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P A N T E X P L A N T

# Optimization of Monitoring Well Placement For Potential RDX Breakthrough Detection in the Ogallala Aquifer

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From Science to Solutions

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# ACRONYMNS AND ABBREVIATIONS

| | |
|---|---|
| 2-D | two-dimensional |
| 3-D | three-dimensional |
| ArgusONE | Argus Open Numerical Environments |
| bgs | below ground surface |
| B&W Pantex | Babcock & Wilcox Technical Services Pantex, LLC |
| CMS/FS | Corrective Measures Study/Feasibility Study |
| DOE | Department of Energy |
| FGZ | fine-grained zone |
| ft/d | feet per day |
| ft/ft | feet horizontally/feet vertically |
| GAM | Groundwater Availability Model |
| GSLIB | Geostatistical Software Library |
| GUI | graphical user interface |
| meters | meter |
| ppb | parts per billion |
| ppm | parts per million |
| PTC | Princeton Transport Code |
| TTU | Texas Tech University |
| TWDB | Texas Water Development Board |

# EXECUTIVE SUMMARY

The Babcock and Wilcox Technical Services Pantex, LLC (B&W Pantex) Environmental Projects and Operations Division is assessing the need for additional monitoring wells to be installed at several locations around the Pantex Plant for early detection of potential groundwater impacts to the Ogallala Aquifer. This effort focuses on the area east of the Plant, where modeling predicted contaminants might migrate beneath the perched groundwater from discharges south of the Plant (BWXT Pantex/SAIC, 2007). The objective of this effort is to identify best locations for up to three new Ogallala Aquifer monitoring wells, using the PlumeFinder technology, and incorporating the results of previous modeling. Due to its widespread occurrence in perched groundwater and relatively high mobility, RDX (a high explosive) was modeled to determine the best locations for the wells. Although source strength and location are not directly measured, insight can be gleaned from the corrective measures study / feasibility study (CMS/FS) (BWXT Pantex/SAIC, 2007) modeling efforts.

The Ogallala Aquifer beneath the impacted perched groundwater is not accessible for investigation, because of the concern that drilling through the perched groundwater may create pathways allowing the spread of contamination. As a result, irreducible uncertainty stemming from a lack of field data is present in the area of interest. The uncertainty specifically pertains to the hydraulic conductivity, potentiometric surface, and the elevation of the redbeds marking the base of the aquifer.

Modeling is combined with optimal estimation techniques to address this uncertainty. Specifically, geostatistical representations of the Ogallala Aquifer hydraulic conductivity fields are coupled with flow and transport simulations to determine the areas of greatest uncertainty in potential RDX plume location. This approach, known as the “PlumeFinder,” is technology which integrates groundwater flow and transport simulation, geostatistical simulation, Monte Carlo simulation, and Kalman filter analysis to optimize monitoring well locations. In the analysis presented here, plume location (plume fringe) is defined as the 1 ppb isopleth contour for RDX and investigated over a 50-year simulation period. The areas of greatest uncertainty in the 1 ppb isopleth location then become candidates for new well locations, which in turn reduce the uncertainty in plume delineation by the maximum amount possible. To locate the leading edge of the RDX plume, both the retardation of RDX and potential biodegradation were ignored. This results in a conservative estimate (shortest travel time) to the fringe of the eastern perched groundwater while identifying the best location for early detection monitoring well placement. The actual travel time for RDX to migrate within the Ogallala Aquifer, if it occurs, is expected to be longer than simulated in this analysis.

The following procedure is used to implement the PlumeFinder technology:

- Gather available information on the groundwater flow and transport properties of the aquifer.
- Gather available information on the current chemistry of the aquifer.
- Use a preliminary groundwater flow and transport model to characterize the movement of groundwater and dissolved contaminants in the aquifer.
- Apply the PlumeFinder technology to baseline the maximum measure of uncertainty from a suspected source area based on the knowledge of the groundwater flow and contaminant transport properties.
- Apply the PlumeFinder technology to assess the maximum measure of uncertainty from a suspected source area based on the knowledge of the groundwater flow and contaminant transport

properties and the existing monitoring well network. This step quantifies the value of the existing monitoring well network as compared to no monitoring wells.

- Use the PlumeFinder technology to generate the next best monitoring well location to gather subsurface information given what is currently known. Constrain the possible locations of future monitoring wells to locations outside the area of impacted perched groundwater.
- Assess the value in the proposed monitoring well with respect to the reduction in the uncertainty in the extent of contamination.
- Update the PlumeFinder observation database with the expected concentration at the new monitoring well location, and repeat the analysis (for up to three wells in the current analysis) to select the next best location for plume fringe location.

The PlumeFinder technology currently requires Princeton Transport Code (PTC) to be used as the numerical code for the flow and transport model. Consequently, to conduct this analysis, a two-dimensional (2-D) model of the Ogallala Aquifer was developed using PTC. This PTC Ogallala Aquifer model was developed by integrating historical information, previous modeling efforts, geostatistical codes, and current field data. Previous models developed for this area include the Pantex BIOF&T3D model and the Pantex Ogallala Aquifer model, both documented in BWXT/SAIC 2007. The latter was a local refinement of the Northern Ogallala Groundwater Availability Model (GAM) (Dutton, Reedy, and Mace, 2001; Dutton 2004). The domain of interest for the PTC model was selected to be an area of approximately 9 square miles (12,000 feet by 24,000 feet) including the southeastern portion of Pantex Plant and areas south and east.

Only sporadic, non-trending, and very low-level (parts per billion [ppb]) detections of RDX have been observed in Ogallala Aquifer monitoring wells. However, RDX detections in the parts per million (ppm) range are routinely observed in perched groundwater above the Ogallala Aquifer. Groundwater simulations show RDX may impact the Ogallala Aquifer in the future (BWXT/SAIC 2007), and the proposed monitoring wells are in response to this potential issue.

Delineation of potential future plumes can be improved by adding three new monitoring wells at locations determined using the PlumeFinder technology in combination with previous modeling results. Installation of new wells, in concert with the existing Ogallala Aquifer monitoring wells, increases the certainty of early plume detection. A new well located using PlumeFinder reduces the maximum measure of uncertainty of plume delineation beyond the fringe of the perched aquifer by 72 %. Two additional wells beyond the eastern extent of perched groundwater provide early detection of potential contamination originating along the fringe of perched groundwater. Since the majority of the projected plume is beneath the perched aquifer, most of the uncertainty in its extent resides there. If the total uncertainty reduction is computed (within and beyond the perched groundwater extent) then the reduction in uncertainty achieved with the addition of a new well located by PlumeFinder is only 16%. This demonstrates the contribution of irreducible uncertainty which results from employing safe investigative practices by imposing the constraint that no wells be drilled through the perched groundwater to investigate a hypothetical plume.

The following specific recommendations are provided upon installation of the additional monitoring wells:

- Assess the groundwater flow field by collecting a complete set of potentiometric surface data to reduce uncertainty in current groundwater flow directions.
- Update the conceptual site model as appropriate (e.g. base of Ogallala Aquifer, lithology, and hydraulic properties).

- Collect analytical data, test for the occurrence of RDX in the Ogallala Aquifer, and assess trends or patterns; compare this with existing information on the sporadic detection of RDX in the Ogallala Aquifer.
- Collect monitored natural attenuation parameters to assess natural degradation rates for RDX with time.
- Compare to previous water table maps, chemical information and expected degradation rates from the CMS/FS. If information is similar (i.e. quasi-stable) then continue long-term monitoring; if not then update the preliminary groundwater model and revise PlumeFinder results to ensure well locations remain adequate for early RDX detection.

# 1.0 INTRODUCTION

## 1.1 BACKGROUND

In 2002, Pantex Plant initiated a comprehensive site investigation and groundwater modeling program to evaluate the extent and potential movement of groundwater and contaminants beneath the Plant. RDX, a high explosive, is one of the most ubiquitous contaminants detected in soils and perched groundwater beneath Pantex Plant. The perched groundwater occurs above the fine-grained zone (FGZ), a series of fining-upward sequences capped by clay layers several feet thick. Near the southern and eastern extent of perched groundwater, site investigation data noted a decrease in clay content and higher permeability of the upper surface of the FGZ. Consistent with the field observations, modeling results showed the potential for low-level RDX impacts to the Ogallala Aquifer in these areas. Due to the concern of spreading RDX contamination by drilling through contaminated perched groundwater and into the Ogallala Aquifer, numerical models were developed to estimate the rate and direction of potential RDX migration.

The detection monitoring capabilities of the existing Ogallala Aquifer monitoring well network can be improved by the installation of additional wells in appropriate locations. To determine the best locations to enhance the detection monitoring network, Pantex Plant requires a tool that links a groundwater flow and transport model and geostatistical techniques to optimize placement of new wells south and east of the Plant. As part of this task, SAIC developed a model to encompass the southeastern and eastern portions of the site and offsite areas, and incorporated an optimization tool to determine the best monitoring well placement.

## 1.2 OBJECTIVE AND TASK DEFINITION

The objective of this effort is to identify best locations for up to three new Ogallala Aquifer monitoring wells using the PlumeFinder technology and incorporating predictions from previous modeling efforts such as the Baseline Human Health Risk Assessment (BWXT Pantex/SAIC, 2006) and CMS/FS (BWXT Pantex/SAIC, 2007). Two potential source areas, one to the south of Pantex Plant and another distributed along the eastern extent of perched groundwater saturation, are evaluated because they are the most likely areas for contaminant breakthrough from the overlying and impacted perched groundwater. These areas were selected based upon site investigation data and prior modeling. The potential source to the south represents the most likely area of breakthrough based upon the current understanding of site conditions and the modeling predictions presented in the CMS/FS. The potential source along the eastern extent of perched groundwater represents the next most likely area of contaminant breakthrough, again, based upon the current understanding of site conditions. Based upon site investigation data, the confining unit underlying perched groundwater is more transmissive along the fringe of perched groundwater than within its interior. So the fringe of perched groundwater is considered a likely area for contamination to migrate to the Ogallala Aquifer. In addition, a constraint is imposed in this analysis that proposed wells not be drilled through perched groundwater.

The best locations are determined by completing a combination of a PlumeFinder assessment of RDX migration from the potential areas of impact to the Ogallala Aquifer and evaluations of well location using results from the CMS/FS modeling.

The outcomes of this task include determining the effectiveness of the current Ogallala Aquifer monitoring well network in the southeastern and eastern Plant areas and recommending placement of three additional monitoring wells. To accomplish these objectives, existing information and modeling results are reviewed to assess where RDX may potentially be migrating to the Ogallala Aquifer. The information required to predict a plume includes:

- Groundwater flow directions and rates, measured and simulated
- Source strength and timing, simulated
- Regulatory / risk-based criteria for plume detection
- Reactions (such as biological) that act to reduce the plume size, measured and simulated

The source locations under consideration are estimated to be in the locations where the FGZ becomes more permeable and groundwater transitions from predominantly horizontal to vertical flow. In this region, vertical flow occurs from the perched groundwater through the FGZ to the underlying unsaturated Ogallala Formation and Ogallala Aquifer. Although source strength and location are not well-defined via direct measurement, knowledge exists from previous site investigations and modeling efforts. The hydrogeologic conditions in the Ogallala Aquifer are also uncertain, specifically the hydraulic conductivity beneath the perched groundwater and the pumping rates from nearby irrigation wells. To address the uncertainty, geostatistical representations of the aquifer hydraulic conductivity are coupled with flow and transport simulations, and the simulation results are used to assess the areas of greatest uncertainty in potential RDX plume fringe location. These areas then became candidates for new well locations that reduce the uncertainty of the groundwater plume fringe location by the maximum amount possible.

## 1.3 DOCUMENT OUTLINE

Section 1 provides an introduction to the effort and work to be accomplished. Section 2 provides an overview of the methodology and modeling approach employed, including a summary of concepts and tools used in this analysis. Section 3 provides detailed information about the model developed and results of the simulations and associated optimization. Section 4 presents the report summary and conclusions. Finally, Section 5 provides a list of references used in this study.

# 2.0 METHODOLOGY

## 2.1 APPROACH

The overall approach to determine the best locations for new wells to enhance the detection monitoring network includes:

1. Develop an understanding of flow and transport conditions in the Ogallala Aquifer beneath the perched groundwater from physical consistency with observed conditions elsewhere.

2. Use the Plume Finder Technology to optimize the early warning detection well network.

The first step was largely completed through recent work at Pantex Plant in support of other Environmental Restoration Program objectives. An extensive hydrogeologic investigation has been completed, and the data collected was used to develop a conceptual model for the site. The results of flow and transport models developed from this framework enhance the understanding of the hydrogeology and provide physically-based estimates of aquifer conditions and properties beneath the perched groundwater. The second step uses the best optimization tools currently available to directly incorporate the results of previous work into the design of the well network. These optimization tools are further described in this chapter.

## 2.2 OPTIMIZATION

Optimization tools are used to guide decisions that are defensible by integrating physics-based simulation models, models based on measured data and observations, and direct incorporation of uncertainty through geostatistics. Simulation models provide a mathematical statement of current and expected future conditions in the subsurface based on the physics of groundwater flow and contaminant transport, but these models are limited by the amount of data available to calibrate the models. By combining the physics and data models, optimization tools provide optimal estimates based on knowledge gained from both the physical simulator and the data. The information content from the different models and associated uncertainty with each is fused through the use of signal processing or formal optimization algorithms. For this project, the uncertainty in predicted plume fringe location is quantified, and the optimum monitoring well locations provide the maximum reduction in this uncertainty.

Optimization tools are extremely useful when limited data are available. For example, this occurs beneath the perched groundwater where investigations have been limited because of the potential for cross contamination to the Ogallala Aquifer as a result of drilling through the FGZ. In this case, optimization tools quantify the uncertainty of a monitoring well network and help determine if our understanding of the subsurface is supported by available data.

## 2.3 PLUMEFINDER

The PlumeFinder is an optimization tool that identifies the optimal locations (i.e., those locations that reduce the uncertainty in contaminant plume location the most) for new monitoring wells. PlumeFinder works by identifying (before sampling) the next sampling location in 2-D (two-dimensional) or 3-D (three-dimensional) space that, when sampled, minimizes the uncertainty of the plume boundary location after the sample has been taken. Sampling activity is prioritized because a new sampling location is proposed only if it provides the maximum amount of information when solving the plume location challenge. Output from the PlumeFinder evaluation consists of a rank-ordered list of sample locations for new monitoring wells that minimize the uncertainty in delineating the plume boundary. The PlumeFinder optimization software is based on well-accepted mathematical and statistical concepts and was developed under the direction of Dr. George Pinder at the Research Center for Groundwater Remediation Design at the University of Vermont, USA (McGrath and Pinder, 1996). It has been extended by Larry Deschaine as part of his PhD work at the Chalmers University of Technology, Sweden.

