Fate and Transport Modeling of Selected Chlorinated Organic Compounds at Operable Unit 1, U.S. Naval Air Station, Jacksonville, Florida

By J. Hal Davis

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Conversion Factors

Multiply	By	To obtain
Length		
inch (in.)	2.54	centimeter
foot (ft)	0.3048	meter
Area		
acre	4,047	square meter
Volume		
liter (L)	1.057	quart
cubic foot (ft^3)	0.02832	cubic meter
Flow rate		
cubic foot per second (ft^3/s)	0.02832	cubic meter per second
cubic foot per day (ft^3/d)	0.02832	cubic meter per day
foot per day (ft/d)	0.3048	meter per day
inch per year (in/yr)	25.4	millimeter per year
Hydraulic conductivity		
foot per day (ft/d)	0.3048	meter per day
Temperature		

Degrees Fahrenheit (°F) may be converted to degrees Celsius (°C) as follows:

°C= (°F-32)/1.8

Vertical coordinate information is referenced to the insert datum name (and abbreviation) here for instance, "North American Vertical Datum of 1988 (NAVD 88)."

Horizontal coordinate information is referenced to the insert datum name (and abbreviation) here for instance, "North American Datum of 1983 (NAD 83)."
Altitude, as used in this report, refers to distance above the vertical datum.

Concentrations of chemical constituents in water are given either in milligrams per liter (mg/L) or micrograms per liter (µg/L).

Acronyms and Abbreviations

d^{-1}	first-order decay rate
DCE	dichloroethene
DPT	direct push technology
µg/L	microgram per liter
MODFLOW	Modular Three-Dimensional Finite-Difference Ground-Water Flow Model
OU1	Operable Unit 1
OU2	Operable Unit 2
OU3	Operable Unit 3
RT3D	Reactive Transport in Three Dimensions Flow Model
TCE	trichloroethene
USEPA	U.S. Environmental Protection Agency
USGS	U.S. Geological Survey
VC	vinyl chloride

Fate and Transport Modeling of Selected Chlorinated Organic Compounds at Operable Unit 1, U.S. Naval Air Station, Jacksonville, Florida

By J. Hal Davis

Abstract

The U.S. Naval Air Station occupies 3,800 acres adjacent to the St. Johns River in Jacksonville, Florida. The Station was placed on the U.S. Environmental Protection Agency's National Priorities List in December 1989 and is participating in the U.S. Department of Defense Installation Restoration Program, which serves to identify and remediate environmental contamination. One contaminated site, the old landfill, was designated as Operable Unit 1 (OU1) in 1989. The major source of ground-water contamination was from the disposal of waste oil and solvents into open pits, which began in the 1940s. Several remedial measures were implemented at this site to prevent the spread of contamination. Recovery trenches were installed in 1995 to collect free product. In 1998, some of the contamination was consolidated to the center of the old landfill and covered by an impermeable cap. Currently, Operable Unit 1 is being reevaluated as part of a 5-year review process to determine if the remedial actions were effective.

Solute transport modeling indicated that the concentration of contaminants would have reached its maximum extent by the 1970s, after which the concentration levels would have generally declined because the pits would have ceased releasing high levels of contaminants. In the southern part of the site, monitoring well MW-19, which had some of the highest levels of contamination, showed decreases for measured and simulated concentrations of trichloroethene (TCE) and dichloroethene (DCE) from 1992 to present. Two upgradient disposal pits were simulated to have ceased releasing high levels of contamination in 1979, which consequently caused a drop in simulated concentrations.

Monitoring well MW-100 had the highest levels of contamination of any well directly adjacent to a creek. Solute transport modeling substantially overestimated the concentrations of TCE, DCE, and vinyl chloride (VC) in this well. The reason for this overestimation is not clear, however, it indicates that the model will be conservative when used to predict concentration levels and the time required for the contamination to move through the system. Monitoring well MW-97 had the highest levels of contamination in the central part of the site. The levels decreased for both the measured and simulated values of TCE, DCE, and VC from 1999 to present. Simulating the source area as ceasing to release high levels of contamination in 1979 caused the drop in concentration, which began in the 1990s at this well.

Monitoring well MW-89 had the highest levels of contamination in the northern part of the site. In order to match the low levels of contamination in wells MW-12 and MW-93, the pit was simulated as ceasing to release contamination in 1970; however, the installation of a trench in 1995 could have caused the source area to release additional contamination from 1995 to 1998. The effect of the additional dissolution was a spike in contamination at MW-89, beginning in about 1996 and continuing until the present time. Results from the last several sampling events indicate that the TCE and DCE levels could be decreasing, but VC shows no apparent trend. Several more years of sampling are needed to determine if these trends are continuing.

Based on the solute transport modeling predictions, TCE, DCE, and VC will have migrated to the vicinity of creeks that drain ground water from the aquifer by 2010, and only relatively low levels will remain in the aquifer by 2015. Because the creeks represent the point where the contaminated ground water comes into contact with the environment, future contamination levels are a concern. The concentration of chlorinated solvents in the creek water has always been relatively low. Because the model shows that concentrations of TCE, DCE, and VC are declining in the aquifer, contamination levels in the creeks also are anticipated to decline.

Introduction

The U.S. Naval Air Station, (referred to herein as the Station) occupies 3,800 acres adjacent to the St. Johns River in Jacksonville, Fla. (fig. 1). The mission of the Station is to provide aerial anti-submarine warfare support, aviator training, and aircraft maintenance. Support facilities include an airfield, a maintenance depot, a Naval hospital, a Naval supply center, and recreational and residential facilities. Military activities have been conducted at the Station since 1909; the Station presently employs about 15,000 people.

The Station was placed on the U.S. Environmental Protection Agency's (USEPA) National Priorities List in December 1989, and is participating in the U.S. Department of Defense Installation Restoration Program, which serves to identify and remediate environmental contamination in compliance with the Comprehensive Environmental Response, Compensation, and Liability Act and the Superfund Amendments and Reauthorization Act of 1980 and 1985, respectively. On October 23, 1990, the Station entered into a Federal Facility Agreement with the USEPA and the Florida Department of Environmental Protection. The agreement designated Operable Units 1, 2, and 3 (U.S. Navy, 1994) (fig. 1) in areas where several sources of similar contamination existed in close proximity, thus allowing the contaminated areas to be addressed in one coordinated effort. Operable Unit 1 (OU1) (U.S. Navy, 1996; 2003) was the Station landfill and has been discussed in a previous study (Davis and others, 1996); it also is the subject of this report. Operable Unit 2 (OU2) was the wastewater treatment plant, which has been remediated. Operable Unit 3 (OU3) (U.S. Navy, 1994) was the Naval Aviation Depot and was discussed in previous studies (Davis and others, 1998; 2000). Since entering into the Federal Facility Agreement, several additional operable units have been designated.

At OU1, several remedial measures were identified that would help prevent the spread of contamination (U.S. Navy 1996). As an initial remedial response, trenches were installed in 1995 to collect free product that was floating on the water table. In 1998, some of the contamination was consolidated to the center of the old landfill and covered by an impermeable cap. A monitoring program began in 1999, in which water-quality samples were routinely collected in designated wells and stream locations. Currently, OU1 is being reevaluated as part of a 5-year review process to determine if the remedial actions were effective. This study is part of that 5-year review process. Tetra Tech NUS, Inc. (Tetra Tech), a contractor for the U.S. Navy, is conducting the review.

Purpose and Scope

A computer model capable of simulating ground-water flow and the fate and transport of trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) at OU1 was needed by the Navy to aid in the remedial decision process. The purpose of this report is to document the development of this model and present the results of the model simulations. Results of this study will increase our understanding of ground-water flow and the movement and fate of contaminants in the Jacksonville area. The methods that have been developed can be applied to other areas to predict contaminant dispersal in hydrologic systems.

The computer modeling effort consisted of: (1) updating an existing regional ground-water model to simulate ground-water flow in the general region at and around OU1, (2) using the updated regional model to establish boundary conditions for a site-specific model centered at OU1, and (3) using the site-specific model to simulate the movement of contaminants and to evaluate the long-term potential for contamination migration to surface waters. The regional ground-water flow model was recalibrated to include more recent data. All of the models referenced in this report were based on work conducted by the U.S. Geological Survey (USGS). All of the water-quality sampling data were collected by Tetra Tech and, thus, the discussion of contamination distribution, history, and movement is based on Tetra Tech data. For a more complete discussion of the methods and results determined by Tetra Tech, see U.S. Navy (2006).

Previous Modeling at the Jacksonville Naval Air Station

The USGS previously developed and calibrated a one-layer regional ground-water flow model that simulated steady-state flow in the surficial aquifer at the Station (Davis and others, 1996). This model used the USGS Modular Three-Dimensional Finite-Difference Ground-Water Flow Model (MODFLOW) software as described in McDonald and Harbaugh (1988). The regional model had 240 rows and 290 columns with a uniform cell size of 100 by 100 ft (feet) and simulated steady-state flow for the entire Station and some surrounding areas. The model was used to determine the direction and velocity of ground-water flow throughout the Station as well as to evaluate the effect of proposed remediation scenarios on ground-water flow at OU1.

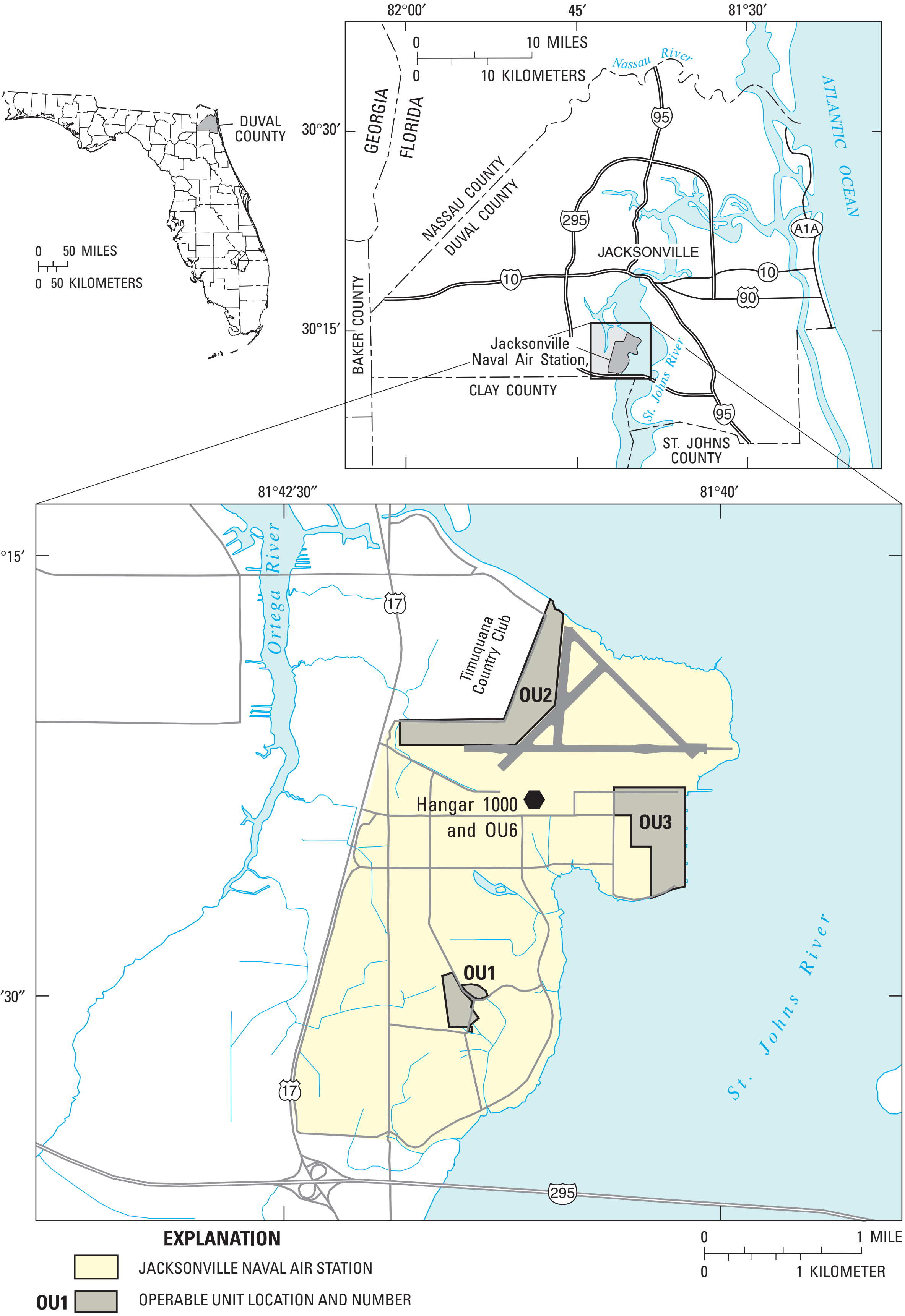


Figure 1. Location of the Jacksonville Naval Air Station.

Hydrogeologic Setting

The climate for Jacksonville is humid subtropical, with an average annual rainfall and temperature of 61 in. (inches) and 78 °F, respectively. Most rainfall occurs in late spring and early summer (Fairchild, 1972). Rainfall distribution during the summer is highly variable because of scattered, intense convective thunderstorms. Winters are mild and dry with occasional frost from November through February (Fairchild, 1972).

Land-surface topography consists of gently rolling hills with elevations ranging from about 30 ft above NGVD 1929 on hilltops to 1 ft above NGVD 1929 at the shorelines of the St. Johns and Ortega Rivers (fig. 1). The study area is in the Dinsmore Plain of the Northern Coastal Strip of the Sea Island District, in the Atlantic Coastal Plain Section (Brooks, 1981). The Dinsmore Plain is characterized by low-relief, clastic terrace deposits of Pleistocene to Holocene age (Brooks, 1981).

The surficial aquifer is exposed at land surface and forms the uppermost permeable unit at the Station. The aquifer is composed of sedimentary deposits of Pliocene to Holocene age (fig. 2), and consists of 30 to 100 ft of tan to yellow, medium to fine, unconsolidated silty sands interbedded with lenses of clay, silty clay, and sandy clay (U.S. Navy, 1994). Pleistocene-age sedimentary deposits in Florida were deposited in a series of terraces formed during marine transgressions and regressions associated with glacial and interglacial periods (Miller, 1986). A generalized geologic cross section through OU1 is shown in figure 3.

SYSTEM	SERIES	FORMATION	HYDROGEOLOGIC UNIT	REGIONAL MODEL
QUATERNARY	HOLOCENE	**Undifferentiated terrace and shallow marine deposits**	**Surficial aquifer**	**Layer 1**
	PLEISTOCENE			
TERTIARY	PLIOCENE			
	MIOCENE	Hawthorn Group	Confining unit	No-flow boundary

Figure 2. Geologic and hydrologic units, and equivalent layers used in the computer model.

The base of the surficial aquifer is formed by the top of the Miocene-age Hawthorn Group (figs. 2, 3), which is composed mainly of low-permeability clays (Scott, 1988). The top of the Hawthorn Group ranges from 30 to 100 ft below land surface across the Station and is about 30 ft below land surface and less than 10 ft below NGVD 1929 at OU1 (fig. 4). The Hawthorn Group is about 300 ft thick and composed of dark gray and olive-green sandy to silty clay, clayey sand, clay, and sandy limestone, all containing moderate to large amounts of black phosphatic sand, granules, or pebbles (Fairchild, 1972; Scott, 1988).

The water-table surface of the surficial aquifer on November 18, 1993, is shown in figure 5. This potentiometric map, prepared by Davis and others (1996), represents one of the most extensive sampling events of water-level data at the Station. In general, the water table slopes east-southeastward toward the St. Johns River or west-northwestward toward the Ortega River. The eastward and westward slopes, however, are modified by the presence of leaky storm drains and small creeks located throughout the study area.

The water-table surface in the vicinity of OU1 is shown in figure 6. As evidenced, the water table slopes toward the small creeks east and southeast of OU1. Ground-water seepage into the creeks provides continuous streamflow throughout the year in most creeks.

Stream-discharge measurements have been taken at irregular intervals in most of the small creeks at the Station since 1992. Average discharges are relatively small, ranging from 0.03 to 0.34 ft^3/s (cubic feet per second) (fig. 7); higher discharges generally occur in the winter when evapotranspiration is low.

Water-level fluctuations in individual wells ranged from 3 to 4 ft between 1993 and 2004 (fig. 8). As with the creek flows, the higher water levels generally occurred in the winter and lower levels occurred in the summer and fall. The lowest water levels (heads) were measured in two wells on April 20, 2004, during an extended dry period.

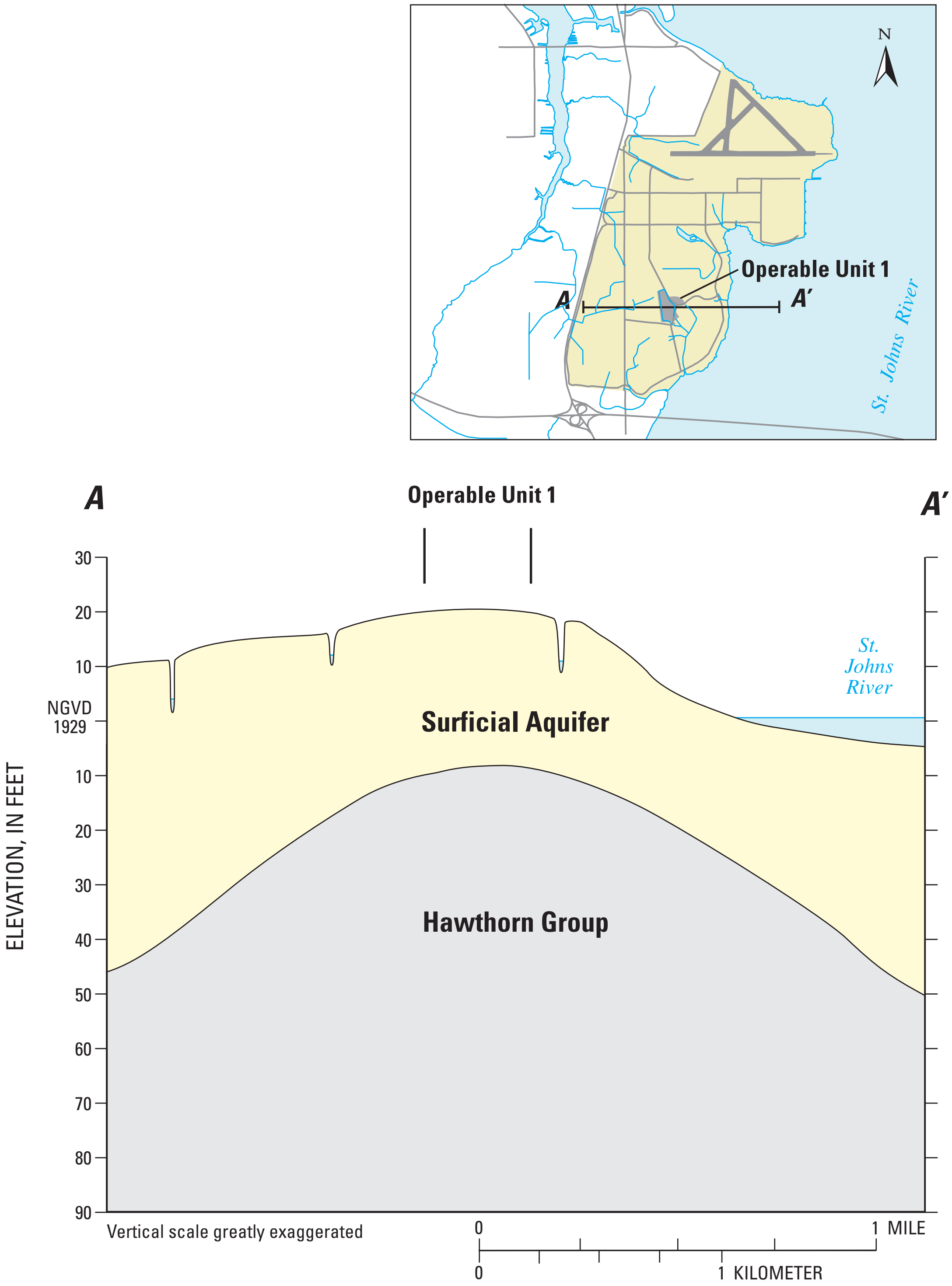


Figure 3. Generalized hydrogeologic section through the study area.

