United States Department of Energy

Savannah River Site

Groundwater Modeling for the Southern Sector of A/M Area (U)

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WSRC-RP-2001-4254

Revision 0

November 2001

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Prepared for U.S. Department of Energy under Contract No. DE-AC09-96SR18500

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-96SR18500 with the U. S. Department of Energy.

EXECUTIVE SUMMARY

A plume of TCE contamination in the Southern Sector of A/M Area appears to have resulted from a former release at the A-014 outfall. A numerical groundwater flow and transport modeling analysis is described that addresses this plume, the existing remedial actions, and potential future remedial actions.

The numerical flow and transport model is based on an understanding of the site that is formed in part by a recent analysis of hydrostratigraphic, head, and chemical data (Rabin 2001) and by a recent groundwater flow modeling analysis that covers a wider area (Aleman and Noffsinger 2001). The numerical model is calibrated to match observed water level measurements within acceptable criteria. The model is also qualitatively calibrated against the observed/inferred shape of the Southern Sector TCE plume. Though the calibration to the observed TCE plume is not perfect, the model is acceptable for comparing various remedial alternatives.

Model simulations indicate that the existing remedial wells, which have been in operation near the A-014 outfall for over ten years, have been effective at removing much of the TCE plume mass. These wells should continue to be effective if operated.

For portions of the TCE plume that are further downgradient, twelve airlift recirculation wells (ARWs) have been installed. These wells withdraw contaminated water in a lower screen, remove a large percentage of the TCE, and reinject the cleaner water through an upper screen. Model simulations indicate that the recirculation wells are effective at cleaning up the middle portion of the plume., but do not remove nearly as much mass as the remediation wells that are nearer the source.

Low concentrations of TCE are found further downgradient than the recirculation wells. A phytoremediation alternative has been suggested for this distal portion of the plume. The phytoremediation alternative would involve withdrawal of contaminated groundwater and treatment of the water via spray irrigation and phytoremediation. A simulation was made to show one possible configuration of withdrawal near groundwater discharge locations. The

simulation showed that the phytoremediation alternative is feasible and would significantly reduce the mass discharge and concentration in seeps near Tims Branch.

Additional simulations were made to show the effect of source reduction on the Southern Sector plume. Two scenarios were considered – complete source removal and 60% reduction in mass flux due to operation of the existing soil vapor extraction/air sparging system.

Overall, the most effective remedial action appears to be the one that was implemented first – the pump-and-treat remediation wells. The existing recirculation wells lower the concentration in the middle portion of the TCE plume. Phytoremediation or monitored natural attenuation (MNA) could be used to ensure that distal portions of the plume are lower that maximum contaminant levels (MCLs). If MNA is relied upon, data will be needed in the seepline wetlands to estimate the appropriate attenuation factor due to natural biodegradation. Source reduction could allow for eventual shutdown of the various water collection systems.

None of the proposed remedial actions address the portion of the Southern Sector TCE plume below the Lost Lake Aquifer Zone (LLAZ). TCE has been observed in the Crouch Branch Middle Sand, where it presumably will flow to distant discharge locations. The Crouch Branch Middle Sand is contained within the Crouch Branch Confining Unit. Another analysis may be needed to show where this portion of the plume is likely to discharge, and whether the concentration of discharge water will be significant. This analysis could probably be done using analytical methods.

The model that is developed and used here can be used in the future to compare remedial alternatives and can be used as a tool to help optimize the operation of various remedial systems. The model may be improved in the future by recalibration following a revised interpretation of the source and/or the TCE plume.

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$\partial c/\partial x_i$	concentration gradient
a_H	horizontal-transverse dispersivity
a_L	longitudinal dispersivity
a_T	vertical-transverse dispersivity
l	decay rate
µg	micrograms
r_b	porous medium bulk density
q	effective porosity
ARW	Airlift Recirculation Well
c	concentration
CAP	Corrective Action Plan
CBAZ	Crouch Branch Aquifer Zone
CBLC	Crouch Branch Lower Clay
CBMS	Crouch Branch Middle Sand
CBRP	C-Area Burning/Rubble Pit
CBUC	Crouch Branch Upper Clay
cm	centimeter
cDCE	cis-1,2-dichloroethylene
c_s	source/sink concentration
d	Day
D_{ij}	dispersion coefficient tensor
DNAPL	Dense Non-Aqueous Phase Liquid
DOE	Department of Energy
FACT	Flow and Contaminant Transport (code)
ft	Feet
g	Grams
GCCZ	Green Clay Confining Zone
GIMS	Geochemical Information Management System
GMS	Groundwater Modeling System
gpm	gallons per minute
h	hydraulic head
HCM	hydrogeologic conceptual model
in	Inches
K_d	sorption coefficient
kg	Kilograms
K_x	horizontal (x-direction) hydraulic conductivity
K_y	horizontal (y-direction) hydraulic conductivity
K_z	vertical hydraulic conductivity
L	Liters
LLAZ	Lost Lake Aquifer Zone
LLLAZ	Lower Lost Lake Aquifer Zone
MAAZ	M-area Aquifer Zone

MAE	mean absolute error
MCL	maximum contaminant level
MNA	monitored natural attenuation
MOC	method of characteristics
MODFLOW	Modular Three-dimensional Finite-Difference Groundwater Flow Model (code)
msl	mean sea level
MT3DMS	Modular Three-Dimensional Multispecies Transport Model (code)
PCE	Tetrachloroethylene
q_s	source/sink groundwater flow per unit volume
RACM	remedial alternative conceptual model
RCRA	Resource Conservation and Recovery Act
RMSE	root mean square error
SRS	Savannah River Site
SRTC	Savannah River Technology Center
SVE/AS	soil vapor extraction/air sparging
TCE	Trichloroethylene
tDCE	Trans-1,2-dichloroethylene
TVD	total-variation-diminishing
ULLAZ	Upper Lost Lake Aquifer Zone
USGS	United States Geological Survey
UTRA	Upper Three Runs aquifer
VC	Vinyl chloride
v_i	Velocity vector
VOC	Volatile organic compound
WSRC	Westinghouse Savannah River Company
yr	Year

1.0 INTRODUCTION

This report documents a numerical modeling analysis of trichloroethylene (TCE) transport in groundwater in the Southern Sector of the A/M Area, Savannah River Site (SRS). The analysis provides a tool for understanding the environmental processes that have shaped the current TCE plume, and a means for assessing the relative effectiveness of different existing and proposed remedial alternatives. The numerical model results and the conclusions derived from this analysis will support other regulatory analyses, including an analysis of the effectiveness of the Phase I Corrective Action Plan (CAP), and will provide technical input to decisions that are being made in support of the Phase II CAP.

The A/M Area is located on the northern[1] part of the SRS (Figure 1.1). Several plumes of trichloroethylene (TCE) exist in the Southern Sector of A/M Area. The TCE plume that extends from the A-014 outfall to local groundwater discharge points along Tims Branch (Figure 1.2) is addressed in the Resource Conservation and Recovery Act (RCRA) Part B permit for the M-area Hazardous Waste Management Facility CAP.

To facilitate the analysis, a numerical model of groundwater flow and solute transport was developed. This numerical model is based on an understanding of the site and environmental processes as presented in section 2 of this report. Many details of this Southern Sector numerical model are derived from a prior regional modeling analysis of A/M Area (Aleman and Noffsinger 2001) and from data provided for this project by Westinghouse Savannah River Company (WSRC) (Rabin 2001). The entire process of constructing and calibrating the Southern Sector numerical model is described in section 3.

Once the Southern Sector numerical model was constructed and calibrated, it was used to predict the future movement of TCE under different scenarios. Section 4 includes the results of this predictive analysis. Predictions were made to show how the TCE plume would have developed if no remedial actions had ever been implemented, if only the existing groundwater extraction

[1] In this report, all relative directions are based on SRS plant coordinates. SRS plant north is 36°22′ west of true north.

wells had been installed, and if only existing actions (groundwater extraction wells and Airlift Recirculation Wells (ARWs)) were continued. These three predictive simulations provide a basis for comparison of various future remedial alternatives. The future alternatives involve existing components and the following additional remedial components:

- Removal of 60% of the source near the A-014 outfall (by air sparging and soil vapor extraction),
- Removal of all of the source near the A-014 outfall,
- Phytoremediation of the distal portion of the plume by well withdrawal and spray irrigation, and
- Monitored natural attenuation (MNA) of the distal portion of the plume.

In section 5, conclusions from this analysis are presented, including an overall assessment of the model and how it can best be used.

2.0 PROBLEM DESCRIPTION

In this section an understanding of the environmental system as it pertains to the Southern Sector TCE plume is described. This understanding was formed from review of prior studies of A/M Area, especially a recent regional numerical modeling analysis (Aleman and Noffsinger 2001), and recent interpretation of hydrogeological data by WSRC (Rabin 2001). The relevant aspects of the physical system include aquifer/aquitard layering, groundwater sources and sinks (including existing remedial systems), and details of the TCE distribution in the Southern Sector area. A hydrogeological conceptual model[2] (HCM) of the site was developed to demonstrate the current understanding of the physical system. Additionally, a remedial alternative conceptual

[2] In this report, a “conceptual model” refers to a general description of the pertinent physical processes. A conceptual model is often illustrated with a simple diagram. A hydrogeologic conceptual model (HCM) describes the general site features, and a remedial action conceptual model (RACM) describes a particular remediation step. The conceptual model(s) form the basis of the “numerical model” (sometimes just called the “model”) which is a detailed mathematical description of groundwater flow and contaminant transport at the site. The Southern Sector

model (RACM) was developed for each potential remediation component under consideration, namely source removal, phytoremediation, monitored natural attenuation, and recirculation wells. The conceptual models that are described in this section form the basis for the numerical model introduced in section 3.

2.1 Prior Studies

Various investigators have produced numerous reports that describe the hydrogeologic setting of SRS and A/M Area. This report relies on information contained in two publications: a South Carolina Department of Natural Resources report on the *Hydrogeologic Framework of West-Central South Carolina* (Aadland et al. 1995), and a WSRC report on the *Classification of Hydrostratigraphic Units at the Savannah River Site* (Aadland and Bledsoe 1990).

Several studies regarding the nature and extent of contamination in the A/M Area have been conducted in support of ongoing restoration efforts. Looney, et al (1992) identified Dense Non-Aqueous Phase Liquid (DNAPL) TCE in the saturated zone beneath the M-area Settling Basin. Jackson, et al (1999) identified DNAPL in the shallow portions if the vadose zone near the A-014 outfall. Looney and Phifer (1994) evaluated conventional pump and treat systems within the Southern Sector. Jackson and Looney (1996) proposed a series of Airlift Recirculation Wells (ARWs) to prevent further migration of a TCE plume. In 1999, a small-scale characterization effort was performed to support future remediation decisions for the Southern Sector (Jerome et al., 1999). Jackson, et al. (2000) described characterization activities along Tims Branch. In addition to these studies, concentration data extracted from the SRS Geochemical Information Management System (GIMS) were used to develop an understanding of the current TCE plume.

Several groundwater-modeling studies have been performed that partially address some of the issues that are the subject of this study. A particle tracking analysis with the FACT model was used to design the ARW system in 1996 (SRTC 1996). This model used eight ARWs and included much of the Southern Sector. A more localized analysis that evaluated the effectiveness

numerical model is used to solve for groundwater head and TCE concentration at discretized points in space and time.

of two of the ARWs was conducted in 1999 (SRTC 1999). A regional MODFLOW model was developed in 2000 to evaluate the effectiveness of the M1 and A2 pump-and-treat systems and the potential for migration of contaminants beyond the northern boundary of SRS (Aleman and Noffsinger 2001). This model encompasses the Southern Sector and was used as a base for the model used in this study.

2.2 Physical Setting

2.2.1 General

SRS is located on the Atlantic coastal plain northeast of and adjacent to the Savannah River. In the study area, the topographic elevation ranges from approximately 375 ft (msl) at M-area to approximately 165 ft (msl) at the lower reaches of Tims Branch. Figure 1.2 shows the location of the Southern Sector and the Southern Sector TCE plume relative to existing site structures, roads, wells, and area water bodies. The TCE plume in this area extends south-southeasterly towards Tims Branch. Jackson et al (2000) investigated regions of plume outcrop along Tims Branch. Tims Branch flows south and discharges to Upper Three Runs Creek outside the study area.

The annual precipitation at SRS is approximately 48 in. Some of the precipitation water evaporates at the surface, some flows overland to area water bodies, and some is taken up by vegetation and evapotranspired. An estimated 12.5 in/yr (Rabin 2001) of the precipitation percolates though the soil and reaches the water table as groundwater recharge. During periods of reduced precipitation, including the prolonged drought of 1999-2000, groundwater recharge is expected to be lower than 12.5 in/yr.

2.2.2 Hydrostratigraphy

The unconsolidated marine and fluvial sediments of the Atlantic coastal plain underlie A/M Area and all of SRS (Aadland and Bledsoe 1990). The sediments vary in age from Late Cretaceous to recent (Figure 2.1). They are a variably stratified, heterogeneous sequence of sand, clay, limestone, and gravel. The uppermost sediments make up the Floridan Aquifer System. The generalized hydrostratigraphy in A/M Area (Figure 2.2) consists of (from surface): 1) the M-Area Aquifer Zone (MAAZ), 2) the Green Clay Confining Zone (GCCZ), 3) the Lost Lake Aquifer Zone (LLAZ), 4) the Crouch Branch Upper Clay (CBUC), 5) the Crouch Branch Middle Sand (CBMS), 6) the Crouch Branch Lower Clay (CBLC), and 7) the Crouch Branch Aquifer Zone (CBAZ).

The CBUC, CBMS, and CBLC make up the Crouch Branch confining unit. The competency of this unit generally decreases moving northward in A/M Area. The LLAZ is generally divided into the Upper Lost Lake Aquifer Zone (ULLAZ) and the Lower Lost Lake Aquifer Zone (LLLAZ). The GCCZ outcrops along Tims Branch, on the eastern side of the study area. The LLAZ is important to this study because it appears to be a primary area of contamination. The LLAZ consists of yellow, tan, orange, and brown, loose to slightly indurated, fine to coarse, moderately to well-sorted, occasionally pebbly sand and minor clayey sand. The LLAZ ranges from 40 ft to 80 ft in thickness within the study area (Rabin 2001).

2.2.3 Source Description

The A/M Area is located in the northern portion of the SRS. M area was a fuel and target fabrication facility from the 1950's to the 1980's. The processes were primarily mechanical and metallurgical, with solvent cleaning and acid/caustic etching used to prepare the materials. The disposal of spent solvents and other liquid wastes through process sewer lines to seepage basins and outfalls resulted in groundwater contamination. It is estimated that some 3.5 million pounds of solvents were released to the subsurface, with groundwater transport creating a plume of TCE. A portion of this plume is located in the Southern Sector of A/M Area, which is the focus of this investigation

Previous characterization, monitoring, and analysis have suggested that the Southern Sector TCE plume is primarily the result of groundwater transport from the A-014 outfall. From 1952 to 1979, large volumes of PCE and TCE were discharged into an unnamed tributary through the A-014 outfall. This discharge has resulted in DNAPLs in the sediments underlying the outfall and dissolved phase contaminants in the groundwater (Rabin 2001).

2.2.4 Plume Characterization

There are numerous groundwater monitor wells in the A/M Area that have been sampled for TCE. TCE concentrations measured in Southern Sector monitor wells were derived from the GIMS database.

Groundwater samples from monitor wells in the Southern Sector indicate an area of TCE contamination extending southeasterly from the A-014 outfall towards Tims Branch. There are other areas of TCE contamination in A/M Area, but the portion of the TCE plume that is apparently emanating from the A-014 outfall is the focus of this study. WSRC (Rabin 2001) interpreted the observed data and delineated a Southern Sector TCE plume that is associated with the A-014 outfall (Figure 2.3). A sizeable portion of this TCE plume has concentrations in excess of 5,000 µg/L. The maximum contaminant level (MCL) for TCE is 5 µg/L.

This plume appears to migrate vertically from the source area through the MAAZ, GCCZ, and ULLAZ into the LLLAZ, where it moves horizontally towards its discharge point along Tims Branch. There is continued downward migration from the LLLAZ into the CBMS, where flow is more southerly.

2.2.5 Groundwater Flow

Groundwater flow directions in the study area are determined from water-level measurements and confirmed by the shape of the TCE plume. Flow directions in the MAAZ appear to generally follow topography. Near the source area, flow is generally downward through the very thin saturated portion of this aquifer. The GCCZ appears to offer restriction to flow in many areas of the study area, but is not continuous near the source area, and hence flow is downward to the LLAZ. Regionally, flow in the LLAZ is generally to the south, but is influenced locally by incisement of Tims Branch near Road 2. The influence of Tims Branch imparts a southeasterly component of groundwater flow in the area between the source and the discharge point. There is also an upward component of flow near Tims Branch.

There is a downward component of flow across the CBUC, CBMS, and CBLC into the CBAZ. Flow in the CBMS and CBAZ is south-southwesterly in much of the study area.

2.2.6 Solute Transport Processes

Dissolved TCE in the groundwater is affected by the processes of advection, diffusion, hydrodynamic dispersion, sorption, and biodegradation. Advection is the process that describes the movement of dissolved TCE along the groundwater flow path, and is often conceptualized as a particle trace. Diffusion is the process of random molecular motion that effectively results in mass flux from areas of high concentration to areas of lower concentration at the pore scale. A much more important process for most solute transport problems is hydrodynamic dispersion, in which a heterogeneous velocity field causes plume-scale mass flux from areas of high concentration to areas of low concentration. Greater velocities result in greater plume spreading. (In the current analysis, as with most groundwater transport problems, diffusion is ignored but hydrodynamic dispersion is considered.) Sorption is the process by which TCE mass is adsorbed to and desorbed from soil particles, effectively retarding the movement of the plume. An equilibrium sorption process is assumed, whereby the concentration of TCE in groundwater is proportional to the TCE concentration on the soil. The proportionality constant is called the sorption coefficient, or K_d, and is dependent on the organic-carbon content of the soil.

Reductive dechlorination of TCE can occur in anaerobic conditions with the presence of microbes, a carbon source, nutrients, and appropriate geochemistry. The result of the process is typically *cis*-1,2-dichloroethylene (cDCE) and inorganic chloride (trans-1,2-dichloroethylene, tDCE, is sometimes formed instead of cDCE). Further reductive dechlorination of cDCE may result in vinyl chloride (VC), then ethylene, or oxidation may result in carbon dioxide (Figure 2.4). The MCLs for cDCE and VC are 5 µg/L and 2 µg/L, respectively. Ethylene and carbon dioxide are environmentally favorable end products of the biodegradation process. The TCE plume in the Southern Sector is typically found in oxygenated zones, and therefore little to no TCE degradation naturally occurs (except near discharge locations, as discussed in section 2.4.5).

TCE and its degradation products are volatile organic compounds (VOCs). They are readily dissolved in air in the unsaturated zone and at the surface of water bodies.

2.3 Hydrogeologic Conceptual Model

The first step in the modeling process is formulation of the site-specific hydrogeologic conceptual model (HCM) of the study area. The HCM is a representation of the groundwater flow and transport system that incorporates a description of the geologic setting, hydrostratigraphic units, hydraulic properties, and system boundaries (such as streams, wells, and other sources and sinks). The HCM helps define the dimensions, layering, property assignments, and boundary conditions of the numerical model. WSRC (Rabin 2001) provided an HCM for this study that is summarized in this section.

Figure 2.5 illustrates the HCM for the Southern Sector TCE plume. The primary TCE source is believed to be in the unsaturated zone beneath the A-014 outfall (DNAPL and dissolved phases) and in bottom sediments of the discharge stream along the A-014 outfall. Flow directions are basically horizontal in the transmissive layers of the LLAZ (ULLAZ and LLLAZ), CBMS, and CBAZ, and more vertical in the confining beds (GCCZ, CBUC, CBLC). TCE contamination is most prevalent in the LLLAZ with decreasing amounts in the CBMS. No significant contamination has been observed in the CBAZ (Rabin 2001). While the CBMS is a transmissive layer in this model, it is not generally considered to be an aquifer, but is rather a part of the Crouch Branch Confining Unit (along with the CBUC and CBLC).

The details of the HCM, including stratigraphic layer elevations, ranges of hydraulic properties, and descriptions of groundwater boundary conditions were provided in a memorandum from WSRC (Rabin 2001), along with monitor well data. This information was used to develop the numerical model of the Southern Sector TCE plume, as described in section 3.

2.4 Remedial Alternative Conceptual Models

The first step toward modeling different remedial alternatives for the TCE plume is to develop a conceptual understanding of the component technologies that make up the remedial alternatives, and to define the specific methods that will be used to numerically model these technologies. These conceptual descriptions and modeling specifications are called remedial alternative conceptual models (RACMs). A RACM for each component technology is discussed below.

2.4.1 Existing Remediation Wells

Several remediation pumping wells are already in operation near the A-014 outfall source (Figure 1.2). These wells are part of the A/M pump-and-treat system. The conceptual model for a remediation well is simply removal of groundwater at a specified withdrawal rate (Figure 2.6). Construction and operation data are used to assign the model location and withdrawal rates for individual wells.

2.4.2 Recirculation Wells

Twelve ARWs were installed in a line near the toe of the Southern Sector plume. The wells are spaced approximately 255 ft apart and are currently in operation. Each well has a lower (withdrawal) screen in the LLLAZ and an upper (injection) screen in the ULLAZ. Withdrawn water is forced upward through the well casing where it becomes aerated. Much of the TCE in the groundwater is volatilized before the water is reintroduced to the aquifer.

Each ARW operates at approximately 30 gpm and has an estimated radius of influence of 160 ft. The TCE removal efficiency of wells SSR-1 through SSR-11 has been estimated at approximately 65% based on performance testing (White 1999). SSR-12 (the northernmost well) is a multi-stage ARW with an estimated removal efficiency of over 90% (Davis Environmental 1998). SSR-9, SSR-10, and SSR-11 will soon be converted to multi-stage ARWs.

An ARW is conceptualized as a well withdrawing contaminated water from a lower aquifer or portion of the aquifer and injecting the cleaner water into the upper aquifer or portion of the aquifer (Figure 2.7). This conceptual model is represented numerically as two wells, one pumping and one injecting. The pumping well withdraws water of prevailing concentration at a specified rate from the aquifer. This water and contamination is effectively removed from the model with the specified flux boundary condition. However, the injection well returns the same quantity of water as was removed, but uses a concentration that is representative of the removal efficiency of the ARW. The concentration is determined by applying a factor to the concentration that was removed by the pumping well. To avoid the need to iterate within the numerical solution, the concentrations injected in a given model time step are based on the concentration withdrawn in the previous time-step (numerical implementation is discussed further in Section 3.1). This approximation is appropriate provided that concentrations do not change considerably from one time step to the next.

In the numerical model, ARW's are specified to have a withdrawal/injection rate of 30 gpm and a removal efficiency of 65% (except SSR-12 which has a removal efficiency of 90%). Sensitivity simulations are used to show how different removal efficiencies affect plume remediation.

2.4.3 Source Reduction

The source area near the A-014 outfall is conceptualized as a distributed area containing contaminants in the unsaturated zone, perhaps in the form of DNAPLs. These contaminants leach out of the source into the saturated zone and have been attributed to development of the portion of the plume that is of interest in this study. The extent of the contamination and behavior of the source are not well characterized. Hence the source area is based on a presumed size resulting from discharge and limited downstream transport from the outfall. Contaminant flux is based on water infiltration and concentrations at (or below) the solubility limit of TCE. The reasonableness of this conceptual model is tested during the calibration phase (sections 3.3 and 3.4) with the objective of matching the general plume shape and concentrations.

For source reduction, the contaminant flux is reduced by lowering the assigned source concentration (Figure 2.8). Two scenarios are considered. First, it is assumed that the soil vapor extraction/air sparging (SVE/AS) system currently in place reduces 60% of the mass flux to the saturated groundwater. For this scenario, the source concentration is multiplied by 0.4. The second scenario considered is complete source removal. Setting the source concentration to zero simulates this action.

Note that although the source term characterization may not be completely accurate due to data limitations, the model gives a reasonable approximation of the relative effectiveness of various levels of source removal.

2.4.4 Phytoremediation

Ex-situ phytoremediation is a remedial alternative currently in use or under consideration for several contaminated sites at SRS, including Southern Sector A/M Area. This alternative entails physical withdrawal of contaminated groundwater via pumping wells (or other methods), and treatment of the water by spray irrigation and phytoremediation by natural vegetation. Volatile organics such as TCE are evaporated or transpired by plants, and it is assumed that none of the contamination or water is reinfiltrated into groundwater. This component technology could be applied anywhere within the TCE plume.

The RACM for ex-situ phytoremediation is identical to the RACM for the remediation wells (Figure 2.6). Groundwater is removed at a specified withdrawal rate. Potential locations and pumping rates for phytoremediation wells are determined in this analysis by trial and error. A well-designed system of phytoremediation wells should have little effect on the regional flow directions, but should intercept as much TCE contamination as possible prior to surface water discharge.

2.4.5 Monitored Natural Attenuation

Natural attenuation refers to processes such as dispersion and biodegradation that can reduce the concentration of TCE in groundwater without human intervention. These natural transport processes are described above (section 2.2.6). The monitored natural attenuation remedial component is simply a method of taking credit for these naturally occurring processes.

The numerical groundwater model that is built from the HCM (section 2.3) already includes the effects of dispersion. Since biodegradation is not occurring naturally in most of the plume area, it is not numerically modeled in the aquifer. However, biodegradation near groundwater discharge areas can be accounted for by adjusting the discharge concentrations by an attenuation factor. Since little site-specific data are available for determining a degradation rate, sediment thickness, or velocity in the sediments, the attenuation factors are estimated based on studies at other areas of SRS and published in the available literature. Reasonable attenuation factors range from 1 (no biodegradation) to 0.01 (hundred-fold concentration reduction). One microcosm study of soils in Southern Sector (Brigmon et al. 1998) suggests that the rate of biodegradation in the study area is fairly low. As an initial guess, an attenuation factor of 0.1 is assumed in this study. Natural degradation is considered as part of the MNA remedial alternative component, and is accounted for my multiplying numerically-modeled discharge concentrations (and discharge mass flux) by the attenuation factor (Figure 2.9). An analysis of observed data from shallow wells in the C-area Burning/Rubble Pit (CBRP) wetlands (GeoTrans 2001) indicated an approximate attenuation factor of 0.011 for TCE at that site. Note that the natural degradation of TCE can result in levels of cDCE and VC that are higher than MCLs.

