MODELING THE INFLUENCE OF THE HETEROGENEOUS SUBSTRATE ON THE TRANSPORT OF THE JET FUEL SOLUTE PLUME, KIRTLAND AIR FORCE BASE, ALBUQUERQUE, NEW MEXICO

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ABSTRACT

A subsurface model was developed to characterize the influence of heterogeneity on solute phase plume migration of the Jet Fuel spill of Kirtland Air Force Base. Core – logs from KAFB boreholes were compiled, and lithology was interpolated across the study area using transition probability geostatistics (T-PROGS). High conductivity materials in the travel path resulted in a faster than average breakthrough time while, if low conductivity materials were placed in the travel path, particles were either forced to divert around the low K material, which added time and changed the direction of travel, or were forced by the hydraulic gradient to move through the materials, which also added travel time. Because these models indicate that material placement and facies dimensions significantly affect particle path, well arrival time, and breakthrough arrival time,
heterogeneity should not be neglected when building groundwater models to predict movement of the KAFB Bulk Fuels Facility saturated plume.
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Introduction

In 1999, Kirtland Air Force Base (KAFB) reported a jet fuel leak from an underground fuel pipe to the New Mexico Environment Department (NMED) (U.S Air Force, 1999). However, as of the submission of this thesis, the aquifer system is still far from being completely understood or remediated. It is important to study the rate and precise direction groundwater will travel, using all available data, in order to understand plume migration.

The U.S. Environmental Protection Agency (EPA) has granted the State of New Mexico the right to implement the Federal Resource Conservation and Recovery Act (RCRA) hazardous waste program, which states that the Kirtland Air Force Base is legally responsible for all clean-up relating to the jet-fuel spill (NMED, 2010; EPA, 2012). KAFB is required to document their plan for clean-up, and actions taken thus far, in quarterly reports available to the public. As part of their monitoring and clean-up, the Kirtland Air Force Base has drilled (as of the KAFB January-March 2015 Quarterly Report) more than two hundred monitoring and vapor extraction wells, one hundred and seventy four of which were used in this study. In June 2015, the first pumping well was completed (NMED, 2015B), with plans to build at least two more in order to collapse the plume (NMED, 2015B). Well-logs from the bulk fuels spill site are available to the public within the quarterly reports and remedial investigation reports online at the New Mexico Environment Department (NMED) and KAFB websites, and contain location data, groundwater levels, chemical data, and borehole lithology. Other core-log data used in this work came from CB&I Federal Services LLC, a consulting company contracting with KAFB, via personal communication.
KAFB contracts with the environmental consulting company CB&I Federal Services LLC, which, along with the EPA, has been creating groundwater flow models (Ellinger, 2013; NMED, 2011; Ellinger, Personal Communication 2015) of the contamination plume. However, the only groundwater flow model draft report released to the public by the EPA assumes a homogenous substrate, and thus no heterogeneity for hydraulic properties (Ellinger, 2013). Due to the complicated underlying geology of the Santa Fe Group Aquifer, these models may not be sufficiently accurate to understand groundwater flow and contaminant transport in the area of the plume. For groundwater modeling, use of homogenous, single hydraulic conductivity values, does not properly account for lithologic types with groundwater flowpaths either much faster or slower than the average. The EPA model assumes Gaussian dispersion, which cannot accurately reflect groundwater transport in a heterogeneous medium like the Santa Fe Group aquifer, and may result in an inaccurate characterization of the movement of the contaminated groundwater plume (e.g., Fogg, 1986; Berkowitz et al., 2000; Weissmann et al., 2004, Klise et al., 2009). To account for that, in this study, the lithologic types present in core data from KAFB boreholes were interpolated across the study site with transition probability geostatistics (T-PROGS), following the methods of Carle and Fogg (1996) and Weissmann et al. (1999), in order to account for heterogeneity in hydraulic properties when modeling the subsurface distribution of lithofacies. The realizations from T-PROGS were then input into the groundwater modeling program MODFLOW, in order to compare rates of contaminant transport of a homogenous “control” model to different heterogeneous T-PROGS realizations.
Boundary conditions for the model were determined by interpolation of hydraulic head data from KAFB and the city of Albuquerque, as well as by comparison to boundary conditions from the EPA’s 2013 model (Ellinger, Personal Communication 2015; Ellinger, 2013). For this study, the use of KAFB core data and modern Rio Grande facies values to build the Markov chain models used in T-PROGS, has allowed for a groundwater flow and solute transport model that might better characterize the behavior of the contaminated plume, and better predict how the plume moving through a heterogeneous substrate will differ from a homogeneous model in its arrival to city water supply wells. The models produced, however, only offer an evaluation of the presence of heterogeneity at the site on the overall plume behavior, and cannot and should not be used to accurately predict arrival times of the contaminant plume to the city wells.

Section I of this thesis will detail a brief history of the KAFB Bulk Fuels Spill and current modeling efforts; Section II will discuss the underlying geology and hydrogeology in the context of the regional geology; Section III will provide an overview of the methodology, including parameters and conditions used for T-PROGS and the groundwater modeling; Section IV will contain the T-PROGS and modeling results, and Sections V and VI will discuss those results and the conclusions reached.
Section I

Overview of the KAFB Spill

KAFB is located in Bernalillo County, New Mexico, just south of Albuquerque city limits (NMED, 2007) (Figure 1). The KAFB Bulk Fuels Facility, which stored diesel, gasoline, and jet fuel (NMED, 2000), finished construction in 1953 (U.S. Air Force, 2014). At some point between 1953 and 1999, at least two underground fuel pipes at the facility began to leak, discharging unknown amounts of jet fuel into the ground (U.S. Air Force, 1999). KAFB officials reported the spill to the New Mexico Environment Department (NMED) in 1999 (U.S. Air Force, 1999). KAFB’s subsequent investigations into the site found several indications that the spill was far more voluminous than initially assumed, when borehole data revealed fuel contamination in the vadose zone at depths of 200 and 310 feet (NMED, 2000). Analysis also showed presence of jet fuel that had not been used since the early nineties (JP-4), as well as ethylbenzene (not used since 1975), indicating that the pipes in question had been leaking for far longer than originally anticipated (NMED, 2000; U.S. Air Force, 2002). The net loss of JP-8 (the fuel then currently in use) alone was estimated at 595 m$^3$ (157,353 gallons) over a five-year period (NMED, 2000).

After removal of the source contaminant, KAFB began an investigation into whether or not the groundwater, 137-152 meters (450 to 500 feet) below the surface of the KAFB Bulk Fuels Facility, had been contaminated, by installing a series of monitoring wells (NMED, 2000). The groundwater north (downgradient) of the site was analyzed for presence of hydrocarbons, volatile organic compounds, and semi-volatile organic compounds (NMED, 2000). Ultimately, it was determined that both the vadose
zone and groundwater below the water table had been contaminated when analyses found 1, 2-dibromoethane (EDB) at levels of 0.21 µ/L (NMED, 2001). EDB has a high aqueous solubility (4325 ppm), and is often added to aviation fuel as an anti-knocking agent (Falta, 2004; EPA, 2014). Exposure above the minimum safe levels determined by the U.S. Environmental Protection Agency (EPA) can damage the respiratory system, nervous system, liver, heart, and kidneys, as well as increase cancer risk (EPA, 2014). According to the federal Safe Drinking Water Program (SDWA), the maximum contaminant level of EDB acceptable in drinking water is 0.05 µg/L (EPA, 2014; NMED, 2015B).

As stage 2 of their abatement plan for the Bulk Fuels Facility, KAFB submitted a proposed remediation plan to NMED in February of 2002 that focused on cleanup of the vadose zone (U.S. Air Force, 2002). The proposed plan involved multiple stages: stage one was to design parameters for soil vapor extraction (SVE) systems to extract volatile organic compounds (VOC) from the vadose zone; stage two was to design the SVE systems; stage three was to implement the SVE systems by installing several monitoring wells, deep soil borings, and shallow SVE wells; and stage four involved additional long-term vapor and water sampling to determine if further action would be required (U.S. Air Force, 2002).

In 2007, 0.44 m (1.44 ft) of light non-aqueous phase liquid (LNAPL) was detected floating on top of the water table in the monitoring well KAFB 1065, requiring KAFB to modify their previously proposed Bulk Fuels Abatement Plan to include more aggressive saturated zone remediation strategies (NMED, 2007). In 2009, NMED determined that the amount of LNAPL (estimated by KAFB to be in the millions of gallons) would take
substantial time and effort to remediate, and if such efforts were not undertaken immediately, there was significant danger to the city of Albuquerque’s water supply wells at the Ridgecrest well field (NMED, 2009) (Figure 1).

Since the implementation of SVE (soil vapor extraction) systems, more than 1,892 m$^3$ (500,000 gallons) of fuel have been recovered (NMED, 2014). However, the groundwater is far from clean, the LNAPL has been mixed and smeared due to a rising water table, and a dissolved solute phase, with EDB as the main concern, is still present in the saturated zone. In 2014, KAFB submitted a new Draft Strategic Plan for the year 2015 (NMED News Release, 2014). This newest proposal outlined a plan to drill sixteen new monitoring wells in order to fill in data gaps, increase the capability of the SVE systems from 90 pounds per hour to 1,500 pounds per hour, and to construct up to seven extraction wells (NMED News Release, 2014; NMED, 2014). The purpose of the extraction well system is to divert the direction of groundwater flow away from Albuquerque and the cone of depression created by the city wells by increased pumping, with the intent to pump and then treat the contaminated groundwater, thus “collapsing the plume” (NMED, 2014; NMED, 2015B). In June 2015, after the SVE wells were temporarily shut down in order to focus work on the new pump and treat system, the first extraction well was completed and began operations (NMED, 2015B). As of November 20, 2015, the extraction well has removed 22,712 m$^3$ (6 million gallons) of water, and about 6,400 µg of EDB (NMED, 2015C). While such interim measures were taking place, long term remediation strategies, such as use of natural or introduced bacteria for bioremediation of the LNAPL, have continued to be field and lab tested (NMED, 2014; NMED 2015B).
Previous KAFB Models

In an effort to better understand the system, the EPA released a groundwater model of the plume area in 2013, which has since been followed up by other EPA models (Ellinger, 2013; Ellinger, personal communication, 2015). However, all of the groundwater models released to the public assume a homogeneous substrate, which is not an accurate representation of the KAFB system due to the complex heterogeneity of the Santa Fe group aquifer (e.g. Hawley, 1992).

The horizontal grid sizes in Ellinger’s (2013) EPA model range from 56.57 m$^2$ to 2,464 m$^2$ (609 ft$^2$ to 265225 ft$^2$), over a total area of 50 km$^2$ (19.26 mi$^2$) and a total depth of 365.76 m (1,200 ft), in eight discreet layers. In its refined center, the groundwater model used grid spacing of 30.48x30.48 m (100x100 ft). Also in Ellinger’s (2013) model, the layers were chosen based on modeling parameters rather than stratigraphy. The top layer began at an elevation of 1,525 m (5,000 ft) above sea level, in order to include the water table, and first five layers went to a depth of 74.9 m (246 ft), in order to contain all parts of the modeled EDB plume (Ellinger, 2013). The next three layers encompassed the remaining 290 m (954 ft), going well below the upper Santa Fe Group, and were necessary to include in the model in order to account for the effects of pumping from the city of Albuquerque’s municipal wells at Ridgecrest.

The original plan for this work was to insert the T-PROGS into Ellinger’s (2013) model. However, even the refined 100X100 foot model cells in Ellinger’s (2013) model were considered too coarse to capture the heterogeneity in a reasonable manner, and modeling a finer grid over the same distance would have resulted in a model too large for computation using code and hardware available for this study. Because of this, it was
decided to build a smaller refined model that conceptualizes the site. The disadvantage of a refined, “conceptual model” (sans particle advection or dispersion), is the inability to predict actual well arrival times or concentration of solute, or to compare model results to known data regarding the location of the EDB plume. To compensate for this, the heterogeneous models in this work were compared to a single homogeneous control model to calculate relative rates of particle transport. Comparison of the heterogeneous models to a homogeneous control (i.e. a model with all of the same boundary conditions and modeling assumptions with the exception of heterogeneity) allowed for the assessment of solely the effect of heterogeneity on transport, to determine if future heterogeneous models would even be necessary to properly predict plume movement. Because the groundwater models were conceptual, it was also decided to run them as a completely saturated system, rather than one just below the water table, to avoid the issues encountered with drying cells not rewetting in MODFLOW while modeling so close to the vadose zone.

For this work, the American measurement system was used in place of the metric system. While the metric system is preferred by the scientific community, all of the data collected from KAFB, as well as other sources such as the Albuquerque Bernalillo County Water Utility Authority, were in units of feet, and projections of New Mexico State Plane (1983) and it was considered much simpler to continue working in those units, rather than converting en masse. To maintain consistency both with the data and its preferred presentation, both units of measurements will be stated.

The groundwater models were built using MODFLOW with GMS (©Aquaveo), which calculates groundwater flow using the finite difference method, and MODPATH
particle tracking was used to determine rate and direction of solute movement.

MODFLOW is currently the most widely used method of groundwater modeling (e.g. Fitts, 2012). In the finite difference method, the area modeled is separated into discreet ‘nodes’ (also known as cells or blocks) and the flowpath of water is modeled using a series of algebraic equations (Harbaugh, 2005), keeping in line with the law of conservation of mass and Darcy’s law. Each cell in the model has its own hydraulic head value, and the physical properties, such as the hydraulic conductivity, are assumed to be homogeneous within each cell. To model heterogeneity, different cells are given different physical properties. The finite difference method was deemed appropriate because it relies on a gridded system, which is also how the resulting facies from T-PROGS are produced.

