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A Multiple-Point Geostatistical Method for Characterizing Uncertainty of Subsurface Alluvial Units and Its Effects on Flow and Transport

By C. Cronkite-Ratcliff, G.A. Phelps, and A. Boucher

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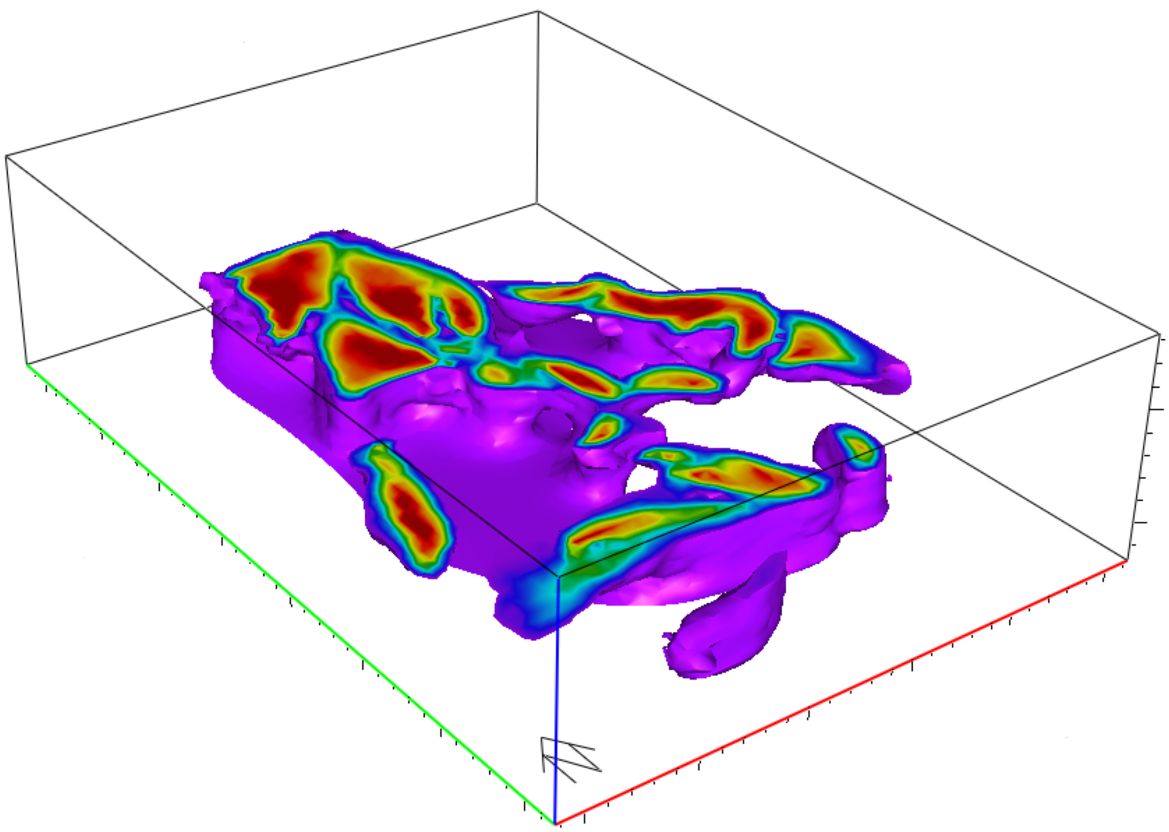

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Abstract

This report provides a proof-of-concept to demonstrate the potential application of multiple-point geostatistics for characterizing geologic heterogeneity and its effect on flow and transport simulation. The study presented in this report is the result of collaboration between the U.S. Geological Survey (USGS) and Stanford University. This collaboration focused on improving the characterization of alluvial deposits by incorporating prior knowledge of geologic structure and estimating the uncertainty of the modeled geologic units.

In this study, geologic heterogeneity of alluvial units is characterized as a set of stochastic realizations, and uncertainty is indicated by variability in the results of flow and transport simulations for this set of realizations. This approach is tested on a hypothetical geologic scenario developed using data from the alluvial deposits in Yucca Flat, Nevada. Yucca Flat was chosen as a data source for this test case because it includes both complex geologic and hydrologic characteristics and also contains a substantial amount of both surface and subsurface geologic data.

Multiple-point geostatistics is used to model geologic heterogeneity in the subsurface. A three-dimensional (3D) model of spatial variability is developed by integrating alluvial units mapped at the surface with vertical drill-hole data. The SNESIM (Single Normal Equation Simulation) algorithm is used to represent geologic heterogeneity stochastically by generating 20 realizations, each of which represents an equally probable geologic scenario. A 3D numerical model is used to simulate groundwater flow and contaminant transport for each realization, producing a distribution of flow and transport responses to the geologic heterogeneity. From this distribution of flow and transport responses, the frequency of exceeding a given contaminant concentration threshold can be used as an indicator of uncertainty about the location of the contaminant plume boundary.

Introduction

Geologic heterogeneity is a significant control on the pathways of groundwater flow and contaminant transport. This heterogeneity is inherently uncertain; characterizing the subsurface necessarily presents an inverse problem because heterogeneity must be characterized from geologic and geophysical data that sample only a portion of the subsurface. Researchers have addressed this problem with geostatistical techniques (Koltermann and Gorelick, 1996; Anderson, 1997; Wolfsberg and others, 2004; Marsily and others, 2005; Eaton, 2006; Renard, 2007). When these methods are used in numerical flow and transport simulations, the uncertainty about the heterogeneity of the subsurface can be related to the uncertainty about predictions of contaminant transport.

The theory of geostatistics is presented by several authors, including Goovaerts (1997), Deutsch and Journel (1998), Chilès and Delfiner (1999), and Remy and others (2009). Geostatistical methods are based on the idea that geologic properties can be considered random variables conditional to the available geologic and geophysical data. When applied through sequential stochastic simulation, geostatistical methods can be used to characterize the spatial distribution of geologic properties by producing a large number of realizations, thereby allowing uncertainty assessment through a Monte Carlo analysis. The advantage of geostatistical methods is that they can both honor the data and characterize heterogeneity according to an assumed model of spatial variability, such as a variogram.

Although traditional variogram-based geostatistical techniques have been widely used, they cannot reproduce the interconnected, curvilinear geometries characteristic of many sedimentary deposits. In the context of flow and transport predictions, which are sensitive to the connectivity of sedimentary facies (Western and others, 2001; Zinn and Harvey, 2003; Knudby and Carrera, 2005), this is a major limitation of variogram-based methods. Multiple-point geostatistics offers a solution to this problem by imitating complex spatial patterns by using a training image (Caers and Zhang, 2004; Hu and Chugunova, 2008). Examples of applications of multiple-point geostatistics in hydrogeology include Feyen and Caers (2006), Ronayne and others (2008), and Huysmans and Dassargues (2009).

This report presents multiple-point geostatistics as a potential tool for characterizing geologic heterogeneity and specifically its impact on uncertainty assessments in contaminant transport predictions. In this study, multiple-point geostatistics is used to produce several stochastic realizations that represent the spatial variation of geologic units in the subsurface. Groundwater flow and contaminant transport are then simulated for each individual realization, producing a distribution of flow and transport responses to the heterogeneity. From this distribution of flow and transport responses, the frequency of exceeding a given contaminant concentration threshold can be used as a measure of uncertainty about the location of the contaminant plume boundary.

This report focuses on the alluvial deposits found in the Basin and Range Province of the southwestern United States. These alluvial basins are an example of an environment with potential applications for the type of analysis presented in this report. They are characterized by considerable heterogeneity in the distribution of hydraulic properties controlling groundwater flow and contaminant transport (Cehrs, 1979; Neton and others, 1994; Koltermann and Gorelick, 1996).

To test the multiple-point geostatistics approach in the alluvial basin environment, a hypothetical geologic scenario is constructed using surface and drill-hole data from the alluvial deposits in Yucca Flat, Nevada, a basin located in the high desert of the southwestern United States (fig. 1). Yucca Flat is located within the Nevada National Security Site (NNSS, previously the Nevada Test Site). Between 1957 and 1992, there were 747 detonations at Yucca Flat, with announced yields of up to 500 kilotons (kt) (Allen and others, 1997). The potential for these detonations to impact the regional water supply has become a topic of interest and the subject of ongoing studies (Shaw Environmental, Inc., 2003).

These ongoing studies examine the release of radionuclides from the detonation sites and the migration of these radionuclides within the regional groundwater system (Federal Facility Agreement and Consent Order, 1996, as amended, 2008; Shaw Environmental, Inc., 2003). Detonations at the NNSS occurred in several different rock units underground, including many in the unconsolidated sediments in Yucca Flat that overlie lithified volcanic and sedimentary rocks within the basin (Bechtel Nevada, 2006). Although a majority of the detonations were carried out in the alluvial deposits (Stoller-Navarro Joint Venture, 2009), many studies do not consider the heterogeneity within the alluvial section (for example, Belcher, 2004). This report presents a method that could potentially be used to incorporate the heterogeneity of these alluvial deposits into future studies of groundwater flow and contaminant transport.