The PlumeFinder works by modeling the information content provided by new sampling locations and quantifies the "maximum measure of uncertainty" in the plume boundary. The procedure is as follows:

1. Build a preliminary flow and transport model for the site. This initial model need not be perfect and does not need rigorous site knowledge to be effective.
2. Generate PlumeFinder statistics.
    a. Geostatistics are used to generate 500 aquifer realizations from observed variations of hydraulic conductivity in the aquifer.
    b. Each aquifer realization is simulated (for a period of 50 years in the current analysis) with the model to create a modeled plume in the aquifer.
    c. Kalman filtering is used to combine the modeled plume realizations with observed data and estimate the uncertainty in plume delineation.
    d. A rank-ordered list of monitoring well locations is created based on their maximum measures of uncertainty.
3. Collect data and add to observation database.
    a. For existing monitoring wells, measured concentration and, if available, hydraulic conductivity, data are included. If measured concentrations are non-detect, a value of one-half the detection limit is assumed.
    b. For future monitoring wells, concentration data is assumed using a value of one-half the plume fringe threshold.
4. Impose the additional constraints; in this case a constraint is imposed that the well not be placed within the extent of perched groundwater.
5. Quantify the confidence in the knowledge of the plume location from the existing Ogallala Aquifer monitoring wells and proposed new monitoring well.

For the transport modeling used in the PlumeFinder analysis presented here a unit source was used, the plume fringe was defined as 1/1000 of the unit source, and RDX concentrations at proposed new monitoring well locations were set at ½ of the plume fringe value (1 part per billion [ppb]). Modeling of the recommended alternative in the CMS/FS (BWXT Pantex/SAIC, 2007) indicated a maximum predicted RDX concentration of 4 ug/l in the Ogallala Aquifer. With the RDX contaminant plume fringe defined as the 0.774 ug/l isocontour, the maximum ratio of plume fringe concentration to potential source in the Ogallala Aquifer is approximately 1/5. No measurements of RDX in the Ogallala Aquifer have been made in the predicted area of breakthrough. Perched groundwater concentrations above this area are on the order of 1 to 4 parts per million (ppm). Therefore, a source to strength ratio of 1000:1 was applied and no retardation or biodecay was applied during the 50-year transport simulation. While conservative, this methodology identified the most likely area of plume migration and the uncertainty with this migration beyond the extent of perched groundwater. The region of uncertainty in a focused area beyond the perched groundwater became the location for the first monitoring well.

## 2.4 MODELING

Numerous challenges exist in developing a modeling approach for this problem. Historical data describing the timing and volume of wastewater releases to the ditches are limited, so the transport of compounds through the upper unsaturated zone to perched groundwater is not well understood. Limited direct observation data are available to determine the timing and mass flux of releases from perched groundwater to the Ogallala Aquifer, including specific flow and transport mechanisms and rates, hydraulic conductivity, and natural attenuation processes in the Ogallala Aquifer. In addition, current and historical withdrawals from the irrigation and water supply wells local to the site are not known with great certainty because the flows are not typically measured at the wellhead nor are detailed operational records kept. These uncertainties are well documented in the Pantex CMS/FS Modeling Report (BWXT/SAIC 2007). In spite of these uncertainties, a method for determining for the best locations for monitoring the potential breakthrough of RDX plumes is needed. The PlumeFinder optimization tool is helpful in developing superior investigation strategies for plume delineation when compared to standard Monte Carlo simulation techniques which merely provide upper and lower bounds on confidence. PlumeFinder uses Monte Carlo and Latin Hypercube techniques and assesses the noise in the concentration signal, compares it on a nodal and model-wide basis to the value of the concentrations samples, and uses Kalman filtering to fuse this information and arrive at the optimal estimate of the plume location.

To implement the PlumeFinder optimization tool, information was obtained and assessed from four primary sources:

- The *Groundwater RCRA Facility Investigation Report* (Stoller, 2004)
- Analytical data available for monitoring wells proximate to the area of interest (from the Pantex Integrated Environmental Database)
- The site-wide BIOF&T3D groundwater flow and contaminant transport model (BWXT/SAIC, 2007)
- The Pantex MODFLOW-SURFACT Ogallala Aquifer model (BWXT/SAIC 2007), which was a local refinement of the Northern Ogallala GAM (Dutton, Reedy, and Mace, 2001; Dutton 2004)

The following tools were used to facilitate this approach:

- Argus Open Numerical Environments (ArgusONE) Modeling Environment – model independent graphical user interface
- Princeton Transport Code (PTC) – finite element flow and transport code
- GSLIB – Geostatistical Software Library
- PlumeFinder – tool that integrates all of the above through optimization algorithms

The PlumeFinder technology currently requires the Princeton Transport Code (PTC) for numerical flow and transport because PlumeFinder includes links to PTC within the ArgusONE modeling environment. Therefore, a 2-D model of the Ogallala Aquifer was first developed using PTC. The PTC Ogallala Aquifer model was developed by integrating historical information, previous modeling efforts, geostatistical codes (GSLIB), and current field data. Previous models developed for this area include the Pantex CMS/FS BIOF&T3D model (BWXT/SAIC 2007) and the Pantex Ogallala Aquifer model (BWXT/SAIC 2007).

The domain of interest includes areas south and east of Pantex (along the fringe of perched groundwater saturation) where (1) investigation data indicate the FGZ becomes more permeable, and therefore introduce likely points of breakthrough to the underlying Ogallala Aquifer and (2) previous modeling results predicted low level impacts to the Ogallala Aquifer.

A transport simulation time of 50 years was selected for the evaluation to support development of the early detection monitoring network.

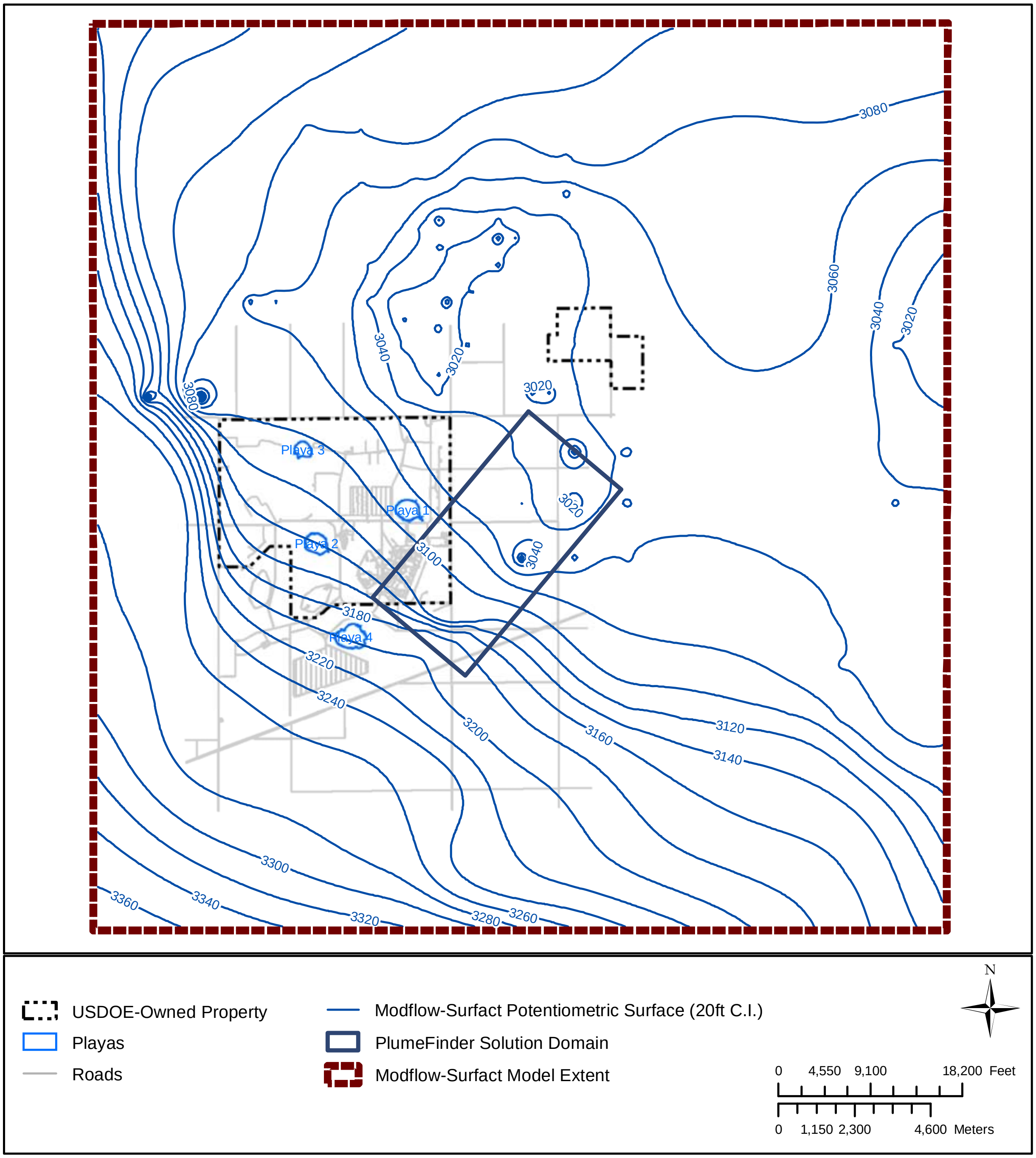



**Figure 2-1. MODFLOW-SURFACT and PTC/PlumeFinder Model Domains**

PlumeFinder differs from standard groundwater flow and transport modeling because in addition to flow and transport, the "information content" is modeled and the worth of new monitoring well data is computed (McGrath & Pinder, 1996). This contrasts the typical approach which simply computes the expected residual mass of RDX. The following example illustrates the PlumeFinder concept.

Given all the unknowns in the above problem statement, if one were to give this problem to 500 different analysts, one could reasonably expect 500 different answers if conventional modeling techniques were used. Each analyst would be free to choose their own interpretation of required information such as historical pumping rates and locations, hydraulic conductivity, and transport process and attenuation parameters. There would be a finite probability that any of the 500 analysts could be correct, but there would be no way to tell which analyst provided the best results using conventional modeling techniques. This is both disconcerting and untenable for decision makers.

Using the PlumeFinder technology, hundreds of different aquifers can be simulated – each with the same probability of being correct. The results from all these simulations are combined, and the areas that have the most uncertainty in the plume concentration are chosen as the best areas to investigate. This approach provides a scientifically-based decision that considers the unknowns.

## 2.5 MODEL CODE AND GRAPHICAL USER INTERFACE

The PlumeFinder technology includes links to the PTC (Pinder, George, F. 1997) numerical flow and transport code. PTC is a 3-D, finite element, saturated flow and single component transport model. PTC has been used for over 20 years, and has been used at major Superfund sites. The PTC model can be accessed through the ArgusONE graphical user interface (GUI) that allows for visualization of models through plug-in extensions. These tools are the interface for the PlumeFinder technology.

PTC is a very robust, accurate, and fast numerical flow and transport solver. This robustness and solution speed is critically important when conducting PlumeFinder integrated modeling and statistical investigations, because 1,500 separate aquifer realizations and subsequent flow and transport simulations are needed to solve the particular optimization challenge presented here. Future modeling needs are also considered satisfied by PTC and the ArgusONE GUI because the possibility of plume migration management exists.

The GSLIB (Deutsch and Journel, 1992) was selected for generating aquifer realizations based on observed variations in hydraulic conductivity data. GSLIB is the industry-standard for geostatistical analysis and the source code is publicly available.

# 3.0 ANALYSIS AND RESULTS

## 3.1 MODEL DEVELOPMENT

A summary of the hydrogeology and current studies of the Ogallala Aquifer are included in the sections below.

### 3.1.1 Hydrogeology

Pantex is situated on the High Plains of the Texas Panhandle. One of the major aquifer systems, the Ogallala Aquifer has more water being pumped from it than any other aquifer in Texas. The Ogallala Formation in which the Aquifer is seated consists of alluvial sands, silt, clay, gravel, and several caliche horizons. An unconfined aquifer in the sands and gravels of the lower Ogallala is the principal source of groundwater in the High Plains region, and is a primary source of potable water for Pantex and the City of Amarillo. In the vicinity of Pantex, this aquifer lies approximately 107 to 130 meters (350 to 425 feet) below ground surface (bgs). The base of the Ogallala is an irregular surface that represents the pre-Ogallala topography, which was influenced by the dissolution of underlying Permian salts and erosion. Consequently, the depth to the base of the Ogallala Formation varies across the Plant from approximately 122 meters (400 feet) below the southwest corner of the Plant to nearly 244m (800 feet) below the northeast corner of the facility. The thickness of the Ogallala Formation in the vicinity of Pantex ranges from approximately 99 to 220 meters (325 to 725 feet), increasing from southwest to northeast. Figure 3-1 shows the water table of the Ogallala Aquifer near Pantex as measured in December 2007.

Regionally, the Ogallala Aquifer water table slopes from northwest to southeast, generally following the regional topographic surface. In the vicinity of Pantex, however, the water table slopes from southwest to northeast, as shown in Figure 3-1, in response to extensive pumping from the City of Amarillo Carson County well field north of Pantex. Figure 3-1 also indicates an area of no saturation in the aquifer on the eastern side of the Texas Tech University (TTU) property. As water levels in the aquifer continue to decline, this area of no saturation will expand.

Groundwater in the Ogallala Aquifer is recharged from downward percolation of water, either from the surface of the High Plains or from the overlying perched groundwater zones. The distribution of recharge is poorly known, with estimates ranging from less than 0.01 inches per year to several feet per year. Higher recharge rates occur where the Ogallala Formation occurs at the surface and where surface water runoff is focused, such as beneath drainage ditches and playas. Lower rates occur for uplands (areas between the ditches and playas). A good summary of the recharge rates is presented in the Subsurface Modeling Report (BWXT/SAIC 2004 and 2007). For this effort, recharge rates were specified based on the MODFLOW-SURFACT model of the Ogallala Aquifer presented in the CMS/FS (BWXT/SAIC 2007).

