Appendix H

NSE Ethylene Dibromide

BNL North Street East EDB Plume

Fate and Transport Modeling Results

November 20, 2018

At the request of BNL's Groundwater Protection Group (GPG), P.W. Grosser (PWGC) performed fate and transport modeling for the North Street East ethylene dibromide (EDB) plume, located south of the BNL property, using the regional groundwater model and the groundwater modeling software Groundwater Vistas, version 7. The lateral and vertical plume extents were provided by the GPG.

Groundwater modeling simulations were performed to estimate the length of time necessary for EDB concentrations to reduce to below the drinking water standard of 0.05 micrograms per liter (µg/L) under the following conditions:

1) natural attenuation;
2) installing and pumping an extraction well at the leading edge of the plume;
3) installing and pumping two extraction wells (one at the leading edge of the plume and one within the plume core); and
4) pumping existing downgradient extraction well NSE-1.

The results of these simulations were compared to aid BNL in determining the most efficient method for meeting BNL's groundwater cleanup goals by 2030.

The work presented in this groundwater modeling memorandum is based upon previously conducted modeling efforts by BNL (**Figures 1 and 2**). PWGC utilized BNL's existing regional three-dimensional numerical groundwater model (Groundwater Vistas Version 7.19 Build 16, 64-Bit, MODFLOW 2000) to create a telescopic mesh refinement (TMR), or sub-regional model, of the North Street East EDB plume and surrounding area within Groundwater Vistas. The local model consists of an area approximately 4,400 ft (east-west direction) by 9,700 ft (north-south direction) around the EDB plume with the plume located in the center north (upgradient area) of the model. This local model was then used to analyze transient flow conditions to predict the fate and transport of the EDB plume utilizing MT3DMS, a modular three-dimensional transport model developed by the United States Geological Survey (USGS) for the simulation of advection, dispersion, and chemical reactions of dissolved constituents in groundwater systems.

Key Assumptions and Model Modifications

The key assumptions made for the modeling effort are:

- The local model inherited hydraulic/hydrogeologic properties from the calibrated regional model. Modifications made to the local model included refining the horizontal grid spacing from 100 ft x 100 ft to 25 ft x 25 ft to obtain higher resolution groundwater head contours and EDB plume concentration contours. Refining the vertical grid consisted of subdividing model layer 3 into two parts, with the lower sublayer set to correlate with the screen zone of proposed well EDB-EW-1 (**Figure 2**). Model layers are defined in **Figure 2**.

- EDB plume conditions were input to Groundwater Vistas using the most recent data available as of August 2018 (**Figures 1 and 2**). Plume concentrations ranged between 0.05 and 1.06 µg/L and were input as three isoconcentration zones: 0.05 - 0.49 µg/L, 0.5 – 0.99 µg/L, and $\geq$1.00 µg/L. The plume was created only in layer 3 of the local model (approximate top elevation of layer 3 = -71 ft relative to mean sea level (MSL) and approximate bottom elevation of layer 3 = -114 to -121 ft MSL). The vertical distribution of the plume was approximated within the layer 3 sublayers (upper and basal) as shown on **Figures 3a-3b**, respectively.

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

- Using MT3DMS, the option for anisotropic dispersion was chosen. Inputs for this dispersion package included longitudinal dispersivity (a_L), transverse dispersivity (a_T) (typically 0.1x a_L), and vertical dispersivity (a_V) (typically 0.01 x a_L). Dispersivity is scale dependent and values will vary with distance, thus the longer the travel distance of the contaminant is the greater its longitudinal dispersivity value will be. Initially, values of a_L =12.5 (i.e., half the grid size), a_T = 1.25, and a_V =0.125 were input to the local model as constants for all model layers and zones.

- Using the equation $a_L = 0.83[\log(L_p)]^{2.414}$ (Xu and Eckstein, 1995), where a_L is the longitudinal dispersivity in feet and L_p is the travel distance in feet, a_L was calculated to be 1.86 for a 25 ft grid. As a sensitivity study, dispersivity values of aL = 1.86, aT = 0.186, and aV = 0.0186 were input to the model and the simulations repeated.

- The chemical reaction package was used to simulate retardation effects. Groundwater Vistas 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 Groundwater Vistas 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. As used in the regional model, all layers were set to have a soil bulk density of 100 lb/ft^3 (as this is a typical or common value for regional sands) and a porosity of 0.24 (which was used in the calibration of the regional model). PWGC calculated a distribution coefficient (K_d) of 0.0006 ft^3/lb for EDB using the following equation:

    - $K_d = K_{oc} \times f_{oc}$ = 0.44 L/kg x 0.08 x 0.0160185 (conversion factor) = 0.0006 ft^3/lb

    Where

    - K_{oc} = 0.44 L/kg, the soil/water partition coefficient of EDB per a National Groundwater Association (NGWA) reference

- o f_{oc} = 0.08, the fraction of organic carbon in typical Long Island sands.

  Applying the appropriate equations and unit conversions K_d was calculated to be 0.0006 ft^3/lb, which was input to Groundwater Vistas. The resulting R value calculated for EDB in the local aquifer is 1.25.

- Groundwater flow contours were generated in MODFLOW using the BNL regional model. **Figures 3a-3b** depict the steady state pumping condition groundwater head contours in layer 3 (upper and basal sublayers, respectively) of the model (the layer where the EDB plume is delineated and the proposed extraction wells were screened for the simulations) and the initial EDB concentrations contours input to Groundwater Vistas.

- Since no active pumping wells were identified within the bounds of the local model, PWGC imported steady-state flow conditions from the regional model as the initial step in the local transient model. Transient conditions were then modeled over a 10- or 30-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.

- EDB plume natural attenuation (i.e., no groundwater extraction or other active remediation) was simulated over the 30-year timeframe to approximate the plume's future location, configuration, and concentrations.

- Remedial extraction of the EDB plume was simulated over a 10-year timeframe in Groundwater Vistas by inputting a well at the leading (southern) edge of the current EDB plume. The screen zone of this proposed well (EDB-EW-1) was placed in the basal sublayer of Layer 3 to fully capture the deeper vertical extent of the plume (approximately -95 to -114 ft MSL). The proposed well was assigned a constant pumping (withdrawal) rate of 100 gpm (19,250 ft^3/d). Groundwater head conditions were held steady throughout the full 10-year MT3DMS modeling period.

- The above conditions were repeated with the addition of a second extraction well, EDB-EW-2, input within the core of the current plume in the Layer 3 basal sublayer and assigned a constant pumping (withdrawal) rate of 100 gpm (19,250 ft^3/d).

- Remedial extraction of the EDB plume was also simulated over a 10-year timeframe by pumping only existing extraction well NSE-1 at 200 gpm (38,500 ft^3/d). This well is located downgradient (south) of the EDB plume; however, it is east of the plume's centerline and its screen bottom is shallower than the current mapped depth of the EDB plume.

Discussion of Model Simulations and Predictions

Several transient modeling simulations were conducted using MT3DMS to evaluate the effects of various parameters on the predicted durations to achieving groundwater concentrations of less than 0.05 µg/L of EDB. These are summarized below.

Scenario 1: Natural Attenuation

The first modeling scenario that was investigated was running MT3DMS with the fate and transport packages active (advection, dispersion and chemical reaction) with no active groundwater extraction. Groundwater flow conditions were held steady throughout the entire model simulation period of 30 years. **Figures 4a-4b** depict the EDB plume at one year after initiation of the modeling simulation. **Figure 4b** indicates that the plume has migrated vertically into Layer 5, the upper portion of the Magothy aquifer. After 15 years the leading edge of the plume has traveled the farthest within the basal sublayer of Layer 3, approximately 5,700 feet south of the current plume location (about four blocks south of Moriches Middle Island Road - **Figure 5a**), and also extends south of Moriches Middle Island Road within Layer 6 (**Figure 5b**). After approximately 30 years, some small areas of EDB concentrations above 0.05 µg/L are still predicted to remain in Layer 6 (approximately 870 feet south of the current leading edge of the plume - **Figure 6**). Under this scenario the model predicts that concentrations of EDB will not be below the groundwater standard of 0.05 µg/L until more than 30 years passes (i.e., beyond the year 2048).

Scenario 2: Groundwater Extraction from a New, Strategically Located Well

The next scenario to be evaluated was installing a new extraction well at the leading edge of the current plume position with the proposed well's screen zone straddling the vertical extent of the EDB plume above 0.05 µg/L. The proposed well (EDB-EW-1) was set to pump continuously at 100 gpm. Running an MT3DMS simulation with the fate and transport packages activated, the model predicts full capture of the plume and a cleanup time of between 7 and 7.1 years. The simulated changes in the plume over time are provided in **Figures 7a-7e**.

Scenario 3: Groundwater Extraction from a Two New, Strategically Located Wells

The next scenario repeated Scenario 2, with a second extraction well (EDB-EW-2) added within the plume core with the proposed well's screen zone straddling the vertical extent of the EDB plume above 0.05 µg/L and set to pump continuously at 100 gpm. Running an MT3DMS simulation with the fate and transport packages activated, the model predicts full capture of the plume and a cleanup time of only 4 years. The simulated changes in the plume over time are provided in **Figures 8a-8e**.

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Scenario 4: Groundwater Extraction from Existing Well NSE-1

The final modeling scenario involved setting existing extraction well NSE-1 to pump continuously at 200 gpm, twice the pumping rate of EDB-EW-1 in the Scenario 2 simulation. Running an MT3DMS simulation with the fate and transport packages activated, the model predicts only partial capture, with EDB plume loss beneath and west of NSE-1 in approximately 8 years (**Figures 9a-9b**).

Dispersivity Sensitivity Study

In addition to the three scenarios summarized above, a quick check on the model sensitivity to dispersivity (D) with regards to the plume's velocity was also performed. Initially, values of a_L =12.5 (i.e., half the grid size), a_T = 1.25, and a_V =0.125 were used for a 10-year natural attenuation simulation. When the Xu and Eckstein equation was applied, a_L was calculated to be 1.86 for a 25 ft grid. As a sensitivity study, dispersivity values of aL = 1.86, aT = 0.186, and aV = 0.0186 were input to the model and the 10-year natural attenuation simulation repeated.

PWGC measured plume migration distances and calculated plume velocities for each run. When the results of the two simulations were compared, no significant differences were identified. Plume velocity was calculated to be 0.985 ft/day with D=12.5 and 0.987 ft/day with D=1.86.

Conclusion

Fate and transport modeling was conducting on the EDB North Street East plume to predict the amount of time needed to reach drinking water standards under four potential remediation scenarios: natural attenuation, capturing and extracting the contaminated groundwater through a new, strategically located well (EDB-EW-1), capturing and extracting the contaminated groundwater using two new strategically located wells (EDB-EW-1 & EDB-EW-2), and by extracting the contaminated groundwater through existing well NSE-1.

