APPENDIX H

MODELING

REPORTS

Memo

SUBJECT	TO
BNL SR-90 Transport Evaluation	Bill Dorsch and Vinny Racaniello

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This memo documents the work performed to simulate the transport of Sr-90 in support of BNL's 5 Year Review. This modeling effort updates work previously conducted by PW Grosser (PW Grosser, 2016) and was completed following an update of the BNL Regional Groundwater Flow Model and the development of a new Sr-90 sub-model.

INTRODUCTION

This modeling effort was performed to evaluate the transport of the Sr-90 groundwater plume emanating from the Former Hazardous Waste Management Facility (FHWMF) and determine when Sr-90 concentrations in groundwater were predicted to fall below the 8 picoCuries/Liter (pCi/L) drinking water standard and predict how far the plume would travel before concentrations fell below the drinking water standard.

This work was conducted in support of the Groundwater Protection Group of BNL's Environmental Protection Division. The modeling software Groundwater Vistas (Version 7.24 Build 70), a graphical user interface which serves as a pre- and post-processor for MODFLOW (McDonald, 1988) and MT3D (Zheng, 1999) models, was used to develop the Sr-90 sub-model, update hydraulic parameters and boundary conditions, and delineate the Sr-90 plume. MODFLOW is the U.S. Geological Survey's modular finite-difference flow model and is used to simulate groundwater flow. MT3D is a modular three-dimensional solute transport model for simulating the movement of contaminant plumes in groundwater.

KEY ASSUMPTIONS AND MODEL MODIFICATIONS

The Sr-90 transport simulations described herein were conducted using a purpose-built sub-model, derived from the recently updated regional groundwater flow model.

The following key assumptions were made for this modeling effort:

- Properties and boundary conditions in the sub-model were inherited from the calibrated and updated Regional Groundwater Flow Model. **Figure 1** shows the layers of the sub-model and the associated horizonal hydraulic conductivities assigned to the sub-model layers.
- Aerial extent of sub-model:
  - Approximately 2900 ft in the east-west direction.
  - Approximately 5400 ft in the north-south direction.

- Following extraction of the sub-model, layer 1 was divided into two layers, with each layer having a saturated thickness of approximately 18 ft in the vicinity of the FHWMF.
- There were no changes made to the sub-model which would alter flow directions or rates of flow predicted by the regional flow model. No new or revised pumping or injection was simulated, and no changes were made to recharge rates or boundary flow conditions.
- Groundwater flow and transport were simulated under steady state conditions.

SUB-MODEL DEVELOPMENT

The sub-model was developed using a process called telescopic mesh refinement (TMR), which enables the development of a sub-model from a larger model while preserving the model parameters, structure, and boundary conditions.

TMR is a well-accepted method for developing sub-models or simply refining more regional scale models in an area of interest. Arcadis developed a simple FORTRAN utility which enables the user to easily create a new model that inherits the properties and boundary conditions from the parent or regional model.

TMR was used to extract a portion of the regional groundwater flow model and modify model grid cell sizes and the discretization of what was formerly regional model layer 1.

The sub-model includes all eight layers from the regional groundwater flow model.

Sub-Model DiscretizatIon

Following development of the sub-model, model layer 1 was modified by splitting the layer in two; **see Figure 1**. This was done to enhance the vertical discretization for the purposes of evaluating the vertical movement of the Sr-90 plume. Following this revision, layers 1 and 2 were each 18-ft thick.

In addition, the model grid was modified to reduce model cell sizes from 100 ft by 100 ft in the regional groundwater flow model to 12 ft by 12 ft in the sub-model.

Model grid and boundary conditions are shown on **Figure 2**.

GROUNDWATER FLOW FIELD

Transport of Sr-90 was simulated under steady state groundwater flow conditions; the groundwater flow field was derived from the recently updated BNL Regional Groundwater Flow Model. The extracted sub-model is bounded by constant head cells (**Figure 2**). The potentiometric surface of the water table within the sub-model is shown on **Figure 3** and indicates that groundwater in the vicinity of the Sr-90 plume is flowing to the south-southeast, with water table elevations ranging from about 40 ft above mean sea level (MSL) near the FHWMF, to about 35 ft MSL at the southern extent of the submodel. These water level elevations are identical to the water table elevations predicted by the regional groundwater flow model over the area of the sub-model.

MT3DMS SETUP

Transport simulations were run using the advection and chemical reactions packages, as described below. Based on previous work simulating the transport of Sr-90, advection with radioactive decay and adsorption are the dominant mechanisms affecting plume transport and attenuation. To provide a conservative estimate of Sr-90 transport, dispersion was not simulated.

Advection Package

During this evaluation, two advection solution schemes were used to complete sensitivity analyses related to the initial concentration distribution of Sr-90 and the impact of the solution scheme on model predictions.

- Total Variation Diminishing (TVD) and
- Finite Difference.

The sensitivity analyses are discussed below.

During the predictive transport simulation, the Method of Characteristics (MOC) was applied. The MOC scheme eliminates numerical dispersion. Given that some dispersion of the plume is expected to occur during transport, use of the MOC scheme results in conservative predictions of plume transport and concentration.

Chemical Reaction Package

MT3D uses the chemical reaction package to define the parameters affecting retardation and adsorption of a dissolved solute. The parameters assignments used for this evaluation were consistent with those applied during previous Sr-90 transport simulations and are summarized in **Table 1**.

Table 1. Summary of Transport Parameters

Parameter (units)	Assigned Value
Soil Bulk Density (lbs/ft^3)	100
Partitioning Coefficient (ft^3/lbs)	0.0168
Soil Porosity (dimensionless)	0.24
Sr-90 half-life (years)	28.81
Sr-90 decay rate constant (1/d)	0.0000659

DISCUSSION OF MODEL SIMULATION AND RESULTS

Initial Conditions Assessment and Sensitivity Analysis

This modeling effort utilized an updated Sr-90 plume distribution to predict plume fate and transport. The updated distribution was developed from historic Sr-90 data and data collected during the 2020 OU I South Boundary Investigation (i.e., temporary well sampling conducted in June/July 2020) which was provided to Arcadis by BNL. During the 2020 investigation, a peak Sr-90 concentration of 689 pCi/L was reported for temporary well GP-40. This concentration was significantly higher than the previously mapped peak Sr-90 distribution of 100 pCi/L (4th Quarter 2019) and suggested that Sr-90 plume distributions previously simulated could have under-represented Sr-90. Recognizing this potential uncertainty in the reported peak concentration, and based on the preference of

BNL to conservatively evaluate Sr-90 fate and transport, two sets of initial conditions were evaluated for the predictive simulations:

1. a peak initial concentration of 1,000 pCi/L, and
2. a peak initial concentration of 750 pCi/L.

The two sets of potential Sr-90 initial conditions are shown in the center and right-hand panels of **Figure 4**. The left-hand panel of **Figure 4** shows the extent of the Sr-90 sub-model against a portion of the BNL basemap. Except for the areas of peak concentration (i.e., 750 or 1,000 pCi/L), the areas of the two plumes and the distributions of Sr-90 concentrations within the plumes are identical. Two 40-year long transport simulations were conducted to evaluate the impact of differing peak concentrations on Sr-90 fate and transport. **Figures 5 – 8** show the model-predicted distribution of Sr-90 after 10, 20, 30, and 40 years of transport, respectively, using the Finite Difference (FD) transport solution scheme. The FD solution scheme was used for this evaluation because it solves quickly. For each of the figures, the left-hand panel shows the extent of the sub-model, and the center and right-hand panels show the model-predicted distribution of Sr-90 resulting from initial conditions with peak concentrations of 1,000 pCi/L and 750 pCi/L, respectively. Following is a summary of the assessment of initial conditions:

- 10 years after the start of the simulation, the peak concentrations in the center and right-hand panels are 128 and 120 pCi/L, respectively. The model-predicted overall plume extents and positions of the plumes are identical.
- 20 years after the start of the simulation, the peak concentrations in the center and right-hand panels are 42 and 40 pCi.L, respectively. The model-predicted overall plume extents and positions of the plumes are identical.
- 30 years after the start of the simulation, the peak concentrations in the center and right-hand panels are 16 and 15 pCi/L, respectively. The model-predicted overall plume extents and positions of the plumes are identical.
- 40 years after the start of the simulation, the peak concentrations in the center and right-hand panels are 5.8 and 5.5 pCi/L, below the drinking water standard of 8 pCi/L and are shown with a red border. The model-predicted overall plume extents and positions of the plumes are identical.

This evaluation demonstrated that using initial concentration distributions with similar overall extents and small areas of differing peak concentrations did not significantly affect the model predicted fate and transport of the plume. Following a review of these results with BNL, the initial concentration distribution with a peak concentration of 750 pCi/L was selected as the starting condition for predictive transport simulations.

Solution Scheme Sensitivity

Two additional transport simulations were conducted to evaluate the impact of the applied transport solution scheme on model-predicted fate and transport. Forty year long, steady state transport simulations were conducted using the third-order Total Variation Diminishing (TVD) and FD solution schemes, using the initial conditions distribution with a peak concentration of 750 pCi/L. TVD is a mass conserving solution method which minimizes numerical dispersion and artificial oscillation. The evaluation indicated that the predicted overall extents of the Sr-90 plumes were similar under the two schemes. However, the TVD scheme generally tended to conserve areas of higher concentration and predicted plumes with sharper boundaries than the FD scheme; the FD scheme tended to smear the plume with time. Following is a summary of the differences in peak plume concentration with time:

- 10 years after the start of the simulation, the peak concentrations predicted by TVD and FD were 250 and 120 pCi/L, respectively.
- 20 years after the start of the simulation, the peak concentrations predicted by TVD and FD were 102 and 40 pCi/L, respectively.
- 30 years after the start of the simulation, the peak concentrations predicted by TVD and FD were 44 and 15 pCi/L, respectively.
- 40 years after the start of the simulation, the peak concentrations predicted by TVD and FD were 17 and 8 pCi/L, respectively.