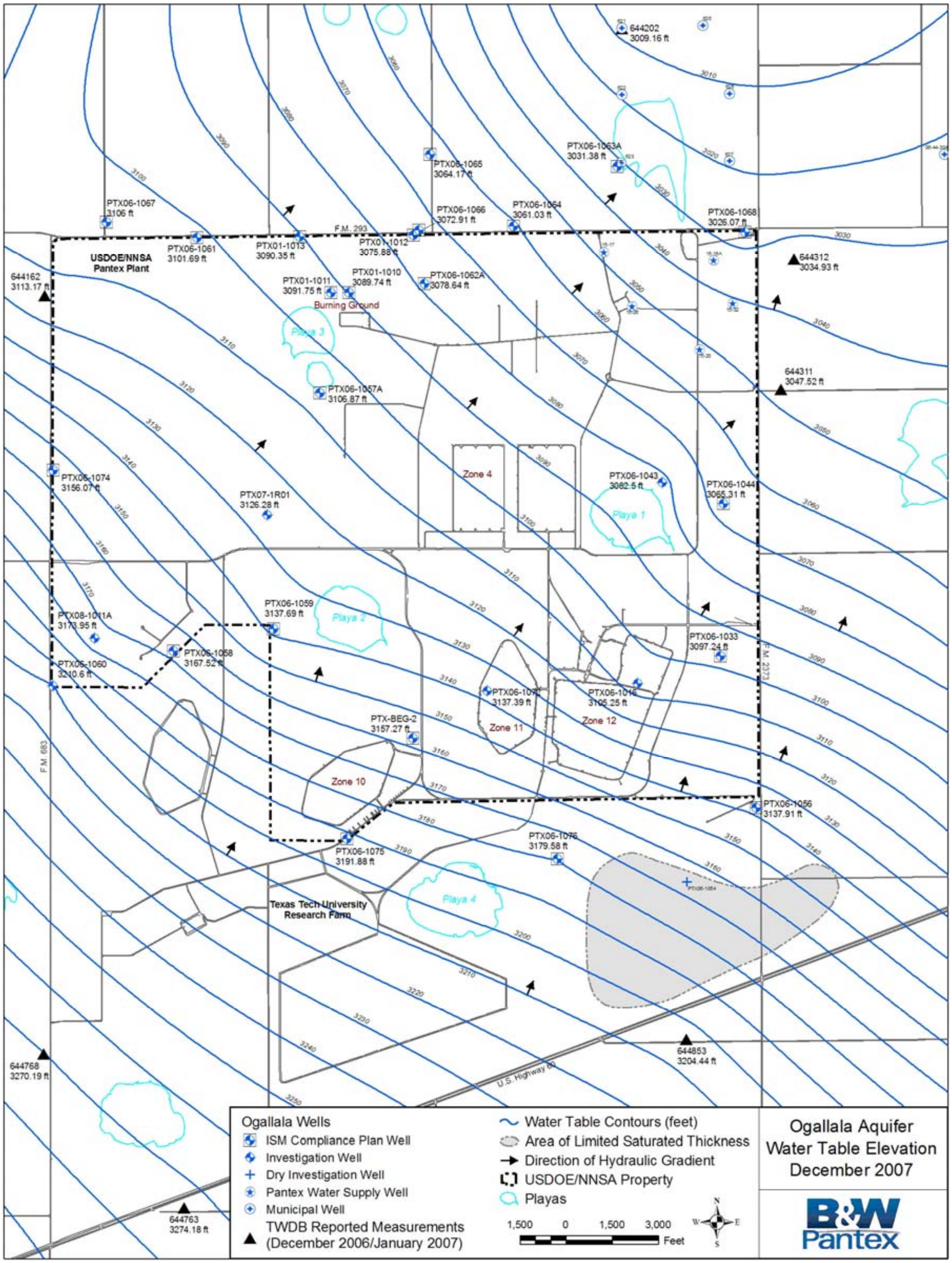



**Figure 3-1. Ogallala Aquifer Water Table, December 2007**

Few site-specific measurements of hydraulic conductivity have been completed in the Ogallala Aquifer at Pantex. As a result, information from regional studies has been used to supplement the site-specific hydraulic conductivity data. Of particular interest in the Bureau of Economic Geology study (Dutton, Reedy, and Mace, 2001) were the tests compiled from Mullican (1997) and from the groundwater database maintained by the Texas Water Development Board (TWDB). Mullican (1997) obtained information on 70 aquifer tests which included high-quality specific-capacity tests. Mullican (1997) were also able to cull data from an additional 1,271 specific-capacity tests in the TWDB groundwater database. To estimate transmissivity and hydraulic conductivity from specific capacity, they used an analytical technique developed by Theis (1963). Hydraulic conductivity was determined by dividing transmissivity by the saturated thickness exposed to the well bore.

Based on results from the data compilation and specific-capacity analysis, the hydraulic conductivity for the Ogallala Aquifer was found to be log-normally distributed (Figure 3-2) with a geometric mean of approximately 14.8 feet per day (ft/d) and a standard deviation that spans from 5 to 44 ft/d. The upper range of the standard deviation (i.e., 44 ft/d) is three times the geometric mean of approximately 14.8 ft/d, indicating variability in hydraulic conductivity. Because of this variability, uncertainty in hydraulic conductivity was evaluated using geostatistical methods to develop 500 equally plausible representations of the Ogallala Aquifer within the Ogallala Aquifer flow model.

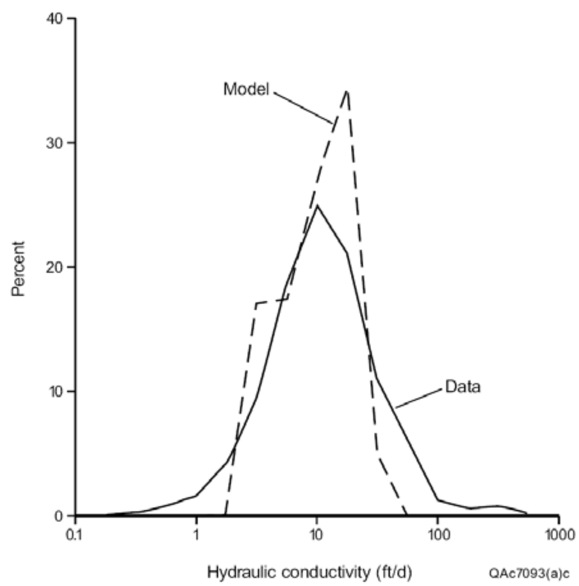



**Figure 3-2. Bureau of Economic Geology Finding of Lognormal Distribution for Hydraulic Conductivity in the Ogallala Aquifer (after Dutton et al, 2000).**

The greatest source of uncertainty in assessing transport is the uncertainty in hydraulic conductivity (Smith and Schwartz, 1981). To illustrate that hydraulic conductivity is the most sensitive parameter for determining plume location, the sensitivity of average groundwater velocity to gradient, porosity, and hydraulic conductivity is evaluated (within the range of values expected at the Plant). Considering Darcy's Law (v=ki/n; where v = velocity, k = hydraulic conductivity, i = hydraulic gradient, and n = porosity), sensitivity to changes in the gradient or porosity changes within the range of measured values at the Plant are relatively small compared to sensitivity to the anticipated range in hydraulic conductivity.

For example, the gradient ranges from 0.003 feet horizontally/feet vertically (ft/ft) beyond the northeast corner of the Plant to 0.012 ft/ft in the vicinity of Zone 12 in the 2007 water table shown in Figure 3-1. The porosity, n, has been measured in a number of samples collected at the Plant and ranges from approximately 29% to 42% based on samples collected from above the water table (SAIC, 2000). Specific yield values can be used to estimate porosity (although they typically underestimate porosity slightly). Specific yield values from 41 test holes scattered throughout the region averaged about 16% (SAIC, 2000). Porosity values published in the literature range from 25% to 35% for the sandy-gravelly sediments (Fetter, 1988) that comprise the Ogallala Aquifer.

Using a constant hydraulic conductivity of 5 ft/d for illustrative purposes, the increase in velocity for the gradient change is by a factor of 4.0 and the decrease in velocity for the porosity change is by a factor of .381. Velocities shown below are in ft/d:

*Gradient Change (using the lower end of the porosity range)*

$v = 5(.003)/.16$ $\qquad$ $v = 5(.0012)/.16$

$v = .094$ $\qquad$ $v = .375$

*Porosity Change (using the mid-point of the gradient range)*

$v = 5(.0075)/.16$ $\qquad$ $v = 5(.0075)/.42$

$v = .234$ $\qquad$ $v = .089$

The change in velocity from varying hydraulic conductivity by the upper and lower end of the standard deviation range, we see an increase in velocity by a factor of 8.8.

*Hydraulic Conductivity Change (using the lower end of the porosity range and the mid-point of the gradient range)*

$v = 5(.0075)/.16$ $\qquad$ $v = 44(.0075)/.16$

$v = .150$ $\qquad$ $v = 1.320$

This example illustrates that the greatest variation is from the hydraulic conductivity field and hence, why it is chosen as the parameter to capture using geostatistics in the PlumeFinder analysis. This example also corresponds with the results by Smith and Schwartz, (1981) that the greatest source of uncertainty is hydraulic conductivity. The remaining transport parameters are as follows:

- Retardation factor: none specified. Retardation refers to the relative velocity of the center of the transport plume to the advective groundwater flow. Neglecting retardation permits the advective portion of the simulated RDX plume to migrate with the same velocity as the groundwater.
- Dispersivity: Dx=50 ft, Dy=5 ft and Dz = 5 ft. Dispersivity refers to the process of the plume spreading in all directions from its centerline. The dispersivity parameters are taken directly from the model reported in the Corrective Measures Study/Feasibility Study (CMS/FS). Smaller values will produce a narrower, focused plume and larger values will produce wider, more disperse plumes with lower peaks values.
- Molecular diffusion: none specified. The process of molecular diffusion (Brownian motion) describes how a concentration of a chemical such as RDX would diffuse from areas of higher concentrations to areas of lower concentrations. This is a slow process, and the dispersion due to the movement outweighs this effect for the Ogallala Aquifer flow system. A non-zero value would results in a practically negligible addition to the dispersive plume front.

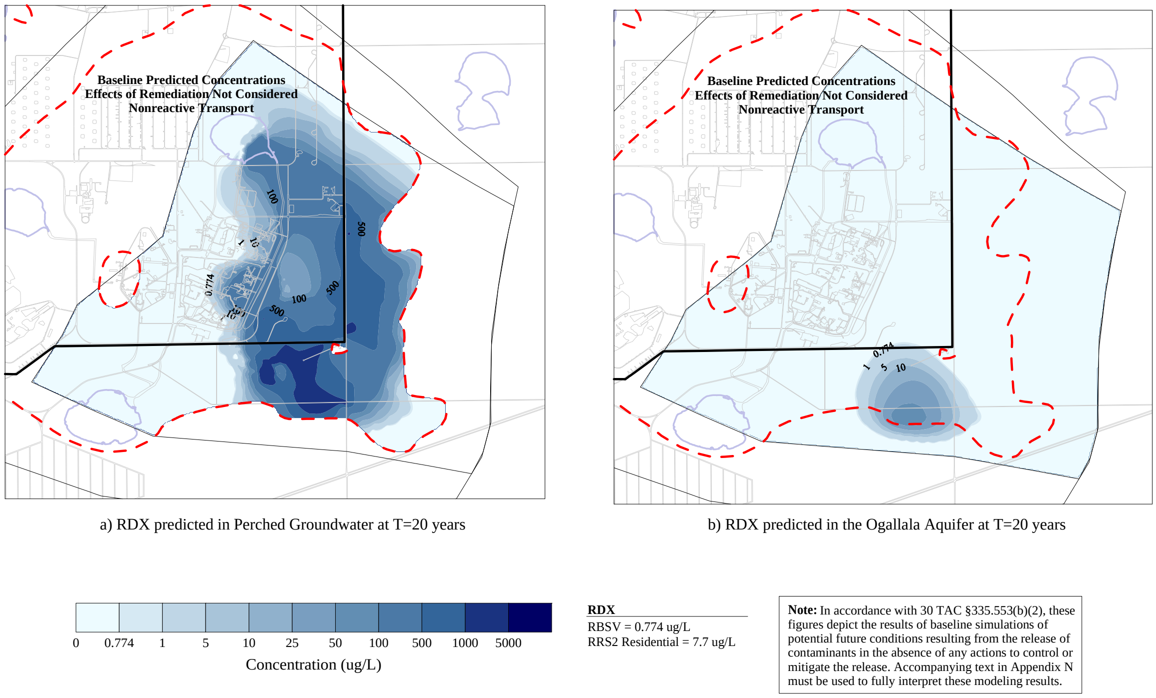
- Biological decay: none specified. The biological decay processes destroy contaminants such as RDX. Neglecting biodegradation allows the simulated RDX to migrate the furthest.
- Porosity: 0.25%. Porosity is the open area of the soils where the water flows. All other parameters being equal and given a fixed flux, higher values of porosity produce slower plume migration and lower values result in faster plume migrations.
- Source strength: constant unit source. In the southeastern portion of the Plant where RDX is projected to migrate from the perched groundwater to the Ogallala Aquifer at detectable concentrations based on CMS/FS modeling a continuous constant unit source is specified. Since the flux through the source area is realization-specific, each simulated aquifer will generate a unique source flux. A second hypothetical source along the eastern fringe of the perched extent is not directly simulated in the PlumeFinder analysis but is evaluated separately.
- Base hydraulic conductivity: specified from the CMS/FS MODFLOW-SURFACT Ogallala Aquifer model (BWXT/SAIC 2007b). This is the base conductivity field used for the geostatistical realizations. It is used directly only in the deterministic case, and varied geostatistically to generate 500 stochastic realizations of the Ogallala Aquifer. The base hydraulic conductivity is not used directly the PlumeFinder fringe calculations.

Finally, variograms from several studies (Clark, 1979; McCuen and Snyder, 1986) show that hydraulic conductivity in the Ogallala Aquifer is spatially correlated. Spatial correlation infers that points that are closer together are more similar to each other than points that are further apart. Fitting a spherical theoretical variogram (Dutton, Reedy, and Mace, 2001) to the experimental variogram resulted in a nugget of 0.12 $[\log(ft/d)]^2$, a sill of 0.22 $[\log(ft/d)]^2$, and a range of 140,000 feet. The range suggests that hydraulic conductivity is spatially correlated within 140,000 feet (26 miles) in the Ogallala Aquifer. The distance correlation is the range (length) beyond which a conductivity measurement no longer has value in predicting local conductivities.

### 3.1.2 <u>Water Quality</u>

Past operational and waste handling procedures have resulted in contamination of the perched groundwater beneath the Plant. Groundwater quality in the Ogallala Aquifer is characterized by groundwater samples collected from monitoring wells installed in the aquifer. Although non-trending sporadic detections of constituents occur in the Ogallala Aquifer at low, non-actionable concentrations below regulatory screening levels, no constituents of concern have been identified in the Ogallala Aquifer based on the current monitoring network.

Modeling conducted as part of the Baseline Human Health Risk Assessment and CMS/FS indicates the potential for contaminants in perched groundwater, particularly RDX, to impact the Ogallala Aquifer in the future (BWXT/SAIC 2006 and BWXT/SAIC 2007). Figure 3-3, taken from the Baseline Human Health Risk Assessment Report, shows modeled concentrations of RDX in the perched groundwater and Ogallala Aquifer after 20 years of transport in the absence of corrective actions. The figure on the left shows that the highest concentrations of RDX in perched groundwater occur south of Pantex Plant beneath TTU property with high concentrations of RDX also found along the eastern boundary of Pantex. The figure on the right shows modeled impacts to the Ogallala Aquifer occur near the southern extent of perched groundwater, beneath the area containing the highest RDX concentrations in perched groundwater. This area was identified as the source area for the PlumeFinder modeling.




a) RDX predicted in Perched Groundwater at T=20 years

b) RDX predicted in the Ogallala Aquifer at T=20 years

**Figure 3-3. Modeled RDX Concentrations in the Perched Groundwater and Ogallala Aquifer**

A second potential source area along the eastern extent of perched groundwater is also considered, although it is not directly included as a source in the PlumeFinder analysis. No impacts exceeding risk based levels to the Ogallala Aquifer were predicted in this area, but the area is considered a potential source because of the high RDX concentrations in perched groundwater coupled with a slightly more permeable FGZ along the fringe of perched groundwater.

RDX is projected to migrate from the perched groundwater to the Ogallala Aquifer. Before entering the Ogallala Aquifer, the RDX must vertically traverse the unsaturated zone between the FGZ and the Ogallala Aquifer water table. In the southeast area this distance is much less than along the eastern extent of saturation. The FGZ is also simulated as slightly less permeable along the eastern extent in the CMS/FS models compared to the southern fringe of perched groundwater. Increased travel time simulated through a thicker unsaturated zone and slightly lower FGZ permeability mitigates predicted impacts to the Ogallala Aquifer hence less impact to the Ogallala Aquifer is expected along the eastern fringe of perched groundwater. However, given the lack of direct data in the Ogallala Aquifer in this area it is prudent to locate monitoring wells capable of detecting RDX migration here.

