A Geologically Based Markov Chain Model for Simulating Tritium Transport With Uncertain Conditions in a Nuclear-Stimulated Natural Gas Reservoir

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Summary
Nuclear-stimulation technology, which used subsurface nuclear detonation to increase permeability of tight natural gas reservoirs, was evaluated in the late 1960s and early 1970s. The Rulison site, located in the Piceance basin, Colorado, is one of three sites in the US where the technology was tested. An increase in exploration and production for natural gas in the basin has led to a need to quantify the extent of radionuclide (mainly tritium) migration after the detonation and potential migration under likely production scenarios. To meet this need, a numerical model was developed to simulate gas flow and tritium transport toward a hypothetical production well. A crucial problem in the model development is that limited on-site data are too sparse to quantify uncertainty of subsurface properties. This problem is partly resolved by using indirect data and information, such as parameter measurements from a nearby site and geological information regarding lithofacies structure. In particular, a geologically based Markov chain model was developed to simulate spatial distribution of the sandstone lithofacies.

This paper presents an application of the numerical model for simulating tritium transport from the nuclear chimney toward the production well at a likely location producing at a rate typical for the basin. The results show that the spatial distribution of lithofacies, especially in regard to the spatial distribution of lithofacies, is critical in controlling tritium transport. The results also show that the parameters of the sandstone and hydraulically fractured sandstone. The parameters become important only when the connectivity of sandstone lenses exists to support tritium transport from the chimney to the production well. The developed modeling framework can be updated as additional subsurface data are collected. The framework can be used to establish the feasibility of drilling restrictions that protect public health and the environment for different production well scenarios.

Introduction
In the late 1960s and early 1970s, subsurface nuclear detonation was considered as a method of increasing the permeability of tight gas reservoirs. Three such reservoirs in the USA (two in Colorado and one in New Mexico) were the subject of feasibility tests. The focus of this paper is the Rulison site in the Piceance basin, located approximately 64 miles northeast of Grand Junction, Colorado (Fig. 1). In 1969 at this site, a 40-kiloton nuclear device was detonated 2568 m below the land surface to fracture low-permeability Cretaceous Mesaverde sandstone. The Rulison site is located in an actively producing gas field in Colorado, and increasing activities of exploration and production have prompted an evaluation of radionuclide migration to ensure that drilling restrictions adequately protect public health and the environment. Among the radioactive isotopes produced by the detonation, tritium, an isotope of hydrogen, is the radionuclide of primary concern because it is produced in abundance and can migrate in both the gas and aqueous phases. The evaluation is hampered by various uncertain conditions in reservoir properties, which increase the challenge of reservoir management. To resolve this problem, a modeling framework was developed for simulating gas flow and tritium transport in the reservoir with uncertain conditions.

This study considers three types of uncertainty in (1) spatial distribution of lithofacies (sandstone and shale), (2) hydraulic parameters of sandstone, and (3) properties of hydraulically fractured sandstone associated with the production well. The first type of uncertainty is aleatory because of spatial variability of the lithofacies; the second type of uncertainty is epistemic because of sparse measurements of lithofacies parameters (primarily permeability and porosity); the third type of uncertainty is also epistemic given by the unknown nature of future hydraulic fracturing. The three types of uncertainty cannot be quantified from the sparse on-site data, which are limited to neutron and gamma logs at two boreholes and a total of 10 measurements of permeability and porosity. This problem is partly resolved by using indirect data and information, including parameter measurements from a nearby similar site, geological information regarding the lithofacies geometry (e.g., mean lengths of lithofacies), and engineering judgment for the hydraulic fractures. This general framework for quantifying uncertainty, especially in regard to the spatial distribution of lithofacies, is equally applicable to other reservoir management problems.

