Appendix H

Western South Boundary Modeling Report

Western South Boundary Groundwater Modeling
Fate and Transport of DCE/TCA and Freon-12

STATE OF NEW YORK PAUL KENNETH BOYCE 074604 LICENSED PROFESSIONAL ENGINEER 03.03.18

Brookhaven National Laboratory

March 23, 2018

Groundwater modeling simulations were performed by P.W. Grosser Consulting (PWGC) to aid Brookhaven National Laboratory (BNL) in estimating how long it will take the Western South Boundary (WSB) VOC (DCE/TCA) and Freon-12 (dichlorodifluoromethane) plumes to attenuate below 5 ppb and to evaluate active pump and treat alternatives that would enable meeting the 2030 cleanup criteria.

The work presented in this groundwater modeling memorandum is based partly upon previously conducted modeling efforts by BNL. PWGC utilized BNL's existing regional 3-dimensional numerical groundwater model (GMS v10.2.4, 64 Bit, MODFLOW 2000) to analyze steady state flow conditions to predict the fate and transport of the WSB DCE/TCA and Freon-12 plumes utilizing MT3DMS a modular three-dimensional transport model for the simulation of advection, dispersion, and chemical reactions of dissolved constituents in groundwater systems developed for the USACE (United States Army Corps of Engineers) by S.S. Papadopulos & Associates, Inc. and the University of Alabama.

Key Assumptions and Model Modifications

The key assumptions made for the modeling effort are:

- The 'onsite' model inherited hydraulic/hydrogeologic properties from the calibrated regional model. Modifications to the original model included converting the regional model to a local or sub-regional model. **Figure 1** depicts the model layering along with associated horizontal hydraulic conductivities assigned to the layers in the vicinity of the Western South Boundary plumes.

- The regional model was converted to a local model so that fate and transport modeling could be conducted. An area roughly 3,700 ft (east-west direction) by 13,200 ft (north-south direction) was delineated around the WSB plume areas and subdivided into a 100 ft by 100 ft grid (see **Figures 2a and 2b**). Constant head boundary conditions were created at the north and south boundaries of the local model to match regional model heads.

- Layer 3 of the local model was divided into two separate layers to more accurately represent and model the DCE/TCA contaminant plume volume. The DCE/TCA plume is divided between the two halves of the split layer with the northern portion of the DCE/TCA being in the lower half or now layer 4 of the sub-regional model and the southern portion of the plume being in the upper half of the divided layer now layer 3 of the local model. More recent vertical profiling data found the presence of an isolated pocket of DCE/TCA at shallower concentrations to the north of the larger portion of the DCE/TCA plume in layer 3 and has subsequently been added to the model. Additionally the Freon-12 plume is also represented by two portions, a northern and a southern portion, but portions are located in layer 6. Recent data allowed the southern portion of the Freon-12 plume to be reduced in areal extent.

- MT3DMS was utilized to create and model the WSB DCE/TCA and Freon-12 plumes. Plume conditions were generated using the most recent data available from vertical profiles performed in 2016 and 2017 in combination with the monitoring well network. DCE/TCA plume concentrations were generated by utilizing the highest observed DCE/TCE values for a given sampling location. This methodology conservatively accounts for the highest individual VOC concentration at each location. These concentrations ranged between 5 and 150 ppb. Concentration values were input individually into model cells within the horizontal extents of the plume boundary (5 ppb contour). The DCE/TCA plume was created in layers 3 and 4 of the local model as described above. The Freon-12 plume was input into layer 6 of the local model. Layer 6 of the local model varies in thickness and elevation with thicknesses at the northern end at 5 ft and the southern portion on the order of 25 ft, see **Figure 1** for layer geometries.

- Fate and transport simulations were run using the advection, dispersion and chemical reaction modeling packages in MT3DMS.

- The advection package solution scheme implemented was the method of characteristics (MOC), this method is the standard method used in BNL modeling scenarios as it can help eliminate numerical dispersion in strongly advection dominated situations as is typically the case. The draw back to this method is it can often produce spurious or artificial oscillations in contaminant mass and concentrations. This was not observed under the current modeling scenario.

- Mechanical dispersion was modeled using the standard hydrodynamic dispersion equations coupled with advection. The main model input for dispersion is the longitudinal dispersivity coefficient which is generally taken as half the grid cell length, or in the case of the current model setup would be 50 ft^2/day. However, a value of 30 ft^2/day was input as this is what has been used in past BNL groundwater modeling scenarios using a grid spacing on the order of 100 ft, it is also a more conservative value by reducing the quantitative effect of dispersion on the fate and transport process. The GMS default values for the ratio of horizontal transverse dispersivity to longitudinal dispersivity and the ratio vertical transverse dispersivity to longitudinal dispersivity were left unaltered at 0.1 and 0.01 as these are typical or standard values and have been successfully utilized in past BNL local models for fate and transport modeling purposes.

- The chemical reaction package was used to simulate retardation effects and adsoprtion. GMS calculates a retardation factor R for each layer based on the distribution coefficient of the specific contaminant and the bulk density and porosity of the material (layer) the contaminant is traveling through. The basic equation used by GMS to calculate the retardation factor is $R = 1 + (\rho_b K_d/n)$ where ρ_b is the soil bulk density, K_d is the distribution coefficient and n is the soil porosity. A soil bulk density of 100 lb/ft^3 was input for all layers as this is a typical or common value for regional sands. K_d was estimated based on actual observed or monitored conditions for VOCs traveling through Upper Glacial materials for the DCE/TCA plume. On site VOC transport observations indicate an R value of around 1.25, this equates to a distribution coefficient value of 0.0006 ft^3/lb when using the calibrated regional model porosity value of 0.24.

A retardation factor or distribution coefficient for Freon-12 was not readily available and had to be researched and calculated. A K_d value of 0.132 L/Kg was obtained from the New Jersey Department of Environmental Protection (NJDEP) soil-water partition equation calculator database. This value was converted to 0.0021 ft^3/lb to produce an R value of 1.88 when using a soil bulk density of 100 lb/ft^3 and a porosity of 0.24.

- Steady state conditions were modeled over a 50 year time period with 4 time steps per stress period (1 year = 1 stress period). One time step equates to 91.25 days or approximately 3 months. A 50 year time period starting January 1, 2018 ends in 2068.
- Plume fate and transport modeling is based on the assumption that there is no continuing source of contamination north of Princeton Avenue.
- A data gap exists between the site boundary and Carleton Drive with regards to the VOC plume. To address this gap in the modeling the higher level plume contours were stretched from the site boundary to midway between the boundary and Carleton Drive.
- In the model output figures that depict the VOC plume towards the bottom lower right of each figure a small blue colored area exists that appears to look similar to the modeled VOC plume. This blue colored area does not change or move with time. The blue area is simply monitoring well identification numbers that based on the scale of the displayed image are illegible and not representative of any VOC plume.

Discussion of Model Simulations and Predictions

The basis for the modeling effort was to optimize the number, location, depth and pumping rates of groundwater extraction wells to accelerate the attenuation of the VOC and Freon-12 plumes associated with the BNL Western South Boundary (WSB) project. The objective of the groundwater modeling was to determine the need for active remediation to meet the cleanup objectives and if required, whether this could be done utilizing the existing groundwater treatment system. Following the determination that natural attenuation would not allow for groundwater cleanup goals to be met, extraction well locations and pumping rates were optimized based on plume size, shape and groundwater flow direction to have the greatest impact with regards to contaminant capture and to achieve the cleanup objective of reaching MCL's in the Upper Glacial Aquifer by 2030. Several simulations were run utilizing various numbers of wells, well locations and depths to achieve a balance of cost efficiency and and plume remediation optimization.

DCE/TCA

Several steady state modeling simulations were conducted using MT3DMS to predict durations to achieving groundwater concentrations of less than 5 ppb of DCE/TCA. The first modeling scenario that was investigated was running MT3DMS with the current DCE/TCA plume configuration under a natural attenuation process until less than 5 ppb are achieved. Under this scenario no new extraction wells are installed and the only existing well that is allowed to run is WSB-1 in layer 3 of the local model at 180 gpm with the treated groundwater being returned to the WSB recharge basin in layer 1. The simulation was carried out over a 50 year time period and after 30 years (year 2048) the model predicts no DCE/TCA concentrations over 5 ppb. **Figures 3** through **7** depict the DCE/TCA plume at 10 year intervals starting at day 1 and ending at year 30.5 (i.e., day 1, years 10, 20, 30 and 30.5). Groundwater velocity in that area of the model in layer 4 is calculated at 139 ft/yr in the portion north of Middle Road and 380 ft/yr for portion south of Middle Road.

A series of modeling simulations were performed by siting several combinations of extraction wells to determine whether the cleanup goal of less than 5 ppb by 2030 can be achieved. Utilizing only one extraction well was ineffective for achieving the cleanup goals and is not discussed. Therefore, two scenarios were investigated, and included either two or three extraction wells installed along the centerline of the DCE/TCA plume. Under both scenarios all wells are installed in layer 4 of the local model, which is where the bulk of the on-site portion of DCE/ TCA plume is initialized. The two well scenario is depicted in **Figures 8** thru **11** and after 16 years (year 2034) the model predicts no DCE/TCA concentrations above 5 ppb either on or off site. Both extraction wells are operating at 112.5 gpm and returning the remediated groundwater to the WSB recharge basin in layer 1. The WSB-1 extraction well under this scenario is assumed to be turned off. WSB-1 is also too shallow and too far to the east to have a significant impact in remediating the present VOC plume so it was turned off during the modeling scenarios.

The three extraction well scenario was run under the same conditions as the two extraction well scenario. All three wells were installed in layer 4 of the local model and located along the centerline of the DCE/TCA plume. Each well was assigned a pumping rate of 75 gpm and all remediated groundwater was returned to the WSB recharge basin in layer 1. The WSB-1 extraction well was again turned off. The model predicts that under a three extraction well scenario the DCE/TCA plume on site is reduced to concentrations less than 5 ppb after 8 years (Year 2026). **Figures 12** through **14** depict the three extraction well scenario starting after 1 year of continuous pumping through year 8 (year 2026) when the on site VOC concentrations are reduced below 5 ppb.

Freon-12

Similar modeling scenarios were run to predict Freon-12 concentrations over time as were done for the DCE/ TCA plume. The first Freon-12 scenario modeled was a 50 year time period to simulate natural attenuation. As in the DCE/TCA scenario no new extraction wells are installed and only the WSB-1 extraction well is running at 180 gpm in layer 3 of the local model and returning remediated groundwater to the WSB recharge basin in layer 1. The notable difference with the Freon-12 model is the plume is created in layer 6 of the local model as opposed to layers 3 and 4 where the DCE/TCA Plume was initialized. **Figures 15** through **20** represent the model output for the Freon-12 natural attenuation simulation starting at day 1 and progressing in 10 year intervals. After 50 years of simulation the model predicts the Freon-12 plume will migrate off site to the industrial park with peak concentrations just over 20 ppb. The slow advance is due to the silty and clayey nature of layer 6 of the local model (see **Figure 1**) as well as the higher retardation factor calculated for the Freon-12. Groundwater velocity in that area of the model in layer 6 is calculated at 59 ft/yr. Due to the fact that the simulation predicted that natural attenuation would not achieve cleanup goals after 50 years it would be not be necessary to prolong the duration of the simulation.

A single extraction well was simulated at the southern end of the Freon-12 plume (along the BNL site boundary) to determine if the year 2030 cleanup objective could be met. Under this scenario, a single extraction well pumping at 75 gpm was installed in layer 6 of the local model with the return water being discharged to the WSB recharge basin in layer 1. The model was run for a 50 year period and after 8.5 years (year 2026) the Freon-12 concentrations are predicted to be reduced below 5 ppb in layer 6, see **Figures 21** through **23**. The northern portion of the Freon-12 plume naturally attenuates to below 5 ppb during this same duration as it starts out at lower concentrations than the southern portion and thus is not needed to be captured by the proposed extraction well.

The model also predicts the presence of Freon-12 in layer 7 of the model, which is the Magothy brown clay (see **Figure 1**). Freon-12 is predicted to enter layer 7 after about 9 months and remain there at low concentrations (highest predicted concentration around 12 ppb) until year 20 (year 2038) when it reduces to less than 5 ppb. During the entire time the model predicts the presence of Freon-12 in layer 7 of the model it essentially does not migrate beyond the site boundary and appears to stall or linger in the same general area. It is believed that this may be a numerical anomaly in the model (likely a result of vertical dispersion) as the clay layer should act more or less as a confining layer and prevent the downward migration of Freon-12 into the Magothy aquifer. The presence of Freon-12 in the confining layer, if any, will not impact the achievement of cleanup goals by 2030 due to it's lack of mobility.

TABLE No. 1 – DCE/TCA and Freon-12 Scenarios Summary

Scenario	Pumping Conditions	Time to Reach Cleanup Objective of < 5 ppb
DCE/TCA Natural Attenuation	No new extraction wells	2048
DCE/TCA 2 Extraction Wells	Two Wells Pumping at 112.5 gpm each	2034
DCE/TCA 3 Extraction Wells	Three Wells Pumping at 75 gpm each	2026
Freon-12 Natural Attenuation	No new extraction wells	50+ years

Scenario	Pumping Conditions	Time to Reach Cleanup Objective of < 5 ppb
Freon-12 1 Extraction Well	One Well Pumping at 75 gpm	2026

Items highlighted in yellow in the above table indicate they meet the ROD cleanup objective of 2030 for the UGA.

Conclusion

Fate and transport modeling was conducting on the WSB DCE/TCA and Freon-12 plumes by converting the regional BNL groundwater model to a local model centered around the western south boundary. The MT3DMS module in GMS was utilized at the local scale to construct and model the plumes.