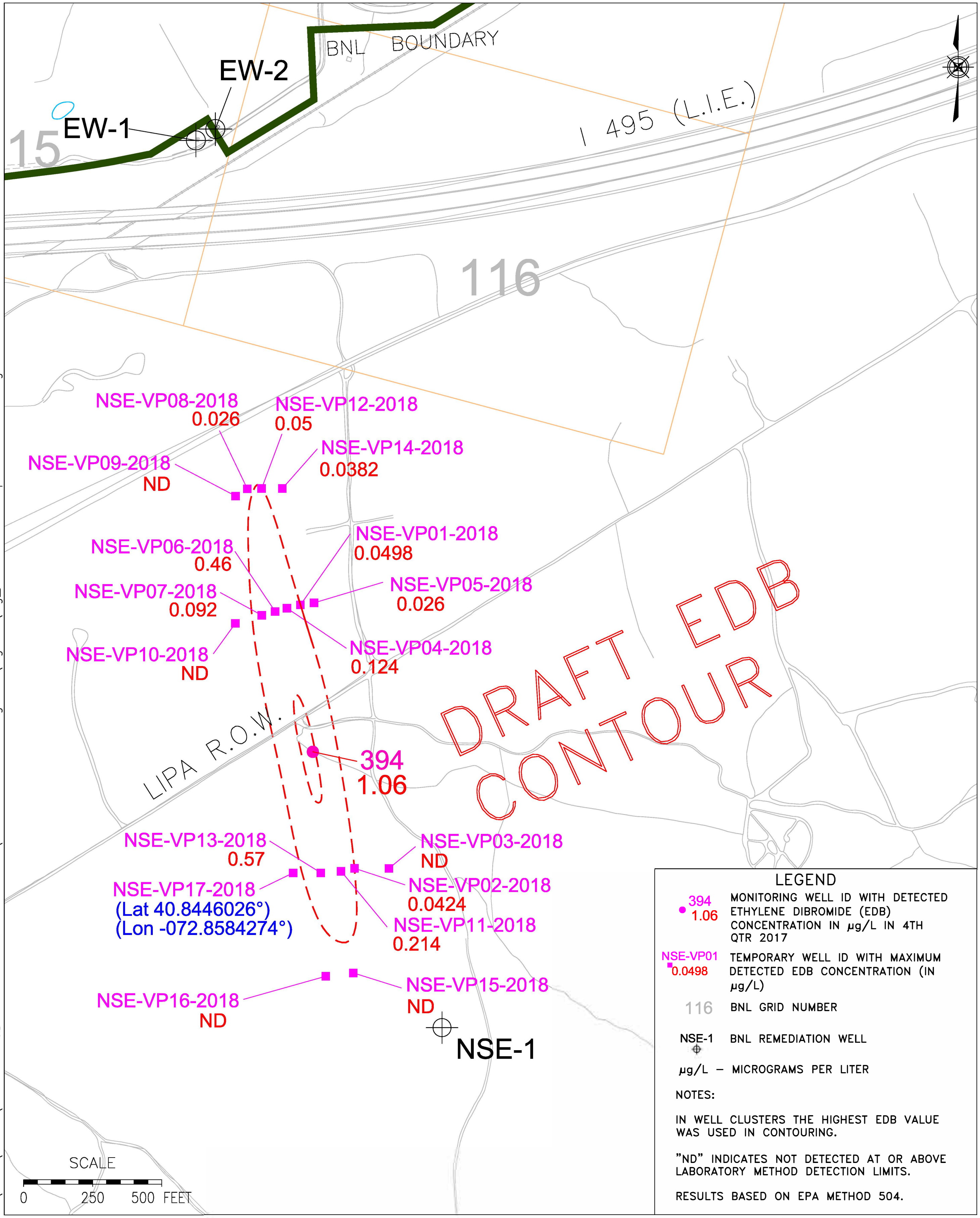
PWGC converted the regional BNL groundwater model to a local model centered around the current extents of the EDB NSE plume (based on August-September 2018 data provided by the GPG. The lateral, vertical and concentration parameters of the plume were simulated in Groundwater Vistas. Various scenarios were run to simulate four possible options being considered to remediate the EDB plume to concentrations below the drinking water standard of 0.05 µg/L and estimate the time needed to reach this goal.

The following is a summary of the various modeling scenario results:

Scenario	Time to Reach Drinking Water Standard
1) Natural Attenuation (Advection, Dispersion, Chemical Reaction; no groundwater extraction)	>30 years (beyond 2048)

Scenario	Time to Reach Drinking Water Standard
2) Groundwater Extraction from a new, strategically placed well, EDB-EW-1. (Advection, Dispersion, Chemical Reaction; proposed well EDB-EW-1 pumping continuously at 100 gpm)	~7 to 7.1 years (~2025)
3) Groundwater Extraction from two new, strategically placed wells, EDB-EW-1 & EDB-EW-2. (Advection, Dispersion, Chemical Reaction; proposed wells EDB-EW-1 and EDB-EW-2 each pumping continuously at 100 gpm)	~4 years (~2022)
4) Groundwater Extraction from existing well NSE-1 (Advection, Dispersion, Chemical Reaction; NSE-1 pumping continuously at 200 gpm)	Capture not achieved

Based on the modeling results, groundwater cleanup goals for EDB are predicted to be achieved by both scenarios 2 and 3. The modeling results for scenario 1, natural attenuation of the EDB plume, predicts that attenuation may extend beyond 30 years and thereby not reach the 2030 cleanup goal. The modeling results for scenario 4 predicts that pumping only NSE-1 will not achieve complete capture of the EDB plume and therefore not meet cleanup goals either. Scenario 2, installation and pumping of one well, is predicted to meet groundwater cleanup goals in approximately 7 years. Scenario 3, installing one new well at the leading edge of the current EDB NSE plume (EDB-EW-1) and a second new well within the plume core (EDB-EW-2) appears to be the most efficient option for EDB remediation, with groundwater cleanup goals predicted to be achieved in 4 years.



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BROOKHAVEN NATIONAL LABORATORY

ENVIRONMENTAL PROTECTION DIVISION

TITLE:

OU III NORTH STREET EAST VP LOCATIONS AND EDB SAMPLE RESULTS

2017 – 2018 NSE INVESTIGATION

DWN:	VT: HZ.:	DATE:	PROJECT NO.:
AJZ	–	06/15/18	–
CHKD:	APPD:	REV.:	NOTES:
JEB	WRD	08/30/18	–

FIGURE NO.: 1

LEGEND

Upper Glacial aquifer
- UG Upper Glacial Sands
- UC Upper Glacial Silts & Clays
- UU Upton Unit

Gardiners Clay
- GL Gardiners Clay
- GS Gardiners Clay – Silt

Magothy aquifer
- MA Magothy Sands and Clay
- MB Magothy Brown Clay
- MC Magothy Clays (undifferentiated)
- MO Magothy – OTHER

000–394 BNL Well ID

ND Indicates not detected at or above laboratory method detection limits

NS Indicates not sampled

.061 Ethylene dibromide (EDB) Concentration (µg/L)

0.05 EDB Contour (µg/L) (Dashed Where Inferred)

Monitoring Well IDs are stacked in order of the depth of the well from shallow to deep

000–???
000–???

µg/L – Micrograms Per Liter

Water Table As Of Nov. 27 – Dec. 1, 2017

Monitoring Well Screen

Extraction Well Screen

NOTES:

1) GEOLOGIC INFORMATION SHOWN IS BASED ON ADDITIONAL EXPLORATIONS (e.g., HYDROPUNCHES, GEOPROBES, VERTICAL PROFILES, AND/OR TEST WELLS) DOCUMENTED IN PREVIOUS, MORE DETAILED REPORTS.

2) EDB EXTENT IS BASED ON FOURTH QUARTER 2017 OU VI SAMPLING EVENTS, SUPPLEMENTED WITH TEMPORARY WELL SAMPLES OBTAINED DURING 2018.

3) RESULTS BASED ON EPA METHOD 504.

4) CONTOUR INTERVAL IS AS SHOWN.

HORIZONTAL SCALE

0 500 1000 FEET

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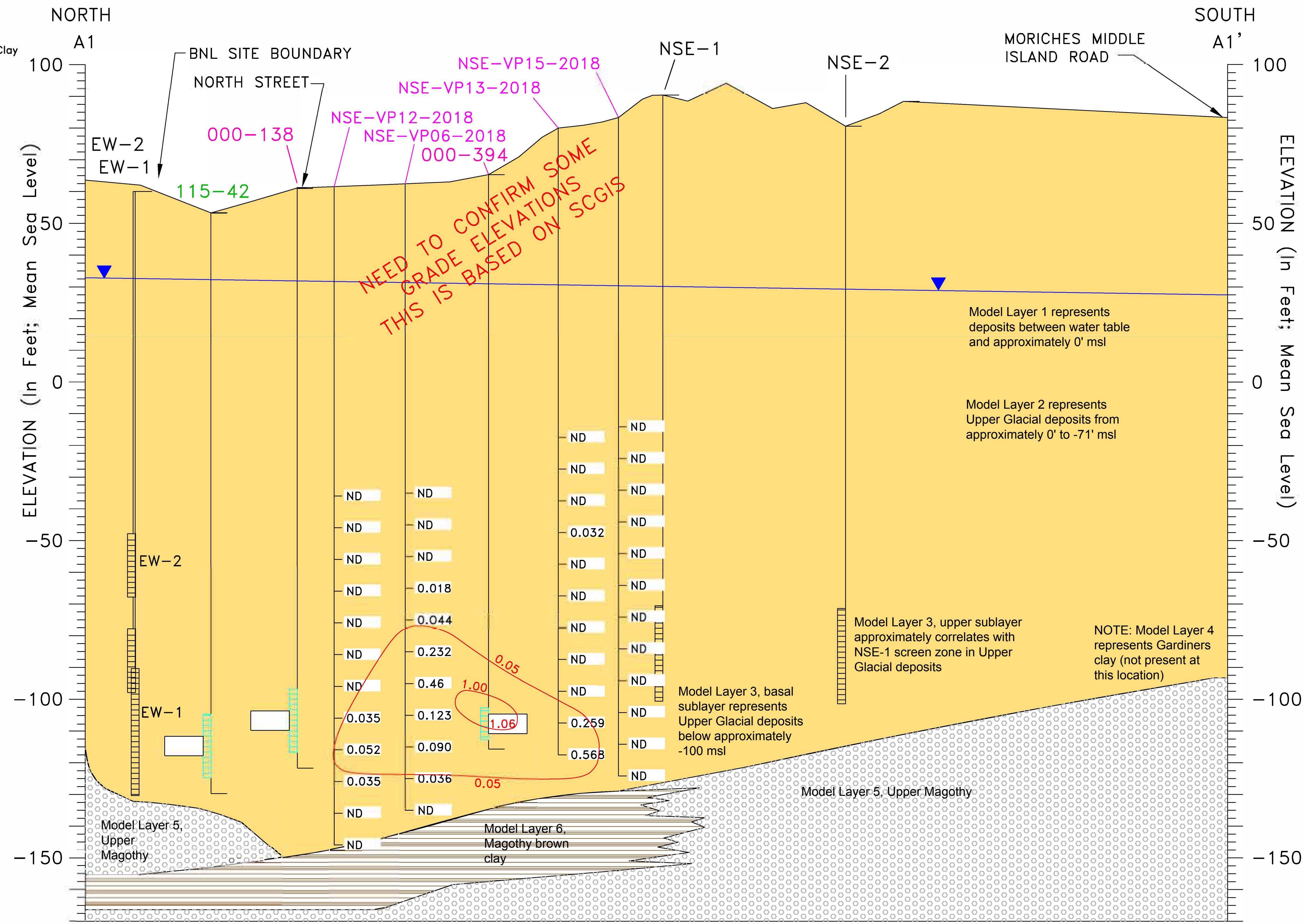

BROOKHAVEN NATIONAL LABORATORY

ENVIRONMENTAL PROTECTION DIVISION

TITLE:

OU III NORTH STREET EAST EDB HYDROGEOLOGIC CROSS SECTION (A1–A1')