Lithofacies. Gas production at the site is primarily from the fluvial section of the Williams Fork formation of the Mesaverde group (Fig. 1). In the Williams Fork formation, two lithofacies—sandstone and shale—were identified on the basis of neutron and gamma logs at the site (Cooper et al. 2007). The shale includes both shale and siltstone, which are lumped together because of their low permeabilities. Gas production and tritium transport occur primarily in the sandstone, making distinctions between shale and siltstone unnecessary in the model. Although the sandstone has very low permeability itself (≈10^{-5} darcies), it is significantly more permeable than the shale and siltstone, whose permeability is ≈10^{-4} darcies (Sandia and CER 1990). The permeability difference of three orders of magnitude warrants modeling the sandstone and shale lithofacies separately.

Characterizing lithofacies heterogeneity can be impeded by a lack of subsurface data, such as those obtained from core measurements and well logs. For example, only two boreholes are available at the Rulison site, and they are insufficient for characterizing the spatial distribution in the horizontal direction. This problem can be partly resolved by incorporating other types of data and information using geostatistical methods (Yamada and Okano 2007) and artificial neural networks (Tang and Ji 2006). The transition probability and Markov chain (TP/MC) method (Carle and Fogg 1996, 1997), a geostatistical method used widely in hydrogeology but seldom in the petroleum industry, was used here. The TP/MC method was used because it can incorporate geological information, such as mean length of lithofacies. This is a useful characteristic of the TP/MC method when data are sparse. As discussed in more detail in the section “Geologically Based Markov Chain Model,” when the transition probability cannot be calculated from
sparse data, the Markov chain model used in the TP/MC method (for describing spatial variability of the lithofacies) can still be obtained from geological information, such as the background lithofacies (i.e., the most abundant lithofacies in this study, which is shale) and mean lengths of the lithofacies. Conversely, if a sample variogram (equivalent to the transition probability) cannot be calculated from sparse data, it is in general difficult to develop a variogram model (equivalent to the Markov chain model). Additionally, the TP/MC can better represent connections of the lithofacies than some conventional geostatistical methods. Lee et al. (2007) found that TP/MC created greater lateral connectivity and better-simulated a pumping test than the sequential Gaussian method. Similar conclusions were drawn by Maji et al. (2006) and Ye and Khaleel (2008) after they compared the TP/MC with ordinary kriging and cokriging, respectively. Lateral connection is of particular importance in this study, because it controls tritium transport toward the production well within sandstone lenses. Detailed comparison between the TP/MC method and other indicator geostatistical methods is warranted in future study.

Sandstone Fractures. Native fractures in the sandstone (in contrast to nuclear-generated and hydraulically generated fractures described below) are important to the successful production of gas in the Williams Fork reservoir (Johnson 1989). The equivalent porous medium approximation is used to incorporate the fractures, with the assumption that every sandstone lens is fractured. It is further assumed that the native fractures terminate at the contact between sandstone and shale, which is consistent with observations in cores and outcrops (Lorenz et al. 1989). This is significant as conductive pathways do not appear to extend into the shale. Fractures in the sandstone are not explicitly modeled because corresponding required parameters (e.g., fracture length, aperture, and network geometry) are not available at Rulison or nearby sites. The effect of the native fractures on sandstone permeability is incorporated by using an anisotropy ratio to increase sandstone permeability along the fracture strike direction, which is approximately east/west (Lorenz et al. 1990). It is conceptualized that the lithofacies structure inherently includes the characteristics of the native fractures in the sandstone by virtue of the permeability range and anisotropy ratio. More discussion on the anisotropy ratio is given in the “Anisotropy Ratio” section.

Nuclear Detonation. The extreme temperature and pressure from the nuclear detonation created a rubble-filled chimney (Fig. 2) estimated to be 23 m in radius and 84 m high (US AEC 1973). Four separate production tests were conducted in an evaluation borehole (located 95 m southeast of the emplacement hole) dur-
Future Gas Production. This study simulates a gas production scenario that begins gas production in 2007 (38 years after the detonation) and stops after 30 years. The production duration and rate were selected on the basis of typical activities in the Piceance basin, and were determined through discussion with operators and the Colorado Oil and Gas Conservation Commission. Production begins at the peak rate of 39,000 thousands of cubic feet of gas (MCFG) per month, and declines to a steady rate of 3,300 MCFG per month from 9 to 30 years. The amount of water produced at the production well is considered modest (Yurewicz et al. 2008). The location of the production well (258 m west of the chimney; Fig. 2) is based on well set-back distances and oriented to be in-line with the preferred fracture direction. The perforation zone and hydraulic fractures associated with the production well are also illustrated in Fig. 2. Before the production starts, tritium transport from the chimney in the aqueous and gas phases occurs by diffusion. After gas production starts, the converging pressure gradient toward the well causes advective flow toward the well.