The objective of the modeling exercise was to determine whether natural attenuation of the contaminants would achieve the cleanup goals, and if not, optimizing additional active remediation to meet the cleanup goal of less than 5 ppb for DCE/TCA and Freon-12 by the year 2030. Allowing the plumes to attenuate naturally will not meet the objective. The DCE/TCA plume will take 30.5 years to attenuate below 5 ppb and the Freon-12 plume is predicted to take in excess of 50 years and migrate off site long before it is reduced to below the cleanup objective.

Three extraction wells pumping at 75 gpm are predicted to meet the cleanup objective for the DCE/TCA plume in 8 years. The wells would be located along the current DCE/TCA plume centerline and screened across the plume vertically at elevations of -80 to -100 AMSL (see **Figures 12** through **14** for modeled well locations).

A single extraction well with the well pumping at 75 gpm combined with natural attenuation of the northern portion of the plume, is predicted to remediate the Freon-12 plume to below cleanup goal criteria within 8.5 years. The well would be located at the extreme southern end of the plume along the western south boundary (see **Figures 21** through **23** for modeled well location). The actual extent of the Freon-12 upgradient of this proposed extraction well location is not well defined, though it has recently been better defined and the data used in this modeling effort. The well would be screened vertically between elevations of -120 to -140 AMSL.

The groundwater modeling performed predicts that neither the VOC or Freon-12 plume will migrate further south than Moriches Middle Island Road under any scenarios (i.e., natural attenuation or pumping). Thus Carman's River, based on the presently modeled and simulated plume conditions is not expected to be impacted by either the VOCs or Freon-12 in the vicinity of the western south boundary of the BNL site.

In conclusion a four well scenario with each of the wells operating at 75 gpm is the optimum scenario predicted to be able to achieve the ROD cleanup objective of 2030 for the VOC and Freon-12 plumes if it is implemented in a timely manner, **Figure 24** depicts the well locations for the four proposed extraction wells. The well locations and pumping rates were optimized utilizing the BNL groundwater model to achieve the cleanup goals in the most efficient and cost-effective manner, while taking advantage of the existing groundwater treatment systems and infrastructure at the Western South Boundary.

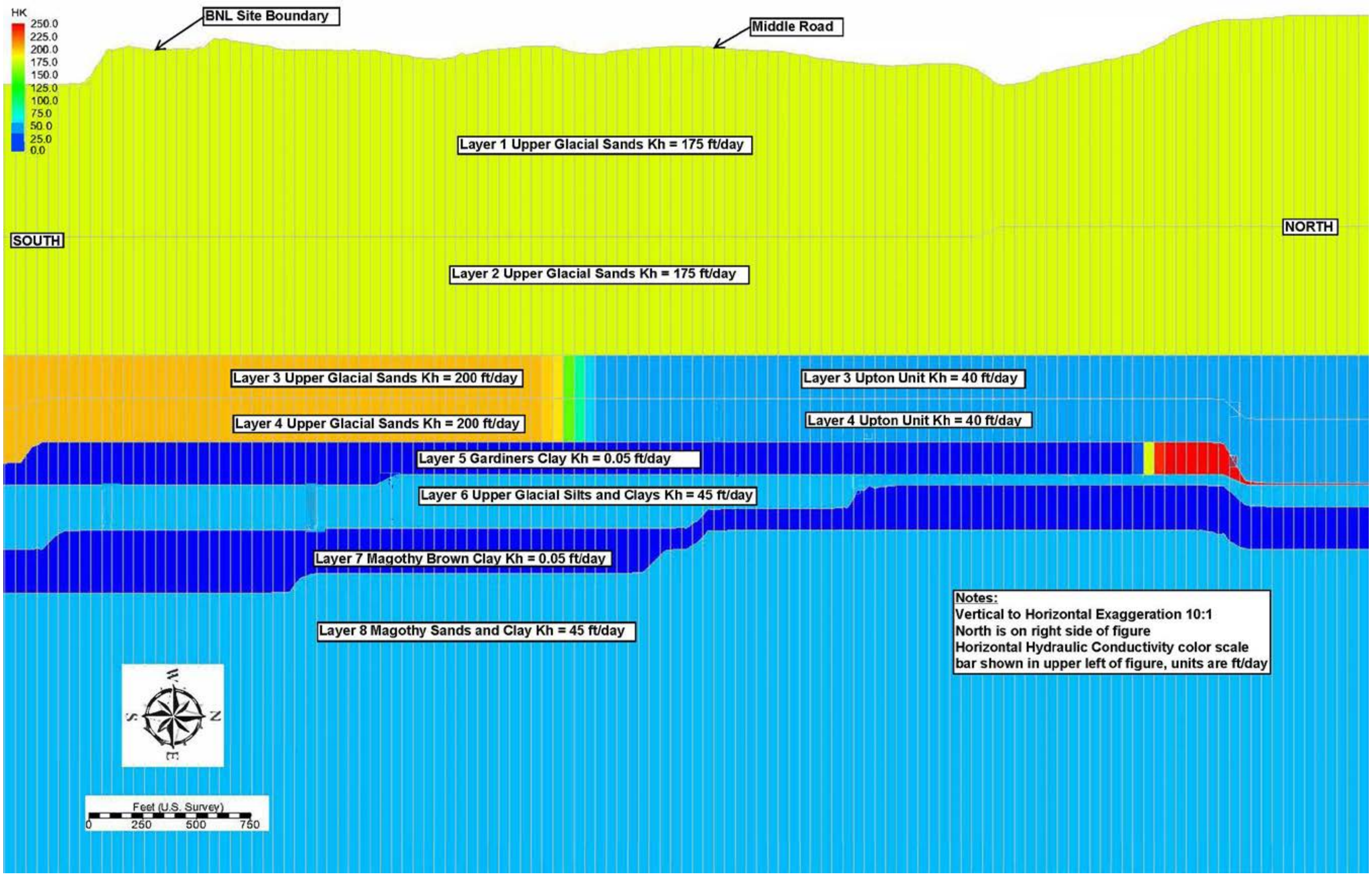
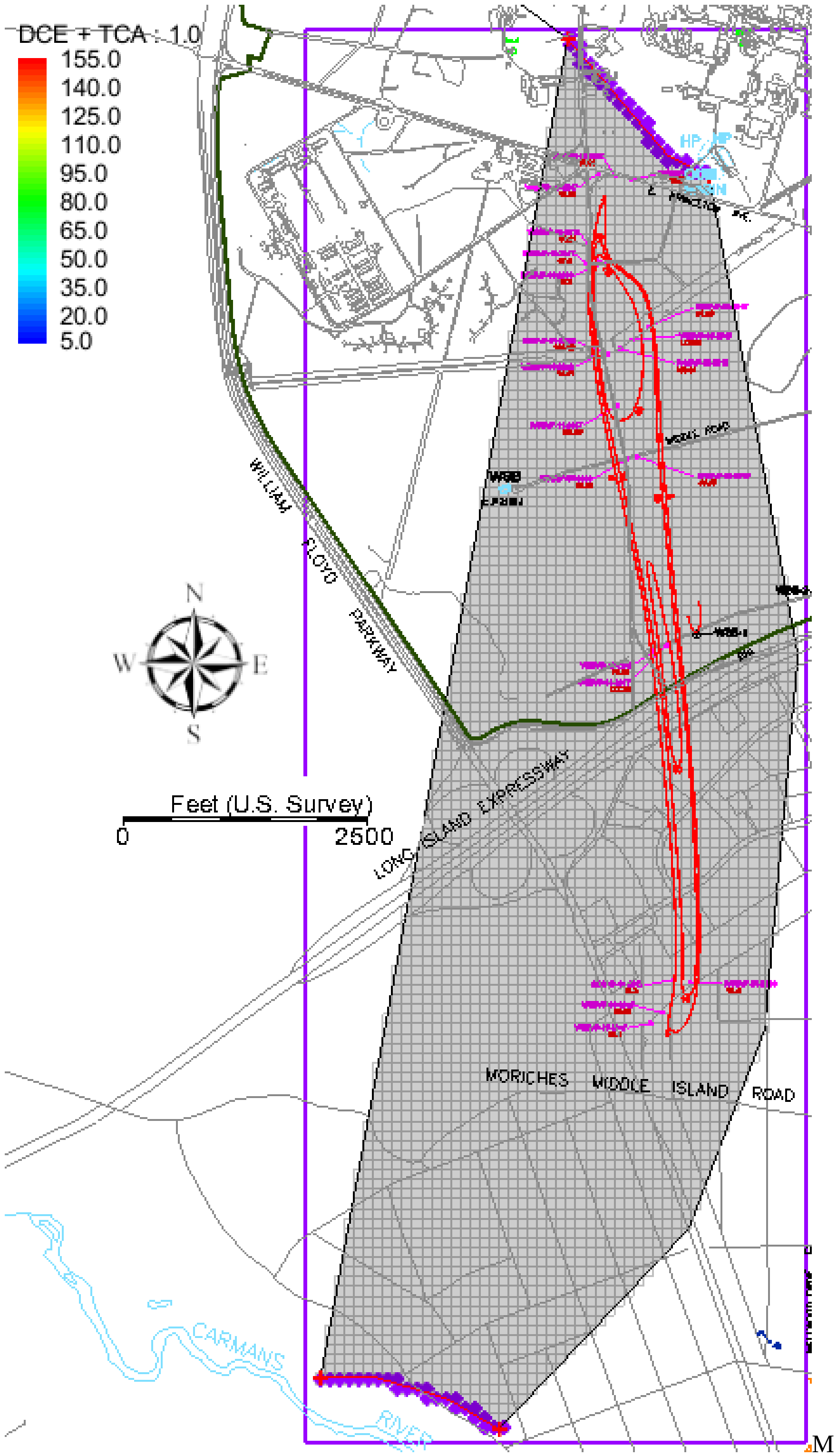


Figure 1 – Model Layering Structure in Vicinity of DCE/TCA and Freon-12 Plumes at WSB – SCALE AS SH



E
Figure 2a – Extents of local model (VOC Plume)

Plume data is from 2016/2017 (VOC Plume - DCE/TCA only)
Local grid spacing is approximately 100' x 100'.

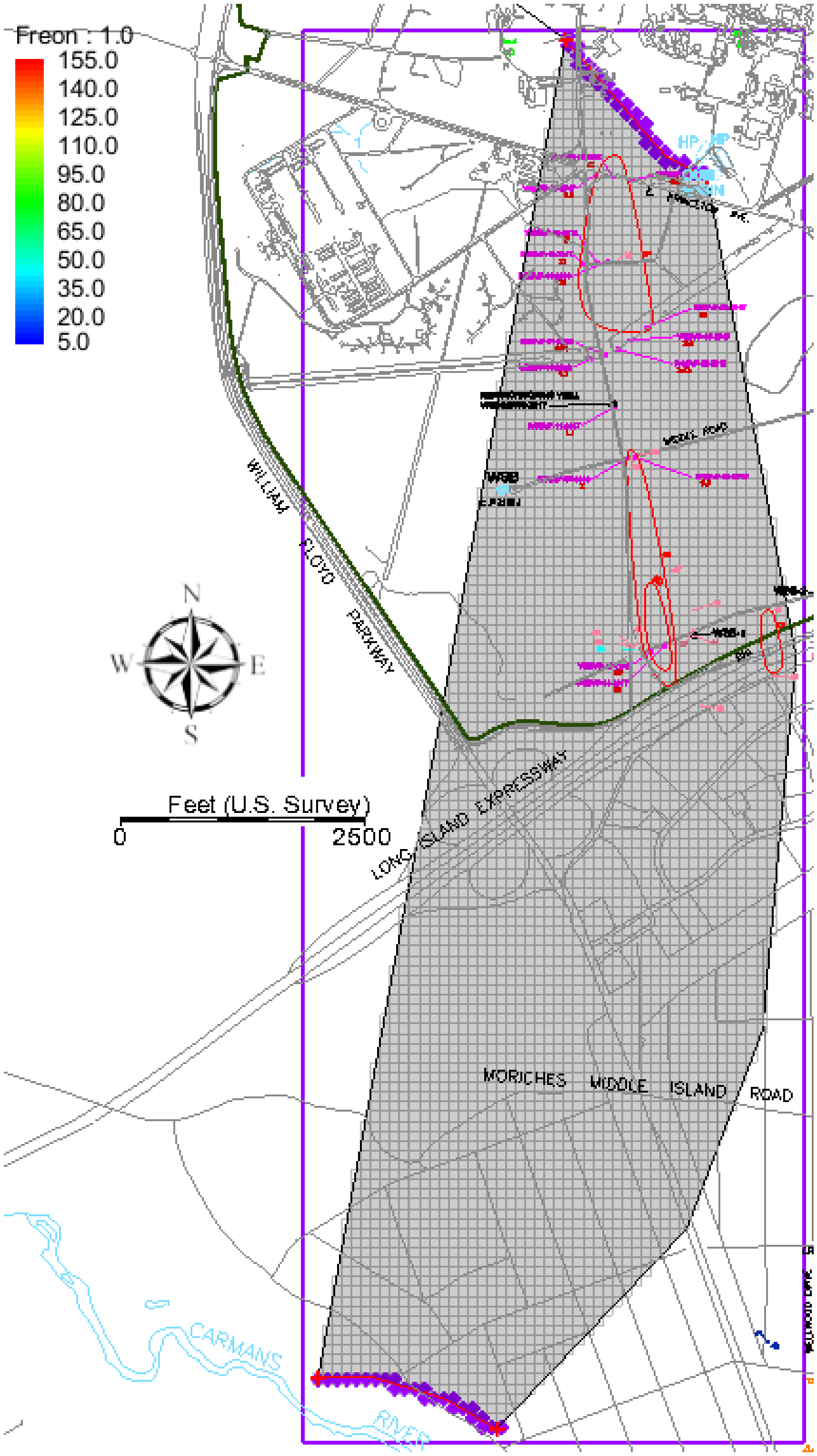


Figure 2b –Extents of local model (Freon-12)

Plume data is from 2016/2017 (Freon-12 Plume)
Local grid spacing is approximately 100' x 100'.