### 3.1.3 <u>Previous Models</u>

Few regional aquifers have been as extensively studied as the Ogallala Aquifer. Models of groundwater flow have been important tools for managing the groundwater resource and evaluating future changes in water level and saturated thickness. At least 15 numerical groundwater flow models have been developed for different parts of the aquifer. Most recently, studies were completed by the Bureau of Economic Geology at the University of Texas on withdrawal projections in the Ogallala Aquifer in the Panhandle Water Planning Area (Dutton, Reedy, and Mace, 2001; Dutton 2004). The studies predicted that by 2050, major areas of the aquifer will have less than 50 feet of remaining saturated thickness and parts of the aquifer in various counties in the Panhandle Water Planning Area may be dry.

Two recent site-specific models have been developed which include the Ogallala Aquifer in the area-of-interest for this study. The motivation for developing these models was to support decision-making that protects the Ogallala and Amarillo well field. Specifically, these are the Pantex CMS/FS BIOF&T3D model and the Pantex MODFLOW-SURFACT Ogallala Aquifer model (BWXT/SAIC 2007).

Ideally, the CMS/FS BIOF&T3D model (BWXT/SAIC 2007) would be integrated with PlumeFinder technology to optimize the proposed well locations. However, execution of one simulation with this model requires approximately 7 to 20 days using computers available in 2007. As part of this study, over 1,500 final simulations were completed during the PlumeFinder analysis. This includes computing flow and transport over a 50-year period, using different – though equally plausible – aquifer conductivity realizations. Years of computational time would be required using the fully 3-D, variable saturated, coupled transient flow and transport model with all the site complexity.

Use of the CMS/FS BIOF&T3D model in a PlumeFinder analysis presented a significant computational hurdle. Therefore, the MODFLOW-SURFACT Ogallala Aquifer model was used to set up a PTC flow and transport model, and then this PTC flow and transport model was applied to the PlumeFinder analysis.

#### 3.1.4 PlumeFinder / Princeton Transport Code (PTC) Model

The first step in the PlumeFinder analysis was to develop the PTC Ogallala Aquifer groundwater flow and transport model from the MODFLOW-SURFACT Ogallala Aquifer model (BWXT/SAIC 2007). The MODFLOW-SURFACT model contains the most recent updates of aquifer properties (including bottom elevation of the Ogallala Aquifer, the hydraulic conductivity and water table information) in the area of interest local to the Plant. It acceptably simulates flow under both steady-state conditions (using reduced pumping rates as described in BWXT/SAIC 2007) and transient conditions. The steady state version was selected for conversion to PTC for computational efficiency. The CMS/FS modeling conducted with the BIOF&T3D model included comparisons of RDX transport results using a declining, transient water table and a steady-state water table for the Ogallala Aquifer. The simulations produced nearly identical results, so the use of the steady-state model is not expected to significantly affect the outcome of the PlumeFinder analysis.

The MODFLOW-SURFACT Ogallala Aquifer steady-state model was used as-is in developing the PTC Ogallala Aquifer model, with the two minor refinements to include a finer grid and modify of two wells. In the final steady-state Ogallala Aquifer model, each model grid cell was 844.8 feet (257.5 meters) wide in the east-west direction and 897.6 feet (273.6 meters) wide in the north-south direction. In the transient Ogallala Aquifer model that was used for predicting future flow conditions, a finer grid cell size was used: 211.2 feet (64.4 meters) in the east-west direction and 224.4 feet (68.4 meters) in the north-south direction. The latter grid resolution was needed to assist in subsequent contaminant transport calculations in PTC, so the withdrawal rates from the steady-state Ogallala Aquifer model were substituted into the finer transient Ogallala Aquifer model grid to obtain the steady-state head solution in the more finely discretized model. During this process, two wells were modified with respect to those included in the final steady-state model. First, one Pantex production was excluded; this well was active c.1994 (i.e., consistent with the time period represented by the steady-state model) but is not active today. Second, one irrigation well that was inadvertently omitted from the final steady-state model was added. This irrigation well lies north of the Amarillo well field, and has insignificant impact on this or previous analyses.

To focus the PlumeFinder calculations, simulations were conducted with the steady-state Ogallala Aquifer model to guide the selection of the PTC model extent. Two unit sources were included. One was an areal source placed in the potential areas of RDX breakthrough to the Ogallala Aquifer predicted by the BIOF&T3D model (BWXT/SAIC 2007) and another was a distributed line source along the eastern fringe of perched groundwater. Transport parameters for RDX were specified consistent with those used in the BIOF&T3D model, with the following notable exceptions:

- Biodegradation is assumed not to occur.
- Retardation is assumed not to occur.
- The source strength in the Ogallala Aquifer is assumed 1000 times greater than the plume fringe (1 ppb) for RDX.

The assumptions are more conservative (result in larger predicted plume extent) than those included (biodegradation & retardation) or simulated (peak concentrations of RDX in the Ogallala Aquifer) from the CMS. For instance, a biodecay rate of 25 years and a retardation factor of approximately 1.7 were assumed in the CMS. This conservatism ensures the PTC model extent is sufficiently large to encompass all realizations produced for the PlumeFinder evaluation. Transport was simulated until the plume produced by both simulated source areas reached steady-state. The source areas and the resulting steady-state plume are depicted in Figure 3-4.

Withdrawals from the Amarillo production wells (generally north and northeast of Pantex) and the local area irrigation wells create cones of depression in the Ogallala Aquifer water table (Figure 3-4) that provide an outer bound for contaminant migration. Consequently, the PTC model domain was specified to extend just beyond this depression, as shown in Figure 3-4. The PTC model domain is substantially smaller than the MODFLOW-SURFACT model domain. This smaller model domain permits the 500 PTC models (i.e. the individual realizations generated after geostatistically varying the hydraulic conductivity) to be executed in about 5 minutes, or less than 1 second per run. The PTC model and the PlumeFinder solution domain cover approximately 9 square miles (12,000 feet by 24,000 feet) including the southeastern portion of the Plant area and the likely points of breakthrough to the south and east.

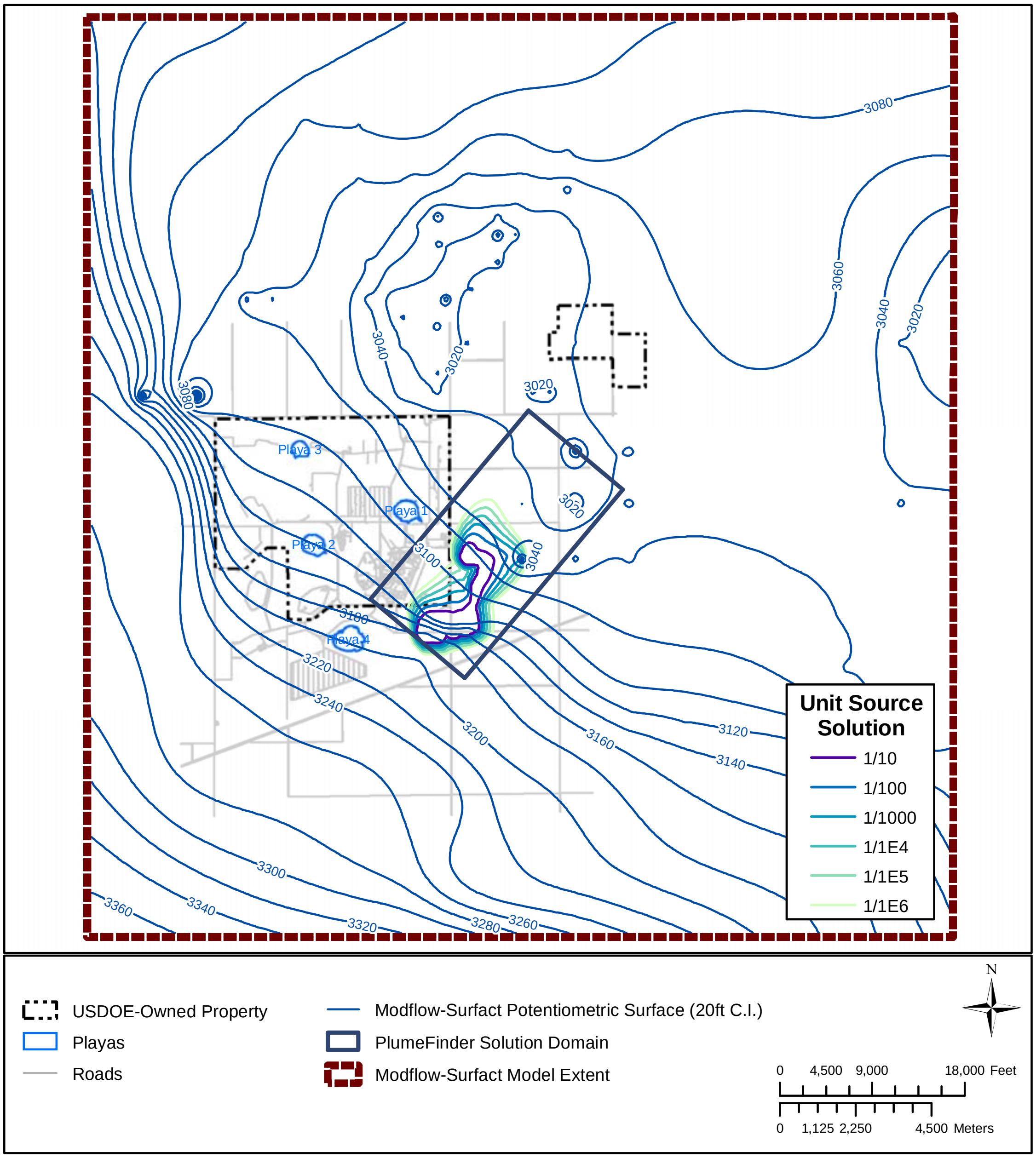



**Figure 3-4. Model Domains and Steady-State Plume**

Simulations were also conducted with the MODFLOW-SURFACT model to assess the sensitivity of contaminant transport to the pumping rate of irrigation wells immediately east of Pantex Plant, nearest the areas of potential breakthrough. Future pumping rates at the wells are unknown; therefore, the wells impart uncertainty on the transport directions in the area of interest. Transport and particle tracking were conducted to assess the sensitivity of results to the pumping rate of the well closest to the potential breakthrough areas. Three sensitivity simulations were conducted with pumping rate reductions of 50%, 75%, and 87.5% for this well. Predicted steady-state heads, steady-state transport results, and particle tracking results for the rate used in the steady-state model are presented in Figure 3-5a. Similar items are presented in Figure 3-5b for a 75% reduction in pumping rate for this well.

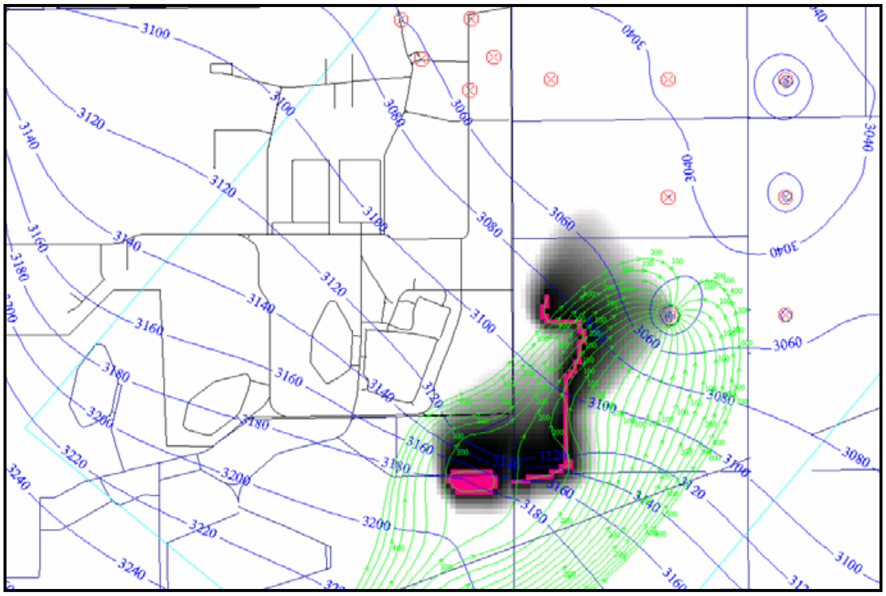



**Figure 3-5a. Unchanged Flow Rate at Pumping Well**

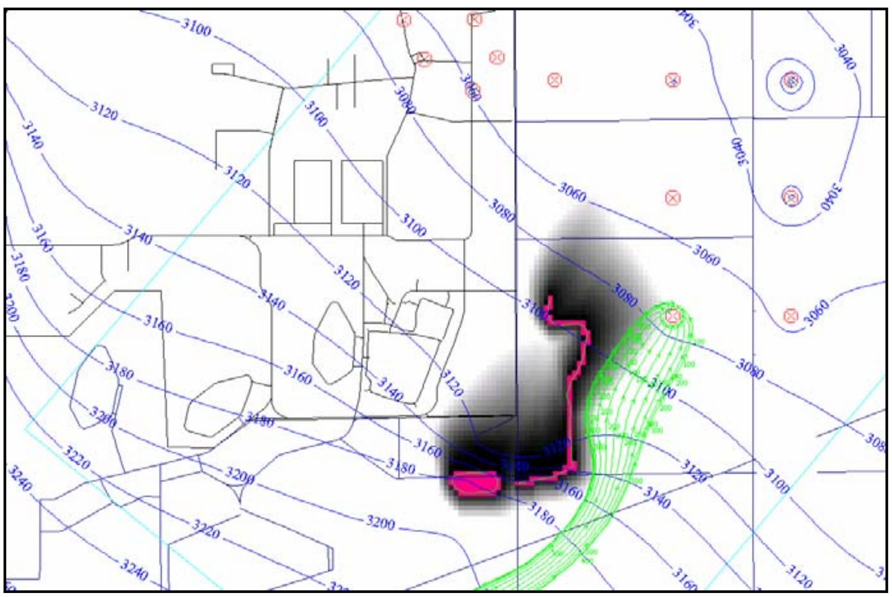



**Figure 3-5b. Reduced Flow Rate at Pumping Well**

**Figure 3-5. Capture Zone and Transport Sensitivity Results**

Comparing the two figures, a diminished capture zone for the well can be seen from the particle tracking comparison. However, impacts on the overall extent of the steady-state plume are not dramatic. Based on this comparison, the decision was made to represent all pumping wells with constant head boundary conditions in the PTC model rather than specify a constant flow rate in each. The constant head boundary condition allows the PTC model to calculate a variable flow rate at each well so that a constant water level is maintained in the cell. Note that much of the RDX release may be captured by a single pumping well. This is plausible but other alternatives cannot be discounted since there is a high degree of uncertainty due to the lack of direct field measurements in this area. Installation of the monitoring wells proposed from this analysis would add direct field measurements for this region and reduce the uncertainty.