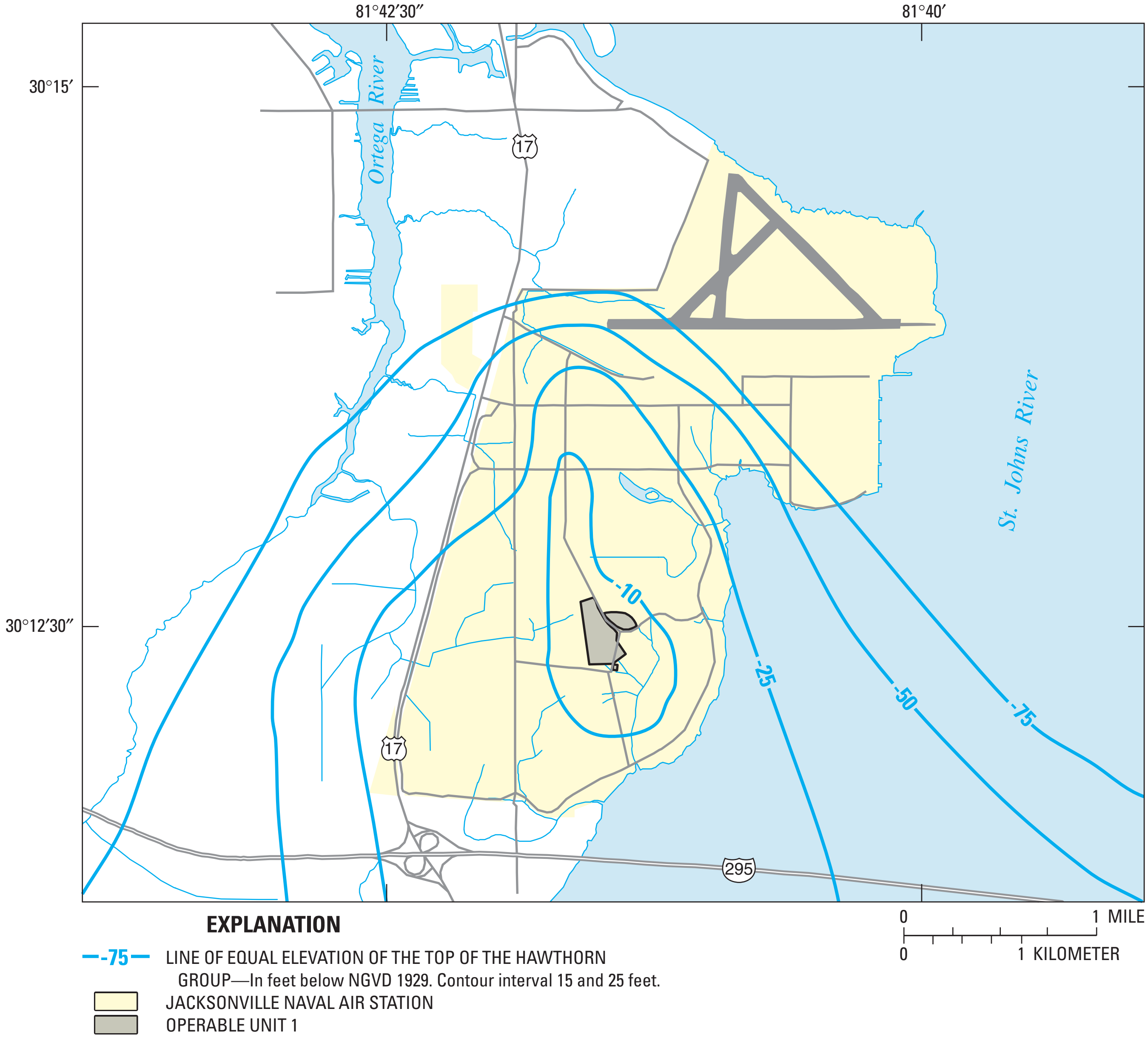


Figure 4. Top of the Hawthorn Group.

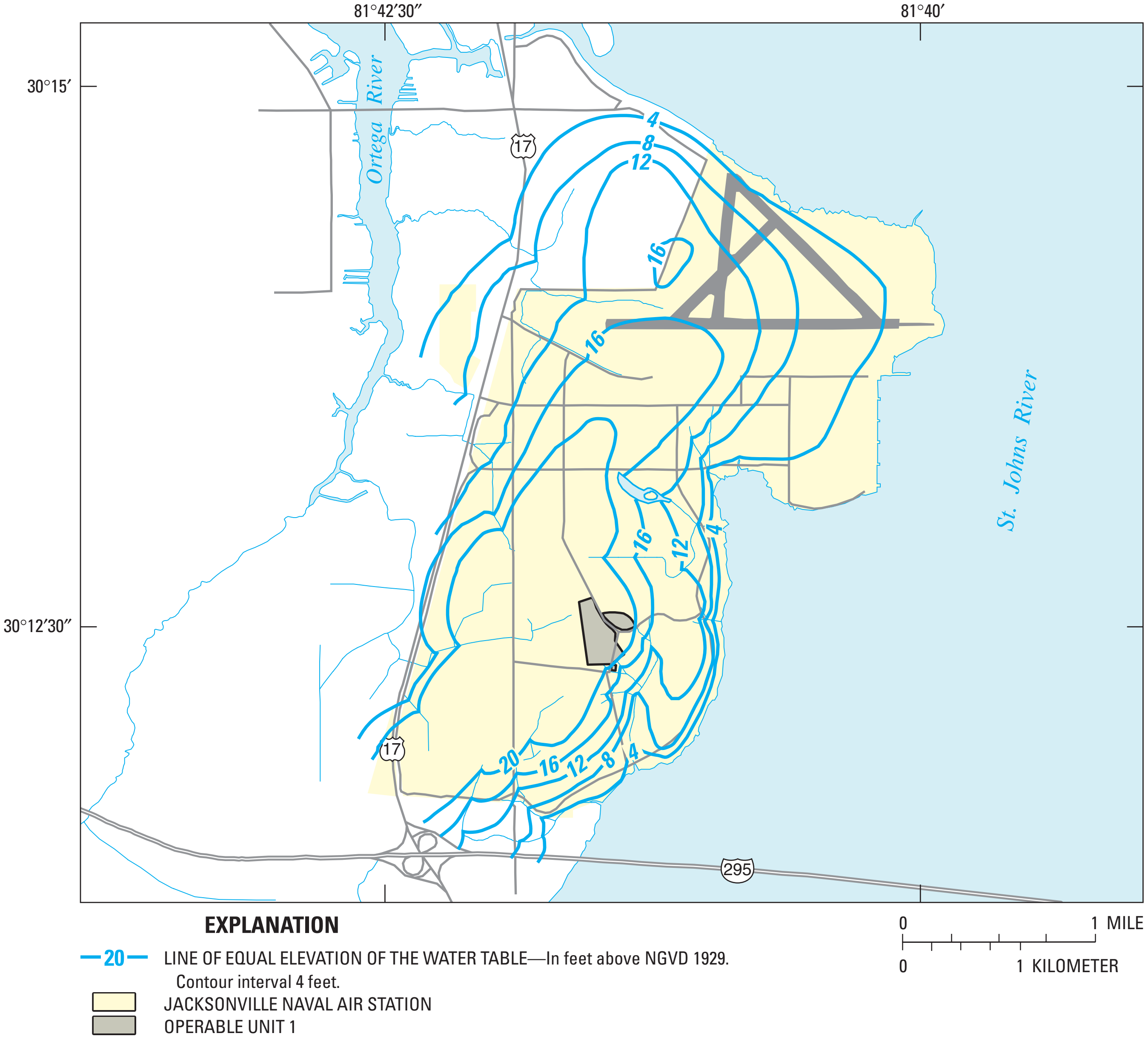
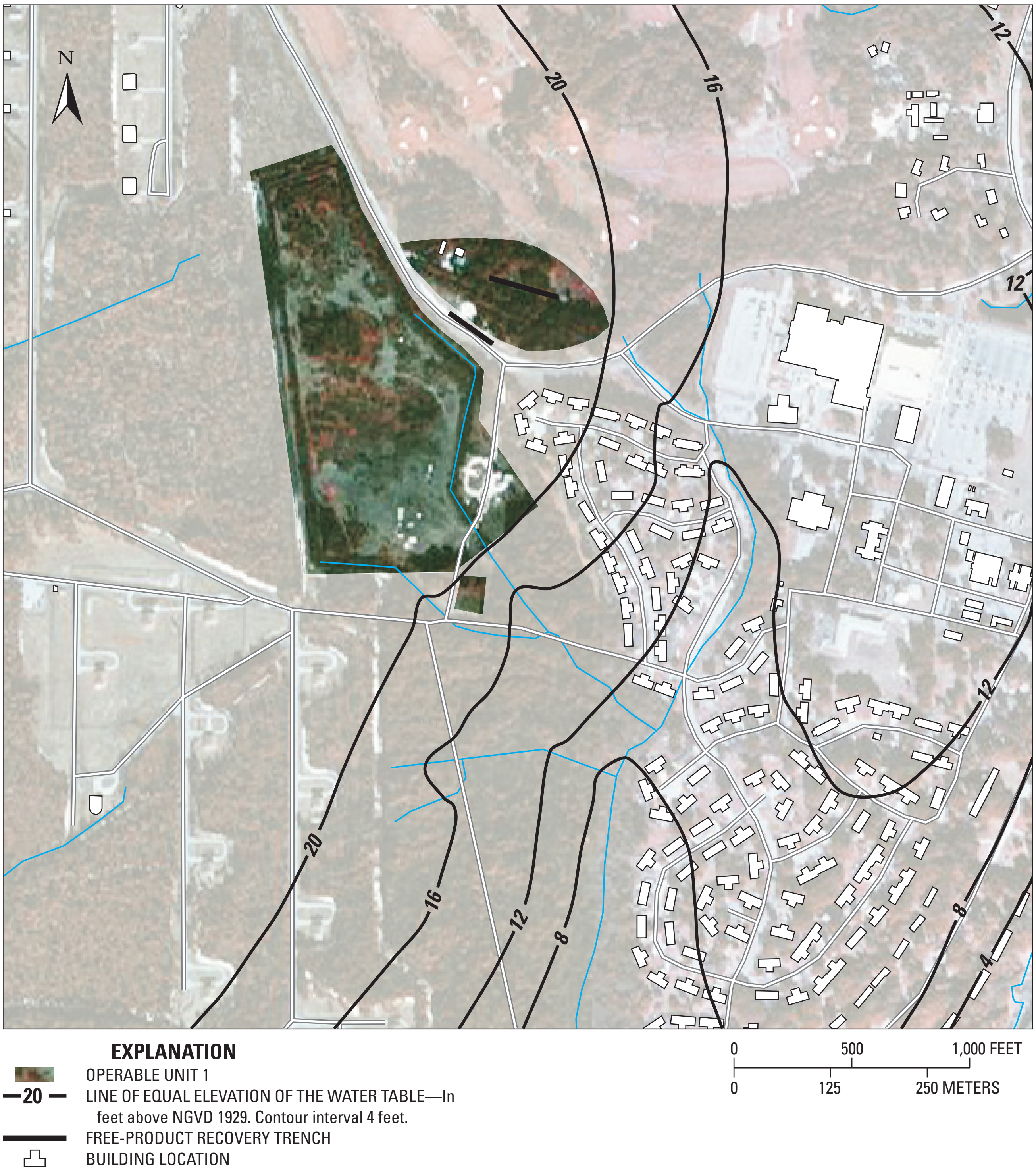


Figure 5. Water-table surface of the surficial aquifer on November 18, 1993, over the entire Station.



Base from Southwest Florida Water Management District digital data, 1992
Universal Transverse Mercator projection, Zone 17, Datum NAD27

Figure 6. Water-table surface of the surficial aquifer on November 18, 1993, in the vicinity of Operable Unit 1.

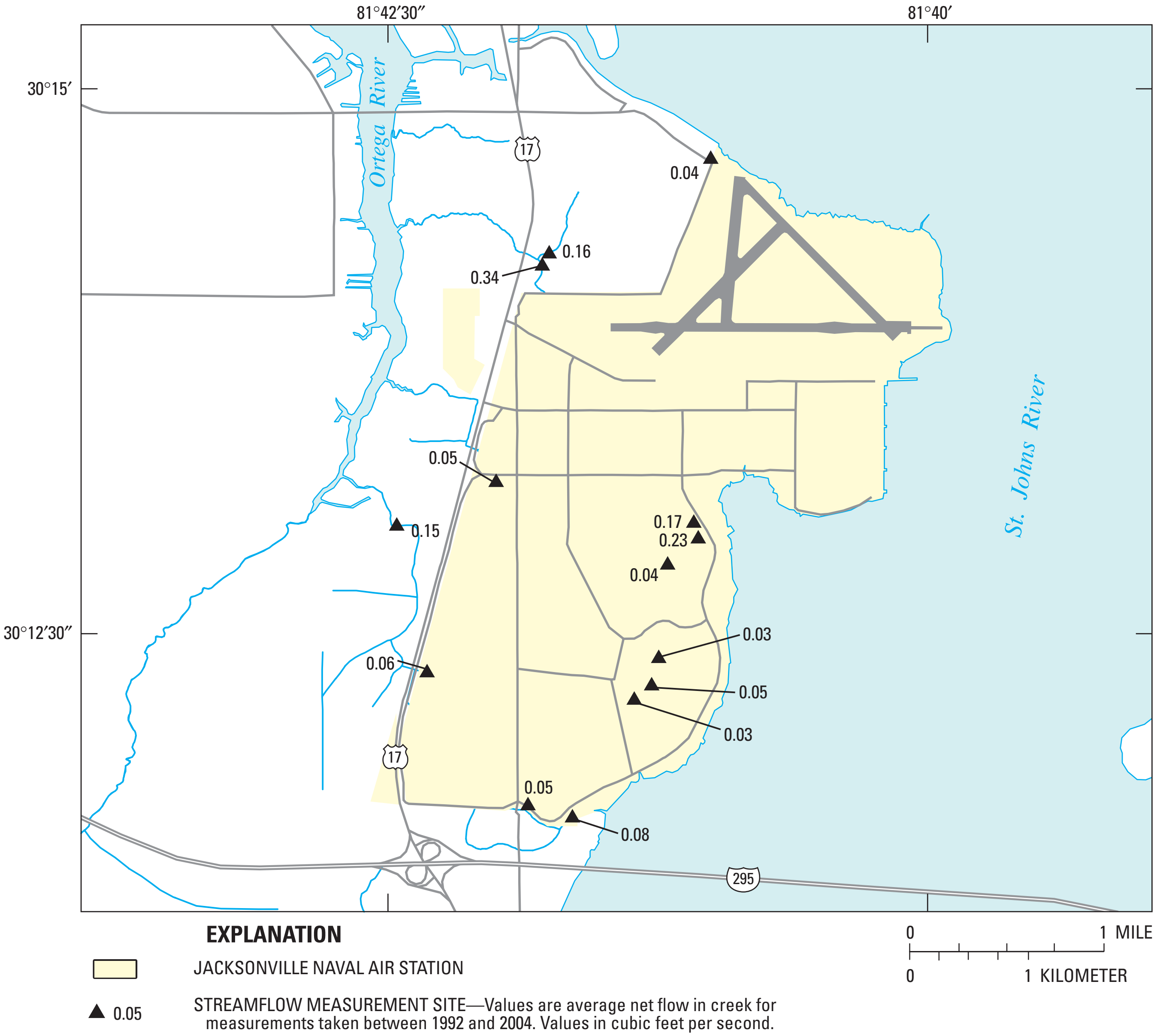


Figure 7. Stream discharges from 1992 to 2004.

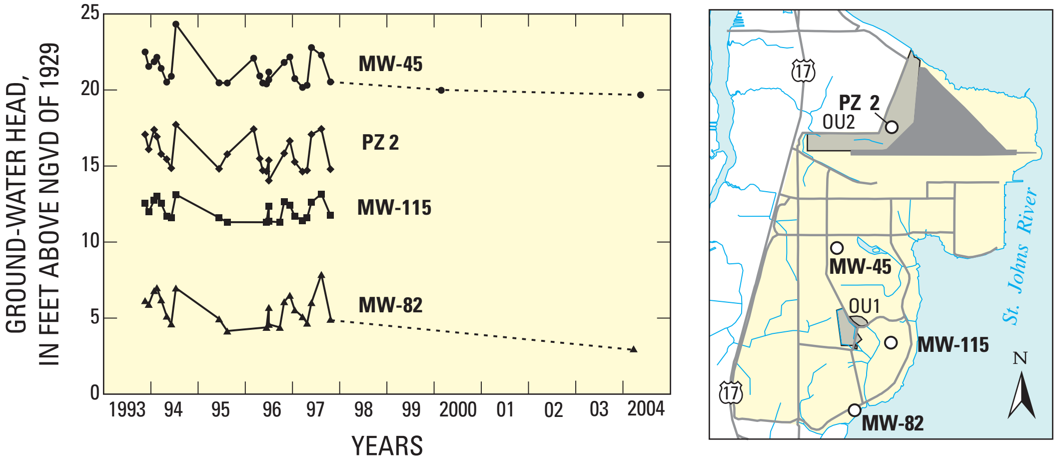


Figure 8. Water-level fluctuations in the surficial aquifer from 1993 to 2004.

Occurrence and Factors Affecting Movement of Trichloroethene, Dichloroethene, and Vinyl Chloride

The primary ground-water contaminants of concern at OU1 are TCE, DCE, and VC. The major source of ground-water contamination occurred as a result of disposing waste oil and solvents in open pits (Cooper and others, 1993; U.S. Navy, 1996). Starting in the 1940s, the Navy used the landfill (which would later become OU1) for the disposal of household and sanitary waste, liquid industrial waste (oil and solvents), and demolition and construction debris. Initially, flammable liquids were burned in the disposal pits; however, burning was discontinued due to air-quality considerations. The disposal of liquids into pits continued until 1978 (U.S. Navy 1996). Although the identity and quantity of waste disposed in each pit are not known, some of the pits received predominately waste solvents and some received both waste solvents and oil. The locations of the waste-solvent pits, waste-solvent and oil pits, and waste-oil plume are shown in figure 9. A total of 105 direct push technology (DPT) samples were collected at OU1 during the initial site investigation (U.S. Navy 1996) to further delineate the contamination. DPT sampling involves pushing a hollow metal rod into the ground to collect geologic samples. Based on the DPT results, approximately 60 ground-water monitoring wells were installed and sampled (U.S. Navy 1996) to further delineate contamination. Later, based on the results of the well sampling, a ground-water monitoring plan was created; only wells with substantial contamination were included in this plan. Wells with no (or low) detections of contamination were abandoned. Because wells near the pit areas fit the no (or low) detection category, they were abandoned. The current 15 monitoring wells (shown in fig. 9) are described in table 1.

Generally, ground water moves from the west-northwest toward the small creeks east-southeast of OU1, as previously discussed. Relatively low levels of TCE and DCE were found in ground water in the vicinity and directly downgradient from the pits; the highest levels of contamination were found approximately halfway between the pits and small creeks, and relatively high levels persisted all the way to the creeks (figs. 10-12). The six shallow monitoring wells are each less than 20 ft deep and are screened across the water table; the nine deep monitoring wells range from 20 to 40 ft deep. The aquifer is composed of interbedded fine sand, silt, and clay, and the different depths represent discrete sampling intervals within one aquifer rather than two separate permeable units. Ground water beneath the disposal pits generally contains relatively low levels of contaminants, indicating that readily dissolved contaminants could have been removed (this might not apply to the most northerly waste-solvent pit 4). High levels of contamination probably continue to exist in the pit areas in the soil matrix. Although concentrations of contaminants in ground water in the vicinity of the pits currently are low, it is not known what these concentrations were during and immediately after disposal; however, they must have been higher to have resulted in the high levels measured farther downgradient.

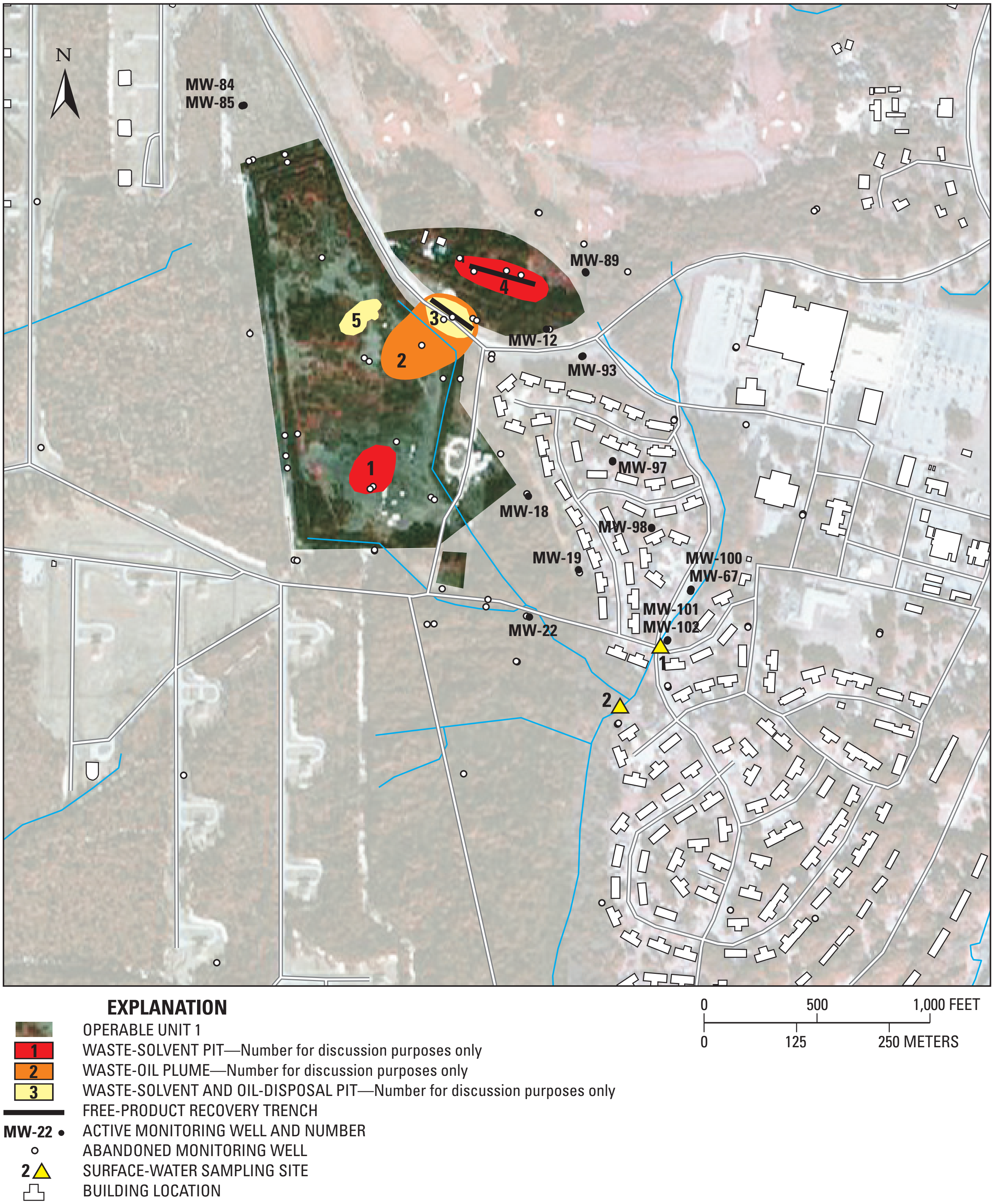


Figure 9. Location of waste oil pits, waste oil and solvent pits, and current water-quality monitoring wells and surface-water sampling sites.