3.0 NUMERICAL MODEL CONSTRUCTION AND CALIBRATION

In this section, development of a numerical groundwater flow and transport model for the Southern Sector TCE plume is documented. The numerical model is based on the HCM of section 2.3 and on data provided by WSRC (Rabin 2001). The construction of the numerical model and calibration to present conditions are discussed in this section. Following calibration, the model is considered to be a useful analysis tool for simulating future conditions (section 4).

3.1 Numerical Methods

In the saturated groundwater, a combination of continuity (mass conservation) and Darcy's Law leads to the following mathematical description of steady-state groundwater flow:

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right)=0 \qquad (1)$$

In this equation, the dependent variable is the hydraulic head, h, which is defined in the traditional (x, y, z) Cartesian coordinate system. The horizontal and vertical hydraulic conductivities (K_x, K_y, and K_z) are known functions. Boundary conditions must also be specified to solve equation 1. The boundary conditions may be specified head (Dirichlet), specified flux (Neumann) or head-dependent flux (Cauchy). It is assumed that groundwater flow is unchanging in time (steady state).

The USGS groundwater flow modeling software MODFLOW (McDonald and Harbaugh 1988) provides a means to solve equation 1 for *h* in a chosen domain, with specified values for hydraulic conductivity and specified boundary conditions. MODFLOW uses the finite difference method to approximate the groundwater flow equation as a set of algebraic equations in a discretized three-dimensional grid of rectangular cells.

The transport of TCE in groundwater is governed by the advection-dispersion-reaction equation, which can be written as follows:

$$(q + r_b K_d)\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(q v_i c) = \frac{\partial}{\partial x_i}\left(q D_{ij}\,\frac{\partial c}{\partial x_j}\right) - l\,(q + r_b K_d)\,c + q_s c_s \qquad (2)$$

In this equation, the Cartesian coordinates are represented by x_i ($i = 1, 2, 3$), and the dependent variable is the TCE concentration in groundwater, *c*. The velocity field (v_i) is determined from the flow solution and Darcy's Law. The effective porosity is q, and the porous medium bulk density is r_b. First order (exponential) decay is assumed at a rate of l. Equilibrium sorption is also assumed, with a sorption coefficient of K_d. TCE sources and sinks are represented by the source/sink groundwater flow rate per unit volume of the aquifer (q_s) and the source/sink concentration (c_s). The dispersion coefficient tensor, D_{ij}, is dependent on the groundwater velocity and specified length scales for dispersion, called dispersivities. Dispersivities are usually specified as longitudinal (along the direction of flow, a_L), horizontal-transverse (a_H), and vertical-transverse (a_T). The initial value of *c* must also be specified in order to solve equation 2.

MT3DMS (Zheng and Wang 1998) is a software program for solving equation 2 that uses the same finite-difference framework as MODFLOW. Once the steady-state values of *h* are determined from MODFLOW, and the independent variables of equation 4 are specified, MT3DMS can be used to solve for TCE concentration (*c*), as a function of space and time, in the modeled domain. For the simulations presented in this report, the standard finite-difference (upstream weighting) solution method is used to simulate solute advection. While this method can lead to numerical error (sometimes called artificial dispersion), it is inherently mass-conservative and typically free of spurious oscillations in the solution. Simulations were attempted with other solution methods including the total-variation-diminishing (TVD) scheme and the method of characteristics (MOC), but these simulations were fraught with numerical instability.

A modification was made to MT3DMS in order to accurately simulate recirculation wells. In its original version, MT3DMS requires that injection-well concentrations be specified before a simulation is executed. A recirculation-well package was added so that an injection-well concentration could be a function of the modeled concentration at a pumping well. The user specifies which injection wells are tied to which pumping wells and the user also specifies a concentration multiplication factor for each pair. The concentration factor reflects the mass-removal efficiency of the recirculation well (e.g., a concentration factor of 0.35 is used to specify a removal efficiency of 65%). In the first model time step, the injection concentration is set to zero. In subsequent time steps, the injection-well concentration is the pumping-well concentration from the previous time step multiplied by the specified concentration factor. This formulation is convenient for handling the recirculation well alternative as presented in section 2.4.2.

Both MODFLOW and MT3DMS are included in the Groundwater Modeling System (GMS) (Brigham Young University 2000) software package (version 3.1; Feb. 1, 2001 build date). GMS is a standard suite of tools for modeling analyses at SRS and other DOE sites.

3.2 Model Design

WSRC (Rabin 2001) provided hydrostratigraphic layer elevations, well data, and boundary-condition specifications for the study area, along with a summary of hydraulic property values determined in prior studies of the site. These data form the primary basis for the construction of the numerical flow and transport model presented here. Additional information, including an initial estimate of boundary conditions at model edges, was taken from a prior numerical model (Aleman and Noffsinger 2001). The prior numerical model covers a large area that includes the entire study area. Both the prior numerical model (Aleman and Noffsinger 2001) and the current numerical model extend vertically from the base of the CBAZ to the water table.

The horizontal domain of the Southern Sector numerical model (Figure 3.1) was chosen to encompass the entire TCE plume and was extended, where possible, to natural groundwater boundaries. Tims Branch is a natural boundary for the MAAZ and portions of the LLAZ to the east/southeast of the plume area. Natural boundaries do not appear within a reasonable distance in other directions from the plume. Therefore, the results of the prior, more regional, numerical model (Aleman and Noffsinger 2001) were initially used to set boundary conditions on most model edges. These model edges were chosen to be relatively distant from the Southern Sector TCE plume (several thousand feet) in order to avoid model accuracy errors due to incorrect specification of boundary conditions.

3.2.1 Model Grid

The Southern Sector model has a maximum horizontal grid spacing of 500 ft by 500 ft, and has cells of 50 ft by 50 ft near the A-014 outfall source and in the main plume area (Figure 3.2). The model has 182 rows and 151 columns. Grid cells to the east of Tims Branch are inactive (outside the modeled domain), as are grid cells outside other chosen model boundaries. The lower left (west) corner of the model has coordinates of 33,880 E and 102,400 N in the SRS plant coordinate system. The model is 20,225 ft by 20,500 ft in the x and y directions, respectively. The grid is rotated 47.7° east of SRS north, which puts the recirculation wells in a single model column (roughly 5 cells apart). Smaller grid spacing is used in the source and plume area so that the resolution of transport results is increased and so that the error in the calculation of the concentration gradient ($\partial c/\partial x_i$) is decreased.

Vertically, the model layering is based on hydrostratigraphic surface elevations provided by WSRC (Rabin 2001). Eight model layers are used, one each for the MAAZ, GCCZ, upper LLAZ, lower LLAZ, CBUC, CBMS, CBLC, and CBAZ (Figure 3.3).

3.2.2 Hydrogeologic Properties

For steady-state groundwater flow, hydraulic conductivity values (K_x, K_y, K_z) are specified in each model cell. The value of hydraulic conductivity is much higher in aquifer zones than in confining zones, and may vary considerably within an aquifer or confining zone. Typically, hydraulic conductivity values are initialized for each hydrostratigraphic layer based on prior studies and the values are adjusted during flow model calibration to achieve a good match between modeled and observed head and/or flux conditions. Section 3.3 provides details on the calibration process used in this study.

Transport modeling also requires specification of values for effective porosity (q) and dispersivity (a_L, a_H, and a_V). The effective porosity (volume-fraction of connected pores in a soil medium) is a factor in determining groundwater velocity (v_i). Effective porosity for natural soils typically varies between 10% and 50%. Dispersivity is a parameter that describes the degree of plume spreading, and is often determined by calibration to an existing plume. Dispersivity values depend on the scale of the plume and are typically higher in highly heterogeneous formations. As a practical rule of thumb, the longitudinal dispersivity (a_L) should be no greater than one-tenth of the problem length scale, the horizontal-transverse dispersivity (a_H) should be about one-tenth of a_L, and the vertical dispersivity (a_V) should be about one-hundredth of a_L. The Southern Sector TCE plume is approximately 7000 ft long, meaning that acceptable values for longitudinal dispersivity are 700 ft or lower. However, prior studies at SRS (e.g., Fogle and Brewer 2000, GeoTrans 2001) suggest that the relatively homogeneous soils at SRS lead to plumes exhibiting much lower dispersivities. Dispersivity is treated as a space-uniform parameter during transport model calibration (section 3.3).

The bulk density (r_b) and sorption coefficient (K_d) determine the degree to which TCE mass is adsorbed to solids in the porous medium (equilibrium sorption is assumed). Greater adsorption effectively results in slower movement of TCE. For TCE, the sorption coefficient is dependent on the organic carbon content in the solids, which is relatively low in the Southern Sector TCE plume area. Estimates of r_b and K_d are taken from an analysis of TCE transport in the similar soils at C Area (Fogle and Brewer 2001). That model uses a uniform bulk density of

4.19 x 10^4 g/ft^3 (1.48 g/cm^3) and a sorption coefficient of 4.52 x 10^{-8} ft^3/g (1.28 x 10^{-3} cm^3/g). Each of these properties is assumed to be uniform in the model domain. Inspection of equation 2 shows that sorption is an unimportant process when the product of r_b and K_d is much lower than the effective porosity (q). For the cited estimates of r_b and K_d, the product (0.0019) is much lower than the porosity range of typical sediments (0.1 to 0.5). It is therefore expected that sorption is not an important transport process for the Southern Sector TCE plume. Nonetheless, sorption is modeled in the transport simulations.

In simulating past and current conditions within the transport model, degradation of TCE is ignored and the decay rate (l) is set to zero. This is justified by the fact that no significant concentrations of TCE degradation products have been observed in the Southern Sector TCE plume. Natural degradation near discharge locations is addressed in the fourth remedial alternative (sections 2.4.4 and 4.5).

3.2.3 Groundwater Flow Boundary Conditions

Flow boundary conditions provide the sources and sinks of groundwater in the model. Three types of boundaries are used in the Southern Sector model – specified head, head-dependent flux, and specified flux boundaries.

Specified head boundaries are used on many sections of the model perimeter (Figure 3.4). The head values that are specified are based on both the results from a prior large-scale groundwater flow model (Aleman and Noffsinger 2001) and extrapolation from observed head values in A/M Area. The adjustment of the specified head values for calibration is discussed in sections 3.3.1 and 3.4.1.

Tims Branch and its tributaries are modeled as head-dependent flux boundaries using MODFLOW's River and Drain packages (Figure 3.4). The tributaries that are modeled with the Drain package can only receive inflow from groundwater. The streams modeled with the River package can either receive inflow from groundwater or provide outflow to groundwater, depending on the relative positions of the water table and stream stage. The creeks modeled with the River package have sufficient surface water inflow to provide a source of water to underlying aquifers. The head-dependent flux boundaries are placed in the uppermost active model layer. In most areas the uppermost layer is layer 1 (MAAZ), but where the GCCZ outcrops the uppermost layer is layer 2, and where the LLAZ outcrops the uppermost layer is layer 3. The wetlands in discharge areas near Tims Branch are not explicitly modeled, but are instead assumed to be part of the head-dependent flux boundaries.

A specified flux is applied at the model top (uppermost active layer) in upland areas to model precipitation recharge (Figure 3.5). A low-recharge condition is applied where surface structures and paved areas exist. A no-flow condition (specified flux of zero) is specified at the model top in discharge areas, and at the model bottom (base of the CBAZ).

Specified flux withdrawal points are also used to model remediation wells that are already in operation (Figure 1.2). For this model, it is assumed that all remediation well pumping began in 1990. Prior to 1990, remediation well pumping is set to zero.

3.2.4 Solute Sources and Other Transport Boundary Conditions

The nature of the A-014 outfall source is described in section 2.2.3. The source is simulated as a mass flux boundary condition in the transport model. A NAPL source is suspected in the vadose zone below the A-014 outfall, with additional TCE appearing to seep downward from the stream east of the outfall.

In the MT3DMS transport model, a relatively high source concentration is assigned to specified-flux (recharge) cells near the A-014 outfall, and lower concentrations are assigned to the head-dependent flux (river) cells at the upper end of the stream (Figure 3.6). This portion of the stream is higher in elevation than the nearby water table; therefore, water seeps vertically from the stream to the groundwater in this area. The source concentrations are assumed to remain constant in time.

The value assigned for source concentration is treated as a calibration parameter for transport (see section 3.3.2). As shown in Figure 3.6, the final source configuration involved a high concentration in four specified-flux (recharge) cells, a moderate concentration in the uppermost four river cells, and a low concentration over a longer stretch of the discharge stream. For reference, the solubility of TCE in groundwater is approximately 1,100,000 µg/L.

Groundwater flow sinks (discharge-area streams and some specified-head boundaries) are TCE sinks, since the water being removed may contain a concentration of TCE. Also, areas of the flow model that are not associated with the Southern Sector plume are made "inactive" for transport. The areas not in the transport model domain include model cells that are far to the north and west of the A-014 source (Figure 3.2). The CBLC and CBAZ (layers 7 and 8) are also made inactive for transport. Initial simulations made with the entire flow-model domain active for transport indicated that the TCE plume was not moving to these areas above MCLs.

3.2.5 Initial Conditions

The initial concentration in the aquifer domain is set to zero to represent pre-contamination conditions. Transport calibration simulations are started some time in the past (within the range of 1960 to 1970) and are terminated in 2000. The starting time of the transport simulations is treated as a calibration parameter (section 3.3.2). The start time is the time when TCE contamination first reaches the saturated groundwater, and should account for some transit time in the unsaturated zone.

Since the groundwater flow is assumed to be at steady state, initial conditions for hydraulic head are not required.

3.3 Calibration Process

The final flow and transport model of the Southern Sector TCE plume is the culmination of a calibration process that was used to increase model reliability. The process involved the setting of calibration goals for flow and transport simulations, and a trial-and-error approach to achieving the calibration goals through multiple parameter value adjustments and simulations. Two phases of model calibration were performed – groundwater flow and solute transport.

3.3.1 Groundwater Flow

The goal of the flow model calibration was to match observed aquifer heads as closely as possible using reasonable hydraulic properties and boundary conditions. Appropriate observed water levels, or head targets, were determined by WSRC (Rabin 2001) through a careful review of historical data. The time period from 1999 to present was selected, and all measured water levels within that time frame were averaged for each well in the model domain. WSRC removed some water level measurements that were obviously erroneous. WSRC provided 374 potential head targets in the model domain, and indicated the aquifer zone for each target.

Contours of the WSRC-supplied target head values, and early flow model calibration simulations pointed out some possible problems with the target data. After careful review, many of the WSRC-supplied targets were removed. First, all targets which were based on only one head measurement were removed. Then, those targets that exhibited a large variation in observed head during the 1999-to-present time frame were removed (standard deviation greater than three feet). Removing these targets, which were probably based on several erroneous measurements, greatly improved model calibration. The remaining 198 targets were used during groundwater flow calibration. These targets range in head from 180 ft to 240 ft.

For each simulation, a head residual (or error) is computed for each head target by subtracting the observed head from the simulated head. The statistics for these residuals are then compared to commonly accepted criteria for groundwater flow model calibration. Specifically, a calibration is sought that has a mean error within 0.5 ft of zero, and has a root-mean-square error (RMSE) less than one-tenth of the observed head range across the area of interest. For this model, the RMSE should be less than five feet (in the plume area, the maximum observed head is 238 ft, and the minimum is 187 ft). The RMSE is calculated by squaring each residual, taking the mean of the squares, and then taking the square root of that mean (when the mean error is zero, the RMSE is the same as the standard deviation). Another measure of calibration quality is the mean-absolute error (MAE), which is calculated as the mean of the absolute value of each residual. The MAE is less affected by extreme outliers. When the MAE is much lower than the RMSE, a few poorly-matched head targets are probably having a large effect on the statistics.

Head calibration alone is usually not sufficient to ensure that a groundwater flow model is a reasonable representation of reality. Another goal of groundwater flow calibration should be to match observed groundwater discharge conditions. For the Southern Sector model, WSRC (2001) provided baseflow measurements at two locations along Tims Branch – one at Road 2 and one at Road C – about 12,000 ft apart. Between these two locations, baseflow in Tims Branch increases from 2.35 cfs to 5.51 cfs. Since the Road C crossing is south (downstream) of the current study area, and since flow from the eastern side of Tims Branch also contributes to its baseflow, the baseflow gain between these stations cannot directly be used as a calibration target. However, the modeled flow to Tims Branch and its tributaries can be checked for reasonableness based on observed conditions. In the study area, groundwater flow to Tims Branch from the western side of the model should probably be about 1 cfs or less.

Calibration was accomplished by adjusting model parameters from their assumed (initial) values, within reasonable limits, until the model matches observed conditions as well as possible. In this analysis, the main parameters are the horizontal and vertical hydraulic conductivities of the different aquifer zones and confining units. Initial values for these parameters (Table 3.1) were based primarily on a prior model study that included the Southern Sector of A/M Area (Aleman and Noffsinger 2001). Those conductivity values were in turn based on the results of field tests (summarized in Rabin 2001) and on calibration of that groundwater flow model. The results of early calibration simulations with the current model pointed out the need for zonation (discrete spatial variation) of hydraulic conductivity in some areas of the model.

Groundwater flow boundary conditions were also adjusted during calibration in order to reproduce observed conditions. Not surprisingly, the initial recharge rate of 12.5 in/yr was found to be too high to match observed conditions in the relatively dry years of 1999-2000. Also, the original specifications for hydraulic head on model boundaries had to be adjusted to allow for calibration. The original values were based on the more regional model (Aleman and Noffsinger 2001). Adjustments were made by extrapolating trends from head targets near model boundaries.

After reproducing the regional-model head field, flow paths from the A-014 outfall source area were verified to coincide with the observed TCE plume location. The flow-path analysis was also used to verify that the travel times for particles through the aquifer were reasonable (i.e., the current extent of the plume could be attained in the period between source release and now). This part of the flow model calibration depends on the assigned values for recharge, hydraulic conductivity, and effective porosity (Table 3.1).

Table 3.1 Model Parameters and Initial Values

Parameter	Initial Value
Hydraulic Conductivity	MAAZ: K_x = 14 ft/d, K_z = 0.7 ft/d GCCZ: K_x = 0.04 ft/d, K_z = 0.002 ft/d ULLAZ: K_x = 44 ft/d, K_z = 2.2 ft/d LLLAZ: K_x = 44 ft/d, K_z = 2.2 ft/d CBUC: K_x = 0.06 ft/d, K_z = 0.003 ft/d CBMS: K_x = 70 ft/d, K_z = 3.5 ft/d CBLC: K_x = 0.06 ft/d, K_z = 0.003 ft/d CBAZ: K_x = 50 ft/d, K_z = 4.0 ft/d
Effective Porosity	20% in aquifer zones 40% in GCCZ, CBUC, CBLC
Dispersivity	25 ft (longitudinal) 2.5 ft (horizontal-transverse) 0.25 ft (vertical)
Bulk Density	4.19×10^4 g/ft^3
Sorption Coefficient	4.52×10^{-8} ft^3/g
Upland Recharge Rate	12.5 in/yr
River & Drain Conductance	5000 ft^2/d/ft
Specified Heads on Model Perimeter	Interpolated from model results of Noffsinger and Aleman (2001)
TCE Source Concentration	1,100,000 µg/L (A-014 recharge) 11,000 µg/L (upper discharge stream) 10 µg/L (middle discharge stream) (See Figure 3.6)
Source Release Date (to saturated zone)	1960

3.3.2 Solute Transport

After calibration of the simulated groundwater flow field, calibration to the current TCE plume was conducted. The observed/inferred concentration contour map (Figure 2.3) provided the target for the transport calibration. The goal was to match this plume shape and magnitude as closely as possible using a specified mass-flux source at the A-014 outfall and at the discharge stream. The calibration was judged by visual comparison of simulated plumes to the plumes in Figure 2.3.

The main transport calibration parameters included source start time, source concentration, effective porosity, and dispersivity. Table 3.1 lists the initial values assigned for these parameters. The source start time refers to the time when significant TCE contamination reached the water table and is some time after 1952, when the A-014 outfall was first used. During calibration, the time was changed to improve the match to the observed plume. The source concentration at the A-014 outfall was initially assumed to be at the solubility limit for TCE (1,100,000 µg/L), with lower concentrations beneath the sediments in the discharge stream. WSRC (Rabin 2001) suggested that the effective porosity of aquifers is approximately 20% and the effective porosity of aquitards is approximately 40%.

3.4 Calibration Results

3.4.1 Groundwater Flow

Groundwater flow calibration was achieved by lowering the recharge rate from 12.5 in/yr to 9 in/yr, by introducing zones of hydraulic conductivity (Figure 3.7), and by adjusting the values of conductivity in these zones. Through trial-and-error simulation, the model was adjusted until a final RMSE of 4.7 ft was achieved (Table 3.2). This value for RMSE is within the calibration goal of 5 ft. Figure 3.8 shows the modeled head field in the aquifer zones, and indicates the location and magnitude of computed head residuals. Plots of modeled vs. observed head and residual vs. observed head are included in Figure 3.9. The overall water budget for this model is shown in Figure 3.10. Tims Branch receives about 0.5 cfs in this simulation.

Particle tracking from the A-014 outfall source in the calibrated model (Figures 3.11 and 3.12) indicated a match to the south-southeasterly flow of the observed TCE plume (more easterly in the shallow aquifers and more southerly in the CBMS). The travel time for the particles from the source to discharge locations varied between 16 years (towards upper reaches of Tims Branch) and 65 years (towards the southern boundary in the CBMS). These are reasonable results given the time period since assumed source presence and the current shape of the Southern Sector plume.

Table 3.2 Head Calibration Statistics

Statistic	Value
Number of Head Targets	198
Mean Error	0.35 ft
Mean Absolute Error (MAE)	3.6 ft
Root Mean Square Error (RMSE)	4.7 ft

3.4.2 Solute Transport

Initial simulations of TCE transport indicated a plume of greater extent than the observed/inferred plume. Adjustments were made, in trial-and-error fashion, to the dispersivity, source start time, and source concentration values. The best calibration was achieved in a simulation that had the source starting in 1970 with the original source concentrations. Relatively low dispersivity values of 5 ft (longitudinal), 0.5 ft (horizontal-transverse), and 0.05 ft (vertical) were used for the final calibration. These values are equivalent to those used in the modeling studies for the C-Area groundwater OU (Fogle and Brewer 2001) and the C-Area Burning/Rubble Pit (GeoTrans 2001).

The modeled plume for 2000, shown in each contaminated aquifer zone in Figure 3.13, is somewhat similar to the observed/inferred plume in Figure 3.8. The match is certainly less than perfect, but is suitable for comparison of remedial alternatives. The over-extensiveness of the low-concentration portion of the modeled plume may be due in part to numerical error (artificial dispersion). This model uses a finite difference solution method for transport, which tends to introduce this type of error when the dispersivities are set to low values (see section 3.1).

In this calibrated transport simulation, the total mass flux into the model from the source is about 420 kg/yr. The model uses a calculated transport time-step size of around 100 days.

3.4.3 Calibrated Values for Model Parameters

The specifications of the calibrated flow and transport model are listed in Table 3.3. This model is considered to be a calibrated model, but it is recognized that other model specifications could also result in a model that is considered to be at least as well calibrated.

Table 3.3 Specifications for the Calibrated Southern Sector TCE Model

Parameter	Value
Hydraulic Conductivity	See Figure 3.7
Porosity	20% in aquifer zones 40% in GCCZ, CBUC, CBLC
Dispersivity	5 ft (longitudinal) 0.5 ft (horizontal-transverse) 0.05 ft (vertical)
Bulk Density	4.19×10^4 g/ft^3
Sorption Coefficient	4.52×10^{-8} ft^3/g
Upland Recharge Rate	9 in/yr
River & Drain Conductance	5000 ft^2/d/ft
Specified Heads on Model Perimeter	Interpreted from measured head in A/M Area and from model results of Noffsinger and Aleman (2001)
TCE Source Concentration	1,100,000 µg/L (A-014 recharge) 11,000 µg/L (upper discharge stream) 10 µg/L (middle discharge stream) (See Figure 3.6)
Source Release Date (to saturated zone)	1970

4.0 NUMERICAL MODEL PREDICTIONS

In this section, the results of predictive simulations are presented. These simulations show the expected future development of the TCE plume under different scenarios. As a base case, a no-action scenario is considered. Then the existing remedial actions – remediation wells and ARWs – are simulated. Finally, several remedial alternatives currently under consideration are modeled to give an idea of their relative effectiveness at reducing the size of the TCE plume, reducing the amount of TCE mass that discharges to Tims Branch, and reducing the maximum concentration of discharging groundwater at potential exposure points.

4.1 No Action

For the Southern Sector TCE plume, the no-action scenario is only a hypothetical case, since several remedial actions have already been put into place, including a pump-and-treat system that has been in operation for over 10 years. However, the no-action scenario is instructive for comparison because it helps to show how effective existing remedial actions are as compared to potential new remedial alternatives.

For the no-action simulation the flow and transport model is re-executed without any remediation well pumping. Also, the end time is extended from 2000 to 2050. The modeled plume in 2050 is shown in Figure 4.1.

4.2 Remediation Wells

The effect of the existing remediation well pumping on the TCE plume is seen by extending the calibration simulation out to 2050 and comparing the results with the no-action simulation. Note that the calibration simulation (as well as this simulation) includes remediation well pumping, beginning in 1990, but does not include the recently-begun recirculation well pumping or any future remedial action.

The future plume for this scenario is shown in Figure 4.2. Note that, relative to the no-action alternative (Figure 4.1), the remediation wells are predicted to effectively remediate the TCE plume.

In Figure 4.3, three types of plots are presented. The top graph shows the mass of the TCE plume in the aquifer over time for the no-action and remediation well scenarios. It shows that the TCE plume mass is significantly reduced by remediation wells.