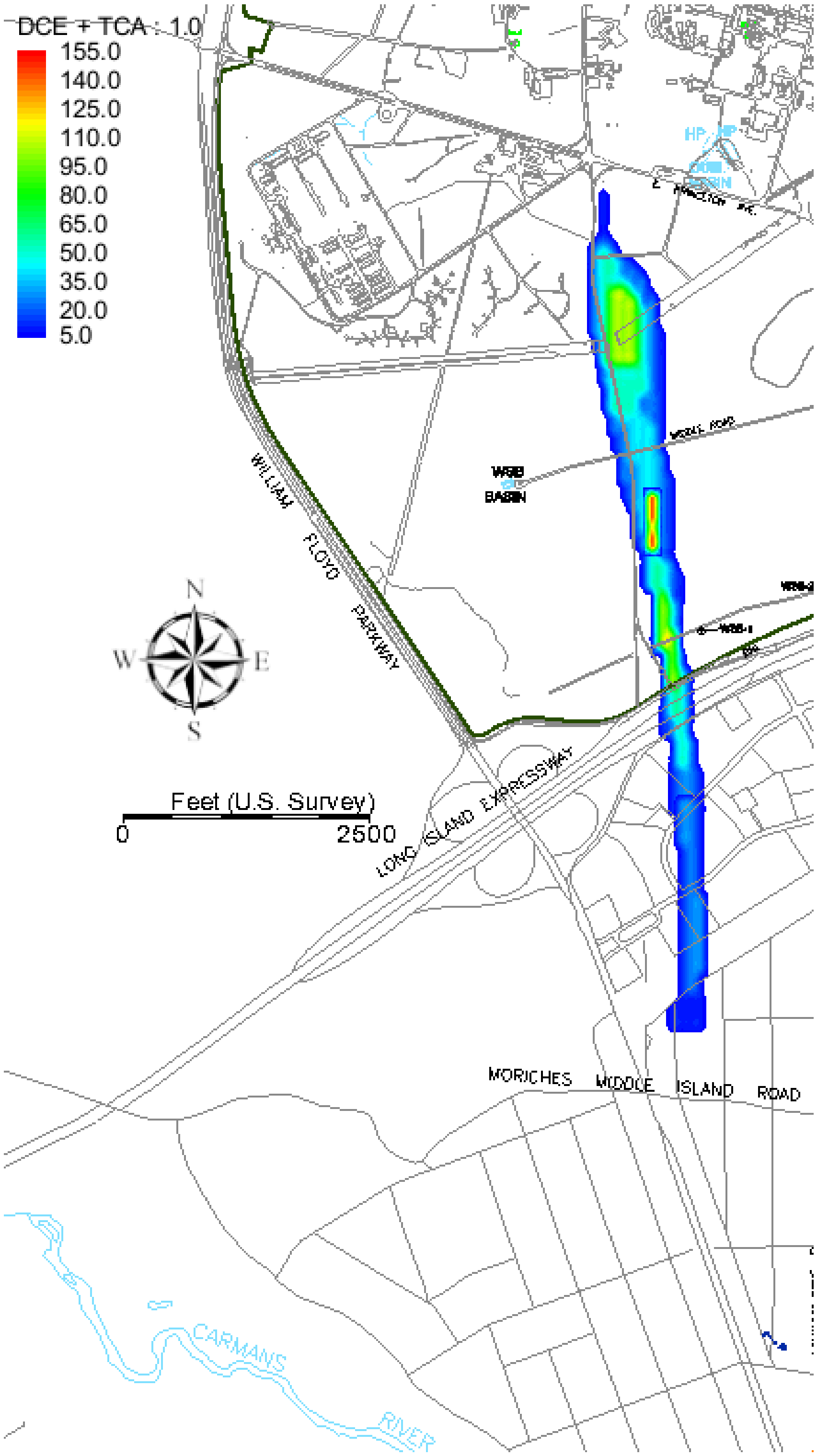


Figure 3 – DCE/TCA Plume Under Natural Attenuation Day 1 (Year 2018)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days

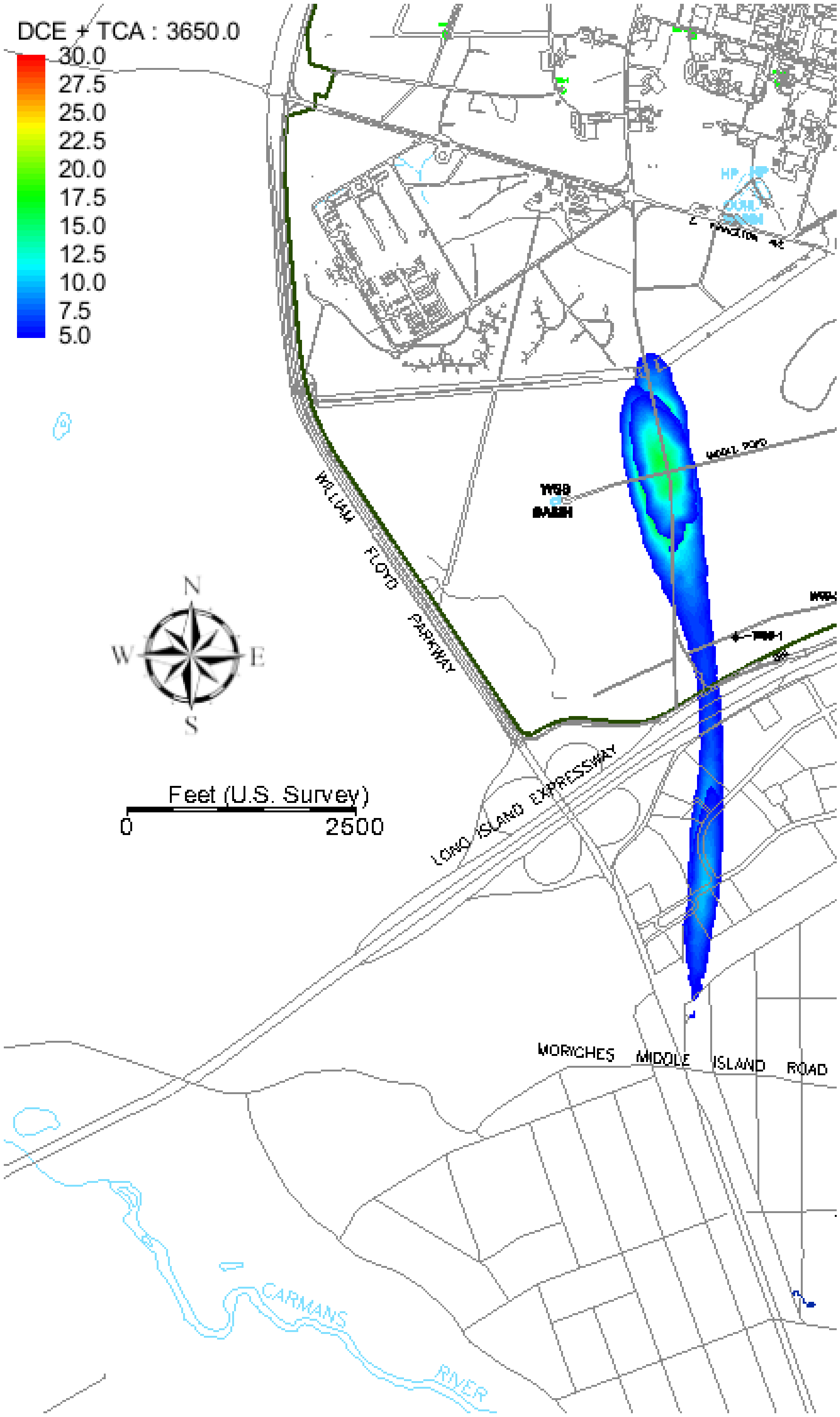


Figure 4 – DCE/TCA Plume Under Natural Attenuation after 10 years (Year 2028)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

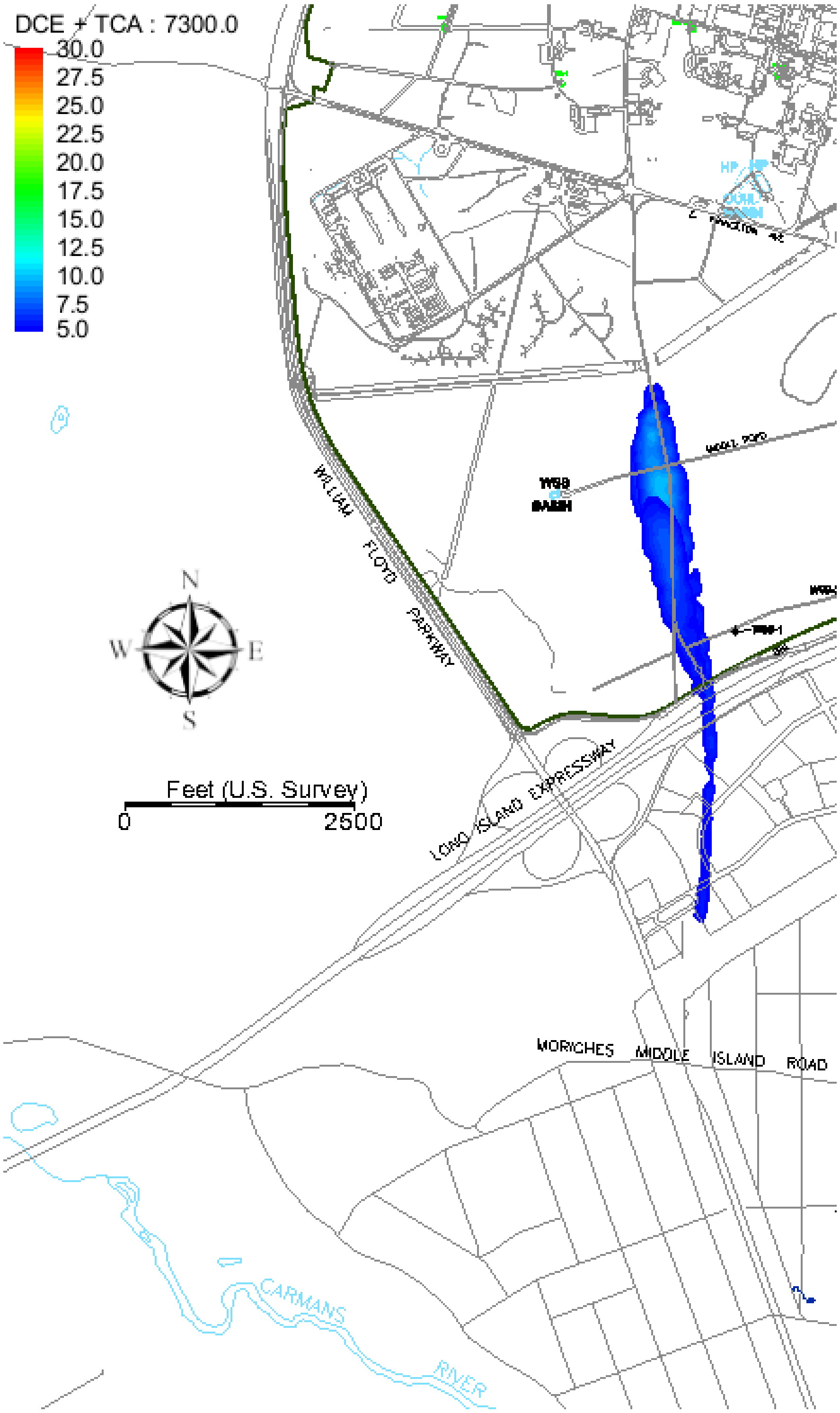


Figure 5 – DCE/TCA Plume Under Natural Attenuation after 20 years (Year 2038)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

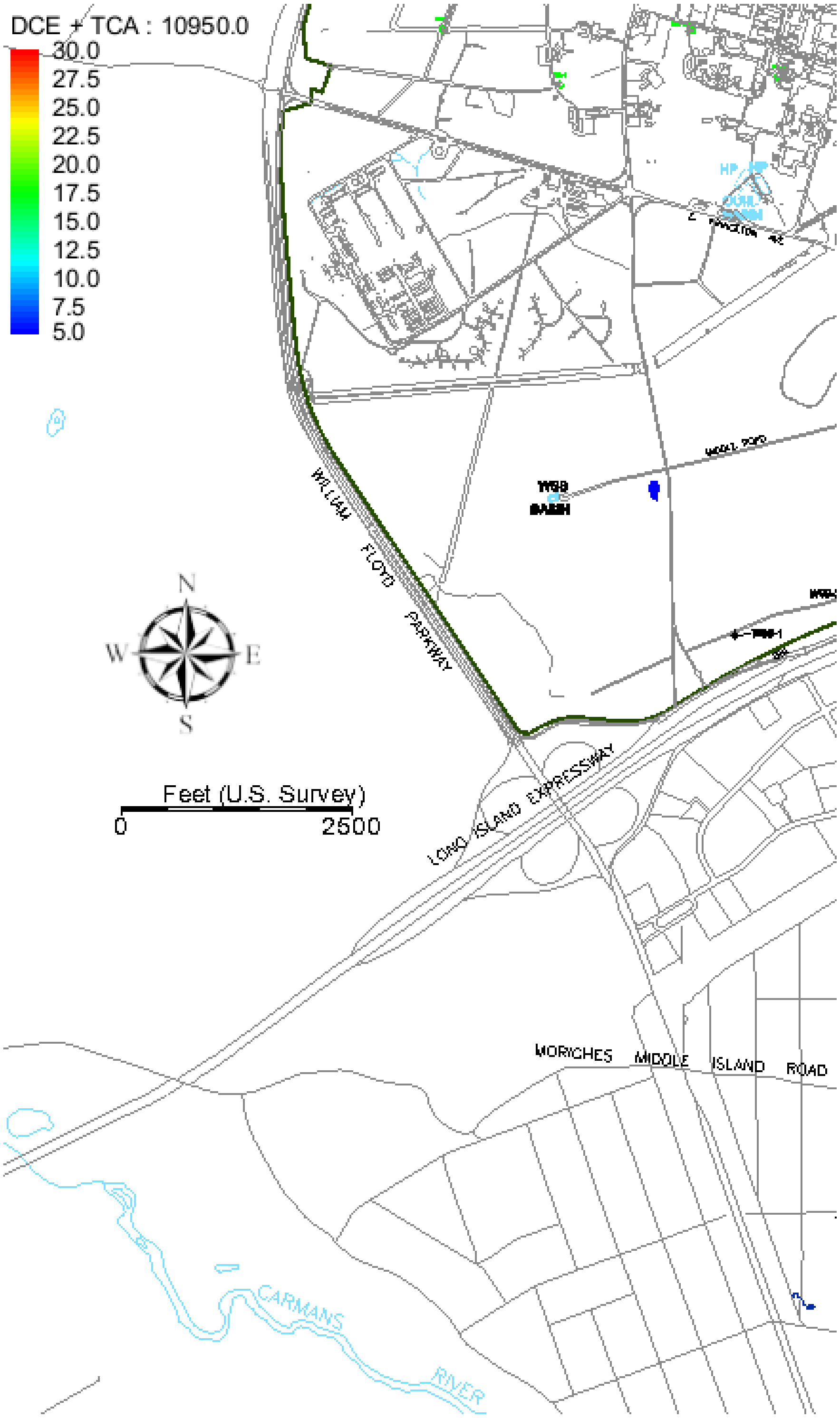


Figure 6 – DCE/TCA Plume Under Natural Attenuation after 30 years (Year 2048)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