Table 1. Monitoring wells completed in the surficial aquifer at Operable Unit 1.

[Depths and screen intervals are with respect to land surface]

Well name	Altitude of top of casing, in feet	Well depth, in feet	Screen interval depth, in feet	Well name	Altitude of top of casing, in feet	Well depth, in feet	Screen interval depth, in feet
MW-12	29.42	35.5	30-35	MW-93	21.00	13.5	3-13
MW-18	23.10	35.0	27-35	MW-95	18.20	13.0	3-13
MW-19	17.00	25.0	19-24	MW-97	19.40	28.0	23-28
MW-22	20.10	30.5	25-30	MW-98	17.10	26.0	21-26
MW-67	11.70	14.0	4-14	MW-100	11.80	22.0	17-22
MW-84	25.50	40.0	35-40	MW-101	12.60	13.5	3-13
MW-85	unknown	13.5	3-13	MW-102	12.40	21.0	17-21
MW-89	25.01	13.5	3-13				

Concentrations of TCE, DCE, and VC were measured in the creeks at two surface-water sampling sites (figs. 9-12). At site 1, concentrations were below detection limits, except for one sampling event in 1999 (fig. 13). At site 2, farther downstream, all three contaminants were detected at low concentrations. The low concentrations (substantially lower than the highest values found in the ground water) are to be expected because of dilution from water from uncontaminated parts of the creek and from diffusion to the air from these shallow creeks (most creeks are only a few inches deep and 2-5 ft wide).

Distribution of DCE in the ground water is shown in figure 11. The source of DCE contamination is probably the result of reductive dehalogenation of TCE and direct disposal of DCE. The compound TCE can degrade in natural environments by reductive dehalogenation and other mechanisms, producing DCE, which can degrade to VC, which can further degrade to ethene. Degradation occurs when a chlorine molecule is removed and replaced by a hydrogen molecule. The rate of degradation can be extremely variable over small distances and depends on the particular compound and the micro-environments within the aquifer. The DCE/TCE ratio appears to increase from about 2 to about 10 between the deep wells near OU1 and the deep wells near the creek. The distribution of VC in ground water is shown in figure 12. The source of VC contamination is likely the result of reductive dehalogenation of DCE.

Biodegradation has been occurring and was documented at OU1. In 1997, Target Environmental Services (1997) analyzed ground-water samples collected from six wells at OU1, and determined that biodegradation was occurring based on the following evidence: (1) a decrease in concentrations of the original contaminants, (2) an increase in the presence of daughter products, (3) a depletion of oxygen and ferric iron, (4) an increase in ferrous iron, and (5) elevated hydrogen levels.

Ground-water quality data (in some wells) have been collected at OU1 since 1992 as part of the original site investigation, and routine water-quality monitoring began in 1999. Four wells (MW-19, MW-89, MW-97, and MW-100) (fig. 9) were chosen for additional discussion because they have some of the highest levels of contamination at the site. Concentrations of TCE and DCE in MW-19 are approximately equal and have been declining sporadically since 1992 (fig. 14). The detection limits for the chemical analysis range from about 0.1 to 1 µg/L (microgram per liter) (Mark Peterson, Tetra Tech, oral commun., March 2005). Concentrations of VC are relatively low compared to TCE and DCE, and have remained relatively constant; VC concentrations declined from 19 to 16 µg/L between 1992 and 2003. Concentrations of TCE and VC in well MW-100 are relatively low (compared to the DCE concentrations) and have been relatively steady since 1999 (fig. 14); the concentration of DCE has been relatively high and also has remained relatively constant. The constant levels are probably because well MW-100 is located far from the pits, so this well would be expected to be the last to show a decline in contamination.

Concentrations of TCE and DCE in well MW-97 have been declining sporadically since 1999 (fig. 15). Concentrations of VC are low compared to TCE and DCE, and have remained relatively constant, ranging between 1 and 2.7 µg/L during 1999-2003. Concentrations of TCE, DCE, and VC in well MW-89 are relatively high compared with other wells at the site. Construction of the free-product recovery trench in waste disposal pit 4 in 1995 could have caused the release of contamination as a result of digging in the pit area, although the high levels detected in well MW-89 in 1994 indicate that the pit could have been releasing higher contaminant levels prior to 1995.

An additional investigation was conducted at waste solvent pit 4 in 2002, to help determine if the trench and free-product recovery system installed in 1995 were effective

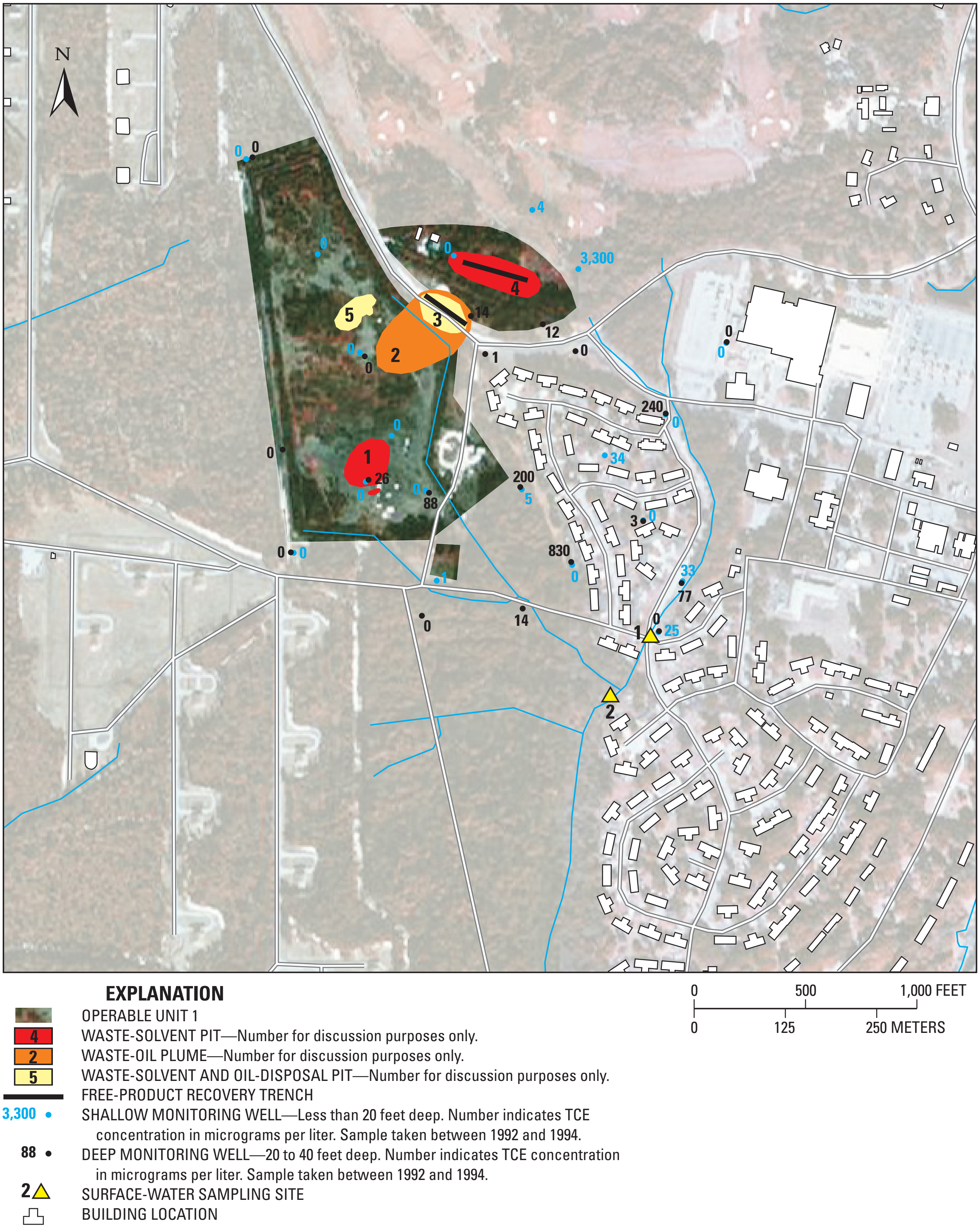


Figure 10. Distribution of trichloroethene (TCE) contamination in the ground water of the surficial aquifer at Operable Unit 1 (composite of samples from 1992 to 1994).

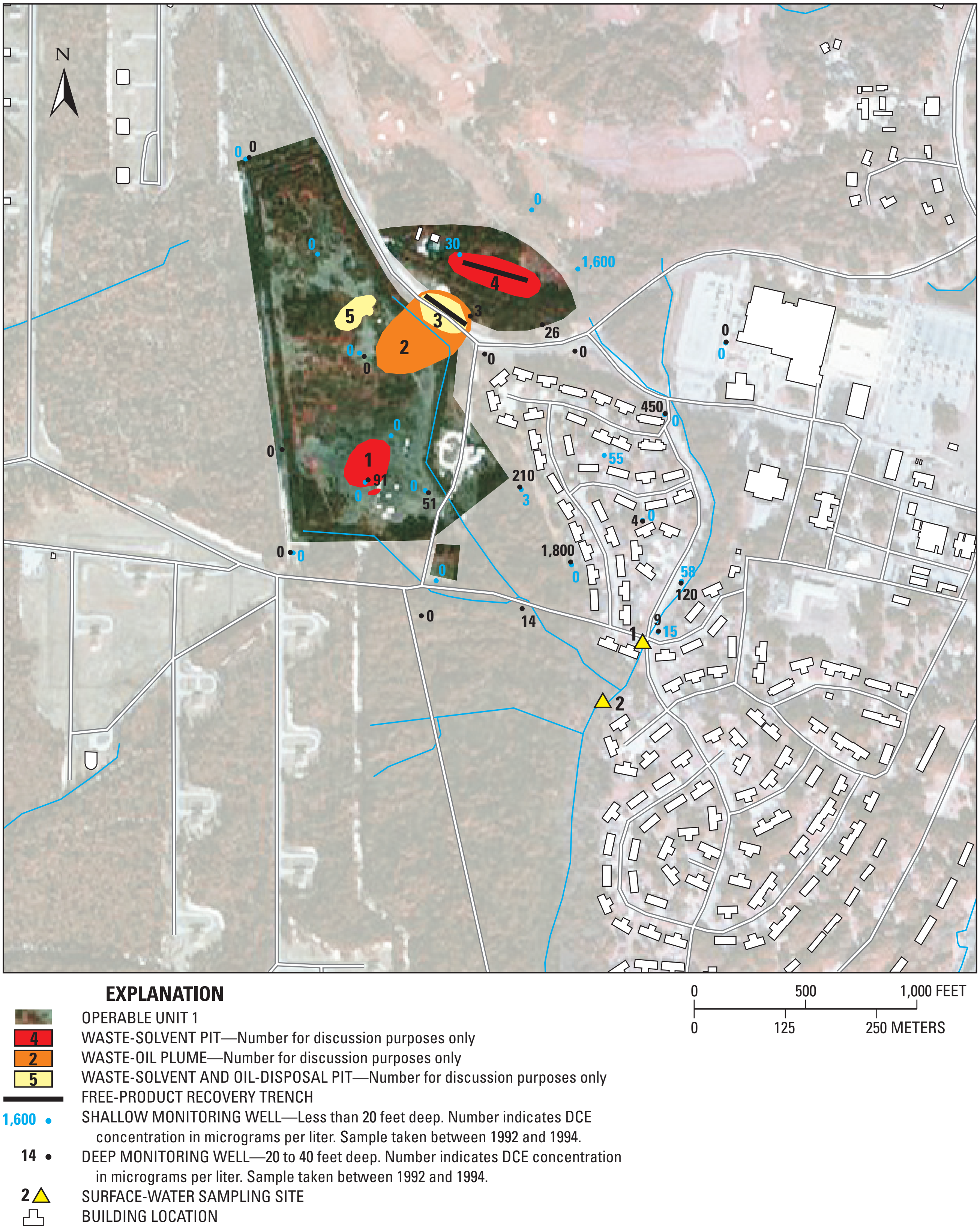


Figure 11. Distribution of dichloroethene (DCE) contamination in the ground water of the surficial aquifer at Operable Unit 1 (composite of samples from 1992 to1994).

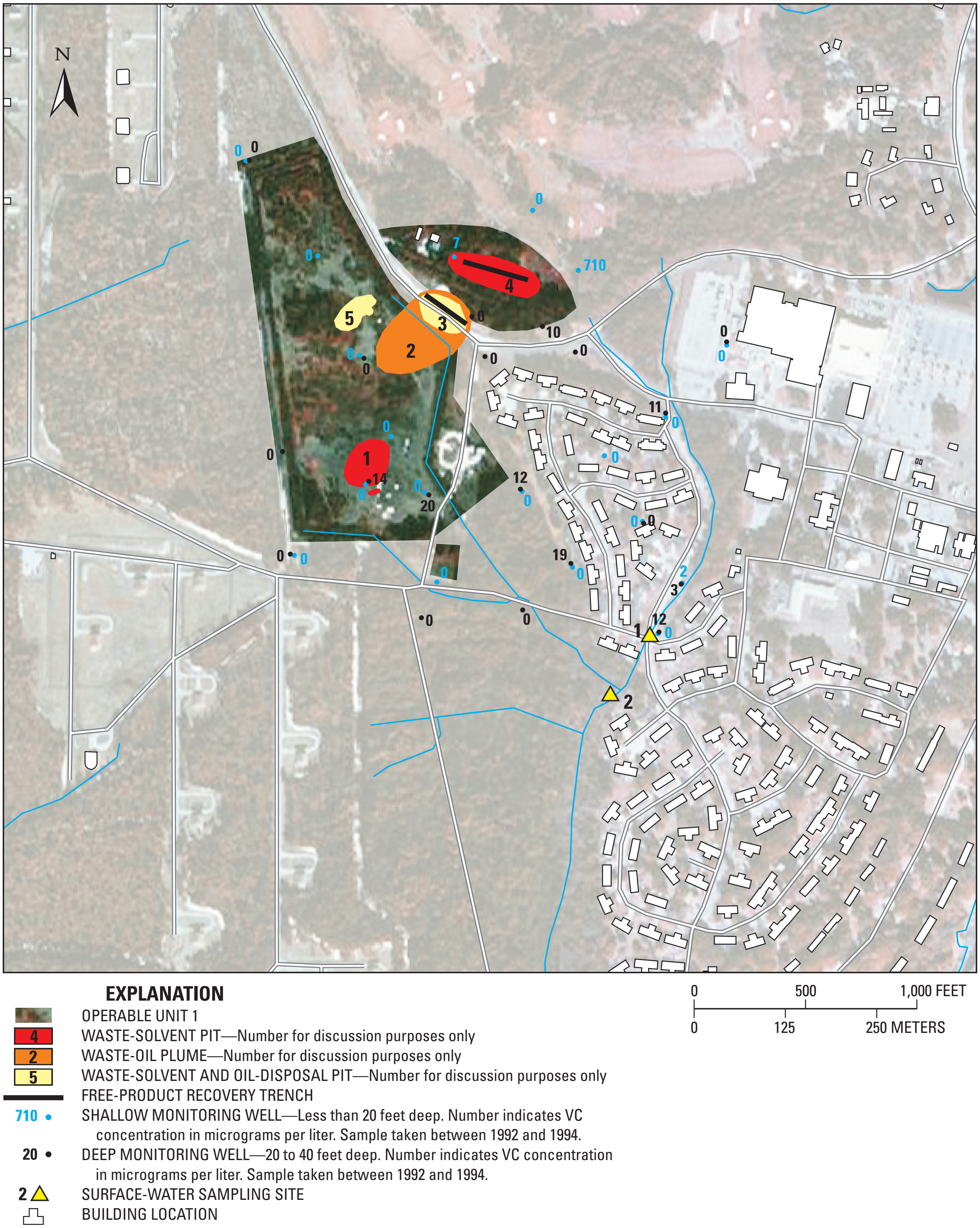


Figure 12. Distribution of vinyl chloride (VC) contamination in the ground water of the surficial aquifer at Operable Unit 1 (composite of samples from 1992 to 1994).

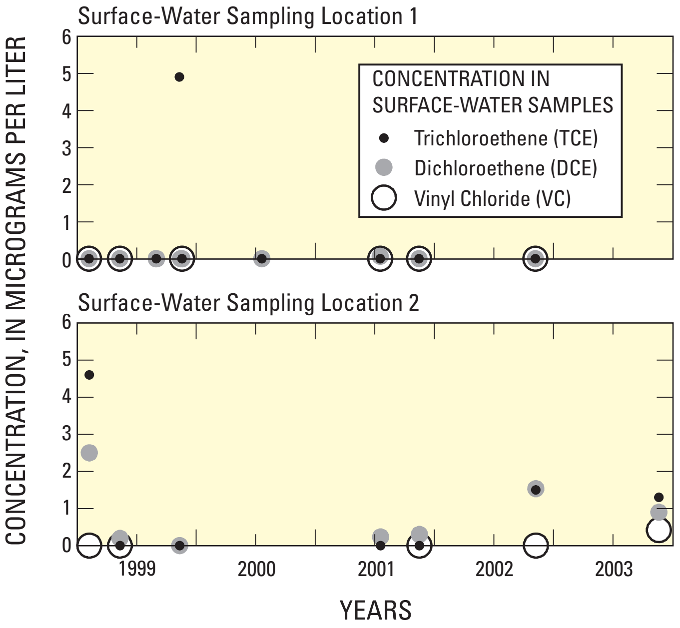


Figure 13. Concentrations of trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) in surface-water sampling locations 1 and 2, 1999-2004.

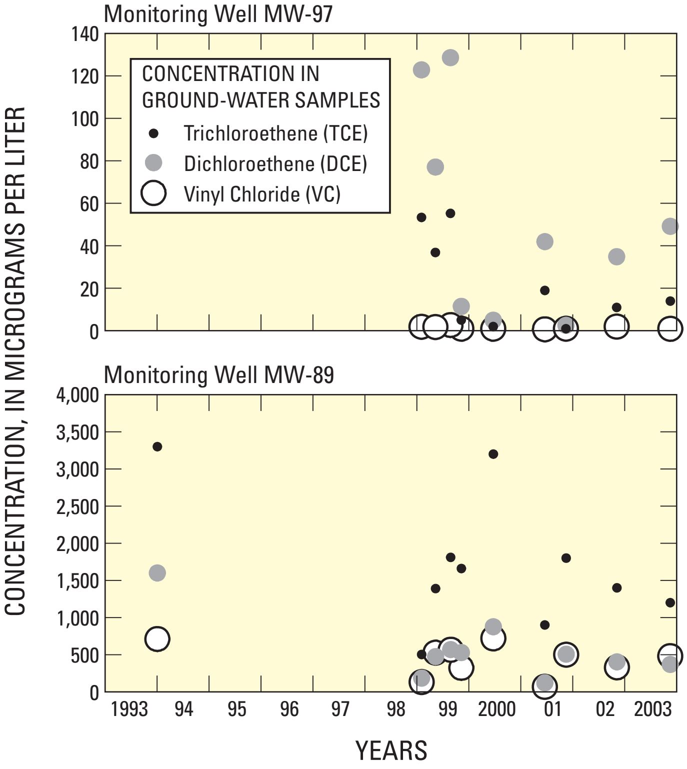


Figure 14. Concentrations of trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) in ground water from monitoring wells MW-19 and MW-100, 1992 to 2003.