Modeling Objective and Steps

In this paper, a comprehensive modeling framework is presented that (1) estimates the extent of diffusive tritium transport from the time of the nuclear detonation to the year 2007 when hypothetical gas production starts, and (2) determines whether tritium could reach the gas production well under a production scenario. Addressing uncertainty in structure and hydraulic parameters of the sandstone lithofacies and hydraulically fractured sandstone is a major component of the framework.

The reservoir simulation and uncertainty assessment are conducted in the following steps:

1. Develop a lithofacies-based geological model on the basis of geophysical logging and geological information from the Rulison site and nearby sites;
2. Generate multiple conditional realizations of the lithofacies (conditioned on borehole lithofacies data) to characterize reservoir heterogeneity and associated uncertainty;
3. Identify probabilistic distributions of hydraulic parameters of the sandstone based on their measurements at the Rulison site and nearby sites;
4. Estimate probabilistic distributions of properties (e.g., length) of hydraulically fractured sandstone on the basis of engineering judgments;
5. Generate multiple realizations of the parameters of the lithofacies and hydraulically fractured sandstone on the basis of the identified probabilistic distributions;
6. Combine the realizations of lithofacies and parameters to support a Monte Carlo simulation;
7. Conduct reservoir simulation and assess predictive uncertainty to facilitate reservoir management and decision making.

The modeling procedure is shown in Fig. 3, and its implementation is given below.

Geologically Based Markov Chain Model. Spatial distribution of the lithofacies is modeled using the TP/MC method. Occurrence of a lithofacies, \( k = \{1, \ldots, K\} \), at location \( x \) can be quantified using an indicator

\[
I_k(x) = \begin{cases} 
1 & \text{if lithofacies } k \text{ occurs at location } x \\
0 & \text{otherwise} 
\end{cases} \tag{1}
\]

Each lithofacies occupies a certain volume proportion, \( p_k \), in the domain and summation of the volume proportion is one,

\[
\sum_{k=1}^{K} p_k = 1. \tag{2}
\]
Using the notation of Carle (1999), transition probability from lithofacies \( j \) at \( x \) to \( k \) at \( x + h \) (\( h \) being lag) along the direction, \( \phi \), is defined as

\[
t(h) = \Pr(k \text{ occurs at } x + h | j \text{ occurs at } x).
\]  

A particularly useful property of the transition probability is that

\[
\frac{\partial t(h)}{\partial h} \bigg|_{h=0} = - \frac{1}{L(\phi)},
\]

where \( L(\phi) \) is the mean length of lithology \( k \) along the direction \( \phi \) (i.e., the total length occupied by \( k \) divided by the number of embedded occurrences of \( k \)). The implication of Eq. 4 is that the tangent of \( t(h) \) at \( h = 0 \) hits the lag at mean length of \( k \) along the direction \( \phi \). The vertical and horizontal directions are considered in this study, and the transition probability matrix in either direction is

\[
\begin{bmatrix}
t_{11} & t_{12} \\
t_{21} & t_{22}
\end{bmatrix},
\]

where the subscripts 1 and 2 denote the sandstone and shale, respectively. For example, \( t_{12} \) is the transition probability from the sandstone to the shale. When a background lithofacies is selected (always the one with the largest volumetric proportion), the embedded TP/MC model can be used, in which the row and column entries involving the background lithofacies do not need to be specified. More explanations of the embedded TP/MC model are referred to Carle and Fogg (1996, 1997) and Carle (1999). In this study, the shale is selected as the background lithofacies, and elements \( t_{12}, t_{21}, \) and \( t_{22} \) are not needed in the matrix, Eq. 5.