To maintain consistency with previous modeling efforts and ensure that the model-predicted transport results minimized dispersion, the Method of Characteristics (MOC) solution scheme was used for predictive transport simulations. This approach provides conservative results, because while the MOC scheme minimizes dispersion, some dispersion is expected to be naturally occurring.

Modeling of Sr-90 Transport

The MOC transport solution scheme was used to evaluate Sr-90 fate and transport by running a steady-state, 60-year long transport simulation to determine when plume concentrations fell to less than the drinking water standard (8 pCi/L). To provide a conservative analysis of plume travel, dispersion was removed from the analysis. The starting conditions for the simulation were based on historical Sr-90 observations supplemented with recently collected groundwater quality data. Initial conditions for the groundwater simulation are shown on **Figure 9**, and the model-predicted Sr-90 distribution 10, 20, 30, 40, 50, and 60 years after the start of the simulation are shown on **Figures 10, 11, 12, 13, 14, and 15**, respectively.

The initial conditions and model-predicted distributions are presented in three-panel figures showing the Sr-90 distribution in model layer 1 (left-hand panel), model layer 2 (center panel), and model layer 3 (right-hand panel). A discussion of the initial conditions and model-predicted distribution of Sr-90 follows:

Initial Conditions

At the start of the simulation, the Sr-90 groundwater plume is limited to model layer 1 (**Figure 9**), with concentrations ranging from 8 to 750 pCi/L. The Sr-90 concentrations in model layers 2 and 3 are 0 pCi/L, therefore, no contours are shown.

After 10 Years of Transport

The model-predicted distribution of Sr-90 10 years after the start of the simulation is shown on **Figure 10**. In model layer 1, the peak Sr-90 concentration has declined from a starting concentration of 750 pCi/L, to about 340 pCi/L. The model predicts that Sr-90 impacted groundwater will move downward into model layers 2 and 3; 10 years after the start of the simulation, the peak concentrations in these layers are about 131 and 5 pCi/L, respectively.

After 20 Years of Transport

The model-predicted distribution of Sr-90 20 years after the start of the simulation is shown on **Figure 11**. In model layer 1, the peak Sr-90 concentration has declined to about 143 pCi/L. The downward migration of the plume continues, and the peak concentrations in model layer 2 and 3 have increased to about 117 and 12 pCi/L, respectively.

After 30 Years of Transport

The model-predicted distribution of Sr-90 30 years after the start of the simulation is shown on **Figure 12**. In model layer 1, the peak Sr-90 concentration has declined to about 72 pCi/L. Downward migration of the plume continues, and the peak concentrations in model layers 2 and 3 have increased to about 127 and 20 pCi/L, respectively.

After 40 Years of Transport

The model-predicted distribution of Sr-90 40 years after the start of the simulation is shown on **Figure 13**. In model layer 1, the peak Sr-90 concentration has declined to about 31 pCi/L. The peak concentration in model layer 2 declined to about 80 pCi/L, and in model layer 3 the peak Sr-90 concentration is virtually unchanged at about 23 pCi/L.

After 50 Years of Transport

The model-predicted distribution of Sr-90 50 years after the start of the simulation is shown on **Figure 14**. In model layer 1, the peak Sr-90 concentration has declined to about 14 pCi/L. The peak concentration in model layer 2 declined to about 38 pCi/L, and in model layer 3 the peak Sr-90 concentration is virtually unchanged at about 23 pCi/L. In all layers, the plume is nearing the BNL property boundary.

After 60 Years of Transport

The model-predicted distribution of Sr-90 60 years after the start of the simulation is shown on **Figure 15**. The plume has crossed the BNL property boundary. In model layer 1, the peak Sr-90 concentration has declined to about 6 pCi/L (less than the drinking water standard of 8 pCi/L). In model layers 2 and 3 the peak concentrations of the off-site Sr-90 plume are about 23 and 11 pCi/L, respectively.

Table 2 and the accompanying line graph summarize the model-predicted distribution of Sr-90 by model layer. The table and graph indicate a steady decline in Sr-90 concentrations in model layer 1, from a peak starting concentration of 750 pCi/L to about 6 pCi/L after 60 years, as the plume is undergoing radioactive decay and moving downward through the aquifer into model layers 2 and 3.

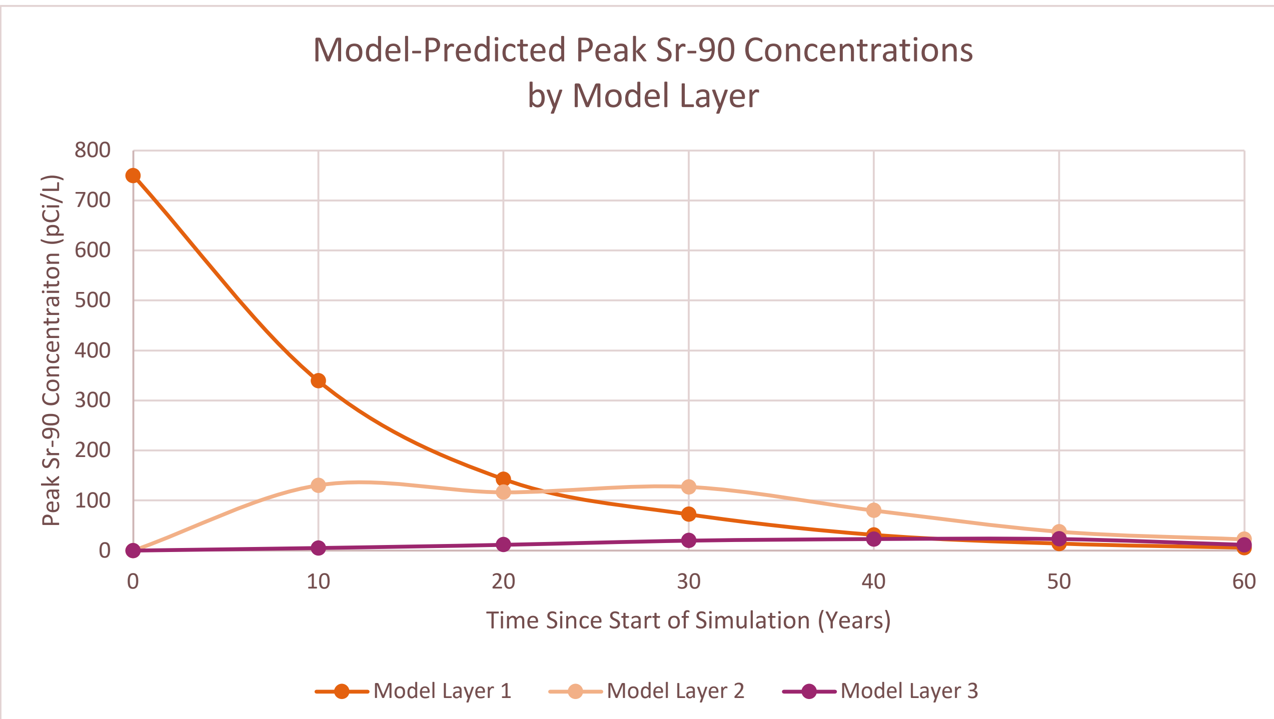
At the start of the simulation, Sr-90 is not present in model layers 2 and 3. Beginning 10 years after the start of the simulation and continuing for another 20 years, the predicted Sr-90 concentration in model layer 2 is maintained at about 130 pCi/L, after which it declines for the remainder of the simulation to about 23 pCi/L after 60 years.

In model layer 3, Sr-90 concentrations increase for the first 30 years of the simulation, then maintains a peak concentration of about 23 pCi/L through year 50 and declines to 11 pCi/L by year 60.

Table 2. Model-Predicted Sr-90 Concentration, Former Hazardous Waste Management Facility, Brookhaven National Laboratory, Upton, NY.

Model	**Transport Simulation Year**						
Layer	**0**	**10**	**20**	**30**	**40**	**50**	**60**
1	750	339	142	73	31	14	6
2	0	131	117	127	80	38	23
3	0	5	12	20	23	23	11

Sr-90 concentrations are presented in pCi/L and rounded to the nearest whole number.



CONCLUSIONS

Based on the shape of the Sr-90 plume and historical plume observations, transport of the Sr-90 plume is believed to be advection dominated and retarded by adsorption and radioactive decay. While it is believed that in a real-world setting dispersion is likely to affect plume transport, dispersion was not included in this analysis so that the transport results would provide a conservative estimate of plume travel and concentration distribution.

Three transport solutions schemes were used to evaluate the fate and transport of Sr-90: TVD, FD and MOC. Although the TVD scheme is considered conservative when compared to the FD scheme, the TVD and FD schemes yielded similar overall predicted plume extents with time. To maintain consistency with previous transport efforts, and to provide a conservative fate and transport estimate, the MOC scheme was applied without dispersion.

Results of the MOC simulation indicate that 60 years after the start of the simulation the Sr-90 plume has crossed the BNL property boundary (i.e., is off site).

- At the water table (i.e., model layer 1), Sr-90 concentrations are less than drinking water standards,
- In middle of the Upper Glacial Aquifer (i.e., model layer 2) the peak Sr-90 concentration is 23 pCi/L, and
- In the lower Upper Glacial Aquifer (i.e., model layer 3) the peak Sr-90 concentration is 11 pCi/L.