**Figure 1. Map of Study Site**

![Map of Study Site](image)
Figure 1 shows a general map of the study site (A) and zoomed in model area (B). The red rectangle indicates the borders of the heterogeneous groundwater model, while the yellow indicates the northern tip of Kirtland Air Force Base. Municipal wells within the model are shown by blue balloons. (Figure modified from GoogleEarth).
Section II

Background

Regional Geology

The city of Albuquerque is located in the Rio Grande rift, which is a late Cenozoic continental rift zone made up of a series of interconnected basins, each with their own unique geologic characteristics. Within the basins, the basic structure is a series of half-grabbens due to the extensive normal faulting (Hawley, 1978; Hawley et al., 1992). The Rio Grande rift is geographically oriented north-south, with tensional stress occurring in the east-west direction (Hawley, 1978), and extends from Colorado to northern Mexico (Hawley, 1978). In southern New Mexico, extension began 36 million years ago and meets with the Basin and Range Province near its southern end (e.g. Grauch et al., 2002). The northern part of the rift, which is narrower and surrounded by mountains on either side, began to extend 26 million years ago (e.g. Grauch et al., 2002). Although the Rio Grande rift is considered its own distinctive geographic province, its formation is closely tied to that of the larger Basin and Range provinces (Hawley, 1986). The major feature of the sediment infill of such an extensional environment are distributive fluvial systems (Gawthorpe and Leeder, 2000; Weissmann et al., 2010). In the case of the Albuquerque Basin, alluvial fan material, eroded from the Sandia Mountains to the east, sits on top of ancestral Rio Grande deposits, which together make up the Upper Santa Fe Group, the upper component of the Santa Fe Group Aquifer (Hawley et al., 1992; Connell, 2007; Connell et al., 2008). Figure 2, modified from Connell (2007), shows an east-west cross section of the Rio Grande rift, with a blue line indicating the approximate location of the
water table, and a red star indicating the approximate location of the KAFB bulk fuels spill saturated-zone plume.

The ages of Santa Fe group materials range from 1 to 30 Ma, with the oldest resting on Oligocene age sedimentary and volcanic bedrock (Hawley et al., 1994). The lower Santa Fe Group, deposited 15-30 million years ago, is mostly finer-grained alluvial fan material (Hawley et al., 1992). When the middle Santa Fe Group sediments were deposited between 15 and 5 million years ago, the basin was at its most tectonically active stage, and deposits from alluvial fans contributed greatly to the infill (Hawley et al., 1992). Finally, the upper Santa Fe Group materials were deposited at the beginning of the Pleistocene, and consist of ancestral Rio Grande deposits and alluvial fan deposits (Hawley et al., 1992; Connell, 2007). Deposition of the Upper Santa Fe unit stopped approximately 1 million years ago, when the ancestral Rio Grande began downcutting into the previously deposited sediments (Hawley, 1994).
Figure 2 (modified from Connell, 2007) shows the approximate location of the water table and the bulk fuels spill in relation to the stratigraphy of the Albuquerque basin. The area is dominated by normal faults and accompanying infill. The Upper Santa Fe Group is composed of Unit I and Unit II (Hawley, 1989), with Unit I (USF1) composed of alluvial materials and Unit II (USF2) composed of ancestral Rio Grande deposits. The fuel spill leached past Unit I and is now spreading north through Unit II of the Upper Santa Fe group. Figure not to scale.
Subsurface Geology

The depth of interest for this study is below the water table beneath the Kirtland Air Force Base bulk fuels facility—150 meters (500 feet) on average (Hawley, 1994). This encompasses only the Upper Santa Fe Group deposits (Hawley et al., 1992), also referred to in the literature as the Sierra Ladrones Formation (e.g. Hawley, 1992; Connell, 1998), and so only these units will be discussed in further detail.

The Sierra Ladrones Formation (aka the Upper Santa Fe Group, see Figure 2) is characterized by interfingering alluvial fan and axial river deposits (Hawley et al., 1992). The alluvial fan deposits extend westward from the Sandia, Manzano, and Manzanita uplifts, and consist of poorly sorted and stratified sand and conglomerates with a silt and clay matrix. These are defined in Hawley et al. (1992) as subunit USF1. The axial fluvial deposits are cross-stratified ancestral river deposits, characterized by alternating pebbly sands and gravels, as well as overbank sediments (fine to medium grained) (Connell, 2010). They are classified by Hawley et al. (1992) as subunit USF2. Subunit USF1 and subunit USF2 can most easily be distinguished from one another by the greater incidence of gravel-sized clasts, as well as the presence of volcanics in USF2.

Connell (2010) approximated the width of the axial ancestral Rio Grande depositional belt as 5-14 km, characterized by multilateral and multistory sand and gravel deposits mostly set east of the modern Rio Grande, and west of the Sandia Mountains. The relative thickness of the Upper Santa Fe unit can range up to 304 to 457 meters (1,000 to 1,500 feet).
Groundwater Setting

Originally, like the modern Rio Grande, the groundwater flow direction beneath Albuquerque was north to south (Thorn et al., 1993). However, as the city of Albuquerque has increased its groundwater pumping, the water table has dropped, and a cone of depression has formed, particularly around the Ridgecrest wells. Figure 3, modified from Thorn et al. (1993) shows a series of maps indicating groundwater levels in the Santa Fe Group aquifer system over time, compared to current, interpolated groundwater elevations. Most recently (Dec, 2008) the Albuquerque Bernalillo County Water Utility Authority has diverted surface water from the Rio Chama, with the San Juan-Chama Drinking Water Project, with the goal to reduce the city’s reliance on groundwater (Koontz, 2014). This decreased pumping has allowed the water table to rise somewhat, but has had little effect on the cones of depression due to continued city well pumping. In essence, the current plume is located in the USF2 unit of the Sierra Ladrones formation (see Figure 2) and the presence of the cone of depression to the north of Kirtland Air Force Base is causing the plume to move northeast, towards the municipal wells.
Figure 3 Area Groundwater Maps

Ground water levels 1960 Santa Fe Group Aquifer system

Modified from Thorn et al., 1993
Ground water levels 1989 Santa Fe Group Aquifer system

Modified from Thorn et al., 1993
Figure 3 (A) shows the change in groundwater elevation, including the development of the cone of depression, between 1960 and 1980 (Modified from Thorn et al., 1993). The blue arrow indicates the general flow of groundwater, and the green star shows the approximate location of the KAFB Bulk Fuels Site. Figure 3(B) shows the current interpolated groundwater elevations from area well data. The stars indicate the Ridgecrest wells and Burton 5, and the red points indicate the locations of KAFB borelogs used to interpolate groundwater levels. The blue box indicates the borders of the groundwater model used in this work. The groundwater elevation interpolation was done in ArcMaps using the Inverse Distance Weighted method.
Section III

Methods

Borelogs

In order to characterize the heterogeneity of the system, lithologic data, as well as geophysical induction logs from many of the same boreholes, were compiled for use in RockWorks 16 and T-PROGS. The borehole data were retrieved from the publically available KAFB Quarterly Reports and other documents, with two exceptions: three core-logs, which were obtained via personal communication with a CB&I representative; and the Trumbull Well Nest data, obtained via personal communication with a representative from the Albuquerque Bernalillo County Water Utility Authority. The three core-logs obtained from CB&I were later released to the public as part of the April-June 2015 KAFB Quarterly Report.

The borelog name, depth of material, USCS code assigned to the material, date of drilling, physical location, groundwater levels, and some water chemistry data, were recorded in Microsoft Excel spreadsheets before being transferred to an Access Database for ease of manipulation. The compiled data are held in appendix IV. Figure 4 shows the location of the borelogs used in this work.

The geophysical logs available on the NMED website were taken in 2010 and 2011 by Jet West and Colog under contract with KAFB (KAFB, 2010; NMED, 2012). For geostatistical analysis, geophysical logs are often preferable to lithology logs due to a lack of continuity errors caused by different drilling methods and different mudloggers categorizing the same materials in different ways (e.g. Lansdale, 2005). However, upon examination, it was found that the geophysical induction logs taken by Jet West and
Colog were consistently very poorly calibrated and unfit for both quantitative and qualitative analysis. A similar conclusion was reached by NMED in a February 2012 communication to KAFB (NMED, 2012), where it was stated that NMED had, “Reviewed the information…and has assessed that the borehole geophysical logs, especially the induction logs generated by Jet West, are not calibrated and not useful.” (NMED, 2012). NMED requested that the induction logs be re-measured (NMED, 2012). However, if this was undertaken, or if any other geophysical induction logs were also later acquired, it is not part of the information currently available to the public on either the KAFB or the NMED websites at the time of the writing of this work.

In contrast with the geophysical logs, the borehole lithology logs were determined to be acceptable for use to increase the general understanding of the system, in order to aid in the decisions regarding the parameters input into T-PROGS. In a system like the Albuquerque basin, there was concern regarding which mean length of facies values would be input into the T-PROGS parameter file due to the fact that the ancestral Rio Grande deposits would have a longer north-south axis and a shorter east-west axis, while alluvial fan deposits from the Tijeras fan would have a longer east-west axis and a shorter north-south axis. To assess if it would be necessary to attempt to model these two very different depositional systems on top of one another, the borehole lithology logs from KAFB were visualized in three dimensions in RockWorks 16, in order to determine the amount of interfingering, if any, present between the alluvial fan material and the ancestral Rio Grande material in the study area at depth.

As discussed in section II, and shown in Figure 2, Hawley et al. (1992) separated the Upper Santa Fe group into two units, defining the alluvial fan material as subunit
USF1, and the axial Rio Grande deposits as subunit USF2. Despite the description of this separation between alluvial fan material and ancestral Rio Grande material, the exact depth where USF1 ended and USF2 began, was not specified. In this study, a 3-D borehole visualization was used to determine an approximate depth of the boundary between USF1 and USF2, in order to ensure that the two units did not meet below the saturated zone.

The 3-D borelog lithology visualization in RockWorks (Figure 5A) showed a clear break between finer grained materials and coarser grained materials at approximately 60 meters (200 feet) below the surface. While it cannot be said that the materials nearer the surface of the borehole visualization had absolutely no coarse grained material, and that the materials at the base of the model near the water table had absolutely no fine-grained material, it was clear that the majority of the materials near the water table, shown in Figure 5B, were coarser grained sands and gravels, while the majority of the materials nearer to the surface, were finer grained muds, silts, and some sands. This delineation is consistent with the type of materials described as alluvial fan material and axial ancestral Rio Grande material from Hawley et al. (1992), and was taken to mean that the vast majority of the materials near the surface were indeed the alluvial fan deposits (i.e. USF1), while the vast majority of the materials near the water table were ancestral Rio Grande deposits (i.e. USF2). This agreed with other studies from the literature (e.g. Hawley et al, 1992; Hawley, 1994) which asserted that the materials present at the water table were only north-south oriented ancestral Rio Grande deposits. Therefore, when constructing realizations in T-PROGS, the Markov chain models were
built using north-south orientations, and mean lengths of facies consistent with ancestral Rio Grande axial deposits.

For building the Markov chain model used in T-PROGS, lithology data were obtained from six boreholes (KAFB-106212, KAFB-106215, KAFB-106218, KAFB-106221, KAFB-106227, and KAFB-106224) (Figure 4) cored through the saturated zone and the water table. It was decided to use core samples only, rather than all of the borehole lithology data for development of the Markov chain models, in order to achieve better precision regarding transitions between and types of materials, with less error caused by drilling method and recording.
Figure 4 shows the borders of the groundwater model used in this work, as well as the city wells and the core and borelogs used to make the model. Only the 6 cores were used to build the Markov chain model (red dots), while the rest (green diamonds) were used to delineate the separation depth between the USF1 and USF2 units of the Upper Santa Fe group.
Figure 5A. Cross Section of Borelog Lithology
Figure 5 (A) shows snapshot looking towards the north, south, east and west, at a vertically exaggerated 3-dimensional analysis of KAFB borehole lithology. Lithologies with low hydraulic conductivity show as cooler colors (blue, green), which grow progressively hotter as hydraulic conductivity of the substance increases. With this visualization, it is clear to see the split between Unit I (alluvial fan material) and Unit II (Ancestral Rio Grande material) of the Upper Santa Fe Group as described in Hawley, 1989. The borehole lithology data was taken from the KAFB quarterly reports appendix D, and analyzed in RockWorks 16.
Figure 5B. Material Types Present at the Water Table

Figure 5B, shows material types present at the water table in 2011 and 2013 (changing due to water table rise from the San Juan-Chama diversion). Like 5A, the data was collected from KAFB borelogs.
Transition Probability Geostatistics: Background

Transition Probability Geostatistics (T-PROGS) is a series of computer programs created as a method for calculating spatial variability of facies in a wide variety of environments using transition probability and Markov chain models (Carle and Fogg, 1996; Carle, 1999). Markov chain models are useful for studies involving facies distributions with multiple categories because, unlike a semi-variogram, which assumes symmetrical distribution, a Markov chain model allows for asymmetrical distributions of categorical data (Carle and Fogg, 1996; Weissmann et al, 1999). Use of transition probability and Markov chain models has been found equivalent to using indicator geostatistics through a semi-variogram for two categories (Carle and Fogg, 1996). In the case of this work, Markov chain models were used to determine the statistical likelihood of hydrofacies placement (based on known sediment types) and continuity in the vertical direction from borehole data. The embedded transition probabilities were then extrapolated in the horizontal direction using mean lengths of facies, following the methods of Weissmann and Fogg (1999), Weissmann et al. (2004), and Engdahl et al. (2010).

In its simplest form, transition probability places data into discreet categories (for example, clay, silt and sand could be chosen as categories 1, 2, and 3, respectively) and then calculates the likelihood of one category appearing after another category (i.e. the “transition probability” between the two) over a set lag distance. In essence, transition probability is determining how often category 1 and 2 will show up in sequence in a preferred direction and different lag distances, vs. 1 and 3, or 2 and 3, or any other combination thereof. A category transitioning to itself is considered an autocorrelation.
and also counted in the probability. With embedded transition probabilities, the transition is a measure of which categories transition to a different category irrespective of lag distance. Mean lengths of facies are added to the calculations to complete the probability map of spatial distributions.

Mathematically, transition probability can be understood as:

\[ T_{jk}(h) = \Pr \{ k \text{ occurs at } x+h \mid j \text{ occurs at } x \} \]

where \( T_{jk}(h) \) = transition probability, \( x \) = a spot in the sequence, \( h \) = a lag distance, and \( k \) and \( j \) refer to different categories (Carle, 1999). Transition probability ultimately comes from the definition for conditional probability, wherein the probability of something occurring at \( B' \) is conditional upon what is present at \( A \) (Carle, 1999). This is written mathematically as:

\[ \Pr\{B'\mid A\} = \frac{\Pr\{A \text{ and } B'\}}{\Pr\{A\}} \]

with \( A = \{j \text{ occurs at } x\} \) and \( B' = \{k \text{ occurs at } x + h\} \)

When measuring transition probabilities for T-PROGS, this likelihood of transitioning from one category to another is done over first small distances (i.e. the “lags”) and then gradually over longer distances (Carle, 1999). A Markov chain model is then fit to these transition probabilities. Figure 6 shows an example of estimated Markov chain models fitted to measured transition probability data.