2017 – 2018 NSE INVESTIGATION

DWN: AJZ	VT:HZ.: 20:1	DATE: 09/25/18	PROJECT NO.: –
CHKD: JEB	APPD: WRD	REV.: –	NOTES: –
FIGURE NO.: 2			

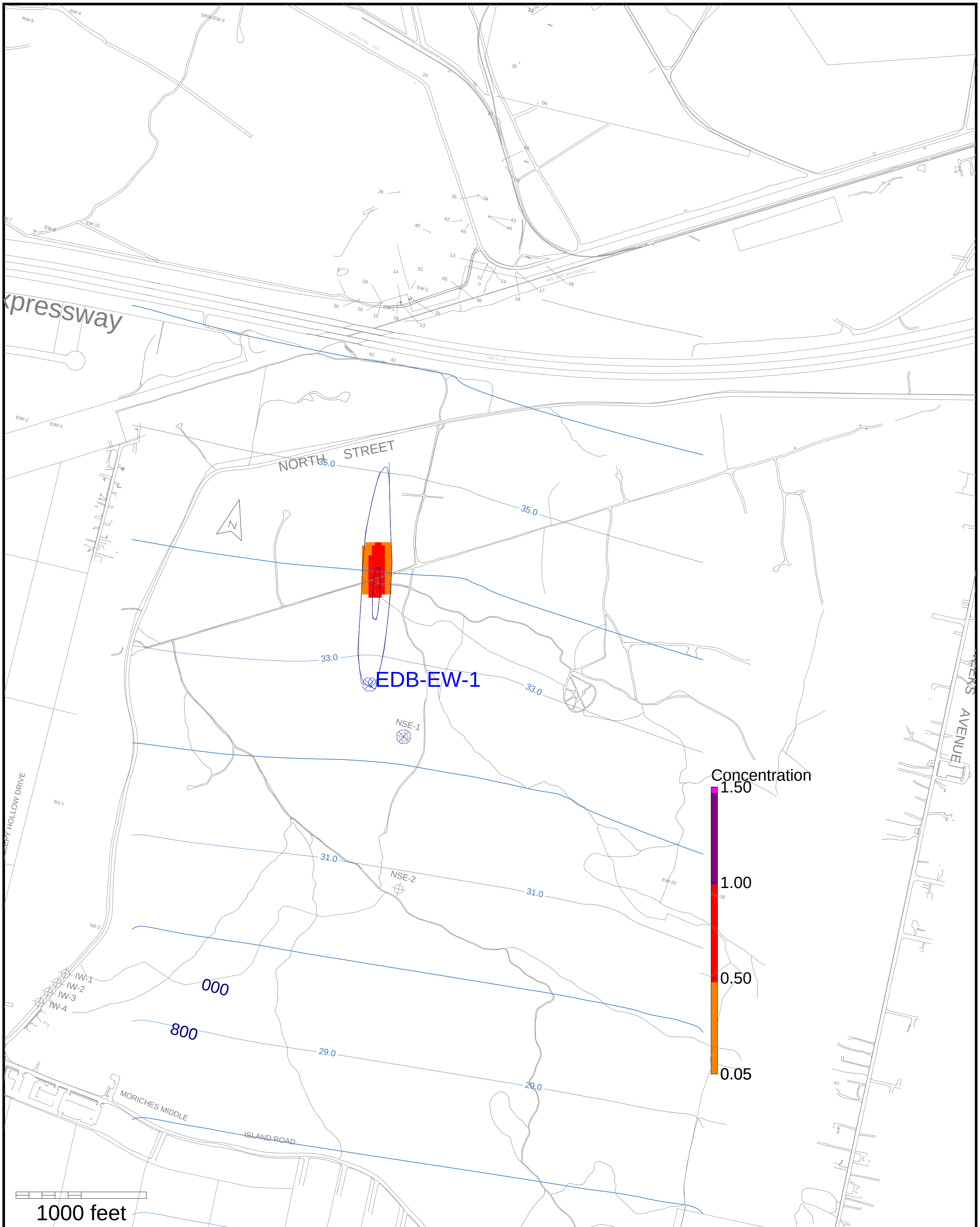

Figure3a

EDB-NSE Initial EDB Concentrations and Groundwater Contours, Layer 3

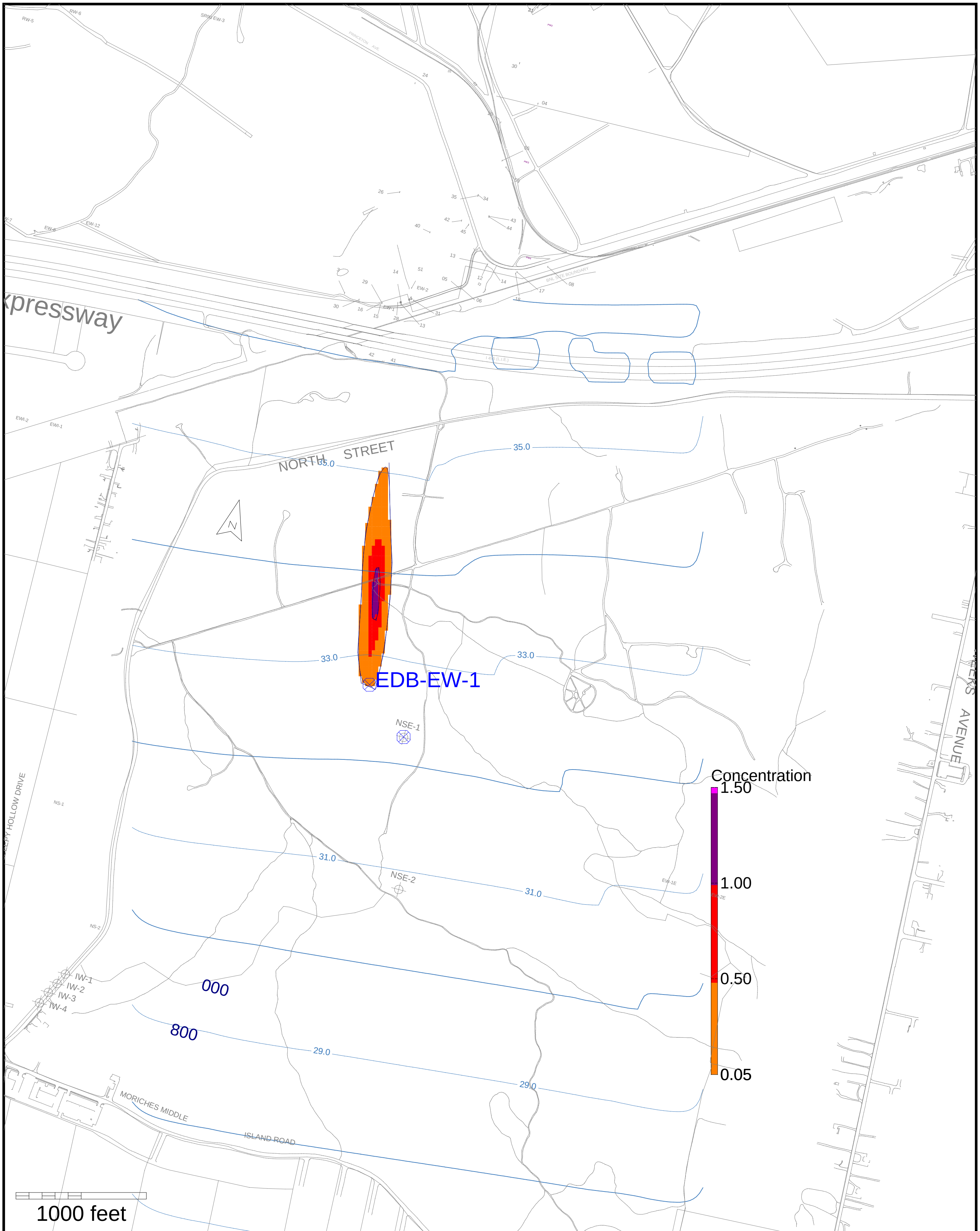

Figure3b

EDB-NSE Initial EDB Concentrations and Groundwater Contours, Layer 3 (basal sublayer)

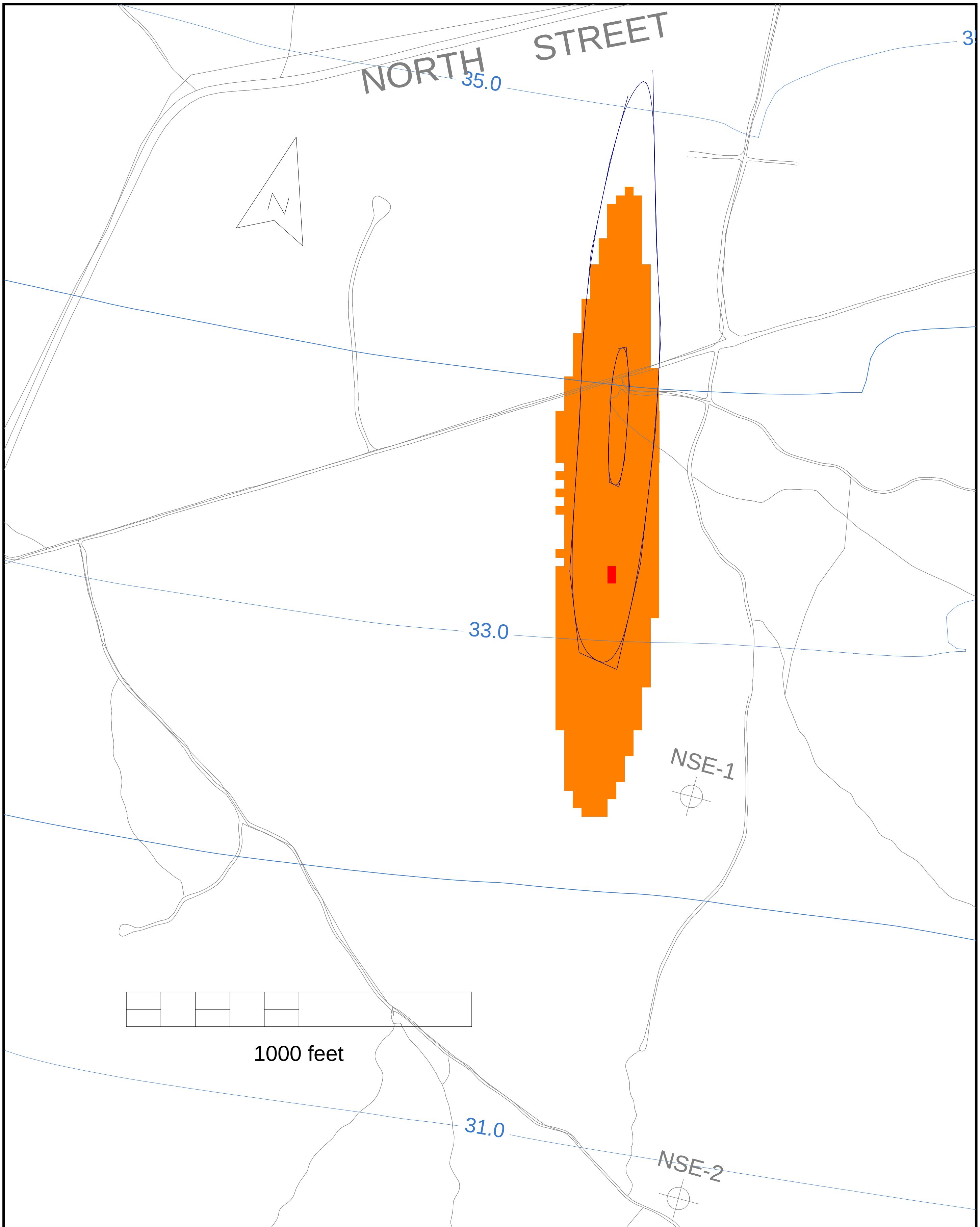

Figure 4a

EDB NSE Natural Attenuation at 1 yr - Layer 3 (basal sublayer)