After establishing the PTC model domain, aquifer properties including hydraulic conductivity, recharge, aquifer top and bottom elevations, and porosity were transferred directly from the MODFLOW-SURFACT model to the PTC model via the ArgusONE numerical modeling GUI. South of the southeast edge of Pantex, a dry area in the Ogallala Aquifer has been observed at one monitoring well. The area is simulated in the MODFLOW-SURFACT model as a partially saturated area, using the value of recharge as the flow in the cell to avoid the dry cell condition. In some areas, the aquifer thickness was less than one foot. Initial testing of the PTC model revealed that realizations with some classes of hydraulic conductivity fields caused the PTC model to fail due to stability limitations in areas with minimal saturated thickness. In these problematic iterations the water table "fell" below the aquifer bottom, causing the hydraulic conductivity in the numerical matrix to go negative and the solver to crash. To prevent these model convergence issues, a confined aquifer configuration was used in the PTC model, and the simulated aquifer thickness was held constant at its initial conditions. This solved the thin aquifer condition and allowed the saturated flow model to be used without requiring a computationally intensive variably saturated flow model or removing the thinner portions of the model domain out of the model. (Removing areas with minimal aquifer thickness was not preferred because the potential RDX source is in these areas.)

The heads from the drawdown of the pumping wells in the steady-state MODFLOW-SURFACT model were transferred into the PTC model and specified as constant head boundary conditions, with specified head values based on the steady-state flow solution. The PTC model boundaries were specified using constant head boundary conditions, again with head values based on the steady-state flow solution. Steady-state flow was then simulated in the PTC model and compared to the MODFLOW-SURFACT model, as seen in Figure 3-6. The comparison shows only minor differences in simulated heads between the two models in the areas of the well fields and at the boundaries with somewhat greater differences underneath the southeastern breakthrough area. The differences can be attributed directly to the combination of both different grid sizes used to solve the model domain, specifically in the area of the wells, and the simplification to apply the approximation of a constant aquifer thickness. The results for the final set of 500 realizations (hydraulic conductivity, head, and concentration) are provided on the attached compact disc.

Figure 3-7 shows the source used in the PTC model and applied to the associated PlumeFinder modeling. This source is placed in the potential area of RDX breakthrough to the Ogallala Aquifer predicted by the BIOF&T3D model (BWXT/SAIC 2007). A unit source strength of 1 ppm was assumed, and the fate and transport solution was calculated with a duration of 50 years. The Plume fringe was defined as the 1 ppb isocontour, and thus the ratio of source concentration to fringe concentration was 1000:1. Neither biodegradation nor retardation was included as a transport process. As a result, the conservative assumptions increased the predicted RDX migration along the likely pathway of the plume and identified the area where RDX from the southern source (breakthrough area) would first migrate beyond the perched groundwater extent.

This PTC model mesh used in the PlumeFinder is shown in Figure 3-8. The dense node arrangement associated with the source ensures accuracy in this critically important region of the model domain and limits numerical dispersion of the transport solution.

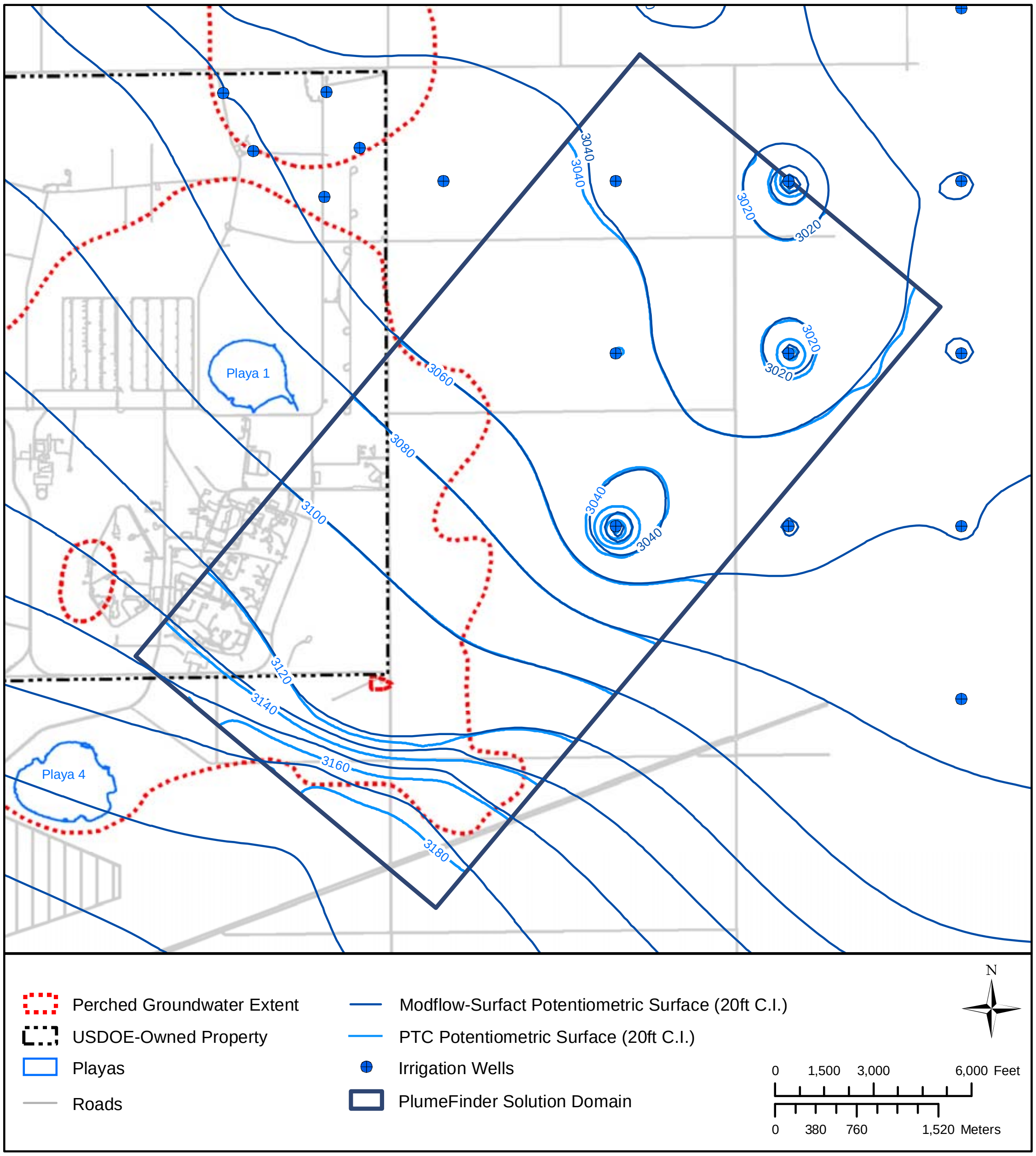



**Figure 3-6. Potentiometric Surfaces Defined in PTC Model and Modflow-Surfact Model**

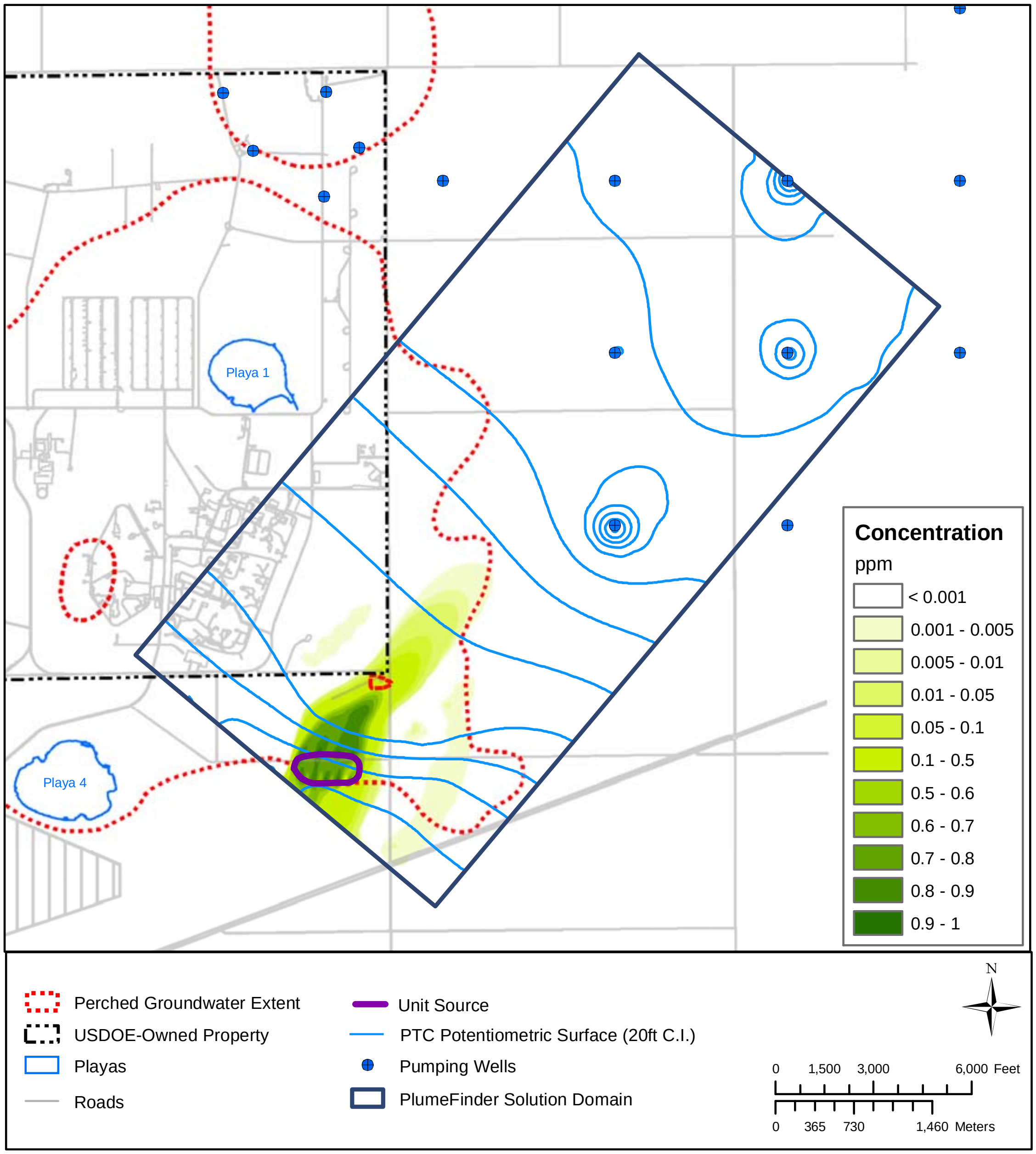



**Figure 3-7. Contaminant Source and 50 year Deterministic Transport Plume in PTC Model**

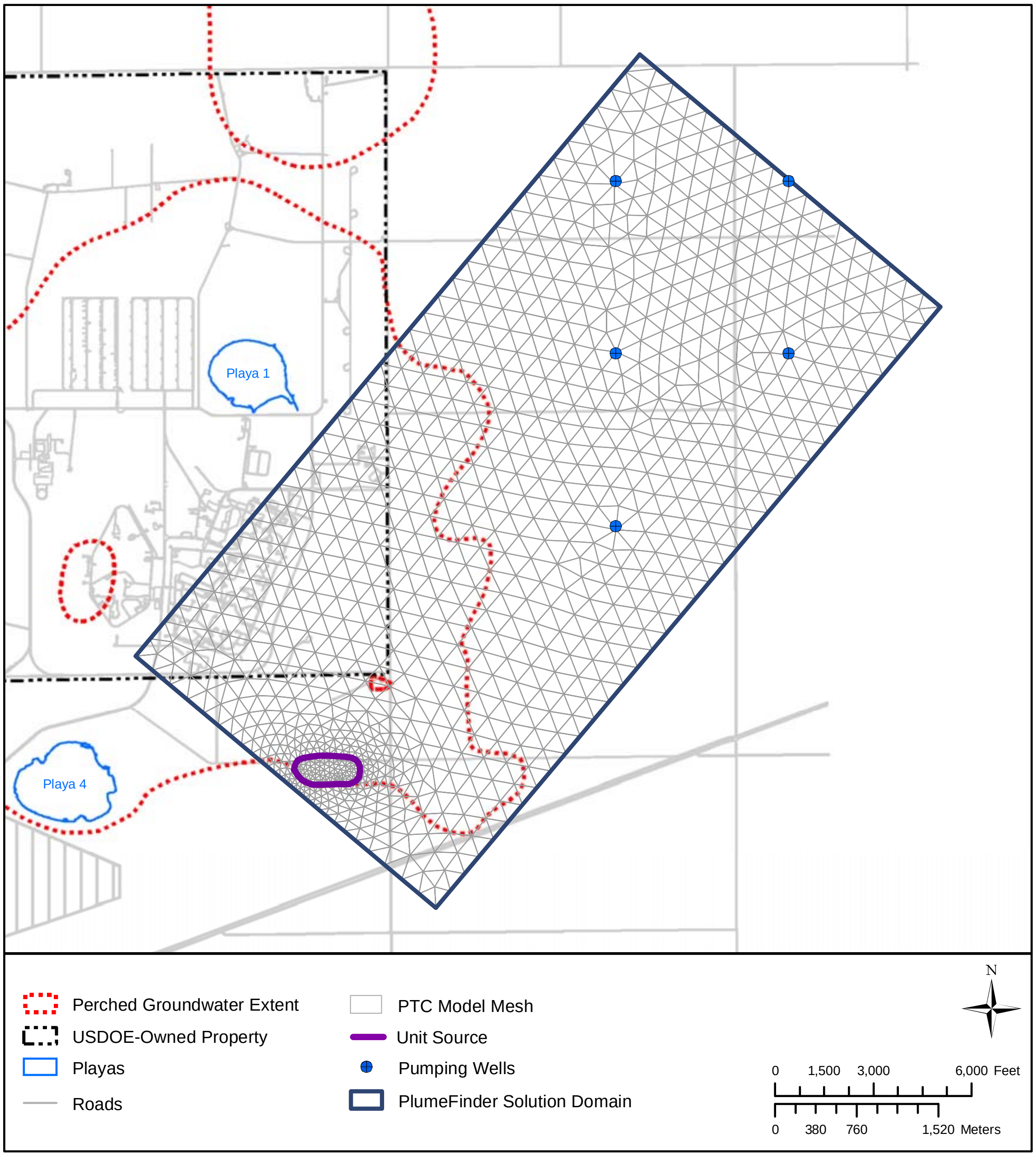



**Figure 3-8. PlumeFinder Computational Mesh in PTC Model**

### 3.1.5 Additional Considerations

Hydraulic conductivity: Hydraulic conductivity is assumed to be locally isotropic; that is, the same in the x and y directions within each element. However, because of uncertainty associated with the hydraulic conductivity and the limited amount of available test data, geostatistics were used to create 500 likely aquifers and the combined results analyzed to provide recommended locations for new monitoring wells. The variogram for the entire Ogallala Aquifer was used as discussed above. The extent the variogram may differ from local conditions is unknown. The variogram provides the best available information from which to base the hydraulic conductivity realizations.

Groundwater flow direction: With the exception of a few monitoring wells, the actual flow patterns beneath the perched groundwater are unknown from direct measurement. The inferred flow directions represent the best estimate from measurements recorded in the Ogallala Aquifer monitoring wells.

Potential Source Locations to the Ogallala Aquifer: The potential source of RDX to the Ogallala Aquifer is inferred. RDX has not been directly measured at any consistent value at any location in the Ogallala Aquifer. RDX is consistently detected in the perched groundwater at values in the mg/l range. The assumed sources used in the PlumeFinder analysis and accompanying qualitative assessment are the best estimates of where RDX could migrate into the Ogallala Aquifer, based upon both site investigation data and previous modeling results.