The spatial distribution of the two lithofacies is simulated using the T-PROGS software (Carle 1999) in the following steps:

1. Estimate indicator data of the lithofacies from Eq. 1.
2. Calculate sample transition probability in the horizontal and vertical directions.
3. Develop the Markov chain model (expressed by the volume proportions and transition probability matrix) by fitting the transition probability. (This is similar to fitting a sample variogram to a variogram model in conventional geostatistics.)
4. Generate multiple realizations of the spatial distribution of the lithofacies conditioned on the on-site indicator data.

On the basis of geophysical logging (not core measurements) at the emplacement and evaluation boreholes, 477 indicator data (i.e., presence of lithofacies of sandstone and shale) were obtained (Cooper et al. 2007). (The estimation from geophysical logging is less accurate than estimating directly from borehole core samples.) The volume proportions (48% for the sandstone and 52% for the shale) are estimated from the indicator data by dividing the number of sandstone or shale occurrences by the total number of indicator data.

Fig. 4 plots the transition probability and fitted Markov chain model in the vertical direction. In the figure, the Markov chain model in Fig. 4a and Fig. 4d decreases from 1 and stabilizes at the volume proportions of the two lithofacies. On the basis of Eq. 4, the fitted mean thickness of the sandstone is 7.5 m, which agrees...
with the observed thickness of 6.1 to 15.2 m at the nearby MWX site (shown in Fig. 1) (Sandia and CER 1990).

The transition probability in the horizontal direction cannot be calculated from the indicator data of the two boreholes. This is a general problem even with more boreholes, because borehole distances are often significantly larger than continuity of the lithofacies. In this case, the Markov chain model is developed on the basis of geological information, specifically the mean horizontal length of the lithofacies. Because the embedded Markov chain model is used, only the mean horizontal length of the sandstone is needed. We use a value of 161.1 m reported by Cole et al. (2004) on the basis of a study of stratigraphically equivalent outcrops at the Piceance basin. Flexibility of incorporating the geological information, such as mean sandstone length, is a useful property of the TP/MC method, especially when data are sparse.

Using the T-PROGS program, 500 conditional realizations of the sandstone and shale structure were generated, conditioned on the indicator data at the two boreholes. Fig. 5 plots two realizations selected arbitrarily for demonstration. Layering structure is depicted in the realizations, because of the small mean thickness and large mean horizontal length of the sandstone. The sandstone and shale are observed at the same horizon, since the mean length of the sandstone is smaller than the domain size. The generated random fields appear similar to those generated using an indicator simulator, because T-PROGS also uses the indicator cokriging technique (Carle and Fogg 1996). T-PROGS differs from conventional indicator kriging in that the cokriging equation is formulated using the Markov chain and not by using indicator variograms.

Probability Distributions of Random Variables of the Sandstone. Table 1 lists the random parameters considered in this study: (1) porosity, permeability, and permeability anisotropy ratio of the sandstone, and (2) permeability and length of the hydraulically fractured sandstone. Details of determining distributions and ranges of the parameter values are given in the sections below. Parameters describing the shale, nuclear chimney, and nuclear-fractured sandstone are treated as deterministic variables either because of their small variability or because they could be estimated from the nuclear test and/or subsequent production testing. Values of the deterministic parameters are given in Cooper et al. (2007). The Latin hypercube sampling (LHS) method (McKay et al. 1979) was used to generate random numbers because it is well known that LHS requires a smaller number of parameter realizations to represent parameter distribution functions. Spatial variability of permeability and porosity was not considered, following the practice of assigning each lithofacies homogeneous parameters (Anderson 1989; Fogg et al. 1998; Zhang et al. 2006; Lee et al. 2007; Ye and Khaleel 2008).