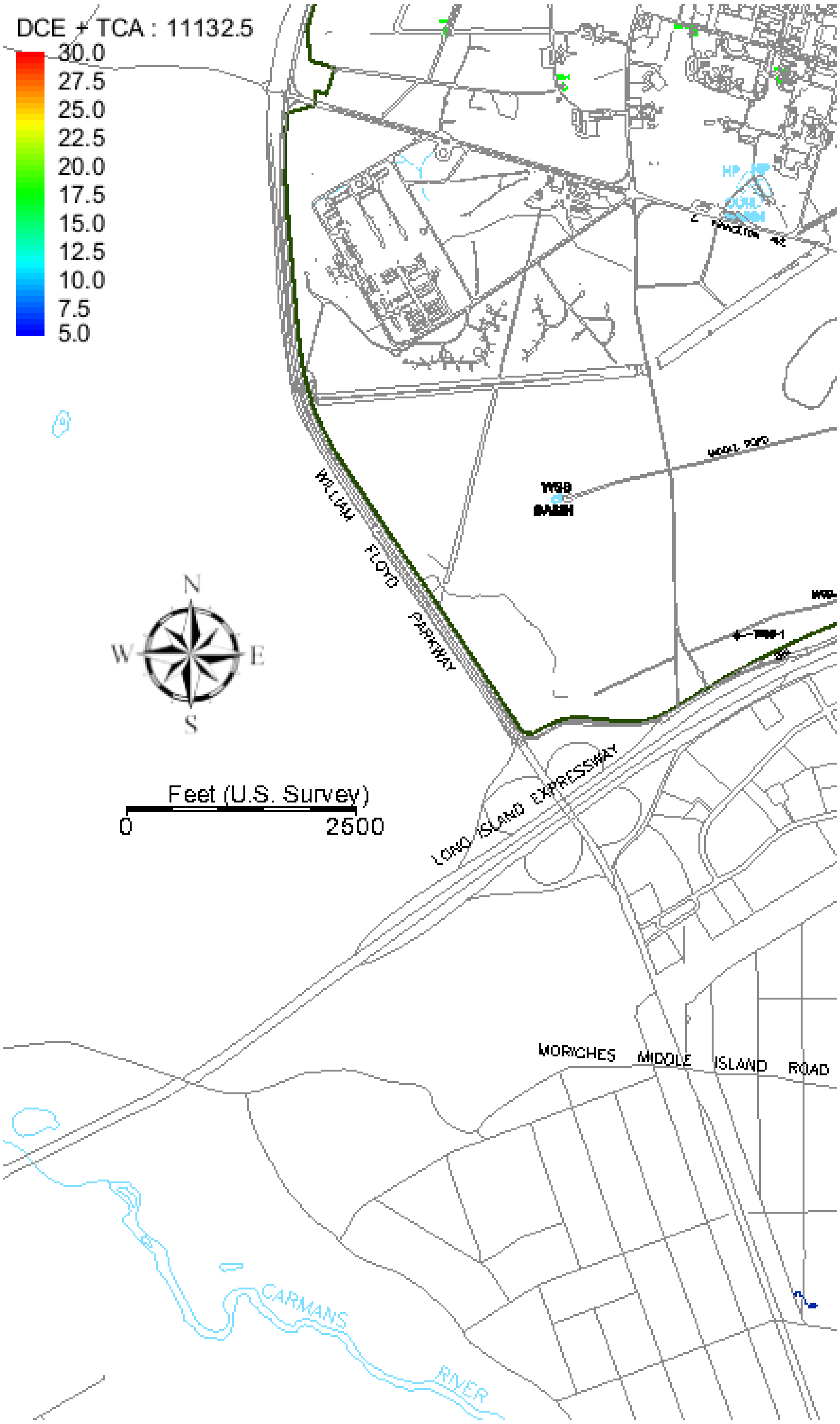


Figure 7 – DCE/TCA Plume Under Natural Attenuation after 30.5 years (Year 2048)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

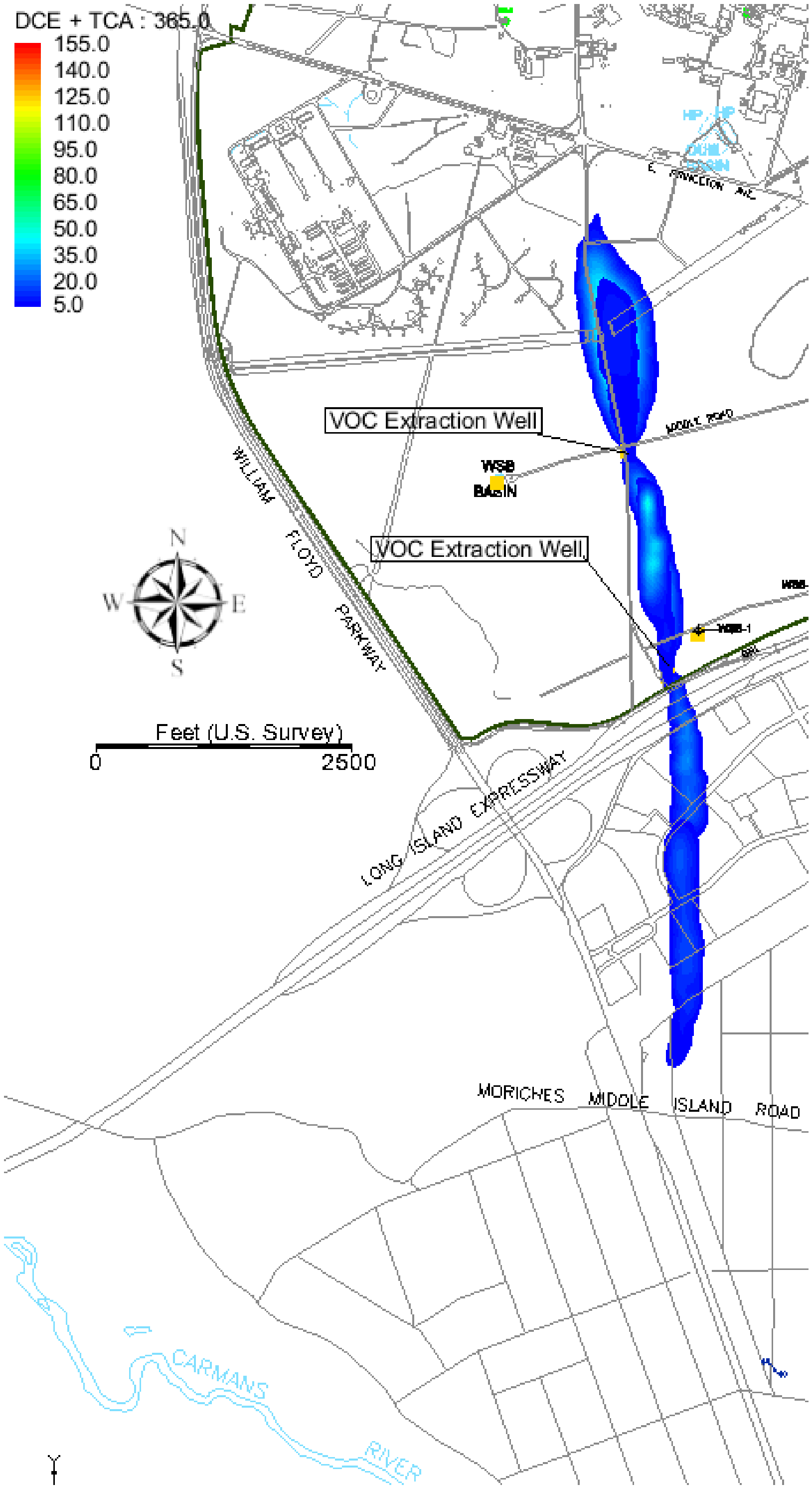


Figure 8 – DCE/TCA Plume Two New Extraction Wells at 112.5 gpm Each – 1 year (Year 2019)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

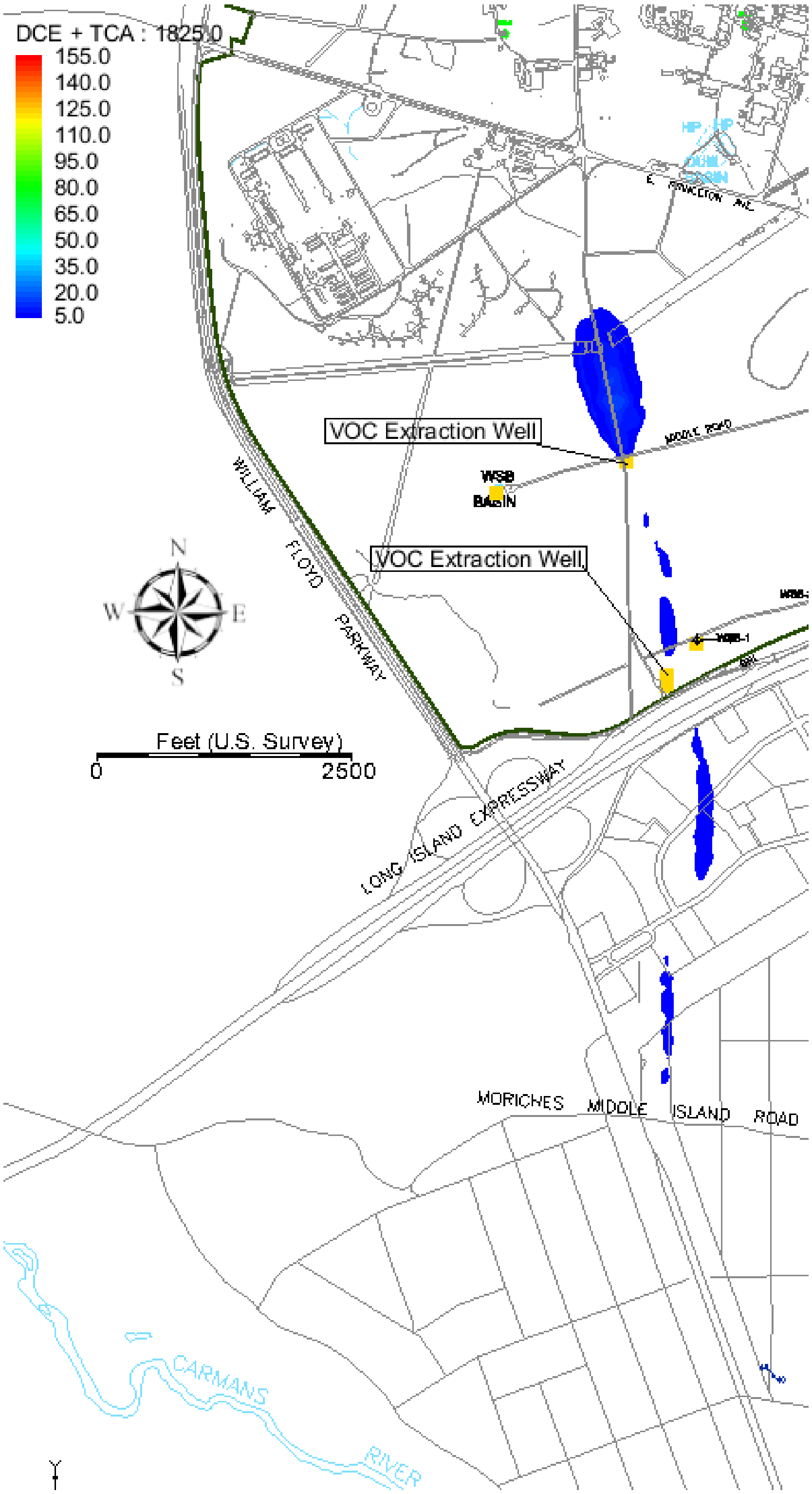


Figure 9 – DCE/TCA Plume Two New Extraction Wells at 112.5 gpm Each – 5 years (Year 2023)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