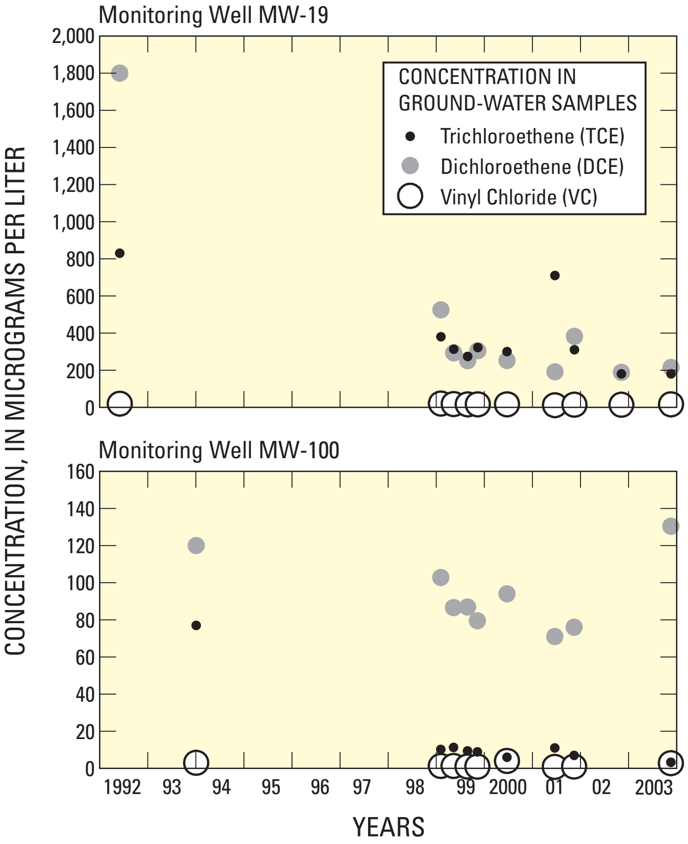


Figure 15. Concentrations of trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) in ground water from monitoring wells MW-97 and MW-89, 1993 to 2003.

(U.S. Navy, 2003). Soil samples collected in the immediate vicinity of the pit (and above the water table) contained elevated levels of petroleum hydrocarbons but had no substantial concentrations of TCE, DCE, or VC. Similarly, ground-water samples showed the same results (although ground water was sampled in just one well). In contrast, high levels of petroleum and chlorinated solvents were present in monitoring well MW-89, which is downgradient from pit 4 (although not directly downgradient). If pit 4 is the source area for the contaminant in well MW-89, then either the distribution of contamination at pit 4 must be variable or the dissolution of chlorinated solvents had been reduced substantially by 2002 when the sampling occurred. An alternate explanation could be the existence of another nearby source area.

The major processes affecting contaminant movement are advection, hydrodynamic dispersion, and retardation as a result of sorption to the sediments. The most important factor affecting contaminant movement at OU1 probably is advection, which is the transport of dissolved constituents with the mean velocity and in the direction of ground-water flow. As previously discussed, the movement of ground water and contamination is from the disposal areas to the southeast, toward the small creeks.

Hydrodynamic dispersion of a dissolved chemical occurs as a result of local variation in ground-water velocity around the mean advective velocity and molecular diffusion. Dispersion will cause a contaminant plume to spread, resulting in lower concentrations away from the plume center. Dispersivities usually are difficult to quantify accurately in the field. Gelhar and others (1992) performed a critical review of field-scale dispersion studies to define reasonable dispersivity values. Using data that these authors described as the most reliable, a reasonable value for longitudinal dispersivity (in the direction of the flow axis) was 7.0 ft for sites similar to OU1. A reasonable value for transverse dispersivity (perpendicular to the flow axis) was 1.3 ft based on the length of contaminant travel.

The rate of movement of a dissolved chemical depends on the ground-water flow velocity and the retardation factor of the particular chemical. The retardation factor is the ratio of the velocity of ground water to the velocity of the chemical. For example, a retardation factor of 1.5 means that ground water moves 1.5 times faster than the dissolved chemical. Retardation of TCE, DCE, and VC occurs because these chemicals are nonpolar, which causes them to partition to the organic matter contained in the aquifer sediments. Therefore, retardation and retardation factors are a function of the fraction of organic carbon content (f_{OC}) of the aquifer. Partitioning is a reversible process; molecules that have partitioned to the organic matter will return to the ground water as relative concentrations change. The retardation factors determined at OU1 were 1.8 for TCE, 1.6 for DCE, and 1.4 for VC (U.S. Navy 1996).

Ground-Water Flow Simulation at the Station

The regional ground-water flow model, originally calibrated for the Station and documented by Davis (1996), was recalibrated and used for this study. The active regional model grid is shown in figure 16. The model consists of one layer with 241 rows and 293 columns; all cells are 100 by 100 ft. The base of the aquifer is the top of the Hawthorn Group (figs. 2-4). The surficial aquifer was modeled as unconfined, and steady-state ground-water flow conditions were assumed. The base of the aquifer is a no-flow boundary.

For calibration purposes, 17 new ground-water-level (head) and 11 stream discharge measurements were obtained from the southern half of the Station. The new heads and all previous head measurements were averaged to approximate the head during average hydrologic conditions; likewise, all of the discharge measurements were averaged. Locations of the previous and new monitoring wells and discharge measurement site locations are shown in figure 16. The recalibration consisted of varying only the recharge rates until the head and discharge values matched the average values. The original 1996 model was calibrated to wetter conditions, so recharge rates were reduced slightly in the new model to simulate the lower rainfall conditions in 1998-2002. The hydraulic conductivity (7.8 ft/d) and riverbed conductances were not altered from Davis (1996). Only the southern half of the model was updated, since that is where the study was concentrated and where new data were collected. Measured and simulated discharge values are listed in table 2. The original strategy for calibrating ground-water levels was to have the simulated heads be within 2.5 ft of the measured heads; the same strategy was used for the recalibrated model. The simulated minus the measured heads equals the residual heads. A graph showing the residuals in relation to the simulated heads is shown in figure 17. Heads at all but 3 of the 32 wells met the ± 2.5-ft criterion.

Recharge rates were determined by model calibration, and ranged from less than 1 in/yr (inch per year) in areas that were largely paved to 13 in/yr at the golf courses. Most recharge rates ranged from 3 to 8 in/yr. The new recharge distribution is shown in figure 18.

Operable Unit 1 Site-Specific Model

The regional model was used to establish boundary conditions for the OU1 site-specific ground-water model. This site-specific model was created to simulate the ground-water flow in the immediate vicinity of OU1 and has a refined grid to improve the resolution. Steady-state ground-water flow conditions were assumed.

Model Construction and Calibration

The OU1 model contains 130 rows and 122 columns of active model cells, all in one layer. All cells are square and are 25 ft long on each side. The location and orientation of the finite-difference grid for the OU1 model is shown in figure 19. The perimeter of the model consists of a no-flow boundary established by following pathlines generated by the regional model—except for a line of specified-head cells that was placed along the upgradient part of the model, where a ground-water divide occurs and the specified-head cells allow water to enter or leave the model as necessary. The model was calibrated to the same data as the regional model. The cap was simulated in both the regional and site-specific model. The head in the specified-head cells was set using the head from the regional model. The small creeks (fig. 19) were simulated using the River Package. Because cell size is smaller in the site-specific model than in the regional model, riverbed conductances needed to be reduced (the riverbed conductance incorporates the length of river that crosses a cell). In addition, some adjustment of the riverbed conductances was required to fine tune the calibration.

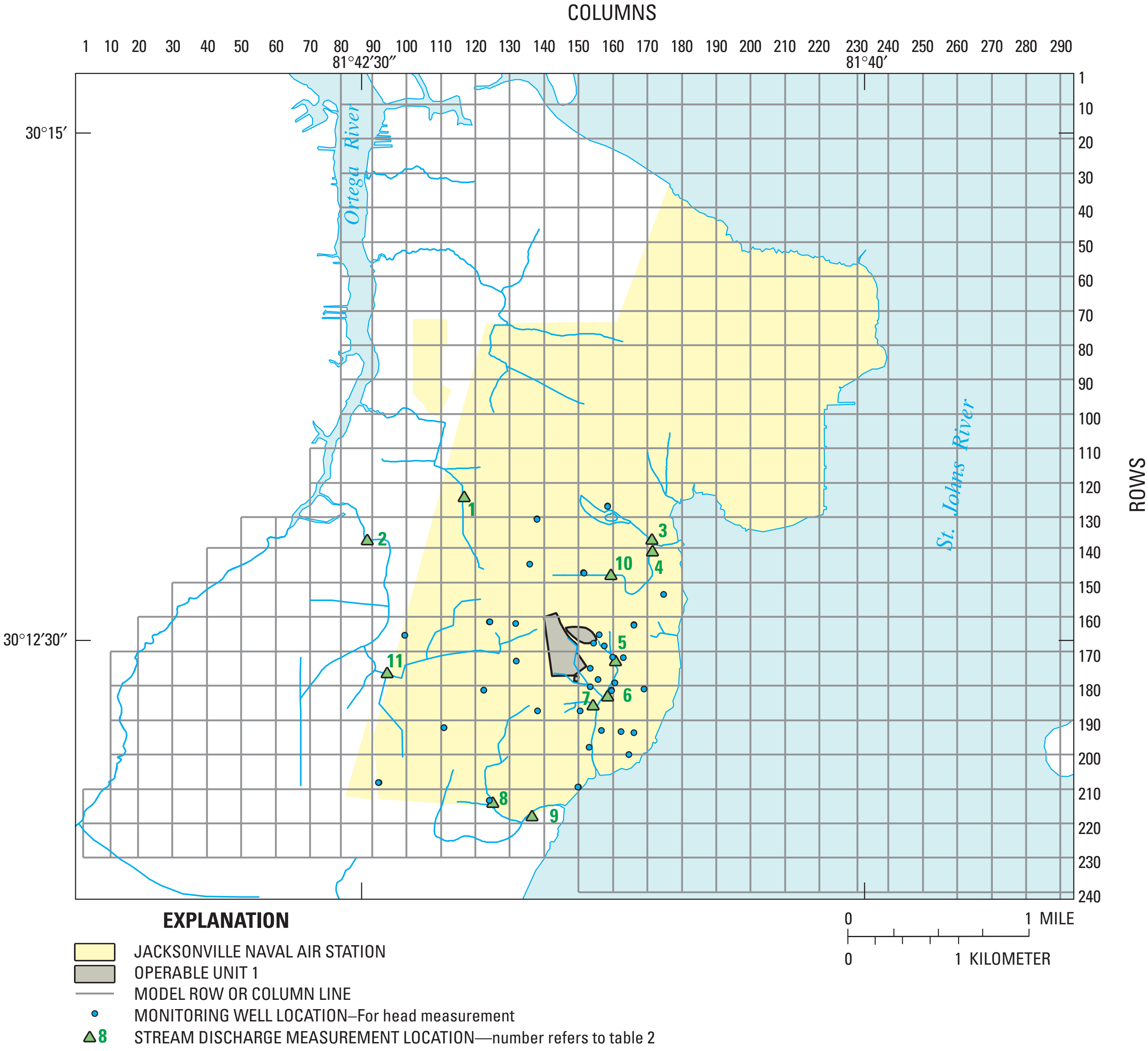


Figure 16. Location of the regional model grid and measurement sites.

The calibration strategy was to match all of the measured heads and discharge rates in the subregion as closely as possible using a trial-and-error approach. After calibration, all of the simulated heads were within 1.5 ft of the measured heads (fig. 20) and all of the discharge rates at streamflow measurement sites 5, 6, and 7 were within 10 percent of the measured rates. Almost all (96 percent) of the simulated ground-water flow was east-southeastward toward the creeks, with only a small part (4 percent) flowing west-northwest toward the specified head cells. Although the riverbed conductances were varied during calibration, hydraulic conductivities and recharge rates were not modified from the regional model values. Model-calculated (simulated) and measured discharge values are shown in table 3. The simulated total discharge was about 1 percent higher than the measured discharge. Most discharge measurements were made under poor conditions, so the measured discharge probably had at least an 8-percent error.

Table 2. Comparison of measured and simulated discharge for the regional model.

Stream discharge measurement site number (fig. 16)	Measured average discharge, in cubic feet per day	Simulated discharge, in cubic feet per day	Percent difference
1	4,320	3,850	-11
2	21,600	23,813	10
3	14,688	12,699	-14
4	19,872	19,756	1
5	2,592	2,837	9
6	4,320	3,850	-11
7	2,592	2,837	9
8	4,320	3,850	-11
9	2,592	2,445	-6
10	3,456	2,763	-20
11	5,184	6,004	16

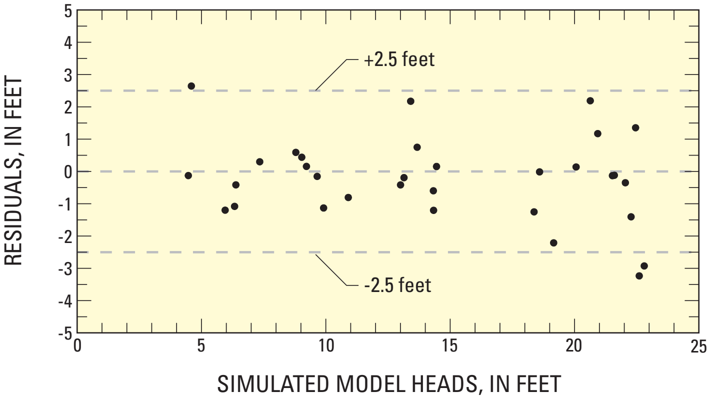


Figure 17. Residuals in relation to the simulated heads for the base-wide model.

Sensitivity Analysis

Sensitivity tests were conducted to determine the effect of changes in model input parameters on the model calibration. Tests were conducted by increasing (or decreasing) each parameter by 50 percent while other parameters remain unchanged. Parameter changes in a simulation resulted in a new distribution of heads and discharge values, and the effect of the parameter change was judged by determining the number of simulated heads that no longer remained within 1.5 ft of the measured values (table 4), and the percent change in simulated discharge at streamflow measurement sites 5, 6, and 7. Input parameters tested were recharge, riverbed conductance, and horizontal hydraulic conductivity.

The model was sensitive to recharge rate changes because recharge was the only source of water to the model. Decreasing the recharge rate by 50 percent caused the simulated heads to drop and the number of simulated heads exceeding the error criterion to increase from 0 to 2 (out of 11); it also caused the simulated discharge values to fall to 43 percent below the measured values. Increasing the recharge rate by 50 percent caused the simulated heads to rise and the number of simulated heads exceeding the error criterion to increase from 0 to 2; it also caused the simulated discharge values to increase to 43 percent above the measured values. Heads in the OU1 site model were relatively insensitive because most of the wells are near creeks, which limit the rise and fall of heads both in the aquifer and in the model.

Decreasing or increasing the riverbed conductance caused little change in the model, probably because the riverbed conductances were relatively high and the creeks only drain water from the aquifer (creeks do not leak water to the aquifer in this model). Changing the conductances by 50 percent did not substantially change the discharge or heads. If the riverbed conductances were lowered sufficiently, heads in the aquifer would begin to rise and the head distribution would be substantially different. Decreasing the river bottom elevation by 50 percent caused all of the heads to exceed the error criterion and caused discharge values to increase by 1 percent. Increasing the river bottom elevation by 50 percent caused all of the heads to exceed the error criterion, but caused discharge to decrease by 9 percent. Decreasing the horizontal hydraulic conductivity by 50 percent caused two heads to exceed the error criterion. An increase of 50 percent in the horizontal hydraulic conductivity caused two of the heads to exceed the error criterion. The simulated discharge values did not change substantially, because the recharge did not change.

Ground-Water Flow Model Limitations

The OU1 site model was constructed to simulate steady-state conditions, because water levels have shown no long-term trend (but did show seasonal variation). The water table generally is close to the land surface, so there is little capacity for a substantial rise in water levels. An extended drought, however, could reduce water levels to below those that were used to calibrate the model. This would result in simulated ground-water flow velocities that would be higher than actual velocities.

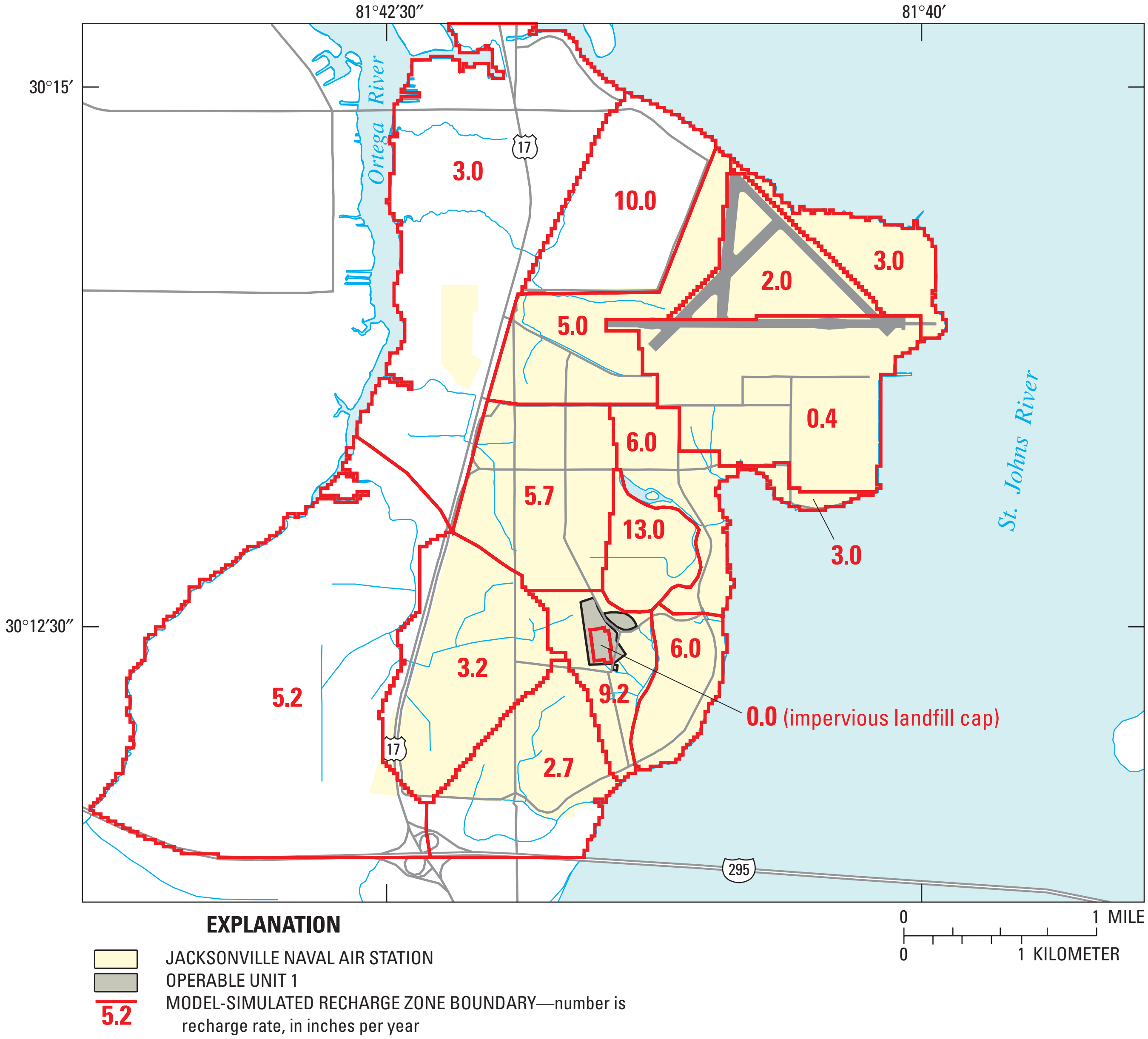


Figure 18. Model-simulated recharge rates for the recalibrated model.

The model uses Darcy's Law, which describes groundwater flow in saturated porous media, to predict the movement of ground water. The accuracy of this model depends on the aquifer fitting the assumptions of this law. Because the aquifer at OU1 is fully saturated and is composed of medium- to fine-grained sediments, the model should fit the assumptions of Darcy's Law.

The surficial aquifer at OU1 was modeled as a single layer, because there were insufficient data to separate the aquifer into multiple layers, and the aquifer appeared to be vertically well connected (there were no significant vertical head gradients at the site). All aquifers have variable permeabilities based on sediment layering and the surficial aquifer is no exception. If high permeability layers carry relatively large amounts of ground water, then the contamination could move through the aquifer system at velocities greater than predicted.