Fifty-year monitoring design period: Fifty years was chosen as a period from which to evaluate the plume fringe uncertainty. Uncertainty grows over time. Sporadic and unreplicated detections of RDX complicate the analysis, as it is uncertain whether or not a plume fringe exists in these monitoring locations. Only three Ogallala Aquifer monitoring wells within the PTC model extent still contain groundwater from which to make assessments.

Irrigation wells (pumping wells): The stochastic analysis of the plume fringe location also addresses the uncertainty associated with the pumping rates of irrigation and water supply wells. Simulations conducted with the MODFLOW-SURFACT Ogallala Aquifer model indicate that flow in the Ogallala Aquifer (and therefore contaminant transport) directions are sensitive to the pumping rates of wells east of Pantex near the areas of potential breakthrough. Future pumping rates at the wells are unknown, and the wells are not under Pantex control. These wells therefore impart substantial uncertainty on the transport directions in the area of interest. Because well pumping rates are allowed to vary with the different aquifer realizations, this uncertainty is somewhat addressed in the PlumeFinder analysis.

One last consideration is that the analysis presented here does not incorporate degradation or biological decay of RDX in the transport calculations. Degradation rates, usually expressed in terms of a first-order kinetic reaction rate, for RDX are well documented in the literature but have not been measured in the Ogallala Aquifer. Because biological reactions are redox-zone specific, the biochemistry is important in assessing the transport of material in the subsurface and will therefore be important in early detection of a plume fringe. As described in the *CMS/FS Modeling Report* (BWXT/SAIC 2007), the degradation rate of RDX is an irreducible uncertainty that can only be addressed over time as information on the redox zones and degradation rates in the Ogallala Aquifer groundwater.

A principled groundwater flow and transport model helps overcome data limitations through accurate representation of the underlying physics. However, a deterministic solution may not capture the variety of possibilities that exist to effectively manage potential migration of RDX. The PlumeFinder technology incorporates the major elements of the uncertainty, and provides a mechanism to support management decisions following a systematic and proven approach. Below are the results of the analysis.

## 3.2 PLUMEFINDER ANALYSIS AND RESULTS

The objective of this analysis is to identify best locations for up to three new Ogallala Aquifer monitoring wells using the PlumeFinder technology and incorporating predictions from previous modeling efforts. PlumeFinder optimally locates wells to better delineate the boundary of a contaminant plume. As noted earlier, PlumeFinder integrates the PTC model, the model GUI (Argus ONE), and geostatistical software into a computer system for guiding the investigation of contaminated aquifers. As discussed in the previous section, PlumeFinder is based on the idea that the best means of delineating a contaminant plume boundary is to place wells in such a manner as to minimize the uncertainty of the boundary location.

The threshold level that defines the RDX plume boundary is 1/1000$^{th}$ of the assumed unit source strength of 1 mg/l. This assumed unit source and plume fringe threshold are conservative. The recommended alternative in the CMS/FS (BWXT Pantex/SAIC, 2007) indicated a maximum predicted RDX concentration of 4 ug/l in the Ogallala Aquifer and a plume fringe defined by the 0.774 ug/l isocontour. An approximately 1/5 ratio produces an area of plume fringe uncertainty much smaller than if a lesser ratio of 1:1000 is used. Despite conservative assumptions in the PlumeFinder analysis, the likelihood that RDX will migrate from the source area to a point beyond the extent of perched groundwater in the east is low in this 50-year design period.

The GSLIB code was used to geostatistically vary the hydraulic conductivity field and generate multiple realizations of the Ogallala Aquifer. The hydraulic conductivity variogram from the Northern Ogallala GAM (Dutton, et al., 2001) was used as input into the model. Because pumping wells are simulated as constant head boundaries, the flow into them varied depending on the geostatistical representation of the aquifer hydraulic conductivity. The analysis consisted of generating 500 aquifer realizations, executing flow and transport simulations for each, and repeating this for each PlumeFinder investigation scenario. Three scenarios were evaluated: no wells, the existing monitoring well network, and one optimally located monitoring well. This resulted in 500 separate flow and transport simulations for each scenario, totaling 1500 simulations. The mathematics underlying PlumeFinder, specifically the Kalman filtering aspect, are explained in Appendix A. The flow and transport mathematics are provided in the PTC textbook and manuals (Pinder, 1997 & 2002). The applied geostatistics are described in the Geostatistical Software Library and User’s Guide (Deutsch and Journel, 1992).

### 3.2.1 Baseline Uncertainty (No Monitoring Wells)

As a first step, the PlumeFinder investigation was executed without monitoring well information to provide a baseline for evaluating the existing well network. The results of the base case can be seen in Figure 3-9. In this figure, darker colors depict greater uncertainty and lighter colors depict higher confidence. The best location to place a well is in the area of maximum uncertainty outside the perched groundwater extent. The value for uncertainty (shown in the legend of Figure 3-9) is a measure of the uncertainty in the value of the RDX concentration in the groundwater when compared to the plume fringe value. The volume underneath the measure of uncertainty value has been normalized to 100%.

- Uncertainty beneath the Perched Groundwater – Most of the plume migration and uncertainty associated with fringe location occurs beneath the perched groundwater, an area for the most part precluded from investigation in the Ogallala Aquifer for reasons of cross-contamination concerns.

- Uncertainty beyond the Extent of Perched Groundwater – Two areas of plume fringe uncertainty occur beyond the extent of perched groundwater saturation, one to the south of the Plant, and one to the east.

- In the area to the south observations show the Ogallala Aquifer to be dry in at least some locations. Investigations in this area are prudent, and B&W Pantex is already planning on further investigations to characterize the Ogallala in this area.
- The area to the east represents the most likely location where RDX could migrate from beneath the perched groundwater extent. The PlumeFinder technology is used to identify the best monitoring well location in this area to the east of perched groundwater saturation.

### 3.2.2 Uncertainty in Current Monitoring Well Network

Figure 3-10 shows the results when the information for the existing three Ogallala Aquifer wells (within the PTC model domain) is added. An assumed concentration of half the plume fringe value (1 ppb) was specified at the three existing well locations. By inspection, information is most lacking in the southeast near the extent of perching groundwater. This finding is consistent with the known uncertainties in the conceptual site model. This analysis shows that the current monitoring well network in the Ogallala Aquifer only reduced the uncertainty in the plume fringe location by 8%.

The reduction in uncertainty is low for several reasons. First and foremost, to avoid the potential for cross contamination, there are only a limited number of monitoring wells (three) installed downgradient of the source area. All are installed through localized areas within the current extent of the perched groundwater where the FGZ projected above the perched groundwater table. PTX06-1033 is outside the area impacted by the source assumed here and has no effect on reducing uncertainty. PTX06-1032 is in an area of low uncertainty with respect to plume delineation and accounts for a minor reduction in uncertainty. PTX06-1056 is directly downgradient of the source area and accounts for nearly all the reduction in uncertainty from the existing Ogallala Aquifer monitoring well network. PTX06-1054, south of the source area, contains insufficient water for sampling and was therefore not included in the PlumeFinder analysis. There are no existing monitoring wells east of the perched groundwater extent capable of characterizing the Ogallala Aquifer near a potential secondary source in that area.

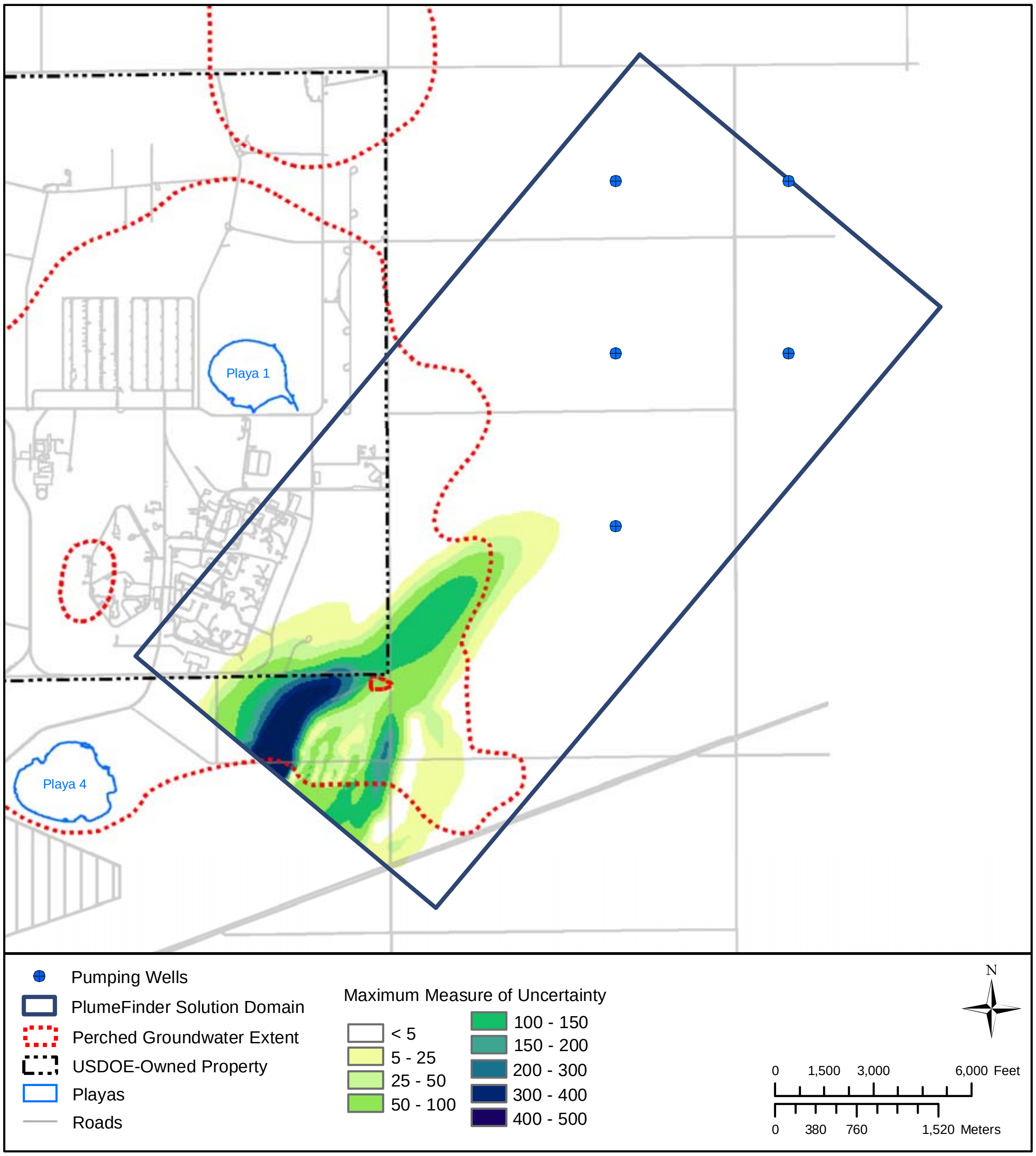



**Figure 3-9. PlumeFinder Rendering of Baseline Uncertainty**

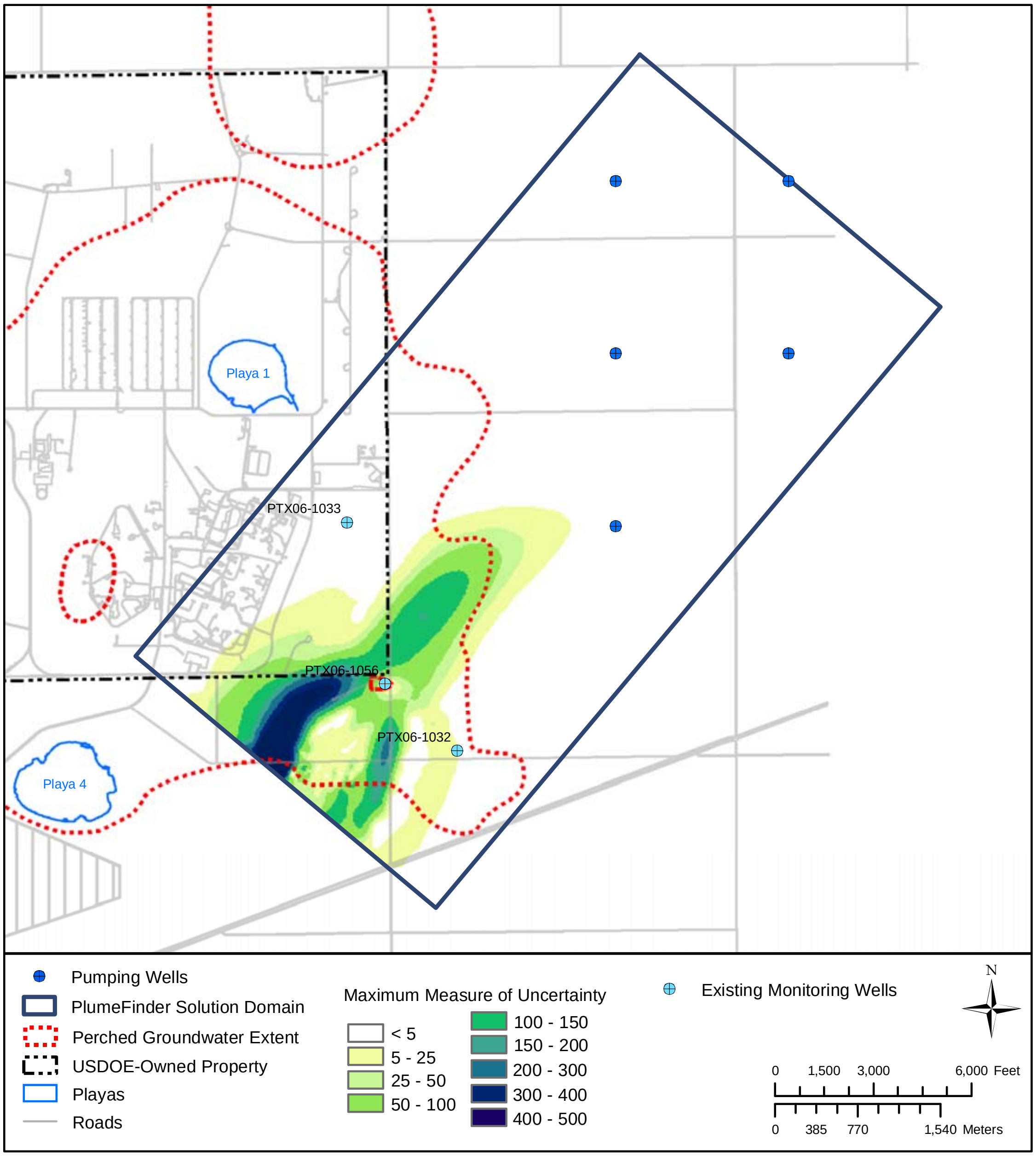



**Figure 3-10. PlumeFinder Rendering of Uncertainty with Existing Pantex Monitoring Wells**

### 3.2.3 Uncertainty with Proposed New Monitoring Wells

A proposed new well is added in the optimal location (i.e., at the location of the maximum value of uncertainty from Figure 3-10) that is to the east of the perched groundwater extent. This location can be seen in Figure 3-11. Assuming the new well detects the plume fringe, Figure 3-11 shows its projected effectiveness in decreasing the uncertainty in plume delineation if installed. This represents a 72% reduction in the volumetric uncertainty beyond the extent of perching from the current case (which assumed the Pantex monitoring well network). Overall, the total uncertainty reduction is 16% when considering the entire volume (below perched, south of Plant, and east of Plant).