On the practical side, T-PROGS is a series of computer programs run in FORTRAN (Carle and Fogg, 1996; Carle, 1999). It treats multi-dimensional spatial data as three separate one-dimensional Markov chain models, which are then simulated in three dimensions through interpolation between these orthogonal directions (Carle, 1999). The process of running a T-PROGS analysis of geological data, such as stratigraphy or facies, involves four main programs: GAMEAS, GRAFXX, MCMOD, and TSIM. A fifth
program, CHUNK, is often used to visualize the simulations from TSIM. However, other visualization software can also be used. In the case of this work, GMS MODFLOW shows the TSIM simulation once T-PROGS is loaded, and was used in place of CHUNK. An in-depth description of each of these programs and parameters used for input into these programs can be found in Appendix I.

Figure 6A. Markov Chain Models and Vertical Transition Probabilities
Figure 6A shows measured vertical transition probabilities and the calculated Markov chains for group A and B, visualized with GRAFXX. It is most important that the calculated Markov chains match the beginning of their measured borehole counterparts. If this is the case, then the calculated Markov chains can be used, with the measured mean lengths of facies (in this case, ancestral Rio Grande deposits), to build the transition probability model.
Figure 6B. Embedded Transition Probabilities

<table>
<thead>
<tr>
<th>Model</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clay</td>
<td>L=45.5</td>
<td>0.018 B</td>
<td>0.058</td>
</tr>
<tr>
<td>Silt</td>
<td>S L=45.5 B</td>
<td>0.0001</td>
<td></td>
</tr>
<tr>
<td>Sand</td>
<td>B B B B</td>
<td>B B B B</td>
<td></td>
</tr>
<tr>
<td>Gravel</td>
<td>S S B L=131</td>
<td>S S B L=1197</td>
<td>0.096 .0001 0.90 1.42</td>
</tr>
</tbody>
</table>

Figure 6B shows an example of the embedded transition probabilities for model A1 for the horizontal and vertical directions. The rest of the embedded transition probabilities can be found in appendix II. S = symmetry assumed, B = background category, L = mean length of facies.
Modeling Ancestral Rio Grande Deposits with T-PROGS

In order to create Markov chain models and run T-PROGS for the KAFB bulk fuels spill site, it was necessary to first obtain certain information about the aquifer system, such as the category ratios and the mean length of facies. As discussed in the previous section, the data used to calculate the vertical Markov chain model were taken from six KAFB drill cores. The boreholes were initially drilled with an air rotary casing hammer to an approximate depth of 137 meters (450 feet), where sonic coring began (U.S. Air Force, 2015). Core was collected to an approximate depth of 174 meters (570 feet), depending on the individual borehole (U.S. Air Force, 2015). The material present in the cores was described using USCS codes, where there was a large variation in material types, ranging from coarse gravel to clay. In order to simplify the wide variety of descriptors, hopefully eliminating some of the error brought on by different recorders using different descriptors for the same materials, the core data were separated into four discreet hydrofacies categories: clay, silt, sand, and gravel. Materials included in each of these categories were estimated to have similar hydraulic properties for use in groundwater modeling. A table of USCS codes and the categories they were assigned can be found in Table 1 below:
Table 1. Core U.S.C.S Codes and Categories

<table>
<thead>
<tr>
<th>U.S.C.S. Code</th>
<th>Material Description</th>
<th>Assigned Hydrofacies Category</th>
</tr>
</thead>
<tbody>
<tr>
<td>NR</td>
<td>No record</td>
<td>N/A</td>
</tr>
<tr>
<td>CL</td>
<td>Lean Clay</td>
<td>1</td>
</tr>
<tr>
<td>CH</td>
<td>Sandy fat Clay</td>
<td>1</td>
</tr>
<tr>
<td>ML</td>
<td>Sandy Silt</td>
<td>2</td>
</tr>
<tr>
<td>MH</td>
<td>Elastic Silt</td>
<td>2</td>
</tr>
<tr>
<td>ML-CL</td>
<td>Elastic silt with lean clay</td>
<td>2</td>
</tr>
<tr>
<td>ML-SP</td>
<td>Elastic Silt with poorly graded sand</td>
<td>2</td>
</tr>
<tr>
<td>ML-SW</td>
<td>Elastic silt with well graded sand</td>
<td>2</td>
</tr>
<tr>
<td>SM</td>
<td>Silty Sand</td>
<td>3</td>
</tr>
<tr>
<td>SW</td>
<td>Well Graded Sand</td>
<td>3</td>
</tr>
<tr>
<td>SP</td>
<td>Poorly Graded Sand</td>
<td>3</td>
</tr>
<tr>
<td>SC</td>
<td>Clayey Sand</td>
<td>3</td>
</tr>
<tr>
<td>CL-SW</td>
<td>well graded sand with clay</td>
<td>3</td>
</tr>
<tr>
<td>SP-SC</td>
<td>Poorly graded sand with clayey sand</td>
<td>3</td>
</tr>
<tr>
<td>SP-SM</td>
<td>Poorly graded sand with Silty sand</td>
<td>3</td>
</tr>
<tr>
<td>SW-CL</td>
<td>well graded sand with clay</td>
<td>3</td>
</tr>
<tr>
<td>SW-MH</td>
<td>well graded sand with elastic silt</td>
<td>3</td>
</tr>
<tr>
<td>SW-SC</td>
<td>well graded sand with clayey sand</td>
<td>3</td>
</tr>
<tr>
<td>SW-SM</td>
<td>well graded sand with silty sand</td>
<td>3</td>
</tr>
<tr>
<td>SWSMS</td>
<td>well graded sand with silty sand</td>
<td>3</td>
</tr>
<tr>
<td>GW</td>
<td>Well Graded Gravel</td>
<td>4</td>
</tr>
<tr>
<td>GM</td>
<td>Silty Gravel</td>
<td>4</td>
</tr>
<tr>
<td>GC</td>
<td>Clay Gravel</td>
<td>4</td>
</tr>
<tr>
<td>GP</td>
<td>Poorly Graded Gravel</td>
<td>4</td>
</tr>
<tr>
<td>GP-GC</td>
<td>poorly graded gravel with clay gravel</td>
<td>4</td>
</tr>
<tr>
<td>GP-GM</td>
<td>poorly graded gravel with silty gravel</td>
<td>4</td>
</tr>
<tr>
<td>GW-GC</td>
<td>Well graded gravel with clay gravel</td>
<td>4</td>
</tr>
<tr>
<td>GW-GM</td>
<td>Well graded gravel with silty gravel</td>
<td>4</td>
</tr>
<tr>
<td>GW-SM</td>
<td>Well graded gravel with silty sand</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 1 shows the USCS code and description from the KAFB quarterly reports, along with the assigned T-PROGS category. Lower hydraulic conductivity materials were categories 1 and 2, while higher hydraulic conductivity materials were categories 3 and 4. For the cores used to build the Markov chain models, if there was no record “NR”, either the data was removed (group B realizations) or the data was assumed to be gravel (category 4) lost during the coring process.
Three different parameter sets were used to build the Markov chain models. The first two, called “A” and “B” differed from each other in their hydrofacies proportions. The percentage of “gravel” present in the cores was lower than in the borehole lithology logs where core was not taken. Thus, it was hypothesized that the not infrequent intervals in the core-logs with “no core collected” might be due to the difficulties of collecting larger gravel pebbles in a sonic drill core. The first hydrofacies proportion set assumed that ‘no core collected’ actually referred to loss of gravel material, and so those numbers were added to the gravel percentages, making for proportions of 11% clay, 1% silt, 77% sand, and 10% gravel. Models run with this first category set are referred to as “Group A”. The second set of hydrofacies proportions simply assumed no data for the instances of ‘no core collected’ and only calculated proportions for those materials that were reported in the logs. The proportions of materials in this second set (‘Group B’) were determined as 12% clay, 1% silt, 83% sand, and 4% gravel.

In T-PROGS, it is possible to set one category as the “background”, where probabilities are set for that category based on probabilities of transition rates in the other categories and the laws of probability. The most abundant category in both cases, sand, was chosen to act as the background category, which the program would then assume was present unless informed otherwise, making the calculation of its transition probability unnecessary.

Vertical transition probabilities were calculated using the measured hydrofacies distribution data from the cores, and Markov chain models were then fit to the data (Figure 6). An example table of the embedded transition probability matrix for one of the Group A models is shown in Figure 6B, with the rest of the tables found in appendix II.
The embedded transition probabilities were used in the horizontal direction, assuming Walther’s law, following the methods of Carle and Fogg (1996) and Weissmann et al. (1999).

Horizontal Markov chain models developed from vertical borehole data are, at best, inexact in describing a system (e.g. Weissmann et al., 1999). Part of the reason, is because it is difficult to identify laterally continuous facies, and thus their mean lengths, with only vertical borehole data. To compensate for this issue, mean facies dimensions taken from an analog site can be used in conjunction with the embedded transition probabilities to obtain estimates used in the Markov chain model (e.g. Weissmann et al., 1999). In the case of this work, the contamination is in the Sierra Ladrones formation which, as discussed in Section II, is comprised of ancestral Rio Grande deposits. Therefore, the mean lengths of facies used needed to be close to those that would have been formed by the ancestral Rio Grande.

To obtain mean lengths of facies, it was assumed that the best analogy for the ancestral Rio Grande deposits were those present on the modern Rio Grande. However, rather than measuring the Rio Grande as it is today, dimensional knowledge of the Rio Grande was taken from aerial photograph data from 1949 and 1961, before the completion of the Cochiti Dam in 1973, due to the dam’s significant impact on natural flooding and thus the river’s evolution and natural depositional patterns (Richard et al., 2005). Ideally, data from even earlier, before the industrialization of Albuquerque would have been used. However, such data were not available.

Over one hundred length and width measurements of bars and channels on the Rio Grande were taken from the aerial photographs. As the facies lengths showed a wide
range of values, the averages of these measurements were separated into bins of ‘small’, ‘medium’, and ‘large’. Examples of these measured aerial images can be found in Figure 7, and tables of the separation bins and their associated mean lengths of facies can be found in Figure 8B. These bins of mean facies length were used to create six realizations in T-PROGS—a small, medium, and large for the Group A category ratios (assuming that “no core collected” meant loss of gravel), and a small, medium, and large for the Group B category ratios (eliminating all “no core collected” percentages).

Fluvial systems like the Rio Grande and its ancestral iterations, are characterized by repeating cycles of erosion and deposition, leading to a wide variety of interspersed channel and bar forms (e.g. Bridge, 2003; Lunt and Bridge, 2004). The factors dictating the ultimate size and stage in river development include, but are not limited to: climate, tectonic setting, gradient, and available sediment type, which can result in fluvial systems that run the gamut from shallow, wide and braided rivers with many channel and bar forms, to narrow channels with simple alternate bars, or even no bars at all (Bridge, 2003). Despite this variation, studies by Holzweber et al. (2014) have shown that the length-width ratio of bars in fluvial systems remains within a constant, power law distribution regardless of bar type (i.e. mid-channel, point, bank-attached, or lateral), basin tectonic setting, catchment and basin climate, gradient, or channel width. Holzweber et al. (2014) found an average range of 0.15-0.35 for the width-length ratio of channel bars. Therefore, regardless of the actual size of the ancestral Rio Grande, the numbers used for the mean length and width of facies in the T-PROGS model of its deposits, were set to follow this same ratio, at least at a first approximation. For this study, the average width-length ratio of the bars measured fell consistently around 0.25.
In Lunt and Bridge (2004), grain size distribution across of a gravelly braid bar was plotted on an aerial photograph, and it was found that smaller grain sizes were located in the center and topographically higher areas of the bars, while cross bar channels tended to have a larger mean grain size than the surfaces of adjacent bars. It should be noted that the Lunt and Bridge (2004) study referred mostly to distribution of sands and gravels. Other literature (e.g. Bridge, 2004) suggests that finer grained materials such as silt and clay, would be found making up the adjacent floodplains. However, it is difficult to quantify mean lengths of floodplain materials, especially once they have been cut through, re-deposited, and buried by an ever-changing river. For assigning mean lengths of facies for the different material categories therefore, bar length and width measurements from the historical aerial photographs of the Rio Grande were input for the clay and silt portions of the Markov chain models (making the assumption that remnant floodplain deposits may take on similar geometries as the bars), while the adjacent river channel width and lengths were used for the gravel category of the Markov chain models. Because sand functioned as the background category in the T-PROGS model, it was not necessary to determine whether using channel measurements or bar measurements for sand in the Markov chain model would have produced a better representation of the grain size distribution in the ancestral Rio Grande.

However, as bar and channel forms visible in a river system can greatly alter depending on the season (e.g. Lunt and Bridge, 2004), these numbers could act only as a starting point for determining the appropriate channel and bar widths for ancestral Rio Grande deposits. Previous work in developing T-PROGS models with mean lengths of facies and borehole data (Rust, 2006) indicated that the mean lengths of facies values
input into the program did not significantly affect the calculation of the T-PROGS model, so long as reasonable values were used. Regardless, in order to test the sensitivity of the model to these lengths scales, one final set of T-PROGS models was built using the Group A category ratios, and bar and channel measurements from Lunt and Bridge (2004), a study of a modern braided river system (the Sagavanirktok River) in Alaska. This is the third parameter set used to build a Markov chain model, and the Markov chain models built with this combination of data is referred to as “Group C”.