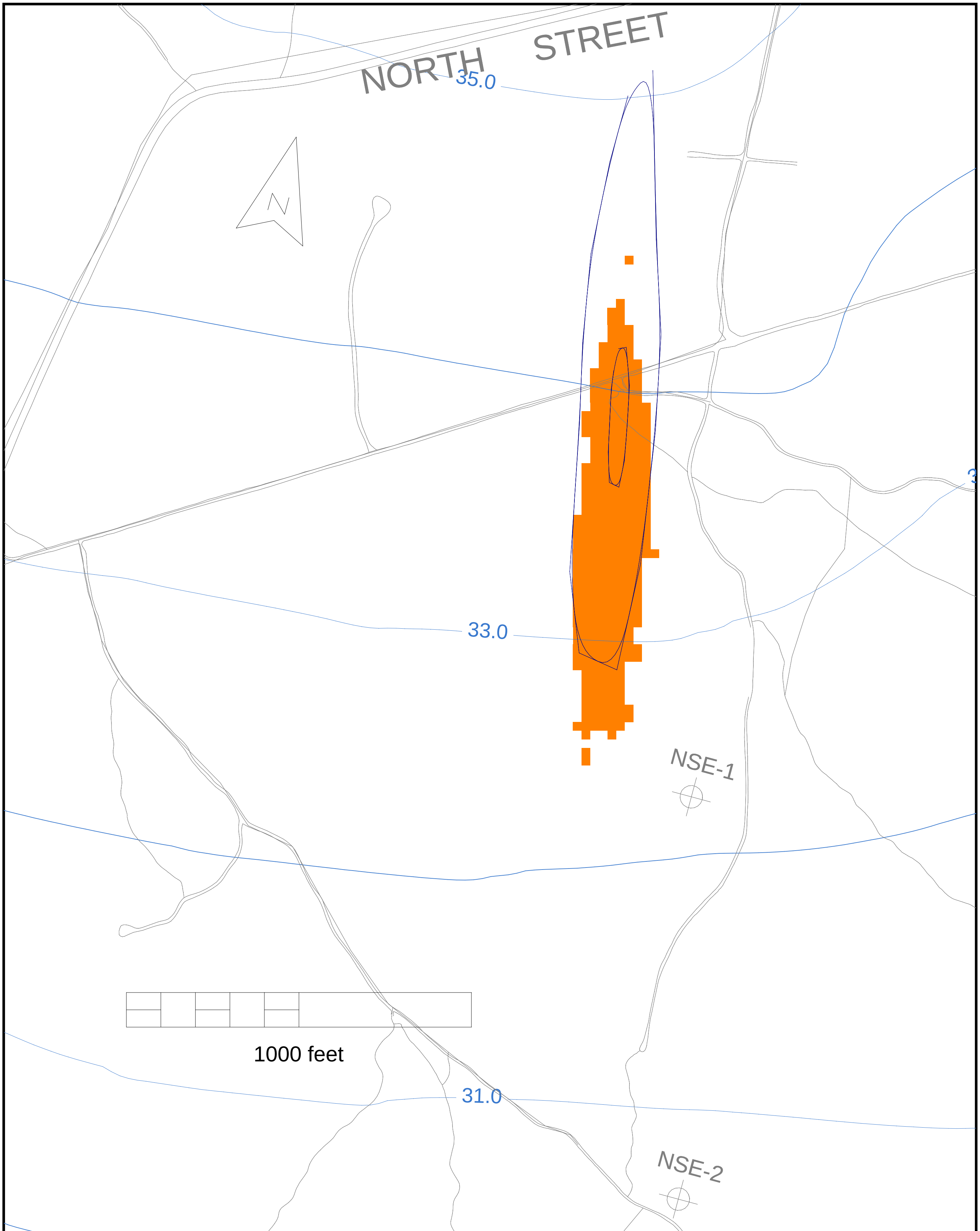

Figure 4b

EDB NSE Natural Attenuation at 1 yr - Layer 5

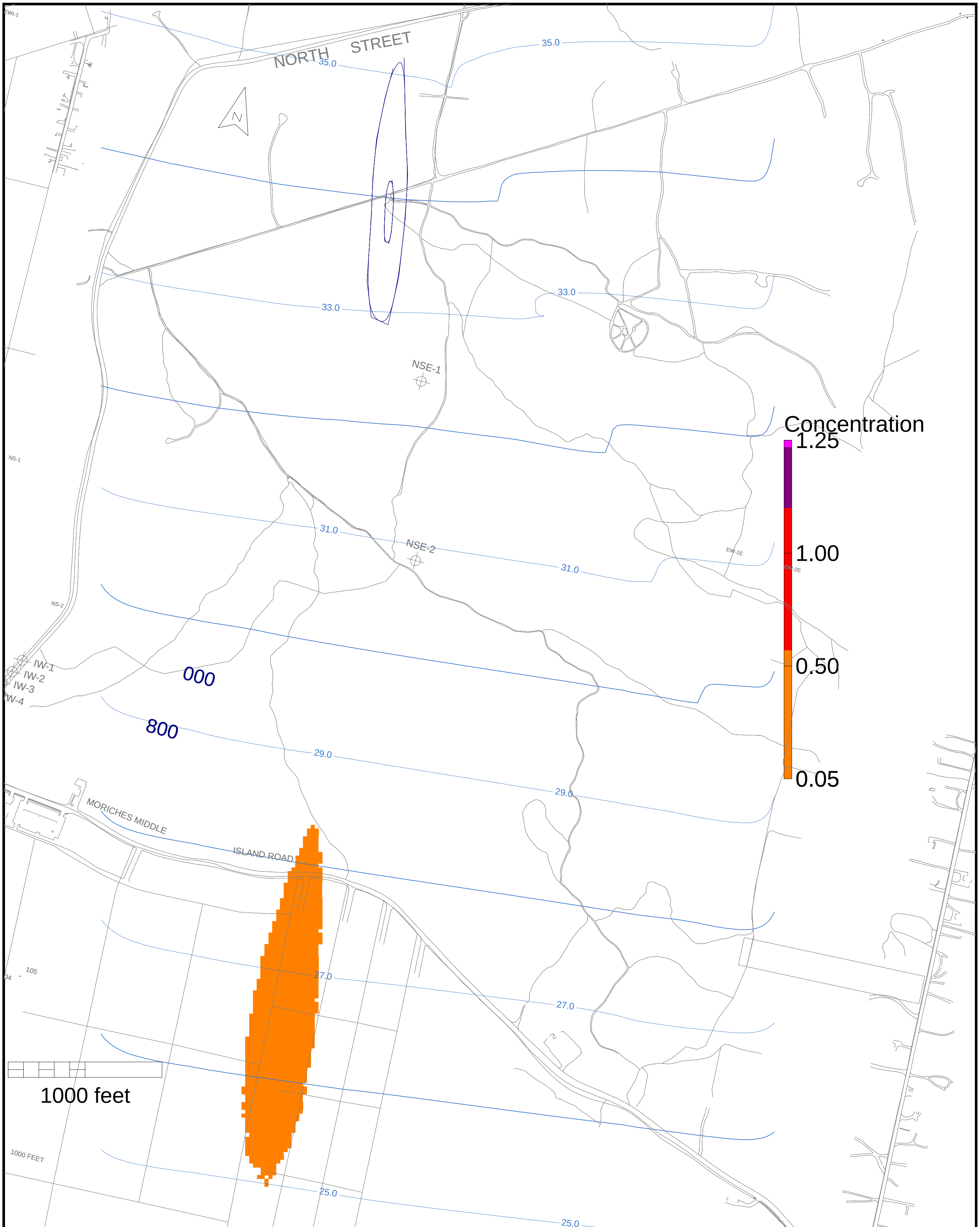

Figure 5a

EDB NSE Natural Attenuation at 15 yrs - Layer 3 (basal sublayer)