Permeability and Porosity. At the Rulison site, there are four estimates of permeability from production tests and six estimates of permeability and porosity from cores. These are insufficient for estimating probability distributions of the two variables. By contrast, the nearby MWX site has abundant permeability and porosity data for the Williams Fork formation (Sandia and CER 1990). Given the similarities in lithology at the MWX and Rulison sites, the extensive data developed at the MWX site are used to estimate the probability distributions at the Rulison site. The MWX data were from the analysis of more than 610 m of core, detailed log analysis and interpretation, and analysis of production testing using both analytic and numerical modeling techniques to match pressure histories. One limitation of the MWX data is that they are
Anisotropy Ratio. In order to incorporate the native fractures in the predominant east/west direction into the equivalent porous medium approximation, the permeability in the x-direction (oriented east to west) was obtained by multiplying the permeability in the y- or z-direction with the anisotropy ratio, \( k_x/k_y \) or \( k_z/k_y \). This is based on the finding of Lorenz et al. (1989) that the system permeability along the fracture strike direction (east/west) is up to 100 times that of the sandstone matrix, while the permeability of other two principal directions is nearly the matrix value. Comparing the matrix permeabilities measured for MWX samples to those estimated for the overall (fractured) reservoir leads to an anisotropy ratio range between 10 and 100 (Sandia and CER 1990); a uniform distribution on the interval \((fractured)\) reservoir leads to an anisotropy ratio range between 10 and 100 (Sandia and CER 1990); a uniform distribution on the interval \((0, 100)\). The 5th and 95th percentiles for length of hydraulically fractured sandstone are 40 and 100 m (Sandia and CER 1990); a uniform distribution on the interval of 10 and 100 is assumed for the ratio. As shown in Fig. 3, random numbers of permeability, \( k_x \) and \( k_y \), and the anisotropy ratio are first generated, and the permeability, \( k_y \), is then calculated by multiplying the anisotropy ratio with the permeability \( k_x \) or \( k_z \). Since \( k_x \) and \( k_z \) follow the lognormal distribution and the anisotropy ratio follows the uniform distribution, \( k_y \) follows the lognormal distribution.

Permeability of Hydraulically Fractured Sandstone. Hydraulic fractures are assumed elongated in the east/west direction, controlled by the in-situ stress state. To reflect the fact that permeability of hydraulically fractured sandstone is larger than the native sandstone, the permeability of the sandstone was multiplied by 100 to yield the permeability of the hydraulically fractured sandstone. The coefficient of 100 was determined ad hoc so that the range of the permeability agrees with the range of 0.01 to 0.1 darcies given by the development data at the MWX site (Sandia and CER 1990). This is illustrated in Table 1. Since sandstone permeability follows lognormal distribution, permeability of the hydraulically fractured sandstone also follows a lognormal distribution.

Production Zone. It is assumed that the perforation interval in the production well extends 5 m in the vertical direction. This appears consistent with industry practice (Sandia and CER 1990; Rutledge and Phillips 2003) and with the general thickness of sandstone bodies encountered at the emplacement and evaluation boreholes. The location of the production interval is different in each realization, depending on the spatial distribution of the sandstone. For each realization, the production interval was located by starting at the same elevation as the working point (the location of the nuclear detonation) to generate the shortest possible flowpath; if shale was present at the location in a given realization, the production interval was moved to the nearest sandstone in the vertical direction. The hydraulic fracture zone around the perforation interval was assumed to have a vertical extent of 10-m above the perforation and 10-m below the perforation. This yields a production zone 25-m high, within which the sandstone is hydraulically fractured but the shale remains unaltered (Wollhart et al. 2005). In practice, a production well would have multiple perforated intervals. These possible producing horizons above and below the production zone are considered to have little to no impact on the pattern of simulated tritium transport. This result is expected because of the natural layering of the Williams Fork formation and the intervening shale barriers between stacked producing intervals.

Length of Hydraulically Fractured Sandstone. The length of hydraulically fractured sandstone was determined on the basis of data from literature (Phillips et al. (2002), Sharma et al. (2003), and Rutledge et al. (2003)) in Texas; Reeves et al. (1999) in Wyoming; Sandia and CER (1990) at the MWX site). The 5th and 95th percentiles for length of hydraulically fractured sandstone are 40 and 160 m, respectively, and are consistent with descriptions by operators in the Piceance basin(1,2). A lognormal distribution is assumed, since it is typical for the length of observed natural fractures in sandstone (Lorenz 2003).