The second plot on Figure 4.3 shows the simulated mass flux to Tims Branch and its tributaries during the simulation, not accounting for biodegradation in wetland sediments. By removing a portion of the aquifer mass, the remediation wells reduce the amount of TCE that discharges to Tims Branch.

The last plot on Figure 4.3 shows the maximum concentration simulated at any discharge location along Tims Branch and its tributaries. This concentration is sometimes used as an exposure-point concentration in risk calculations, because it is the maximum concentration that would reach a surface water body or an environmental receptor at the ground surface. The remediation wells also reduce the predicted discharge concentrations relative to the no-action case. The TCE concentrations shown in this plot may be much higher than the actual TCE concentrations at discharge locations, because the natural degradation of TCE has not been taken into account (see section 4.6).

4.3 Recirculation Wells

Airlift recirculation wells are essentially in-well pump and treat systems. Contaminated groundwater is drawn into a lower screen, passed upward through an in-well air stripper or carbon absorption unit, and reinjected via an upper screen. Twelve ARWs are now in operation in the Southern Sector TCE plume (Figure 1.2).

In the numerical model, ARWs are modeled as two wells – one pumping and one injection. An additional module, called the recirculation-well package, was added to the MT3DMS code so that injection-well concentrations could be made a function of pumping-well concentrations (see section 3.1).

The twelve ARWs were added to the Southern Sector model to simulate current conditions. Figure 4.4 shows the simulated capture zones (in each aquifer zone) for the ARWs and the remediation wells in this scenario. When the twelve ARWs are included in the model (from 2000 to 2050), the resulting plume is less extensive (Figure 4.5) than in the prior scenarios.

In this simulation, eleven of the recirculation wells have an assumed TCE removal efficiency of 65% and the remaining well, SSR-12, has an assumed removal efficiency of 90%. The total mass removal by this system of ARWs is shown in Figure 4.6. The graph shows that the ARWs remove significantly less mass than the upgradient remediation wells.

Additional simulations were made to show the effect of changing SSR-9, SSR-10, and SSR-11 to multi-stage ARWs (assumed 90% efficiency), and to test the effect that higher assumed efficiencies (80% for SSR-1 through SSR-7, 95% for SSR-9 through SSR-12) would have. These changes had only a small effect on the simulated aquifer mass, discharge flux, and discharge concentrations (Figure 4.7). Overall, the simulations indicate that the recirculation wells provide a small improvement in remediation effectiveness relative to remediation wells only.

4.4 Source Reduction

Two source-area remediation scenarios were considered – complete source removal, and 60% effective SVE/AS. In each case, the existing remediation wells and recirculation wells are simulated (the base-case ARW efficiencies are used). Source removal is simulated by setting all source concentration values to zero, and 60%-effective SVE/AS is simulated by setting the A-014 outfall source concentration to 440,000 µg/L. The resulting plumes for these two simulations are shown in Figures 4.8 and 4.9. Figure 4.10 shows the effect of the source remediation alternatives on plume mass, mass discharge, and discharge concentration.

4.5 Phytoremediation

Physical withdrawal of water from the Southern Sector plume near Tims Branch is also a potential remedial action. The groundwater would be withdrawn from the aquifer and the TCE treated by ex-situ phytoremediation. This could be accomplished by spray irrigating vegetation, promoting volatilization and phytoremediation.

In the model, this phytoremediation action is simulated via pumping wells. Various different pumping scenarios were tested, using different well locations and different pumping rates, with the goal of reducing discharge concentrations and keeping aquifer drawdown to a few feet or less.

The best scenario involved 16 phytoremediation wells pumping a total of 450 gpm from the ULLAZ. The simulated capture zone for this phytoremediation system is shown in Figure 4.11. The resulting TCE plume is shown in Figure 4.12. Note that this scenario also includes the remediation wells and ARWs (but no source remediation). Because the phytoremediation wells are located in a low-concentration area, the rate of mass removal is low (Figure 4.13) compared to other alternatives. The mass, mass-flux, and concentration vs. time curves for this scenario are shown in Figure 4.14.

4.6 Monitored Natural Attenuation

Natural degradation of TCE to cDCE and other organic compounds is likely occurring in the shallow sediments near discharge points at Tims Branch. Analytical data in these areas are needed to clearly show this and to estimate the appropriate attenuation factor (see the RACM discussion in section 2.4.4). Any remedial alternative that involved monitored natural attenuation (MNA) would take credit for this degradation.

In order to account for MNA, no additional numerical simulations are made. Rather, the model-predicted discharge concentrations and discharge mass flux are adjusted to account for TCE degradation in the wetland sediment. As a first guess, the attenuation factor is assumed to be 0.1.

Note however that site-specific data are needed to justify any attenuation factor, and that dechlorination of TCE can result in higher levels of cDCE, tDCE, and VC.

Figure 4.14 shows the effect that an assumed 0.1 attenuation factor would have on two of the modeled scenarios. If the attenuation factor is shown to be 0.1 or lower, and other remedial actions are continued or implemented, then it is likely that discharge concentrations of TCE along Tims Branch will be below the MCL of 5 µg/L.

5.0 CONCLUSIONS

This numerical model of TCE transport in the Southern Sector of A/M Area uses reasonable assumptions and is qualitatively calibrated to the existing TCE plume. It is used here, and can be used in the future, to give an indication of the effectiveness of different remedial alternatives. The results can also be used to perform a risk analysis for TCE exposure.

Uncertainties exist for many of the site conditions that define the model input parameter values. Fortunately, many of the parameters that are least defined by the model calibration (such as sorption coefficient) have little effect on the predicted results.

The transport model calibration shown in this report is less than ideal, and therefore the predicted future TCE plumes should be recognized as rough estimates. The transport calibration suffers due to lack of information about the source area, an inexact interpreted plume representation that is used as the calibration target (interpretation of this plume may be complicated by other nearby sources), and perhaps numerical error resulting from the finite-difference method of solution (other methods were attempted to limit this error, but none proved satisfactory). While there is considerable uncertainty in the exact size, shape, and concentration of the future Southern Sector TCE plume, the simulated relative effectiveness of the different modeled scenarios is valid.

The remediation wells that have been in operation for over 10 years near the A-014 outfall source are capturing much of the TCE plume and helping to reduce the mass of TCE in the aquifer. According to the model results, this pump-and-treat system has been and will continue to be an effective remedial action for the Southern Sector plume.

The ARWs that began operation more recently are effective at remediating TCE in the LLAZ groundwater downgradient of the remediation wells. These ARWs are not as effective as the remediation wells in removing mass because the plume concentrations are lower near the ARWs.

Cleanup of the A-014 outfall source area would have benefits in the long term. As long as a source is present, remedial action in Southern Sector is likely to continue. If the source is effectively remediated, then it may become feasible to shut off some or all of the remediation wells and ARWs. If complete source removal is not feasible, then a vadose-zone extraction action may be useful to minimize the release of TCE into the saturated groundwater. Indeed, an SVE/AS system is already in operation in the area for this purpose.

Though not indicated on the observed/inferred TCE plume maps from WSRC (Rabin 2001) (Figure 2.3), TCE has been observed near the seepline at Tims Branch (Jackson et al. 2000), and the model predicts current and future discharge of TCE near Tims Branch. One proposed remedy for this distal portion of the Southern Sector plume is ex-situ phytoremediation. Model simulations were made to show that removal of water just prior to discharge would significantly lower the mass discharge and discharge concentration of TCE in seeps along Tims Branch. In the model, 16 wells were used, with a total pumping rate of 450 gpm. It is likely that an optimized collection system could be equally effective at a lower withdrawal rate.

Data to demonstrate the occurrence of natural biodegradation are unavailable for this site. Experience at other areas of SRS (e.g., C-Area, GeoTrans 2001) suggests that TCE biodegradation may be an important process in the wetland sediments of discharge areas. An MNA remedial action would take credit for this natural process of TCE degradation, which could reduce discharge concentrations by a factor of 10 to 100. But until appropriate data are collected and analyzed, MNA cannot be a defensible alternative.

The portion of the TCE plume that has reached the CBMS, below the LLAZ, is unaffected by any of the proposed remedial actions. This part of the plume may pose little risk of exposure since it does not outcrop in the local area, and would therefore be dispersed significantly. However, it seems reasonable to attempt to ascertain the eventual fate of this portion of the plume, perhaps using analytical calculations.

Additional data collection, source characterization, and plume delineation will be essential for improving the understanding of solute transport at A/M Area. The site is complicated by multiple sources, which are not fully understood, and by co-mingling of the groundwater contamination plumes. Further data analysis would also help to optimize the operation of remedial systems such as pump-and-treat systems, ARWs, and phytoremediation. The model developed here could also be used as a tool in the optimization process. The process would help define when certain remedial components should be started up and/or shut down.

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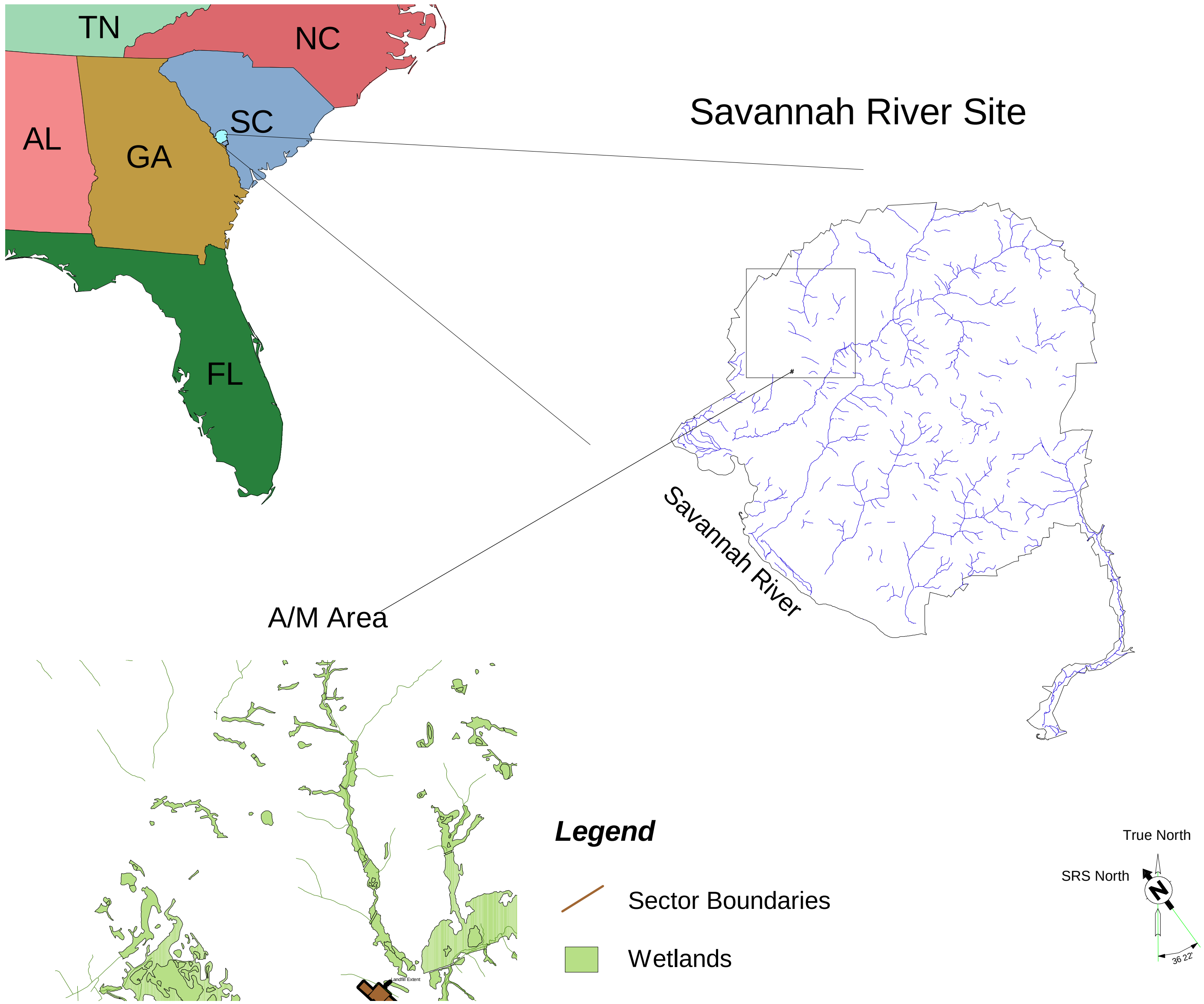


Figure 1.1 A/M Area Southern Sector Site Location

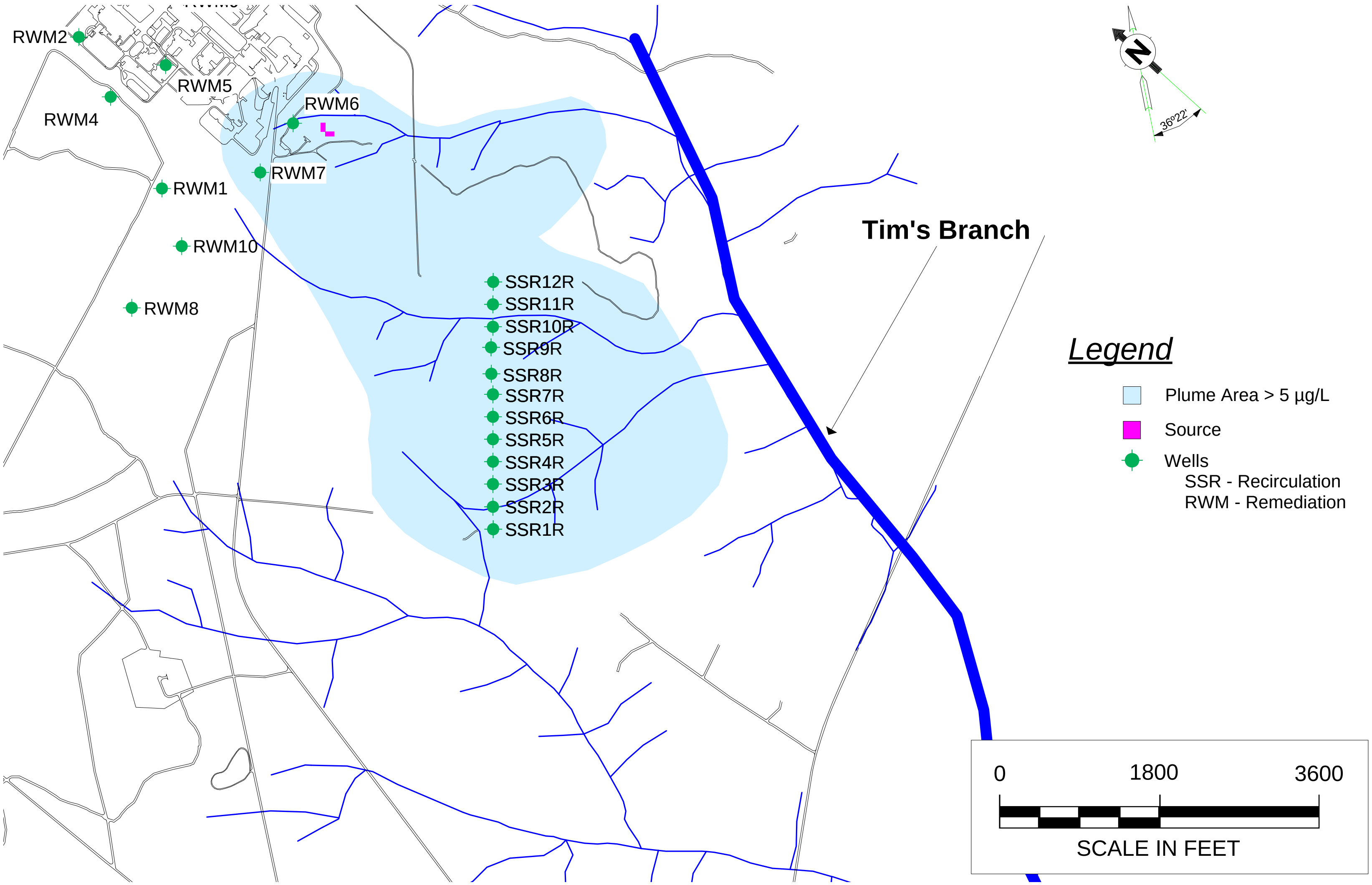
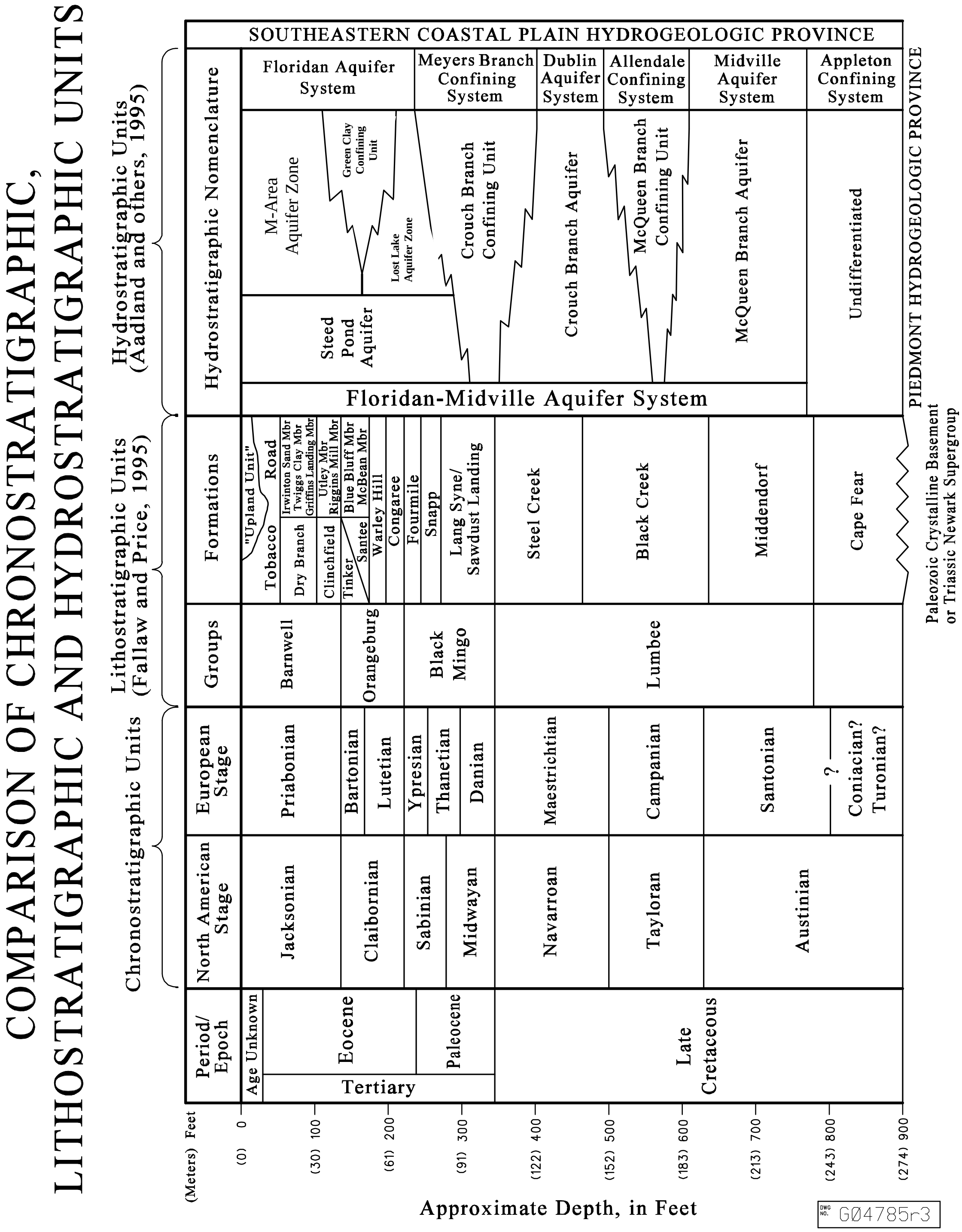


Figure 1.2 Southern Sector TCE Plume Area



Note: From Fogle and Brewer (2001)

Figure 2.1 SRS Geologic Stratigraphy

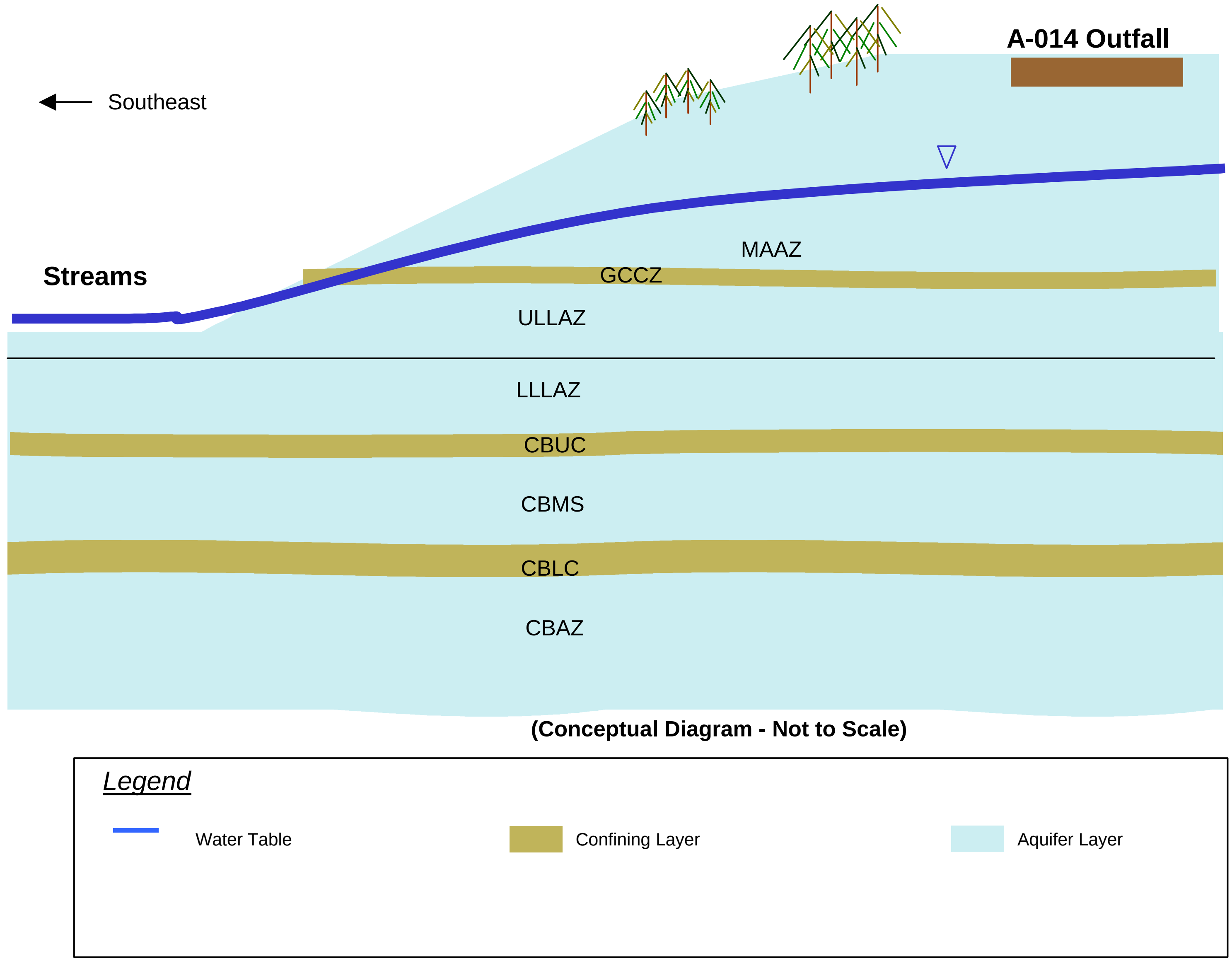


Figure 2.2 Modeled Hydrostratigraphic Layers

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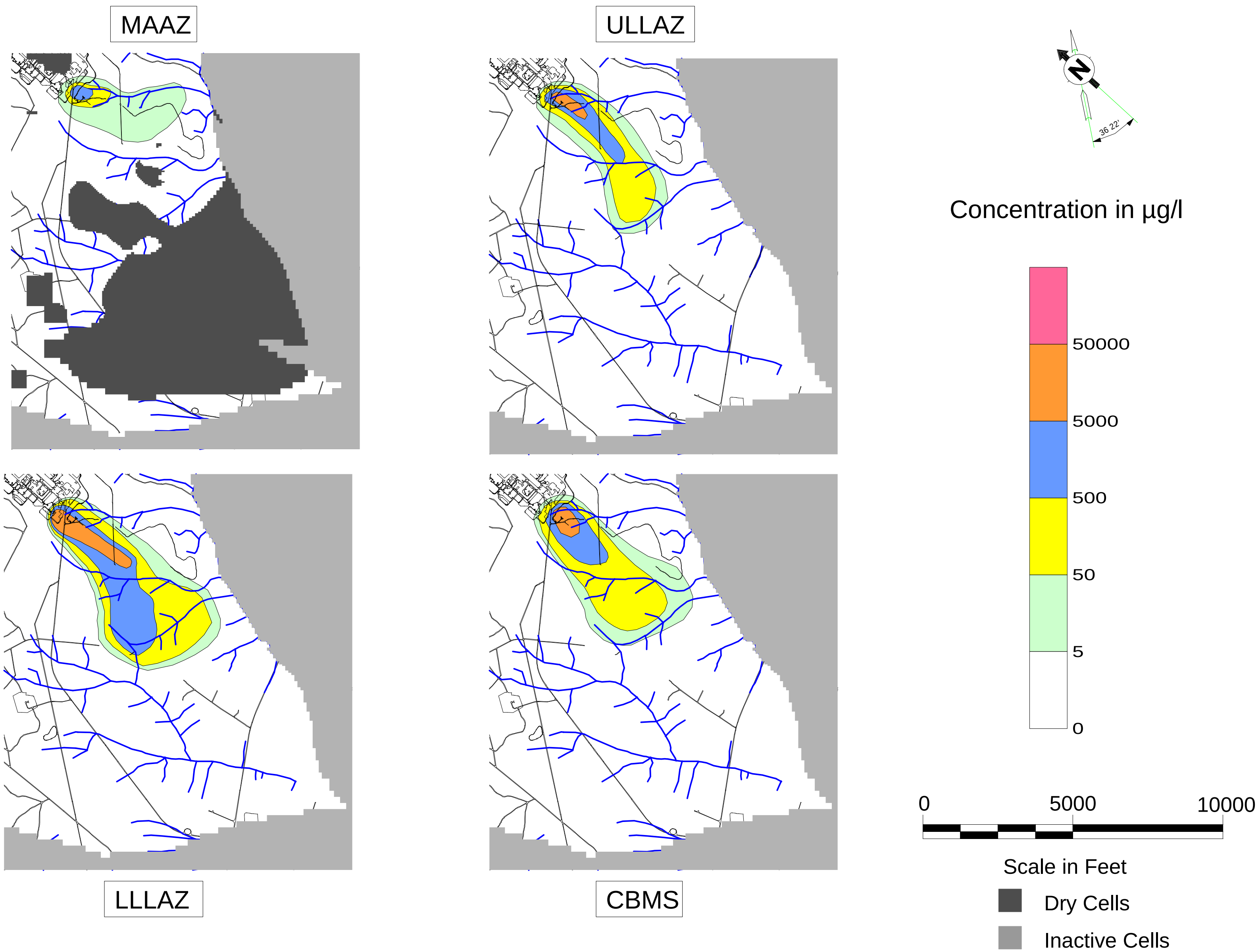