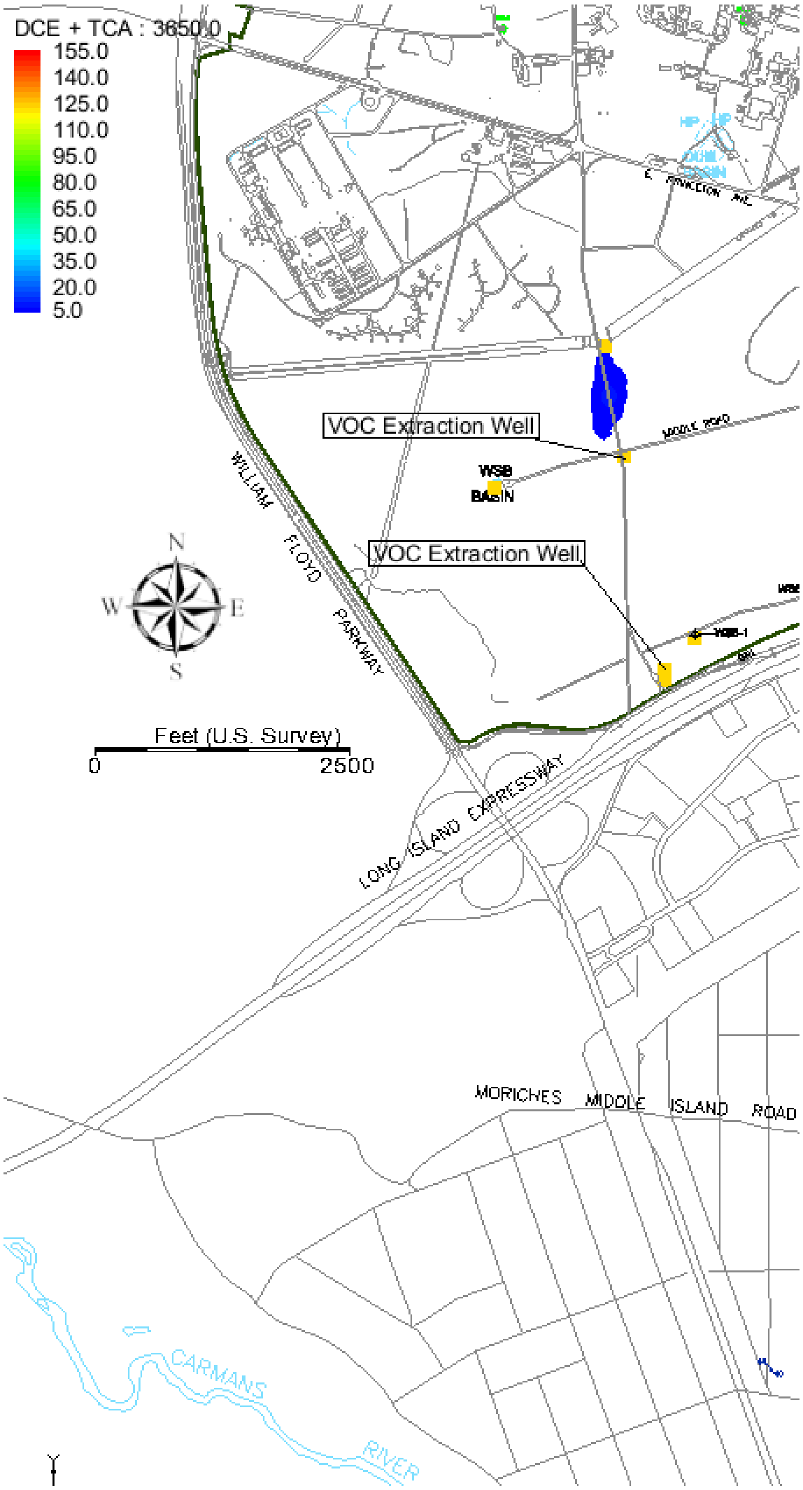


Figure 10 – DCE/TCA Plume Two New Extraction Wells at 112.5 gpm Each – 10 years (Year 2028)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

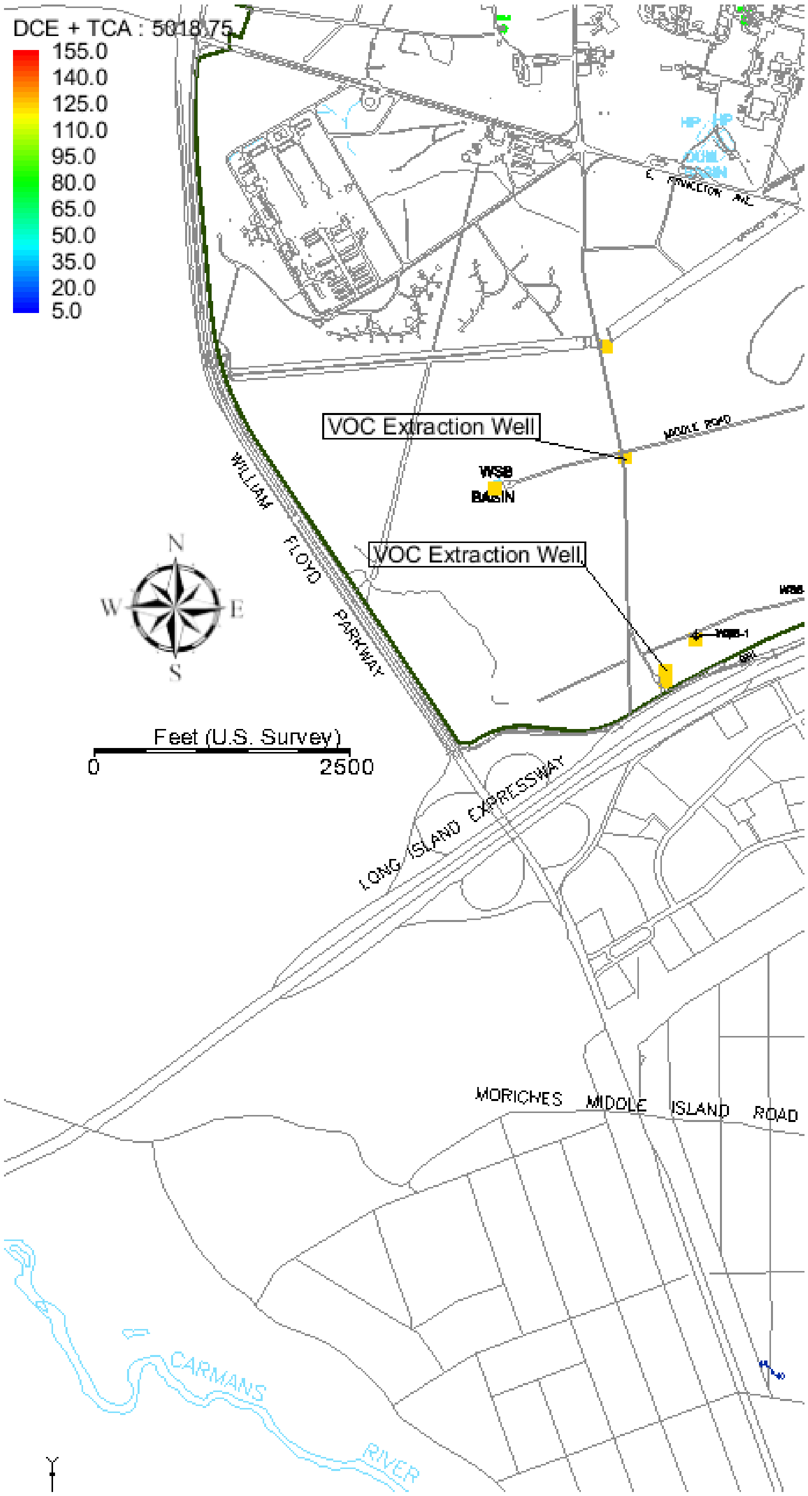


Figure 11 – DCE/TCA Plume Two New Extraction Wells at 112.5 gpm each – 13.75 yrs (year 2031)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

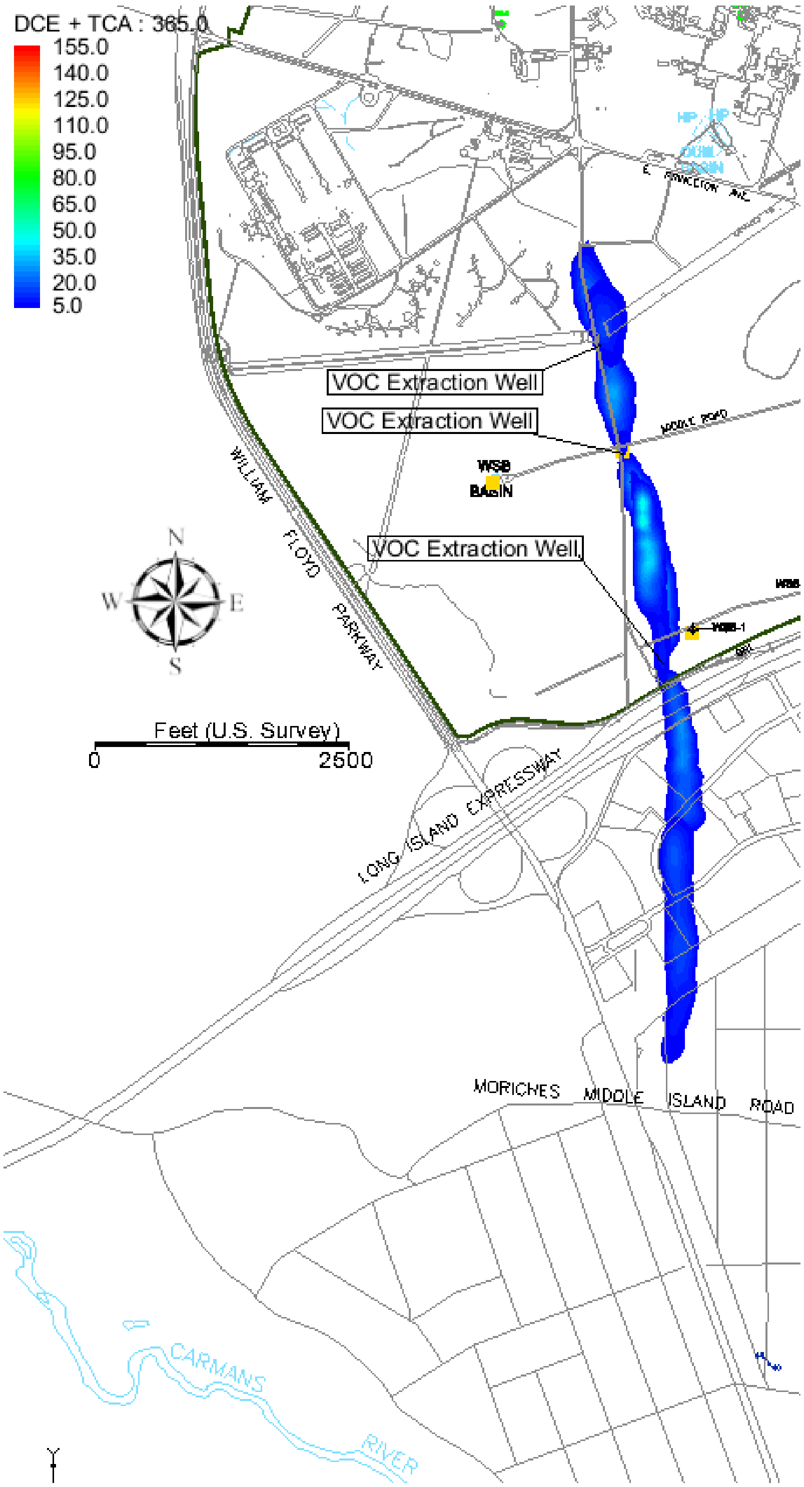


Figure 12 – DCE/TCA Plume Three New Extraction Wells at 75 gpm Each – 1 yr (Year 2019)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

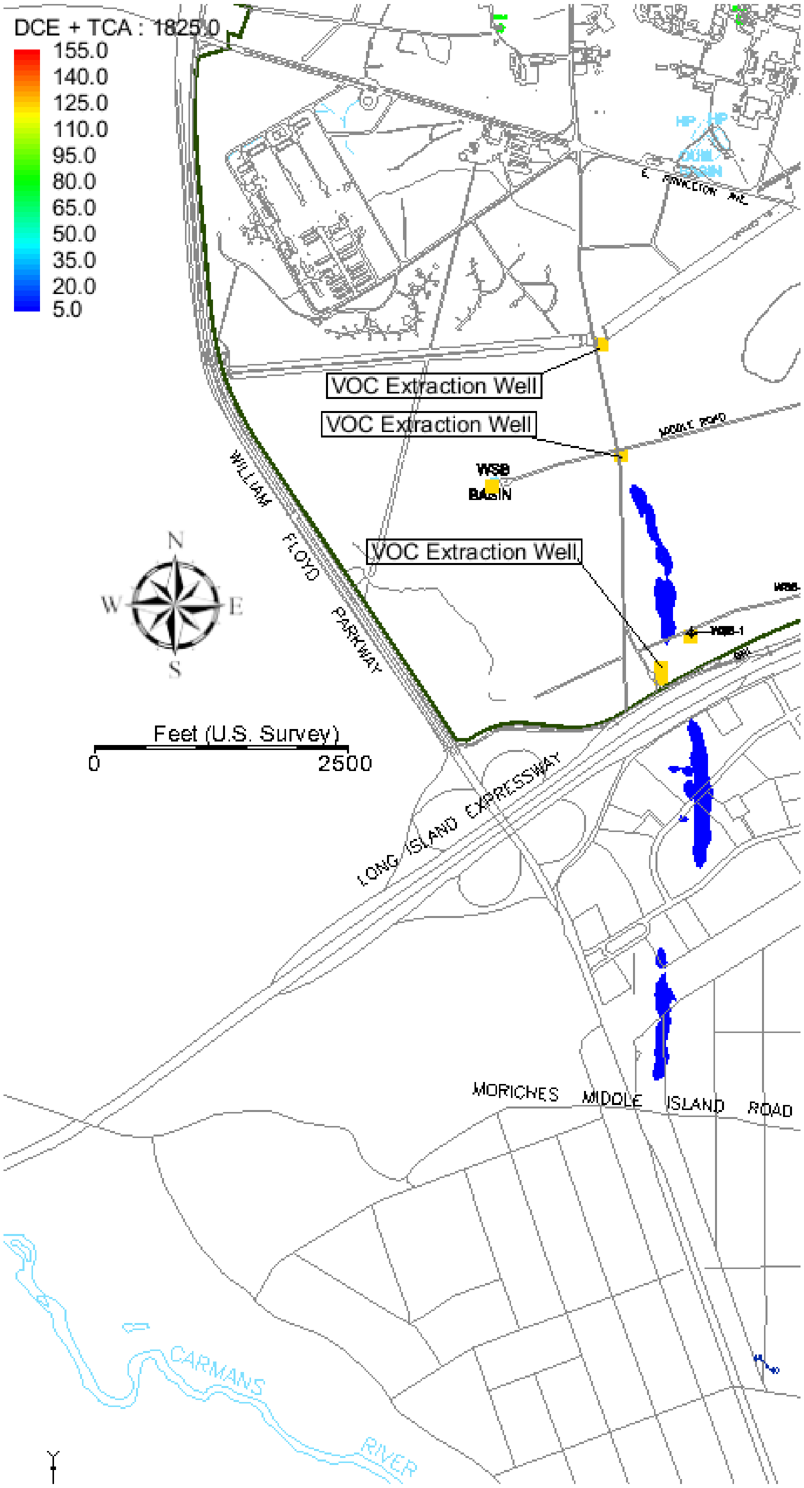


Figure 13 – DCE/TCA Plume Three New Extraction Wells at 75 gpm Each – 5 yrs (Year 2023)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