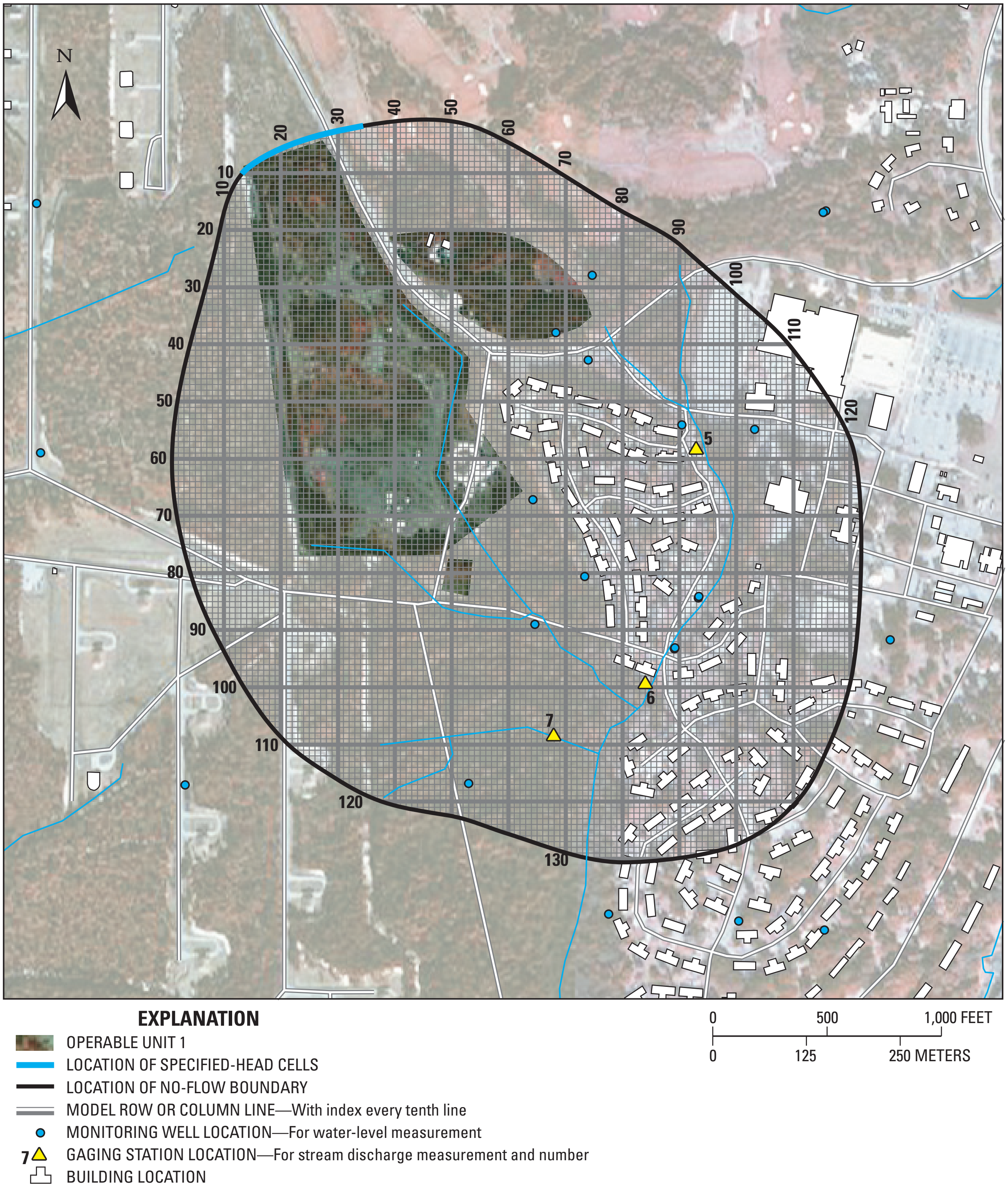


Figure 19. Location and orientation of the subregional model finite-difference grid.

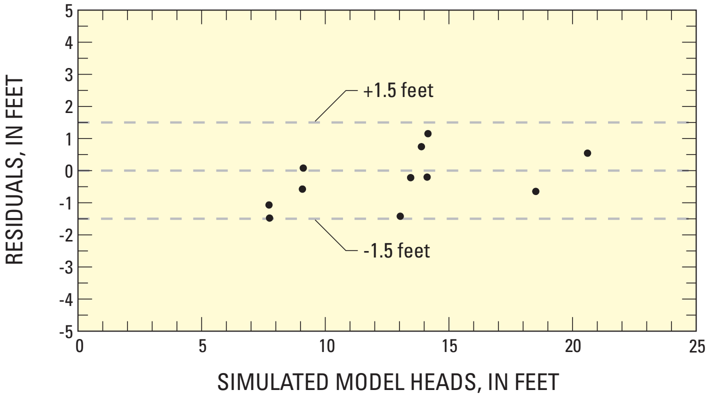


Figure 20. Residuals in relation to simulated model heads for the Operable Unit 1 model.

Table 3. Comparison of simulated and measured stream discharge for the Operable Unit 1 model.

Stream discharge measurement site number (fig. 16)	Measured average discharge, in cubic feet per day	Simulated discharge, in cubic feet per day	Percent difference
5	2,592	2,859	10
6	4,320	4,122	-5
7	2,592	2,657	3
Total	9,504	9,638	1

Table 4. Summary of sensitivity analyses for the recalibrated Operable Unit 1 site-specific model.

[*, indicates parameter is multiplied by the number to the right. Measured discharge values were: 2,592 ft^3/d (cubic feet per day) at site 5, 4,320 ft^3/d at site 6, and 2,592 ft^3/d at site 7]

Parameter changed	Number of simulated heads that exceeded the calibration criterion of 1.5 feet	Simulated discharge (cubic feet per day)			Percentage of discharge values above (+) or below (-) measured discharge
		Stream discharge measurement site 5	Stream discharge measurement site 6	Stream discharge measurement site 7	
Calibrated model	0	2,859	4,123	2,657	+1
Recharge * 0.5	2	993	3,093	1,322	-43
Recharge * 1.5	2	4,654	5,071	3,884	+43
Riverbed conductance * 0.5	0	2,924	4,078	2,678	+2
Riverbed conductance * 1.5	0	2,859	4,123	2,657	+1
River bottom elevation * 0.5	11	4,338	2,757	2,530	+1
River bottom elevation * 1.5	11	840	5,561	2,240	-9
Horizontal hydraulic conductivity of upper layer * 0.5	2	3,144	3,014	2,484	-9
Horizontal hydraulic conductivity of upper layer * 1.5	1	2,408	5,142	2,265	+3

Fate and Transport Simulations of Trichloroethene, Dichloroethene, and Vinyl Chloride at Operable Unit 1

Fate and transport modeling at OU1 was conducted to help understand how contaminants move in the ground-water flow system and specifically to estimate how long it could take for the contaminants to move through the system. The previously discussed OU1 flow model was used in combination with the modeling computer code, Reactive Transport in Three Dimensions (RT3D), developed by Clement (1997), for the fate and transport modeling. This code was used because it can simulate the degradation of TCE to DCE to VC.

The objective of the fate and transport modeling calibration was to match, as closely as possible, the known temporal and spatial distributions of TCE, DCE, and VC using a trial-and-error approach. Although the disposal of solvents at OU1 began in the 1940s, ground-water quality sampling did not begin until 1992. The calibration strategy consisted of varying the effective porosity, dispersivity, retardation, chemical decay rate, and start and stop times of dissolution from the disposal pits until simulated concentrations matched the measured concentrations as closely as possible. The OU1 flow model was modified slightly for the fate and transport modeling. The model was changed from steady state to transient so that the installation of the impermeable cap at OU1 in 1998 could be simulated. The simulated recharge was included in the cap area before 1998 but not after. The specific yield of the aquifer was assumed to be 0.1, which is between the range of expected values of 0.01 to 0.3 (Freeze and Cherry, 1979); effective porosity was assumed to be 22.5 percent. For each simulation, all other model parameters were constant; degradation and sorption were constant along a flow path, and degradation occurred in both the dissolved and sorbed phases. After calibration, the fate and transport model was used to simulate future concentrations. The ground-water flow model simulated the period from January 1, 1945, to January 1, 2020. This period was divided into two stress periods: from January 1, 1945, to January 1, 1998, and from January 1, 1998, to January 1, 2020. During the second stress period, the recharge at the impervious cap was changed from 9.2 to 0.0 in/yr to simulate cap installation.

The contaminant transport model simulations were divided into five stress periods: from January 1, 1945, to January 1, 1970; from January 1, 1970, to January 2, 1979; from January 2, 1979, to July 1, 1995; from July 1, 1995, to January 1, 1998; and from January 1, 1998, to January 1, 2020. The purpose of dividing the simulations into these stress periods was to facilitate the simulation of the release of contaminants at the times of disposal (as discussed below) and the simulation of installation of the impervious cap. The stress periods were further divided into time steps. The time steps were determined by the model code and were 13.5 days each.

Conceptual Model of Contaminant Movement

The disposal of oil and solvents at OU1 began in the 1940s. The disposal pits would have begun releasing contaminants to the ground water immediately, and the contaminants would have migrated southeast toward the small creeks that drain water from the surficial aquifer. Travel of the contaminants to the creeks was relatively slow, because ground-water flow was slow, and because organic matter in the aquifer also retarded the movements of contaminants. Contaminant concentrations also would have declined due to dispersion as the contaminant moved farther from the source. The spread of contamination probably reached its maximum extent in the 1970s; during the late 1970s, disposal at the pits was discontinued. The monitoring well sampling, which occurred from 1992 to 1994, gave the first look at the distribution of contamination in the ground water at the site (figs. 10, 12, and 13). As previously discussed, ground water in the vicinity and directly downgradient from the pits had relatively low contaminant levels; the highest levels were found about midway to the creeks. For this distribution to occur, the dissolution of contamination from the pits would have had to decline substantially at some point in the past.

The reduction in dissolution could be caused by two mechanisms; either the source of the solvents was dissolved away or the easily dissolved solvents were depleted while the solvents that were contained in less permeable parts of the aquifer (with sluggish or little ground-water flow) remained. Exactly how rapidly the pits would transition from releasing high levels of contaminants to low levels is difficult to access accurately. Hartog (2004) injected a 50-L (liter) mixture of trichloromethane (5 L), TCE (22.5 L), and PCE (22.5 L) into a shallow, uniformly sandy aquifer. The downgradient concentration of TCE remained high until 80 percent of the TCE was dissolved, then the concentration declined rapidly. The time between injection and TCE depletion was 2 years. Because the ground water beneath and downgradient from the pits is relatively clean, a similarly rapid decline in concentrations is possible.

In Hartog's study, the injected contaminants were believed to have completely dissolved. This result presumably occurred because the aquifer is uniformly sandy, allowing flowing ground water to come into close contact with the free product. The aquifer at OU1 is more complex, consisting of interbedded fine sands, silts, and clays. The mechanism by which TCE, DCE, and VC were distributed through the aquifer indicates that during the period when dumping occurred, a continuous supply of free product was in contact with flowing ground water. Once the dumping stopped, the free product in contact with moving ground water was dissolved. According to Hartog's study, the downgradient concentrations would have remained high until a substantial amount of the TCE and DCE that was readily dissolvable was consumed. After the readily dissolvable amount was depleted, concentrations in the ground water around the pits would have decreased. Because of the complex aquifer lithology, a large quantity of free product could remain in the pit areas but would be isolated from the readily moving ground water.

Once dissolution was reduced substantially, ground-water quality in the aquifer near the pits would improve. The dissolved contaminates would eventually travel through the aquifer to discharge to the small creeks. As seen in figures 10 to 12, this process was underway at the site when the investigations began in the 1990s. Free-product recovery trenches were installed in pits 3 and 4 in 1995. The goal of using the trenches was to collect free product, which was continually pumped out and removed from the site; however, this disturbance could have caused pits 3 and 4 to once again become a source of ground-water contamination by allowing residual free product access with actively flowing ground water.

Fate and Transport Modeling Overview

The model simulated a time period that began in 1945. The waste-disposal pits were simulated as specified concentration cells. The period of time that a pit acted as a source of ground-water contamination and the concentration levels of TCE, DCE, and VC at the pit during the simulations is given in table 5. These times and concentrations were determined during model calibration (and are discussed later). Pit 4 could have acted as an important source twice; the first time was during the period when solvents were being disposed, and the second time was immediately after the free-product recovery trench was installed, assuming that this disturbance allowed for additional dissolution of contaminants. When a simulation began, RT3D assigned particles to specified concentration model cells and each particle represented a cell volume-weighted mass of contamination. The movement of particles was tracked during each step in the simulation. The sum of the masses of all the particles in a cell equaled the total mass of contamination for that cell. The cells in the pit areas were modeled with specified concentrations during model steps (although the concentrations varied from one step to the next). Because the free-product phase of the contaminants is denser than water, it is not possible to know exactly where in the aquifer the free product could be located, so it was simulated throughout the full thickness (although this probably resulted in simulating more dissolved product than actually existed).

Advection of ground water is the most important factor governing the transport of these chemical compounds. The direction of ground-water flow was determined from the intercell flow velocities, which were part of the output from MODFLOW. The intercell flow velocities were divided by the effective porosity to calculate the ground-water velocity. In addition to advection, the effects of retardation, hydrodynamic dispersion, and chemical decay were added to the simulation. The effects of retardation due to sorption caused the contaminant to move slower than the ground water, and these effects were specified by the retardation factor. The effect of hydrodynamic dispersion, as specified by the dispersivity, caused the plume to spread.

Table 5. Time periods and contaminant concentrations used in waste-disposal pit simulations.

[Concentrations are in micrograms per liter]

Pit number	Simulation start date	Simulation stop date	Trichloroethene	Dichloroethene	Vinyl chloride
1	1945	1979	10,000	10,000	0
1	1979	End of simulation	25	25	0
2	1945	1979	10,000	10,000	0
2	1979	End of simulation	10	10	0
3	1945	1979	2,500	2,500	0
3	1979	End of simulation	10	10	0
4	1945	1970	30,000	30,000	0
4	1970	1995	10	10	0
4	1995	1998	30,000	30,000	0
4	1998	End of simulation	10	10	0
5	1945	1979	10,000	10,000	0
5	1979	End of simulation	10	10	0

Chemical decay, as specified by a half-life, dictated how rapidly the compounds degraded naturally in the aquifer. The compound TCE degrades into DCE; DCE degrades into VC; and VC can degrade into ethene (VC can biodegrade to other nonhazardous compounds). Anaerobic dechlorination occurs by sequential removal of chlorine atoms. In this case, TCE consists of two double-bonded carbon atoms surrounded by three chlorine atoms and one hydrogen atom. As a result, TCE is transformed to DCE when one of the chlorine atoms is replaced by a hydrogen atom. Subsequently, DCE is transformed into VC when one of the two remaining chlorine atoms is replaced by another hydrogen atom. For a more complete discussion of contaminant transport, refer to Zheng and Bennett (1995).

Calibration to Current Distributions of Trichloroethene, Dichloroethene, and Vinyl Chloride

Disposal into the pits began in 1945, but the investigation into ground-water quality did not begin until the 1990s. So about 45 years passed for which there are no data to aid in model calibration. The overall calibration strategy was as follows: (1) set the simulation period to begin in 1945, when leaching of TCE and DCE to the ground water began; (2) simulate the movement of TCE and DCE in the aquifer, as well as the degradation of TCE to DCE to VC to nonhazardous compounds; and (3) adjust the starting levels of TCE and DCE and the time when the pit stopped releasing contaminants such that the model best matches the downgradient trend in TCE, DCE, and VC levels in the monitoring wells.

The simulated concentration of TCE in 1970 is shown in figure 21. In this scenario, the pits have been leaching since 1945 and the concentrations probably represent nearly the maximum extent of contamination and are approaching steady state.

The simulated extent of TCE and DCE contamination in 1994 is shown in figures 22 and 23, respectively. At the end of the simulation period, all of the pits were releasing low levels of contaminants. In 1979, pits 1, 2, 3, and 5 transition from releasing high levels of TCE and DCE to low levels. This transition was necessary to match the low levels of contamination at and downgradient from the waste-disposal pits. In turn, the pits were simulated as releasing higher levels of contamination prior to 1979 in order to match the higher levels of contamination farther downgradient and in the vicinity of the creeks.

The simulated extent of VC contamination in 1998 is shown in figure 24. At the end of the simulation period, pits 1, 2, 3, and 5 were releasing low levels of contaminants. Free-product recovery trenches were installed in pits 3 and 4 in 1995. This disturbance could have caused the area around these pits to once again become a source of ground-water contamination (the reason for the high concentrations shown on the figure in the vicinity of pit 4). Therefore, this area was simulated as a source from 1995 to 1998. Only the eastern part of pit 4 was simulated as a renewed source of contamination, because the installed trench was filled with gravel (the surficial aquifer is silty sand) and the ground-water table slopes eastward. Consequently, ground water would be expected to flow into the trench on the western end and out of the trench on the eastern end. Another possibility is that the digging could have rearranged the distribution of sediments, which would have allowed some free product to once again come into contact with actively flowing ground water. The pits would be expected to release contaminants until the contaminant source was depleted. Routine ground-water sampling did not begin until 1999, so no data exist to verify the simulation. Because there is no water-quality sampling evidence that pit 3 began releasing contaminants again, it was not modeled as doing so (although it is a possibility).

The simulated extent of TCE, DCE, and VC contamination and the measured values from ground-water sampling in 1999 (the earliest routine sampling event) are shown in figures 25, 26, and 27, respectively. Simulated and measured time-series plots for wells MW-19, MW-100, MW-97, and MW-89 are shown in figures 28, 29, 30, and 31, respectively. A key consideration during model calibration was to match wells with the highest levels of contamination but, as a result, the models tend to overpredict contaminant levels at wells where the concentrations are low. This was considered acceptable, however, because the data indicate that the model prediction is conservative; that is, maximum contamination levels are predicted at the wells with low concentrations.

Monitoring well MW-19 had the highest levels of contamination in the southern part of the site. The levels currently are decreasing for both the measured and simulated TCE and DCE concentrations (fig. 28). In the model simulation, waste disposal pits 2 and 5 transitioned to releasing low levels of contamination in 1979, causing the drop in simulated concentrations in the 1990s.

Monitoring well MW-100 had the highest levels of contamination of any well directly adjacent to a creek (fig. 29). The model overestimated the concentrations of TCE, DCE, and VC in this well. Although the reason is unclear, this indicates that the model will be conservative (will overpredict) when used to predict concentrations and the time required for the contamination to move (flush) through the system.

Monitoring well MW-97 had the highest levels of contamination in the central part of the site. The levels have been decreasing since 1999 for measured TCE, DCE, and VC concentrations, and simulated concentrations reflect the same pattern (fig. 30). The simulation of the transition of waste disposal pit 3, in 1979, to releasing low levels of contamination, caused the decrease in simulated concentrations in the 1990s at this well. Based on this simulation, the contaminant concentrations had declined substantially by the time water-quality sampling began; presently, the plume has almost completely passed this well.

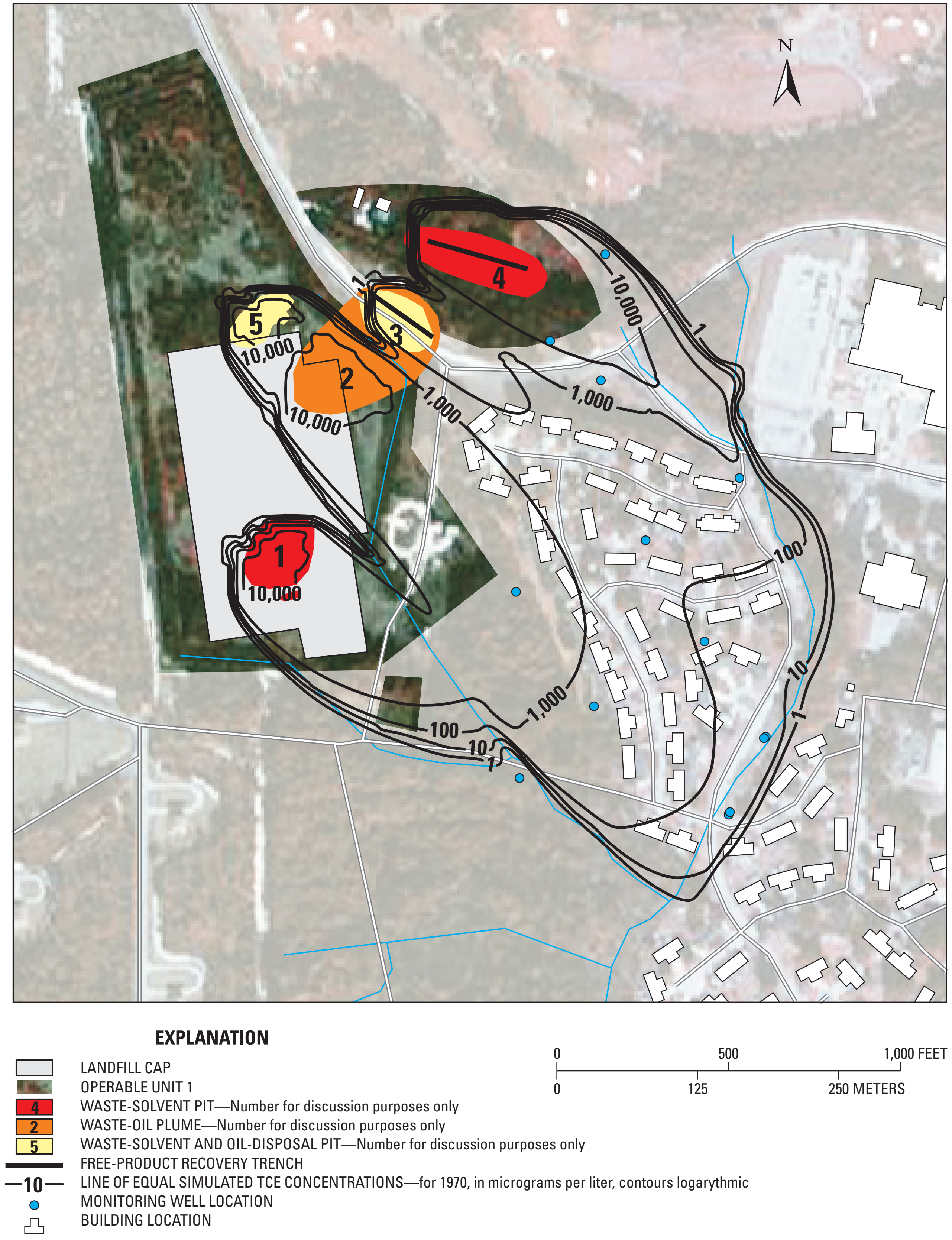


Figure 21. Simulated trichloroethene (TCE) concentrations for 1970.