Figure 2.3 Observered/Inferred TCE Plume in the Southern Sector of A/M Area

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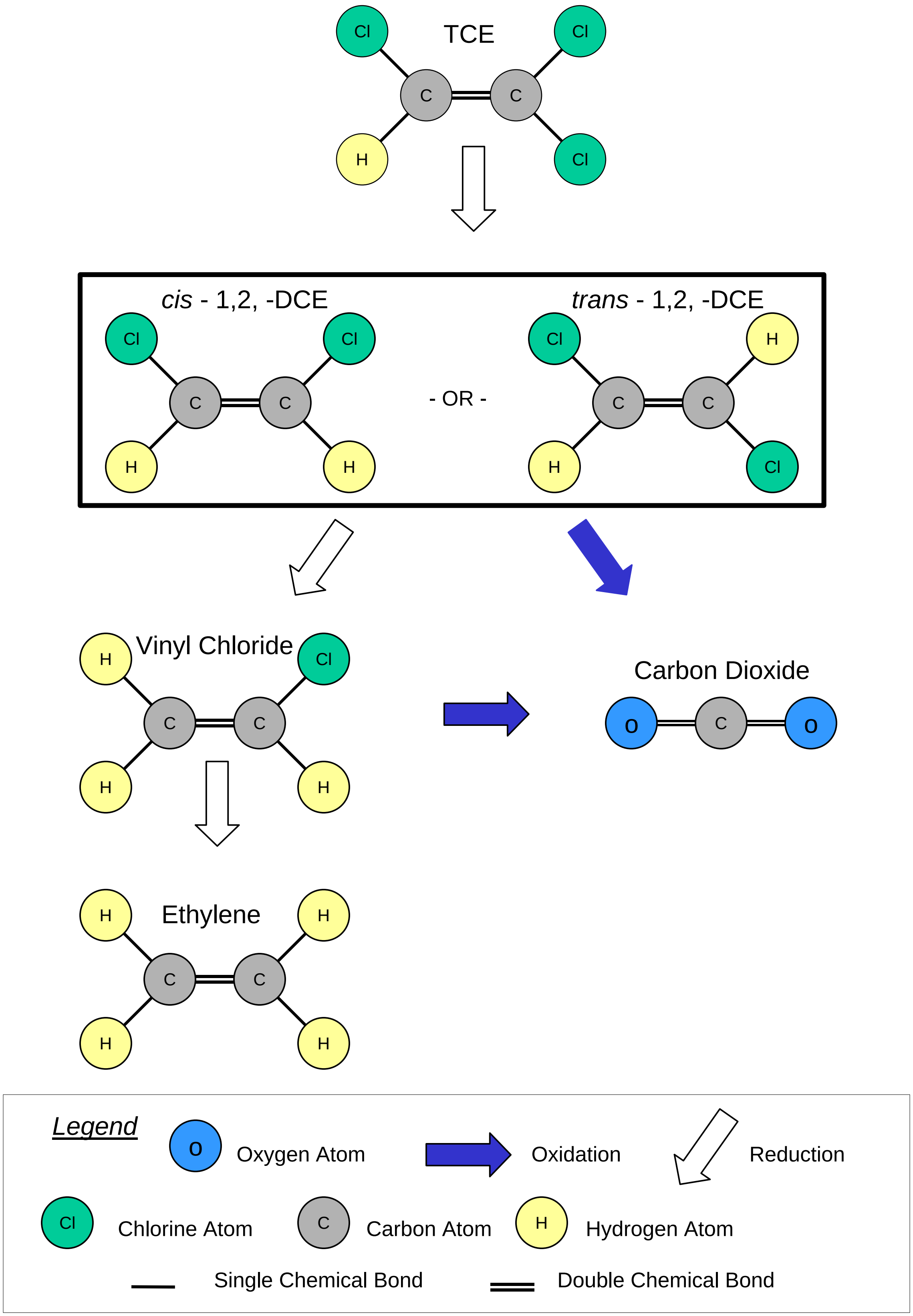

Figure 2.4 Biodegradation Steps for TCE

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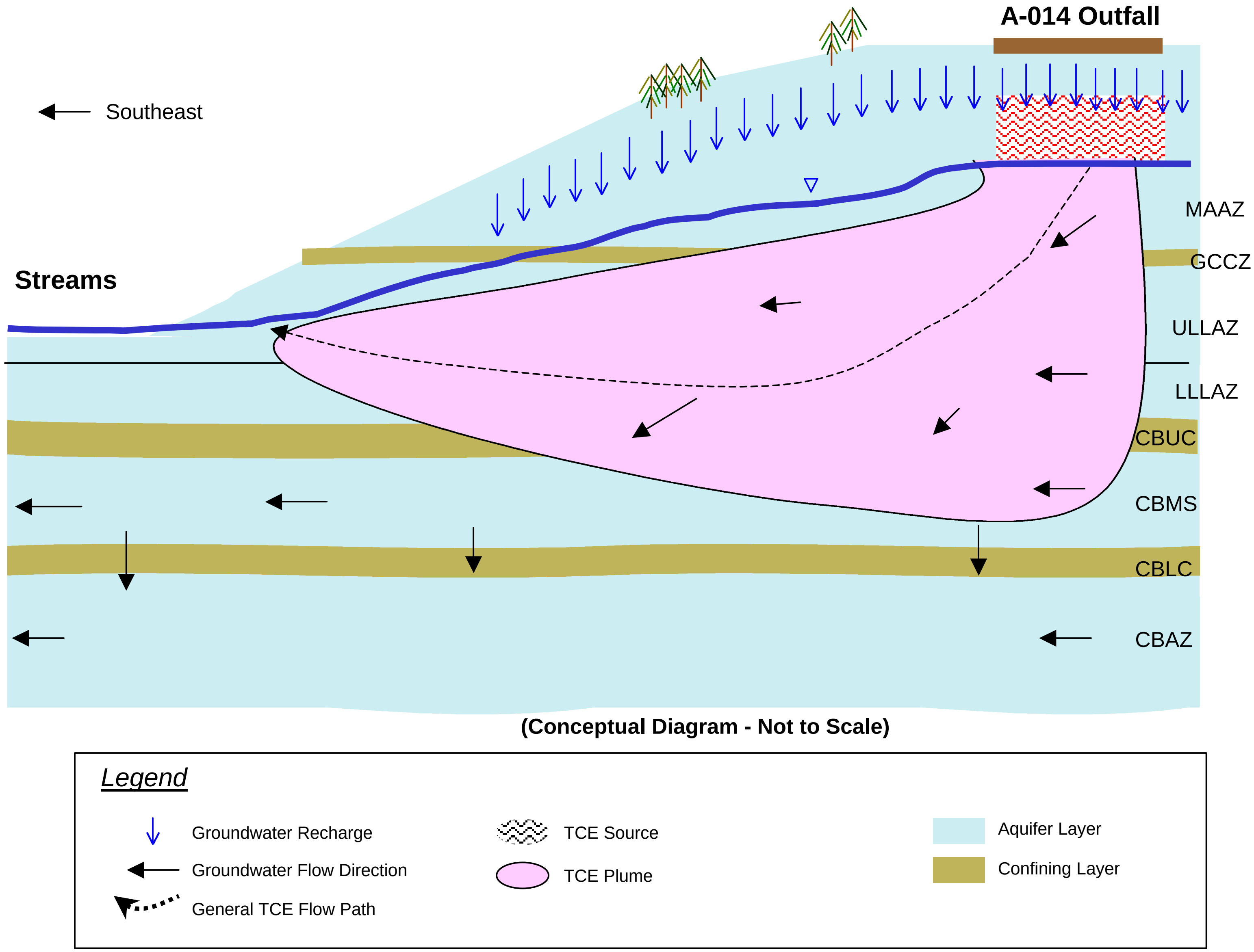


Figure 2.5 Hydrogeologic Conceptual Model for the Southern Sector of A/M Area

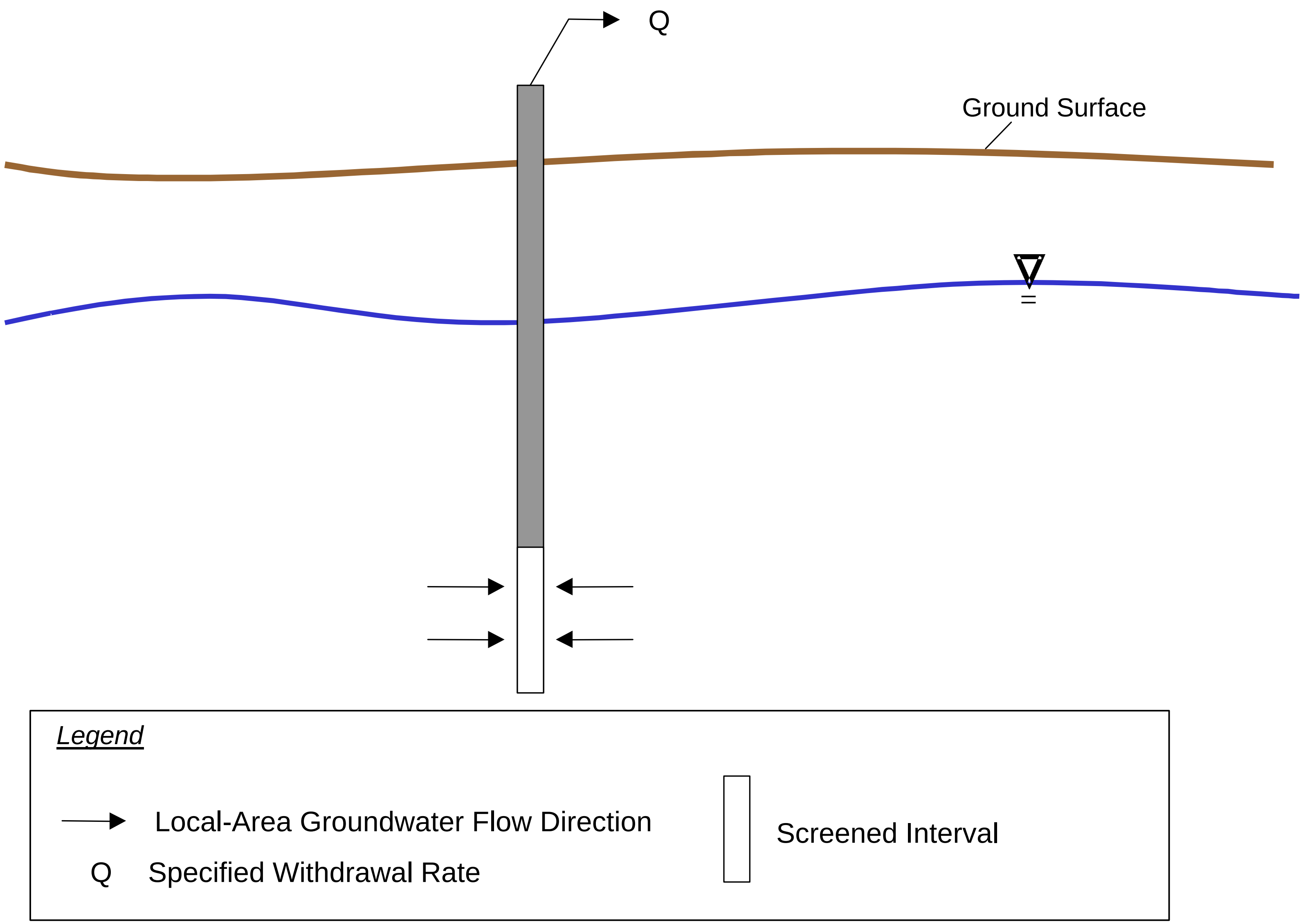


Figure 2.6 Remedial Alternative Conceptual Model for Remediation/Phytoremediation

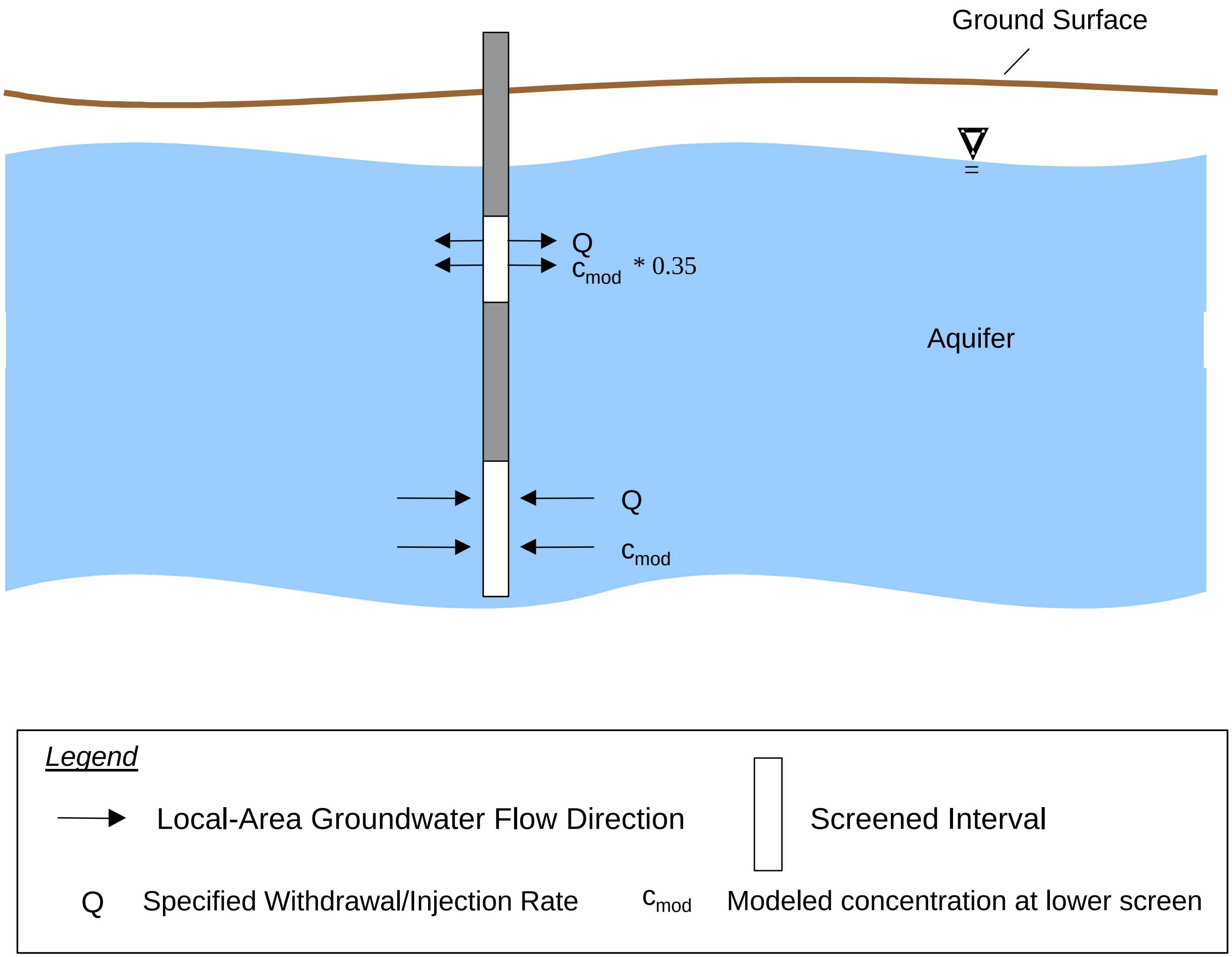
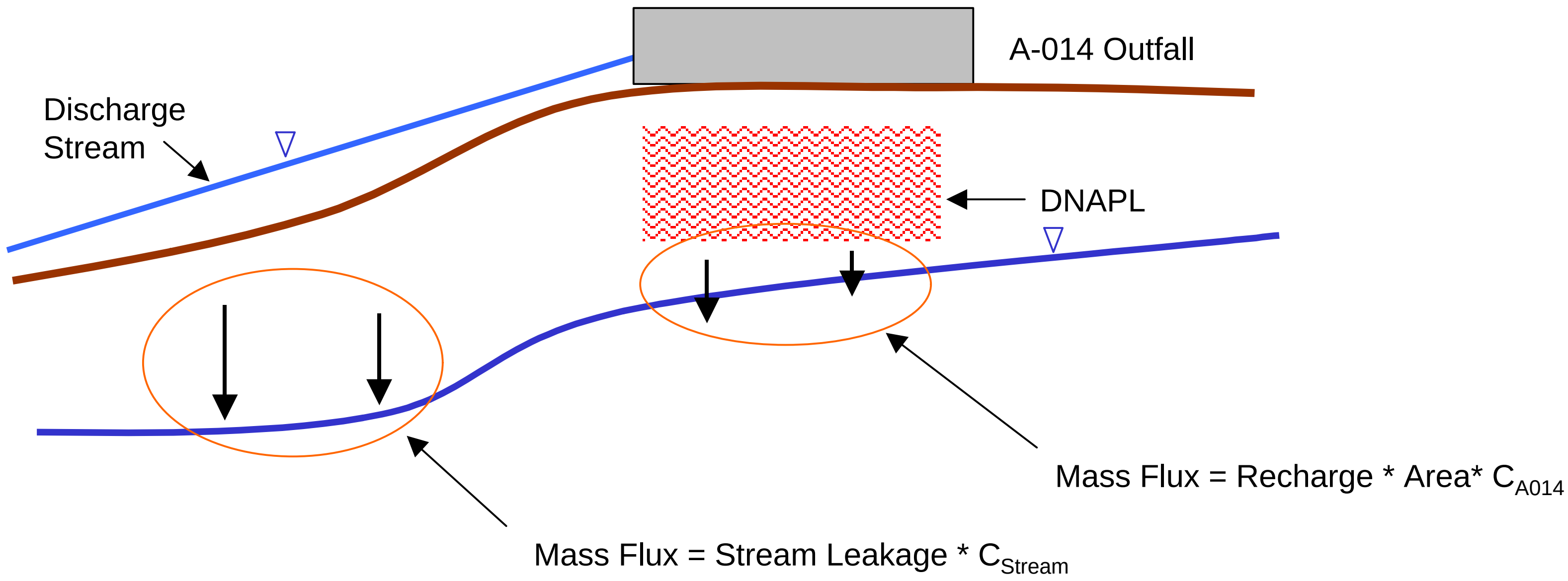


Figure 2.7 Remedial Alternative Conceptual Model for a Recirculation Well



Source Removal : $C_{A014}^{(new)} = 0, C_{Stream}^{(new)} = 0$

Source Reduction : $C_{A014}^{(new)} = C_{A014} \times 0.4$

Legend

→ Mass Flux

C_{A014} Modeled source concentration at A-014 Outfall

C_{Stream} Modeled source concentration at Stream

Figure 2.8 Remedial Alternative Conceptual Model for Source Reduction

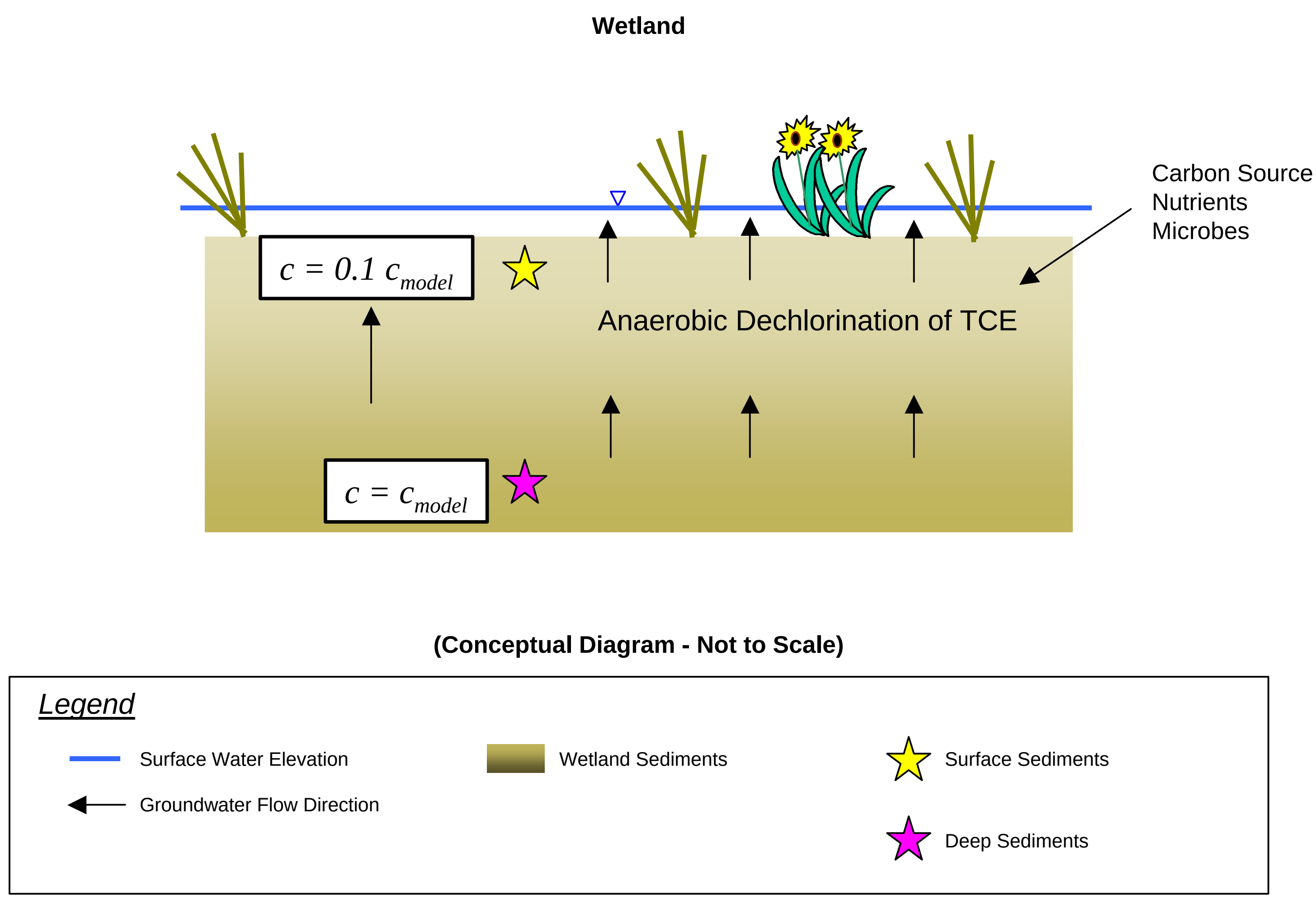


Figure 2.9 Remedial Alternative Conceptual Model for Monitored Natural Attenuation