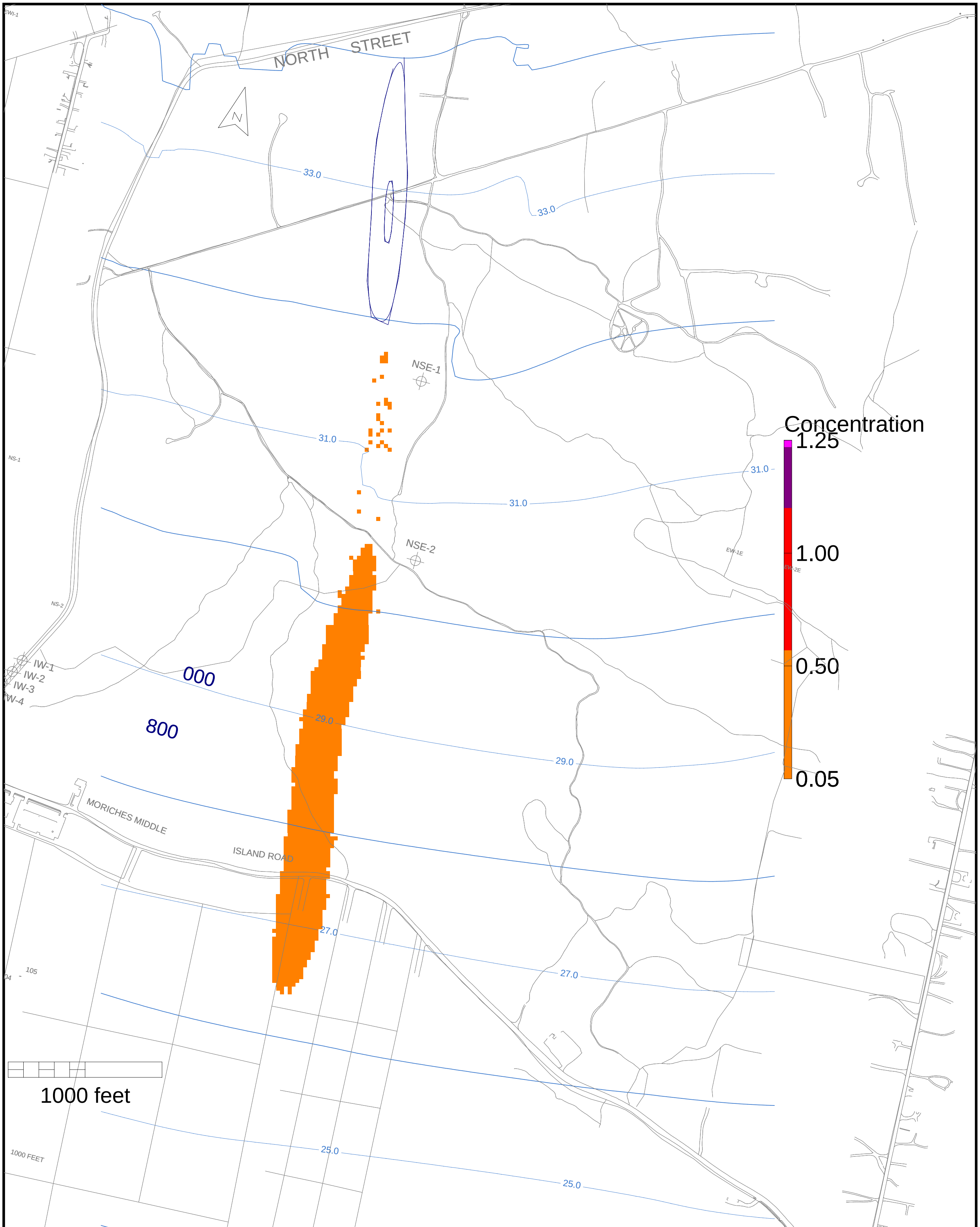

Figure 5b

EDB NSE Natural Attenuation at 15 yrs - Layer 6

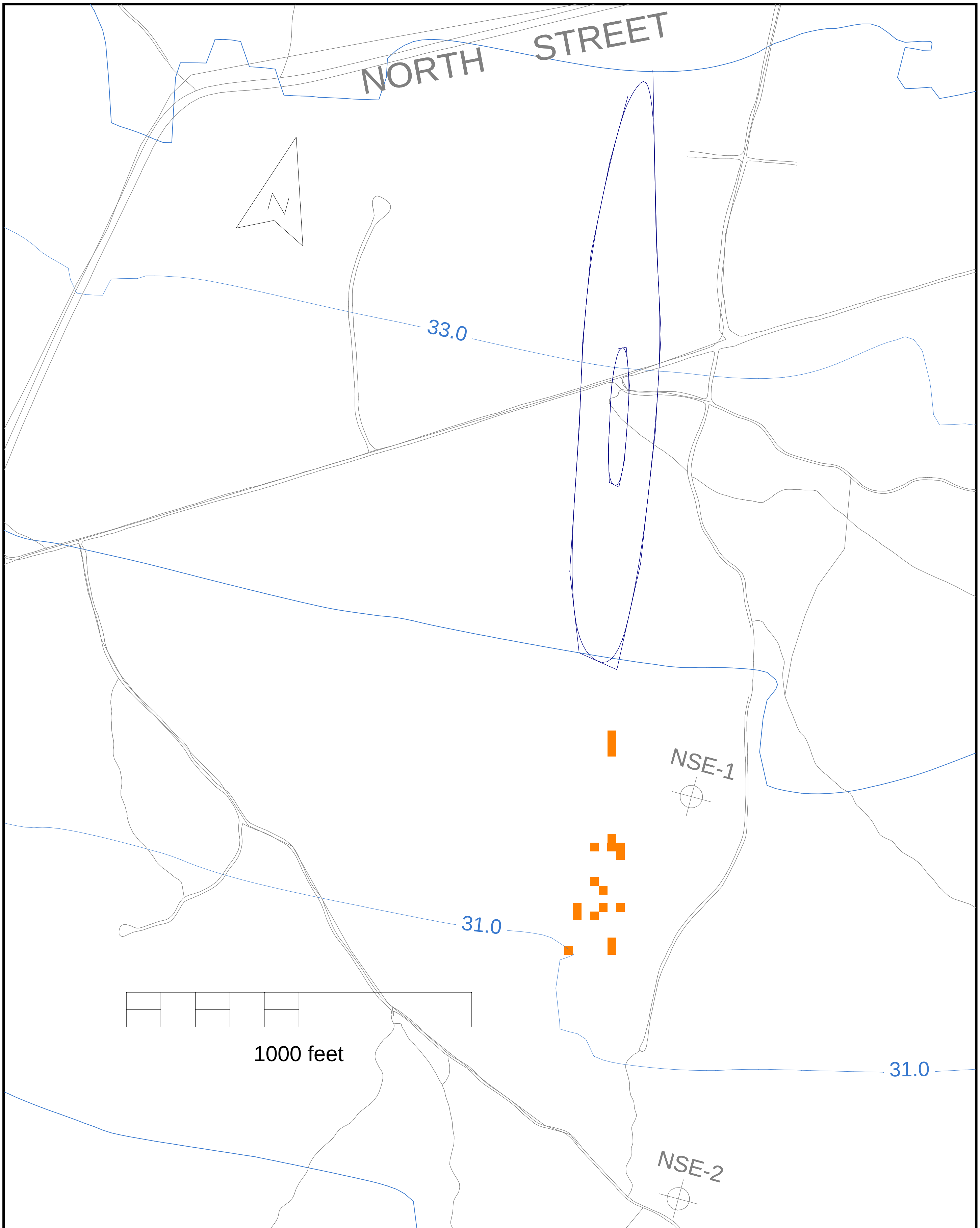

Figure 6

EDB NSE Natural Attenuation at 30 yrs - Layer 6

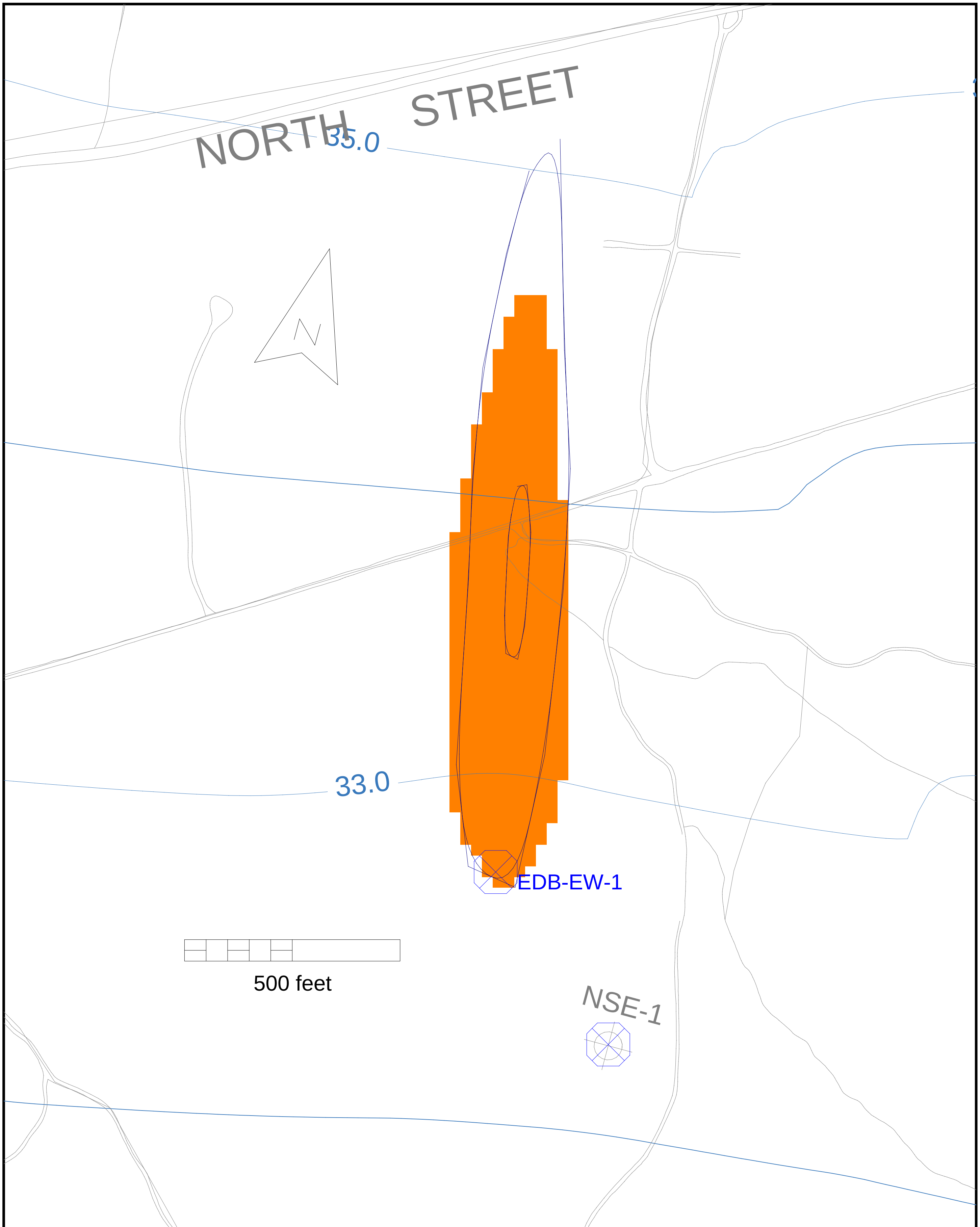

Figure 7a

EDB-NSE Pumping EDB-EW-1 at 100 gpm for 1 yr, Layer 3 (basal sublayer)