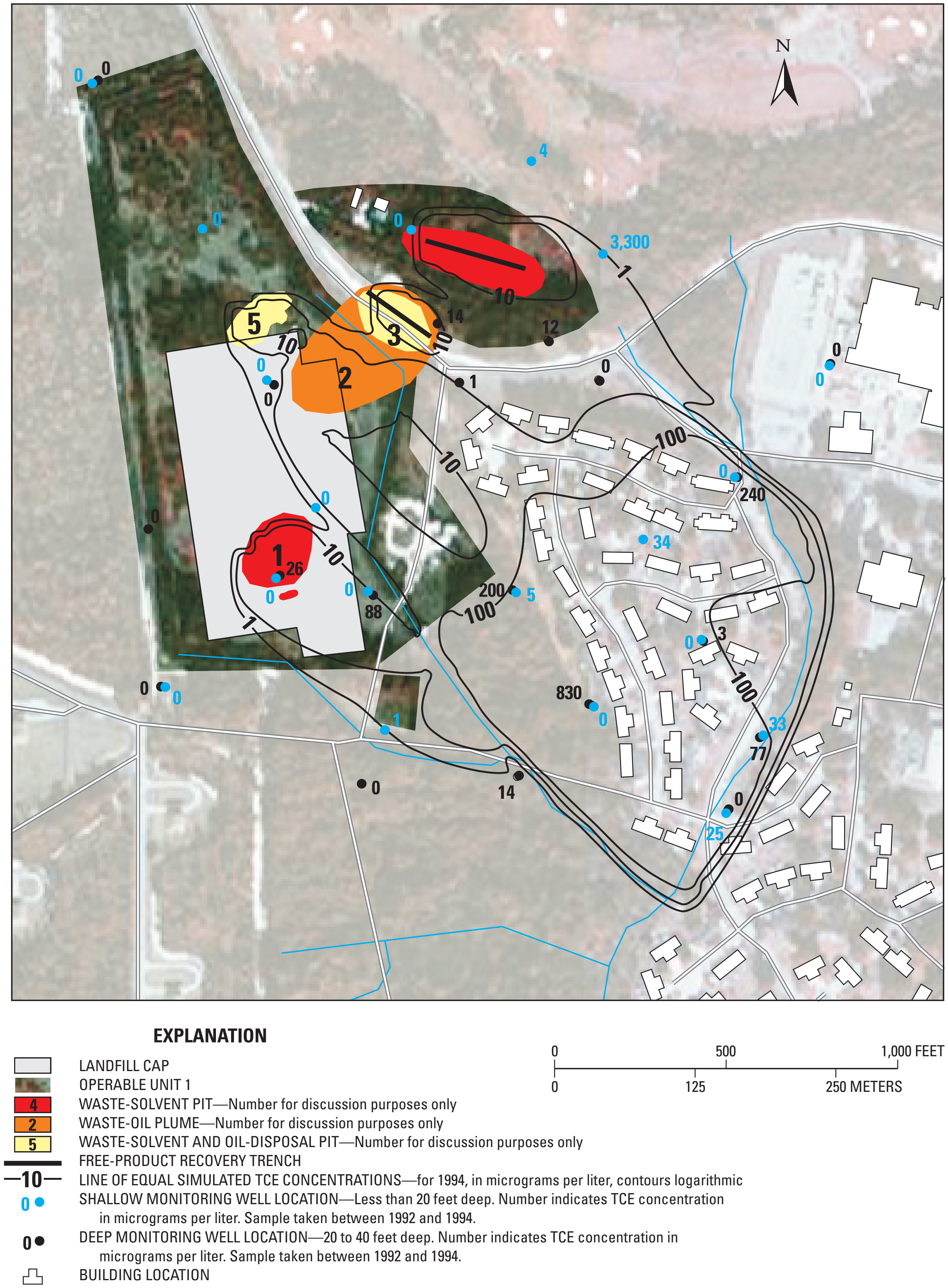


Figure 22. Simulated trichloroethene (TCE) concentrations for 1994 and measured concentrations from 1992 to 1994.

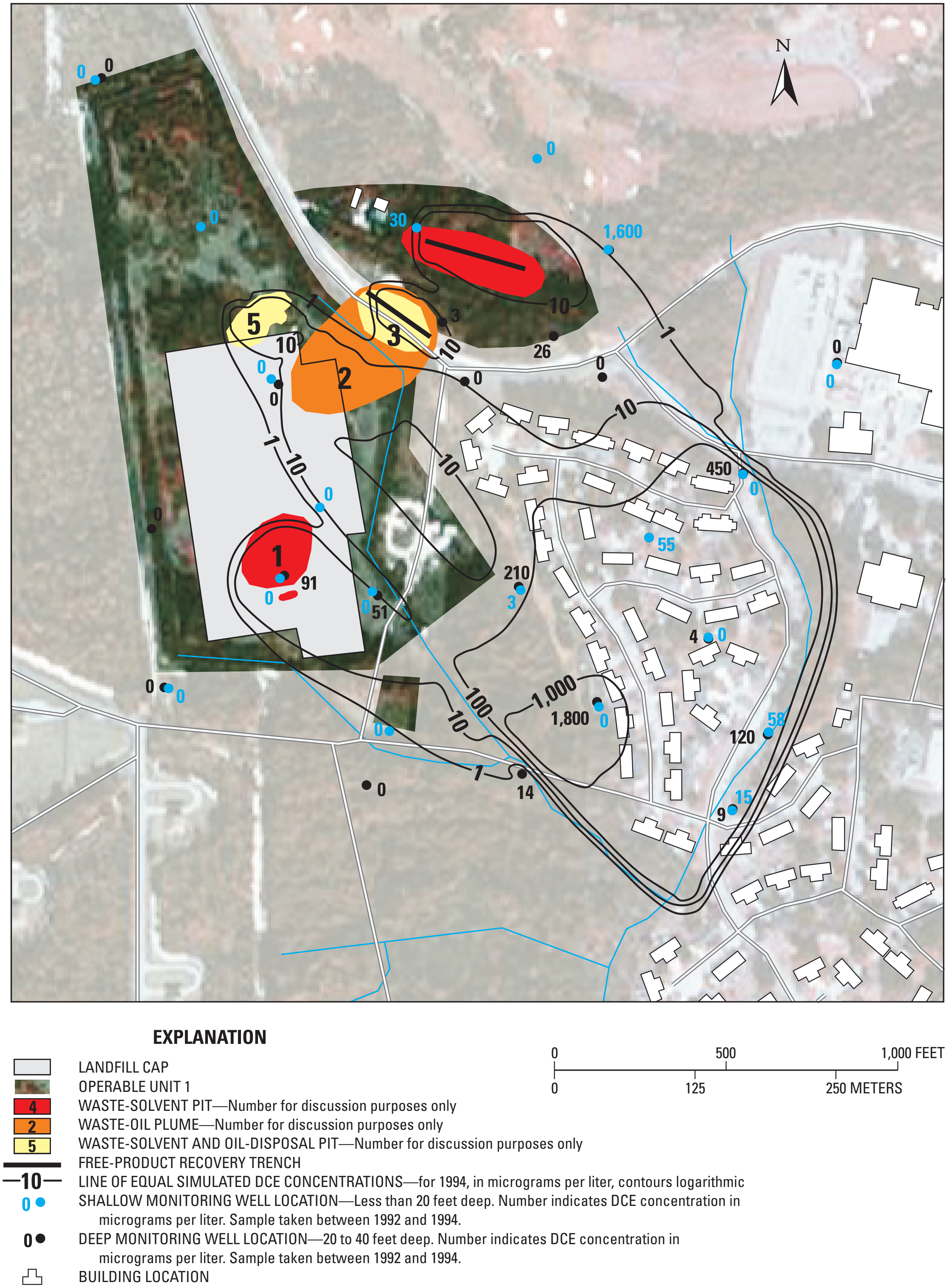


Figure 23. Simulated dichloroethene (DCE) concentrations for 1994 and measured concentrations from 1992 to 1994.

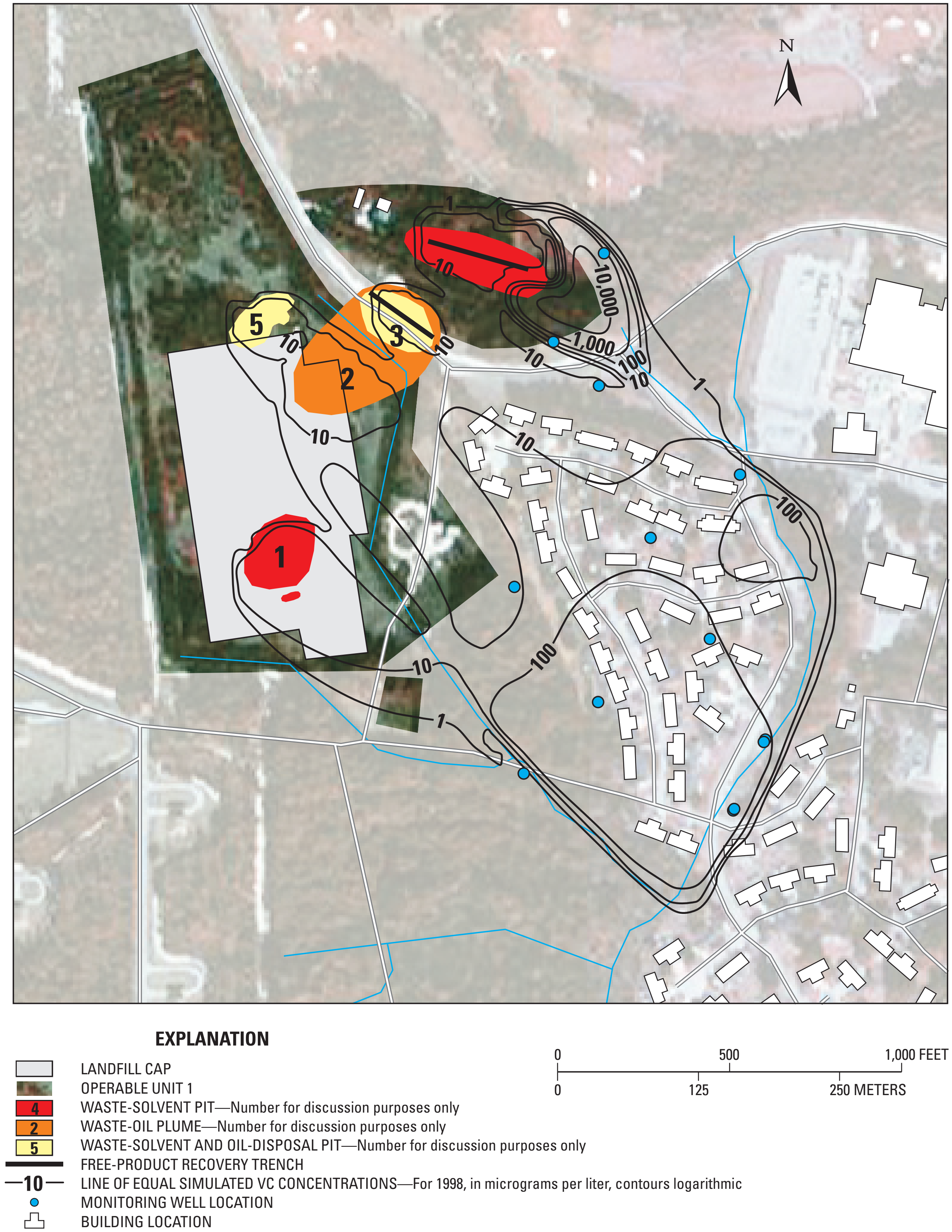


Figure 24. Simulated extent of vinyl chloride (VC) contamination in 1998.

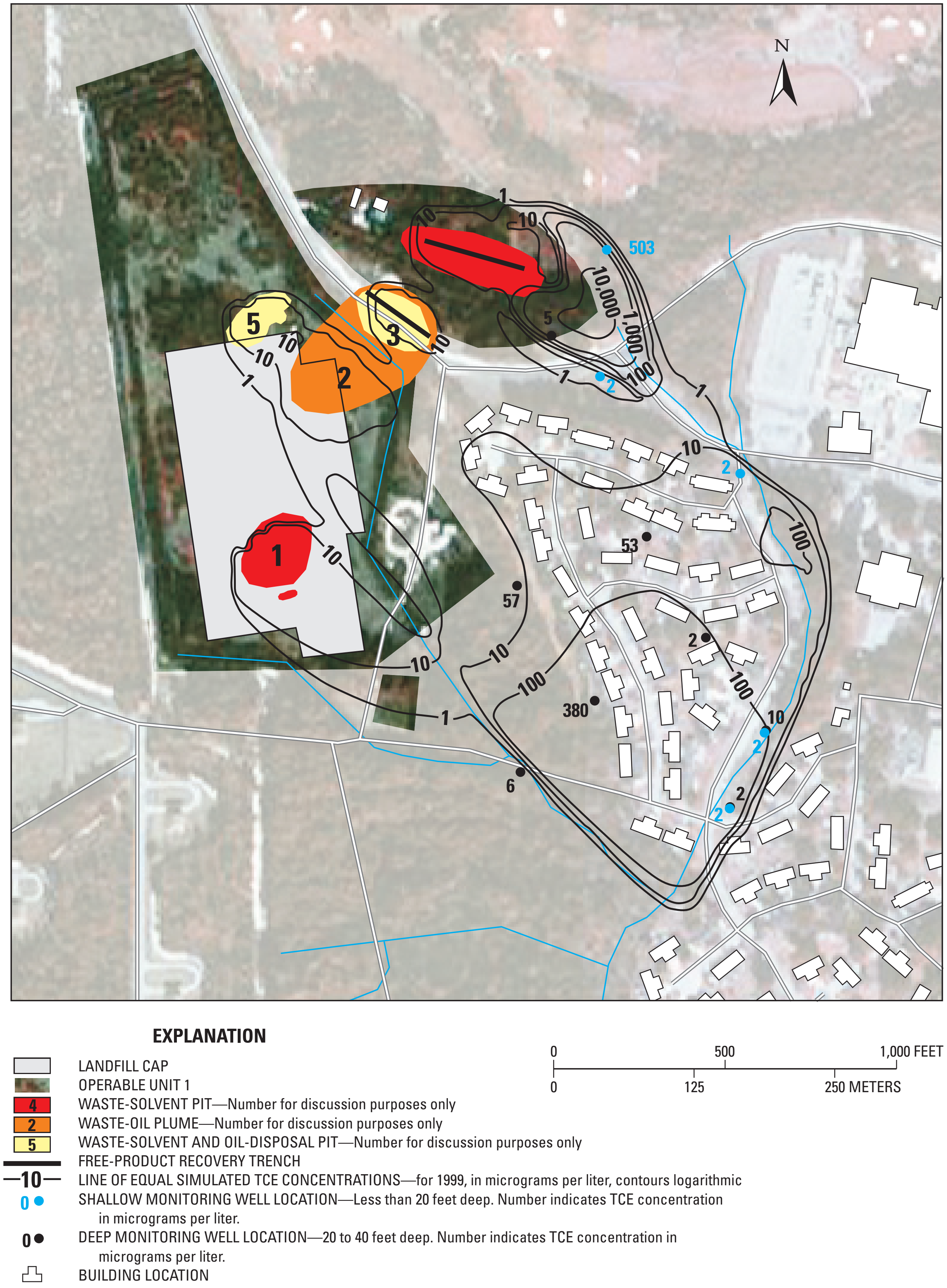
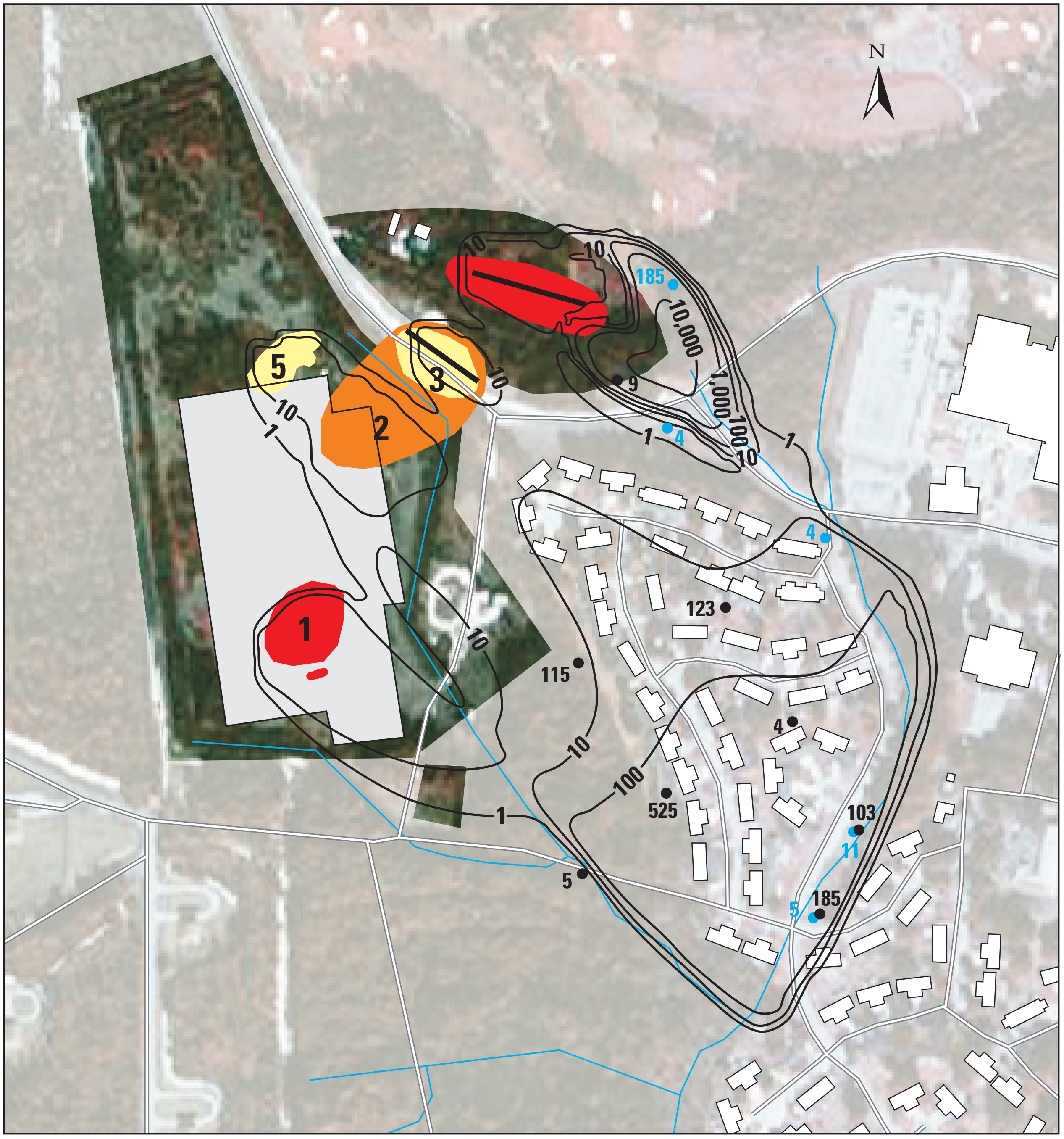


Figure 25. Simulated trichloroethene (TCE) concentrations for 1999.



EXPLANATION

▭	LANDFILL CAP
▨	OPERABLE UNIT 1
🟥 4	WASTE-SOLVENT PIT—Number for discussion purposes only
🟧 2	WASTE-OIL PLUME—Number for discussion purposes only
🟨 5	WASTE-SOLVENT AND OIL-DISPOSAL PIT—Number for discussion purposes only
▬	FREE-PRODUCT RECOVERY TRENCH
—10—	LINE OF EQUAL SIMULATED DCE CONCENTRATIONS—for 1999, in micrograms per liter, contours logarithmic
0 ●	SHALLOW MONITORING WELL LOCATION—Less than 20 feet deep. Number indicates DCE concentration in micrograms per liter.
0 ●	DEEP MONITORING WELL LOCATION—20 to 40 feet deep. Number indicates DCE concentration in micrograms per liter.
⌂	BUILDING LOCATION

Figure 26. Simulated dichloroethene (DCE) concentrations for 1999.

EXPLANATION

▭ LANDFILL CAP

▨ OPERABLE UNIT 1

4 WASTE-SOLVENT PIT—Number for discussion purposes only

2 WASTE-OIL PLUME—Number for discussion purposes only

5 WASTE-SOLVENT AND OIL-DISPOSAL PIT—Number for discussion purposes only

▬ FREE-PRODUCT RECOVERY TRENCH

—10— LINE OF EQUAL SIMULATED VC CONCENTRATIONS—for 1999, in micrograms per liter, contours logarithmic

0 ● SHALLOW MONITORING WELL LOCATION—Less than 20 feet deep. Number indicates VC concentration in micrograms per liter.

0 ● DEEP MONITORING WELL LOCATION—20 to 40 feet deep. Number indicates VC concentration in micrograms per liter.

⌂ BUILDING LOCATION

Figure 27. Simulated vinyl chloride (VC) concentrations for 1999.