Purpose

This study has two purposes – one is to demonstrate a method for characterizing geologic heterogeneity by using multiple-point geostatistics, and the second is to show that this method can be used for analyzing the uncertainty in the results of flow and transport simulations. This method and the ensuing uncertainty analysis are demonstrated using a “test case” representing the general geologic characteristics of alluvial basins. Although this test case is developed by using data from the study volume in Yucca Flat, it is intended to be a generic example, with the study volume serving potentially as an analog for other alluvial basins.

The aim of using data from a real site is to test the integrated geostatistical model and flow and transport simulation with geologic heterogeneity on a basin-wide scale and with parameters drawn from a well-studied region. As noted by Huysmans and Dassargues (2009), applications of multiple-point geostatistics to real-world cases in hydrogeology are scarce; one objective of using data from Yucca Flat is to demonstrate the use of multiple-point geostatistics in a context with potential practical hydrogeologic applications. The data from Yucca Flat also present a common challenge for 3D geologic modeling, where vertical (1D) subsurface data must be combined with horizontal (2D) surface data to develop a 3D model of the subsurface geology.

Because this study focuses on the heterogeneity of alluvial deposits, the geologic structure was simplified to include only alluvial units, excluding local structural complexities known to be present. These complexities include faults that intersect the study volume and volcanic and carbonate rock units present at depth in some places within the volume. Incorporating these complexities would require scientific interpretation beyond the scope of this project. Although the results of this report are intended as a "test case" to demonstrate the method presented in this study, they are not suitable as an analysis of flow and transport for the selected part of Yucca Flat. For flow and transport modeling studies related to the ongoing corrective action investigation of Yucca Flat, the reader is referred to Shaw Environmental, Inc. (2003), Bechtel Nevada (2006), and Stoller-Navarro Joint Venture (2006, 2007, 2009).

Geology

Yucca Flat is a topographically closed Cenozoic basin that drains to a playa at its southern end (Bechtel Nevada, 2006). The basin consists of a thick Pliocene and Quaternary alluvial section overlying Miocene volcanic rocks, which in turn overlie a thick section of stratified Paleozoic rocks. At its deepest point, the alluvial section is more than 900 m thick (Bechtel Nevada, 2006). Examination of drill-hole samples from the alluvial section has revealed that alluvial geologic units of similar character to those found at the surface have been deposited throughout much of the history of the basin. This finding implies that the depositional environment has remained constant throughout this period, and that the surface Quaternary geology can inform models of the subsurface Pliocene and Quaternary alluvial geology. A map of the surface geology of Yucca Flat is shown in figure 2.

Structurally, Yucca Flat is cut by multiple normal faults, as is typical of basin and range structures, with the Carpetbag Fault (Slate and others, 1999) having the greatest amount of throw at approximately 1 km. The Carpetbag Fault forms the western boundary of the deepest sedimentary basin within Yucca Flat. It has been active in the Quaternary Period, but observation does not indicate Holocene activity. The Yucca Fault (Slate and others, 1999), a major north-trending fault east of the Carpetbag Fault, is an active Holocene fault with a maximum estimated throw of 400 m (Sweetkind and Drake, 2007a). These two major faults and several minor faults and fault splays offset underlying rock units and sediments. Although this study focuses on characterizing the geologic complexity of alluvial units in the subsurface, the structural complexities introduced by alluvial basin topography and faulting are not considered. Such an effort would require a complete examination of all of the alluvial samples within the study area, a task beyond the scope of this study.

This study focuses on the uncertainty introduced into flow and transport modeling by heterogeneous alluvial deposits. The alluvial section in Yucca Flat is particularly important in terms of contaminant transport because it hosted a majority of the underground detonations, extends throughout the basin, and typically is hundreds of meters thick. Previous 3D models of the alluvial deposits have either assumed the alluvial material was homogeneous and that hydraulic conductivity is a function of depth (for example, Belcher, 2004), or incorporated lithology and grain size information from drill-hole descriptions combined with a simple nearest-neighbor interpolation model to generate a volumetric model of the alluvium (Sweetkind and Drake, 2007b).

Quaternary alluvial units in the southwestern United States can be described and mapped using generalized soil chronosequences (Miller and others, 2009), a combination of surface morphology, grain size, soil development and landscape position. Slate and others (1999) used this approach to map Quaternary geologic units at the surface on the NNSS, and Menges and others (1996) used this approach to map alluvial units and investigate paleoseismic activity in the vicinity of Yucca Mountain. Nimmo and others (2009a) performed laboratory measurements of hydrologic properties of these units in the Mojave Desert, recording a range of hydraulic conductivity for each unit.

Study Volume

The 3D study volume is located in the north-central part of Yucca Flat. It extends 5 km east-west, 7 km north-south, and 760 m below ground surface (bgs). In UTM coordinates, the southwest corner of the study volume is located at 11U 580400 4106700. Surface elevations range from 1,280 m in the southeast corner to 1,379 m in the northwest corner. The surface geology of the study volume (fig. 3) is characterized by several different depositional environments, including alluvial fan deposits, central wash deposits, and playa deposits. The alluvium within the region of the study area is potentially cut by several faults, including the Yucca Fault, which runs north-south through the eastern part of the study volume. Qai, Qay, and QTa units (see table 1) collectively make up 97 percent of the units mapped at the surface of the study volume. Within the study volume, the alluvial section extends up to 700 m bgs, attaining its maximum depth in the southeastern part of the study area.

The study volume serves as a data source for the hypothetical “test case” developed in this study. This specific study volume was chosen because the alluvial section within the study volume consists of deposits from several different depositional environments with a large amount of available drill-hole data. Several of the drill-holes analyzed by Sweetkind and Drake (2007b) are located within the study volume. The size of the study volume was determined to be large enough to allow the modeling of large-scale variations in geologic units and the corresponding flow and transport response. The similarity of the alluvial deposits, depositional environment, and climate to alluvial deposits and environments throughout the southwestern United States make this volume an excellent source of data for developing analogs for other basin-fill systems in arid environments.

Method

Overview

The method presented in this report is executed in three steps: (1) geologic data acquisition, (2) geostatistical modeling, and (3) flow and transport modeling. In the geologic data acquisition step, surface geologic map information is evaluated for suitability of extrapolation to mapping the subsurface for flow and transport modeling. In the geostatistical modeling step, this surface geologic information is combined with vertical drill-hole data to develop a geostatistical model for the spatial variability of the geologic units in the subsurface.

The purpose of the geostatistical modeling step is to generate a series of alternative 3D geologic models stochastically, all of which honor the available data and are based on a consistent geologic interpretation. In the flow and transport modeling step, a 3D numerical model is used to simulate flow and transport for each realization. The purpose of the flow and transport modeling step is to produce a distribution of flow and transport responses to the set of alternative 3D geologic models.

The method is applied on a modeling domain (fig. 4) that matches the physical dimensions of the study volume. The coordinates of the data used in the modeling domain correspond to the equivalent coordinates of the data sources within the study volume of Yucca Flat. The modeling domain is discretized into a regular grid of 51 by 71 by 39 nodes, connecting along the x, y, and z axes, respectively, to form a mesh of 50 by 70 by 38 cells. Nodes are spaced regularly, such that each cell (or element) is 100 m by 100 m by 20 m.

This study considers permeability as the only parameter that varies between the different geologic units. Furthermore, permeability is considered uniform within each geologic unit. Assigning a different uniform value for permeability to each unit ensures that the flow and transport response depends on the configuration of geologic units as characterized by the geostatistical model. Differences in the flow and transport response can then be evaluated as the effect of differences in the geologic heterogeneity between each realization.

Geologic Data Acquisition

The objective of the geologic data acquisition step is to determine if the alluvial units mapped at the surface in Yucca Flat persisted through time as the Yucca Flat basin gradually filled with sediment, and if the hydrologic properties of these units could be estimated based on existing data.

The alluvial units at the surface in Yucca Flat consist of poorly to moderately consolidated, poorly sorted mixtures of sediment, with particle sizes ranging from clay to boulders, derived from local mountain ranges (Bechtel Nevada, 2006). The sediment is deposited on alluvial fans that subsequently are modified physically and chemically over time by soil formation processes (Gile and others, 1966; McFadden and others, 1984; Wells and others, 1987; Reheis and others, 1995). These modifications allow geologic units to be distinguished from one another by degree of soil development, surface morphology, grain size, and landscape position, and were used by Slate and others (1999) to map the surface alluvial units within Yucca Flat. Similar Quaternary geologic units have been described and mapped throughout the Mojave Desert (Menges and Miller, 2007; Menges and others, 2001).