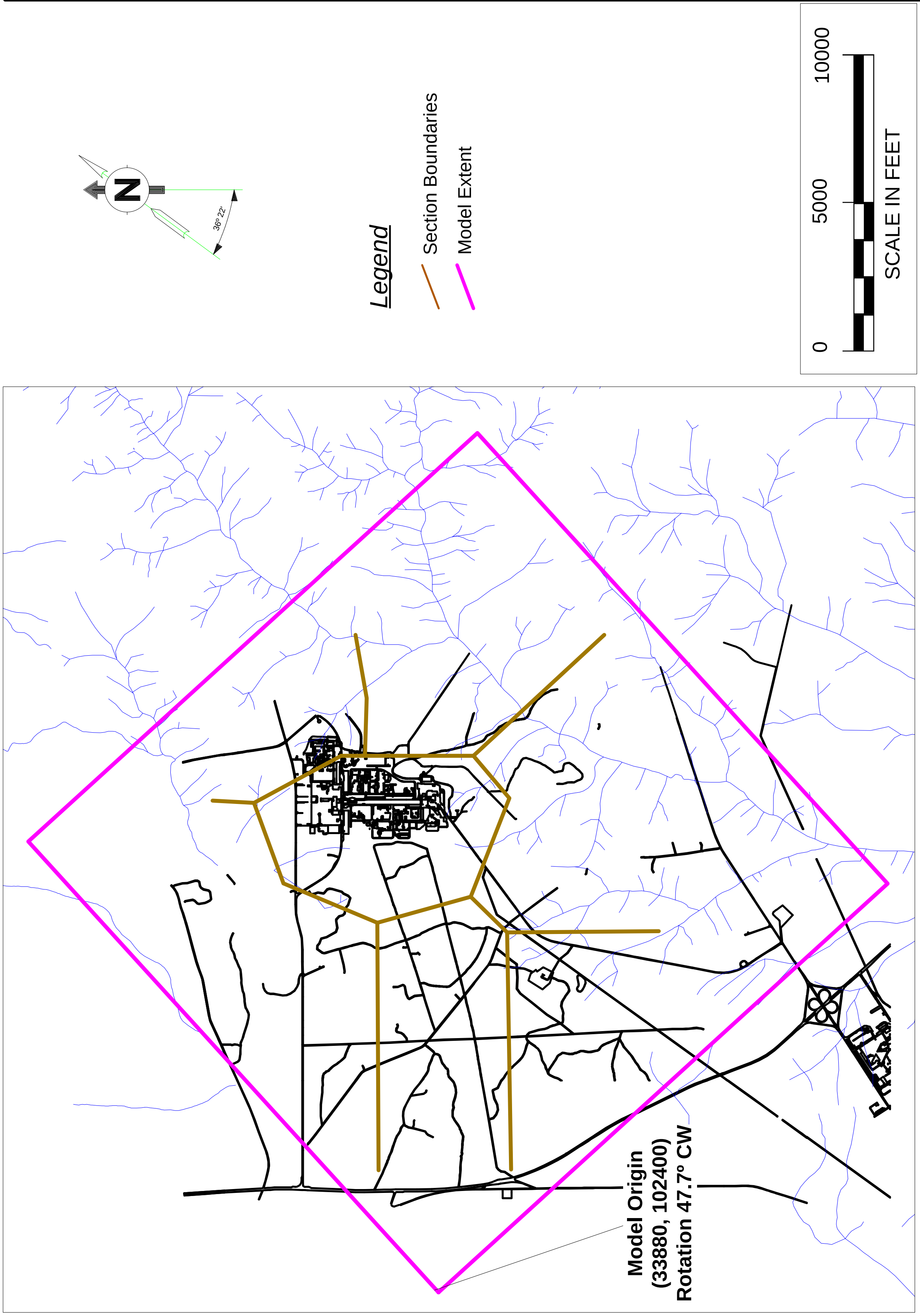


Figure 3.1 Location of the Numerical Model

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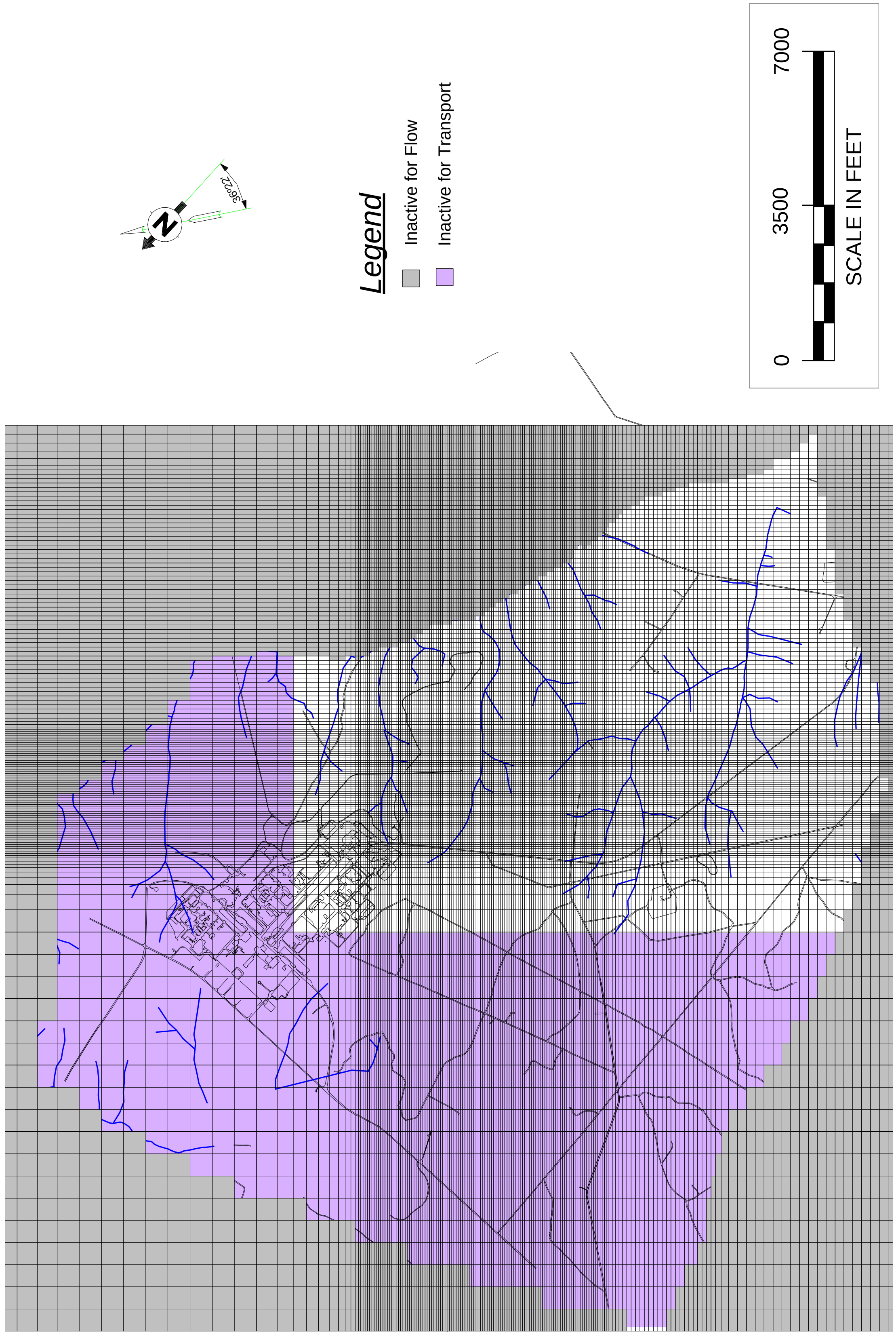