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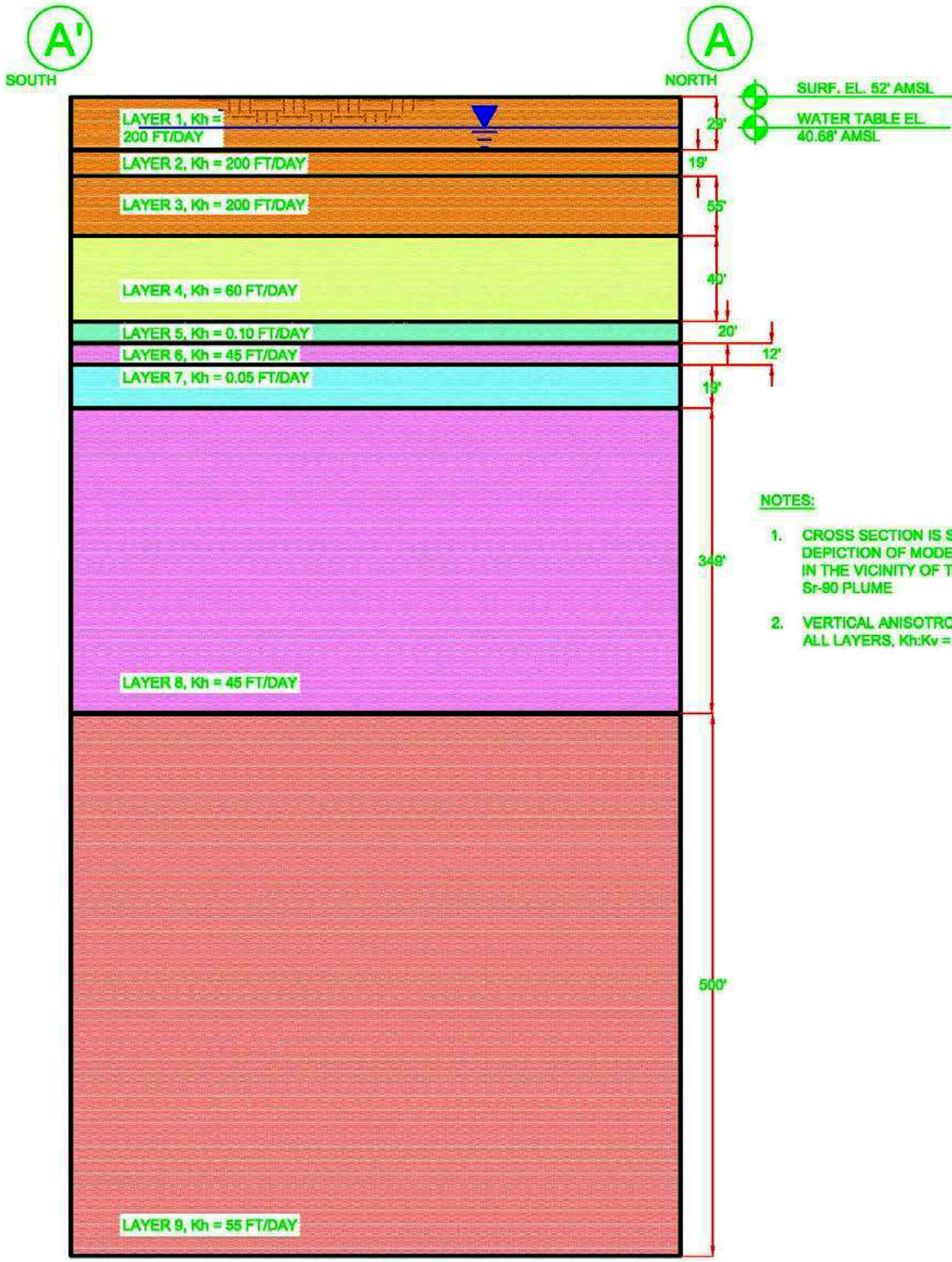
Arcadis, Regional Groundwater Model, Brookhaven National Laboratory, Upton, New York. Prepared for Brookhaven National Laboratory, Associated Universities, Inc. November 1996.

Arcadis, 1999 Regional Groundwater Model Update, Brookhaven National Laboratory, Upton, New York. Prepared for Brookhaven National Laboratory, Brookhaven Science Associates. July 30, 1999

P.W. Grosser Consulting, Groundwater Modeling Report, Former Hazardous Waste Management Facility (FHWMF) Groundwater Modeling, Fate and Transport of Sr-90 Plume – Rev 04. June 3, 2016.

McDonald, Michael G. and Arlen W. Harbaugh. 1988. A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model. Techniques of Water-Resources Investigations of the United States Geological Survey, Chapter A1.

Zheng, C. and Wang, P.P. 1999. MT3D a Modular Three-Dimensional Multispecies Transport Model. Strategic Environmental Research and Development Program. US Army Corps of Engineers. November 1999.



NOTES:

1. CROSS SECTION IS SCHEMATIC DEPICTION OF MODEL LAYERS IN THE VICINITY OF THE FHWMF Sr-90 PLUME
2. VERTICAL ANISOTROPY IS 10 IN ALL LAYERS, Kh:Kv = 10:1

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CROSS-SECTIONAL VIEW OF MODEL

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FIGURE 1

SCALE IN FEET

0 1000 2000

CONSTANT HEAD BOUNDARY

SUB-MODEL GRID
CELLS ARE 12 FT X 12 FT

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SUB-MODEL GRID AND
BOUNDARY CONDITIONS

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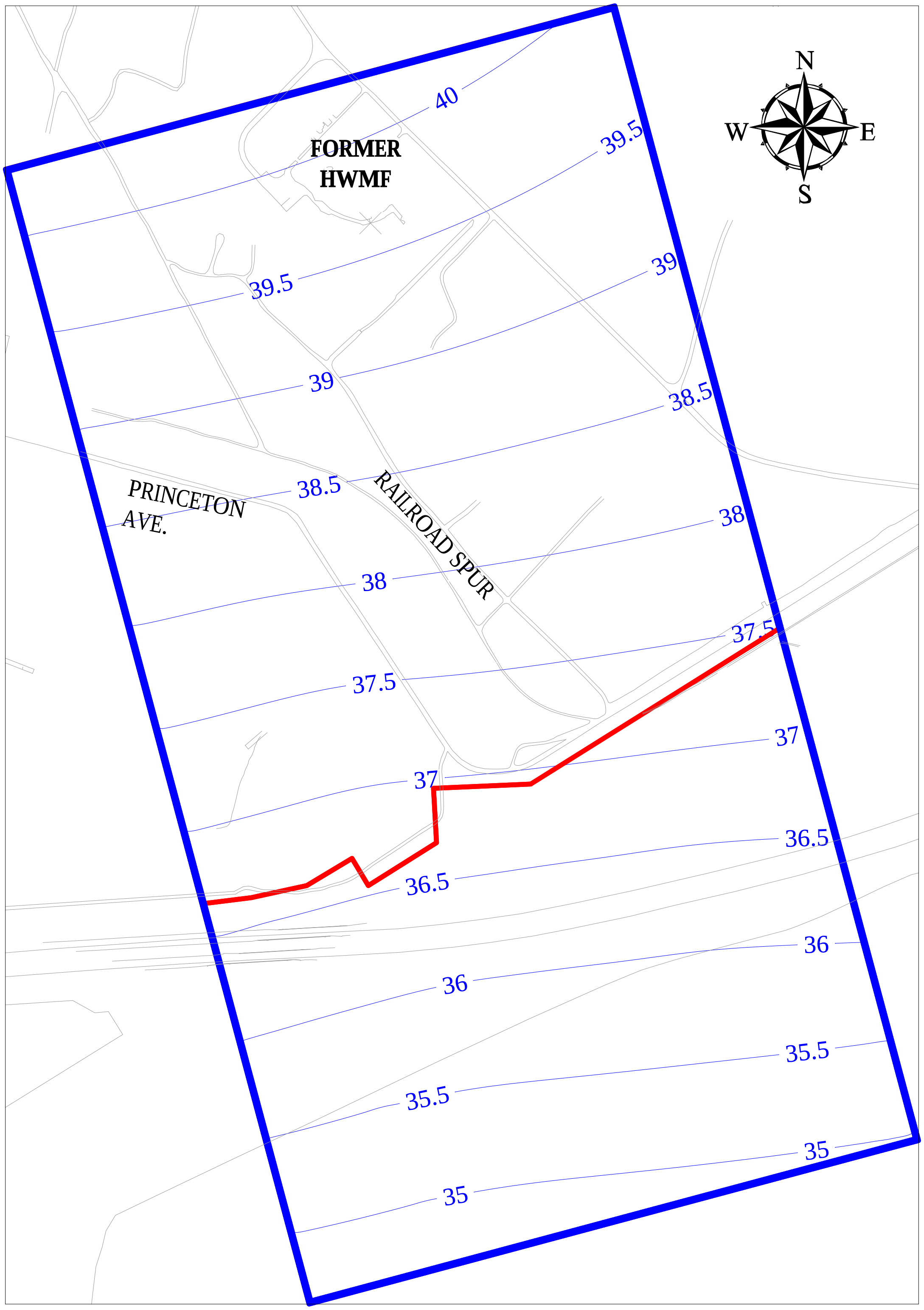
FIGURE