To explore the subsurface alluvial sediments, drill-hole samples were examined specifically for soil development characteristics to use in classifying the samples according to the geologic mapping schema used to map the surface alluvial units. The distinction between the Holocene and Pleistocene units identified in the drill-hole samples particularly is important because of the lower hydraulic conductivity of the Pleistocene units. Fourteen drill-holes, each sampled at intervals of 25 or 50 ft, were logged across the Yucca Flat basin; seven of these holes were within the study area. The drill-hole data consistently showed soils similar to those observed at the surface, indicating that the climate and depositional environment are factors that have not changed significantly through the Holocene and Pleistocene records sampled by the drill-holes. Proportions also were similar to the areal proportions observed at the surface, with the exception that fewer soils resembling early to mid-Pleistocene soils were identified. This finding is likely an artifact of sampling because these early to mid-Pleistocene soils typically are preserved close to mountain range fronts, and few of the drill-holes sampled met this criterion.

Although less likely, the absence of these soils in the drill-hole samples may indicate more rapid basin subsidence in the past, or a tendency for these soils not to be preserved. No absolute dating of the samples was attempted, so the exact span of time is uncertain, but based on the preserved soil types, the records should extend at least 140-300 ka into the past (Miller and others, 2009). The alluvial units logged in the drill-holes were used as a hard constraint for subsequent stochastic modeling of the subsurface geology.

Nimmo and others (2009a) measured the hydraulic conductivity of alluvial units in the eastern Mojave Desert, which are similar to the primary alluvial units present in Yucca Flat. Because hydraulic conductivity is directly proportional to permeability for a fluid of constant density and viscosity, the hydraulic properties of the alluvium can be effectively estimated and used for subsequent modeling.

The alluvial units present on the surface geologic map of Yucca Flat were used in the modeling effort. Some of these units are not present at the surface within the study area, but they are observed elsewhere within Yucca Flat; therefore, although no playa deposits exist at the surface within the study area, it is possible that local topographic lows may have led to playa deposits within the study area in the past. Six alluvial units have been mapped at the surface in Yucca Flat (table 1). The different geologic map units are shown in terms of permeability in figure 5.

QTa, Qai, and Qay collectively constitute 97 percent of the alluvial units on the surface geologic map of Yucca Flat. Playa deposits compose nearly all of the remaining 3 percent, with QTc and Qeo present only in minor amounts. It is assumed that the proportions observed in the surface geologic map are represented throughout the study volume; that is, because QTa, Qai, and Qay make up 97 percent of the mapped alluvial units, they make up the same proportion of the volume. This assumption is consistent with the areal extent and proportions of similar Quaternary geologic units described initially by McFadden and others (1984) and shown subsequently by extensive mapping on alluvial fans across the eastern Mojave Desert (Menges and Miller, 2007; Menges and others, 2001). The spatial relationship between the volumetrically dominant units, QTa, Qay, and Qai, is expected to have the greatest control on flow and transport.

Geostatistical Model

In the geostatistical modeling step, the SNESIM algorithm (Strebelle, 2002), modified with search tree partitioning (Boucher, 2009), is used to characterize the geologic heterogeneity of the alluvial deposits from the study volume. The same method was applied by Phelps and others (2011). The multiple-point geostatistical method is applied here because flow and transport are expected to be affected significantly by the shape and connectivity of sedimentary deposits.

Remy and others (2009) provide a review of current multiple-point geostatistical methods. Multiple-point methods characterize the spatial relations between data from a training image, rather than from a variogram. A training image is a conceptual illustration of the general shapes, orientations, and arrangements of the geologic environment. In some respects, the training image can be considered an analog for the region being modeled. The SNESIM algorithm scans the training image and stores the patterns found in the training image in a search tree. Patterns that occur more frequently are assigned a higher probability of occurrence. For example, oxbow lakes commonly occur near, but disconnected from, their source rivers, so this spatial configuration might receive a high probability of occurrence in a model of a river valley.

The resulting modeled geology likely would have oxbow lake-shaped features that do not connect to the adjacent river features.

As with variogram-based methods, training image-based methods require an assumption of stationarity: the patterns recorded in the training image are expected to be repeated everywhere in the region being modeled. This assumption could be violated if, for example, a geologic region of interest extends from a mountain front to a distant valley floor, where thick, coarse debris flow deposits are expected near the mountain front, and broad, braided channels are expected far from the mountain front. In this case, debris flow deposits and braided channels are not expected uniformly across the region. If such a region were used as a training image, debris flow sedimentation patterns would be mixed in with braided channel sedimentation patterns across a subsequent model, and the model would violate geologic principles of depositional environments. Modeling such a region using multiple-point geostatistics would require using two separate training images, one with braided channels and one with debris flows, resulting in two separate geologic models that would need to be "stitched" together. It is possible, however, to use a non-stationary training image, as is done in this study, and also to build non-stationary geologic models. In this case, the training image and (or) region to be modeled must be separated into stationary regions.

Geologic models (realizations) are generated by using the SNESIM algorithm. The study area of interest is discretized into a grid of pixels (equivalent to cells in the modeling domain), and values (representing discrete categories, such as geologic map units) are assigned to each grid cell in sequential order. At each grid cell in the sequence, a discrete category is assigned randomly based on the surrounding conditioning data and the patterns stored in the search tree. Readers are referred to Strebelle (2002) for a detailed description of the SNESIM algorithm.

Modeling the geologic heterogeneity of a 3D volume using the SNESIM algorithm requires some representation of heterogeneity in all three dimensions. This representation of heterogeneity would give information on the 3D configuration of alluvial units, similar to those assumed to be in the subsurface of Yucca Flat. Three-dimensional training images can be generated using object-based simulation methods (for example, Deutsch and Wang, 1996), where simple shapes (for example, channel deposits generated using sine waves, or lobate flow units generated using an ellipse) are placed within a training image volume. Object-based methods, however, have a number of limitations in terms of matching hard data and realistically representing geologic heterogeneity (Feyen and Caers, 2006). Surface geologic maps, which record the patterns describing natural geologic heterogeneity, are readily available for use as training images, but are limited to two dimensions.

A 2D horizontal training image was combined with 1D vertical variograms to characterize the geologic heterogeneity in three dimensions. The 2D training image was derived from the surface geologic map by Slate and others (1999), and the 1D variograms were derived from vertical drill-hole logs.

The 2D training image used is the surface Quaternary geologic map of Yucca Flat (Slate and others, 1999). The Quaternary geologic map records several depositional environments, including alluvial fan deposits, central wash deposits, and playa deposits. Each environment has unique patterns and scales governing geologic heterogeneity and, thus, does not exhibit the stationary patterns required for a training image. To overcome the lack of stationarity in the geologic map, the training image is partitioned into several stationary regions called "partition classes" (Boucher, 2009). Partition classes are internally stationary, and the patterns unique to each partition class are stored efficiently within an imbricated search tree. The ability to partition a training image into several stationary regions not only allows more complex training images to be used, but also enables more geologically complex realizations to be generated. Readers are referred to Boucher (2009) for a detailed description of the search tree partitioning method. The advantage of using the search tree partitioning method is that it allows a non-stationary image – such as the geologic map of Yucca Flat, a map with several regions of distinct geologic patterns (older units along mountain fronts, alluvial washes channeling flow down the valley axis, a playa at the southern end of the basin) – to be divided into stationary portions that can be used in simulation.

The first step in the search tree partitioning method is to separate the training image into partition classes. To separate the training image using the Quaternary geologic map, an assumption is made that the Quaternary geologic units within Yucca Flat are related to the topography. Topographic variables, in this case gradient, aspect, map distance to bedrock, and elevation of source, are related directly to the training image and can be used to develop partition classes. Using topographic variables to develop partition classes allows the surface geologic map to be separated into regions that share similar topographic characteristics. By using the *k*-means algorithm (MacQueen, 1967), the four topographic variables were divided into 15 partition classes, which were then overlain with the training image to divide it into partition classes. Each partition class was incorporated into its own search tree, resulting in 15 imbricated search trees. During the simulation, these search trees were available to define unique patterns for distinct regions of the model volume.

Next, these 2D simulations needed to be combined to generate a single 3D realization. The training image was combined with the vertical variograms during the implementation of the SNESIM algorithm. Vertical variograms were derived from the drill-hole data described in the previous section. A single 3D realization was generated one layer at a time, with subsequent layers incorporating the previously modeled layer as hard data. The vertical variograms were used to modify the probability of the occurrence of a given category based on previously simulated layers. At each grid cell, two probabilities are available to simulate a geologic unit: (1) the conditional probability obtained using the search tree partitioning method, in the horizontal direction, and (2) the conditional probabilities obtained using the 1D vertical variograms and indicator kriging method in the vertical direction (Deutsch and Journel, 1998). The two probabilities are combined using the tau model (Krishnan and others, 2005; Krishnan, 2008), which provides a solution for integrating partially redundant data. The geologic unit is then assigned by drawing a discrete category from the resulting posterior probability distribution. This procedure allows spatial continuity to be maintained in the vertical direction and the horizontal direction.