Figure 3.2 Model Grid

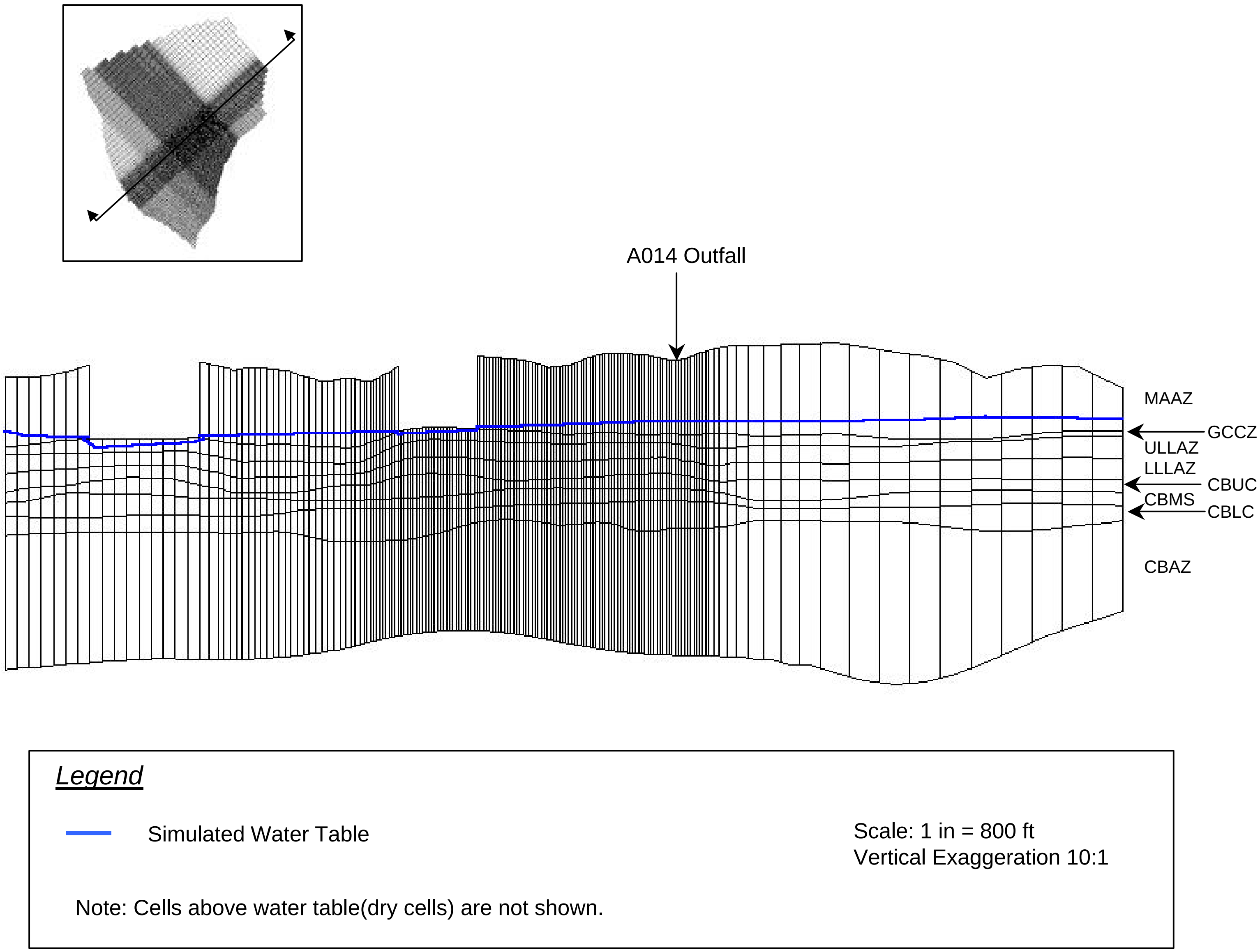

Figure 3.3 Representative Cross-Section Through Column 43

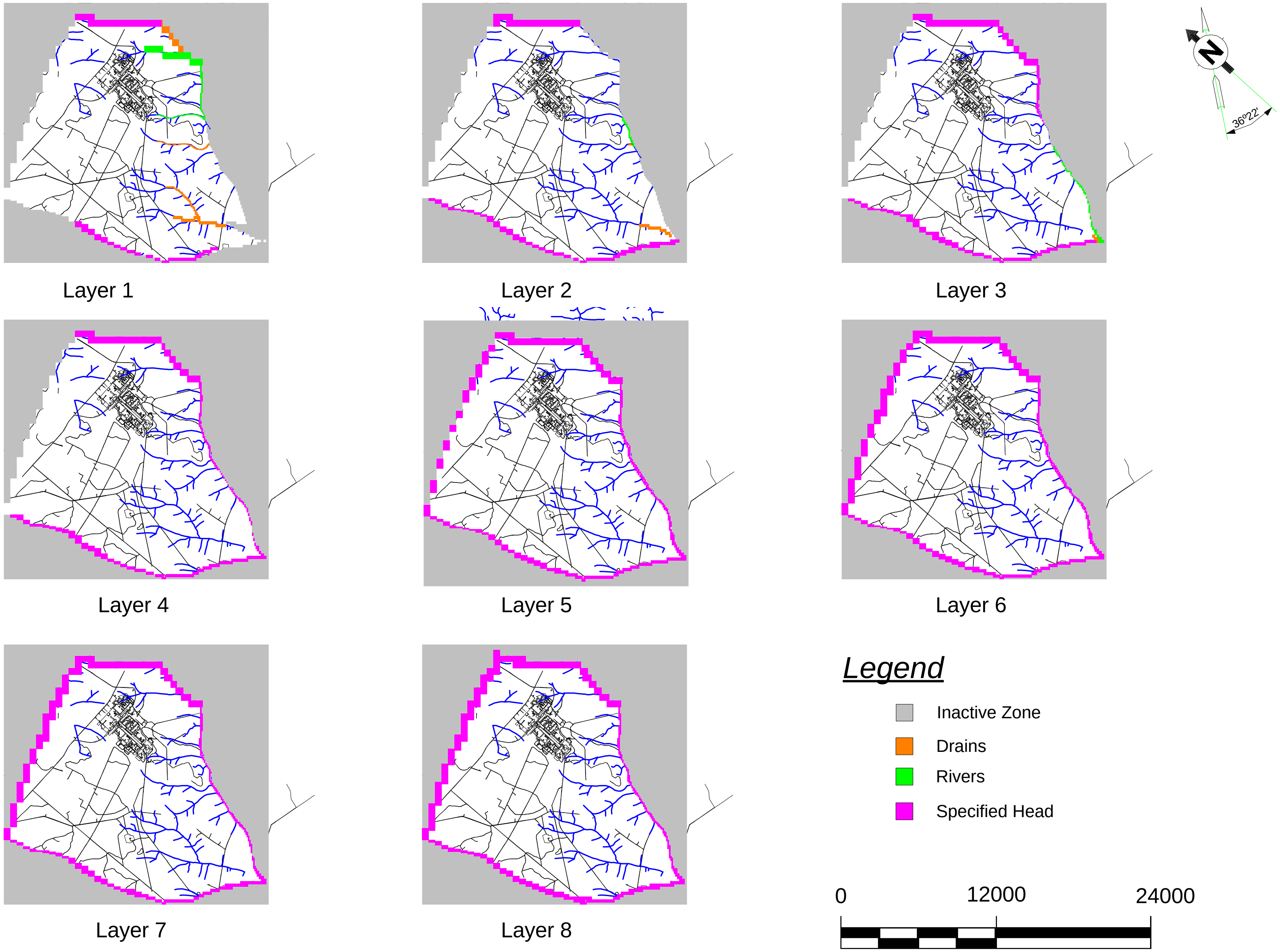

Figure 3.4 Specified-Head and Head-Dependent Boundary Conditions

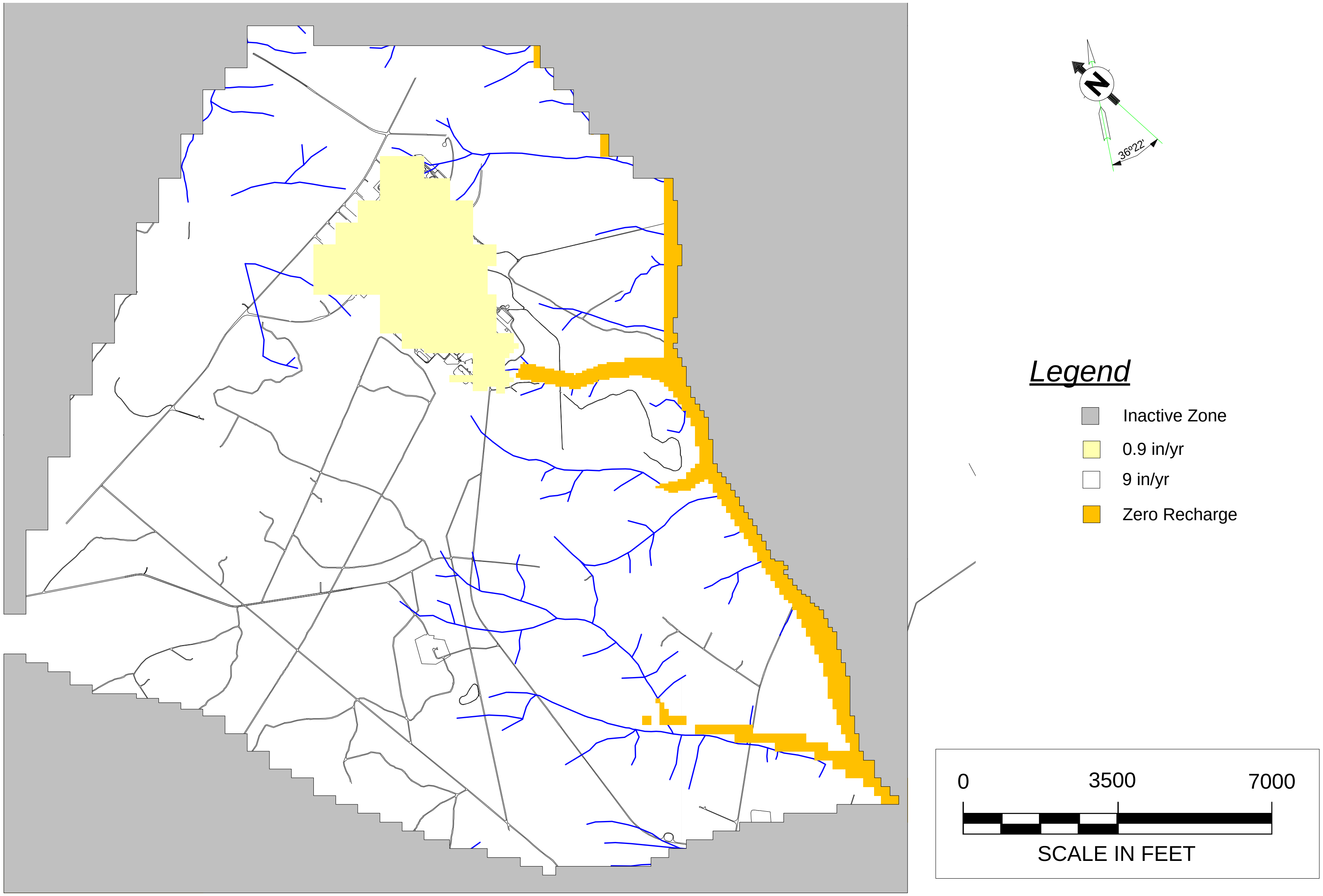

Figure 3.5 Recharge Zones

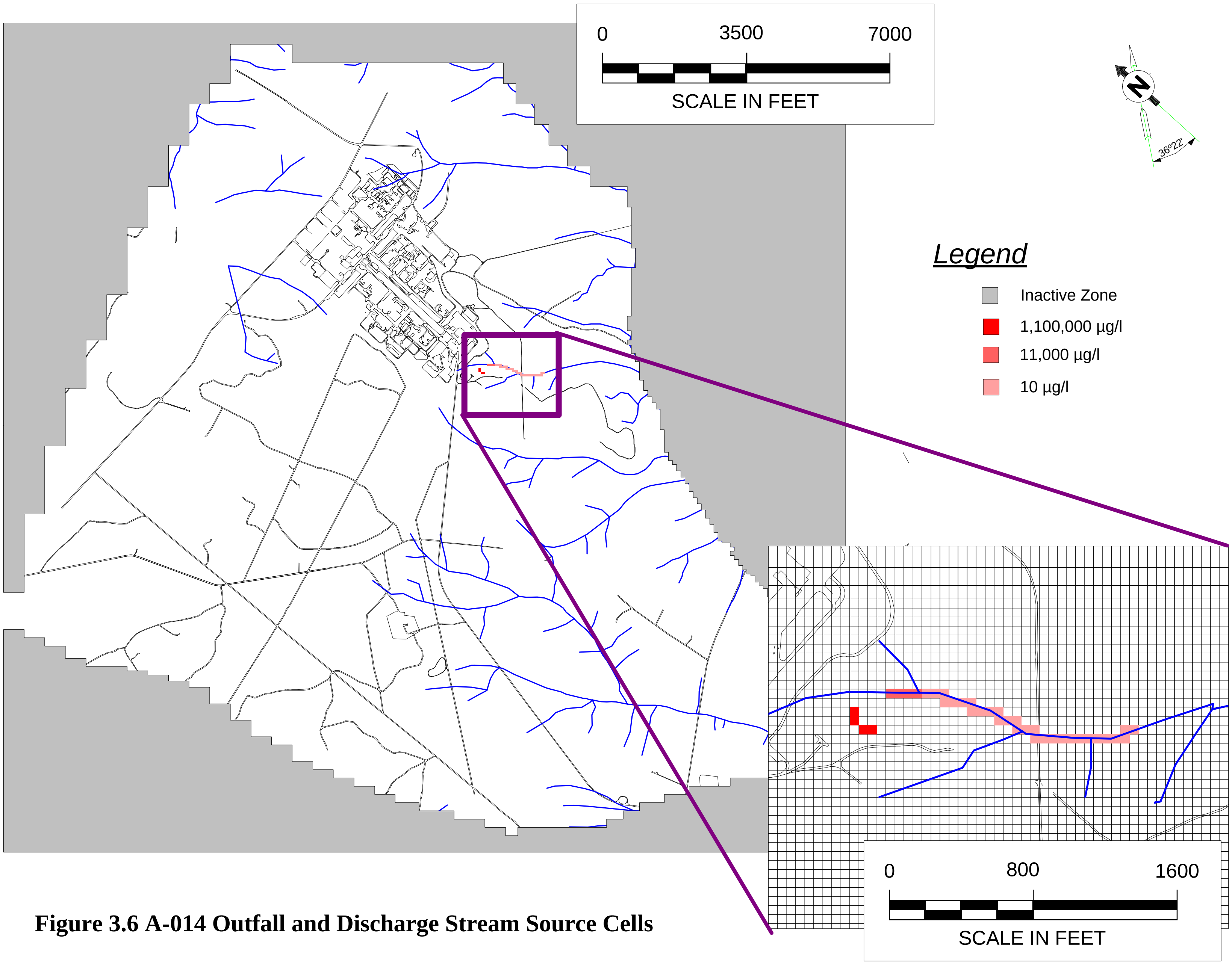

Figure 3.6 A-014 Outfall and Discharge Stream Source Cells

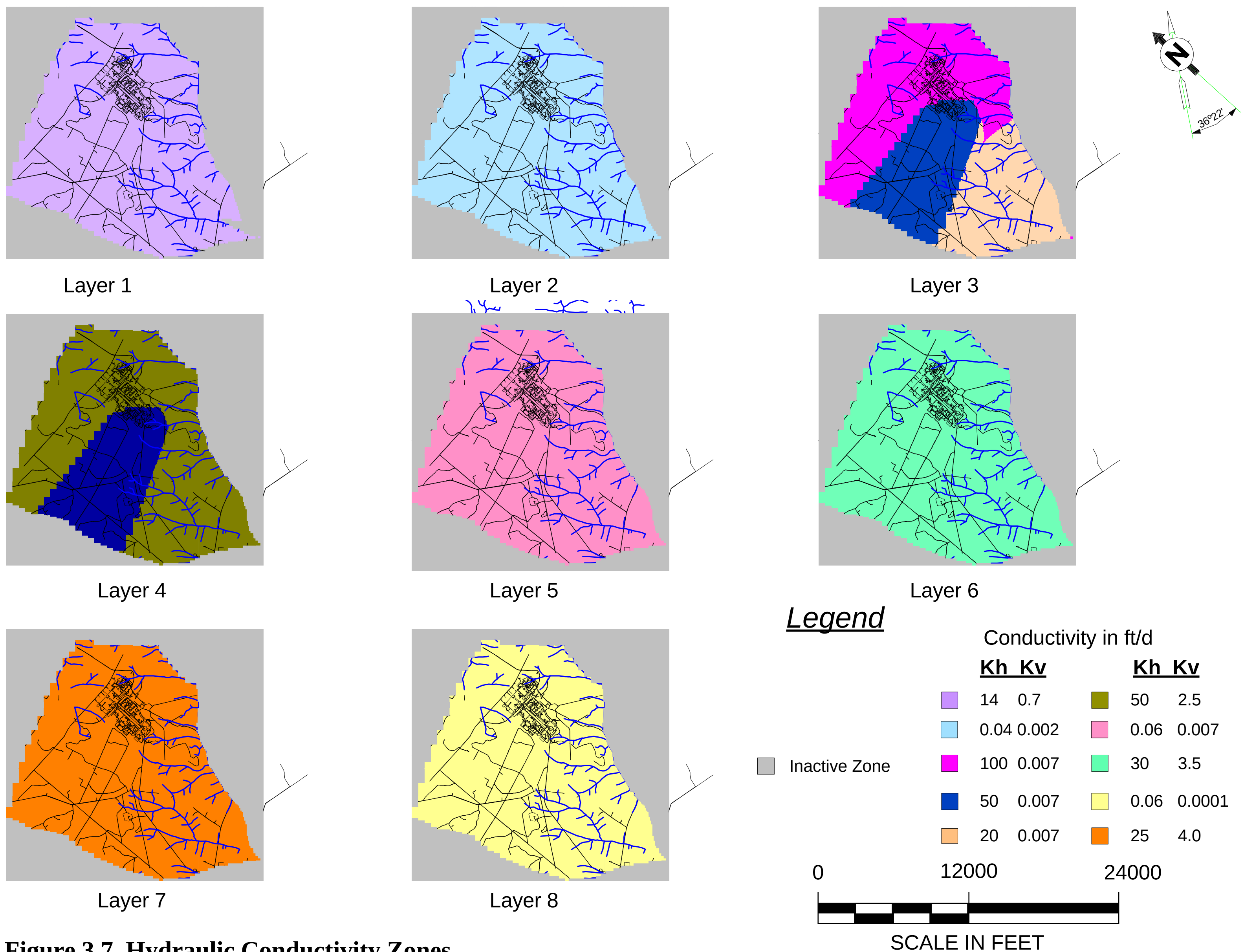

Figure 3.7 Hydraulic Conductivity Zones

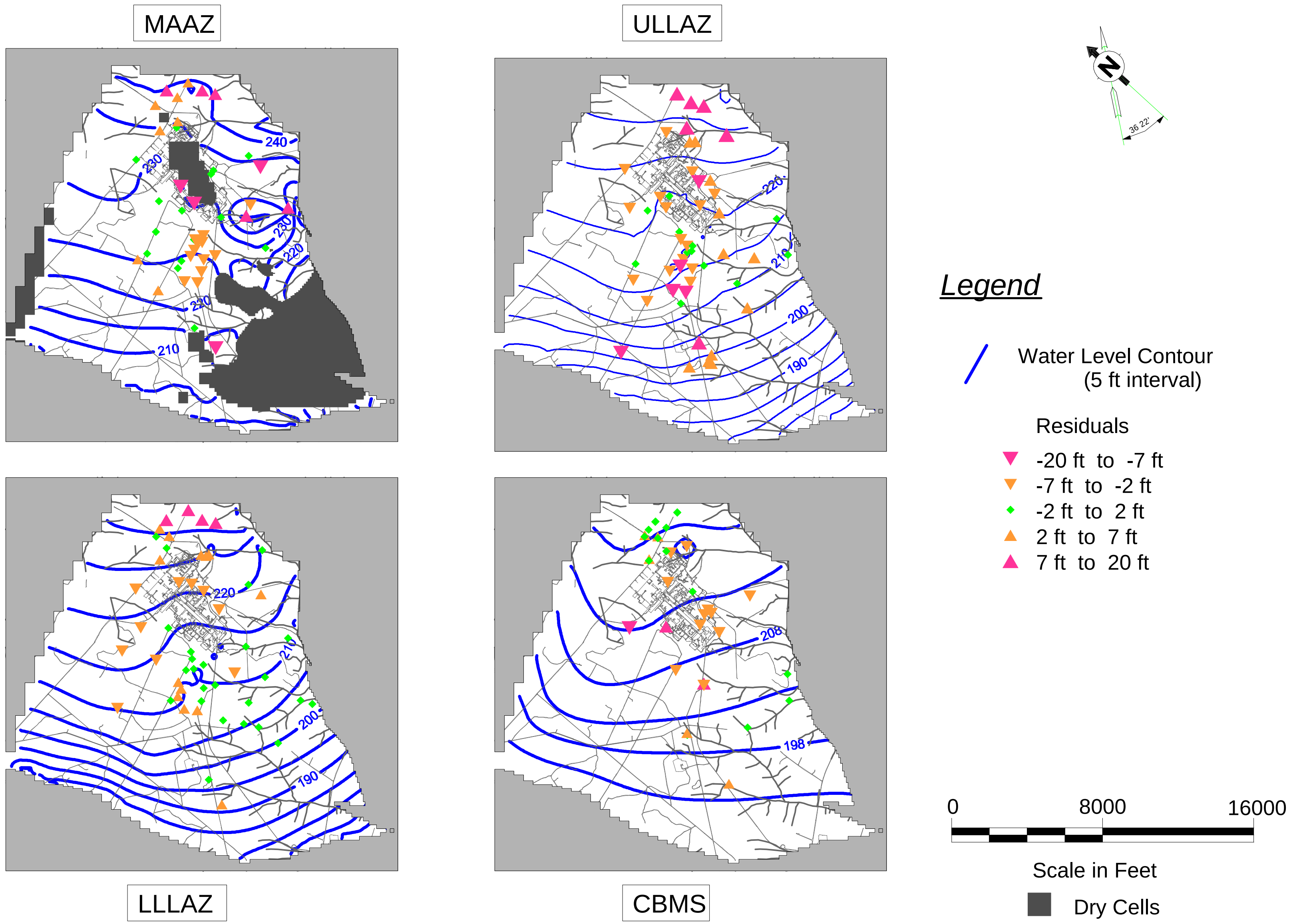

Figure 3.8 Calibrated Model Head and Head Residuals

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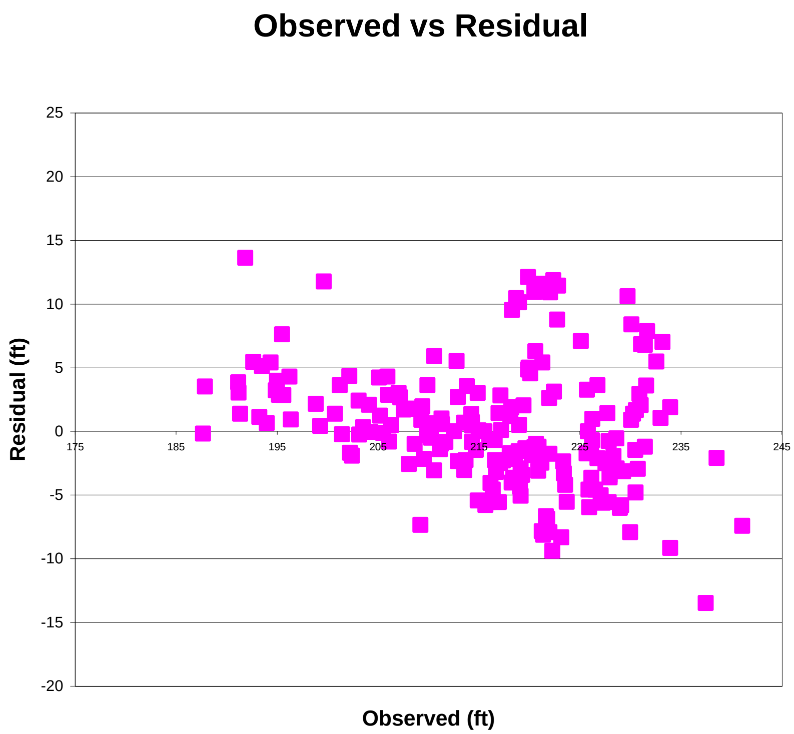

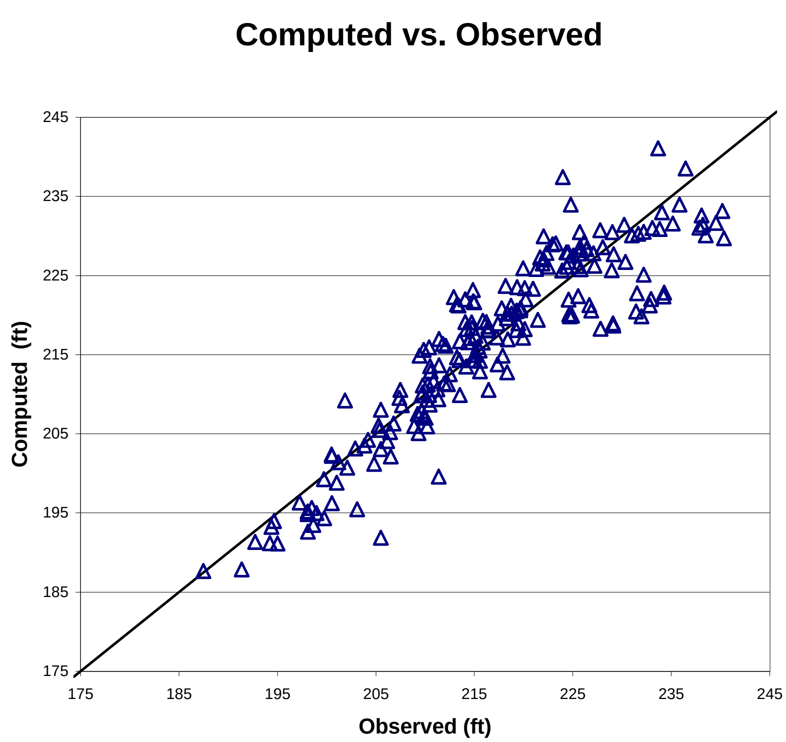

Figure 3.9 Comparison of Modeled Head and Head Residuals to Observed Head

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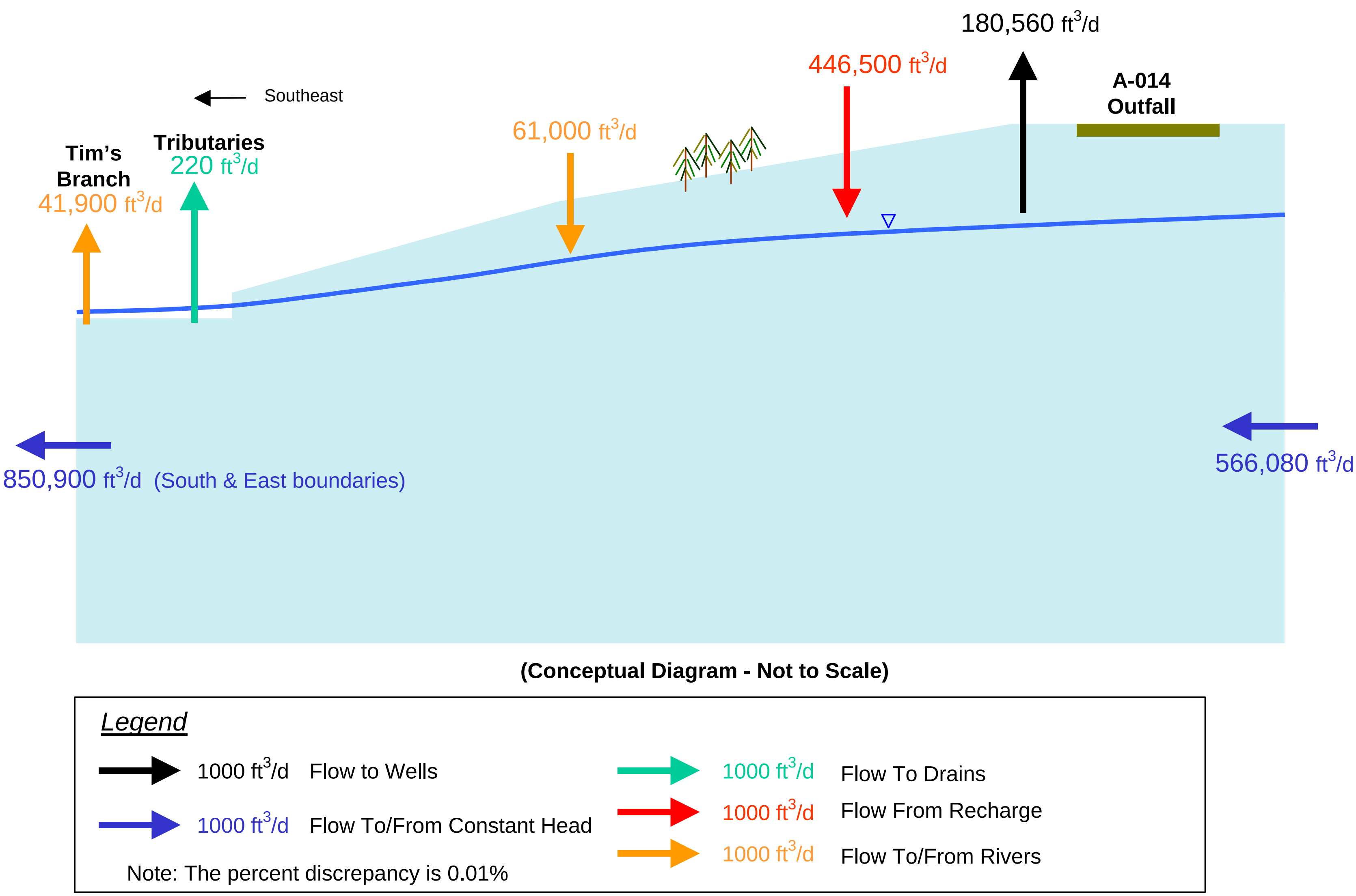

Figure 3.10 Calibrated Model Water Budget

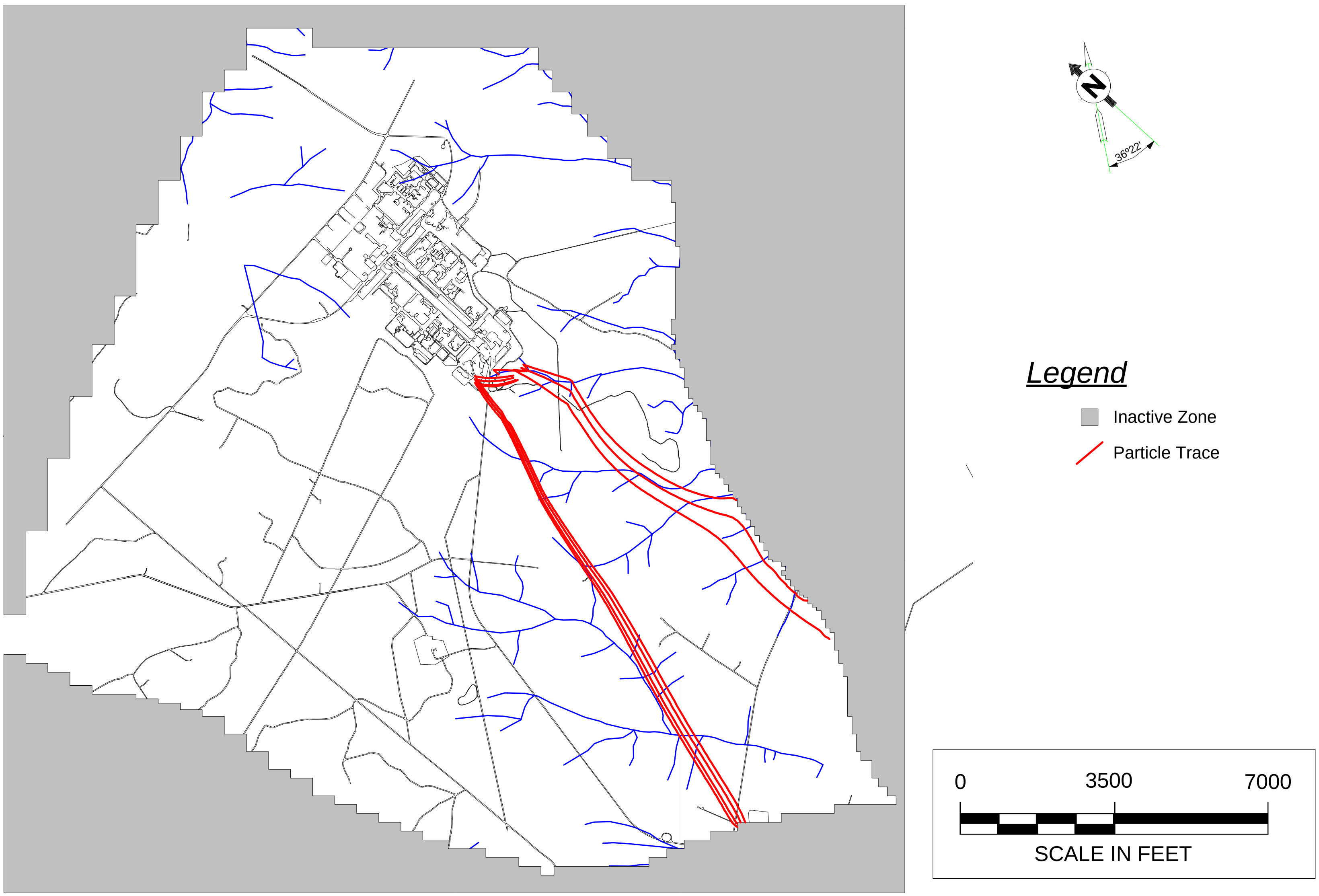

Figure 3.11 Modeled Particle Traces from the A-014 Source (Plan View)

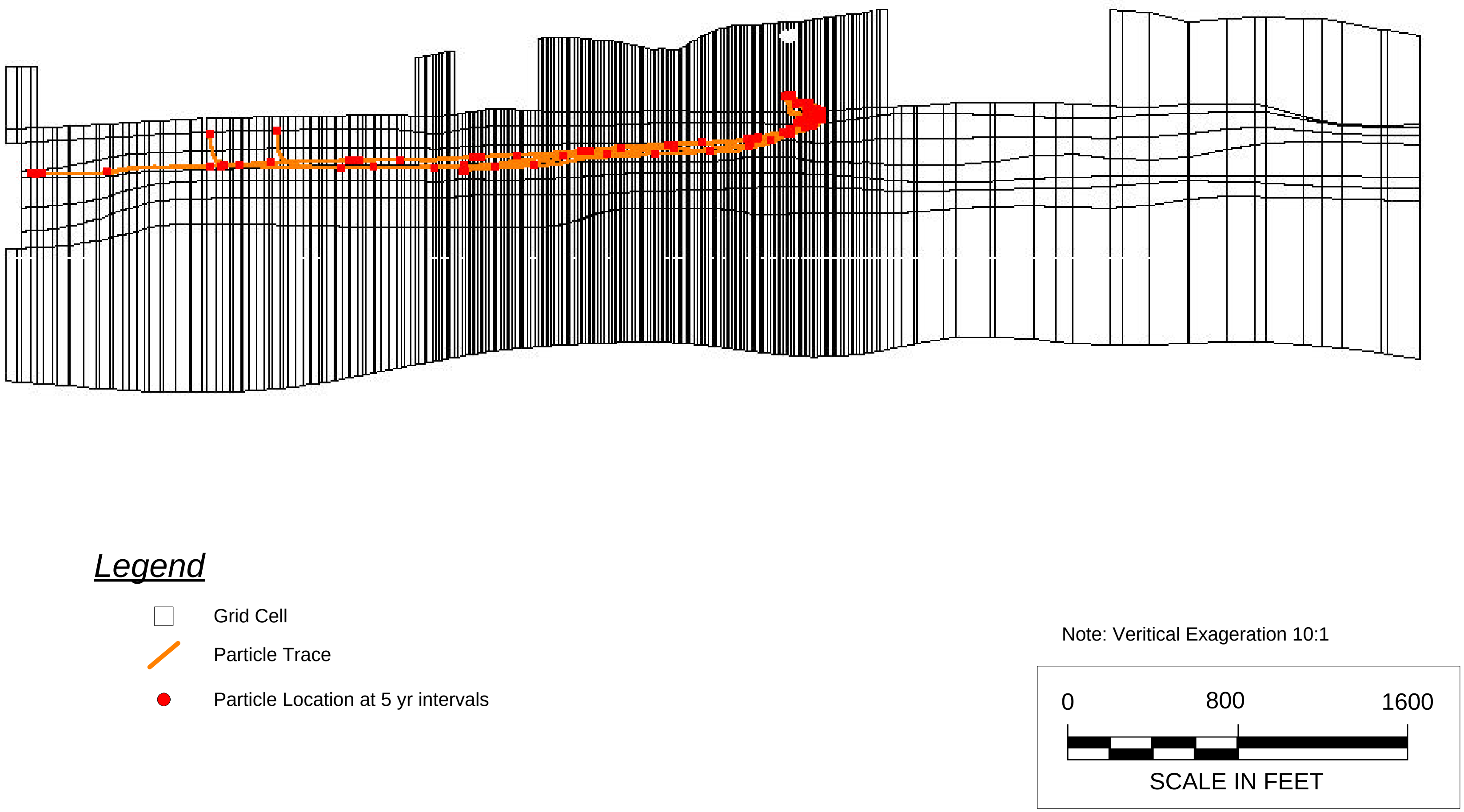

Figure 3.12 Modeled Particle Traces from the A-014 Source (Cross Section View)

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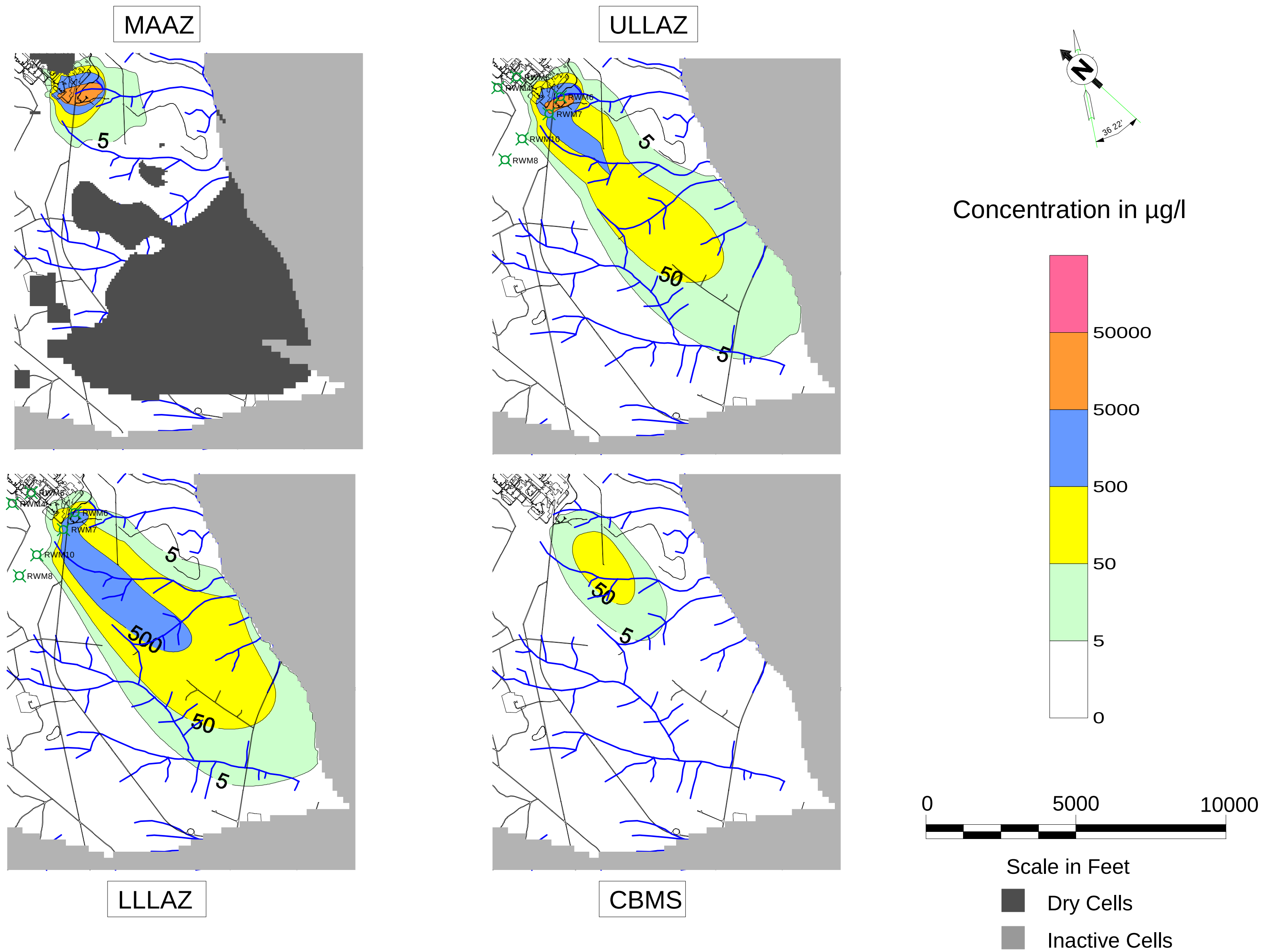

Figure 3.13 Modeled TCE Plume 2000

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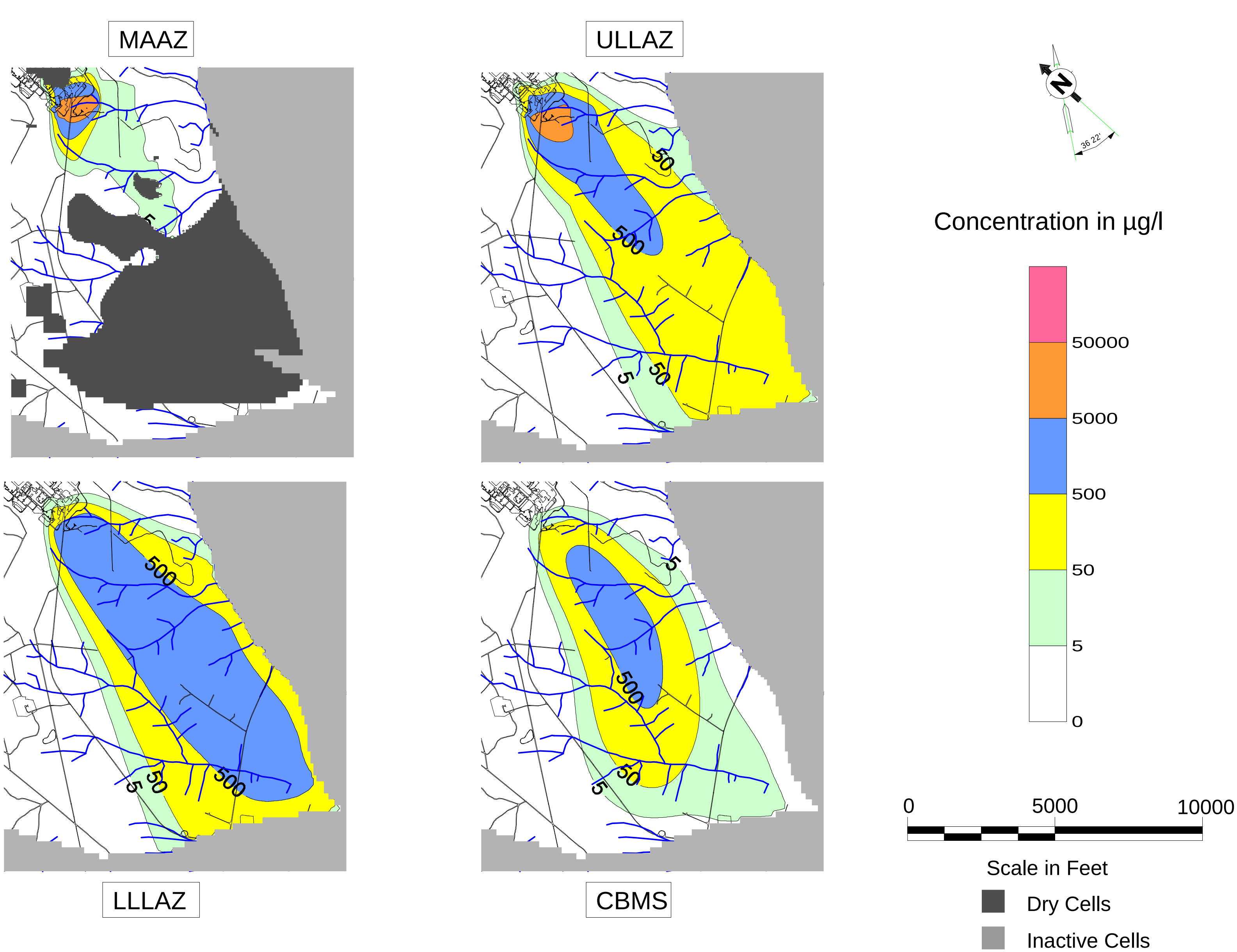