The majority of the remaining uncertainty exists beneath perched groundwater and constitutes irreducible uncertainty due to the constraint that wells not be drilled through areas of perched groundwater containing RDX. As such, it is more desirable to place two additional wells slightly downgradient of the extent of perched groundwater rather than to drill through the perched groundwater to install monitoring wells. The locations of these well are shown on Figure 3-12. They are placed based on insight from the CMS/FS and associated BIOF&T3D modeling. They are not placed by the PlumeFinder analysis. The purpose of these two wells is early warning detection of RDX from the eastern portion of the perched groundwater, as opposed to farther field plume detection from the potential RDX source area beneath perched groundwater. They are located as preliminary investigation wells to gather subsurface information in these areas. PF-2 is where the extent of perched groundwater extends the least when compared to the surrounding area to assess the potential for downward migration (see Figure 3-3a) , and PF-3 is at the point where there is a decreasing area of RDX in the perched groundwater (also Figure 3-3a). These placements are motivated by an understanding of the physics of the 3-D flow and transport system. They are not positioned simply by placing them between potential receptors, for example. Installation of these wells will provide key observation data to better understand the flow and transport properties in this area and to assist in making informed decisions regarding potential RDX migration.

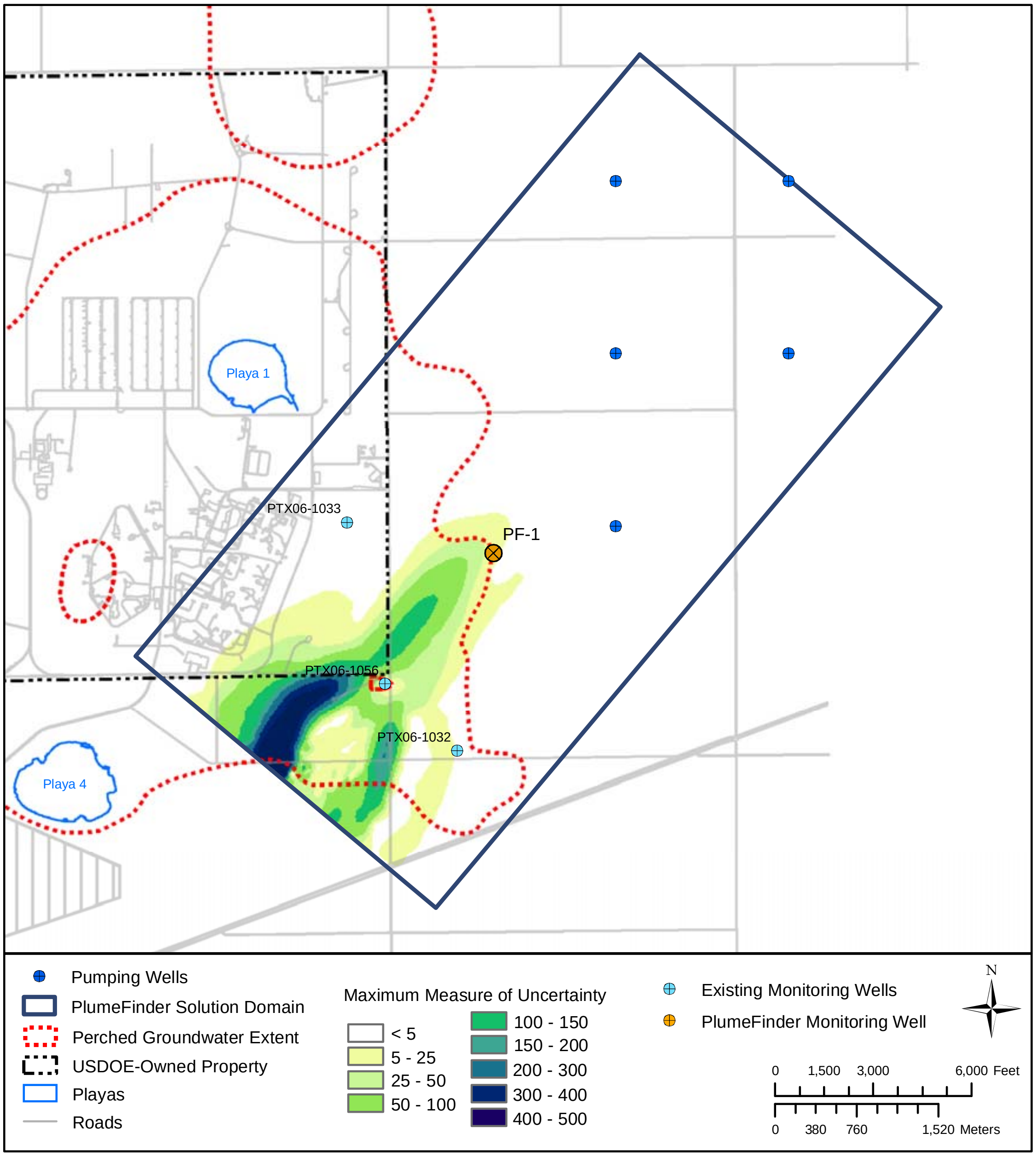



**Figure 3-11. PlumeFinder Rendering of Uncertainty with First New Well Installed**

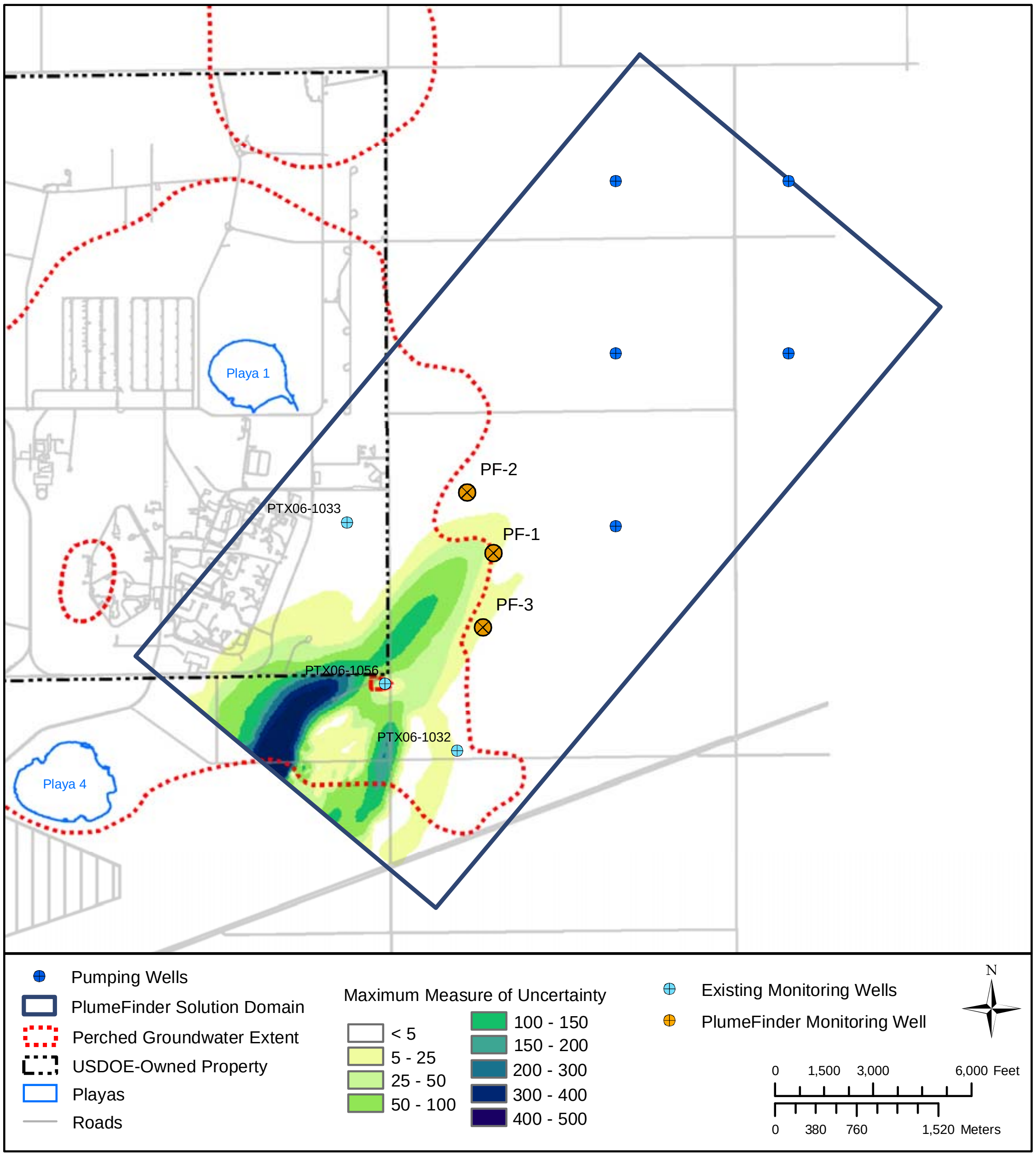



**Figure 3-12. PlumeFinder Rendering of Uncertainty with Second and Third New Wells Installed**

### 3.2.4 Summary of PlumeFinder Results

The first monitoring well, PF-1, details the effect of uncertainty from a potential RDX source area in the southeastern portion of the Plant derived from contamination in the overlying perched groundwater. Proposed wells PF-2 and PF-3 additionally help to provide early warning detection at the fringe of perched groundwater, and are based on professional judgment since the reduction in uncertainty computed from the PlumeFinder analysis indicated minimal value beyond the one monitoring well for reducing uncertainty from the potential source in the southeast. These three locations are based on the optimization performed with PlumeFinder combined with understanding the 3-D flow and transport physics to provide early warning detection for RDX derived from vertical flow near the extent of perched groundwater. Important points to consider are:

1) The fluxes from the perched groundwater vary with location and over time as the perched groundwater slowly drains into the Ogallala Aquifer.

2) Remediation is underway which is designed to minimize the risk that RDX enters the Ogallala Aquifer.

3) Placement of groundwater monitoring wells directly adjacent to the perceived extent of perched groundwater might cause a failure to identify RDX migrating to the Ogallala Aquifer due to the lack of direct observations in this area.

4) Placement of monitoring wells too far from the perched groundwater extent reduces their usefulness as an early warning system.

5) Currently, there are no Ogallala Aquifer monitoring wells east of the perched groundwater extent (second source); and therefore, there is no way to determine if the Ogallala Aquifer has been impacted in this area. Modeling results from the risk assessment and CMS/FS indicate only very low (ppb range) potential impacts in this area.

Hence, the proposed monitoring well network provides a balance of these complexities and the one well (PF-1) is optimal for detecting plume fringes from a potential source in the southeast area within a 50-year time period. The other two wells, PF-2 and PF-3, are good locations to assess migration of RDX along the eastern fringe of perched groundwater. For the monitoring well network to be workable, the well screens must be long enough to account for the documented and projected decline in the Ogallala Aquifer water table.

Note that in this analysis precise knowledge of the flow and transport system is not necessary, but is very helpful in making good decisions about well placement. The PlumeFinder assesses the ability of a monitoring location to provide information valuable to determining where the plume fringe resides. The conclusions for the PlumeFinder analysis for RDX in the Ogallala Aquifer are as follows:

- The existing monitoring network was established by installing monitoring wells through the FGZ. Although this was done using safe installation criteria, the existing network has limited value for RDX detection beneath the perched groundwater. It demonstrates the amount of irreducible uncertainty to safely investigate beneath the perched groundwater.

- Better delineation of the plume fringe can be achieved by adding three new wells outside the eastern extent of perched groundwater. The wells, however, do little to reduce the uncertainty in RDX plume fringe delineation beneath the perched groundwater.

- A periodic review of the flow directions and a regular sampling regimen, including both target and monitored natural attenuation parameters, is warranted.

- This analysis can be updated pending installation of the three proposed wells, collection of water table data, hydraulic conductivity, and RDX concentrations, if warranted.

# 4.0 SUMMARY

## 4.1 RESULTS OF WELL PLACEMENT OPTIMIZATION

A significant benefit in understanding the potential plume migration, as well as plume fringe delineation, can be gained by this analysis. Adding three new monitoring wells provides for a solid increase in understanding the groundwater flow and transport in this eastern area – an area currently devoid of Ogallala Aquifer monitoring wells. It also shows the irreducible uncertainty in knowledge of plume migration beneath the perched groundwater when safe investigation practices limit the amount of available data. The locations for three new monitoring wells are shown in Figure 4-1. PF-1 has been established using the PlumeFinder technology while PF-2 and PF-3 are recommended based on previous modeling efforts and site investigation data. With the high cost of monitoring well installation and sampling in the Ogallala Aquifer, it is prudent to collect additional subsurface characterization data before more new wells are installed beyond the three recommended. Additional valuable information includes verifying the presence or absence of RDX in the aquifer, determining the flow direction variation with time, and determining natural attenuation parameters over time and distance. This data will reduce the uncertainty in the information used to locate additional wells, if needed. A summary of the volume under the measure of uncertainty for RDX is presented in Table 4-1. The corresponding percentage reduction in far field plume fringe uncertainty from the current conditions is shown in parenthesis.

The reduction in uncertainty shown in Table 4-1 indicates that the first proposed monitoring well network has been well designed and reduces the uncertainty in plume location beyond the extent of perched groundwater for RDX by 72%. This translates into a total reduction of uncertainty for the entire plume (to the south and beneath the perched groundwater) of only 16%. Increasing the uncertainty reduction more would require drilling through the perched aquifer, which is not recommended. Hence, this 16% improvement also represents the irreducible uncertainty in understanding the flow and transport system. The installation of the second and third wells is for early warning detection of RDX originating along the eastern fringe of perched groundwater.

- PF-1: This is a dual-purpose monitoring well. This location resolves the greatest portion of uncertainty from the southeastern perched groundwater area and provides early warning detection for RDX emanating from the eastern fringe.

- PF-2 and PF-3: These serve as early detection wells for RDX emanating from the eastern fringe, and are derived from the physics-based understanding of 3-D flow and transport and the conceptual site understanding.

**4-1. PlumeFinder RDX Results Summary**

| PlumeFinder Simulation | Overall Measure of Uncertainty Residual (reduction) |
|---|---|
| Baseline<br>(No Wells Installed) | 100% |
| Current Conditions<br>(Existing Well Network) | 92% (8% reduction) |
| Add One New Well<br>(improvement from current conditions) | 84% (16% reduction) |
| Add One New Well<br>(improvement from current conditions east of perched groundwater) | 28% (72% reduction) |

The results of this analysis are significant because they document the baseline condition, quantify the value of the existing well network, and provide insight for optimally refining the well monitoring network. Adequate knowledge of the plume location is important to conducting good site investigations and making good plume management decisions. The PlumeFinder technology used in this study quantifies the plume fringe location even when data is limited and uncertain, so informed decisions can be made to ensure that long term monitoring or remediation activities are optimally located. The PlumeFinder technology applied here provides one new well location recommendation to produce the maximum reduction in plume uncertainty using proven mathematical and geostatistical principles. It also shows and quantifies the residual uncertainty beneath the perched groundwater. Above all, plume management needs to be done in a cost-effective manner with a focus on collecting information with demonstrated value to decision-makers. An improvement in the Ogallala Aquifer monitoring system can be made and the corresponding management risk associated with the decision to commit funds to implement additional wells for that purpose is clarified and quantified as a result of using the PlumeFinder technology.