With the addition of Group C, there were seven Markov chain models built in total: three each for Groups A and B (with mean lengths of facies from the Rio Grande in average groups of small, medium, and large), and one more (i.e. “Group C”) with mean lengths of facies from Lunt and Bridge (2004) and the same hydrofacies proportions as Group A. Table 2 shows the naming scheme for each Markov chain model:

<table>
<thead>
<tr>
<th>Mean Length of Facies</th>
<th>Group A Hydrofacies Proportions</th>
<th>Group B Hydrofacies Proportions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small</td>
<td>A1</td>
<td>B1</td>
</tr>
<tr>
<td>Medium</td>
<td>A2</td>
<td>B2</td>
</tr>
<tr>
<td>Large</td>
<td>A3</td>
<td>B3</td>
</tr>
<tr>
<td>Lunt and Bridge (2004) values</td>
<td>C1</td>
<td></td>
</tr>
</tbody>
</table>

Ten (10) equally probable T-PROGS realizations were developed for each geologic scenario, with each realization referred to in this work as a ‘Trial”, or “T” (e.g, T1, T2, etc.), in addition to a homogeneous control, for a total of seventy-one (71) T-PROGS realizations. Group C (e.g., with measurements from Lunt and Bridge 2004) was
added in order to compensate for the imperfect analogy of using the modern Rio Grande as a substitute for the ancestral Rio Grande, in order to test the sensitivity of the model to the geologic assumptions.

Figure 7: Aerial Photographs of pre-Cochiti Dam Rio Grande
Figure 7 (modified from cabq.gov) shows aerial photographs of the pre-dam Rio Grande. Bar and channel dimensions were measured in order to incorporate them into the horizontal Markov chain models.
The hydrofacies category ratios obtained from the KAFB cores were separated into two groups: group ‘A’ where a record of ‘no core collected’ was assumed to mean gravel loss during the coring process, and group ‘B’ where areas of no core collected were removed from the category ratios. The main difference between groups A and B is the percentage of gravel; group A has 6% more gravel than group B.

<table>
<thead>
<tr>
<th></th>
<th>Groups A &amp; C</th>
<th>Group B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>11%</td>
<td>12%</td>
</tr>
<tr>
<td>Silt</td>
<td>1%</td>
<td>1%</td>
</tr>
<tr>
<td>Sand</td>
<td>77%</td>
<td>83%</td>
</tr>
<tr>
<td>Gravel</td>
<td>10%</td>
<td>4%</td>
</tr>
</tbody>
</table>
The mean widths and lengths of facies, measured from historical Rio Grande photographs, were separated into bins of small, medium, and large. With the sand set as the background category, the bar lengths and widths were set for the clay and silt, while the channel lengths and widths were set for the gravel, following cross channel grain size distribution of a braided stream discussed in Lunt and Bridge (2004). In addition to the three Rio Grande bins, a fourth bin was set, using bar and channel measurements from photographs of the Sagavanirktok River in Alaska from Lunt and Bridge (2004). This was done in order to ascertain if the ‘soft’ facies data used to build the Markov chain models noticeably affected the outcome.

<table>
<thead>
<tr>
<th>Bin 1 (small)</th>
<th>X-length (ft)</th>
<th>Y-length (ft)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>45.5</td>
<td>160.3</td>
</tr>
<tr>
<td>Silt</td>
<td>45.5</td>
<td>160.3</td>
</tr>
<tr>
<td>Gravel</td>
<td>131</td>
<td>1197</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bin 2 (medium)</th>
<th>X-length (ft)</th>
<th>Y-length (ft)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>120</td>
<td>463</td>
</tr>
<tr>
<td>Silt</td>
<td>120</td>
<td>463</td>
</tr>
<tr>
<td>Gravel</td>
<td>201</td>
<td>1686</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bin 3 (large)</th>
<th>X-length (ft)</th>
<th>Y-length (ft)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>305</td>
<td>1211</td>
</tr>
<tr>
<td>Silt</td>
<td>305</td>
<td>1211</td>
</tr>
<tr>
<td>Gravel</td>
<td>367</td>
<td>2527</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Lunt and Bridge (2004) Sagavanirktok River</th>
<th>X-length (ft)</th>
<th>Y-length (ft)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>501</td>
<td>1210</td>
</tr>
<tr>
<td>Silt</td>
<td>501</td>
<td>1210</td>
</tr>
<tr>
<td>Gravel</td>
<td>426</td>
<td>1259</td>
</tr>
</tbody>
</table>
Incorporating T-PROGS realizations in MODFLOW

For this project, the challenge was to model a comparable area to Ellinger’s (2013) model, while still achieving a meaningful degree of heterogeneity and refinement.

Table 3 shows the model and cell dimensions used in this work:

Table 3. Model Dimensions

<table>
<thead>
<tr>
<th>Grid Origin (NM State Plane)</th>
<th>1538428.807 E 1472301.512 N</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-length</td>
<td>4653.4 m (15267 ft)</td>
</tr>
<tr>
<td>Y-length</td>
<td>3739.6 m (12269 ft)</td>
</tr>
<tr>
<td>Z-depth</td>
<td>301 m (988 ft)</td>
</tr>
<tr>
<td>Cell X</td>
<td>15.24 m (50 ft)</td>
</tr>
<tr>
<td>Cell Y</td>
<td>15.24 m (50 ft)</td>
</tr>
<tr>
<td>Cell Z</td>
<td>0.46 m (1.5 ft)</td>
</tr>
<tr>
<td>Total Area</td>
<td>17.4 km² (6.7 mi²)</td>
</tr>
</tbody>
</table>

These dimensions resulted in 305x245 cells in the XY plane. The T-PROGS results were inserted into MODFLOW following the methods of Rust (2006) to cover the total model area 17.4 km² (6.7 mi²), and a depth of 13.7 m (45 ft).

As a depth of 13 m (~45 ft) below the water table would be far too shallow to account for the well screens for the municipal production wells, an additional 287.4 m (943 ft) of homogenous material was added below the heterogeneous material, to make for a total of 301 m (988 ft) in the Z-direction. There were a total of 32 cells in the Z-direction, 31 of which were heterogeneous. An additional single (and much thicker) layer of cells was added below the heterogeneous cells, to accommodate the deep municipal pumping wells, for a total of 2,391,200 cells. Stratigraphically, this base layer of
homogeneous cells includes material from the Middle and Lower Santa Fe groups, and therefore the Markov chain models developed with data from the Upper Santa Fe group would not have been applicable at those depths. The top of the model was set at 1482.65 m (4865 ft) above sea level, and the base elevation was set at 1195.12 m (3921 ft) above sea level. Figure 9 shows a comparison of Ellinger’s (2013) model dimensions to the model used in this work, as well as an illustration of model dimensions and a 3-D cartoon interpretation.

In MODFLOW, general head boundaries were set at the north, south, east, and west sides of the model. The boundary conditions were taken from head values from KAFB wells, and Albuquerque municipal wells. The well-data water levels were interpolated in ArcGIS using Inverse Distance Weighted (IDW), and the general head boundaries for the model were obtained by determining what the interpolated head values were where they crossed the borders of the model. The head values changed depending on where along the model borders they were located, and so rather than a uniform general head boundary for each of the four borders, a gradient general head boundary was used. The values used were corroborated with the head boundaries in Ellinger’s (2013) model, received via direct communication with Dr. Scott Ellinger of the EPA, and used with his permission. Because of the interpolation, the values used can only be considered an estimate of the head. The head values estimated from the IDW interpolation (Table 4) were:
Table 4. Interpolated Hydraulic Heads for Model General Head Boundaries

<table>
<thead>
<tr>
<th>Boundary</th>
<th>General Head (feet)</th>
<th>General Head (feet)</th>
</tr>
</thead>
<tbody>
<tr>
<td>North</td>
<td>4847 (west)</td>
<td>4822 (east)</td>
</tr>
<tr>
<td>South</td>
<td>4866 (west)</td>
<td>4847 (east)</td>
</tr>
<tr>
<td>West</td>
<td>4866 (south)</td>
<td>4847 (north)</td>
</tr>
<tr>
<td>East</td>
<td>4847 (south)</td>
<td>4822 (north)</td>
</tr>
</tbody>
</table>

However, when these boundaries were input into the model, the model was unsuccessful due to the issue of cells drying out and failing to rewet. To compensate for this, it was decided to maintain the gradient along the boundaries while saturating the model. As such, the model was saturated while the head boundary gradients were maintained, and these values were applied to the general head boundaries:

Table 5. Interpolated Hydraulic Gradients for Model General Head Boundaries

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Gradient (per 1000 feet)</th>
</tr>
</thead>
<tbody>
<tr>
<td>North</td>
<td>1.64</td>
</tr>
<tr>
<td>South</td>
<td>1.24</td>
</tr>
<tr>
<td>West</td>
<td>1.06</td>
</tr>
<tr>
<td>East</td>
<td>3.59</td>
</tr>
</tbody>
</table>

Unfortunately, even with these new boundaries, the heads did not converge successfully within a reasonable number of iterations (<300). Hypothesizing that the issue was due to the high number of cells, in addition to the large difference between the lowest head value and the highest value, a gradient of 3.59 per 1000 feet, the highest head was
gradually lowered until the model would run. The models converged successfully with head gradients of:

**Table 6. Altered Hydraulic Gradients for Model General Head Boundaries**

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Gradient (per 1000 feet)</th>
</tr>
</thead>
<tbody>
<tr>
<td>North</td>
<td>1.64</td>
</tr>
<tr>
<td>South</td>
<td>0.98</td>
</tr>
<tr>
<td>West</td>
<td>1.06</td>
</tr>
<tr>
<td>East</td>
<td>3.10</td>
</tr>
</tbody>
</table>

Because Ellinger (2013) found that no unique set of boundary conditions existed that resulted in successfully calibrated heads, and he interpreted that a range of head boundaries could result in successful head calibration, these changes were deemed acceptable for a “conceptual” model, (i.e. one that is not a true representation of the system).

The conductance for the general head boundaries was calculated as $C = \frac{KA}{dx}$ with $K$ the mean hydraulic conductivity value (21.3 m/day or 70 ft/day), Area = 6.9 m$^2$ (75 ft$^2$) and $dx = 1600$ m (5250 ft) to allow for sufficient room for flow outside the cones of depression near the edges of the grid boundaries for the model to converge. The conductance was set at 0.3 m/day (1 ft$^2$/day), because this was the best conductance value that allowed for all of the heads of all of the models to successfully converge. The model was run as a steady state system following the method of Ellinger (2013).

The hydraulic conductivities of the materials and other flow properties were taken from a variety of sources including KAFB slug test results from the KAFB Quarterly Reports, values used in Ellinger (2013’s) model, and other values (for silt and clay) taken
from the literature (e.g. Fitts, 2012) if no other sources were available. The weighted arithmetic mean of the hydraulic conductivity values used in this model was 21.3 m$^2$/day (70 ft$^2$/day) for the runs with gravel added in place of ‘no core collected’ values, and 65 ft$^2$/day for runs that eliminated the ‘no core collected’ values. These were reasonably similar to the average hydraulic conductivities used by Ellinger, which was 21.9 m$^2$/day (72 ft$^2$/day) (Ellinger, 2013). Porosity values were taken from the literature (e.g. Fitts, 2012). The average values used in Ellinger (2013) were assigned to the fifth “homogeneous” category, used for the homogeneous control model, as well as entered below the T-PROGS calculated heterogeneity to give an appropriate depth for the municipal pumping well screens.

Table 7. Assigned Hydraulic Conductivity Values

<table>
<thead>
<tr>
<th>Material</th>
<th>K (m/day)</th>
<th>K (ft/day)</th>
<th>Porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>0.00001</td>
<td>0.000328</td>
<td>0.2</td>
</tr>
<tr>
<td>Silt</td>
<td>0.01</td>
<td>0.0328</td>
<td>0.25</td>
</tr>
<tr>
<td>Sand</td>
<td>21.3</td>
<td>70</td>
<td>0.3</td>
</tr>
<tr>
<td>Gravel</td>
<td>45.7</td>
<td>150</td>
<td>0.45</td>
</tr>
<tr>
<td>Homogeneous</td>
<td>21.9</td>
<td>72</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Currently, the City of Albuquerque’s groundwater usage creates a sizable cone of depression that causes the groundwater under KAFB to flow north towards the cluster of municipal wells (see Figure 3). As such, the wells in question were an integral part of the groundwater model, particularly the Ridgecrest wells, which are predicted to be in the path of the plume (Ellinger, 2013). The Ridgecrest Wells and the Burton 5 Well data, including well depth, well screen depth, and pumping values, were received via direct...
communication with Fredrick Shean of the Albuquerque Bernalillo County Water Utility Authority. The well data input into MODFLOW is described in table 8 below:

Table 8. Model Well Values

<table>
<thead>
<tr>
<th>Well Name</th>
<th>Z (m)</th>
<th>flow rate (cmd)</th>
<th>screen top elev(m)</th>
<th>screen base elev(m)</th>
<th>screen length (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RIDGECREST_1</td>
<td>1482.85</td>
<td>-6077.8</td>
<td>1464.87</td>
<td>1274.67</td>
<td>190.19</td>
</tr>
<tr>
<td>RIDGECREST_2</td>
<td>1482.85</td>
<td>-15181</td>
<td>1428.29</td>
<td>1193.60</td>
<td>234.70</td>
</tr>
<tr>
<td>RIDGECREST_3</td>
<td>1482.85</td>
<td>-12583</td>
<td>1452.37</td>
<td>1203.66</td>
<td>248.71</td>
</tr>
<tr>
<td>RIDGECREST_4</td>
<td>1482.85</td>
<td>-15508</td>
<td>1454.51</td>
<td>1198.47</td>
<td>256.03</td>
</tr>
<tr>
<td>RIDGECREST_5</td>
<td>1482.85</td>
<td>-15742</td>
<td>1434.08</td>
<td>1190.24</td>
<td>243.84</td>
</tr>
<tr>
<td>Burton_5</td>
<td>1482.85</td>
<td>-14936</td>
<td>1442.62</td>
<td>1259.74</td>
<td>182.88</td>
</tr>
</tbody>
</table>

A step-by-step explanation of the T-PROGS to MODFLOW process is described in appendix I. Once T-PROGS heterogeneity was inserted into MODFLOW, MODPATH particle tracking was used to determine potential rate and path of the contamination. (It should be noted that MODPATH only models advection of the particles, not dispersion or diffusion). In MODPATH, one hundred particles were released from the body of the layer one cell matching the geographic location of the former KAFB Bulk Fuels Facility.
Figure 9A compares between Ellinger’s (2013) groundwater model and the model used in this work, indicated by the red box. The smaller size allowed for the computations necessary for a more refined grid. In its center, Ellinger’s (2013) model has 100X100 feet cells, while the entire model used in this work has cell dimensions of 50X50 feet in the X and Y, and 1.5 feet in the Z.
Figure 9B. Groundwater Model Dimensions

Figure 9B shows the model dimensions. The red dots indicate the location of the core logs used to build the vertical Markov chain models, while the green stars indicate the city wells. The models cells used in this work were 50x50x1.5 feet. The model area was 12,269x15267 feet, and covered a depth of 988 feet—46.5 feet of which were heterogeneous Upper Santa Fe group material modeled with T-PROGS.
Section IV
Results

There were three Group A realizations (with mean lengths of facies, small, medium, and large), three Group B realizations (with mean lengths of facies small, medium, and large), and one Group C realization (mean lengths of facies from the Sagavanirktok River (Lunt and Bridge, 2004), and hydrofacies percentages the same as the A Group). For each realization, ten equally statistically likely models, or “trials” were run in TSIM and transferred into MODFLOW. These will be referred to here as “realization sets”. With the addition of the homogeneous control model, a total of 71 different MODFLOW model runs were successfully conducted.