To generate a geostatistical realization of modeled alluvial units within the modeling domain, the volume is filled one layer at a time, from top to bottom. The first layer is the surface geologic map and is known. The next layer is simulated using the search tree partitioning method, conditioned to the drill-hole data. Vertical continuity is maintained with the layer above by using the vertical variograms to constrain the outcomes of the partitioned search tree, imitating the tendency of an alluvial fan depositional environment to remain constant over time, and only occasionally avulsing and abruptly changing the depositional environment. The following layers are simulated in the same manner, until the volume is filled. The final realization is a volume filled with simulated alluvial units that match all available drill-hole data, the vertical variogram information, and the complex patterns found in the partitioned training image.

Twenty realizations were generated according to this method. Each realization represents one possible subsurface map unit configuration, and all realizations are assumed to be equally probable. The collection of realizations characterizes the potential variability of alluvial units in the subsurface and, therefore, represents the uncertainty about the configuration of geologic units within the volume.

Flow and Transport Model

A 3D, finite-element numerical model is developed using SUTRA (Voss, 1984) to simulate flow and transport within the modeling domain. Each geostatistical realization is incorporated into a flow and transport simulation; for every realization, each grid cell corresponds directly to an element in the finite-element mesh. The finite-element mesh has dimensions and discretization equivalent to those used in the geostatistical modeling step. The coordinates of the nodes are adjusted to match elevations from the corresponding digital elevation model (DEM) (Gesch, 2007; Gesch and others, 2002).

Contaminant transport is simulated with a conservative, non-sorbing tracer with the basic physical properties of tritium (^{3}H). Radioactive decay is not considered. This tracer is continuously released from 224 point sources located at nodes corresponding to the “working point” of each underground test, defined by Stoller-Navarro Joint Venture (2006) as the emplacement location of each nuclear device. The values for concentration at each point source are considered mass fractions equal to the approximate yield equivalent in tons divided by 10^{7}, and effectively are arbitrary.

Uniform values for permeability were assigned to each geologic map unit. Approximate values were based on the ranges provided by Phelps and others (2011), in which hydraulic conductivities are assigned to the geologic map units by using a combination of field measurements (Nimmo and others, 2009a, b) and petrophysical relations derived from grain size distributions considering particle packing in sediment mixtures (Koltermann and Gorelick, 1995). The flow and transport model assumes that permeability is isotropic for all media (permeability is not greater in one direction than in another). A uniform effective porosity is assumed to be 31.0 percent.

Figure 6 demonstrates that the modeled geologic units are translated directly into permeability. Note that the geology (fig. 6*A*), and hence the permeability distribution (fig. 6*B*), is dominated by the three most prevalent units: QTa, Qai, and Qay. Although all realizations have the same surface geology, they can be distinguished by significant variation in the distribution of subsurface geologic units. Based on the values assigned, QTa is the least permeable major unit and is expected to act as the greatest barrier to flow; Qay is the most permeable major unit and is expected to enhance flow. The permeability of Qai lies between the permeability of QTa and the permeability of Qay. The less abundant units (QTc, Qeo, and Qp) have more extreme values, but are present only in minor amounts.

Transient flow and transport are simulated for a time period representing 50 years. Initial conditions consist of specifying a pressure distribution corresponding to an estimated potentiometric surface (D’Agnese and others, 1998), and specifying contaminant concentrations at each source node. Hydrostatic pressure head is specified at the lower boundary, and an infiltration rate of 3.15 mm per year is specified at the upper boundary. Boundary conditions and contaminant concentrations at source nodes are held constant. During the simulation, the modeling domain is partially saturated down to depths ranging from 350 to 650 m bgs, below which the domain is fully saturated. Measurable contaminant transport results were produced only in the saturated portion of the domain.

Results

The results of the flow and transport simulations show significant variability in the size, shape, and orientation of plumes generated by the flow and transport model. The differences between individual flow and transport simulations are the result of variations in geologic heterogeneity between realizations.

Results from four of the twenty flow and transport simulations are presented in figure 7; these four simulations were selected to display the range of variability in size, shape, and orientation of the contaminant plumes produced in each simulation. Plumes are defined as the body of groundwater with contaminant mass fractions above 10^{-4}, an arbitrary cutoff level selected to allow for visual comparison between the results of each simulation. The plumes are displayed in plan view to allow identification of the main features and relative locations of each plume. The simulations have predicted plumes in a variety of configurations, ranging from a large plume extending across much of the region to several smaller localized plumes within the region.

In geologic media characterized by a heterogeneous permeability distribution, flow is directed through high permeability units and diverted around low permeability units. A direct spatial correlation between contaminant concentration and the permeability of co-located geologic media does not reveal the specific pathways of flow and transport required to understand the effect of geologic heterogeneity on flow and transport pathways. However, the simulations produced some examples where this relationship can be examined visually. Figure 8 compares modeled permeability distributions to the configuration of simulated contaminant plumes for a co-located slice of the subsurface for two different simulations. In figure 8*A*, a relatively homogeneous distribution of high permeability allows separate plumes to co-mingle, while in figure 8*B*, the presence of a low permeability abandoned alluvial deposit (QTa) maintains several hundred meters of separation between two smaller plumes, preventing the same co-mingling behavior.

Figure 9 shows the frequency of exceeding the threshold contaminant mass fraction of 10^{-4} everywhere within the modeling domain, based on the results of all 20 simulations. These maps show significant variability in the boundaries of the simulated contaminant plumes. Although points with at least a 50 percent frequency of exceeding a concentration of 10^{-4} form generally separate clusters, the points with at least a 10 percent frequency of exceeding a concentration of 10^{-4} extend throughout the central portion of the modeling domain. These results indicate that the extent and direction of the simulated plumes can vary by several hundred or even thousands of meters between realizations.

Discussion

Uncertainty in the configuration of geologic map units in the subsurface is characterized by generating a series of realizations stochastically using multiple-point geostatistics. The 3D geostatistical model used in this study combines both 2D and 1D data, drawing directly upon both geologic map data and drill-hole data to develop a 3D model of spatial variability. The set of realizations approximates a distribution of possible spatial configurations of geologic units below the surface. Groundwater flow and contaminant transport is then simulated for each realization, producing a distribution of flow and transport responses to the range of spatial configurations. From this distribution of flow and transport responses, the frequency of exceeding a given contaminant concentration threshold can be used as an indicator of uncertainty about the location of the contaminant plume boundary.

Successfully developing a 3D geostatistical model of this geologically complex alluvial basin environment depended on several key resources. One key component was the surface geologic map of Yucca Flat, which provided a range of spatial patterns describing geologic units in alluvial basins. Another key component was the availability of quality drill-hole data that enabled the identification of the alluvial units in the subsurface. These data provided critical information on the distribution of alluvial units in the subsurface and evidence that these units were similar to those at the surface and that the geologic map was appropriate for use as a training image. A third key factor was the use of the search tree partitioning method, which separated the training image into internally stationary regions and reconstructed these regions in each realization.

Conclusions and Recommendations

This study has presented a method for characterization of geologic heterogeneity and investigating its effect on uncertainty in contaminant transport predictions. The method uses data from Yucca Flat to develop a test case for application to geologically complex alluvial basins in arid regions. This study has gone beyond previous studies of arid alluvial basins in several respects by: (1) defining and examining the subsurface in terms of Quaternary geologic units mapped at the surface, (2) developing a geostatistical model of the subsurface that adheres to observed geologic patterns at the surface and continuity of geologic units with depth, (3) simulating groundwater flow and contaminant transport, and (4) characterizing the variability of flow and transport owing to geologic heterogeneity.

However, this report represents a work in progress on several accounts. In order to apply this method to the corrective action investigations for Yucca Flat, additional geologic information must be considered. This information includes the location of the volcanic and carbonate units within the basin and information on structural geology, including faults and the displacement of units across faults. There are also many ways in which the flow and transport model could be improved, such as making changes to the scale and resolution of the model, the assigned flow and transport parameters, and the physical setup of the numerical model. More detailed data would need to be included to account for the spatial variability in flow and transport parameters, an accurate simulation of variably-saturated flow, the realistic behavior of multiple mobile contaminants, and an accurate characterization of the hydrologic and radiologic source terms. Additional steps would need to be taken to develop constraints on the flow and transport simulation and to incorporate geologic modeling into these constraints.