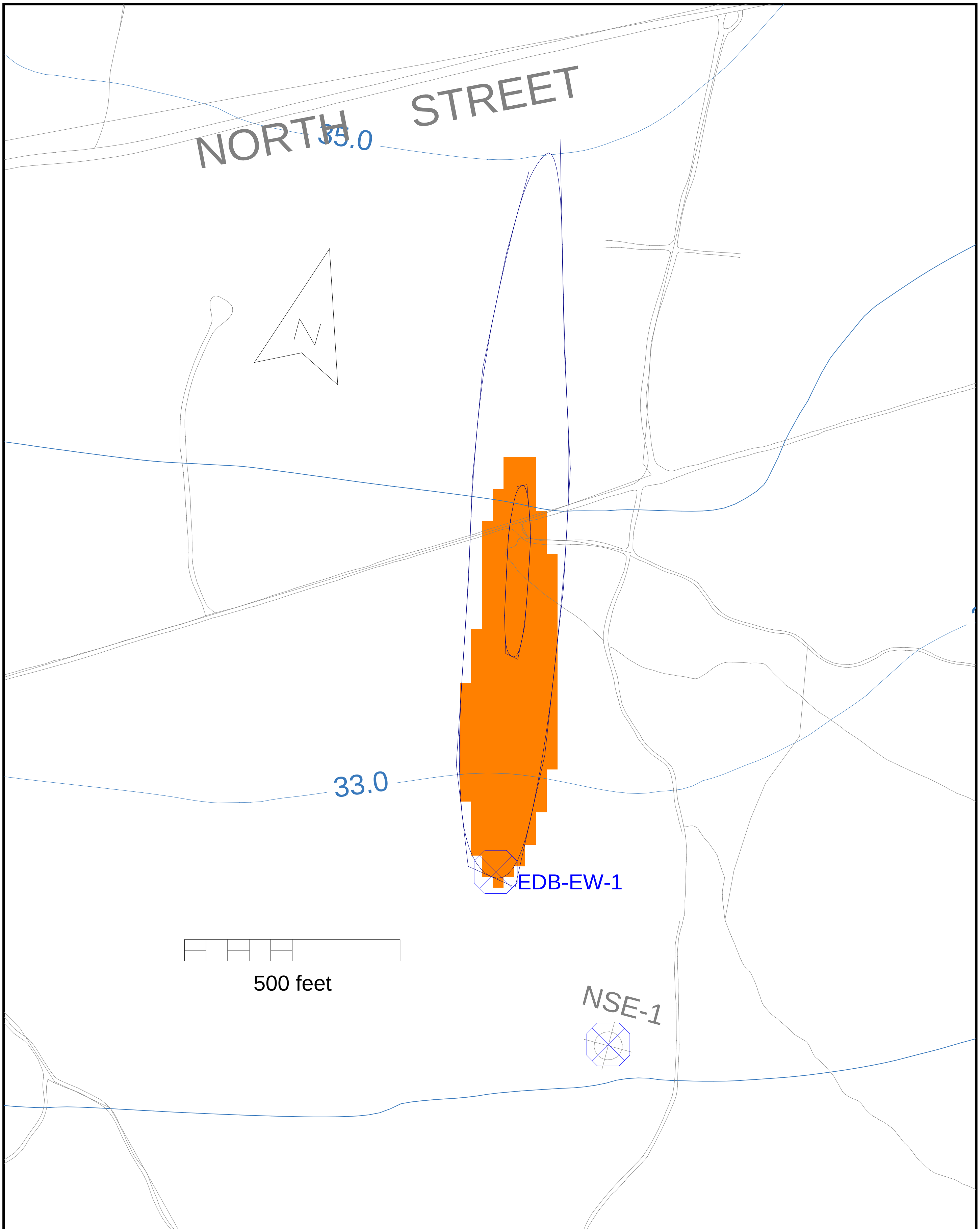

Figure 7b

EDB-NSE Pumping EDB-EW-1 at 100 gpm for 1 yr, Layer 5

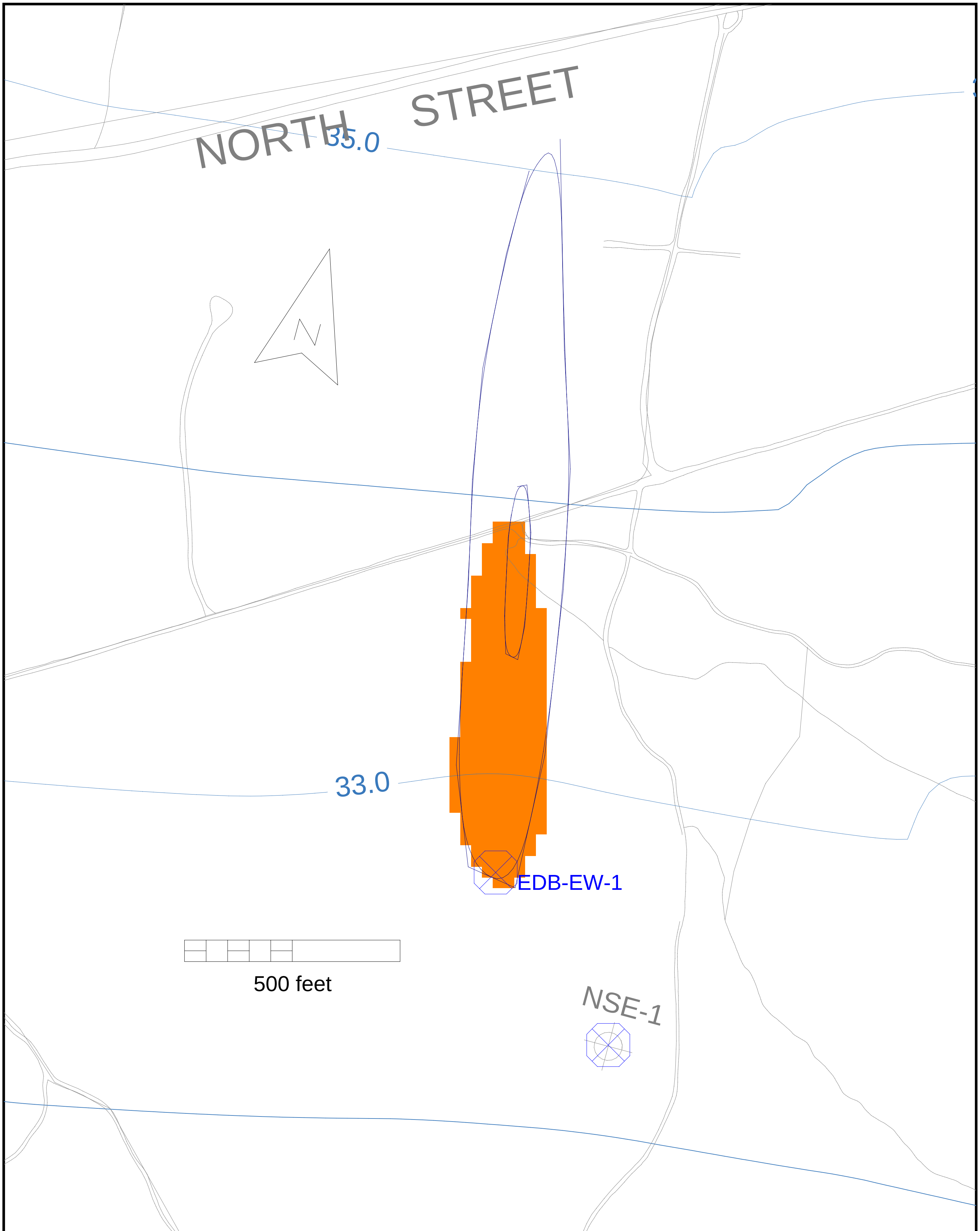

Figure 7c

EDB-NSE Pumping EDB-EW-1 at 100 gpm for 3.5 yrs, Layer 3 (basal sublayer)