2



SCALE IN FEET

0 1000 2000

36.5 POTENTIOMETRIC SURFACE CONTOUR AND WATER LEVEL ELEVATION IN FEET

SUB-MODEL BOUNDARY

SITE BOUNDARY

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WATER TABLE CONTOURS

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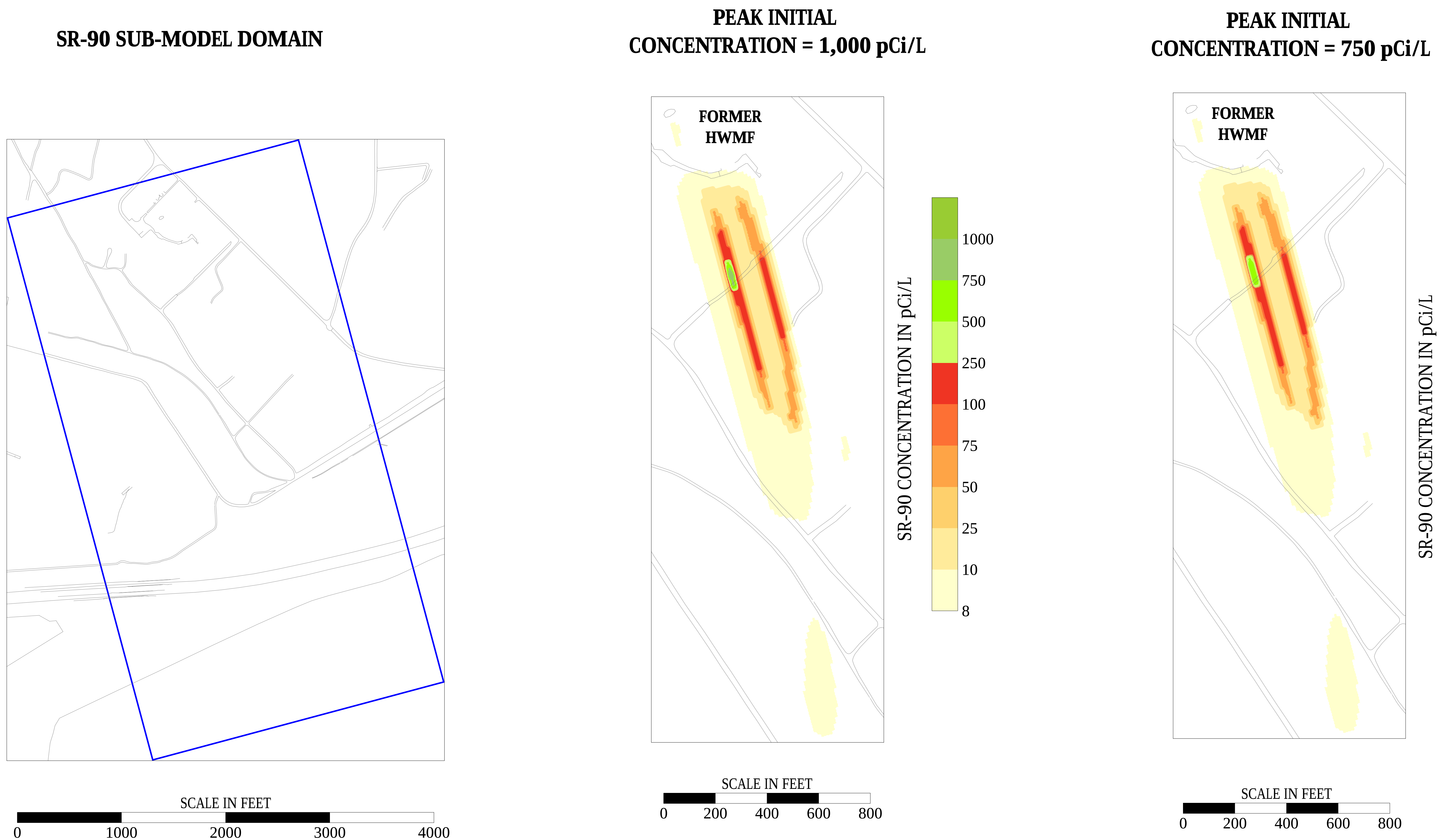
FIGURE 3



Max Concentration Center Panel: 1,000 pCi/L
Max Concentration Right Panel: 750 pCi/L

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SR-90 INITIAL CONDITIONS

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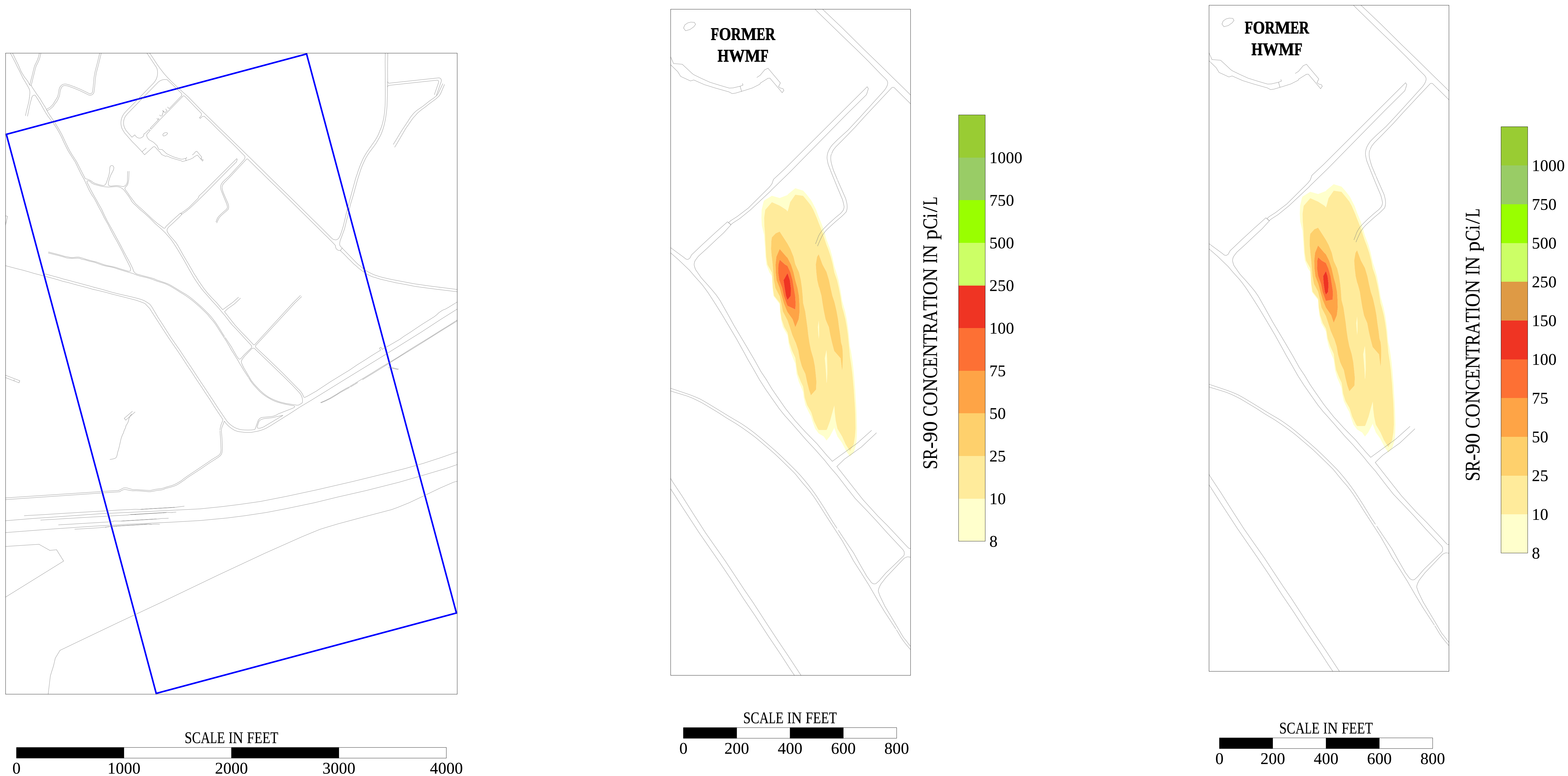
FIGURE
4

SR-90 SUB-MODEL DOMAIN | **PEAK INITIAL CONCENTRATION = 1,000 pCi/L** | **PEAK INITIAL CONCENTRATION = 750 pCi/L**



Max Concentration Center Panel: 128 pCi/L
Max Concentration Right Panel: 120 pCi/L

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MODEL PREDICTED SR-90
DISTRIBUTION AFTER 10 YEARS

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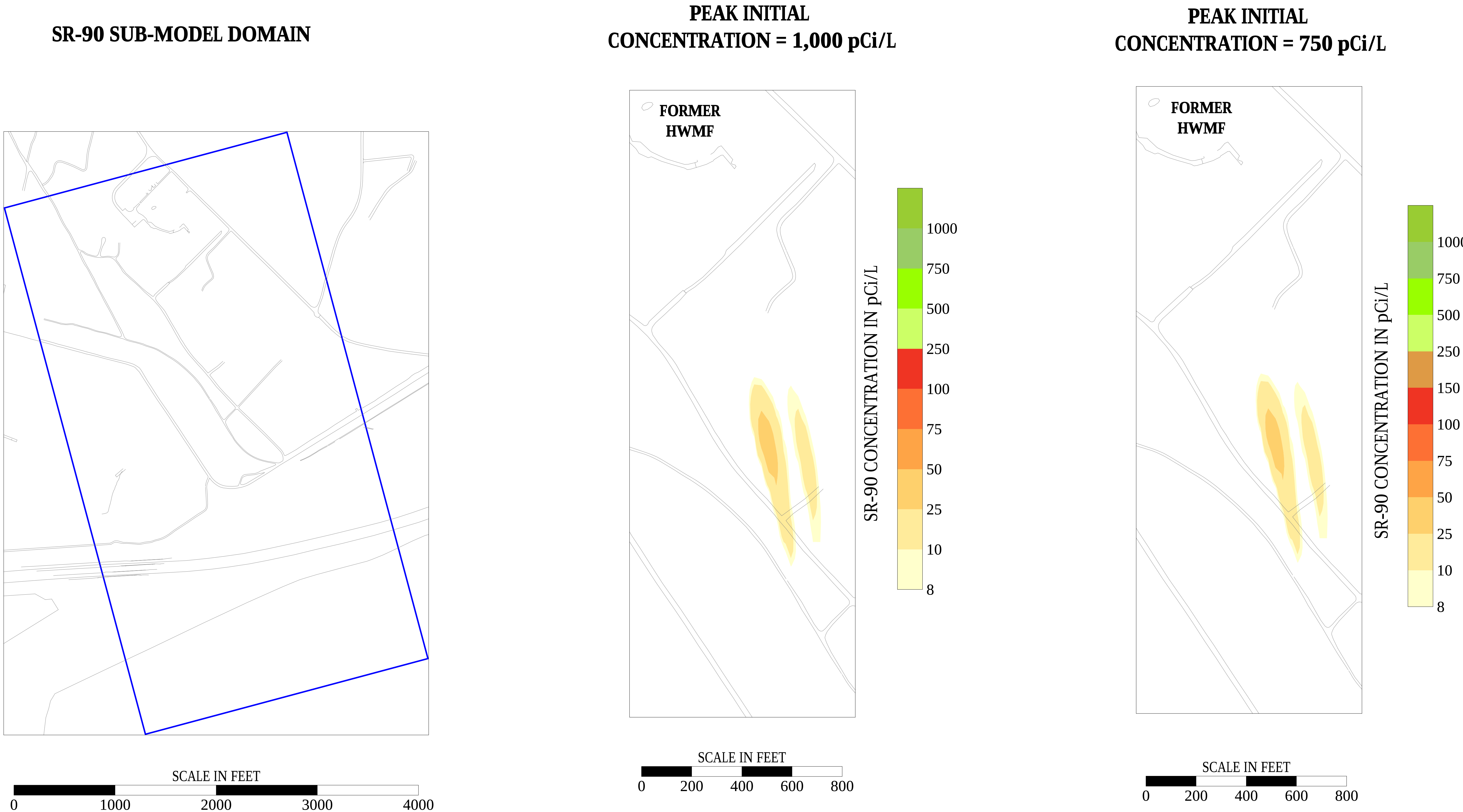
FIGURE
5