Although this study has focused on the applicability of multiple-point geostatistics, the wide range of problems involving subsurface geologic heterogeneity may require a toolbox that uses a variety of geostatistical methods. In order to become more practical for potential users, methods for combining geostatistical modeling with flow and transport simulation need to be further developed. In particular, efforts should be made to further develop tools for uncertainty analysis that can be applied practically where informed decision analysis or risk assessments are required.

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Figures

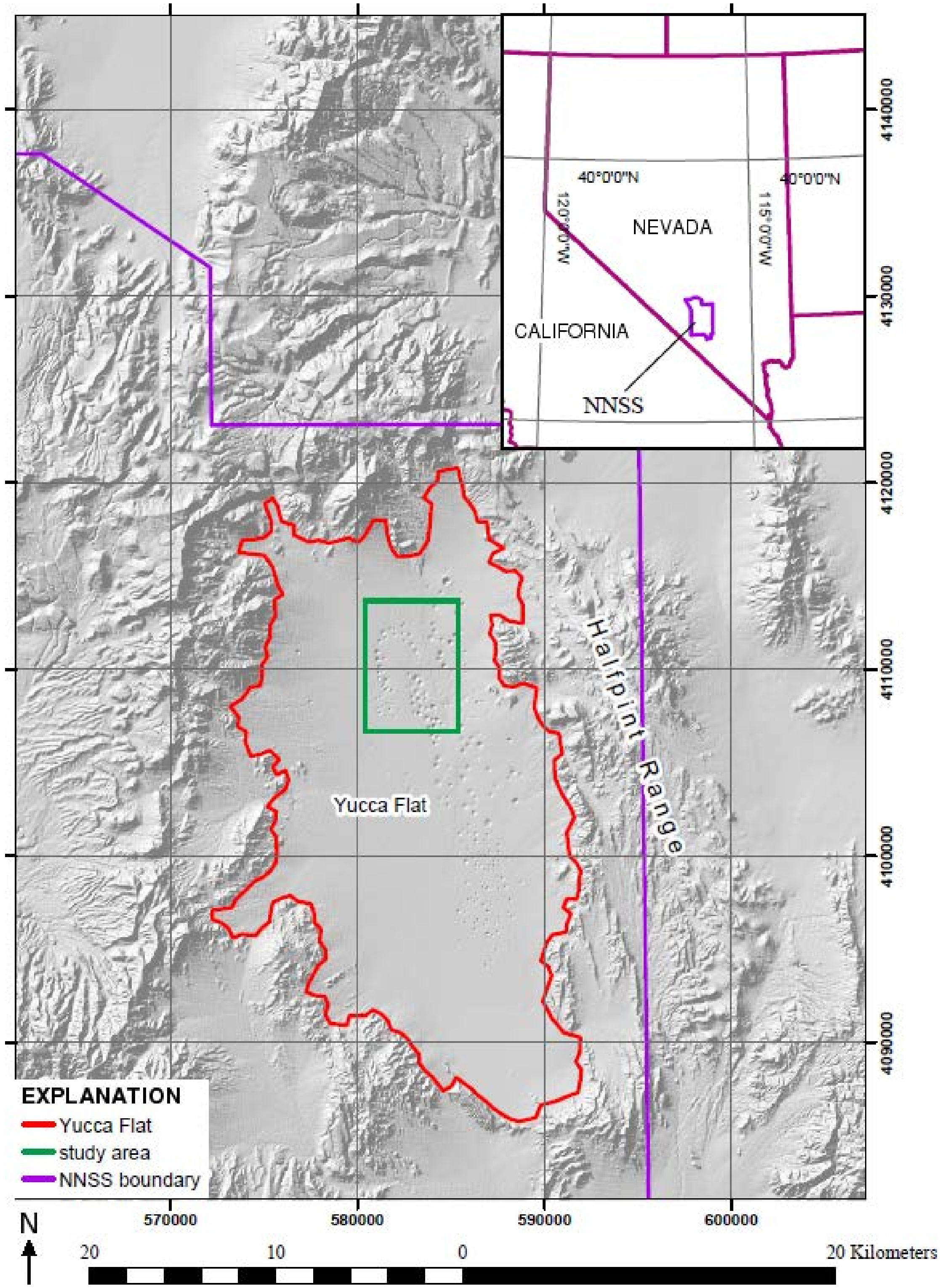

Figure 1. Location of the study area within Yucca Flat, Nevada. Location of the Nevada National Security Site (NNSS, previously the Nevada Test Site) is shown inset. Base map is a merged 30 m digital elevation model (Gesch, 2007; Gesch and others, 2002).

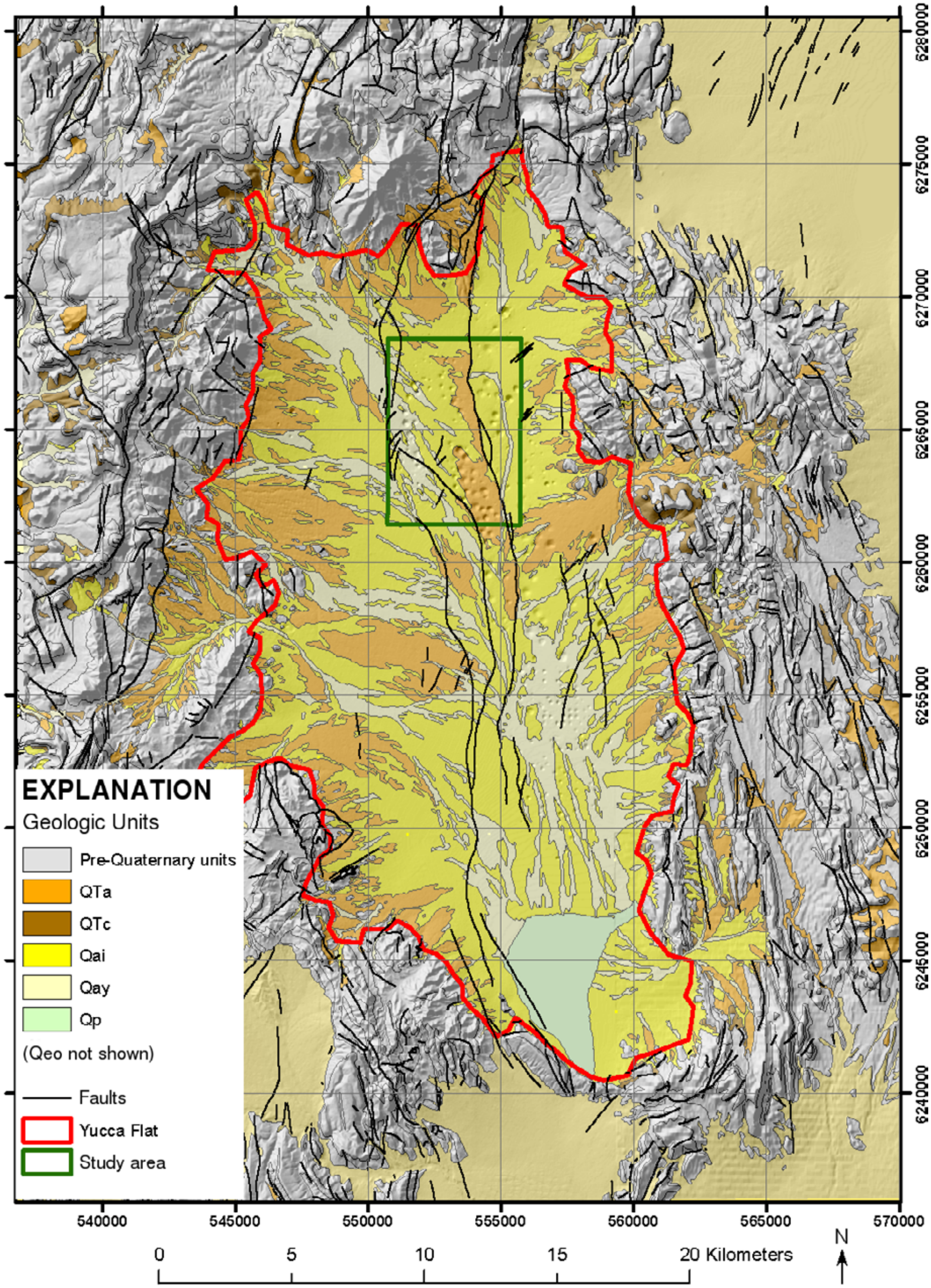

Figure 2. Location of the study area in Yucca Flat, Nevada shown with the surface geology (Slate and others, 1999; see table 1 of this report for geologic units).