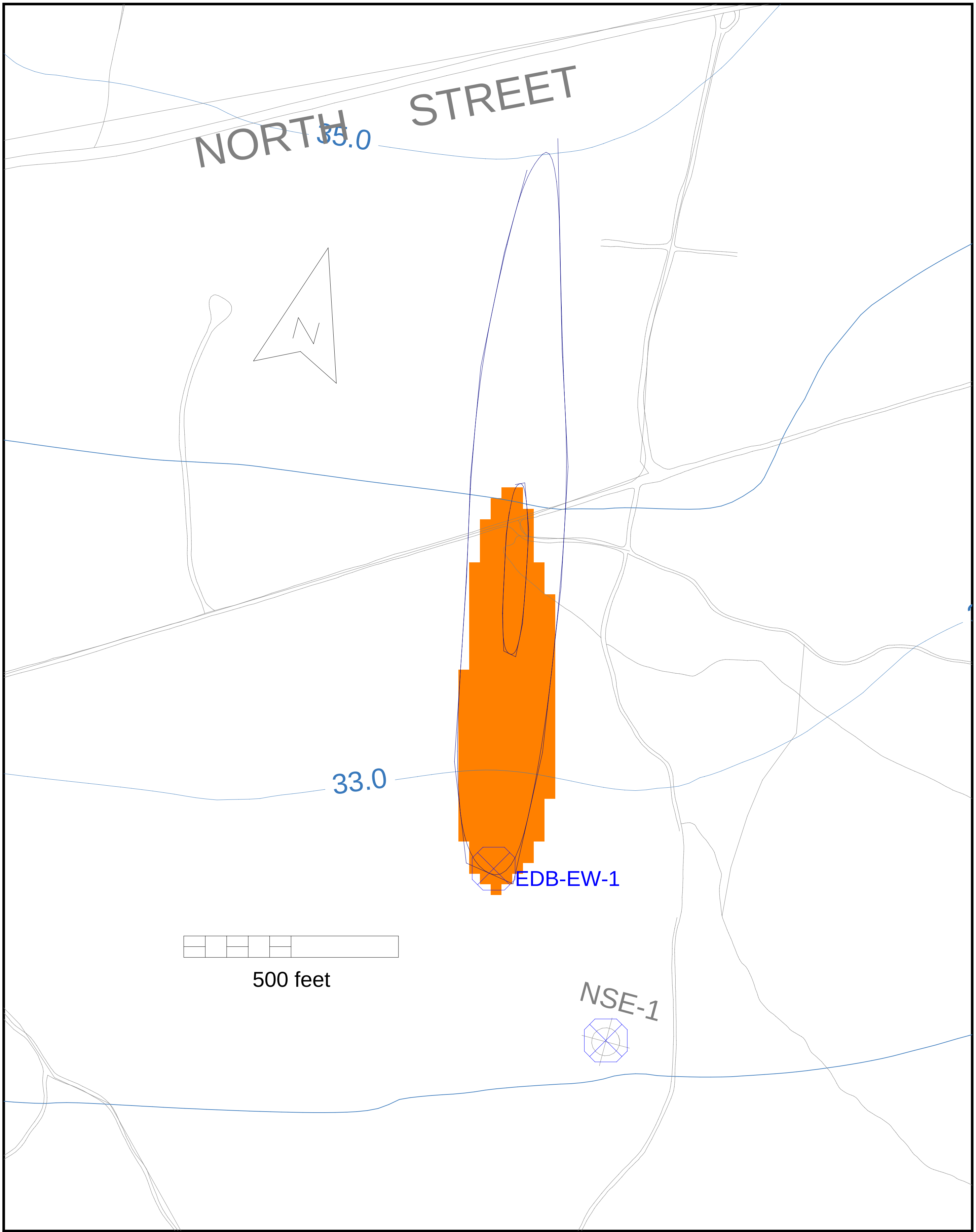

Figure 7d

EDB-NSE Pumping EDB-EW-1 at 100 gpm for 3.5 yrs, Layer 5

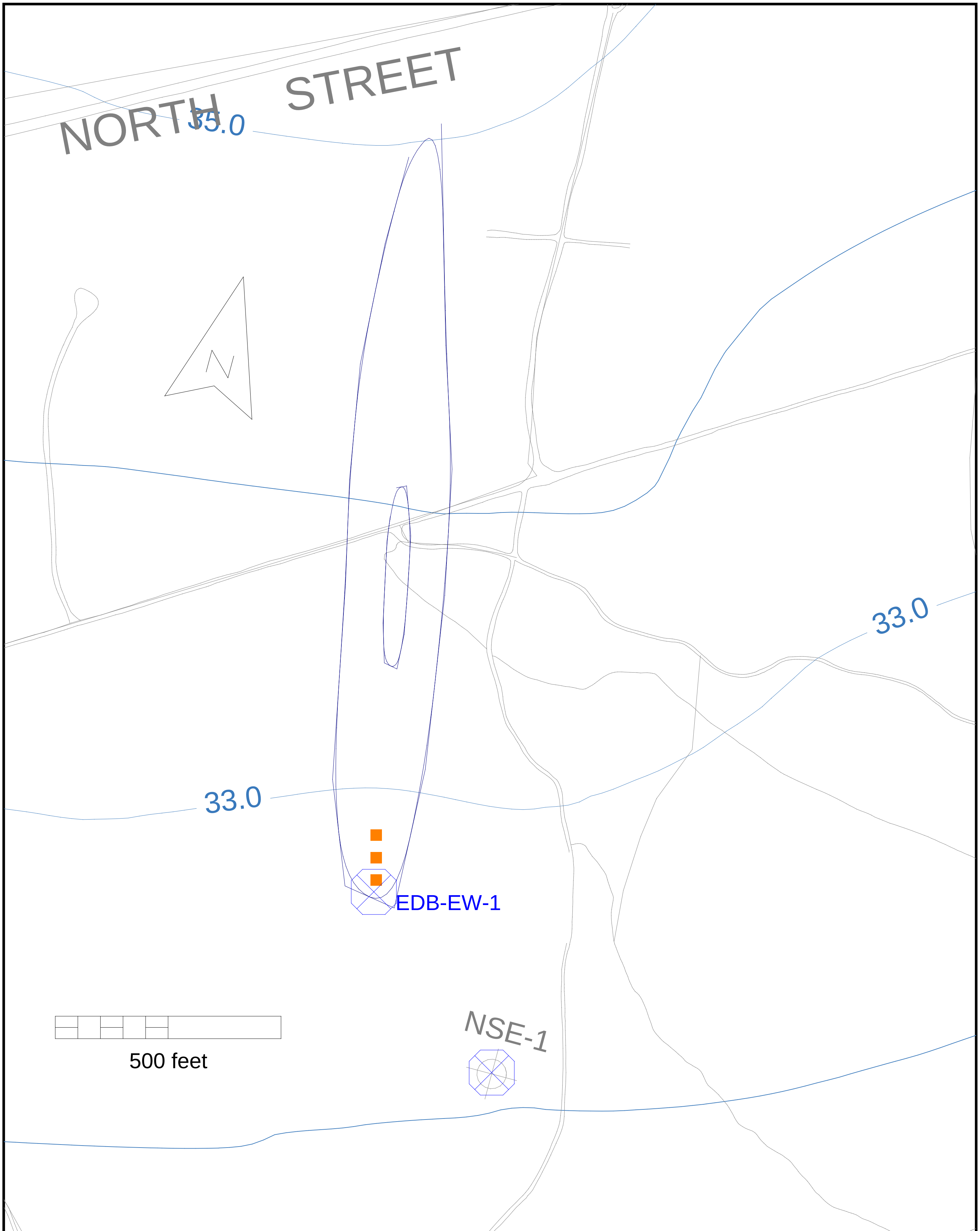

Figure 7e

EDB-NSE Pumping EDB-EW-1 at 100 gpm for 7 yrs, Layer 5

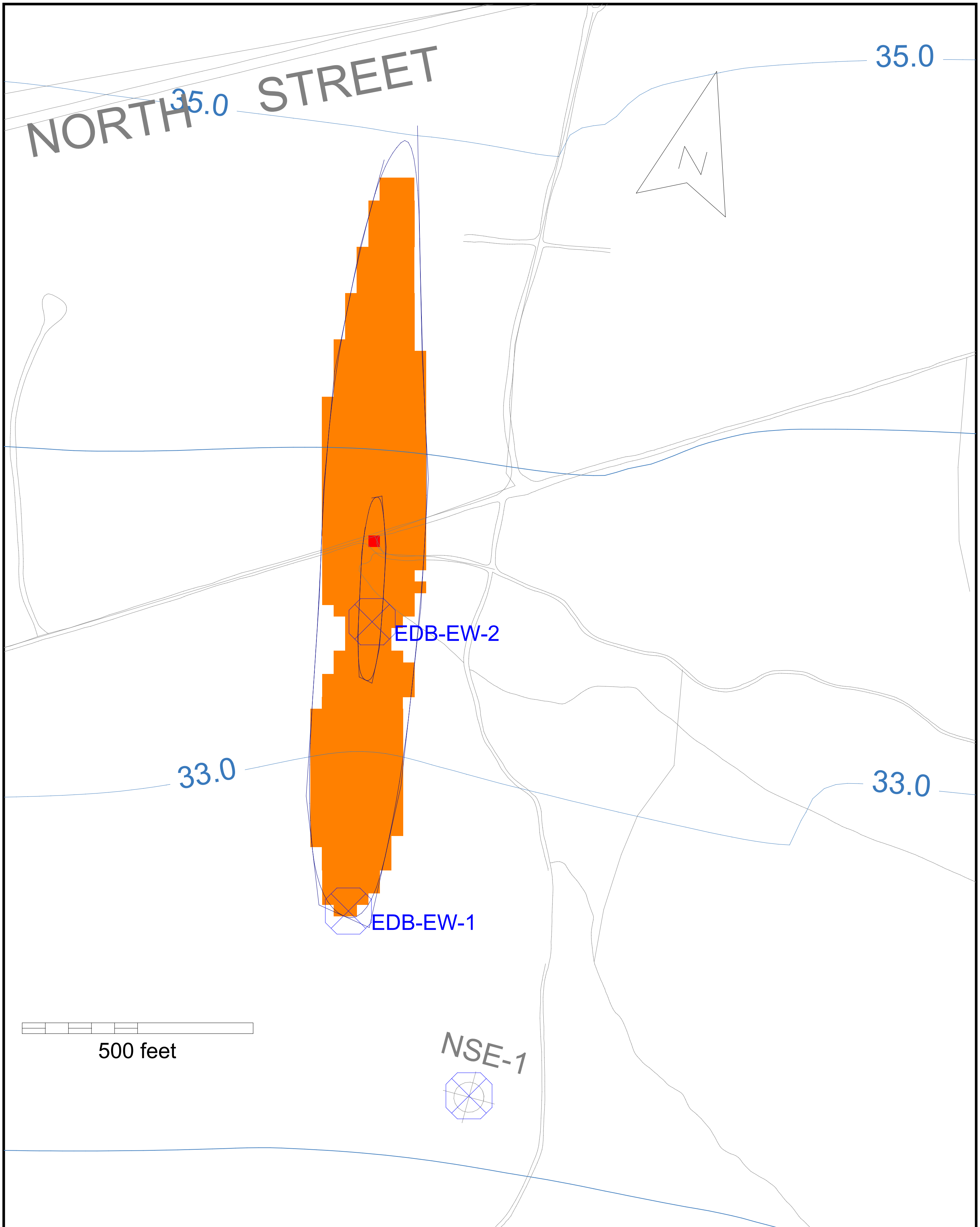

FIGURE 8a

Pumping EDB-EW-1 and EDB-EW-2 at 100 gpm for 91 days Layer 3 (basal sublayer)

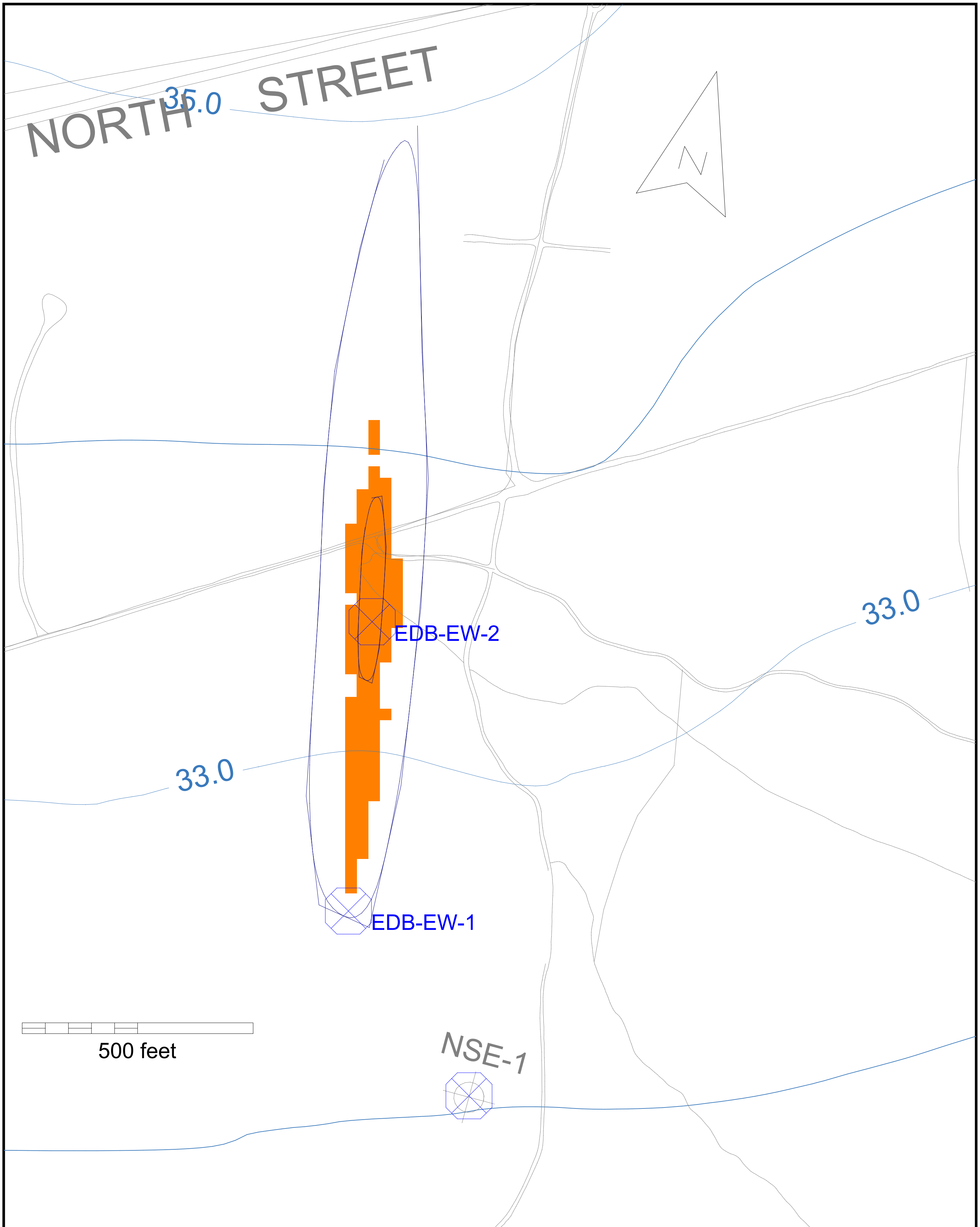

FIGURE 8b

Pumping EDB-EW-1 and EDB-EW-2 at 100 gpm for 91 days Layer 5

FIGURE 8c

Pumping EDB-EW-1 and EDB-EW-2 at 100 gpm for 2 yrs Layer 3 (basal sublayer)