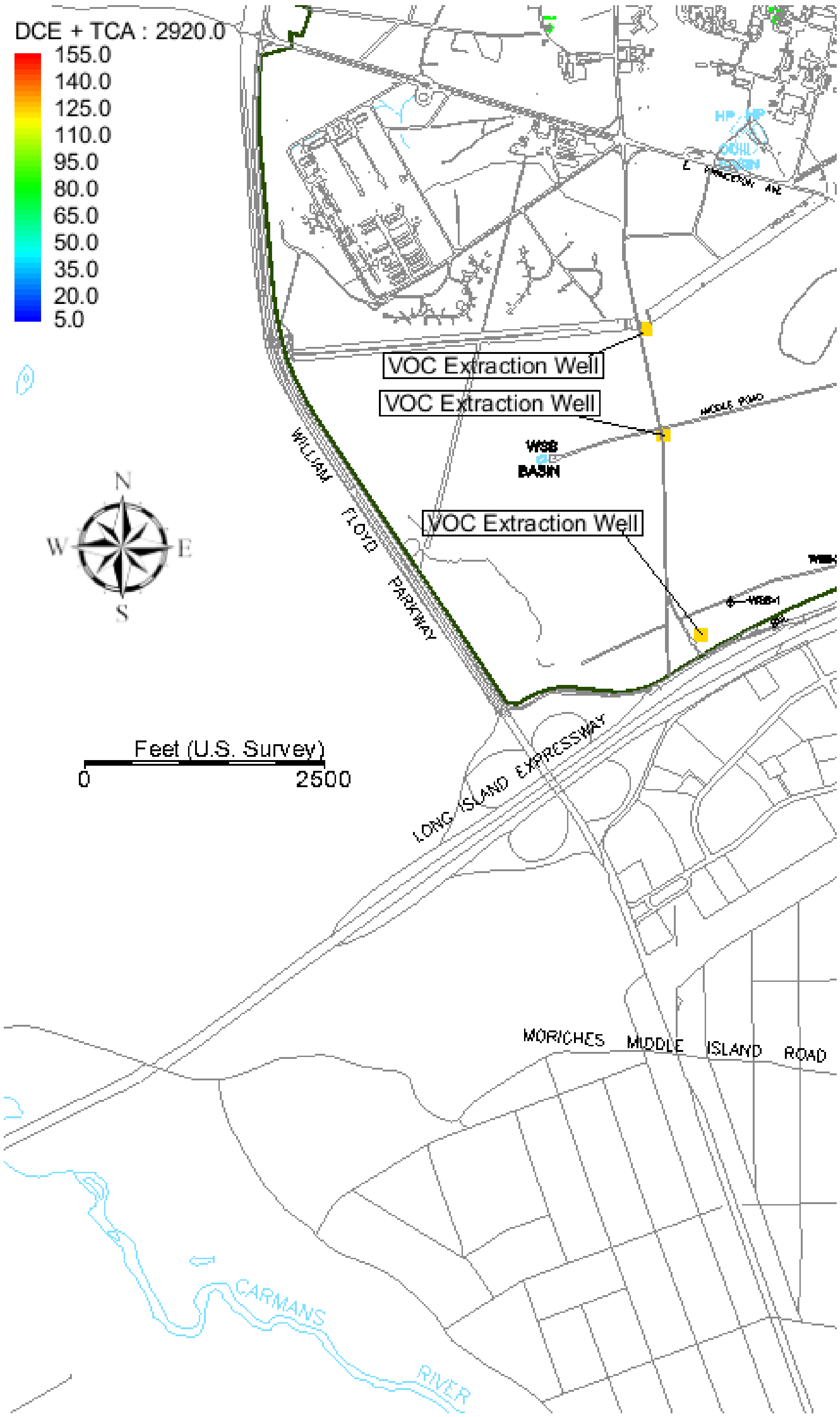


Figure 14 – DCE/TCA Plume Three New Extraction Wells at 75 gpm Each – 8 yrs (Year 2026)

Color scale in upper left corner represents DCE/TCA concentrations in ppb.
Number following DCE/TCA above color scale in upper left corner is time in days.

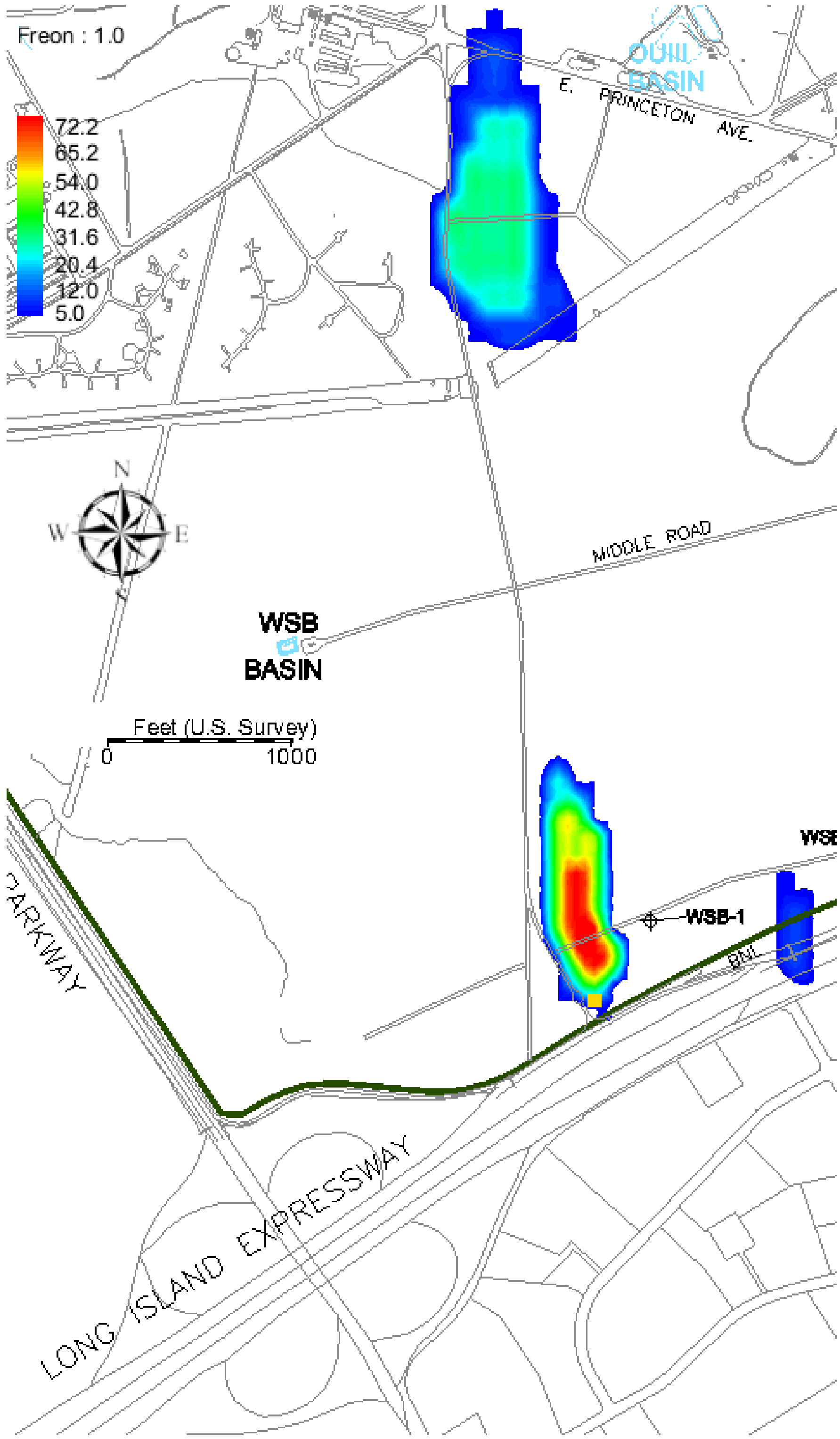


Figure 15 – Freon-12 Plume Under Natural Attenuation day 1 (Year 2018)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

Figure 16 – Freon-12 Plume Under Natural Attenuation after 10 years (Year 2028)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

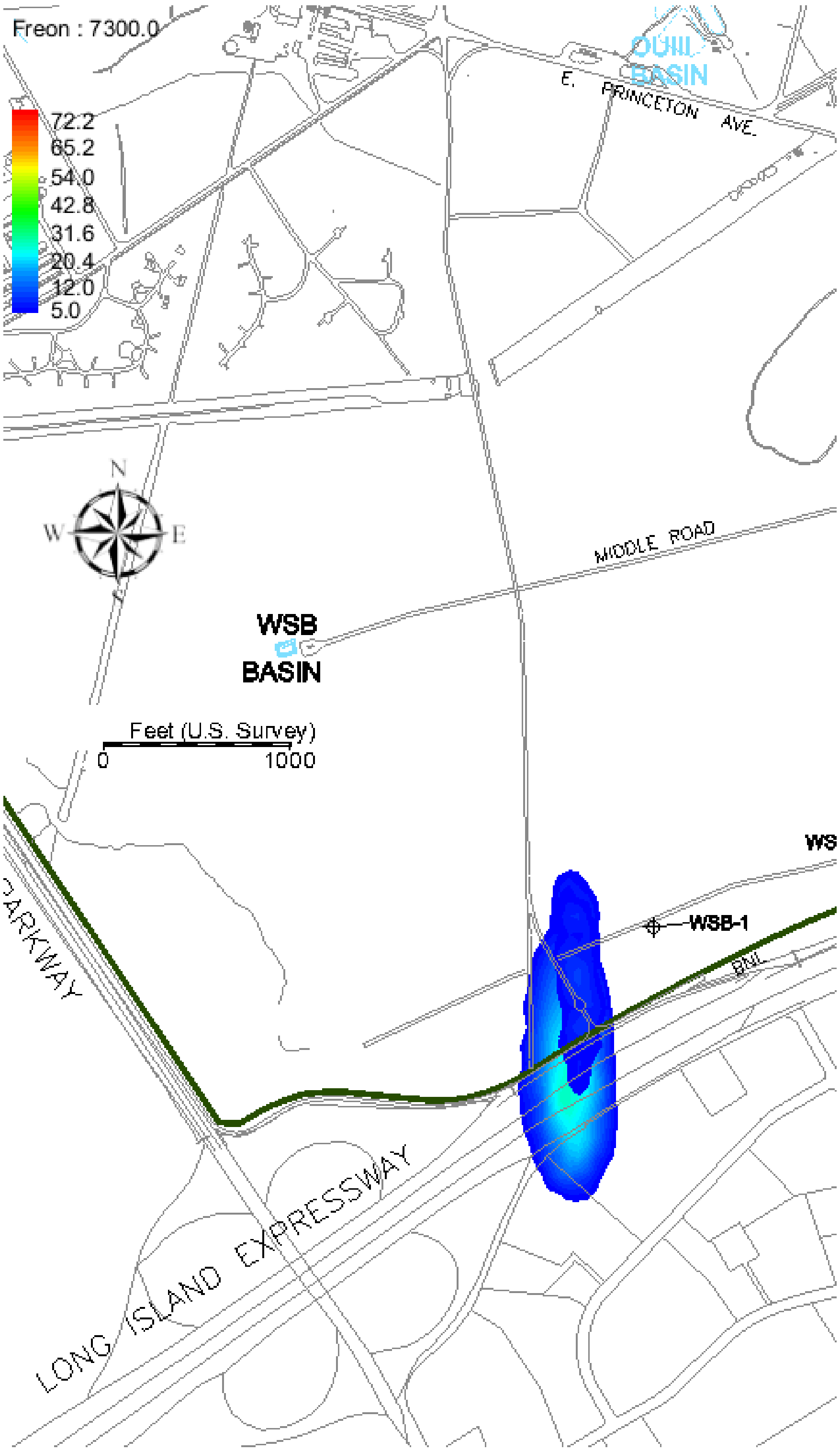


Figure 17 – Freon-12 Plume Under Natural Attenuation after 20 years (Year 2038)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