Max Concentration Center Panel: 42 pCi/L
Max Concentration Right Panel: 40 pCi/L

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MODEL PREDICTED SR-90
DISTRIBUTION AFTER 20 YEARS

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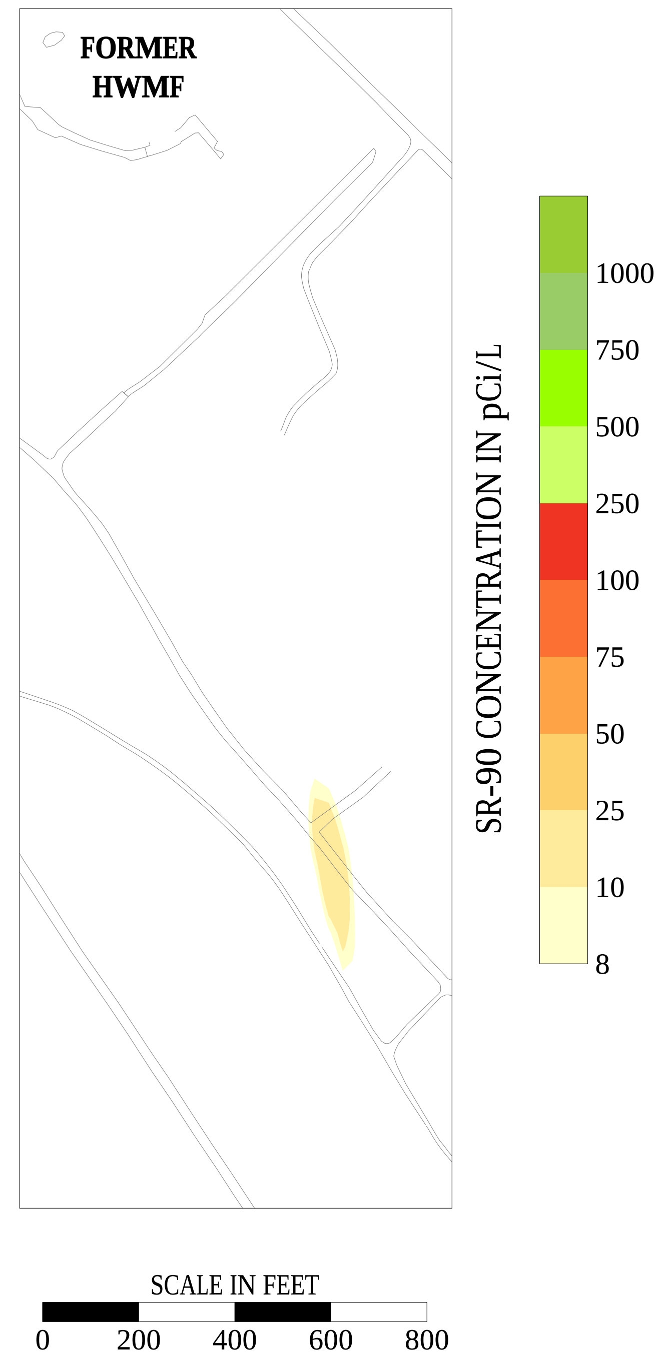
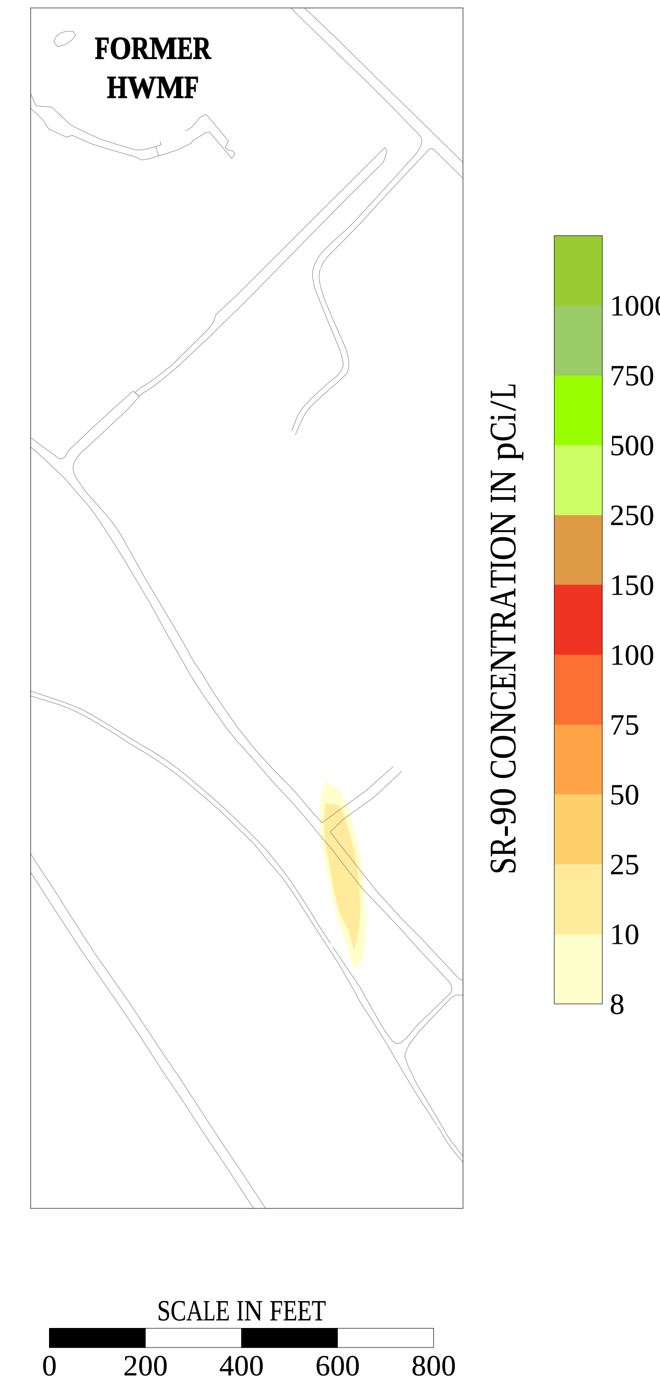
FIGURE
6