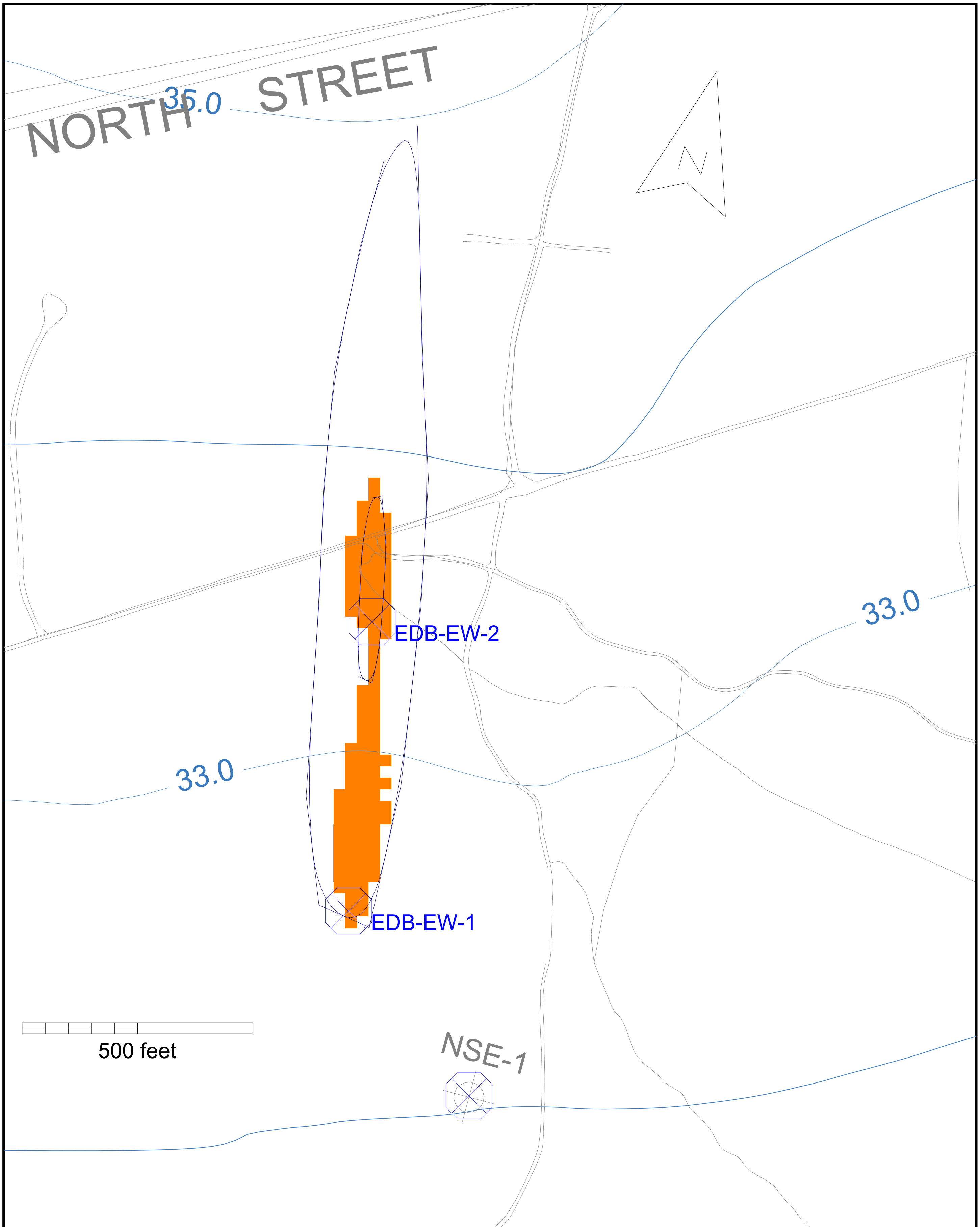

FIGURE 8d
Pumping EDB-EW-1 and EDB-EW-2 at 100 gpm for 2 yrs Layer 5

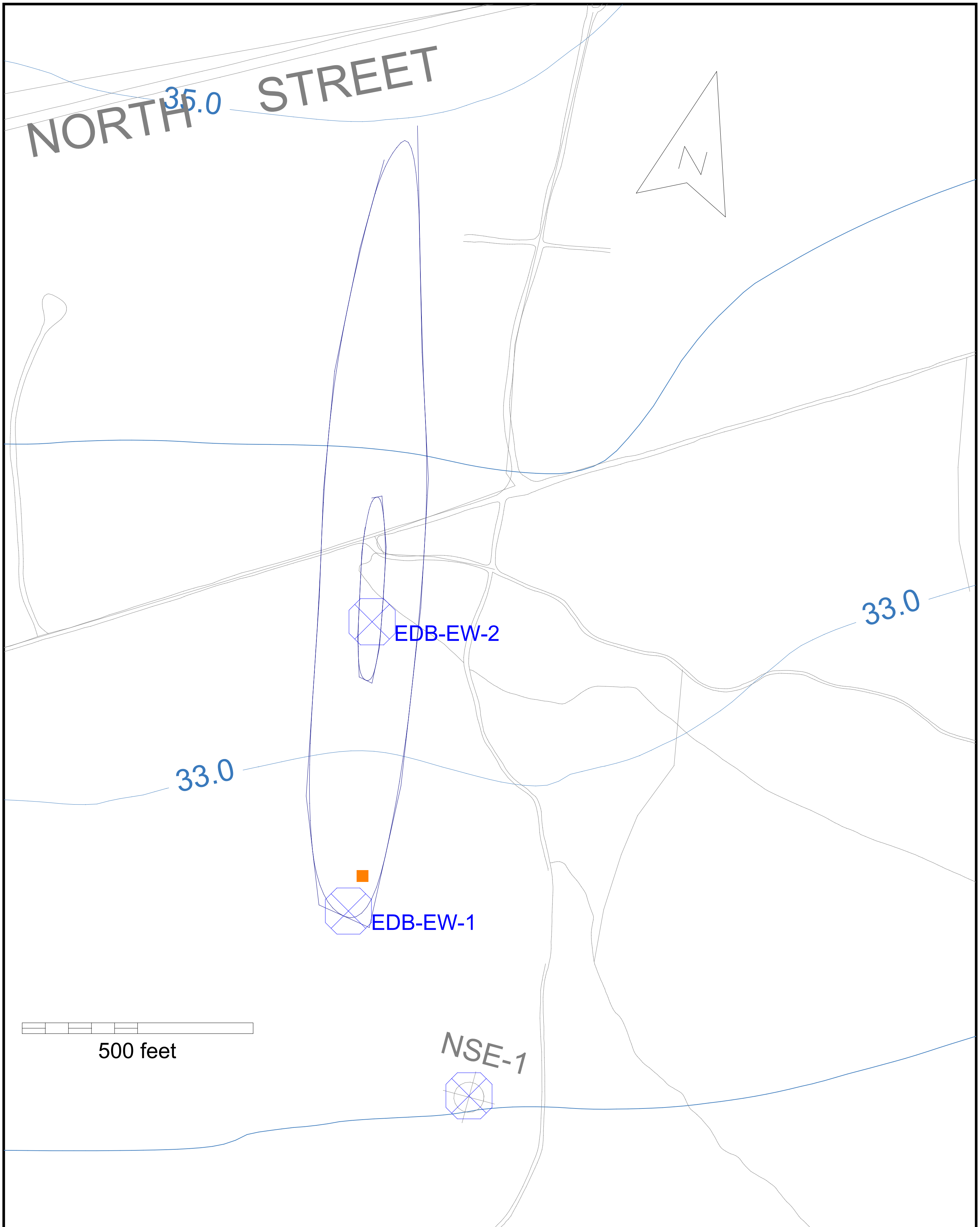

FIGURE 8e
Pumping EDB-EW-1 and EDB-EW-2 at 100 gpm for 4 yrs Layer 5

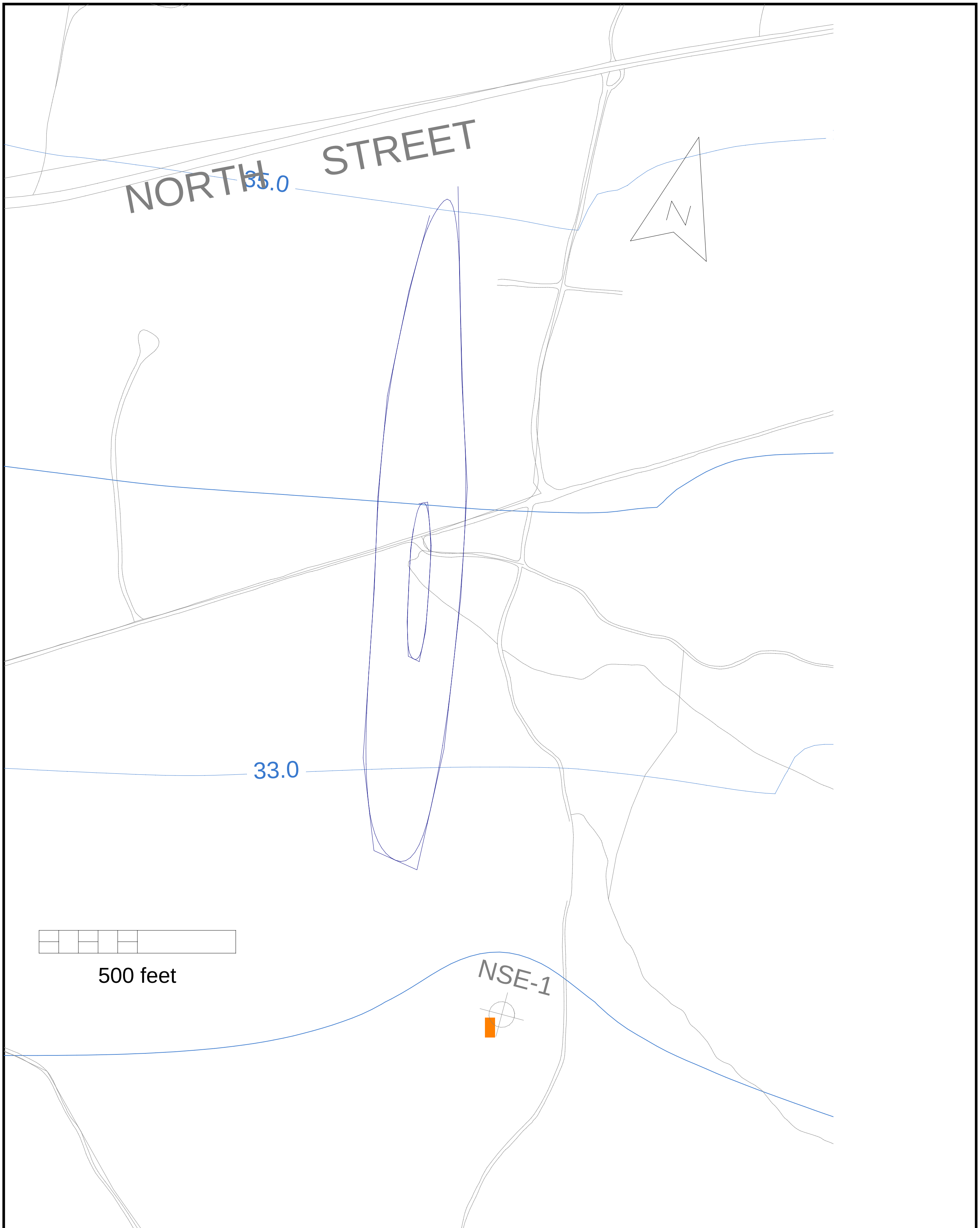

FIGURE 9a

EDB NSE Pumping NSE-1 at 200 gpm for 8 yrs, - Layer 3 (basal sublayer)

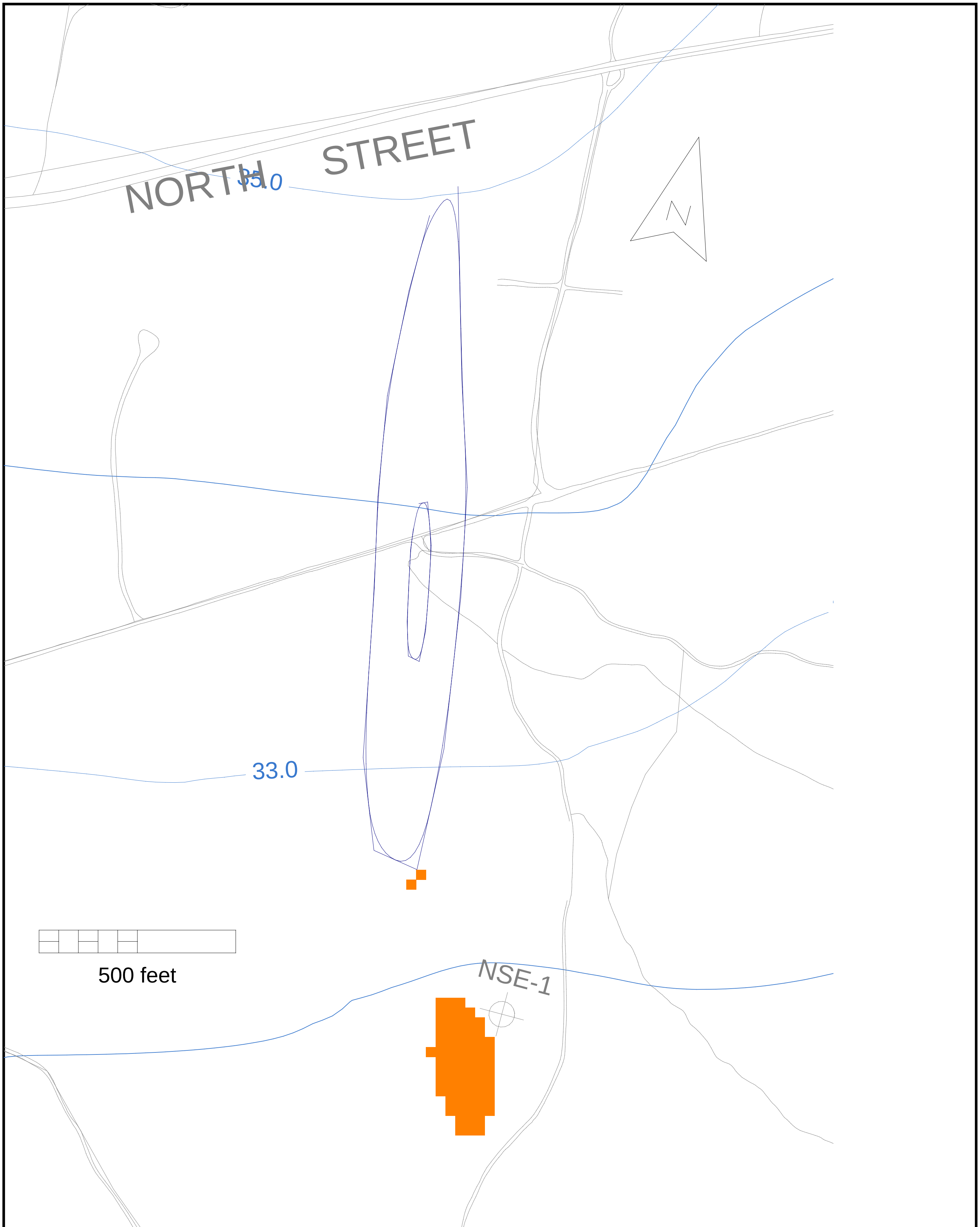

FIGURE 9b

EDB NSE Pumping NSE-1 at 200 gpm for 8 yrs, - Layer 5