The particles for the homogeneous realization reached Ridgecrest 5 with an initial arrival of 69 model years after release. Visually, the MODPATH run for the homogeneous model shows the particles moving straight towards Ridgecrest 5, showing no particle dispersion (Figure 16). All of the particles for the homogeneous realization intersected the well within the same year, with a mean arrival time of 69.3 years, and a median arrival time of 69.3 years, with a standard deviation of 0.19. The small differences in arrival time can be attributed to the particles being released from different points within the body of the source cell. It should be noted that because the model is not a true representation of reality (due to the flooded cells, boundary conditions, and other factors), '69 model years' is not the true measure of time it will take for the contamination from the KAFB site to reach Ridgecrest 5. Therefore, '69 model years’ will be considered the metric that the heterogeneous realizations are measured against, rather than an actual measure of time to the well.
For the heterogeneous models, the realization set with the quickest particles to reach Ridgecrest 5 was A2 (see Table 2 for model delineations), with the fastest particles on an individual trial reaching Ridgecrest 5 only 60.3 model years after release, 12% faster than the rate predicted by the homogeneous model. If *average* initial arrival times are considered, the lowest average initial Ridgecrest 5 arrival was also for realization A2, with ten trials resulting in an average initial arrival time of 70.2 model years, followed by A3 (70.4 model years) and A1 (71.63 model years) (Figure 10a). These predictions are between 2-4% slower than the initial arrival time predicted by the homogeneous model (Table 9). The initial breakthrough of the ‘B’ group realizations were, on average, 5-9% slower to reach Ridgecrest 5. The ‘C’ group, with dimensional values for the facies taken from Lunt and Bridge (2004) and material ratios the same as the A group, had the slowest average initial arrivals, reaching the Ridgecrest 5 well 11% later than predicted by the homogeneous model.

Figure 10a compares the initial arrival times of the seven heterogeneous realization sets to the homogeneous realization. All of the *averaged* initial Ridgecrest 5 heterogeneous arrivals were between 2-11% slower than the homogeneous realization. However, there were *individual* trials with breakthrough arrival times that reached Ridgecrest 5 faster than predicted by the homogeneous model. The most notable, Trial 7 from model group A2 (A2 T7), had particles that hit Ridgecrest 5 12% faster than the homogeneous model, indicating that while average initial arrival times might be slower than those predicted by the homogeneous model, that does not preclude the possibility of contamination reaching Ridgecrest 5 before the homogeneous prediction.
While all of the particles for the homogeneous model reached Ridgecrest 5 in one peak, the heterogeneous models had much larger ranges of well arrival times. Further examination of the data reveals that all of the heterogeneous models calculated a standard deviation of greater than 10, indicating a very widespread range of data in comparison to the homogeneous realization, where \( \sigma = 0.19 \). While the standard deviation fails to capture how skewed the distribution is, histograms of well arrival time for each set of realizations (Figures 11a-g) clearly show the long tails typical of non-Fickian distribution, which has been shown to follow a power law distribution (e.g. Benson et al., 2000; Berkowitz et al., 2000). Due to these long tails present at the end of the heterogeneous realizations, with some arrival times more than 400 years after the peak arrival times, mean values of the entire distribution of a run were found not to provide a good understanding of any subtler differences between A, B, and C group realizations.

Additionally, none of the particles arrived at Ridgecrest 5 at the exact same time, which made it difficult to calculate the actual mode (or “peak”). However, if the arrivals are grouped into bins, such as they were for the histograms, then the peak arrival times for

<table>
<thead>
<tr>
<th>Group</th>
<th>A1</th>
<th>A2</th>
<th>A3</th>
<th>B1</th>
<th>B2</th>
<th>B3</th>
<th>C1</th>
<th>Homogeneous</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Initial Arrival (model years)</td>
<td>71.63</td>
<td>70.2</td>
<td>70.4</td>
<td>73.59</td>
<td>72.57</td>
<td>75.3</td>
<td>76.72</td>
<td>69.0</td>
</tr>
<tr>
<td>Percent Difference from Homogeneous Rate</td>
<td>4%</td>
<td>2%</td>
<td>2%</td>
<td>7%</td>
<td>5%</td>
<td>9%</td>
<td>11%</td>
<td>N/A</td>
</tr>
<tr>
<td>Standard Error of the Mean</td>
<td>0.8</td>
<td>1.5</td>
<td>1.5</td>
<td>0.7</td>
<td>0.8</td>
<td>2.4</td>
<td>1.8</td>
<td></td>
</tr>
</tbody>
</table>
the bins can be considered. Table 10 shows the average peak arrival times to Ridgecrest 5 for the seven realizations. Group A realizations’ peak arrivals were 5-8% slower than the homogeneous arrival, while group B realizations’ peak arrival times were 10-13% slower. Group C’s average peak arrivals were similar to the upper end of Group A, at 8% slower than the homogeneous arrivals. As Group A and C used the same percentages of hydrofacies when calculating their Markov chain models, this similarity in peak arrivals seems reasonable, and what one would expect.

**Table 10. Ridgecrest 5 Average Peak Arrivals (“Modes”)**

<table>
<thead>
<tr>
<th>Model</th>
<th>Average Peak Bin (“Mode”)</th>
<th>Average Percent of Particles</th>
<th>Percent Difference to Homogeneous</th>
<th>Standard Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>78</td>
<td>44%</td>
<td>8%</td>
<td>0.89</td>
</tr>
<tr>
<td>A2</td>
<td>75.6</td>
<td>53%</td>
<td>5%</td>
<td>0.72</td>
</tr>
<tr>
<td>A3</td>
<td>78.8</td>
<td>56%</td>
<td>8%</td>
<td>2.60</td>
</tr>
<tr>
<td>B1</td>
<td>81.2</td>
<td>31%</td>
<td>11%</td>
<td>1.37</td>
</tr>
<tr>
<td>B2</td>
<td>80.4</td>
<td>37%</td>
<td>10%</td>
<td>1.26</td>
</tr>
<tr>
<td>B3</td>
<td>83.1</td>
<td>39%</td>
<td>13%</td>
<td>3.51</td>
</tr>
<tr>
<td>C1</td>
<td>78.6</td>
<td>51%</td>
<td>8%</td>
<td>1.89</td>
</tr>
</tbody>
</table>

There were somewhat unexpected results however, when the averaged median arrival times were examined. Table 11 shows the range of the averaged ten median arrival times for each model realization, and Figure 10b plots the median arrival times compared to each other and the homogeneous realization. Examining table 11 and Figure 10b it can be seen that averaged median arrival times for all of the heterogeneous realizations are 6-18% later than as predicted by the homogeneous realizations. However, similar to the
averaged initial arrival times discussed above (table 9 and Figure 10a), a later average median arrival time does not preclude the possibility of individual trials with median arrival times faster than the predicted median homogeneous arrival time. As seen in Figure 10b, realizations A2, A3, and B3 all showed instances of median Ridgecrest 5 arrival times faster than the predicted homogeneous median arrival time. Here, it should also be noted that unlike for the peak arrival times, while Group C used the same category ratios as Group A, its median arrival times more closely resembled the B Group than the A Group.

Table 11. Ridgecrest 5 Average Median Arrival Times

<table>
<thead>
<tr>
<th>Group</th>
<th>A1</th>
<th>A2</th>
<th>A3</th>
<th>B1</th>
<th>B2</th>
<th>B3</th>
<th>C1</th>
<th>Homogeneous</th>
</tr>
</thead>
<tbody>
<tr>
<td>Median Ridgecrest 5 Arrival (avg)</td>
<td>77.2</td>
<td>74.1</td>
<td>75.5</td>
<td>82.4</td>
<td>80.0</td>
<td>81.7</td>
<td>78.4</td>
<td>69.3</td>
</tr>
<tr>
<td>Percent difference from Homogeneous rate</td>
<td>10%</td>
<td>6%</td>
<td>8%</td>
<td>16%</td>
<td>13%</td>
<td>18%</td>
<td>12%</td>
<td>N/A</td>
</tr>
<tr>
<td>Standard error</td>
<td>0.8</td>
<td>1.1</td>
<td>1.5</td>
<td>1.7</td>
<td>1.7</td>
<td>3.5</td>
<td>2.3</td>
<td></td>
</tr>
</tbody>
</table>

Unlike the homogeneous model, where 100% of the particles reached Ridgecrest 5, particles from thirteen of the heterogeneous realizations bypassed Ridgecrest 5, and were instead drawn into Ridgecrest 4, a well slightly to the northeast of Ridgecrest 5 (see Figure 1 for well locations). The only MODFLOW models with MODPATH trials that hit Ridgecrest 4 were A3 (Trials 1 and 8), B3 (Trials 1, 3, 6, 7, 9, and 10), and C1 (Trials 2, 3, 4, 5, and 9). Although these results cannot be compared to a homogeneous control, they can be compared to one another, to determine if there are any similarities or patterns.
Logically, as Ridgecrest 4 is farther away from the source contaminant than Ridgecrest 5, the median time until Ridgecrest 4 was reached was longer than for Ridgecrest 5. Shown in Table 12, the averaged median Ridgecrest 4 arrival time for A3 was 98.96 model years, while B3 was 107.74 model years, and C1 was 111.56 model years. This follows the same pattern as median arrivals to Ridgecrest 5, with median arrival times for the B and C groups occurring slightly later than those for the A group, although again, due to the nature of the MODFLOW model, these numbers should not be considered as measures of actual time to well, and should only be considered in terms of relative comparison.

Table 12. Ridgecrest 4 Arrivals

<table>
<thead>
<tr>
<th>Realization</th>
<th>A3</th>
<th>B3</th>
<th>C1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean (model years)</td>
<td>103.05</td>
<td>110.90</td>
<td>138.11</td>
</tr>
<tr>
<td>Median (model years)</td>
<td>98.96</td>
<td>107.74</td>
<td>111.56</td>
</tr>
<tr>
<td>Initial Arrival</td>
<td>93.80</td>
<td>81.18</td>
<td>97.13</td>
</tr>
<tr>
<td>Last Arrival</td>
<td>131.86</td>
<td>479.55</td>
<td>207.30</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>21.13</td>
<td>35.36</td>
<td>287.05</td>
</tr>
</tbody>
</table>

For the models with particles that hit Ridgecrest 4, only on two trials (Group A3 Trial 1 and Group B3 Trial 3) did 100% of the particles reach Ridgecrest 4. Otherwise, if the particles hit Ridgecrest 4, they tended to be split between Ridgecrest 4 and Ridgecrest 5, as shown in table 13: 
Table 13. Ridgecrest 4 vs Ridgecrest 5 Arriving Particle Ratio

<table>
<thead>
<tr>
<th>Run</th>
<th>% of Particles Reaching Ridgecrest 4</th>
<th>% of Particles Reaching Ridgecrest 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>A3 (T1)</td>
<td>100</td>
<td>0</td>
</tr>
<tr>
<td>A3 (T8)</td>
<td>86</td>
<td>14</td>
</tr>
<tr>
<td>B3 (T1)</td>
<td>80</td>
<td>20</td>
</tr>
<tr>
<td>B3 (T3)</td>
<td>100</td>
<td>0</td>
</tr>
<tr>
<td>B3 (T6)</td>
<td>52</td>
<td>48</td>
</tr>
<tr>
<td>B3 (T7)</td>
<td>12</td>
<td>88</td>
</tr>
<tr>
<td>B3 (T9)</td>
<td>49</td>
<td>51</td>
</tr>
<tr>
<td>B3 (T10)</td>
<td>79</td>
<td>21</td>
</tr>
<tr>
<td>C1 (T2)</td>
<td>20</td>
<td>80</td>
</tr>
<tr>
<td>C1 (T3)</td>
<td>32</td>
<td>68</td>
</tr>
<tr>
<td>C1 (T4)</td>
<td>89</td>
<td>11</td>
</tr>
<tr>
<td>C1 (T5)</td>
<td>44</td>
<td>56</td>
</tr>
<tr>
<td>C1 (T9)</td>
<td>61</td>
<td>39</td>
</tr>
</tbody>
</table>

For table 13, T* refers to the particular trial that showed those results in the set.

Qualitatively, diversions from the Ridgecrest 5 path to the Ridgecrest 4 path seem to occur when there is a deposit of low hydraulic conductivity material early enough in the path for the particles to have the time and space to spread out and be diverted north, away from the influence of Ridgecrest 5’s cone of depression. In realization B3 Trial 10 (Figure 14) there is a large clay deposit in layer 1 immediately after the particles are released, with an elongate north-south shape that sets them on a more northerly path that goes around Ridgecrest 5 and hits Ridgecrest 4 instead. In another trial (A3 Trial 1) a series of elongate north-south clay and silt deposits in layer six (Figure 15) to the north and west of Ridgecrest 5, also seem to cause the particles to spread and divert northerly enough to be away from the influence of Ridgecrest 5, and captured by Ridgecrest 4. The
cross sections in Figures 14 and 15 also show that the particles tend to stay within the top 5-10 layers for the majority of the time, showing mostly horizontal movement until they travel closer to the wells and are forced down.