Figure 4.1 Modeled TCE Plume 2050 with No Action

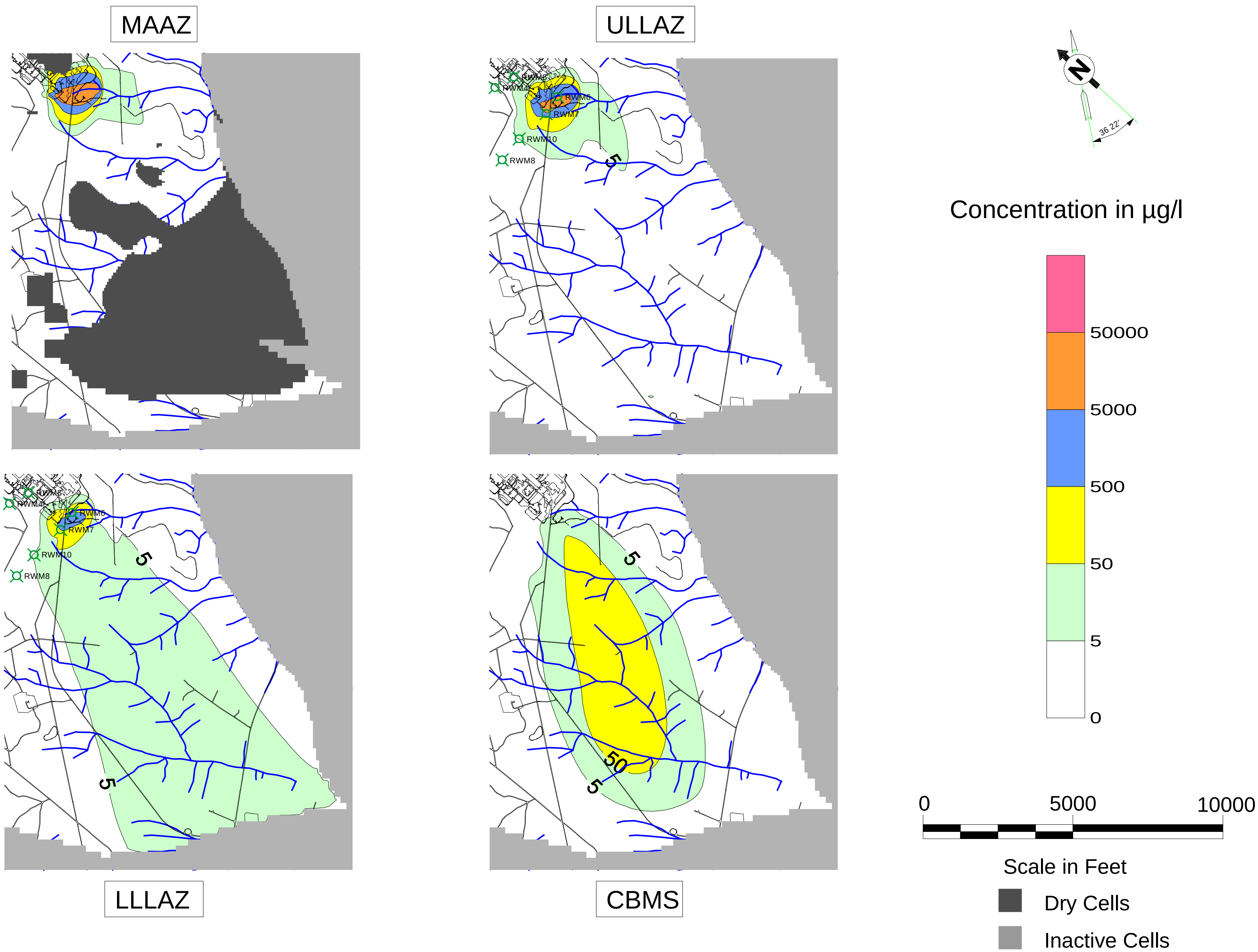

Figure 4.2 Modeled TCE Plume 2050 with Remediation Well Pumping

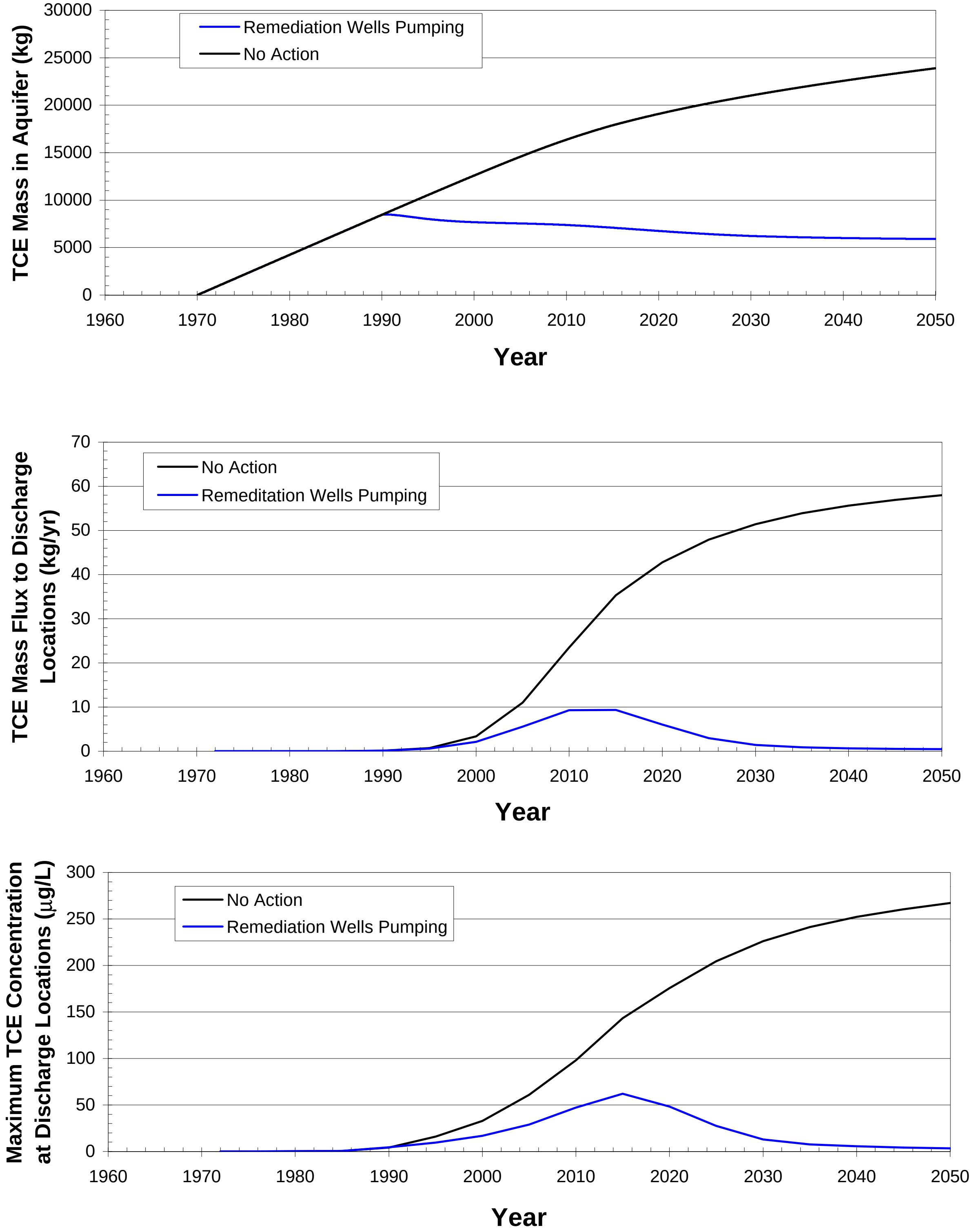

Figure 4.3 Simulated TCE Plume Mass, Mass Discharge, and Discharge Concentration for the No Action Scenario and Remediation Well Pumping Scenarios

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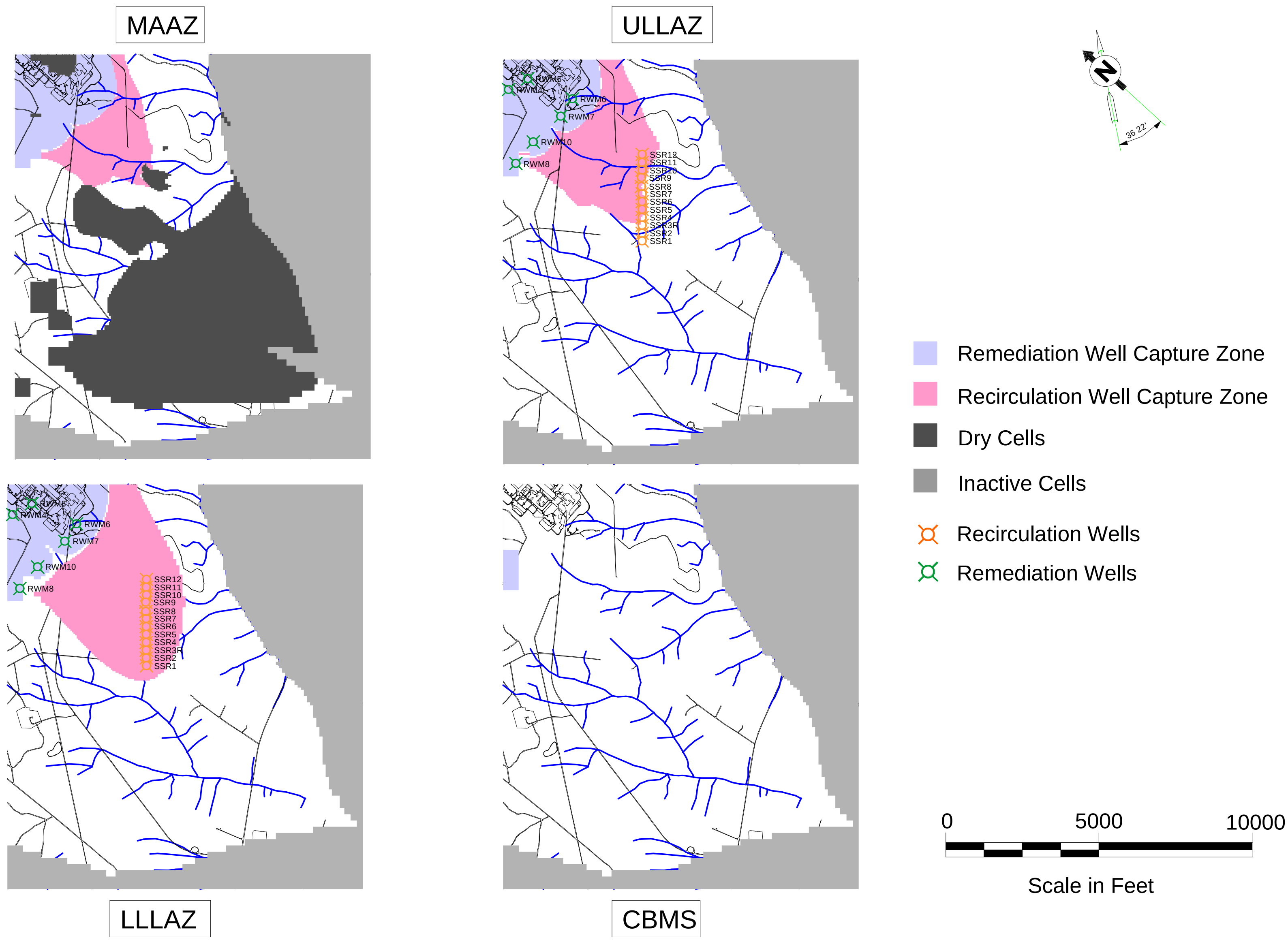

Figure 4.4 Modeled Capture Zones for the Recirculation Wells

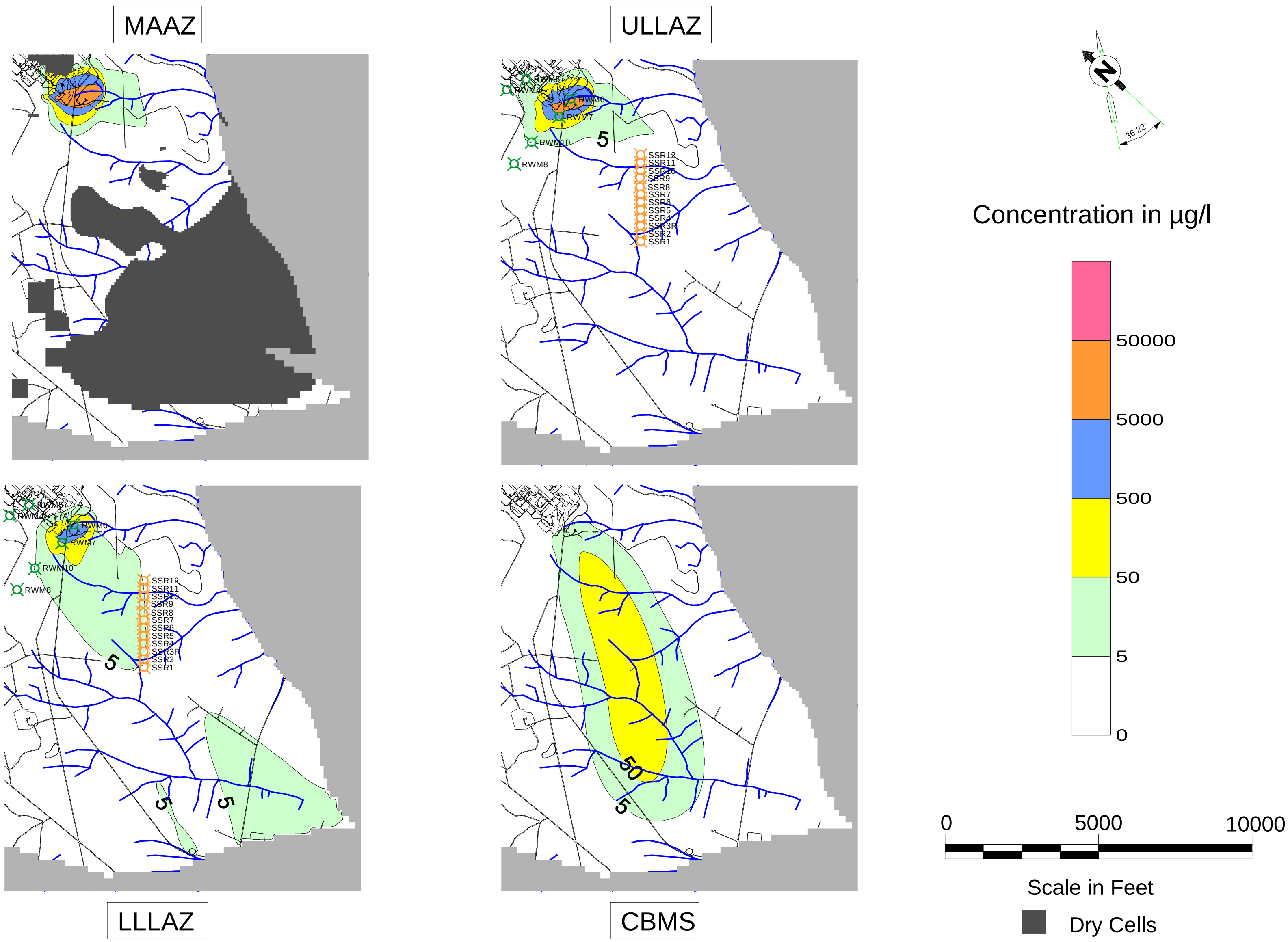

Figure 4.5 Modeled TCE Plume 2050 with Recirculation Wells

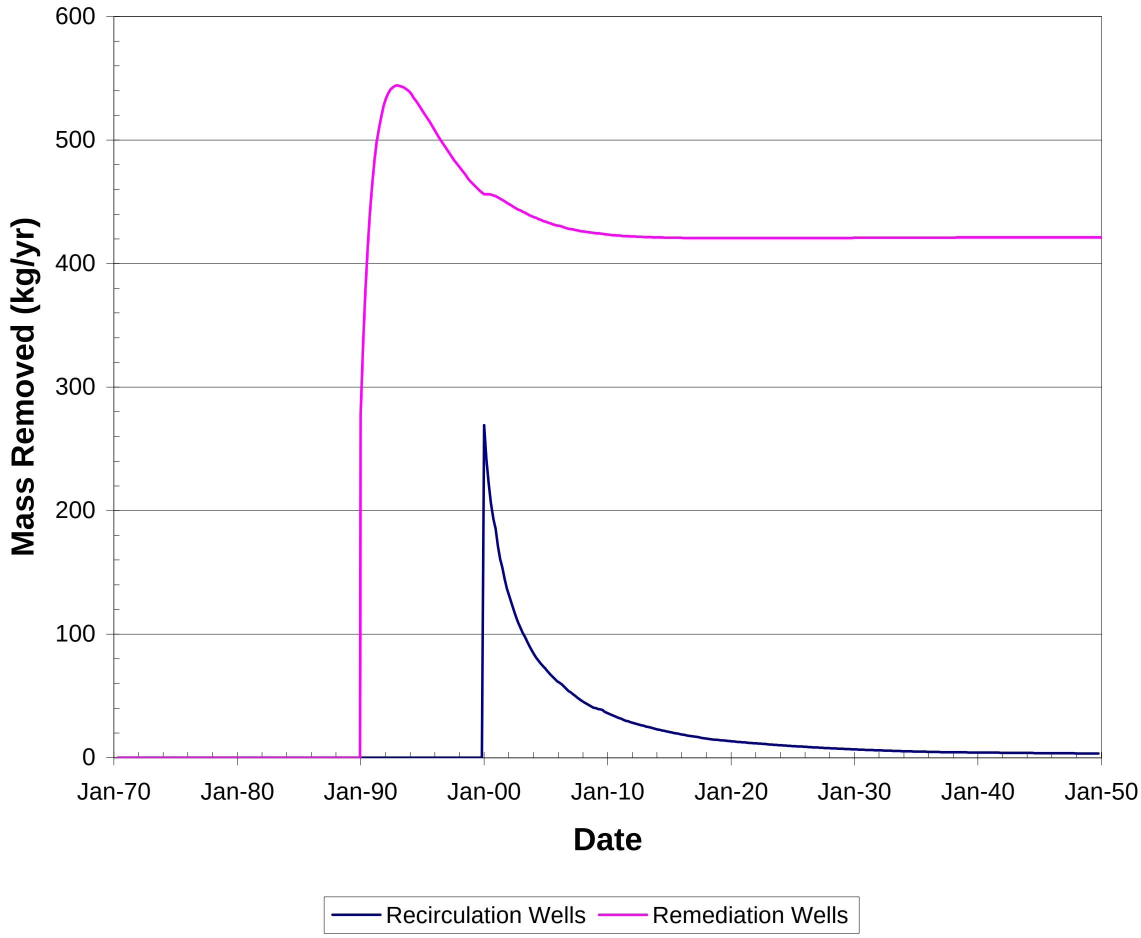

Figure 4.6 Modeled Mass Removal by Remediation and Recirculation Wells

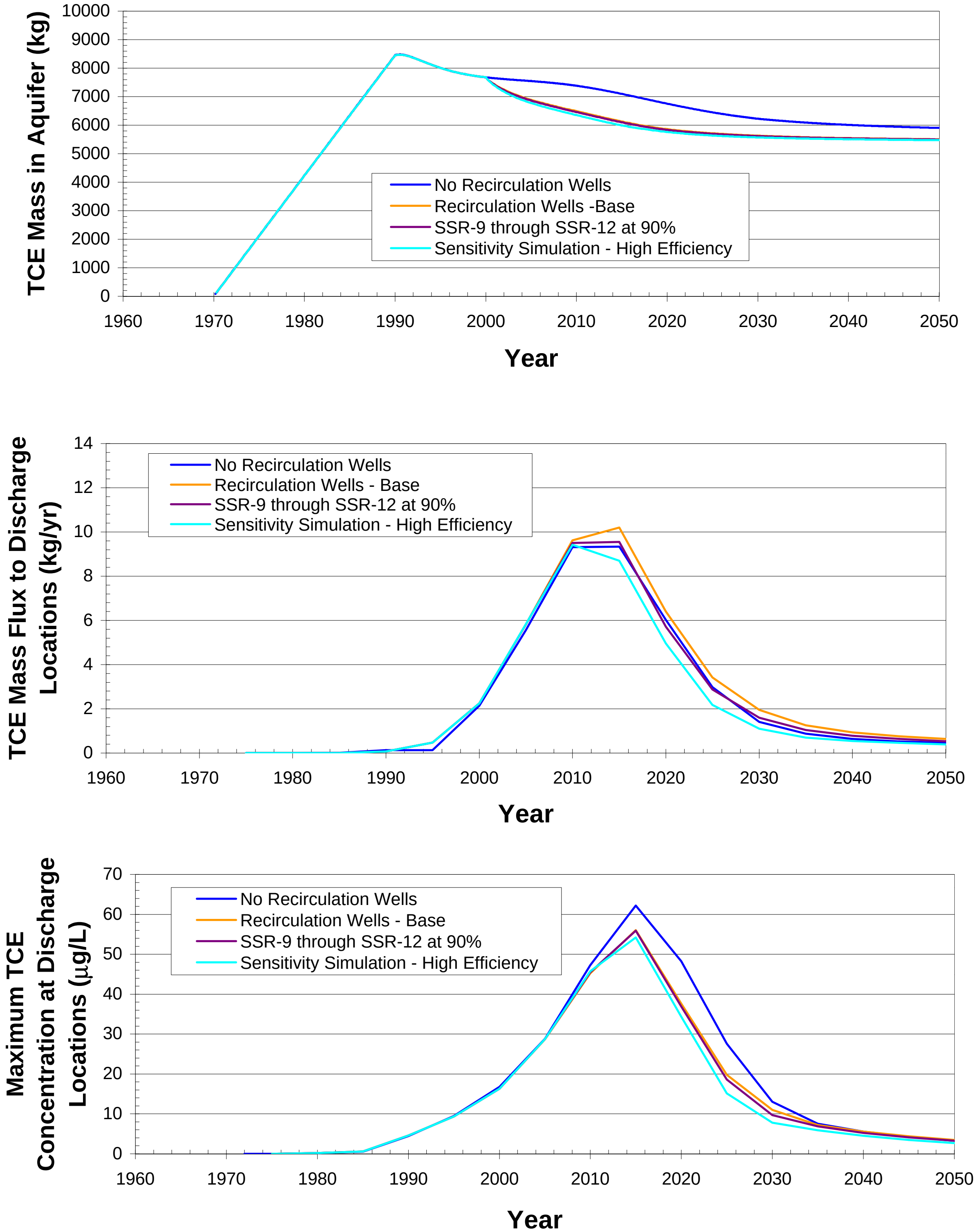

Figure 4.7 Simulated TCE Plume Mass, Mass Discharge, and Discharge Concentration for the Recirculation-Well Scenarios

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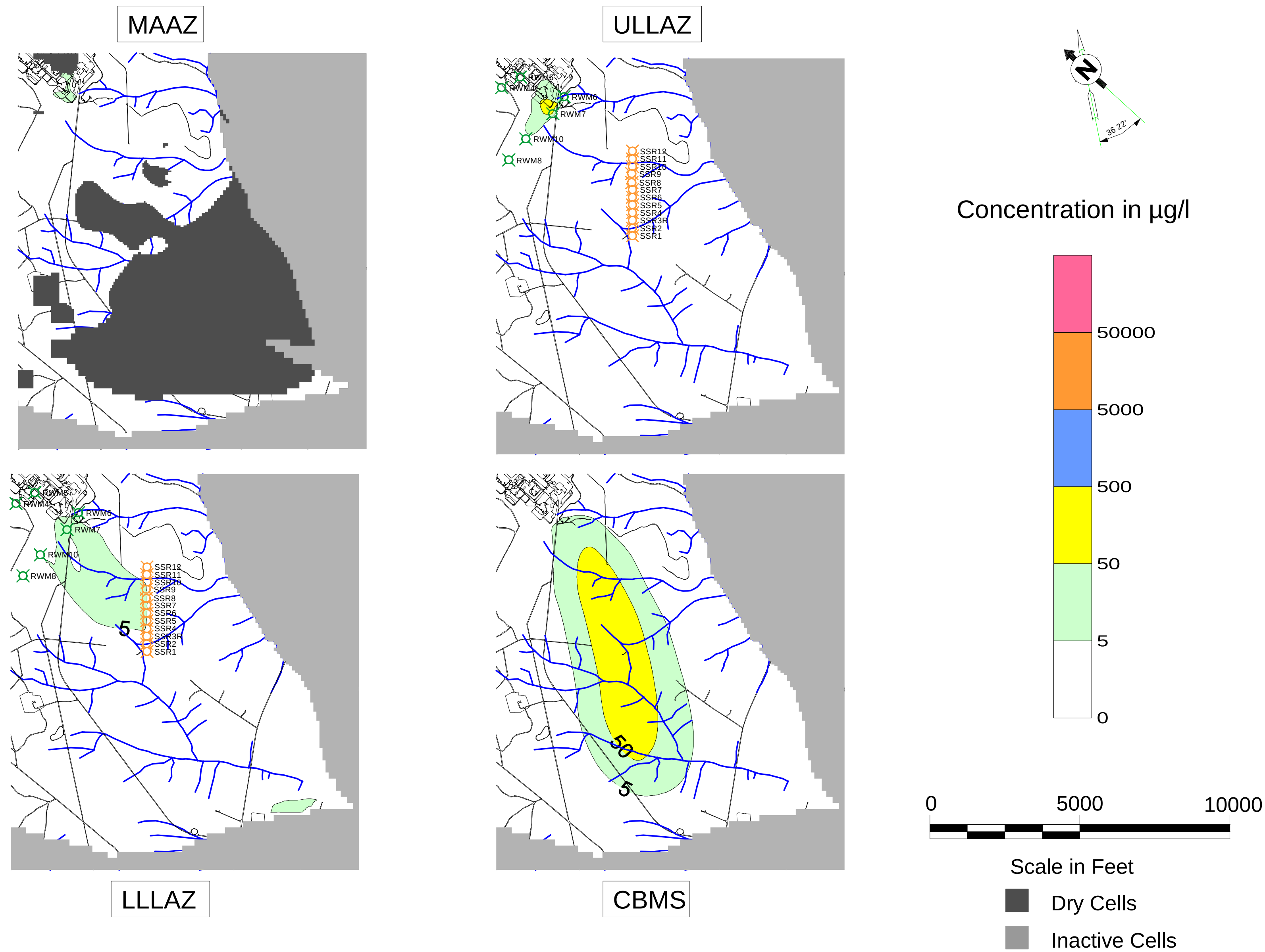