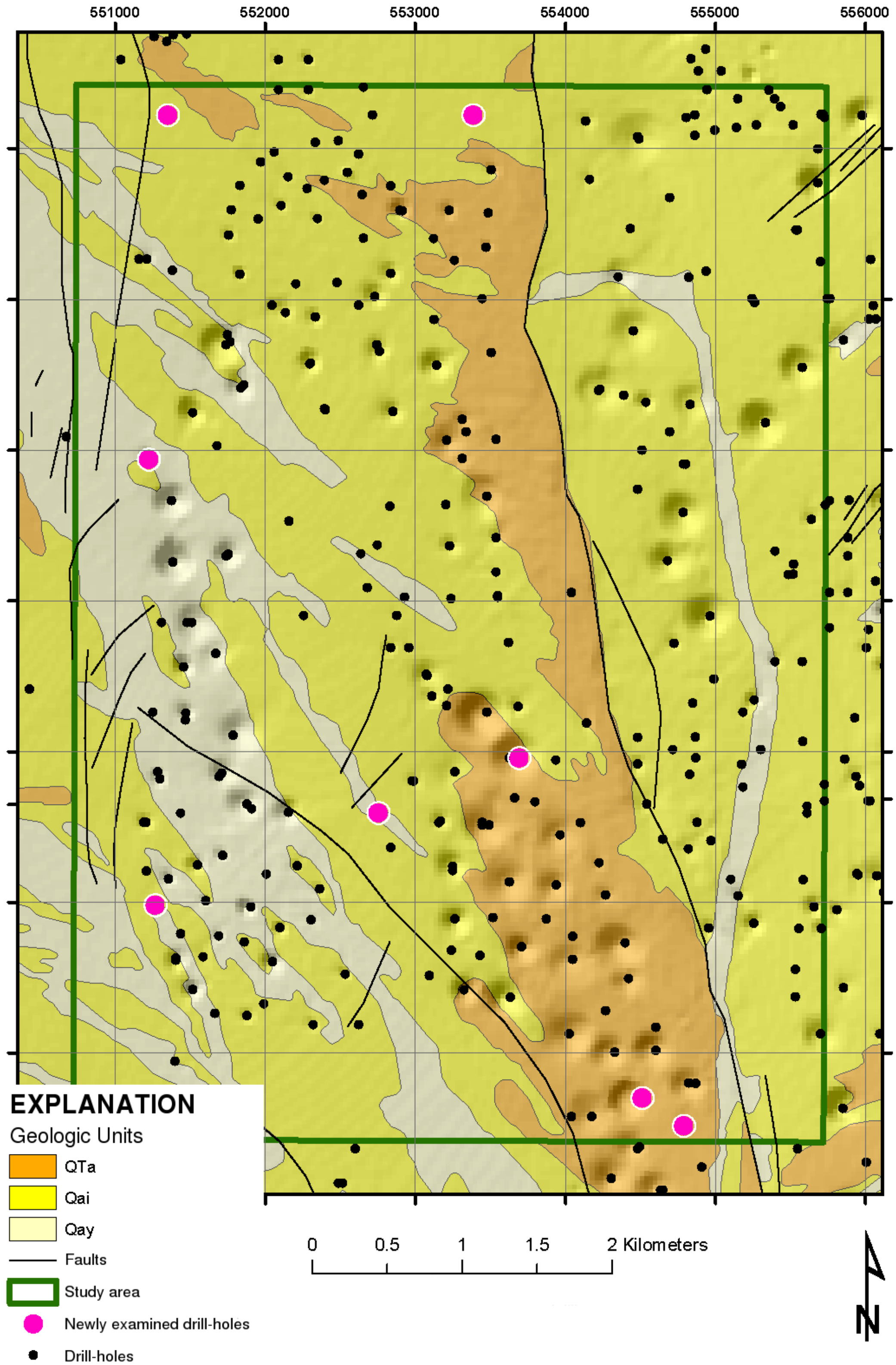

Figure 3. Surface geologic map of study area in Yucca Flat, Nevada, showing the drill-holes used to characterize the subsurface heterogeneity of the alluvial deposits (see table 1 for geologic units).

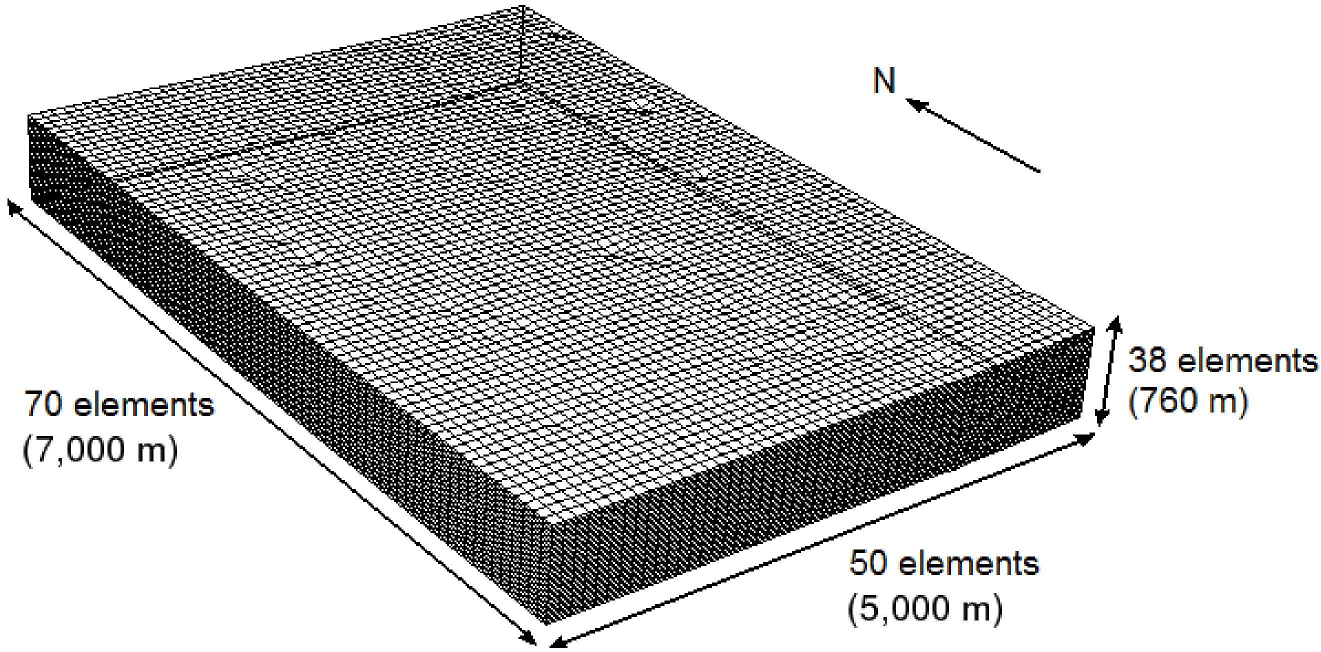

Figure 4. This figure shows the discretization of the modeling domain into a regular grid of cells (elements) with nodes at the corners of cells.

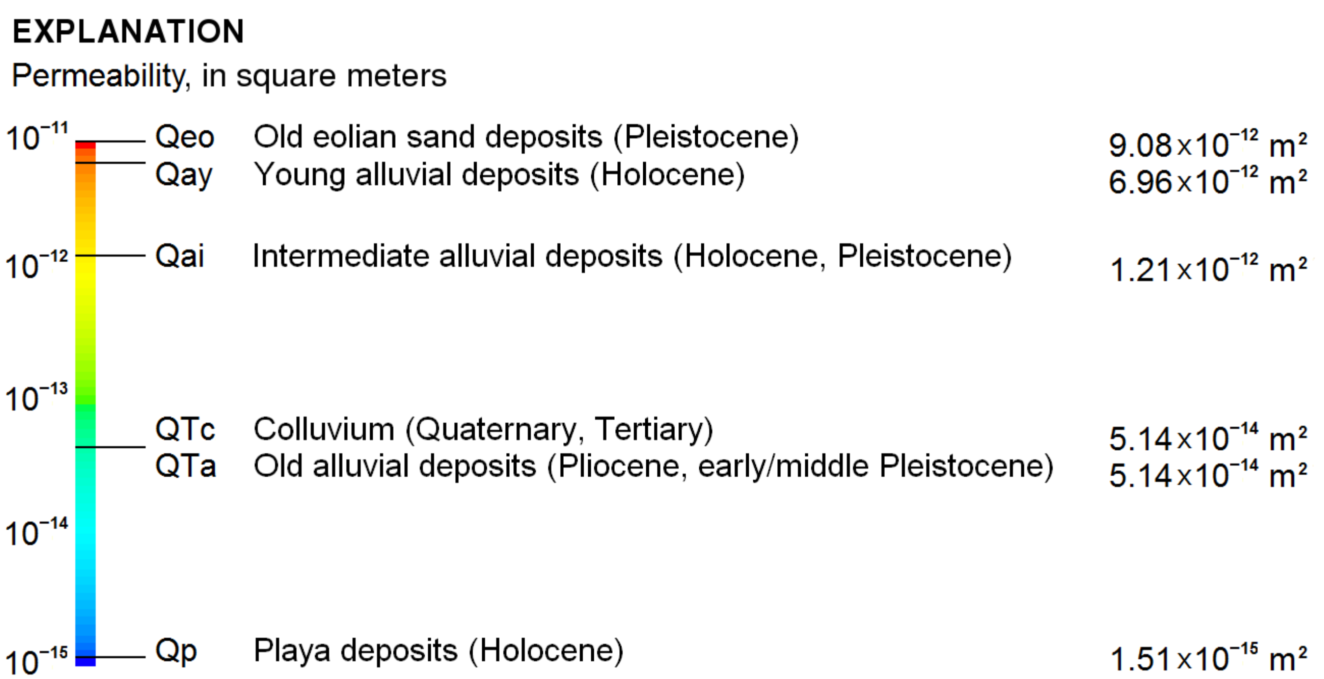

Figure 5. This figure uses a logarithmic scale to display the relationship between the different geologic map units in Yucca Flat, Nevada, in terms of their permeability (see table 1).