If the low hydraulic conductivity materials are closer to the wells than the contamination site, such as they are for realization B3 Trial 4 (model layer 5, Figure 13), then the particles will still be affected, shown by their diverting north and spreading out, but they will not have enough distance from Ridgecrest 5 to be drawn into Ridgecrest 4 instead, and will eventually be forced by the hydraulic gradient to return to Ridgecrest 5.

Essentially, the results for the heterogeneous models show that adding substrate heterogeneity to a homogeneous groundwater model does change the outcome for both when the particles reach a well, in addition to, in some cases, which well the particles will actually go to. There are noticeable differences in rate and direction of travel between models built by Markov chains using different percentages of material and the same facies values (i.e. Groups A1 and B1, A2 and B2, and A3 and B3), as well as models built by Markov chains using the same percentages of materials and different facies values (i.e. the A and C groups). As such, the models must be examined to determine what factors caused some particles to reach the Ridgecrest wells faster or slower than others, as well as why some particles were drawn to Ridgecrest 4 over Ridgecrest 5.
Figure 10. Box and Whisker Plots of Particle Arrival Times
Figure 10 shows a box and whisker plot of the averaged initial arrival times to Ridgecrest 5 (10A) and the averaged median arrival times to Ridgecrest 5 (10B) compared to the homogeneous realization (the red line). Although the median arrival times tend to be slower than the homogeneous, there are several instances of the contaminant arriving years before predicted by the homogeneous realization.
Figure 11. Ridgecrest 5 Particle Arrival Histograms

A

Realization A1

percent frequency

years until ridgecrest 5 arrival

Homogeneous
T2
T11
T10
T9
T8
T7
T6
T5
T4
T3
T1

B

Realization A2

percent frequency

years until ridgecrest 5 arrival

Homogeneous
T11
T10
T9
T8
T4
T3
T2
T1
T12
T6
T5
T1
C

Realization A3

Percent Frequency

Years until Ridgecrest 5 Arrival

D

Realization B1

Percent Frequency

Years Until Ridgecrest 5 Arrival
Figure 11 (A-G) show Ridgecrest 5 arrival histograms of all ten trials per T-PROGS model, compared to the homogeneous control model. The most noticeable differences between the homogeneous and heterogeneous runs are that the average peak arrivals times for the heterogeneous trials are generally later than the homogeneous control. Additionally, the homogeneous trial shows a Gaussian distribution, while the heterogeneous trials all show non-Fickian distribution, with long tails.
Section V

Discussion

Due to the limitations of a conceptual model, the results discussed above cannot be taken literally; that is, they are not predictive of the actual length of time it would take the plume from the KAFB bulk fuels spill to reach the Ridgecrest wells. Additionally, these models only take advection into account, and not diffusion or dispersion below the scale of model cells, and so even comparison to current knowledge regarding the plume’s location cannot be taken as a direct analogy. The model was simplified in order to examine only the effect that heterogeneity might have on plume movement. Instead of actual plume travel time, the results instead should be considered as percent difference of travel time relative to a homogeneous control model.

For all seven heterogeneous models, averaged peak arrival times were 5-13% slower than the homogeneous peak arrival time, and averaged median particle arrival times of all the realizations varied to be between 6-18% slower than the predicted homogeneous median arrival time, which is encouraging for the current situation. However, due to the nature of the EDB contamination, which is highly soluble in water (4325 ppm) and is poisonous in small doses (Falta, 2004), the initial breakthrough time is more important to consider than averaged peak or median arrival times. Figure 10a shows that while averaged initial arrival times at Ridgecrest 5 are later than the predicted homogeneous averaged initial arrival, there are individual instances of initial breakthrough arrivals up to 12% faster than the homogeneous prediction. To determine the cause of this, the T-PROGS heterogeneity was examined in conjunction with the
resulting MODPATH movement in models that showed either unusually fast well arrival
times or unusually slow well arrival times.

Figure 12 shows the T-PROGS heterogeneity in comparison to the MODPATH
particle movement for Model A2 Trial 8, which had an initial arrival time 12% faster than
predicted by the homogeneous initial arrival and 14% faster than predicted by the average
initial arrival time for the A2 group. In Figure 12’s cross-section, it can be seen that after
their initial release, the particles remained in the upper 5-10 layers and traveled mainly
through gravels and sands, which could account for the relative rapidity of the particles to
Ridgecrest 5, and were not drawn down into lower layers until they moved closer to the
wells. In layer six (Figure 12) it can be seen that the particles did encounter some lower
hydraulic conductivity materials and did spread out a little, but were seemingly too close
to Ridgecrest 5 and its cone of depression to be drawn into Ridgecrest 4.

Similarly, model B3 Trial 4 (Figure 13) had an initial particle arrival time 18%
faster than the average initial arrival times for the B3 group, and 10% faster than the
predicted homogeneous average initial arrival. The T-PROGS and MODPATH
comparison of B3 T4 (Figure 13) also show a large section of gravel directly in the path
of particles towards the well, after which there is only sand for the particles to travel
through until they reach a clay deposit in layer 6 (Figure 13) which caused some
spreading. Like in model A2 Trial 8, the particles tended to stay in the top 5-10 layers,
until they were drawn down by the wells.

On the other end of the spectrum, model group B3 Trial 10 had an initial arrival
time 17% slower than group B3’s mean initial arrival time, and 28% slower than the
predicted homogeneous initial arrival time. The T-PROGS and MODPATH comparison
of B3 Trial 10 (Figure 14) shows a large section of clay immediately next to the contamination site cell that the particles, travelling in the upper 5 layers, first attempted to go around, and then were forced through by the hydraulic gradient. This initial diversion and then path through the clay likely played a large part in the slowdown of the particle movement. In addition, 80% of the particles released for B3 T10 hit Ridgecrest 4 instead of Ridgecrest 5. Examining Figure 14 further, it appears as though the initial diversion of the particles from the path the homogeneous particles would have taken, forced them further north than they otherwise would have been (i.e. as compared to the homogeneous model—Figure 16) where, closer to the Ridgecrest wells, the particles encountered more clay deposits that continued to cause spreading and directed the majority of them past Ridgecrest 5 and into Ridgecrest 4 instead. The few particles that made it to Ridgecrest 5 only did so once they were outside of the clay deposit, and in a sand deposit instead.

On a comparable note, Model A3 Trial 1’s particles also moved into Ridgecrest 4 instead of Ridgecrest 5. In this case as well (Figure 15), a later series of clay and silt deposits in layer 6, to the west and north of Ridgecrest 5, seems to have diverted the particles towards Ridgecrest 4.

Although it is most noticeable with the outliers, the pattern of faster particle travel times when sand and gravel is present along the flowpath, versus slower particle travel times when clay is present and the flowpath is diverted around the clay (as in B3 T10 and A3 T1) and/or slowed by the flowpath going through the low K bed (as in B3 T10) holds for the majority of the models (see appendix V for all MODFLOW models). Extrapolated further, this theme of fast-path gravel and slow-path clay could account for the differences in particle rate between the A group and the B group (recall that the A group
has 6% more gravel than the B group). As illustrated in Table 14, for each facies bin (aka small, medium, large), the comparable models for A and B (example, A1 and B1) showed the A group with faster average initial arrivals than the B group.

### Table 14. Ridgecrest 5 Average Initial Arrivals (‘Model Years’)

<table>
<thead>
<tr>
<th>Mean Facies Length</th>
<th>A (10% gravel)</th>
<th>B (4% gravel)</th>
<th>C (10% gravel)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small</td>
<td>71.63</td>
<td>73.6</td>
<td></td>
</tr>
<tr>
<td>Medium</td>
<td>70.2</td>
<td>72.6</td>
<td>76.2 (facies values from Lunt and Bridge (2004))</td>
</tr>
<tr>
<td>Large</td>
<td>70.4</td>
<td>75.3</td>
<td></td>
</tr>
</tbody>
</table>

Possibly more interesting than the differences in initial arrival times between the A and B groups, is the difference between the A group and the C group. Despite using the same percentages of materials as the A group, the C group average initial arrival is later than both the A group and the B group. Recall that the only difference between the A and C groups was the facies dimensions used to build the Markov chain models. The C group, rather than taking facies length values from the pre-dam modern Rio Grande, used facies length values from Lunt and Bridge’s (2004) study of the Sagavanirktok River, a braided river system in Alaska. If only the hydrofacies percentages could affect the rate of groundwater movement, then the Group C results should have been similar to the Group A results, as the percentages used therein were the same. That they were not suggests that the bar and channel dimensions used in the Markov chain model are just as important for solute transport. In other words, the dimensions of the materials had just as much of an effect on particle transport as the proportions of material. Previous work (Rust, 2006) had suggested the opposite conclusion (that hydrofacies lengths used in the Markov chain
models were essentially inconsequential so long as reasonable values were used), so this result was unexpected.

While initial breakthrough times are extremely important for contaminant monitoring in the near future, the non-Fickian distribution of the heterogeneous well arrival times (aka the long tails) also has implications regarding the contaminant travel path and KAFB’s proposed pump and treat plan. In previous works, Benson et al. (2000), Berkowitz et al. (2000) and Klise et al. (2009) report the occurrence of particle tailing due to transport through heterogeneous media, with faster initial arrivals resulting from particles taking a more direct path through pathways of connected higher conductivity materials, and slower arrivals resulting from particles taking a less direct path, and therefore having more interaction with lower conductivity materials. As seen in the histograms in Figure 11, as well as in the plot shown in Figure 17, where the whiskers on the box and whisker plot of all of the model runs show very long tails in comparison to their median arrival times, all of the heterogeneous models showed this non-Fickian transport. Using the same reasoning as the above discussion, wherein materials with low hydraulic conductivity slowed down particle transport, it would make sense to attribute the long tails here to some of the particles getting stuck in the clay and silt deposits on the way to wells, while others were able to avoid those deposits and traveled mainly through sands and gravels.

The model with the longest tail was B2 Trial 7. When examined (Figure 18), B2 Trial 7 does show areas where the released particles released start out all travelling along the same path until they encounter materials with different hydraulic conductivities juxtaposed to one another and are split. If some of the particles are allowed through
gravel, when others adjacent are stuck in clay, it could account for the long tails, with the particles that moved through higher conductivity materials getting to the well much more quickly than particles that were forced through lower conductivity materials. However, despite the fact that B2 Trial 7 does show instances of particles being separated along different travel paths, this is not at all unique to this particular model; all of the previous heterogeneous models (Figures 12-16) also show instances of particles splitting due to encounters with juxtaposed high and low conductivity materials. Therefore, the exact conditions or mechanisms that lead to longer or shorter tails remains unclear, and a heterogeneous model that goes beyond conceptual, and also accounts for dispersion, would be helpful in better predicting the type of tail that will occur in the KAFB system. In the interim however, it can be assumed that any heterogeneous model will show some degree of tailing, while a homogeneous model will not.

Understanding the specificities of the tail is important for future work because if the EDB contamination has the potential to get stuck in the clays, this could have implications not only for well arrival time, but also for KAFB’s proposed pump and treat system: if KAFB intends to “collapse” the plume, and yet part of the plume is mired in low hydraulic conductivity materials, then it will likely take longer than planned for the pump and treat system to fully collect all of the contamination.

When viewed from the side, all of the MODFLOW models (Figures 12-15) show generally horizontal particle movement, until the particles are drawn down by the wells. The Albuquerque municipal wells are screened deep in the aquifer (approximately 600-800 feet depending on the well), while the models in this work show that the saturated plume tends to remain in the upper level of the Sierra Ladrones formation. This infers that
the vertical heterogeneity in areas immediately surrounding the city wells may be important to characterize in order to understand downward migration to these screened intervals. Additionally, if the well construction is faulty (e.g., poor anular seal), there is potential for EDB contaminated water to enter the wells before actually hitting the well screens via the aquifer materials.

For the KAFB system, the results for the heterogeneous models underscore the need for more knowledge regarding type and placement of ancestral Rio Grande materials. For example, if a stratigraphic unit of higher conductivity material is in the correct location and has the correct dimensions, initial arrival times of the particles to the wells will be much more rapid than as predicted by a homogeneous model. Likewise, if a low conductivity material is located in the way of the transport path, there is potential both for a decrease in travel rate, and path diversion. As the situation stands currently, there is not sufficient data to model the jet fuel contamination in the Santa Fe Group aquifer to the degree of accuracy needed for a heterogeneous model that can truly describe the system.
Figure 12. T-PROGS and MODPATH for model A2 T8

A2 T8
Layer 1
Figure 12 shows the MODPATH particles’ path through the T-PROGS generated heterogeneity. Model A2 Trial 8 had an initial arrival time 12% faster than predicted by the homogeneous initial arrival and 14% faster than predicted by the average initial arrival time for the A2 group. Here, it can be seen that from the beginning, the particles travel mainly through gravels and sands in the upper layers, which could account for the relative rapidity of the particles to Ridgecrest 5. When the particles reach clay deposits in layer 6, they do spread and divert slightly north, but not enough to be captured by Ridgecrest 4 instead of Ridgecrest 5.
Figure 13. T-PROGS and MODPATH for model B3 T4

B3 T4
Layer 1
Figure 13 shows the MODPATH particles’ path through the T-PROGS generated heterogeneity for model B3 Trial 4. This trial had an initial particle arrival time 18% faster than the average initial arrival times for the B3 group, and 10% faster than the predicted homogeneous average initial arrival. The MODPATH particles travel mostly through sand and gravel at the start and in the top layer. As the particles drop down to layer 5 (7.5 feet), they encounter clay, which causes them to divert and slow. The zoomed in east-west transects (MODPATH particles shown in purple) shows that the particles tend to stay within the top ten layers, moving generally horizontally, until they are forced into the lower layers due to well pumping.
Figure 14. T-PROGS and MODPATH for model B3 T10

B3 T10
Layer 1
Figure 14 shows the MODPATH particles’ path through the T-PROGS generated heterogeneity for model B3 Trial 10. The MODPATH particles for this model had an initial arrival time 17% slower than group B3’s mean initial arrival time, and 28% slower than the predicted homogeneous initial arrival time. Here there is a large section of clay immediately next to the contamination site cell that the particles first attempt to go around, and then through. This initial diversion and then path through the clay likely played a large part in the slowdown of the particle movement, as well as path diversion. In layer 5, the particles are forced through even more clay deposits, further spreading out and north, towards Ridgecrest 4 instead of Ridgecrest 5.
Figure 15. T-PROGS and MODPATH for model A3 T1