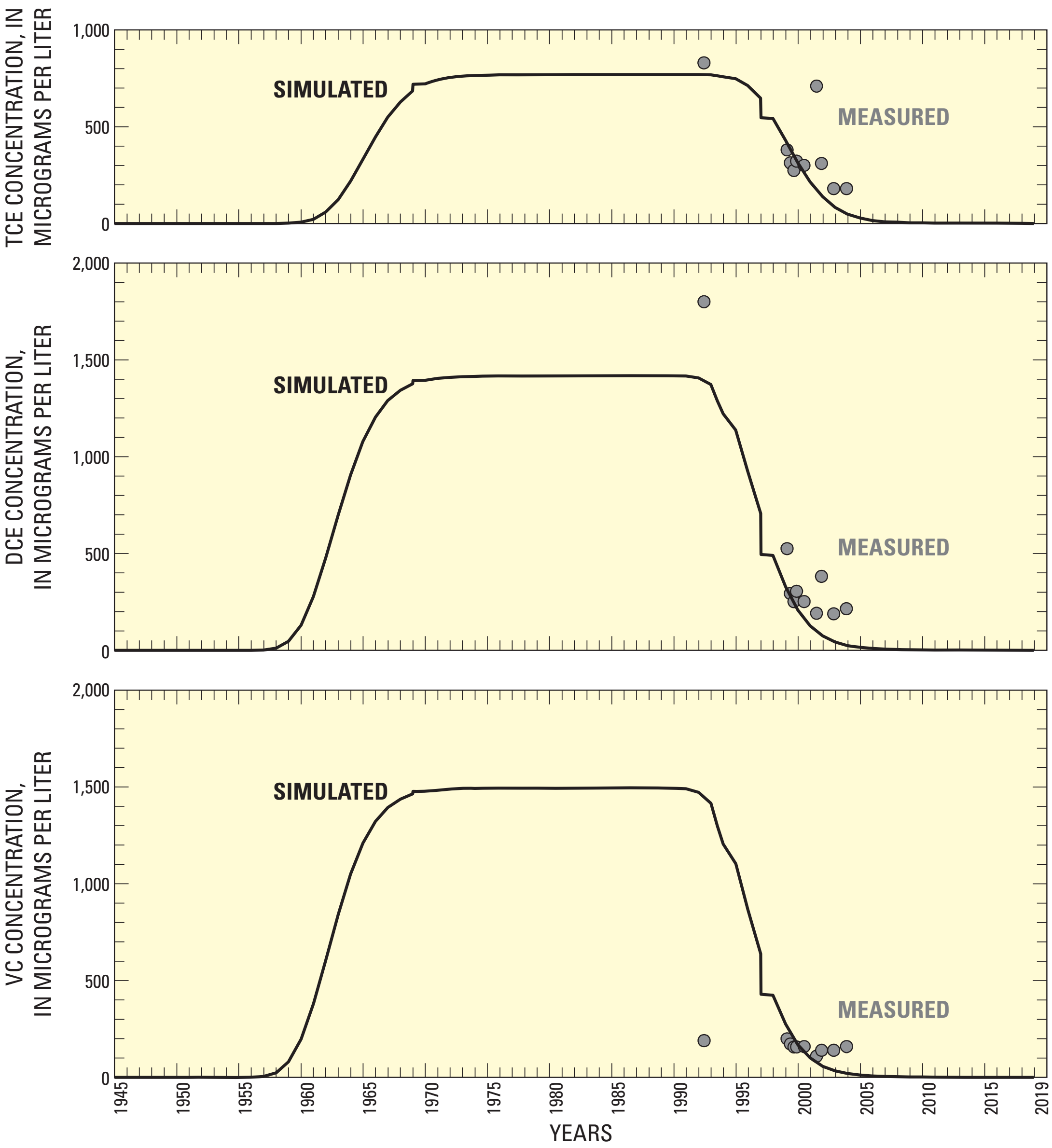


Figure 28. Simulated and measured concentrations of trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) in monitoring well MW-19, from 1993 to 2004.

Monitoring well MW-89 had the highest levels of contamination in the northern part of the site. Simulated waste-disposal pit 4, as it transitioned to the release of low levels of contamination in 1970, was required to match the low levels of contamination in wells MW-12 and MW-93. However, it appears that the installation of the trench through waste disposal pit 4 in 1995 (fig. 9) could have caused the source area to release additional contamination from 1995 to 1998, as previously described. The effect of the additional source period is a spike in contamination at MW-89 beginning in about 1996 and continuing until the present time (although the high level detected in 1994 indicates that this source area could have been releasing higher levels prior to 1995 because of some other disturbance). Concentrations of TCE calculated from the last several sampling events indicate that TCE could be decreasing. This trend also could be true for DCE, but VC shows no apparent trend. Several more years of sampling are needed to determine if these trends are accurate and continuing.

Discussion of Model Calibration Parameters

Matching the measured concentration values in the wells was accomplished by varying: (1) concentrations being released to the aquifer at the source areas, (2) timing of the release at the source areas, (3) dispersivity, and (4) first-order decay rates of TCE, DCE, and VC. The dispersivity values that gave the best match were: longitudinal 7.0 ft, transverse 1.3 ft, and vertical 1.3 ft. These dispersivity values fall within the expected range (1-10 ft for longitudinal and 1-2 ft for transverse dispersivity) described by Gelhar and others (1992).

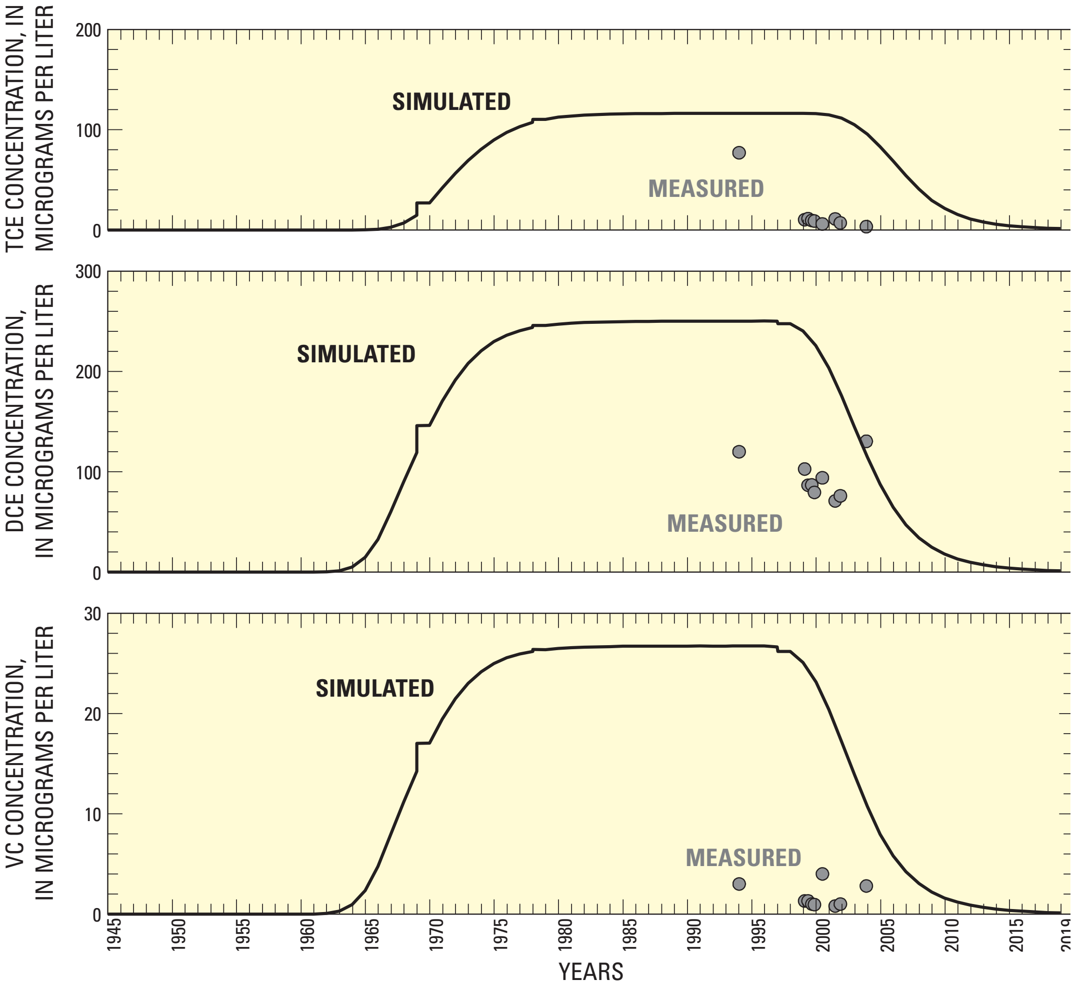


Figure 29. Simulated and measured concentrations of trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) in monitoring well MW-100, from 1993 to 2004.

The model was relatively insensitive to dispersivity because the discharge point was close to the source. Dispersivity has the greatest effect on contaminant concentrations when the contamination has a long distance to travel, and thus, a long period to affect the plume. The first-order decay rate (1 perday, or d^{-1}) for TCE that resulted in the best match was 0.0003 d^{-1}. At a similar site (Operable Unit 3), first-order decay rates of 0.0007 to 0.0002 d^{-1} were derived from 10 years of TCE concentration data (U.S. Navy, 1998). The expected range of values for TCE is 0.0002 to 0.08 d^{-1} (U.S. Environmental Protection Agency, 1998). At this site, the simulated degradation rate of TCE that gave the best match was at the slow end of the expected range. The calibrated first-order decay rate was a 0.0003 d^{-1} for DCE and 0.002 d^{-1} for VC. The expected range of values for VC is 0.0006 to 0.08 d^{-1} (U.S. Environmental Protection Agency, 1998). A relatively high decay rate (but still within the expected range) for VC was required to match the low concentration values measured at the site. At Cecil Field, located about 10 mi west of the Jacksonville Naval Air Station, a low TCE decay rate and a high VC decay rate also were measured and attributed to mildly oxidizing conditions (Frank Chapelle, U.S. Geological Survey, written commun., 2002).

Prediction of Future Trends

Waste disposal pits 1, 2, 3, and 5 appear to be releasing low levels of contaminants to the aquifer, as could be pit 4. Based on this assumption, future concentrations of TCE, DCE, and VC were predicted with the model. By 2010, most of the contamination probably will have migrated to the vicinity of the creeks (figs. 32, 33, and 34).

By 2015, only relatively low levels of TCE are predicted to remain and these will be directly adjacent to the creeks (fig. 35). Concentrations for DCE and VC show similar trends. By 2020, contamination is predicted to be nearly nonexistent, except for very low levels remaining next to the creeks.

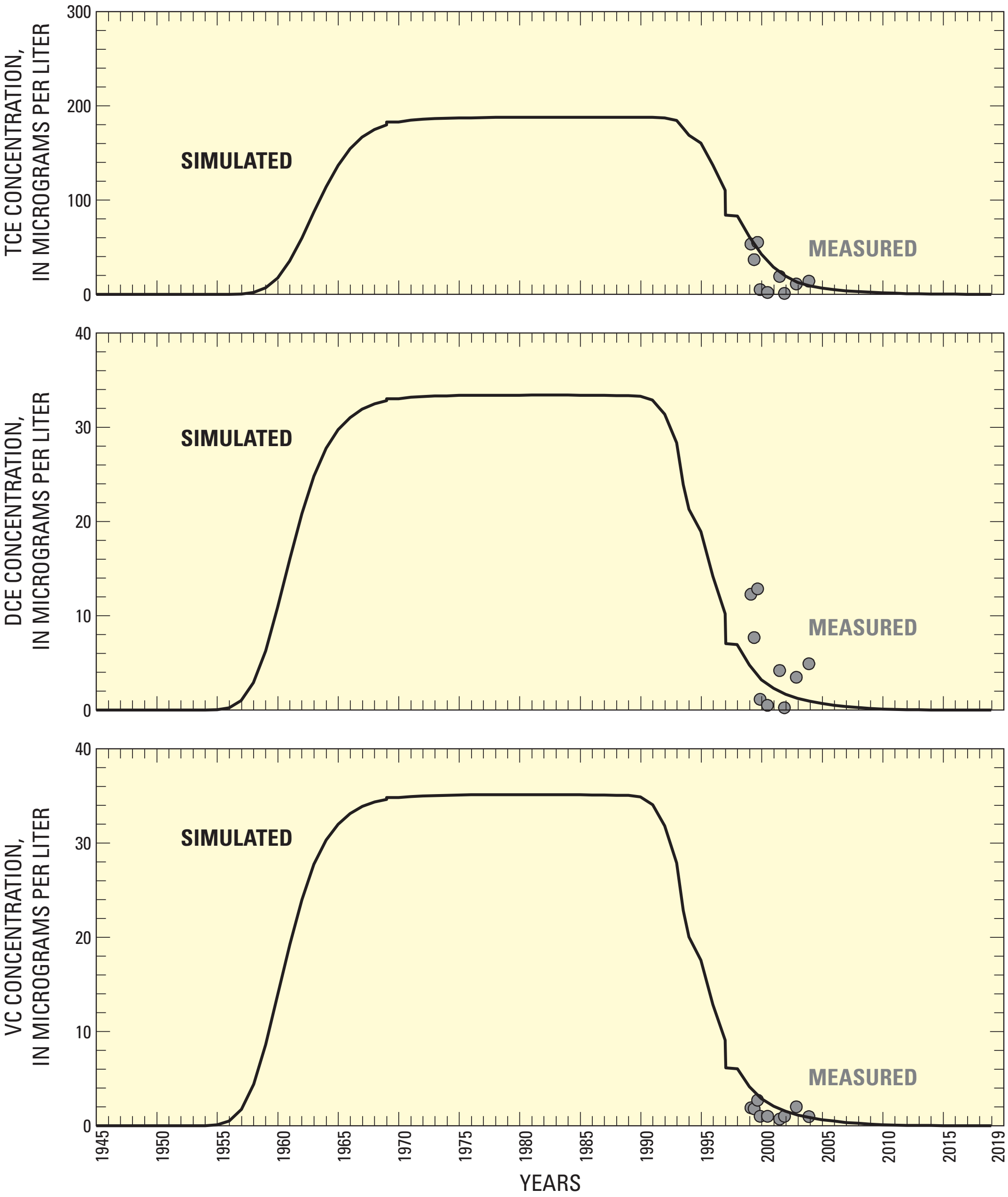


Figure 30. Simulated and measured concentrations of trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) in monitoring well MW-97, from 1993 to 2004.

Tetra Tech is monitoring the concentrations of contaminants in the small creeks at the two surface-water sampling sites and the 17 monitoring wells shown in figure 9. The creeks represent points where the contaminated ground water comes into contact with the environment. The concentration of chlorinated solvents in the streamwater has always been relatively low (fig. 11). It is not possible by simulation to directly predict contamination levels in the creeks caused by ground-water flow, because the creeks are shallow (a few inches deep in most areas) and the loss of volatile contaminants to the atmosphere will, therefore, be high. Because the modeling has simulated declining values of TCE, DCE, and VC in the ground water seeping into the creeks, it is anticipated that contamination levels in the creeks also will decline.

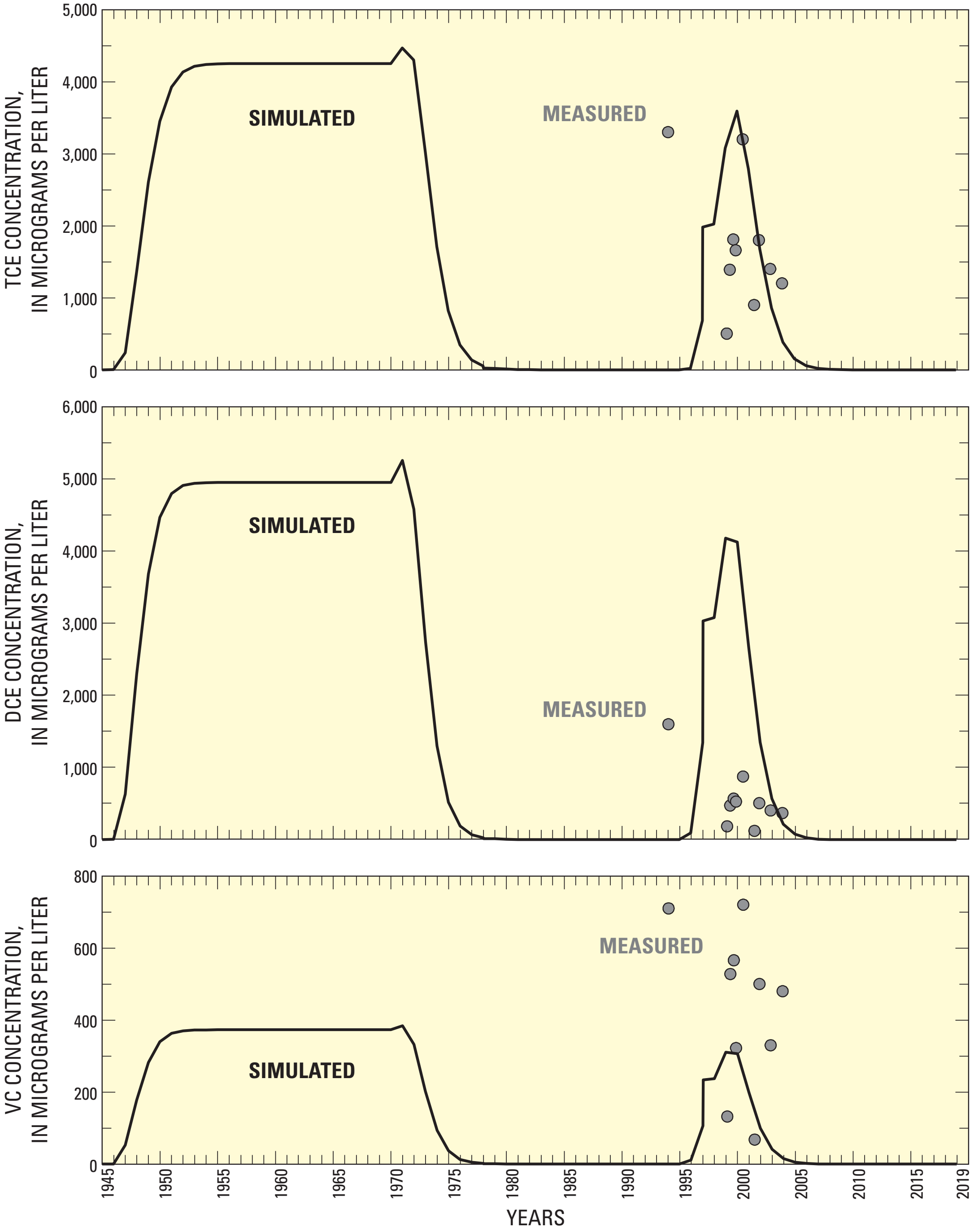


Figure 31. Simulated and measured concentrations of trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) in monitoring well MW-89, from 1993 to 2004.

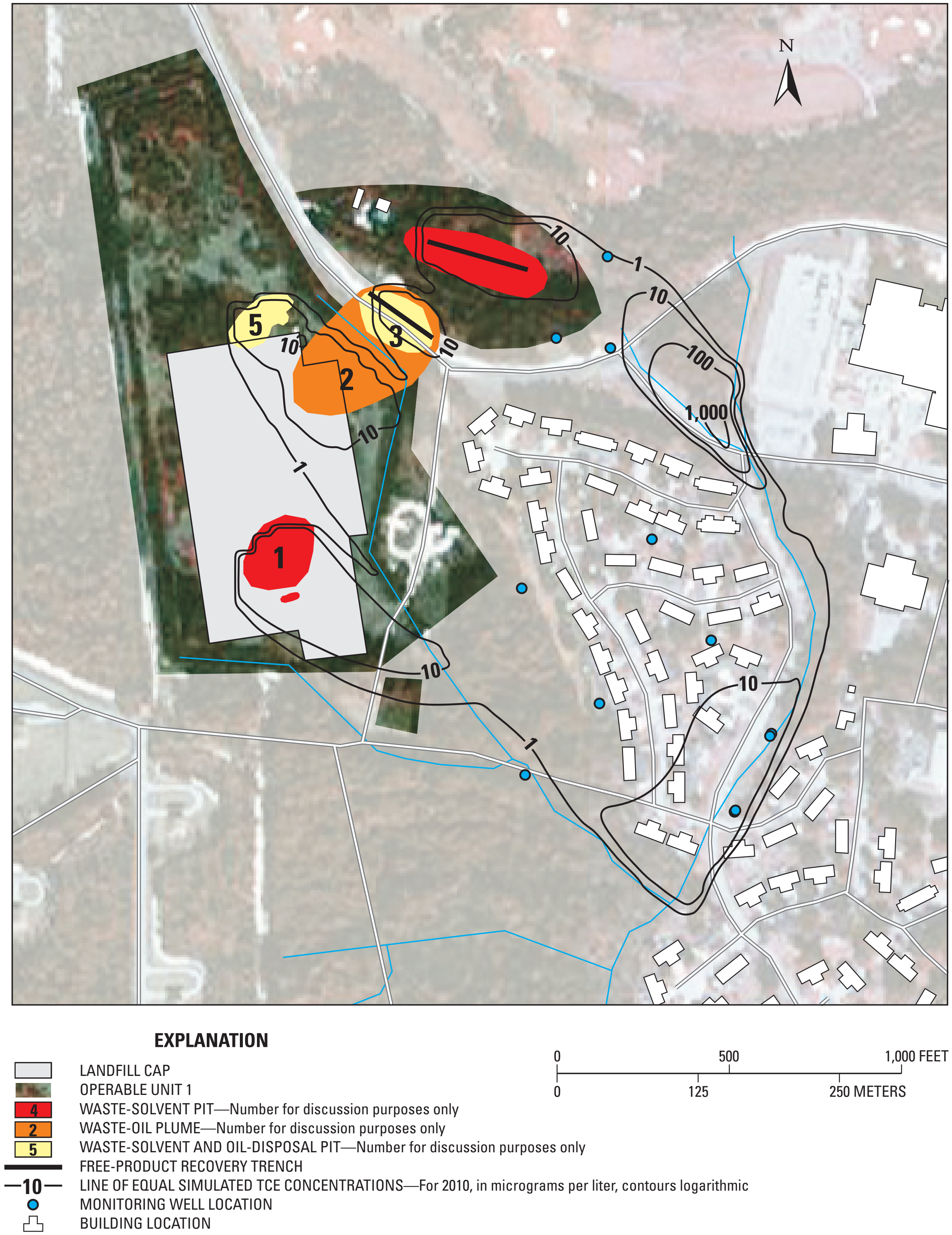


Figure 32. Simulated trichloroethene (TCE) concentrations for 2010.

