uncertain and could benefit from further characterization. The U20az model demonstrates that simplified detonation-damage zonation, with geometry based on estimated yield, may be sufficient to perform predictive modeling of gas breakthrough timing at a foreign site. However, any site-specific information, such as rock type, geologic setting, fracture information, or saturation conditions, should be included if available for flow and transport parameter estimation. Some previous work has relied on building the permeability structure around UNEs from hydrodynamic simulations of rock damage (Jordan et al., 2014, 2015), which allows the inclusion of distinct features, such as detonation-induced fractures. As discussed, a limitation of the present model may be the simplicity of the damage zone structure. Future work is planned to perform gas migration modeling using a mesh and permeability field based on a hydrodynamic simulation, which is under development for the Barnwell test at U20az. Successful development of this model...
will allow an evaluation of the relative benefits of a more complex damage structure with the idealized damage structure used in the present model.

This work also provides a basis for understanding how barometric pumping controls the rate of gas migration. Barometric pressure conditions with high amplitude swings from high to low on a multiday scale, such as evident in the December 1989 record, may be sufficient to pull gas from the working point to the ground surface without the additional drive provided by increased temperature and pressure at the working point, although these will certainly facilitate gas migration. This effect was demonstrated by successfully matching the observed gas seepage following the Barnwell event without additional drivers for transport using a calibrated model of the site that also predicted the absence of surface seepage from barometric pumping alone during the 2013 NGME. The absence of surface breakthrough of injected tracers due to barometric pumping alone during the NGME is probably a consequence of starting the experiment during the summer months when barometric pressure changes were of smaller amplitude and higher frequency. The results of this work show that if similar tracer injection experiments were performed during a period with more dramatic pressure lows, such as the winter months, tracer breakthrough at the ground surface may have occurred. Overall, the results of the simulations provide evidence that under the right conditions, barometric pumping may explain the arrival of radioactive gas at the ground surface after a UNE. Additionally, the heterogeneous hydrostratigraphy may influence the subsurface gas migration pathways.

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References

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Weeks, E.P. 1978. Field determination of vertical permeability to air in the unsaturated zone. Prof. Pap. 1051. USGS, Denver, CO.