SR-90 SUB-MODEL DOMAIN

PEAK INITIAL CONCENTRATION = 1,000 pCi/L



PEAK INITIAL CONCENTRATION = 750 pCi/L



Max Concentration Center Panel: 16 pCi/L
Max Concentration Right Panel: 15 pCi/L

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MODEL PREDICTED SR-90 DISTRIBUTION AFTER 30 YEARS

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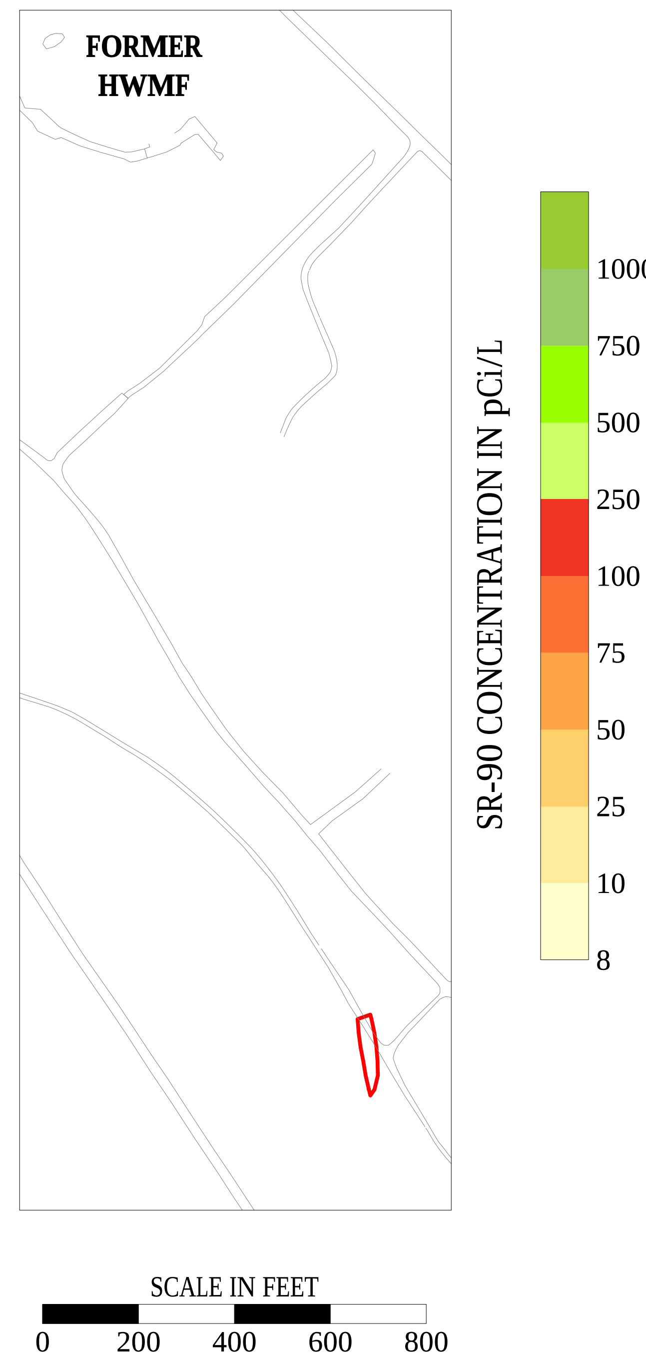
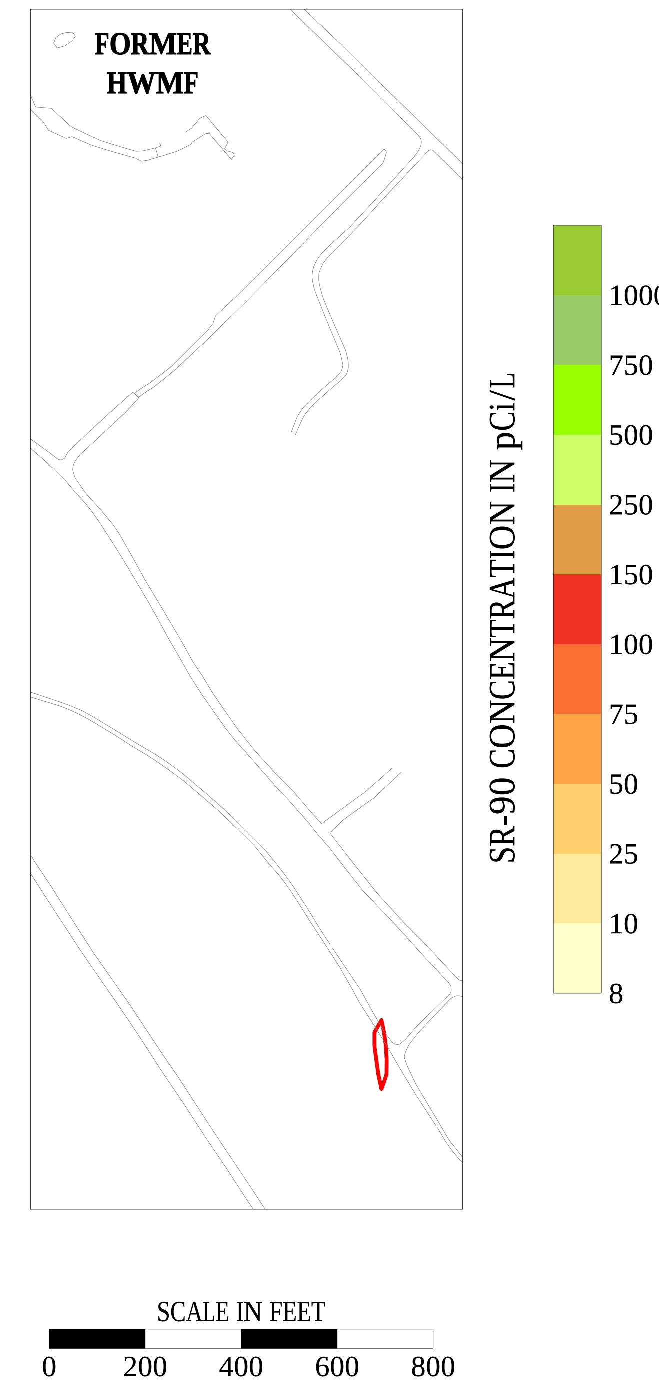
FIGURE 7

SR-90 SUB-MODEL DOMAIN

PEAK INITIAL CONCENTRATION = 1,000 pCi/L



PEAK INITIAL CONCENTRATION = 750 pCi/L



Max Concentration Center Panel: 5.8 pCi/L
Max Concentration Right Panel: 5.5 pCi/L
5 pCi/L contour shown

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MODEL PREDICTED SR-90 DISTRIBUTION AFTER 40 YEARS

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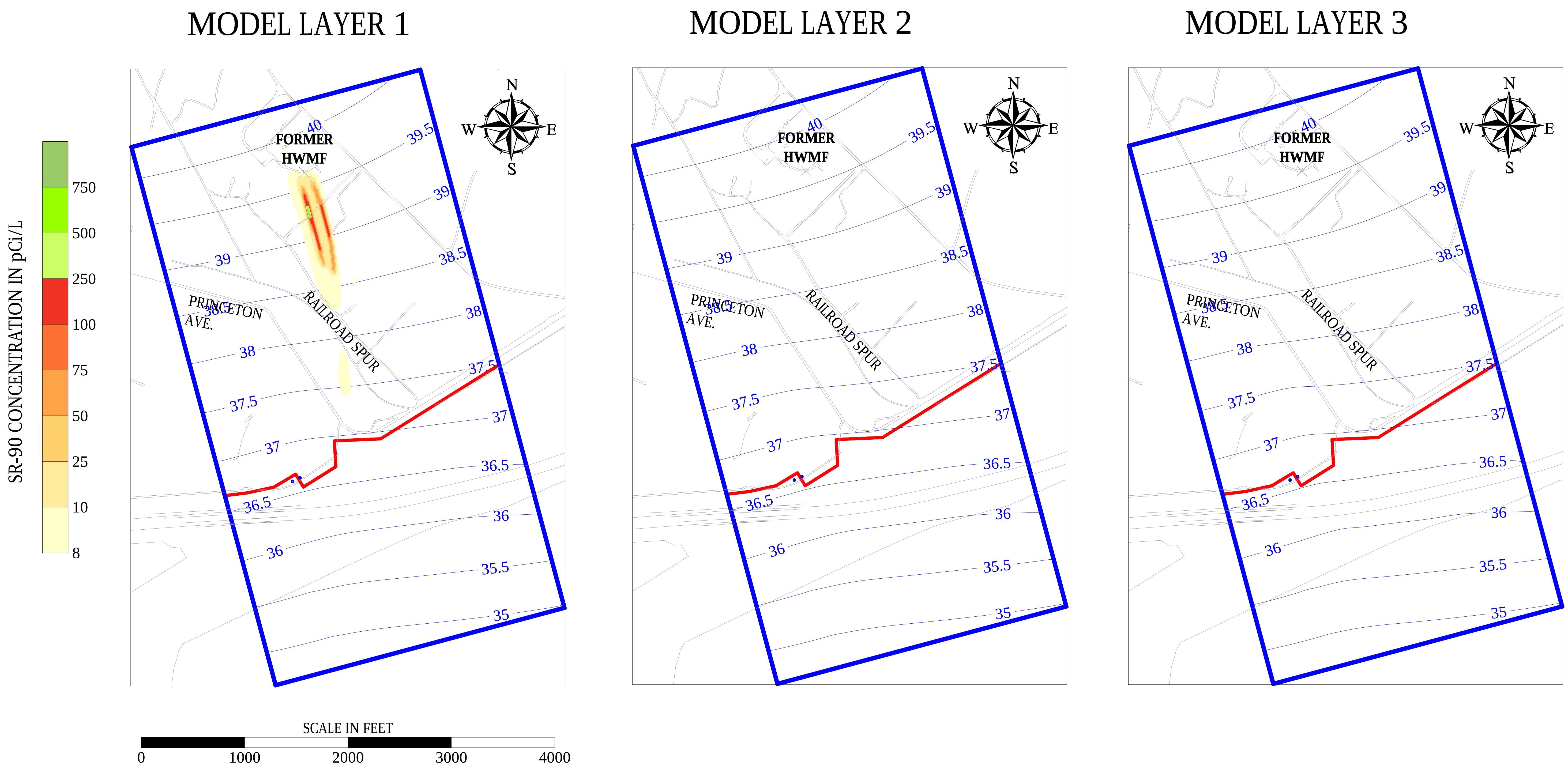
FIGURE 8



36.5 POTENTIOMETRIC SURFACE CONTOUR AND WATER LEVEL ELEVATION IN FEET

SUB-MODEL BOUNDARY

SITE BOUNDARY

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MODEL PREDICTED SR-90 INITIAL CONDITIONS