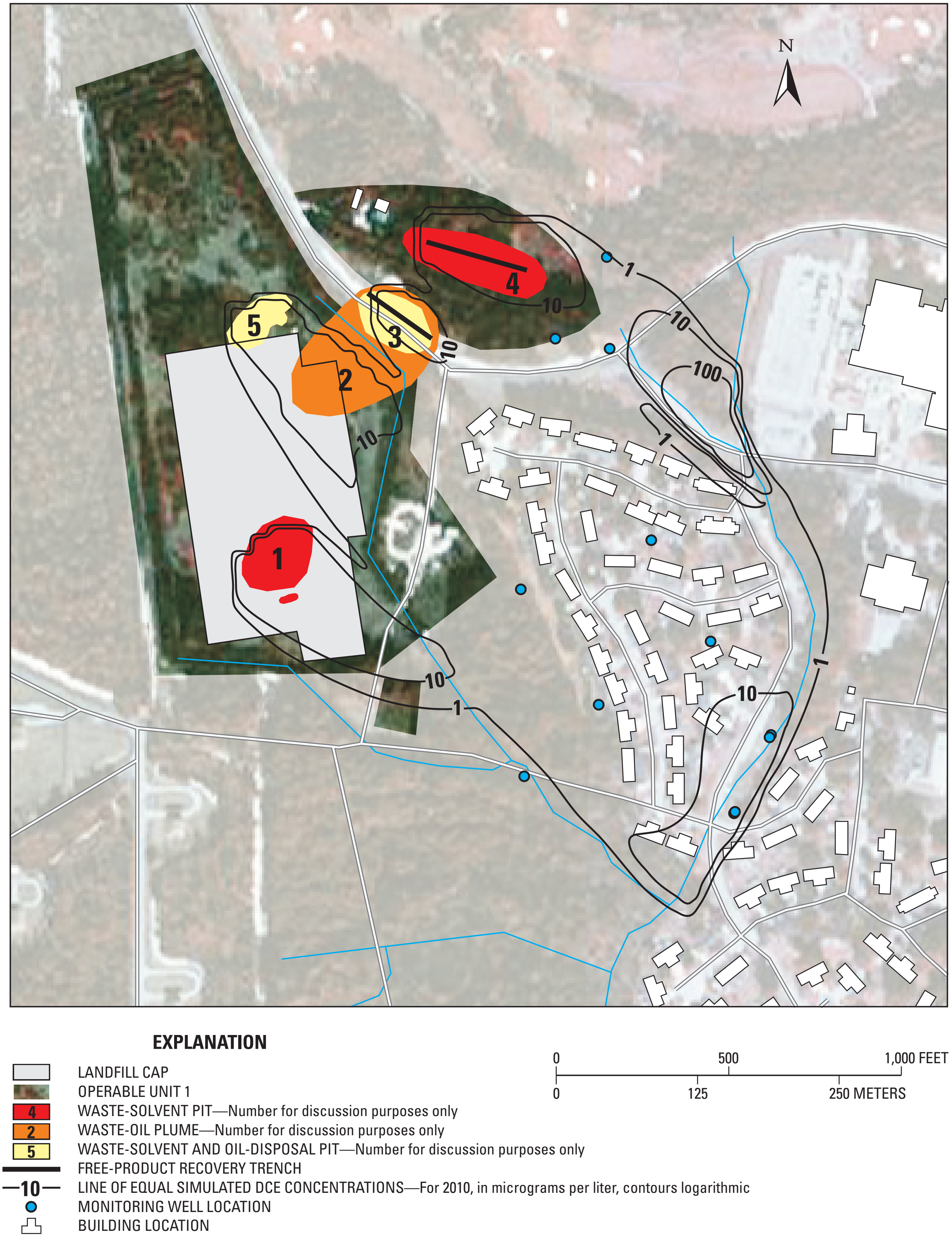


Figure 33. Simulated dichloroethene (DCE) concentrations for 2010.

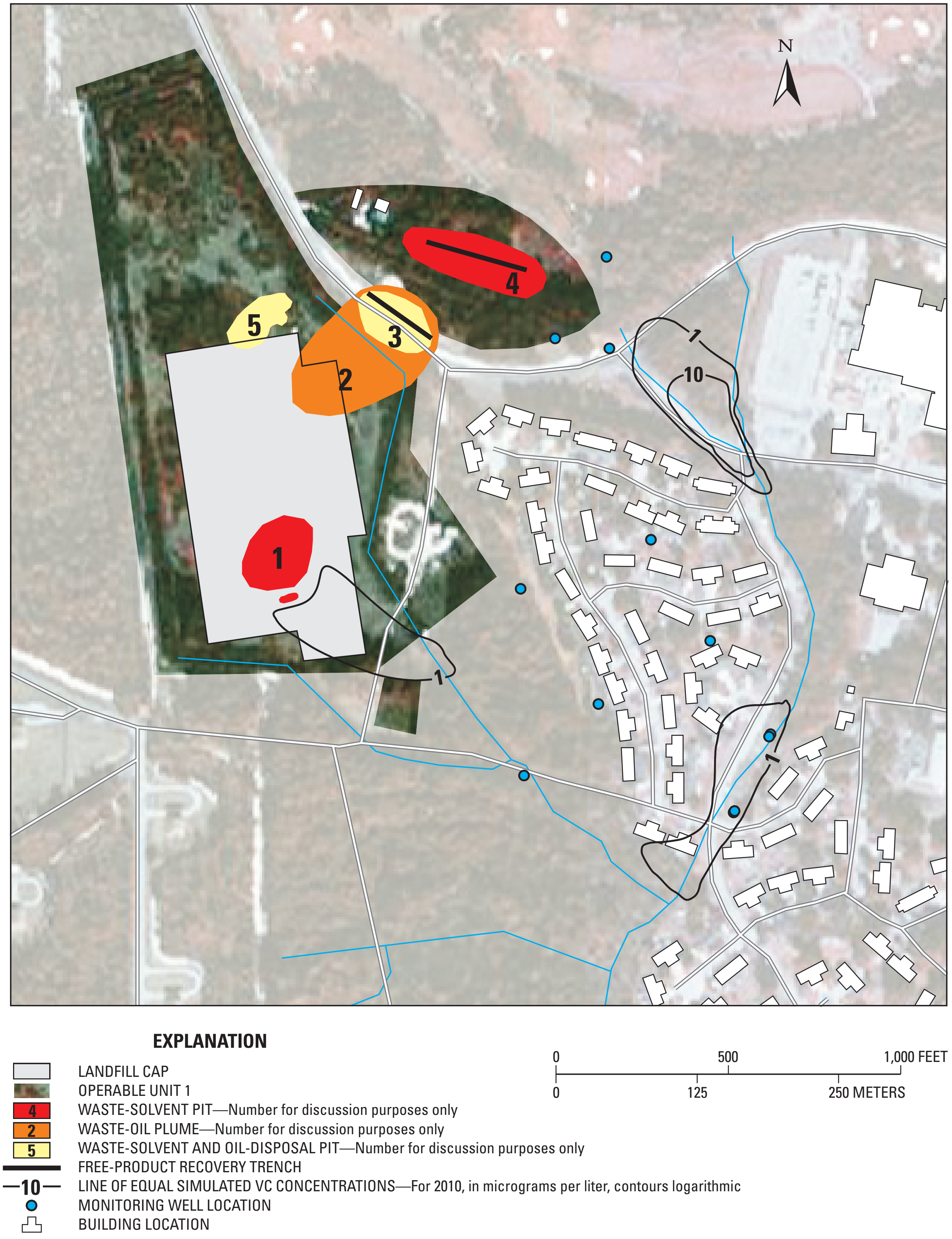


Figure 34. Simulated vinyl chloride (VC) concentrations for 2010.

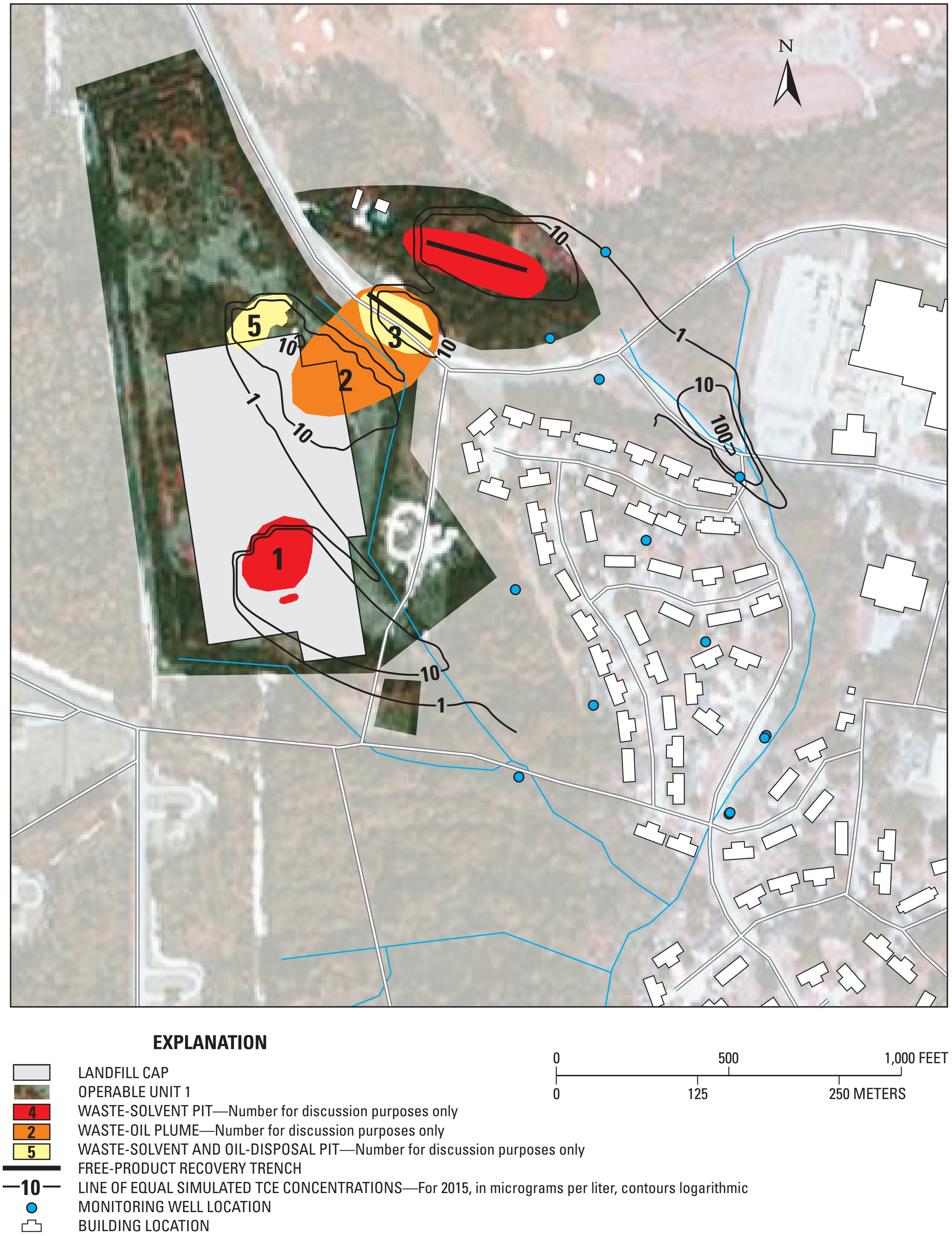


Figure 35. Simulated trichloroethene (TCE) concentrations for 2015.

Measurement Error and Effect of Parameter Variation on Fate and Predictive Transport Modeling

The simulation of future contaminant concentrations and the times of arrival at the creeks are subject to three major sources of error: (1) the simulated ground-water flow velocities might not accurately reflect the actual flow velocities; (2) the measured concentrations might not fully characterize the contaminant concentrations in the aquifer; and (3) the model input parameters might not accurately characterize the transport mechanisms.

Ground-water velocity probably is the most important factor when predicting the traveltime from the source area to the creek. If the actual ground-water velocities are greater than the simulated velocities, then the contaminants will move toward and into creeks faster than predicted. If the simulated velocities are slower, then contaminants will remain in the aquifer longer and arrive at the creeks later than predicted. Simulated contaminant concentrations discharging to the creeks are related directly to initial concentrations at the source. If the simulated concentrations in the source area are substantially higher than the actual concentrations were, then the model-predicted concentrations discharging to the creeks will be too high; however, the plumes were generally well defined laterally and vertically, and were characterized using data from several wells, making it less likely that substantially higher concentrations existed.

Model parameters such as retardation, hydrodynamic dispersion, porosity, and chemical degradation have a strong influence on the simulated movement and concentration of contaminants. Variations in each of these parameters can affect the model-simulated fate and transport of contaminants. The effect of retardation on contaminant movement is straightforward. If the retardation factor is doubled, then the rate of travel of the contaminant is halved. Conversely, if the retardation factor is halved, then the rate of travel is doubled. Similar to the retardation factor, the effective porosity affects the movement of contaminants in a linear fashion. If the porosity is doubled, then the traveltime of the contaminants also is doubled. If the porosity is halved, then the traveltime is halved.

The simulated first-order rates of chemical degradation were 0.0003, 0.0003, and 0.002 d^{-1} for TCE, DCE, and VC, respectively. Because a similar rate of degradation for TCE (0.0002) was documented at a similar site nearby (U.S. Navy, 1998), using this rate has some justification and adds to the appropriateness of the solution. The rates for DCE and VC, however, are simply model-calibration parameters (although they fall within expected values) that resulted in the best calibration for the model. If the actual rates of degradation are substantially different (or if they vary over time), then the simulated concentrations also could vary. Additionally, the initial concentrations and simulated concentrations in the aquifer are correlated, thus making a unique prediction more difficult. For example, if the initial concentration were too high and the first-order decay rate too low, then a match to the measured values is still possible. Errors in the simulated flow velocities also will substantially affect the contaminant concentrations arriving at the creeks. Faster flow velocities will result in less time for biodegradation, and thus, higher concentrations in the aquifer.

Summary

The U.S. Naval Air Station occupies 3,800 acres adjacent to the St. Johns River in Jacksonville, Florida. The mission of the Station is to provide aerial antisubmarine warfare support, aviator training, and aircraft maintenance. Support facilities include an airfield, a maintenance depot, a Naval hospital, a Naval supply center, and recreational and residential facilities. The Station was placed on the U.S. Environmental Protection Agency's National Priorities List in December 1989, and is participating in the U.S. Department of Defense Installation Restoration Program, which serves to identify and remediate environmental contamination.

One contaminated site, the old landfill, was designated as Operable Unit 1 (OU1) in 1989. Several remedial measures were implemented at this site to prevent the spread of contamination. Free-product recovery trenches were installed in 1995 to collect free product. In 1998, some of the contamination was consolidated to the center of the old landfill and covered by an impermeable cap. A monitoring program was begun in 1999 in which water-quality samples were routinely collected in designated wells and stream locations. Currently, OU1 is being reevaluated as part of a 5-year review process to determine if the remedial actions were effective.

The primary ground-water contaminants of concern are trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC). The source of ground-water contamination occurred as a result of disposing waste oil and solvents in open pits. Starting in the 1940s, the Navy used the landfill for the disposal of household and sanitary waste, liquid industrial waste (oil and solvents), and demolition and construction debris. Concentrations of TCE, DCE, and VC have been measured at two locations in creeks downgradient from OU1 from 1992 to present . At one location, the concentrations have been below the detection limit except for one sampling event in 1999. At a second location, downstream from the first, all three contaminants have been detected at low concentrations.

Ongoing biodegradation has been documented at OU1. Target Environmental Services in 1997 analyzed ground-water samples from six wells at OU1. Biodegradation was determined to be occurring based on the following evidence: (1) decrease in concentrations of the original contaminants, (2) increase in the presence of daughter products, (3) depletion of oxygen and ferric iron, (4) increase in ferrous iron, and (5) elevated hydrogen levels.

The USGS developed and calibrated a one-layer regional ground-water flow model that simulated steady-state flow in the surficial aquifer at the Station and some surrounding areas. This model had 241 rows and 293 columns with a uniform cell size of 100 by 100 ft. This regional model was then used to set the boundary conditions for a site-specific OU1 solute transport model. The OU1 site-specific model contains 130 rows and 122 columns of active model cells; the model has one layer and all cells are 25 ft on each side. Fate and transport modeling was done using the computer code Reactive Transport in Three Dimensions (RT3D).

All fate and transport model simulations began in 1945. The waste-disposal pits were simulated as specified concentration cells. The period of time that a pit acted as a source of ground-water contamination and the concentration levels at the pit were determined during model calibration. The northernmost disposal pit could have acted as a source twice—the first when the solvents were being disposed and again immediately after the free-product recovery trench was installed.

Simulations indicated that the concentration of contaminants would have reached the maximum extent by the 1970s, after which the concentrations generally declined because the pits had ceased releasing high levels of contaminants. In the southern part of the site, monitoring well MW-19, which had some of the highest levels of contamination, showed decreases for both the measured and simulated TCE and DCE concentrations from 1992 to present. To match the decline in measured concentrations, it was necessary to simulate two upgradient disposal pits as transitioning from releasing high levels of contamination prior to 1979 to releasing low levels after 1979.

Monitoring well MW-100 had the highest levels of contamination of any well directly adjacent to a creek. The model overestimated the concentrations of TCE, DCE, and VC in this well. The exact reason is not clear; however, the overestimation shows that the model will be conservative (will overpredict) when used to predict concentrations and the time required for the contamination to move (flush) through the system at this location.

Monitoring well MW-97 had the highest levels of contamination in the central part of the site. The levels decreased for both the measured and simulated TCE, DCE, and VC values from 1999 to present. Simulating the source area as ceasing to release high levels of contamination in 1979 caused the decline in concentration, which began in the 1990s at this well. Based on the simulations, it appears that the concentrations had decreased substantially by the time water-quality sampling began; the plume has now almost completely passed this well.

Monitoring well MW-89 had the highest levels of contamination in the northern part of the site. To match the low levels of contamination in wells MW-12 and MW-93, waste disposal pit 4 (source area) had to be simulated to cease releasing high levels of contamination by 1970. It appears, however, that the installation of a trench in 1995 could have caused the source area to release additional contamination from 1995 to 1998. The effect of the additional release is a spike in contamination at MW-89, beginning in about 1996 and continuing to the present time. Concentrations of TCE calculated from the last several sampling events indicate that TCE could be decreasing. This trend could also be true for DCE, but VC shows no apparent trend. Several more years of sampling are needed to determine if these trends are accurate and continuing.

The dispersivity values that gave the best match to simulated organic concentrations using a trial-and-error approach were: longitudinal 7.0 ft, transverse 1.3 ft, and vertical 1.3 ft. The model was relatively insensitive to dispersivity because the discharge point was close to the source. Dispersivity has the greatest effect on contaminant concentrations when the contamination has a long distance to travel, and thus, a long period to affect the plume. The first-order decay rate for TCE that resulted in the best match was 0.0003 d^{-1} (first-order decay rate). This simulated degradation rate was at the slow end of the expected range. The calibrated first-order decay rate was 0.0003 for DCE and 0.002 d^{-1} for VC. The expected range of values for VC is 0.0006 to 0.08 d^{-1}. A relatively high decay rate (but still within the expected range) for VC was required to match the low concentrations measured at the site.

Based on predictive simulations, TCE, DCE, and VC will migrate to the vicinity of the creeks by 2010. By 2015, only relatively low levels of TCE are predicted to remain and these will be directly adjacent to the creeks. By 2020, contamination is predicted to be nearly nonexistent, except for low levels remaining directly next to the creeks.

The creeks represent the points where contaminated ground water comes into contact with the environment. The concentration of chlorinated solvents in the streamwater has always been relatively low. Because the modeling shows that TCE, DCE, and VC concentrations are declining, it is anticipated that contamination levels in the creek should show a declining trend.

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