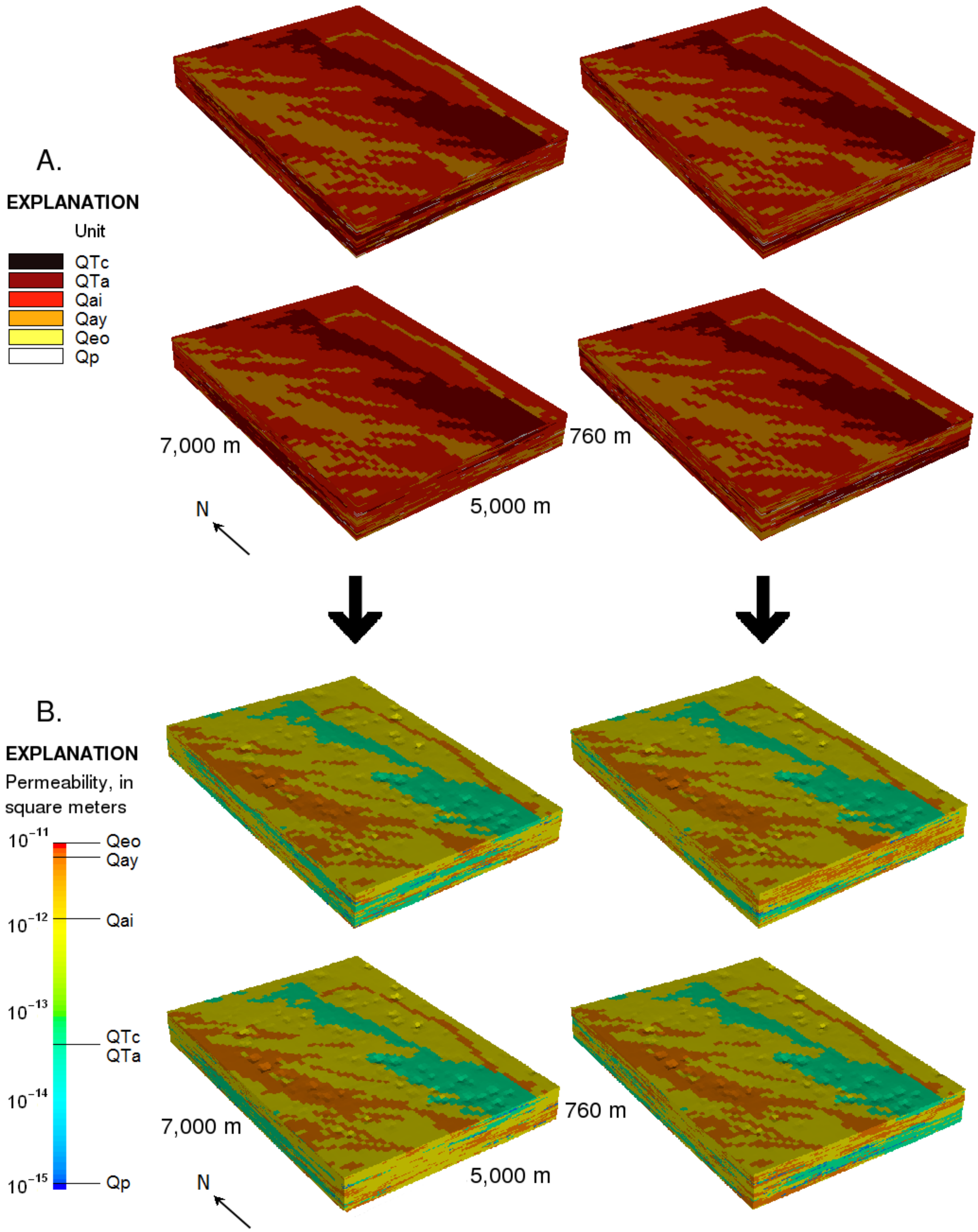

Figure 6. Distribution of modeled geologic units from the modeling domain. *A*, Four of 20 realizations from the geostatistical model. *B*, Corresponding distribution of permeability for the four realizations.

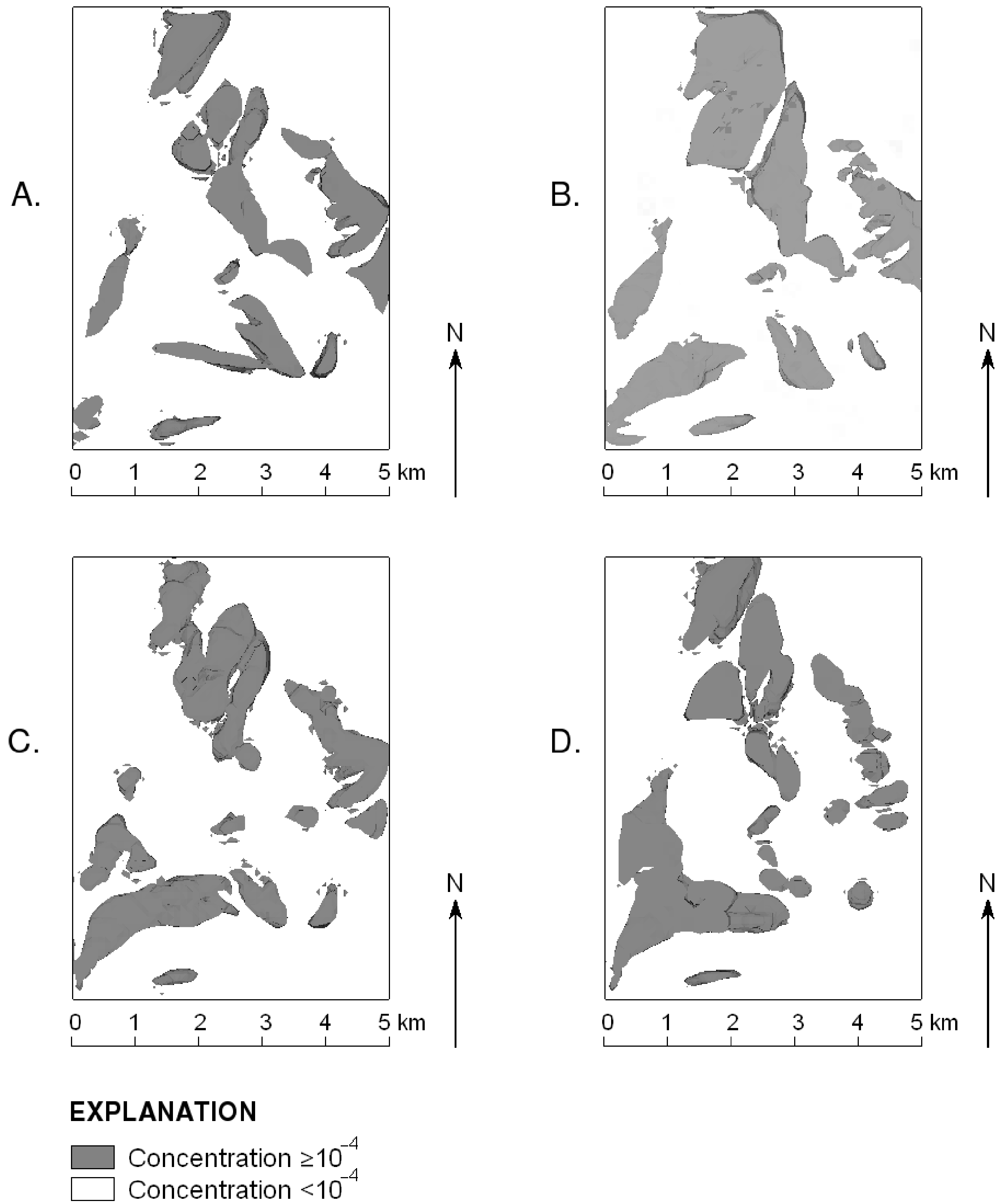

Figure 7. This figure shows contaminant plumes from four (*A*-*D*) of the 20 flow and transport simulations for the modeling domain.