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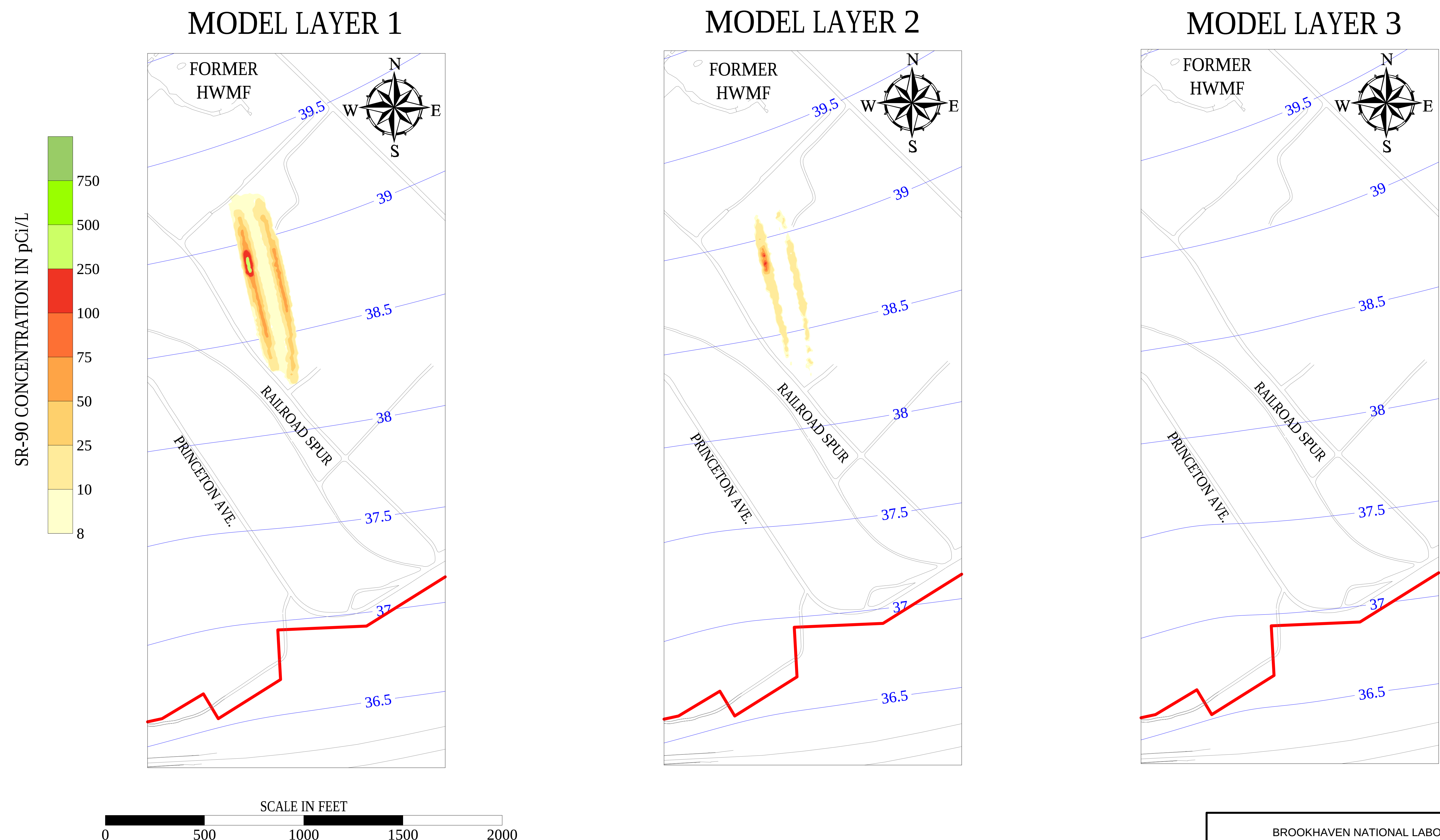
FIGURE 9



36.5 POTENTIOMETRIC SURFACE CONTOUR AND WATER LEVEL ELEVATION IN FEET

SITE BOUNDARY

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MODEL PREDICTED SR-90 DISTRIBUTION T=10 YEARS

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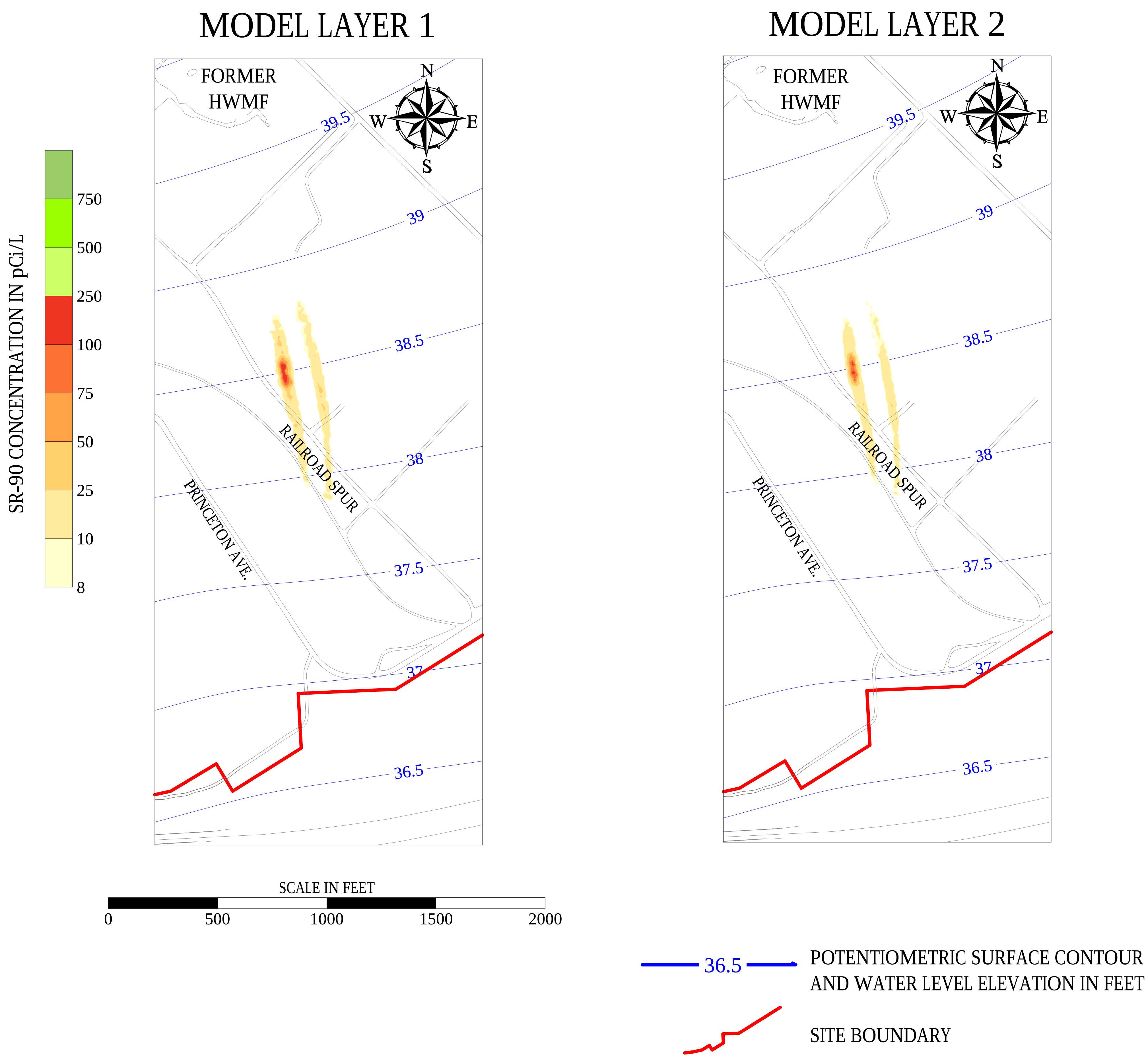
FIGURE 10



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MODEL PREDICTED SR-90 DISTRIBUTION T=20 YEARS

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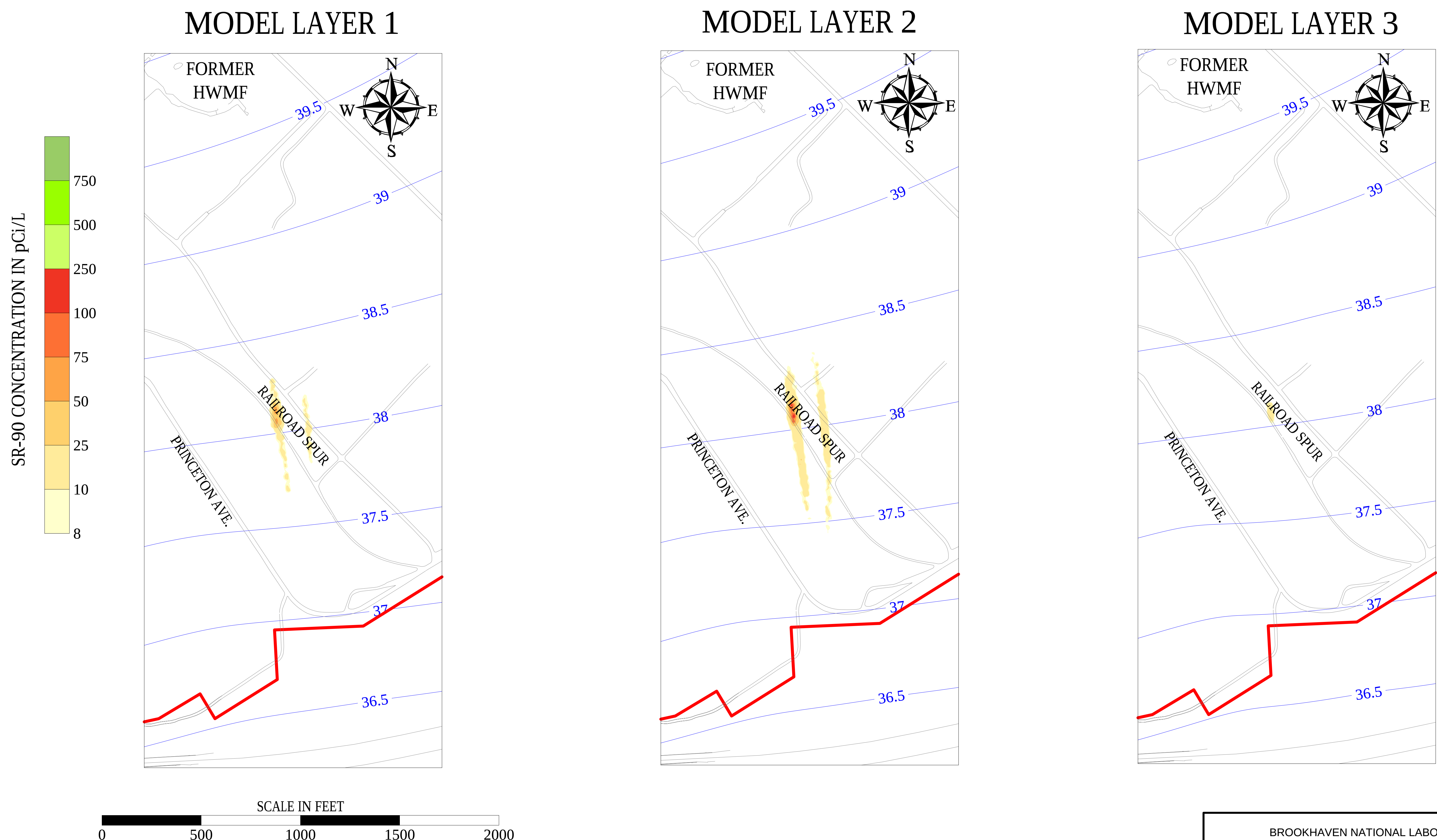
FIGURE 11