**Numerical Modeling.** A conceptual model of the multiphase flow and transport problem was developed on the basis of conservative conditions and the principle of parsimony. The model is conservative in favoring tritium transport toward the production well to err on the side of protecting human health. For example, the correlation between permeability and porosity was not considered so that a combination of large permeability and small porosity values would be possible to result in fast transport. The model is parsimonious because it is simple but able to explain observed physical and chemical processes; sparse data at the site does not support a more complex model, such as one describing discrete fracture networks. Details of the conceptual model and its numerical implementation can be found in Cooper et al. (2007). After the detonation and before the production of natural gas, THO migrates in the reservoir through diffusion in the aqueous and gas phases as a result of the concentration gradient resulting from the production of tritiated water by the detonation. The possible impact of gas production on tritium migration is modeled by introducing a pressure gradient toward the well, which results in an advective flow component to the transport analysis. Retardation processes include radioactive decay and exchange of THO between the liquid and gas phases. Fig. 3 illustrates the modeling process, starting with steady-state flow simulation before the nuclear detonation. After the nuclear detonation, the chimney and nuclear fractures were included in the model to simulate tritium transport from the chimney. The gas production begins 38 years after the detonation and stops after 30 years of production (68 years after the detonation),

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**TABLE 1—RANGES AND DISTRIBUTIONS OF RANDOM PARAMETERS OF THE NATIVE SANDSTONE AND HYDRAULICALLY FRACTURED SANDSTONE**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Minimum</th>
<th>Mean</th>
<th>Maximum</th>
<th>Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity (%)</td>
<td>0.08</td>
<td>5.29</td>
<td>10.5</td>
<td>Normal</td>
</tr>
<tr>
<td>Intrinsic permeability of ss* in y- and z-direction (darcy)</td>
<td>(2.42 \times 10^{-3})</td>
<td>(2.63 \times 10^{-3})</td>
<td>(3.27 \times 10^{-3})</td>
<td>Log normal</td>
</tr>
<tr>
<td>Anisotropy ratio ( (k_x/k_y) )</td>
<td>10</td>
<td>55</td>
<td>100</td>
<td>Uniform</td>
</tr>
<tr>
<td>Intrinsic permeability of ss in x-direction (darcy)</td>
<td>(2.70 \times 10^{-1})</td>
<td>(1.50 \times 10^{-4})</td>
<td>(2.95 \times 10^{-3})</td>
<td>Log normal</td>
</tr>
<tr>
<td>Intrinsic permeability of hfs* in y- and z-direction (darcy)</td>
<td>(2.42 \times 10^{-5})</td>
<td>(2.63 \times 10^{-4})</td>
<td>(3.27 \times 10^{-1})</td>
<td>Log normal</td>
</tr>
<tr>
<td>Intrinsic permeability of hfs in x-direction (darcy)</td>
<td>(2.70 \times 10^{-3})</td>
<td>(1.50 \times 10^{-2})</td>
<td>(2.95 \times 10^{-1})</td>
<td>Log normal</td>
</tr>
<tr>
<td>Length of hfs</td>
<td>36.10</td>
<td>71.96</td>
<td>132.98</td>
<td>Log normal</td>
</tr>
</tbody>
</table>

* Native sandstone is ss and hydraulically fractured sandstone is hfs.
while the simulation continues for a total time of 500 years after the detonation. The hydraulically fractured sandstone is included in the model at the beginning of the production period.

**Results**

Following the modeling process shown in Fig. 3, 500 Monte Carlo simulations were conducted. Simulation results for one realization are first shown to illustrate factors controlling tritium migration, followed by the composite Monte Carlo results. Tritium concentration is expressed as mass fraction of tritiated water in either the aqueous or gas phases, $X_{THO}$ or $X_{THO}^{*}$ (i.e., the density of THO in a phase per density of the phase). Background values of tritium mass fraction in the liquid and gas phases are $10^{-18}$ g THO/g liquid H$_2$O and $10^{-20}$ g THO/g gas (methane and water vapor), respectively (Cooper et al. 2007).