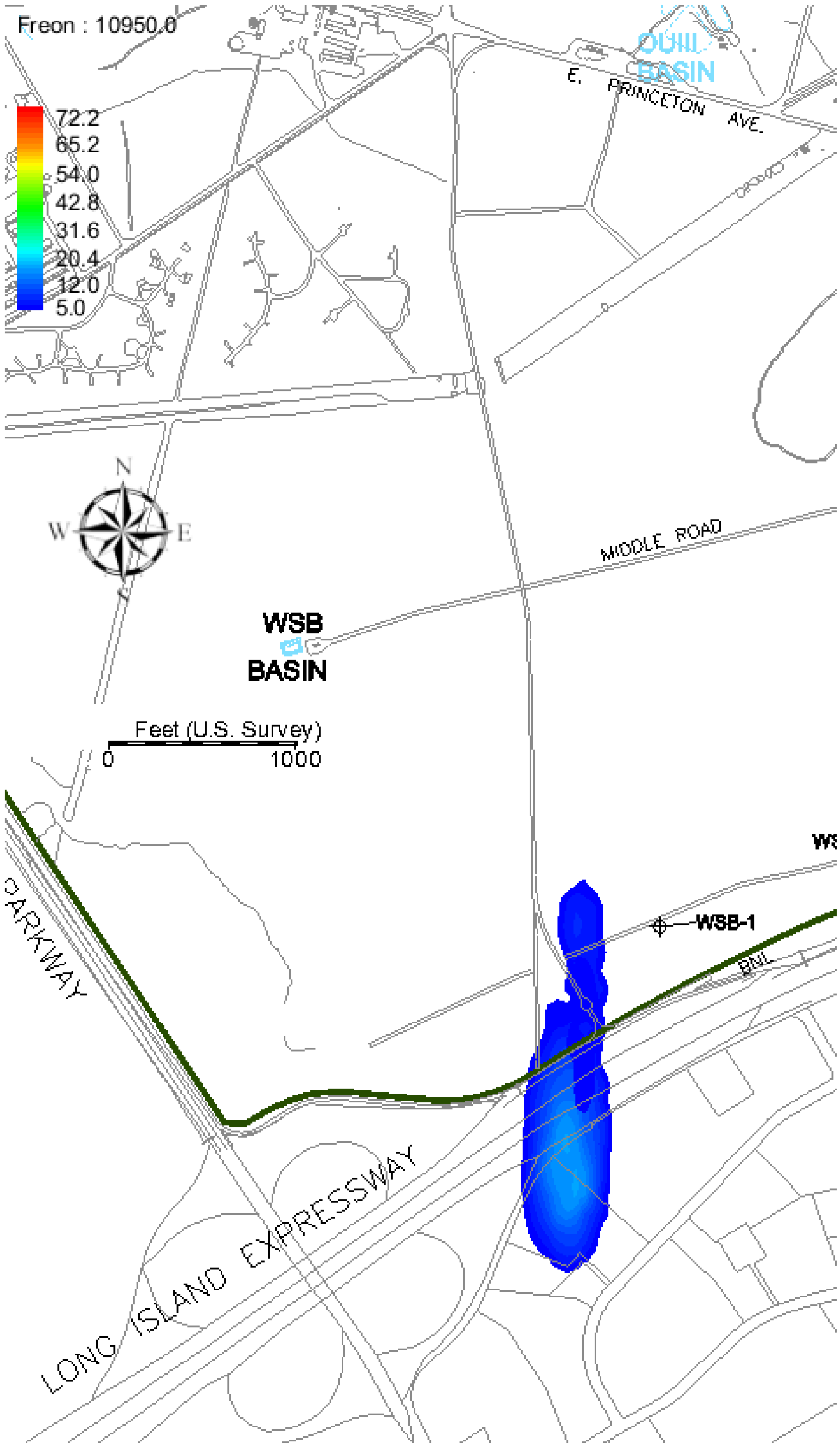


Figure 18 – Freon-12 Plume Under Natural Attenuation after 30 years (Year 2048)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

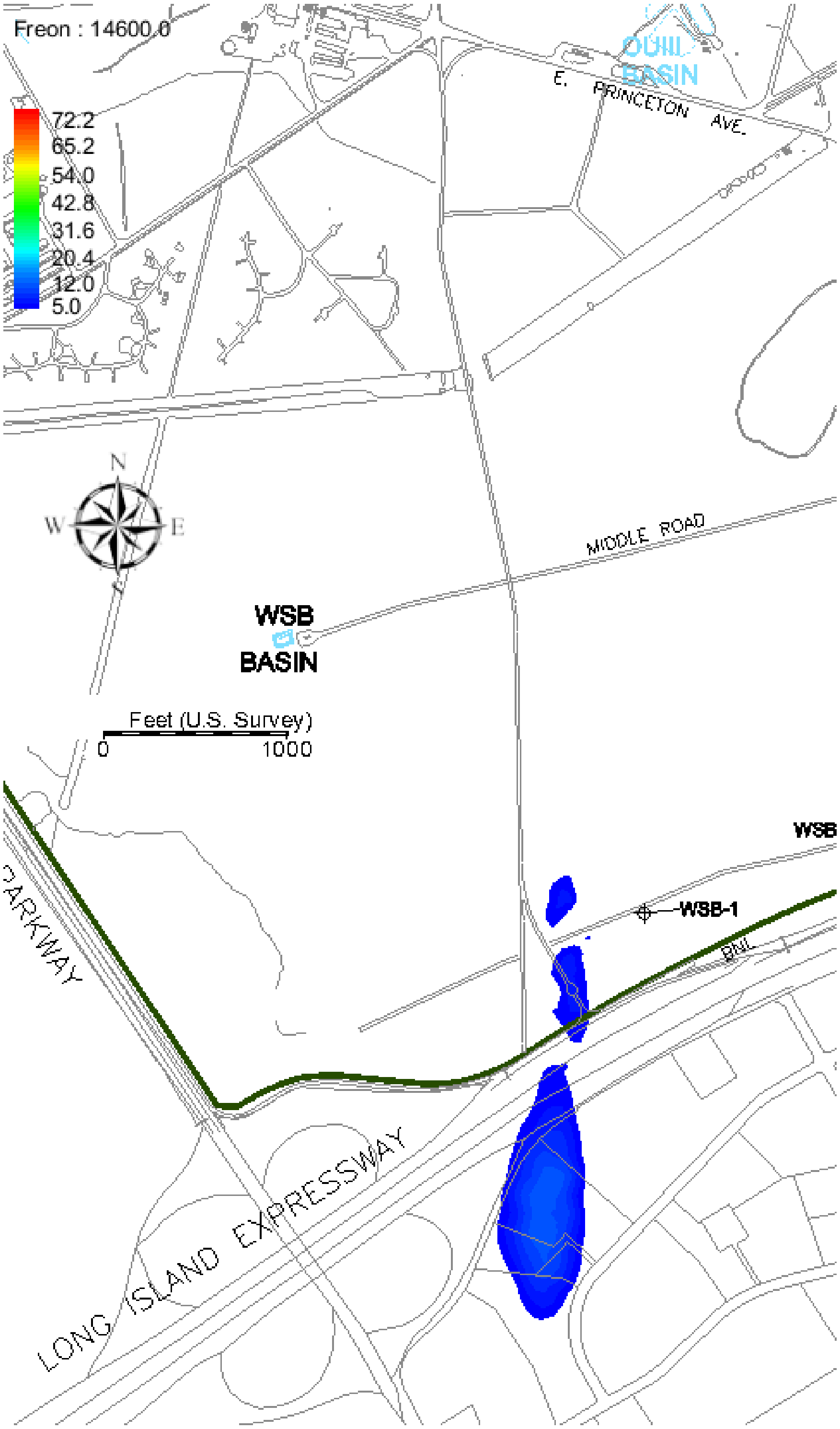


Figure 19 – Freon-12 Plume Under Natural Attenuation after 40 years (Year 2058)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

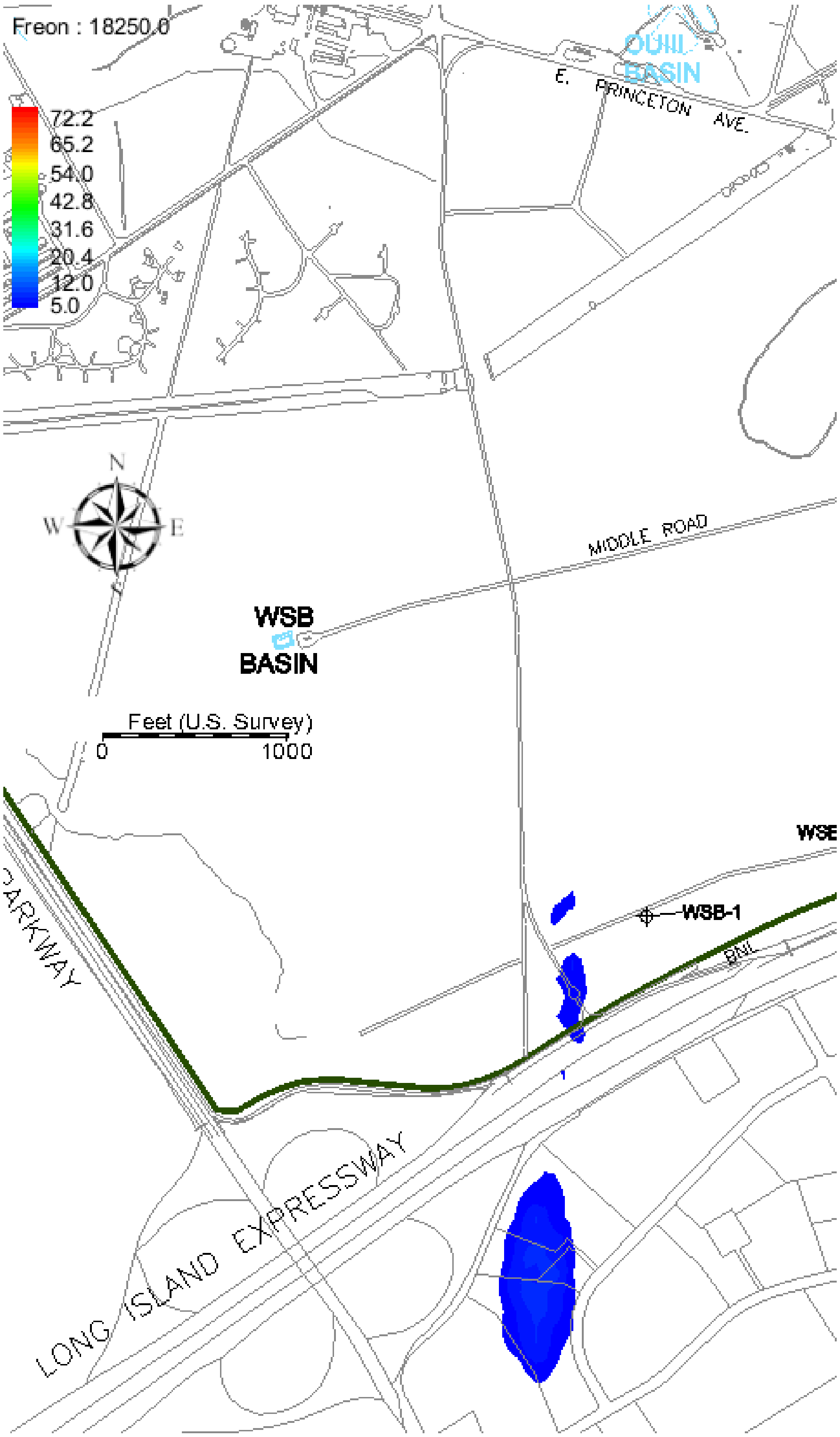


Figure 20 – Freon-12 Plume Under Natural Attenuation after 50 years (Year 2068)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

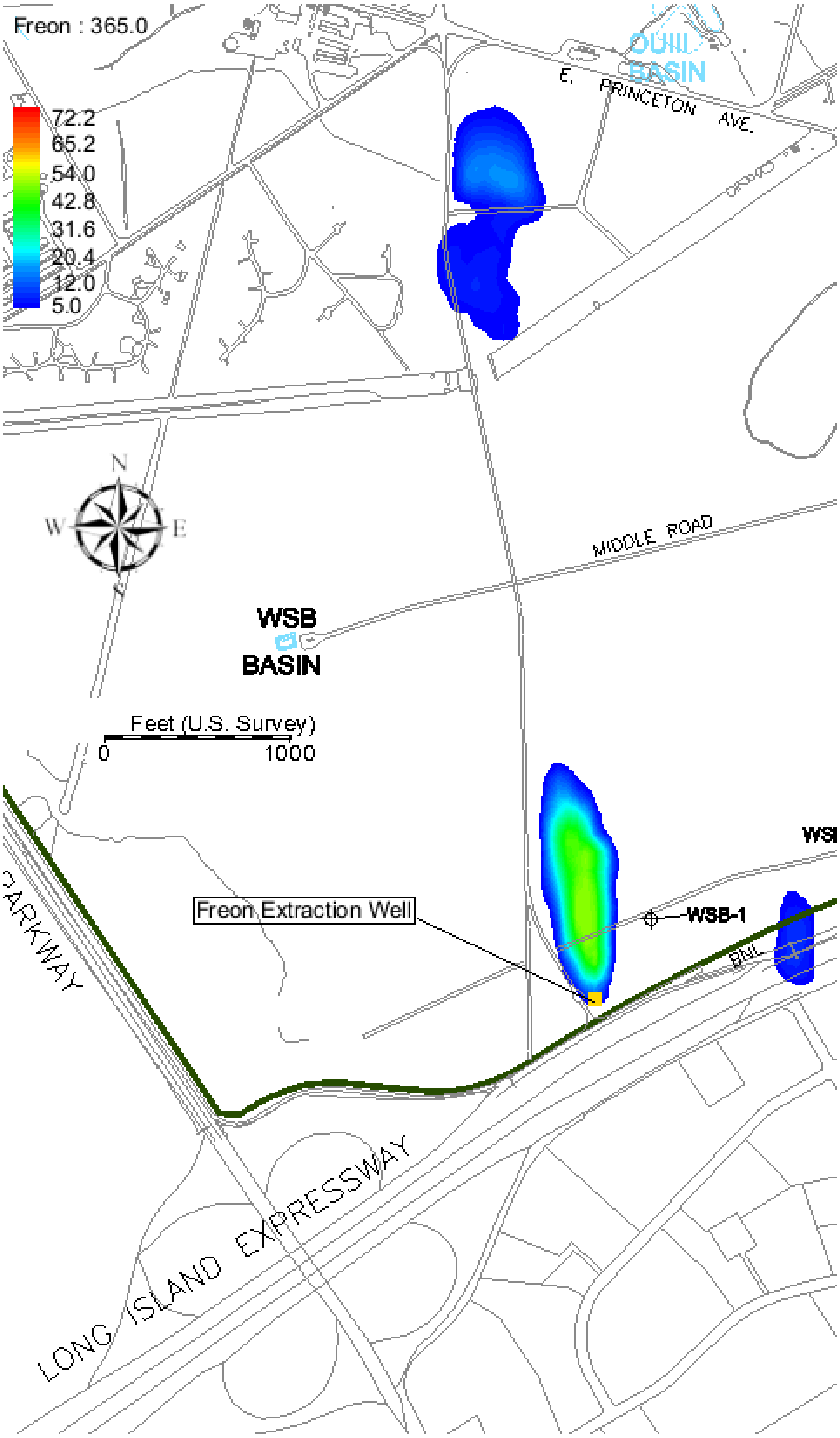


Figure 21 – Freon-12 Plume One New Extraction Well at 75 gpm – 1 year (Year 2019)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