Figure 4.8 Modeled TCE Plume 2050 with Source Removal

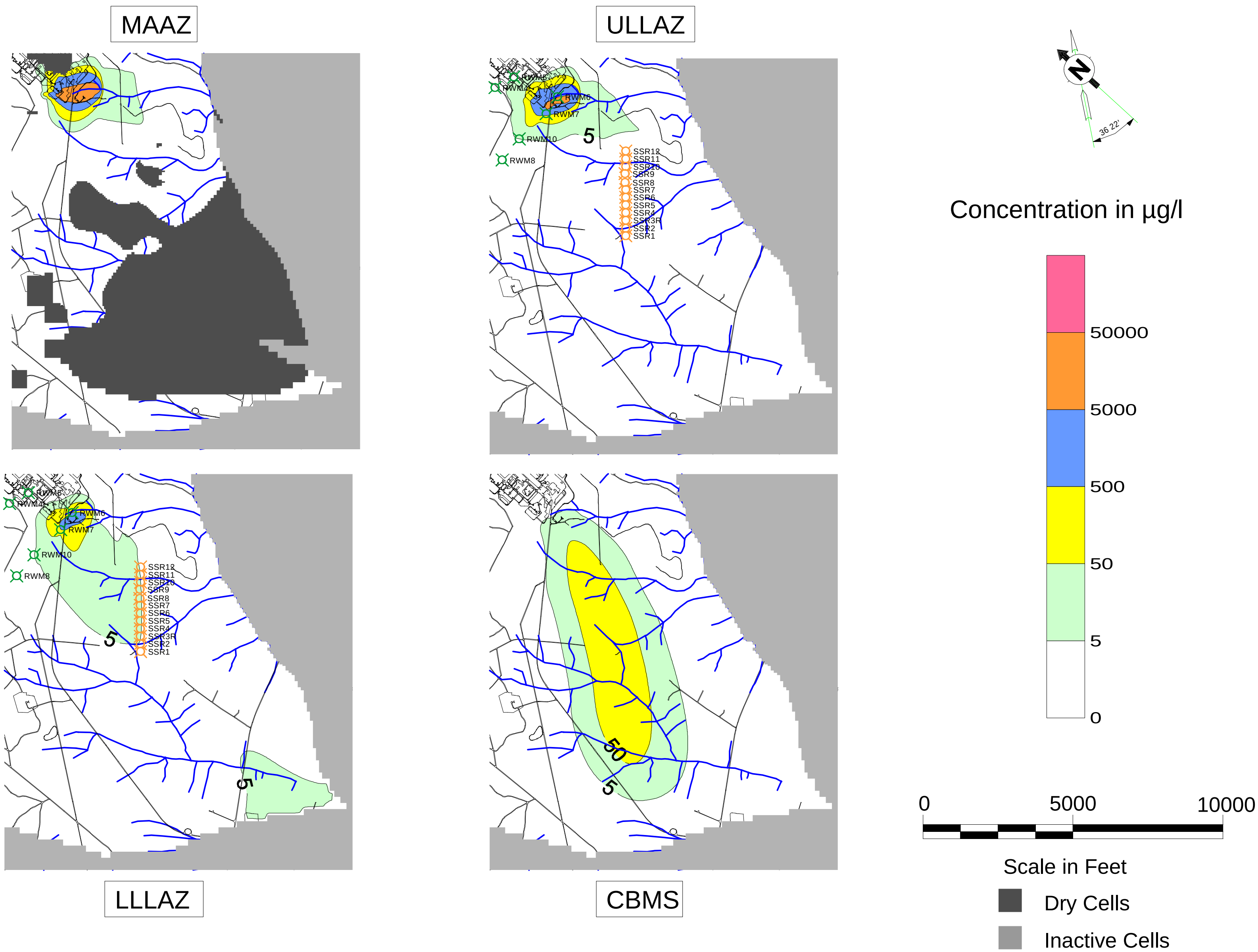

Figure 4.9 Modeled TCE Plume in 2050 with 60% Source Removal

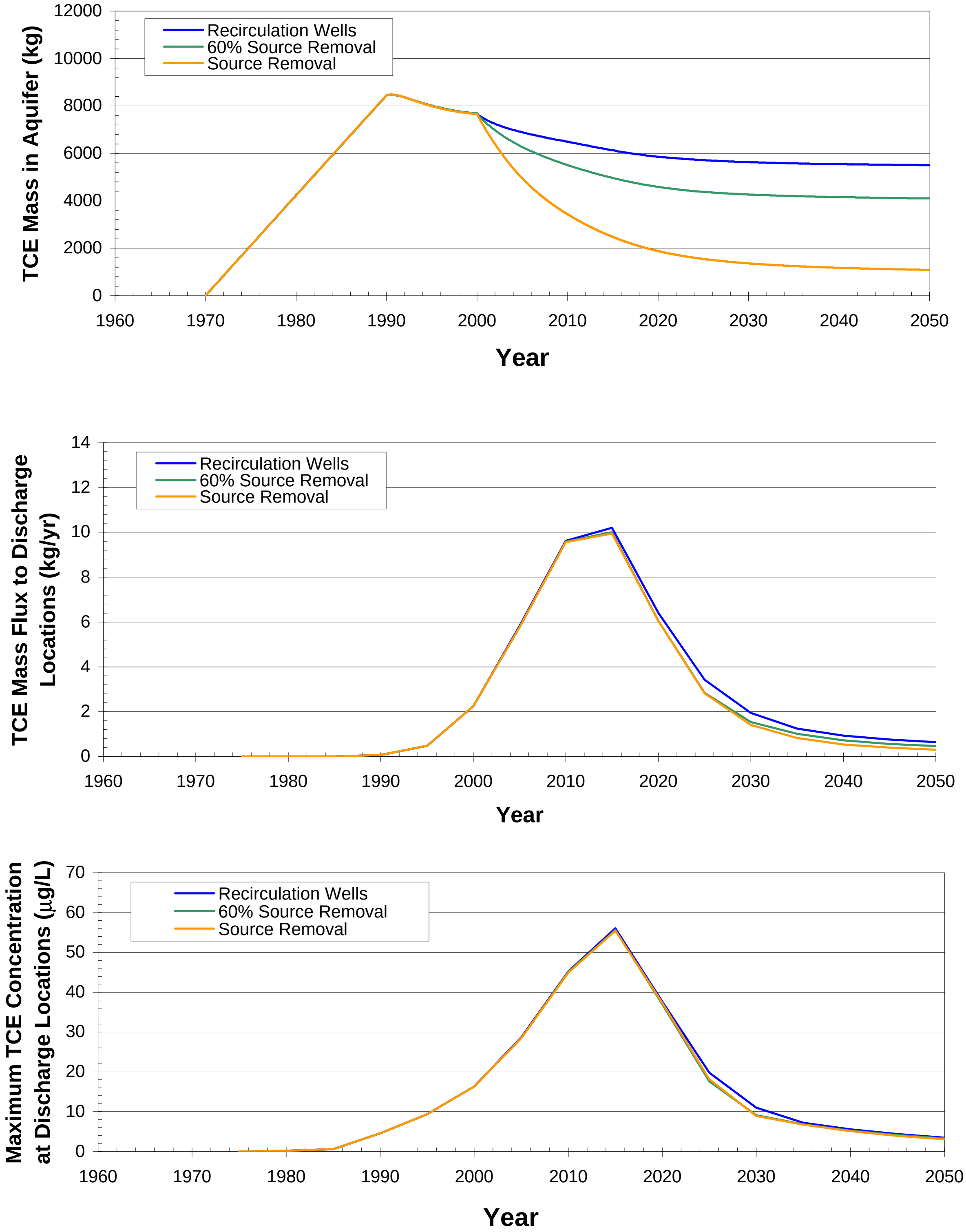

Figure 4.10 Simulated TCE Plume Mass, Mass Discharge, and Discharge Concentration for the Source Reduction Scenarios

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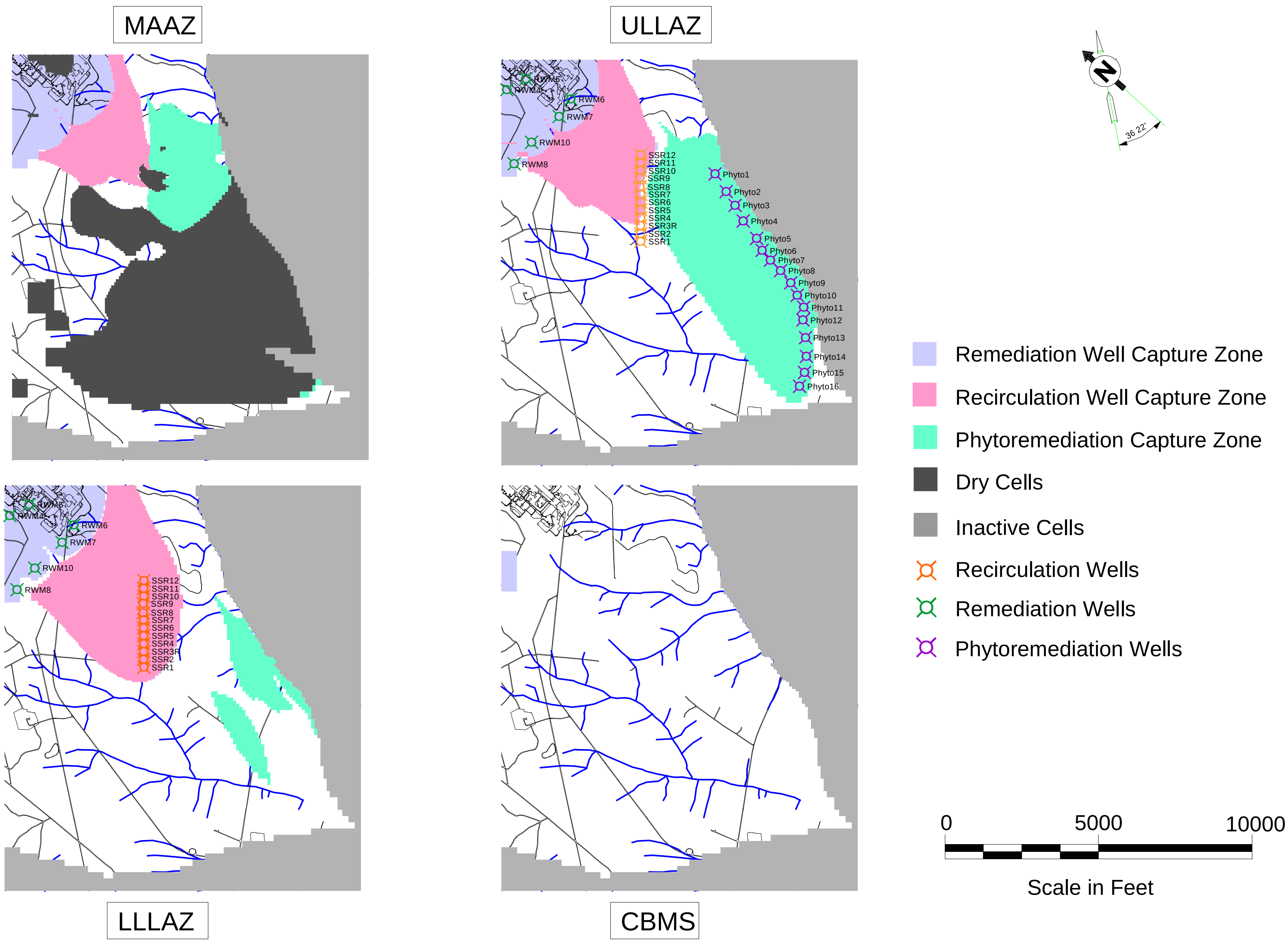

Figure 4.11 Modeled Capture Zones for the Phytoremediation Wells

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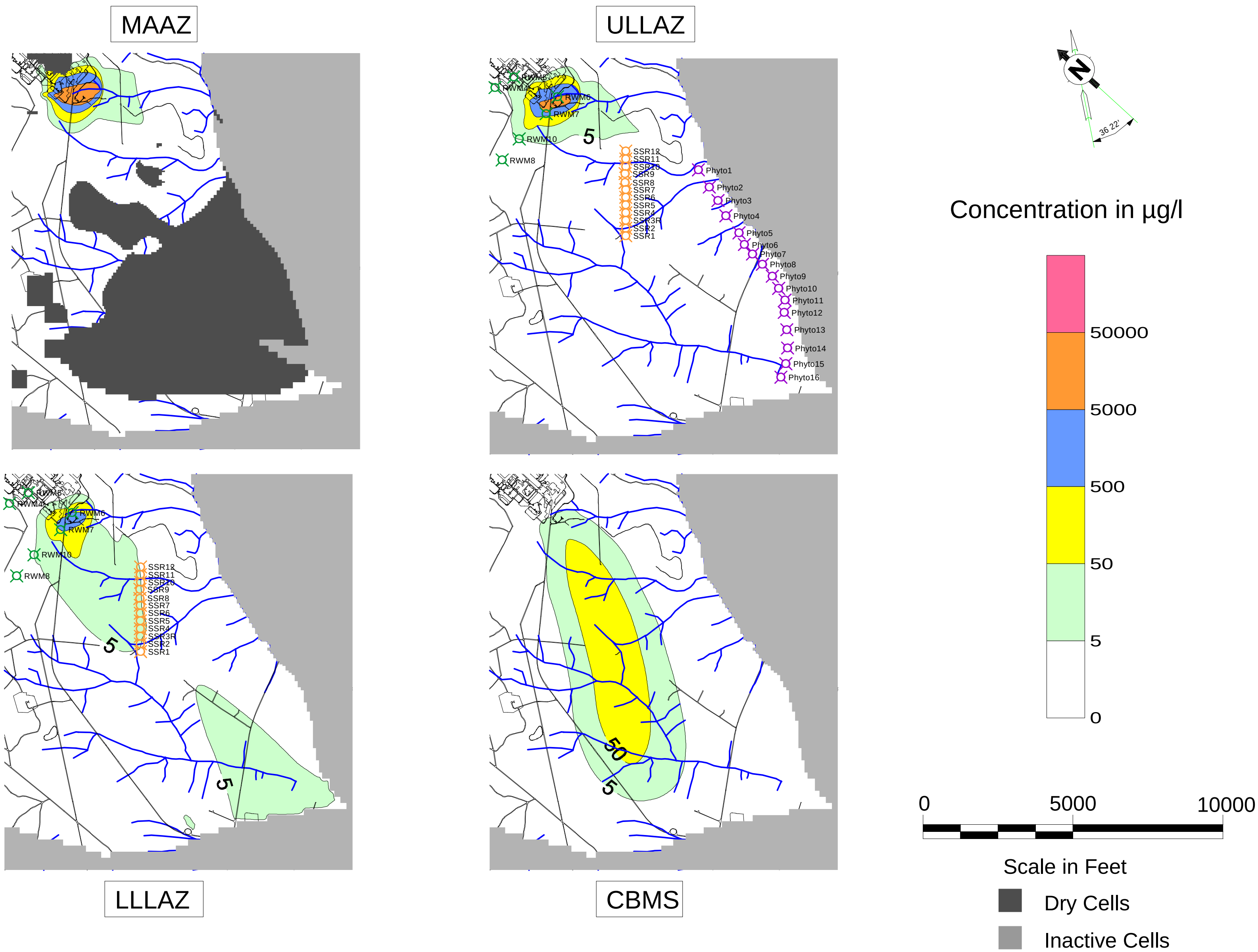


Figure 4.12 Modeled TCE Plume in 2050 with Phytoremedition Wells

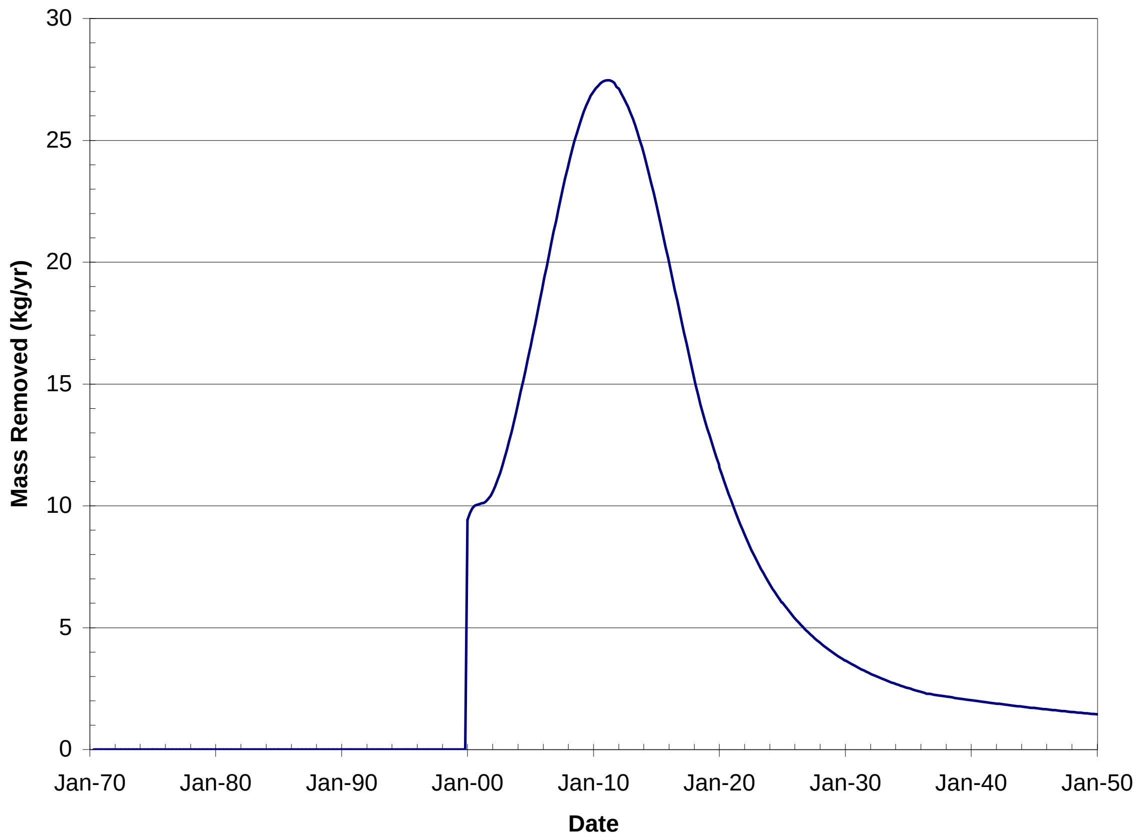


Figure 4.13 Modeled Mass Removal by Phytoremediation Wells

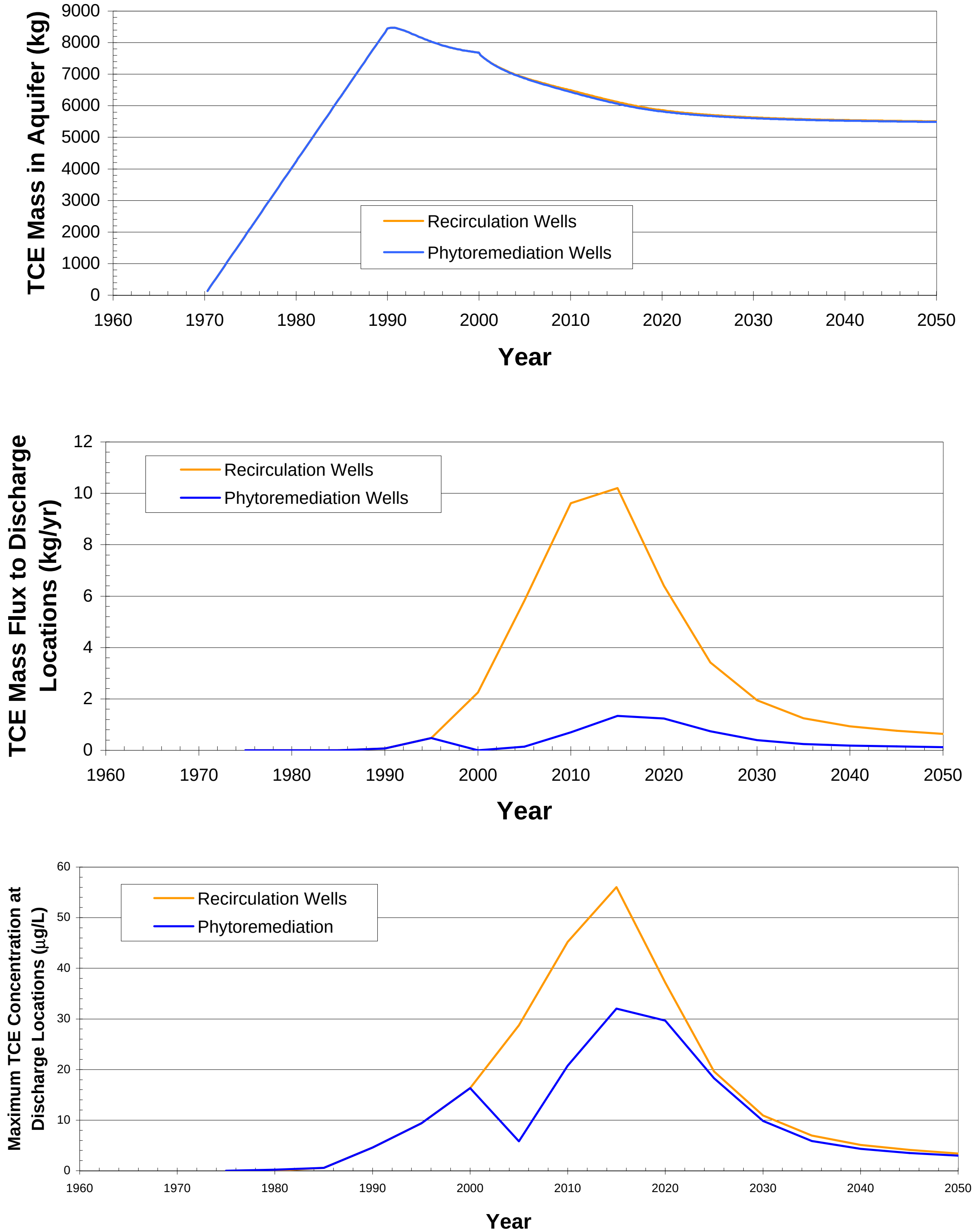
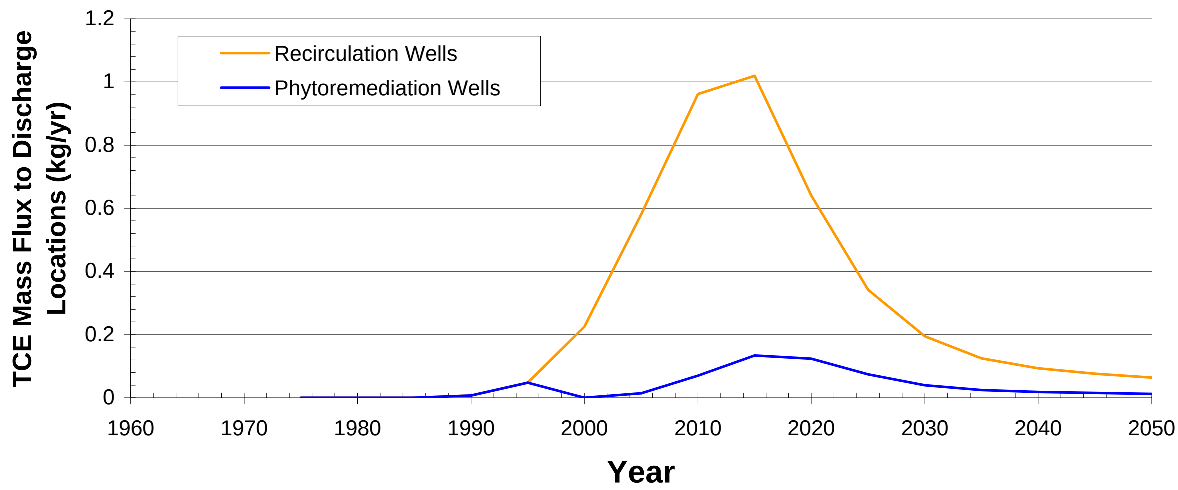
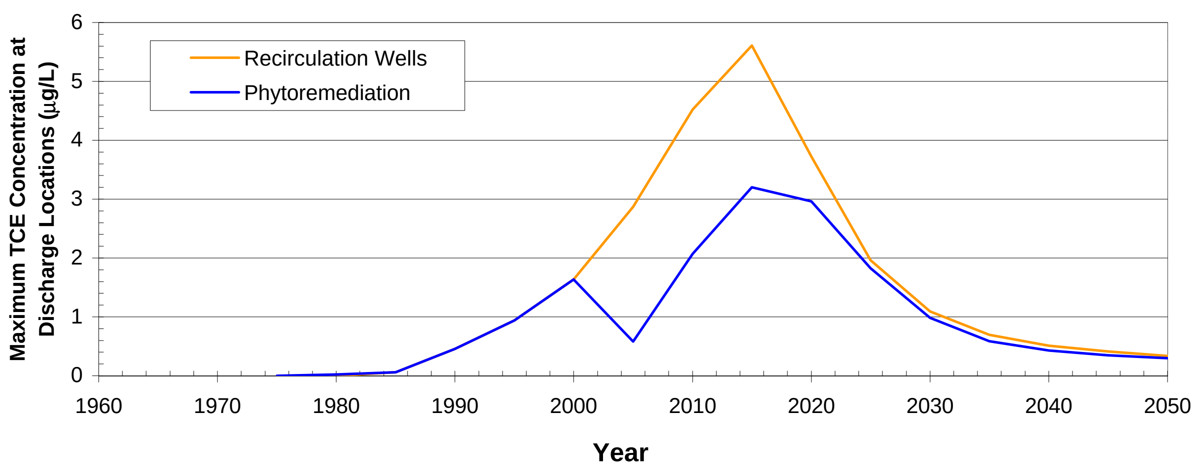


Figure 4.14 Simulated TCE Plume Mass, Mass Discharge, and Discharge Concentration for the Phytoremediation Scenario





Note: Attenuation of 0.1 Assumed

Figure 4.15 Potential Discharge Mass Flux and Concentration with MNA