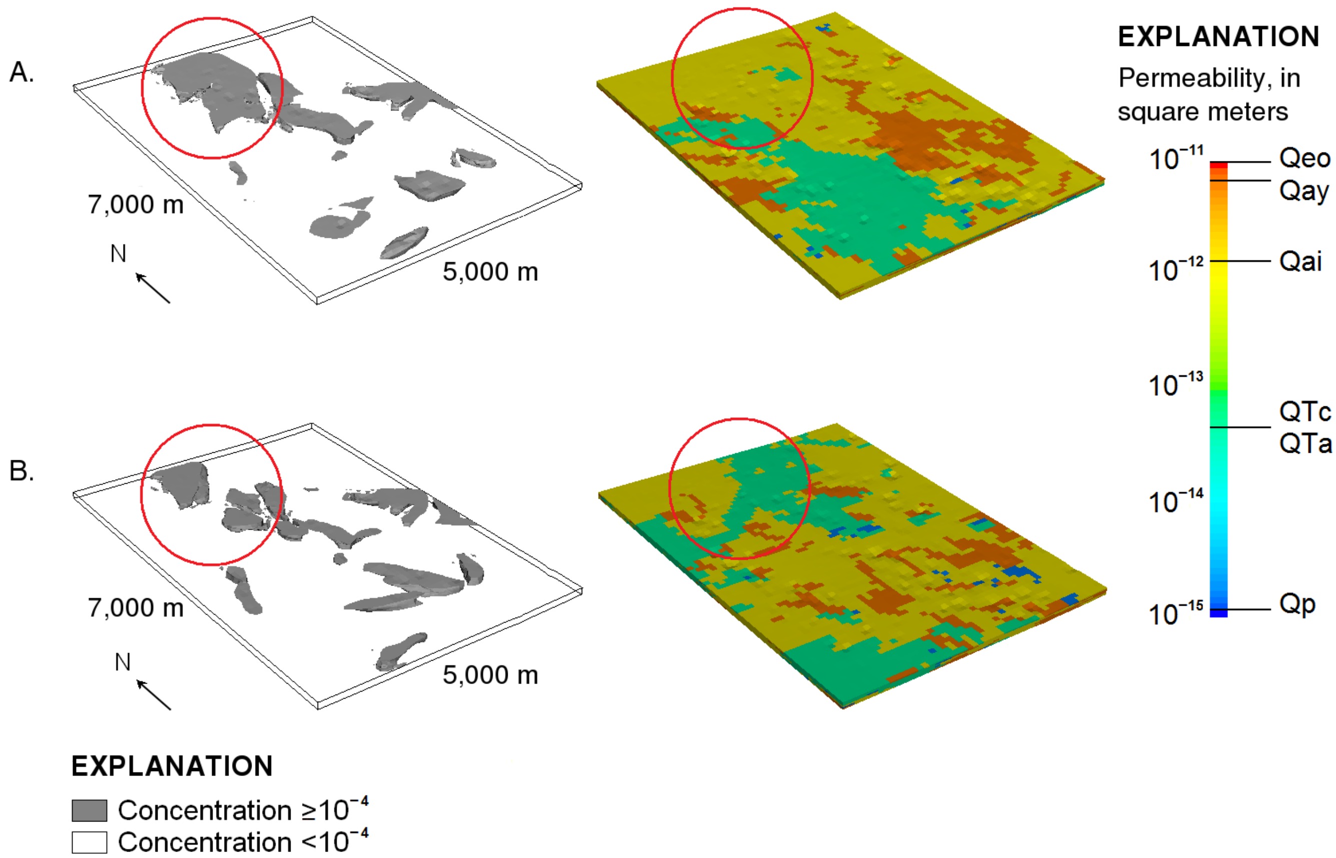

Figure 8. This figure shows results from two different simulations (*A* and *B*) from the same slice of the modeling domain located between 560 and 580 m bgs; the location of simulated contaminant plumes (left) can be compared to the modeled permeability distributions (right). The circled region provides an example of the difference between the results of the two simulations.

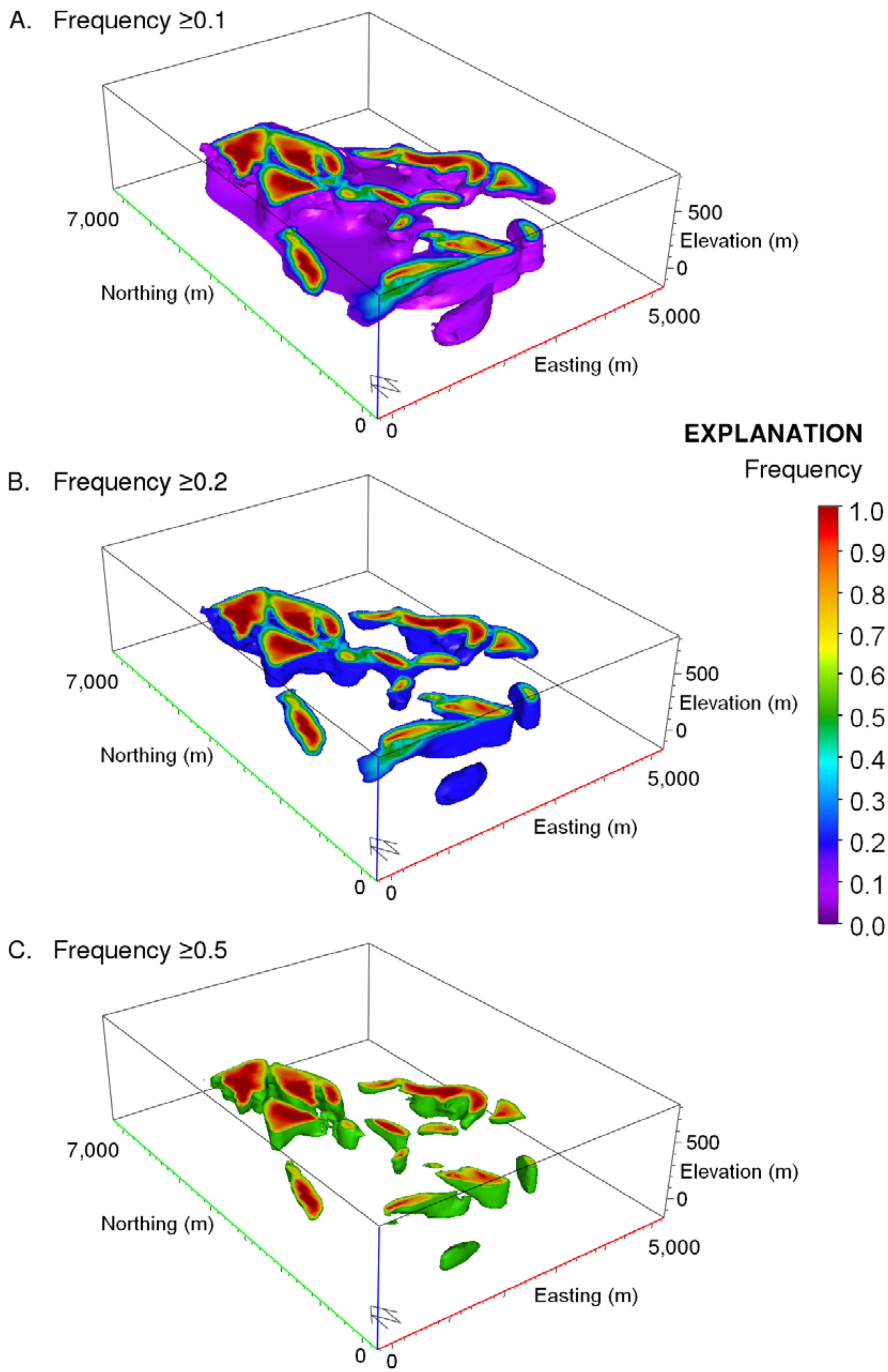

Figure 9. Map of frequency of exceeding a contaminant mass fraction of 10^{-4} in the modeling domain. Frequencies above *A*, 10 percent; *B*, 20 percent; and *C*, 50 percent, are shown.

Tables

Table 1. Alluvial units mapped at the surface in the study area in Yucca Flat, Nevada.

Unit	Description	Permeability, in square meters
QTc	Colluvium (Quaternary, Tertiary)	5.14×10^{-14}
QTa	Old alluvial deposits (Pliocene, early/middle Pleistocene)	5.14×10^{-14}
Qai	Intermediate alluvial deposits (Holocene, Pleistocene)	1.21×10^{-12}
Qay	Young alluvial deposits (Holocene)	6.96×10^{-12}
Qeo	Old eolian sand deposits (Pleistocene)	9.08×10^{-12}
Qp	Playa deposits (Holocene)	1.51×10^{-15}