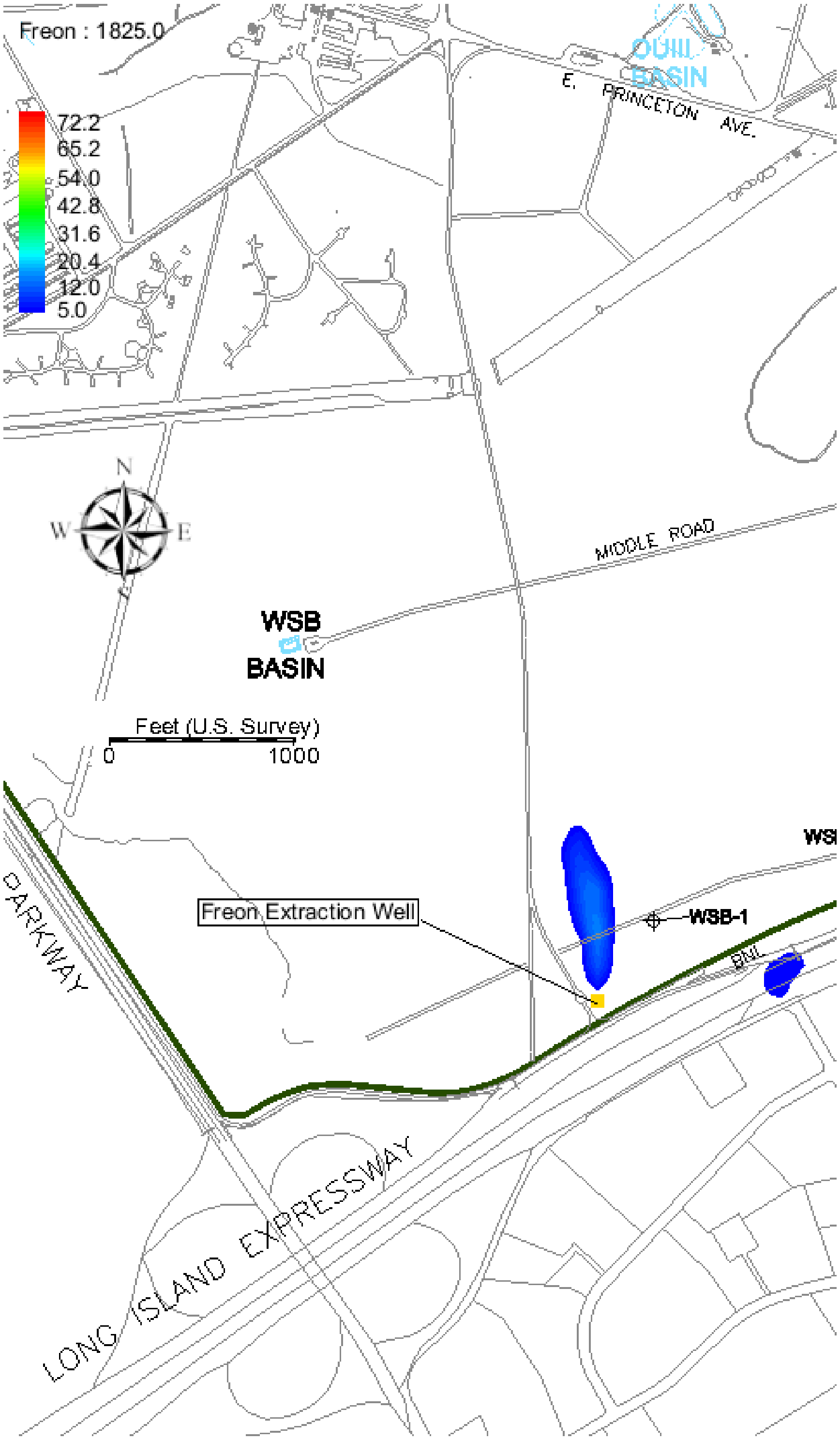


Figure 22 – Freon-12 Plume One New Extraction Well at 75 gpm – 5 years (Year 2023)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

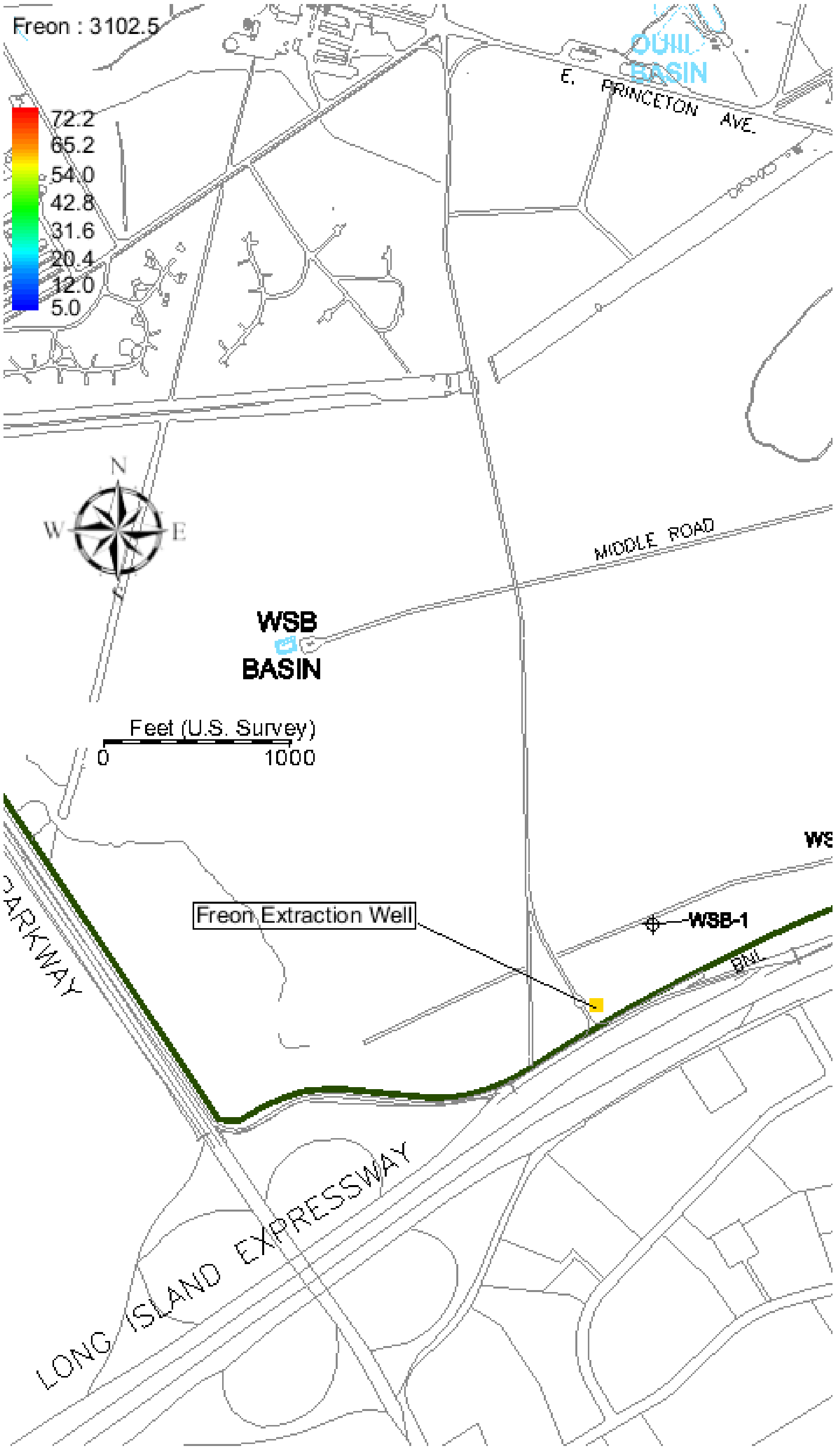


Figure 23 – Freon-12 Plume One New Extraction Well at 75 gpm – 8.5 years (Year 2026)

Color scale in upper left corner represents Freon-12 concentrations in ppb.
Number following Freon-12 above color scale in upper left corner is time in days.

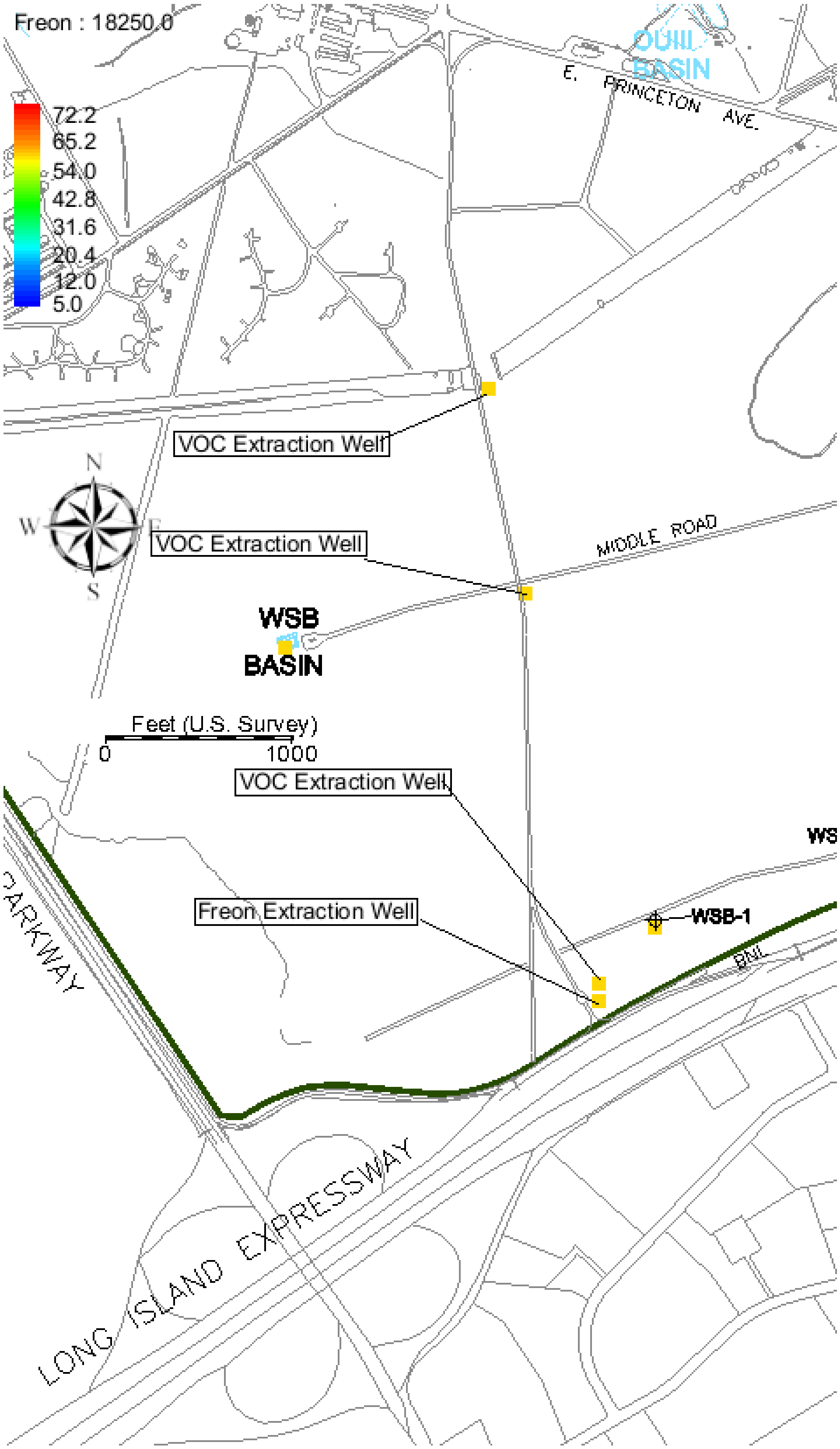


Figure 24 – Locations of 4 Proposed Extraction Wells

Prepared for:

BROOKHAVEN NATIONAL LABORATORY

Groundwater Protection Group
Brookhaven National Laboratory

Prepared by:

PWGC
Strategic Environmental Engineering Solutions

(March 2018)