## 4.2 RECOMMENDATIONS

The reduction in uncertainty from this analysis is relatively low when compared with other studies, and is driven by the inaccessibility of the areas of highest uncertainty beneath the perched groundwater. Therefore, the following recommendations supplement this analysis:

- A periodic evaluation of flow directions and regular sampling of chemical parameters, including both target and monitored natural attenuation parameters, is needed. The groundwater flow field should be assessed by careful examination of potentiometric data and water chemistry in this area.

- Following installation of the three new Ogallala Aquifer monitoring wells, data gleaned from the new wells should be compared with historical Ogallala Aquifer water table and chemical information, and an assessment of natural attenuation should be performed.

- The new field data should be compared with the current model assumptions, and any updates / refinements implemented, as merited.

- Future new well locations, if warranted, should be assessed using the PlumeFinder technology.

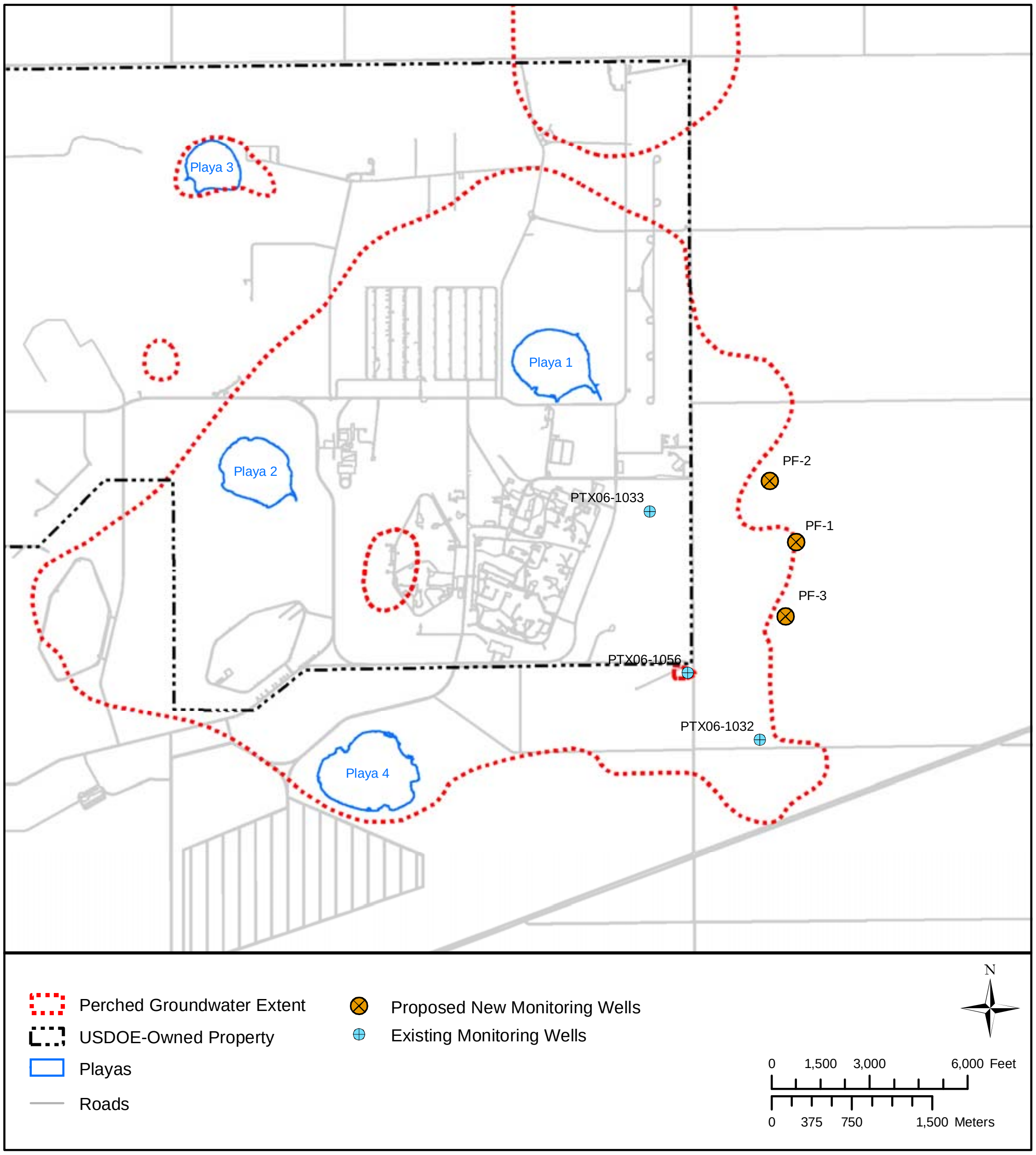



**Figure 4-1. Proposed New Well Locations based on PlumeFinder Results**

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# Appendix A

# Kalman Filtering used in the PlumeFinder Analysis

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# LIST OF EQUATIONS

## 1.0 OPTIMAL ESTIMATION VIA KALMAN FILTERING

The goal of optimal estimation is to be able to develop an estimate of the subsurface conditions with respect to flow and transport. This estimate then becomes the state of the system for optimization and decision-making under uncertainty. As discussed in the report, the costs associated in collecting information content about the subsurface results in only sparse knowledge available for analysis. To estimate how the subsurface conditions may vary, geostatistics are used to generate representative realizations. These realizations are used as inputs to the computational fluid dynamic models. This results in a distribution of subsurface conditions, as opposed to a single valued estimate. We now have a quandary: we have predictions of the subsurface condition from models, and we also have data from field surveys. While the role of information theory in this problem is conceptually enlightening, the most important part of this problem is solving the input/output representation of a linear or non-linear system. This generates a probability distribution function for the unknown (e.g., concentration of contaminate in groundwater), and the associated entropy reveals a certain measure of the uncertainty of it. This type of problem falls into the general field of optimum filtering and the stochastic signal extraction from noisy data.

Common parameter estimation in the geo-sciences groundwater modeling community consist primarily of: Bayesian estimators, cokriging estimators, geostatistical inverse methods, Kalman filtering, least squares methods, maximum likelihood methods, and pilot point techniques. McLaughlin and Townley (1996) showed that all these methods are special cases of the Gaussian maximum a posteriori estimator. Additionally, it is shown that using equivalent assumptions, the Kalman filter is equivalent to the least squares estimate, maximum likelihood estimate and the maximum a posteriori estimate. See for example: *Applied Optimal Estimation* (Gelb 1974), *Optimal Estimation with an Introduction to Stochastic Control Theory* (Lewis 1986), *Optimal Control and Estimation* (Stengel 1994). A nice overview of the extended Kalman filter is found in *Stochastic Methods in Subsurface Contaminant Hydrology* (Govindaraju 2002).

The first references found using Kalman filtering in groundwater investigations appeared in 1990s. Techniques have been developed to integrate the information content from both the predictive models and the observed measurements. The technique used in this work was integrating the computational fluid dynamic model (PTC) with a Kalman filter, as it has been demonstrated to provide the best unbiased estimate of the subsurface conditions integrating the uncertainty in the simulator and field data.

## 2.0 EXTENDED KALMAN FILTERING

The extended Kalman filter is a method to combine the information from samples that are available at discreet time and space with the predictions of a subsurface simulator to provide the minimum error estimate of subsurface conditions.

For extended Kalman filtering to be effective, a stochastic representation of the aquifer is necessary. Stochastic aquifer realizations were conducted using the GSLIB geostatistical package. This approach used the GAMS variogram to generate 500 aquifer realizations; the set of these realizations is called the ensemble. The concept here being that the deterministic representation is difficult to be precisely accurate, so one is always dealing in stochastic nature and uncertainty when developing predictions of subsurface behavior, specifically of the Ogallala Aquifer beneath the Pantex Plant.

The filter used in the analysis is comprised of essentially two parts:

1. The propagation component that specifies how the conditional moments (i.e., hydraulic head, contaminant distribution, flow velocity fields) evolve between times information is available (via sensor measurements). This component performs what a subsurface flow and transport simulator typically perform in conventional groundwater flow and transport projects.

2. The updating component incorporates the new information and specifies how the propagated moments are modified. This component performs the activity typical of a parameter estimation algorithm

The key benefit that the Kalman filter performed is the formal way to integrate the information from the physical PTC simulator and the monitoring well field data. But rather than do these separately, the Kalman filter updates both the mean and the covariance of the model state and associated parameters. Because the conditional statistics are used as the uncertainty measure— as opposed to the spatial variability—the assumption of ergodicity is not required. Ergodicity refers to a stationary random function and its ability to tend towards the stationary mean of its cdf. This concept is used widely in geostatistical analysis. This is an important point. At the scales that are of interest in most flow and transport studies, the conditional hydrobiogeochemical moments are most likely non-stationary and, hence, nonergodic. It should be noted that the updated estimates need not be mass conservative, but the best representation of the mass available given the uncertainty of the information available about the system and its performance.

The Kalman filter is a recursive algorithm. It is a convenient way to fuse the predictions between a subsurface simulator and field data. It estimates the state variables in a linear system by optimally combining the information content of the model and data, incorporating uncertainty. In linear systems, the Kalman filter estimate is the true conditional mean —the truly optimal (minimum variance) estimate. The Kalman filter must be extended to handle non-linear systems, such as most groundwater flow and transport challenges. Linearizing the state equation around the latest parameter estimates to approximate the conditional mean does this. Essentially, this formulation is like a series of linear batch filters. Practice has shown that even with this reduced dimensionality and linearization, the extended Kalman filter will provide an estimate that is close enough to the conditional mean and mode.

To explain this concept, the mathematical explanation that follows is essentially taken from *Stochastic Methods in Subsurface Contaminant Hydrology* (Govindaraju 2002), with insight added to help bring out the value of this approach. The state and parameter equations for a flow and transport simulator were presented above. Here, we focus on the equations of the Kalman filter and the state-parameter moment update equations:

**Equation 1. Kalman Filter**

$$K(x,t) = P_{xx}(x,x^{'},t)H^{T}(x^{'},t)[H(x,t)P_{xx}(x,x^{'},t)H^{T}(x^{'},t) + R(x,x^{'},t)]^{-1}$$

K (x, t) is the Kalman gain matrix. This matrix provides the weighting between the expected values from the simulations and the measured values at the sensor locations.

$P_{xx}$ (x, x’, t) is a first order approximation of the conditional covariance between two variables and two locations, denoted as x and x’ at time t. Conditioning makes the stochastic analyses more site specific for the Pantex Plant / Ogallala Aquifer flow and transport system. The variables are properties typically measured in the field such as hydraulic head, conductivity, chemical concentrations, and the like. The Pantex heads and concentrations were measured in the monitoring wells, and the conductivity information from the local and GAMS modeling studies. The conditional mean of the variable's random field is the minimum variance unbiased estimate of the actual site-specific distribution. The conditional variance measures the uncertainty of this estimate. The conditional covariance relates to the behavior between different variables.

H (x', t) is an operator in space and time. It specifies the relationship between the augmented state vector and the measurements made in the field. The augmented state vector contains the stochastic simulator – the heads, velocities, concentrations, and the uncertain parameters such as conductivities, retardation, biochemical degradation, source strength. The assumptions of these are provided in the main body of the report.

R (x, x', t) is the measurement covariance matrix covariance between two variables and two locations, denoted as x and x' at time t.

The second key equation relates how the augmented state vector [X (x, t)], the vector that contains the stochastic simulator – the heads, velocities, concentrations, and the uncertain parameters (such as conductivities, retardation, biochemical degradation, source strength, etc.) is updated after a measurement is made. Since we are placing a hypothetical monitoring well, we have no direct measurement. We assume it will detect a value of half the plume fringe value, but that neither hydraulic conductivity nor heads are known. This minimizes the possibility biasing the results based on estimates from the regional Ogallala model. After actual monitoring well installation, the concentration, water levels and hydraulic conductivity should be measured.

**Equation 2. Augmented State Vector Update**

$$\hat{X}^{+}(x,t) = \hat{X}^{-}(x,t) + K(x,t)[Z(x,t) - H(x,t)\hat{X}^{-}(x,t)]$$

$\hat{X}(x,t)$ is the first-order approximation of the conditional mean, given all measurements. The (-) sign indicates the estimate before the new measurement information is given, and the (+) indicates the estimate after the new information is analyzed.

Z (x, t) is the measurement vector. It is equal to H (x, t) X (x, t) + V (x, t). H and X are defined above, and V (x, t) is a measurement error vector, with zero mean, Gaussian white noise. It relates to the fact that when a measurement is made, the uncertainty about the value of the measurement at that point in time is reduced to zero plus the measurement error.

The third key equation relates how the first order approximation of the conditional covariance between two variables and two locations, denoted as x and x' at time t [$P_{xx}$ (x, x', t) ] is updated after a measurement is made:

**Equation 3. Conditional Covariance Update**

$$P_{xx}^{+}(x,x',t) = P_{xx}^{-}(x,x',t) - K(x,t)H(x,t)P_{xx}^{-}(x,x',t)$$

The Kalman filter performs as follows:

- Equation 1 defines the Kalman filter.

- Equation 2 states that the best linear unbiased estimate (minimum variance) of the augmented state vector [ $\hat{X}^{+}(x,t)$ ] is a linear combination of the model prediction [ $\hat{X}^{-}(x,t)$ ] and the field measurement [Z (x, t)]. This is how the predictive model information and field measurements are used in concert to provide the best estimate of the subsurface conditions. In general, subsurface simulators are coded to conserve mass. By adding the information content of the field data, the mass conservation is not guaranteed. This is, however, the best estimate of the subsurface conditions when the information is imperfect. It has a correction for the field data reliability, for if the measurements are unreliable, the measurement covariance matrix [R (x, x', t)] will be large. Because this term appears as an inverse in the Kalman gain matrix, K (x, t) will be small. Because K (x, t) weighs the observations, the best estimate will be close to the model estimate. If the measurements are of high accuracy, then this equation ensures that the estimate is consistent with the observed field data. This functionality allows for optimization of allowable measurement error: do you collect a lot of data with low fidelity? A few highly accurate data points or some combination of both is an optimal investigation design question. For this investigation, only formal monitoring wells are considered.

- Equation 3 is the heart of the optimal sampling design approach. The first order approximation [$P_{xx}$ (x, x', t)] of the updated conditional covariance between two variables and two locations, denoted as x and x' at time t, does not depend on any new observations. Note that all the terms rely on knowledge we currently have – denoted by (-), as opposed to (+). This equation is linearized around the most recently updated estimate of X (x, t), the augmented state vector – which depends on measurements to date but not the future. This provides insight to how the Kalman filter will behave and its accuracy before any new samples are taken. Because this equation is the difference between two positive definite matrices, the difference most also be positive definite. This says that the value of adding information (taking samples) is quantifiable, and the updated covariance matrix will always be less than or equal to the forecast covariance matrix. Of course, if the measurement covariance matrix [R (x, x', t)] goes to infinity, the second term of this equation will go to zero. This means that the samples have no value, which is consistent with why the matrix goes to infinity (unreliable samples).

These important attributes of the Kalman filter provided great value in finding the best location for a monitoring well in the Ogallala Aquifer just slightly beyond the eastern extent of perched groundwater at Pantex Plant.

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