Controlling Factors for Predicted Tritium Transport. Fig. 6 shows the results for one realization in which THO reaches the production well. Figs. 6a and 6b are the vertical and horizontal cross sections showing the spatial distribution of sandstone and shale and locations of the chimney, nuclear fractured zone, and hydraulically fractured zone. The continuous and extensive sandstone between the nuclear and hydraulic fractures is clearly shown in the two figures, especially in Fig. 6b. Fig. 6c shows that for the 38 years before the start of gas production, tritium (plotted as $X_{THO}^{*}$) diffuses radially away from the chimney through the surrounding rocks. In Fig. 6d, after 10 years of gas production, tritium reaches the production well, which is represented by the vertical red line. It is obvious that in the absence of a regional gradient, advective tritium transport is triggered by the production of gas at the well, and that transport is largely through the sandstone. The extent of tritium migration is controlled by the spatial distribution of the sandstone as well as its permeability and porosity. For this realization, the sandstone permeability, $k_x$, is $2.04 \times 10^{-18}$ darcies, close to the mean value listed in Table 1, and the sandstone porosity is 0.42%, approximately one order of magnitude less than the mean value but one order of magnitude greater than the minimum value listed in Table 1.

Evaluation of the individual realizations indicates that the lithofacies structure is more critical in controlling tritium transport than the permeability and porosity values alone. Parameters of the sandstone and the hydraulically fractured sandstone become important only when the nuclear- and hydraulically-generated sandstone is connected by native sandstone. The importance of hydraulic fracture length also depends upon the lithofacies structure in that the sandstone must provide a pathway between the nuclear and hydraulic fractures for the hydraulic fractures to be important. This is confirmed by Fig. 7, which is a plot of $X_{THO}^{*}$ (20 years after the gas production) at the production well against sandstone permeability along the $x$-direction ($k_x$), sandstone porosity, hydraulically fractured sandstone permeability along the $x$-direction ($k_x$), and length of the hydraulically fractured zone for all 500 realizations. Fig. 7 shows nearly zero correlation between the simulated mass fraction and each of the parameter values. Taking the $k_x$ as an example, while the small $k_x$ values correspond to small $X_{THO}^{*}$ values, the large $k_x$ values correspond to average $X_{THO}^{*}$ values. A trend is slightly evident for porosity in that smaller porosity values correspond to larger $X_{THO}^{*}$ values, whereas there is no trend between the hydraulic fracture length and $X_{THO}^{*}$. The parameters have an impact on the results only in the context of the lithofacies distribution. Note that mass fractions less than the background value of $10^{-20}$ have only numerical meaning, not physical meaning, for the sensitivity analysis. In other words, only mass fractions larger than $10^{-18}$ are considered meaningful for decision making.

Predictive Uncertainty of Tritium Transport. Predictive uncertainty of tritium transport is assessed on the basis of the 500 realizations using the 5th, 50th, and 95th percentiles of predicted tritium mass fractions. While the 5th and 95th percentiles (also called uncertainty bounds) are often used in uncertainty analysis, they exclude extreme
In risk analysis, the first and 99th percentiles are also used to include the extreme events, if necessary. We do not use the mean and variance of the mass fraction fields since the simulated mass fractions are non-Gaussian because of the combination of the various distributions listed in Table 1. The 5th, 50th, and 95th percentiles are expected to contain more information regarding uncertainty than the mean and variance. Figs. 8 and 9 below plot only the 50th and 95th percentiles for convenience of presentation, because the 5th percentile has only small values of mass fraction and is not of interest for site management.