A3 T1
Layer 1
Figure 15 shows the MODPATH particles’ path through the T-PROGS generated heterogeneity for model A3 Trial 1. Here, a series of clay and silt deposits in layers 5 and 6 to the northwest of Ridgecrest 5, are hypothesized to have diverted the particles towards Ridgecrest 4 instead. MODPATH particles shown in purple.
Figure 16 shows MODPATH particle movement for the control homogeneous model. Compared to the heterogeneous models, there is no path dispersion, and all of the particles reached Ridgecrest 5 in a single peak.
The plot for Figure 17 shows Ridgecrest 5 particle arrival times for all of the models, demonstrating the long tails resulting from non-Gaussian distribution. It is hypothesized that the long travel times are due to particles getting stuck in low conductivity materials. If contamination has the potential to get stuck in clay, this could have implications for both well arrival time and KAFB’s proposed pump and treat system.
Figure 18A. T-PROGS and MODPATH for model for B2 T7

B2 T7
Layer 1
Figure 18B. T-PROGS and MODPATH for model for B1 T9

B1 T9
Layer 1

Figure 18 shows the MODPATH particles’ path through the T-PROGS generated heterogeneity for model B2 T7, which the longest tails of all the models run, and B1T9, which had one of the shortest tails of all the models run. In B2T7, it can be seen that some MODPATH particles end up traveling through a high hydraulic conductivity material, while their immediately adjacent neighbors are forced through lower hydraulic conductivity materials therefore becoming significantly slowed. This wide range of particle rate ultimately results in particle tailing. If contamination can become mired in the clay, this could have implications for well arrival time and the proposed pump and treat system. If part of the plume is stuck in low hydraulic conductivity materials, then it will take longer for the pump and treat system to fully collect all of the material. However, comparing B2T7 to a model with a much shorter tail, such as B1T9, shows that the occurrence of juxtaposed high and low conductivity material that the particles must travel through is not unique to models with longer tails. Therefore, while all the models show tails, indicating that the existing heterogeneous substrate will also cause tailing, the exact mechanism behind longer or shorter tails is still unclear.
Section VI

Conclusion

A conceptual, numerical groundwater model of the area affected by the KAFB bulk fuels spill showed clearly that the addition of heterogeneity had an effect on both particle travel time and particle travel path. While particles released during a control homogeneous run arrived at Ridgecrest 5 in a single spike after release, all of the heterogeneous realizations showed averaged median arrival times 6-18% later than the homogeneous prediction, and averaged initial arrival times 3-9% later than the homogeneous prediction, as well as long tails following a power-law slope, indicative of non-Fickian transport. The heterogeneous realizations also showed instances of breakthrough arrival times to Ridgecrest 5 as much as 12% earlier than the predicted homogeneous arrival time, if the heterogeneity in that particular model allowed for the particles to travel through mainly high conductivity materials on the way to Ridgecrest 5. In addition to gravel placement affecting particle travel, clay placement was also shown to be significant. If clay was placed in the travel path, particles were either forced to divert around it, which added time and changed the direction of travel, or forced to move through it, which also added to travel time and caused the particles to spread out from one another. The occurrence of adjacent clay and gravel bodies along the travel path was also hypothesized to explain the non-Fickian distribution of arrival times; if some particles ended up in sand or gravel, while their neighbors were mired in clay, that could result in some particles reaching the well fairly quickly, while others were significantly slowed, resulting in wide range of arrival times and therefore, the long tails. While the exact mechanism behind shorter or longer tails in this particular aquifer system is still
unknown, what is known is that as the Sierra Ladrones formation is heterogeneous, there will be particle tailing in the EDB plume. As such, well-monitoring and clean-up time projections should be adjusted accordingly.

The differences in arrival times between the A and B groups was attributed to the reduced gravel in the B group, lowering the model sets’ overall hydraulic conductivity and thus slowing the rate of particle travel. However, despite using the same category ratios as Group A, the averaged initial arrival time of the Group C runs was 11% slower than the initial arrival time of the homogeneous run while, as comparison, the A group showed averaged initial arrival times only 2.6% slower than the homogeneous run. In fact, Group C, with slower median arrival times and shorter tails, tended to resemble Group B more so than Group A. With the category ratios between the A and C groups set the same (10% gravel), the differences in initial arrival time here was hypothesized to be due to the mean lengths of facies used in the Markov chain model, as the Group A and Group B Markov chains were calculated using bar and channel dimensions from the modern Rio Grande, while the Markov chains for Group C were calculated using bar and channel dimensions from Lunt and Bridge’s (2004) study of a braided river in Alaska. These findings are taken to indicate that in addition to material ratios, the facies dimensions used in the Markov chain model can also have a significant effect on model heterogeneity, and thus particle travel time.

If material placement and facies dimensions were inconsequential to particle travel time and path, then a homogeneous model of the KAFB system would be sufficient to model the plume, with the caveat that as heterogeneity is present in the system, a small possibility of early contaminant arrival does exist, and it would be prudent to monitor
accordingly. However, because material placement and hydrofacies dimensions were found to have an effect on particle path and well arrival time, and especially breakthrough arrival time, heterogeneity should not be neglected. Efforts should be made to at least interpret, if not model, the actual size and placement of ancestral Rio Grande bars and channels in the plume area, and to continue monitoring plume direction for changes. A heterogeneous model would also be advantageous for determining the type of tail most likely to occur in the KAFB system due to the issue that, if particles are stuck in clays, this could significantly raise the pumping time needed for KAFB’s proposed pump and treat system to fully remove all of the contamination.

The hydrofacies and their placements used in this work are not representative of what is actually in the subsurface; they are statistically likely possibilities. Therefore, if further work is to be done, then additional data regarding the geometry and location of the heterogeneity present in the aquifer is necessary. For example, further core and geophysical data would be useful in constraining the material ratios, sizes and locations of the deposits.

It is clear from the results of this work that further studies should be done to understand and model the heterogeneity of the KAFB bulk fuels spill system. However, the challenge lies not only in collecting additional data from cores and other sources, but also in modeling to a reasonable size and resolution, given the limits of the technology available. While scant or only general information regarding category ratios, and bed size and placement will not accurately portray the effect that heterogeneity will have on a particular system, neither will a model that cannot model the study area to a reasonable
resolution and size, and all of these issues must be considered when building the next heterogeneous groundwater model of the KAFB bulk fuels spill saturated plume.
## List of Appendices

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Appendix I

T-PROGS PROGRAMS

Background

GAMEAS, which is used to compute bivariate geostatistics, is run first. For GAMEAS, the raw data, in this case borehole lithologies, is recorded and separated into discreet categories. Then, the transition probability from one category to another over a set distance interval (for example, every 0.25 meters or every 0.5 meters) is calculated and saved as a .eas file, which is what GAMEAS will refer to when running. In the case of this work, the data input into GAMEAS was from six KAFB core logs, and four categories (clay, silt, sand, and gravel) were chosen over an interval of 0.25. An annotated example of the GAMEAS parameter file can be found in appendix III.

The second step of TPROGS is to take the measurements computed by GAMEAS and model their spatial variability as a Markov chain model using the program MCMOD. In addition to the GAMEAS output file, MCMOD also requires the ratio of the categories to each other, as well as the mean width and length of facies for each category. An example of the MCMOD input file can be found in appendix III.

Before generating a conditional 3-D simulation with the MCMOD results, the data from GAMEAS is compared to the developed Markov chain models from MCMOD using the program GRAFXX (annotated parameter file in appendix III), which visualizes the Markov chain models next to the raw, GAMEAS data. Only after the Markov chain model and the actual data are determined to sufficiently resemble one another can the MCMOD data be put into the program TSIM (annotated parameter file in appendix III), which will generate a conditional 3-D simulation of the data based on the Markov chain.
model. In order to rationalize the application of transition probabilities from vertical successions in the horizontal direction, Walther’s law was assumed, following the method of Weissmann et al (1999). The TSIM data is then visualized using either CHUNK or another program. The TSIM output file can be manually inserted into MODFLOW run files, so that the groundwater modeling program can read the heterogeneity.
MODELING T-PROGS IN MODFLOW

Integrated T-PROGS into GMS (Rust, 2006 Master’s Thesis)
Edit → Units → Feet

To create the grid frame in GMS:
In the map icon → Feature Objects → Grid Frame
1. Double click frame, enter x, y, z for the origin
   a. X = 1538428.807 (Easting of SW node)
   b. Y = 1472301.512 (Northing of SW node)
   c. Z = 3921
2. Enter Dimensions (i.e. total x, y, z lengths)
   a. X-length = 15,267 feet
   b. Y-length = 12,269 feet
   c. Z-length = 988 feet

To create the 3-D grid:
In the 3-D grid module → Grid → Create Grid
1. Origin and lengths may have to be reset
2. Set cell numbers
   a. X = 305
   b. Y = 245
   c. Z = 32
3. Highlight 3D Grid data → Grid → Redistribute Layers
4. Edit grid elevation top (4865 feet) and elevation bottom (3921 feet)
5. Assign starting head for all grid layers to 4865 feet
6. Edit the fraction for layers 1 through 31 each to 0.001518219, layer 32 should be 0.952935223 (this is to include the effects of the deep city wells). Select okay.

Create the conceptual model:
1. Under “Map Module” right click and select “new conceptual model”. Name the new model.

Initialize MODFLOW:
1. Highlight 3-D Grid Module/MODFLOW → Select: New Simulation
2. Attributes used in the model
   a. Wells
   b. General Head Boundary
3. With 3-D grid Data highlighted, go to Modflow → select LPF –Layer Property Flow from the dropdown. Change Layer Property Entry Method from “Use data arrays” to “Use material ID’s.”
4. Select “Material Properties”. Change the properties accordingly:

<table>
<thead>
<tr>
<th>Material</th>
<th>Horizontal K (ft/day)</th>
<th>Horizontal Anisotropy</th>
<th>Vertical Anisotropy (Kh/Kv)</th>
<th>Porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>0.000328</td>
<td>1</td>
<td>0.1</td>
<td>0.2</td>
</tr>
<tr>
<td>Silt</td>
<td>0.0328</td>
<td>1</td>
<td>0.1</td>
<td>0.25</td>
</tr>
<tr>
<td>Sand</td>
<td>70</td>
<td>1</td>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
<td>Gravel</td>
<td>150</td>
<td>1</td>
<td>0.1</td>
<td>0.45</td>
</tr>
<tr>
<td>Homogeneous</td>
<td>72</td>
<td>1</td>
<td>0.1</td>
<td>0.3</td>
</tr>
</tbody>
</table>

**Head Boundaries:**

a. Right click the Conceptual Model → Select New Coverage
b. Label the new coverage “Head”. Select the General Head Boundaries box. Set for layers 1-32, with an elevation of 4865.
c. In this model, there are four General Head boundaries, one for each side. The system is saturated to avoid technical issues with wetting and drying cells. A depth of 75 feet of water was added to each boundary to maintain the gradient while saturating the system.

a. The conductance for the general head boundaries was calculated as $C = \frac{KA}{dx}$ with K the mean hydraulic conductivity value (21.3 m/day or 70 ft/day), Area = 6.9 m² (75 ft²) and dx = 1600 m (5250 ft) to allow for sufficient room for flow outside the cones of depression near the edges of the grid boundaries for the model to converge. The conductance was set at 1 ft²/day
b. To create each head boundary:
   i. Arc Tool. Click next to one corner of the boundary, make sure the resulting line goes through all of the boundary cells, double click at the end of the boundary to finish the arc.
   ii. Arc Select tool → Highlight the arcs/boundaries now created → right click Properties → Dropdown menu to “General Head Boundaries”. Change Conductance.
   iii. Select the nodes with the node select tool and then right click → attributes → select head values:
      1. North boundary set at: (left) 4922- (right) 4897
      2. South boundary set at: (right) 4935- (left) 4930
      3. West boundary set at: (base) 4930- (top) 4922
      4. East boundary set at: (base) 4935- (top) 4897

**Import Well and Other Data:**
This was modeled under steady state conditions, with and without pumping the new KAFB well, so a single flow rate under each Ridgecrest Well and Burton 5, was assumed.
1. Under Map Module ➔ Conceptual Model (previously created?) ➔ create a new Coverage Area. Rename it “Well Data”
   a. Within each coverage ➔ Set-up select Wells from Source ➔ Sink ➔ Coverage list
   b. Apply to all layers (1 to 32) and define a default elevation
2. Data can be imported from *.txt file [well name no spaces, x, y, z, screen length, top of screen elevation, bottom of screen elevation, flow rate]. Flow rate should be negative since water is being extracted.
3. In GMS go to File ➔ Open select the *.txt file with the well data
   a. Set GMS data type as Wells
   b. Assign correct file header type to each data column
   c. Finish (Wells should appear on the correct points)
4. To Import the fuel spill location, go to File ➔ Open select the *.txt file with the bulk fuels facility location data [name, easting, northing]. Import data as “2D scatter points”.

Map Data to MODFLOW:
1. Highlight “Map Module” go to Feature Objects ➔ Map ➔ MODFLOW/MODPATH
   a. Do NOT select “all applicable coverages” DO select “Active Coverage Only” (or else TPROGS won’t load).

Run MODFLOW:
1. First Check Simulation to check for errors.
2. Ignore warning re: grid sizes
3. If no errors, save first, then run Modflow. Should only be a few iterations, which will create a folder of files. The .msf file will be altered in order to insert TPROGS.

Importing TPROGS into MODFLOW
1. Close out of GMS. It will ask if you want to save. Don’t save (or else TPROGS won’t load)
2. Use the .ascii output file from TSIM and modify so that there are no negative values (i.e. absolute values only).
3. Locate the *.mfs file from MODFLOW output. Replace the ‘DMAT 1” line with “MAT”. Below the new “MAT” line, copy-past the .asci TSIM output file (sans the X, Y, Z cell dimensions at the very top). Add 74,725 “5”’s (i.e. X number of cells by Y number of cells) to the bottom of the copied *.asc, to account for the single homogeneous layer below the TPROGS. Save and close. Reopen GMS and the model, and TPROGS should now be loaded.
Run MODFLOW
1. With TRPOGS now installed, MODFLOW should run through several iterations before completion. In order to run Modflow, the TPROGS must first be mapped to MODFLOW/MODPATH by right clicking the conceptual model and selecting Map to Modflow/Modpath → Active coverage only. Check the model. If no errors, run MODFLOW. Before running, the program will ask if you would like to save. Select yes (otherwise it won’t read the TPROGS).
2. If the model doesn’t converge, go to MODFLOW → PCG2, and select. Alter the iterations as necessary for the heads to converge (200 and 250 seemed to work for maximum number of outer and maximum number of inner iterations respectively).

Run MODPATH
1. With 3D Grid Data highlighted, go to the cell with the previously loaded “Bulk Fuels Spill Location”. Highlight the cell.
2. Go to MODPATH → Generate Particles at Selected Cells.
3. Generate between 50-100 particles inside the selected cell

TROUBLESHOOTING
Issue: When running MODFLOW for the first time, the cells become red.
Solution: The cells have dried out. Change the starting head for the grid so that it’s closer to the head boundaries, to ensure that the cells remain flooded.

Issue: TPROGS has loaded but MODFLOW doesn’t read it.
Solution: The new TPROGS has not been mapped to the MODFLOW. Map to MODFLOW, then run again.

Issue: When running MODFLOW, the heads will not converge
Solution: Change the number of iterations and/or (for General Head Boundaries) change the conductance and/or change the head gradient so there is not a huge difference between the highest and lowest head boundary values
## Appendix II

### Embedded Transition Probabilities for T-PROGS

L = Facies length (feet)

S = Symmetry/Same

B = Background category (sand)

<table>
<thead>
<tr>
<th>Model</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>Clay L=45.5 0.018 B 0.058</td>
<td>L=160.3 0.018 B 0.058</td>
<td>1.068 0.018 0.92 0.058</td>
</tr>
<tr>
<td></td>
<td>S L=45.5 B 0.0001</td>
<td>S L=160.3 B 0.0001</td>
<td>0.68 2.78 0.32 0.0001</td>
</tr>
<tr>
<td></td>
<td>Sand B B B B</td>
<td>B B B B</td>
<td>0.61 0.012 4.84 0.38</td>
</tr>
<tr>
<td></td>
<td>Gravel S S B L=131</td>
<td>S S B L=197</td>
<td>0.096 0.0001 0.90 1.42</td>
</tr>
<tr>
<td>A2</td>
<td>Clay L=120 0.018 B 0.058</td>
<td>L=463 0.018 B 0.058</td>
<td>1.068 0.018 0.92 0.058</td>
</tr>
<tr>
<td></td>
<td>S L=120 B 0.0001</td>
<td>S L=463 B 0.0001</td>
<td>0.68 2.78 0.32 0.0001</td>
</tr>
<tr>
<td></td>
<td>Sand B B B B</td>
<td>B B B B</td>
<td>0.61 0.012 4.84 0.38</td>
</tr>
<tr>
<td></td>
<td>Gravel S S B L=201</td>
<td>S S B L=1686</td>
<td>0.096 0.0001 0.90 1.42</td>
</tr>
<tr>
<td>A3</td>
<td>Clay L=305 0.018 B 0.058</td>
<td>L=1211 0.018 B 0.058</td>
<td>1.068 0.018 0.92 0.058</td>
</tr>
<tr>
<td></td>
<td>S L=305 B 0.0001</td>
<td>S L=1211 B 0.0001</td>
<td>0.68 2.78 0.32 0.0001</td>
</tr>
<tr>
<td></td>
<td>Sand B B B B</td>
<td>B B B B</td>
<td>0.61 0.012 4.84 0.38</td>
</tr>
<tr>
<td></td>
<td>Gravel S S B L=367</td>
<td>S S B L=1968</td>
<td>0.096 0.0001 0.90 1.42</td>
</tr>
<tr>
<td>B1</td>
<td>Clay L=45.5 0.019 B 0.0685</td>
<td>L=160.3 0.019 B 0.0685</td>
<td>1.07 0.019 0.91 0.0685</td>
</tr>
<tr>
<td></td>
<td>S L=45.5 B 0.0001</td>
<td>S L=160.3 B 0.0001</td>
<td>0.677 2.79 0.323 0.0001</td>
</tr>
<tr>
<td></td>
<td>Sand B B B B</td>
<td>B B B B</td>
<td>0.85 0.015 6.58 0.149</td>
</tr>
<tr>
<td></td>
<td>Gravel S S B L=131</td>
<td>S S B L=197</td>
<td>0.132 0.0001 0.868 1.65</td>
</tr>
<tr>
<td>B2</td>
<td>Clay L=120 0.019 B 0.0685</td>
<td>L=463 0.019 B 0.0685</td>
<td>1.07 0.019 0.91 0.0685</td>
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<td>S L=120 B 0.0001</td>
<td>S L=463 B 0.0001</td>
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<tr>
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<td>Sand B B B B</td>
<td>B B B B</td>
<td>0.85 0.015 6.58 0.149</td>
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<td>Gravel S S B L=201</td>
<td>S S B L=1686</td>
<td>0.132 0.0001 0.868 1.65</td>
</tr>
<tr>
<td>B3</td>
<td>Clay L=305 0.019 B 0.0685</td>
<td>L=1211 0.019 B 0.0685</td>
<td>1.07 0.019 0.91 0.0685</td>
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<td></td>
<td>S L=305 B 0.0001</td>
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<td>0.677 2.79 0.323 0.0001</td>
</tr>
<tr>
<td></td>
<td>Sand B B B B</td>
<td>B B B B</td>
<td>0.85 0.015 6.58 0.149</td>
</tr>
<tr>
<td></td>
<td>Gravel S S B L=367</td>
<td>S S B L=1968</td>
<td>0.132 0.0001 0.868 1.65</td>
</tr>
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<td>C1</td>
<td>Clay L=501 0.018 B 0.585</td>
<td>L=1210 0.018 B 0.585</td>
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</tr>
<tr>
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<td>S L=1210 B 0.0001</td>
<td>0.68 2.78 0.32 0.0001</td>
</tr>
<tr>
<td></td>
<td>Sand B B B B</td>
<td>B B B B</td>
<td>0.61 0.012 4.84 0.38</td>
</tr>
<tr>
<td></td>
<td>Gravel S S B L=426</td>
<td>S S B L=1259</td>
<td>0.096 0.0001 0.90 1.42</td>
</tr>
</tbody>
</table>
Appendix III

Annotated T-PROGS Parameter Files

A. Example .par file for GAMEAS

START OF GAMEAS PARAMETERS for MCcore_1 Dummy line of text
..\TPROGS_Files_KAFB\Run_TPROGS\MCcore_1\GAMEAS_MCcore_1.eas input
data file (.eas file)
1 2 3 Column numbers in data files of x, y, z locations of data
4 4 5 6 7 Number of categories plus column of category
-1. 2. Minimum and maximum values to screen extreme data
..\TPROGS_Files_KAFB\Run_TPROGS\MCcore_1\GAMEAS_MCcore_1_output.eas
GAMEAS Output file for use in MCMOD
100 Number of lags for calculated bivariate spatial statistics
0.25 Lag spacing
0.15 Lag tolerance i.e. distance allowed for defining data pairs
1 Loop of “ndir” directions (TPROGS manual suggests keep at 1)
0.0 90 1 -90 4 0.2 Azimuthal direction, tolerance and bandwidth; dip direction,
tolerance, and bandwidth
16 Number of cross correlations
1 1 11 Remaining: tail variable, head variable, index for type of bivariate statistic
1 2 11
1 3 11
1 4 11
2 1 11
2 2 11
2 3 11
2 4 11
3 1 11
3 2 11
3 3 11
3 4 11
4 1 11
4 2 11
4 3 11
4 4 11
### B. Example .par file for MCMOD. Part I – Develop Vertical Markov Chain Models to Determine Embedded Transition Probabilities in Z-direction

4 Number of categories
0.113074E+00 0.1060E-01 0.7738E+00 0.9541E-01 proportions for each category 1 2 3 4
3 background category
../../../TPROGS_Files_KAFB/Run_TPROGS/MCcore_1/MCcore1_mcmmod.dbg debugging file name
../../../TPROGS_Files_KAFB/Run_TPROGS/MCcore_1/MCcore1mcmmodotpt.bgr output 3D model file name
../../../TPROGS_Files_KAFB/Run_TPROGS/MCcore_1/MCcore1mcmmod_det.bgr output 3D model determinant file name used later in TSIM
0.01 0.02 0.1 X Y Z lateral extent in 3D model in terms of determinant (debug file no. of lags should be 10-20)
10 10 1 X Y Z lag spacing for 3D model in terms of determinant
../../../TPROGS_Files_KAFB/Run_TPROGS/MCcore_1/MCcore1mcmmod_x.eas output file name for parameters for 1D x-direction model
200 1. X direction number of lags. Lag spacing
3 X direction modeling approach
45.5 .34 0.5 row 1 entries for x-direction transition rate matrix
-1 45.5 0.03 row 2 entries for x-direction transition rate matrix
0 0 0 0 row 3 entries for x-direction transition rate matrix
-1 -1 0 200 row 4 entries for x-direction transition rate matrix
../../../TPROGS_Files_KAFB/Run_TPROGS/MCcore_1/MCcore1mcmmod_y.eas output file name for parameters for 1D y-direction model
200 1. Y direction number of lags. Lag spacing
3 Y direction modeling approach
160.3 .34 0.05 row 1 entries for y-direction transition rate matrix
-1 160.3 0.03 row 2 entries for y-direction transition rate matrix
0 0 0 0 row 3 entries for y-direction transition rate matrix
-1 -1 0 1653 row 4 entries for y-direction transition rate matrix
../../../TPROGS_Files_KAFB/Run_TPROGS/MCcore_1/MCcore1mcmmod_z.eas output file name for parameters for 1D z-direction model
20 0.5 z-direction number of lags, lag spacing
2 z-direction modeling approach
../../../TPROGS_Files_KAFB/Run_TPROGS/MCcore_1/GAMEAS_MCcore_1_output.eas TPROGS data file
3 lag number for developing Markov chains from TPROGS data
C. Example .par file for MCMOD. Part II – Embedded Transition Probabilities in X, Y, and Z-directions

4 Number of categories
0.113074E+00 0.1060E-01 0.7738E+00 0.9541E-01 proportions for each category 1 2 3 4

3 background category

..\MCcore_1\MCcore1_mcmo.dbg debugging file name
..\MCcore_1\MCcore1_mcmo.det.dbg output 3D model file name
..\MCcore_1\MCcore1_mcmo.det.dbg output 3D model determinant file name used later in TSIM

0.05 0.5 0.001 X Y Z lateral extent in 3D model in terms of determinant (debug file no. of lags should be 10-20)

10 10 1 X Y Z lag spacing for 3D model in terms of determinant

..\MCcore_1\MCcore1_mcmo_x.eas output file name for parameters for 1D x-direction model

200 1 X direction number of lags. Lag spacing

3 X direction modeling approach

45.5 0.02 0.2047 row 1 entries for x-direction transition rate matrix
-1 45.5 0.03 row 2 entries for x-direction transition rate matrix
0 0 0 0 row 3 entries for x-direction transition rate matrix
-1 -1 0 131 row 4 entries for x-direction transition rate matrix

..\MCcore_1\MCcore1_mcmo_y.eas output file name for parameters for 1D y-direction model

200 1 y direction number of lags. Lag spacing

3 y direction modeling approach

160.3 .34 0 .05 row 1 entries for y-direction transition rate matrix
-1 160.3 0 .03 row 2 entries for y-direction transition rate matrix
0 0 0 0 row 3 entries for y-direction transition rate matrix
-1 -1 0 1197 row 4 entries for y-direction transition rate matrix

..\MCcore_1\MCcore1_mcmo_z.eas output file name for parameters for 1D z-direction model

20 0.5 z-direction number of lags, lag spacing

3 z-direction modeling approach

1.07 0.02 0.058 row 1 entries for z-direction transition rate matrix
0.67 2.78 0 .001 row 2 entries for z-direction transition rate matrix
0 0 0 0 row 3 entries for z-direction transition rate matrix
.10 .0001 0 1.42 row 4 entries for z-direction transition rate matrix
D. Example .par file for TSIM

4 Number of categories
0.113074E+00 0.1060E-01 0.7738E+00 0.9541E-01 Proportions
../MCcore_1/MCcore1_sim.asc Output file for grid
2 Output format (ASCII)
1 Debugging level (higher = more info)
../MCcore_1\MC1tsim.dbg Debugging file name
4175 Seed for random number generator
1 Number of simulations
1543793.9 -3949 46.5 x center; negative number of nodes in +/- x-direction; x-node size
1477962.316 -5814 50 y center; negative number of nodes in +/- y-direction; y-node size
4840 -25 1 z; number of nodes on z-direction; z-node size
1 4 Min and max number of data points used for cokriging estimates
1 Basis function for cokriging estimates (1=transition probability)
0.001 Value for defining singularities in singular value decomposition
../mcmod/lnl_tp_xyz.bgr Transition probability model file name (from MCMOD)
../MCcore_1/MCcore1mcmod_det.bgr Determinant file name (from MCMOD)
../MCcore_1/GAMEAS_MCcore_1.eas Input data file name
0. 0. Fixed azimuths: coordinate system; stratigraphic
0. 0. Fixed dips: coordinate system; stratigraphic
junkaz.bgr Specified azimuth direction file
junkdip.bgr Specified dip direction file
4 9.98341748397e-005 -1 Quenching parameters: max# of iterations; tolerance;
1=closest lags only, 1=weight
0.40 Determinant value prescribing spatial limit of quenching lags
Appendix IV

Electronic

All Borelog Data Access Database

Appendix IV is an access database containing all of the borelog and water data used in this work. The data was collected from electronic PDFs from the Kirtland Air Force Base Quarterly Reports. As such, its accuracy cannot be guaranteed.

As of the writing of this work, the Quarterly Reports can be accessed under the “Project Documents” section at www.kirtlandjetfuelremediation.com.
Appendix V

Electronic PDF

All T-PROGS/MODFLOW Models

Appendix V is an electronic pdf of images of all of the T-PROGS models. The T-PROGS models all show layer one T-PROGS, layer one MODFLOW hydraulic heads, and MODFLOW particle tracking through all layers.
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ArcMap© 2010. ESRI


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