Fig. 8 plots the 50th and 95th percentiles of tritium mass fraction in the gas phase ($X^\text{TBO}_g$) at 38 and 48 years after the detonation (at the start, and 10 years after the start, of gas production). Since the percentiles are estimated as ensemble variables over the 500 realizations, the tritium distribution is less heterogeneous than that observed in an individual realization. As shown in Figs. 8a and 8b for the period when diffusion controls tritium transport, predictive uncertainty of tritium transport is negligible because the 50th and 95th percentiles are visually identical. Figs. 8c and 8d show that the uncertainty dramatically increases after gas production starts, and the 95th percentile has a significantly larger plume size than the 50th percentile. After gas production ceases, the production effect dissipates and diffusion again begins to control tritium transport, which results in negligible expansion of the plume size. In addition, the plume size shrinks with time caused by radioactive decay (the half-life of tritium is 12.3 years). As a result, the $X^\text{TBO}_g$ contours of the 50th and 95th percentiles become similar with time (Cooper et al. 2007).

Fig. 9 is a plot of the 50th, 95th, and 99th percentiles of the 500 breakthrough curves at the production interval against parameter (a) intrinsic permeability of sandstone along the x-direction ($k_x$), (b) porosity of sandstone, (c) permeability of hydraulically fractured sandstone along the x-direction ($k_x$), and (d) hydraulic fracture length. Results are shown for 58 years after the detonation (20 years after the gas production).

Conclusions

One of the challenges of modeling tritium transport at the Rulison site is that sparse on-site data cannot adequately quantify the uncertainty of subsurface properties. This problem is partly resolved by using indirect data and information, such as parameter measurements from a nearby site and geological information regarding lithofacies geometry. For example, the on-site geophysical logging from the emplacement and evaluation boreholes can be used to develop the Markov chain model in the vertical direction, but not the Markov chain model in the horizontal direction. The horizontal model is constructed by incorporating geological information from outcrop studies that provide the mean horizontal length of the sandstone. Using the geological information for the Markov chain model in the horizontal direction is of particular importance, since spatial distribution of the sandstone is critical in controlling tritium transport. Distributions of hydraulic parameters of the sandstone and properties of the hydraulically fractured sandstone were developed primarily by using the parameter measurements from the MWX site. Parameter values are of secondary importance to transport in comparison to the lithofacies structure, as they become important only when the nuclear and hydraulic fractures are connected by the sandstone.

The modeling framework developed for the Rulison site allows for the evaluation of possible production scenarios under uncertain conditions. As ongoing gas exploration continues nearby, some of the uncertainties considered may be better quantified, which leads to overall uncertainty reduction. For example, the TP/MC model can be readily updated by conditioning on additional new well logs, reducing uncertainty in the lithofacies structure.

Sensitivity analysis is needed in future study to investigate the following issues. The first one is to determine the sensitivity of predictive uncertainty to the combination of lithofacies structure
and parameters of lithofacies. In this study, after 500 realizations of lithofacies structures and parameters are generated, they are combined through random permutation before running the Monte Carlo simulation. Predictive uncertainty may change for other combinations of lithofacies structures and parameters. Secondly, a sensitivity analysis is needed to quantitatively measure importance of various random variables to the predictive uncertainty of tritium transport and to guide additional data collection. In addition to the random parameters listed in Table 1, other parameters (e.g., diffusion coefficient, tortuosity, mass transfer coefficient, and initial and boundary conditions) may also significantly affect the results of uncertainty assessment (predictive uncertainty will increase as more uncertain parameters are incorporated in the simulations). A sensitivity analysis would shed light on selection of the random parameters. Because of the random lithofacies structure, unconventional statistical quantities are indispensable for measuring sensitivity of predictive uncertainty to the parameters.

Nomenclature

\[ I_k(x) \] = indicator data of lithofacies \( k \) at location \( x \)

\[ L_{k,\phi} \] = mean length of lithology \( k \) along direction \( \phi \)

\[ p_k \] = volume proportion of lithofacies \( k \)

\[ f_{j,k}(h_{\phi}) \] = transition probability from lithofacies \( j \) to \( k \) at lag \( h_{\phi} \), direction \( \phi \)
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References


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