36.5 POTENTIOMETRIC SURFACE CONTOUR AND WATER LEVEL ELEVATION IN FEET

SITE BOUNDARY

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MODEL PREDICTED SR-90 DISTRIBUTION T=30 YEARS

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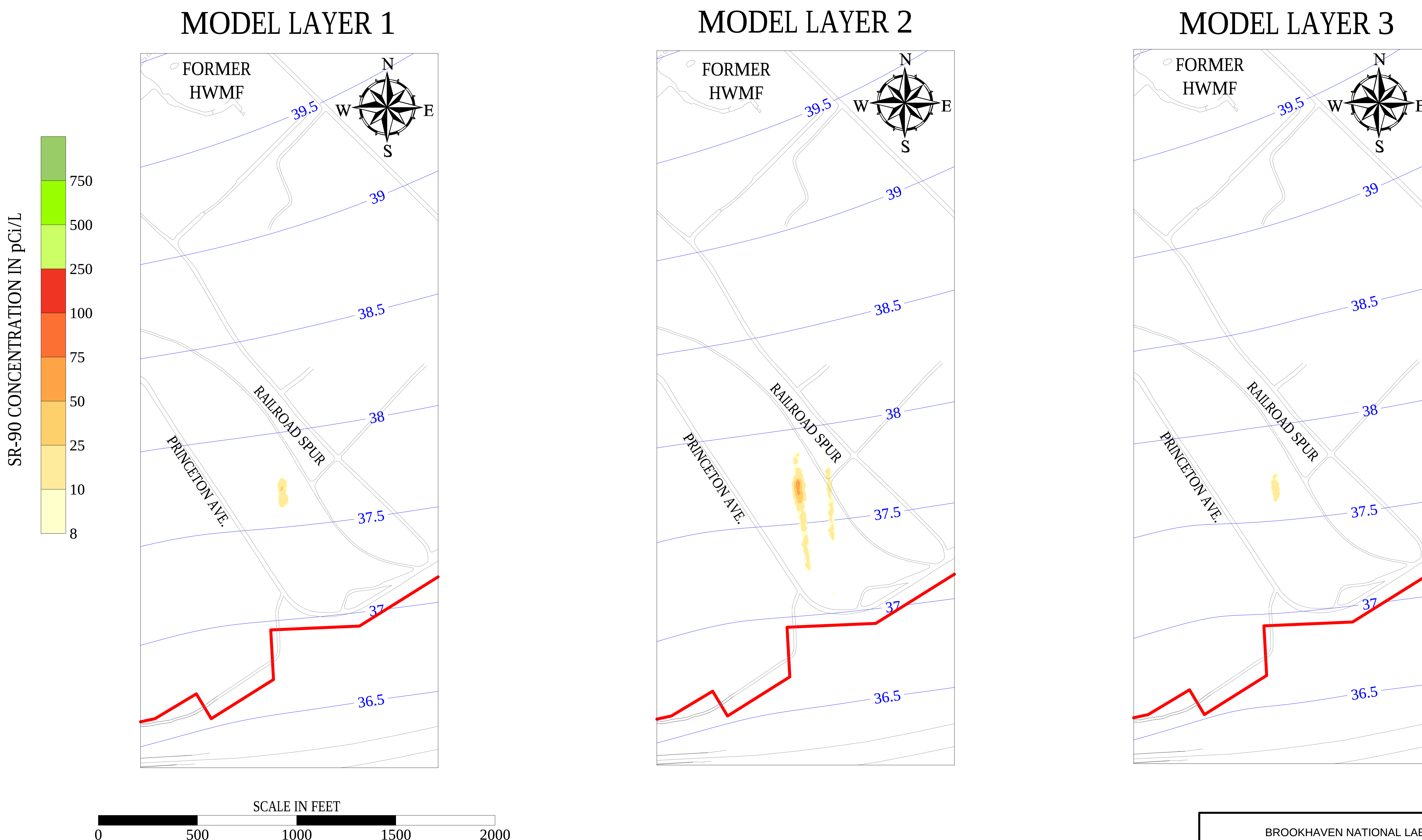
FIGURE 12



36.5 POTENTIOMETRIC SURFACE CONTOUR AND WATER LEVEL ELEVATION IN FEET

SITE BOUNDARY

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MODEL PREDICTED SR-90 DISTRIBUTION T=40 YEARS

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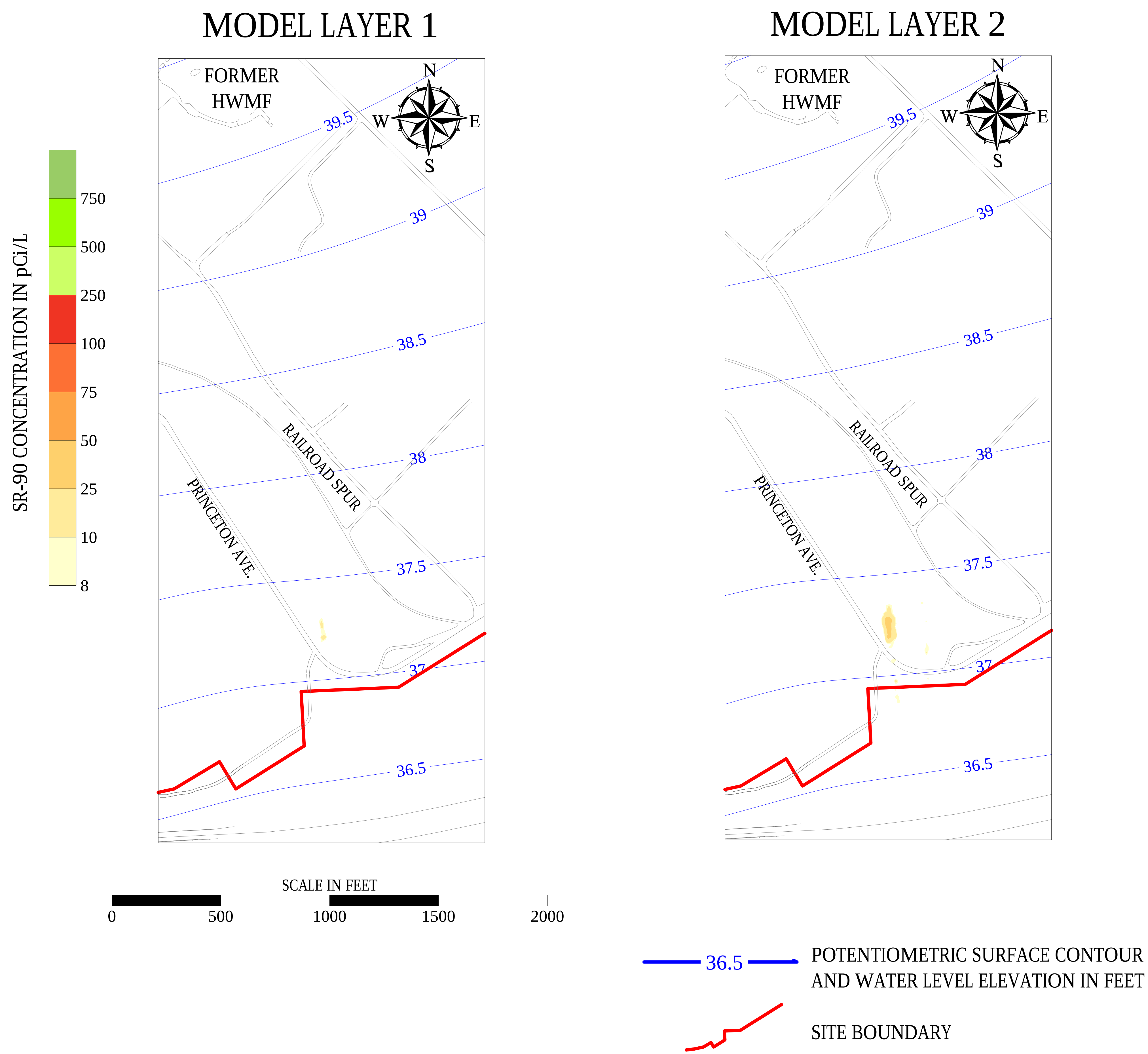
FIGURE 13



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SR-90 TRANSPORT SIMULATION

MODEL PREDICTED SR-90 DISTRIBUTION T=50 YEARS

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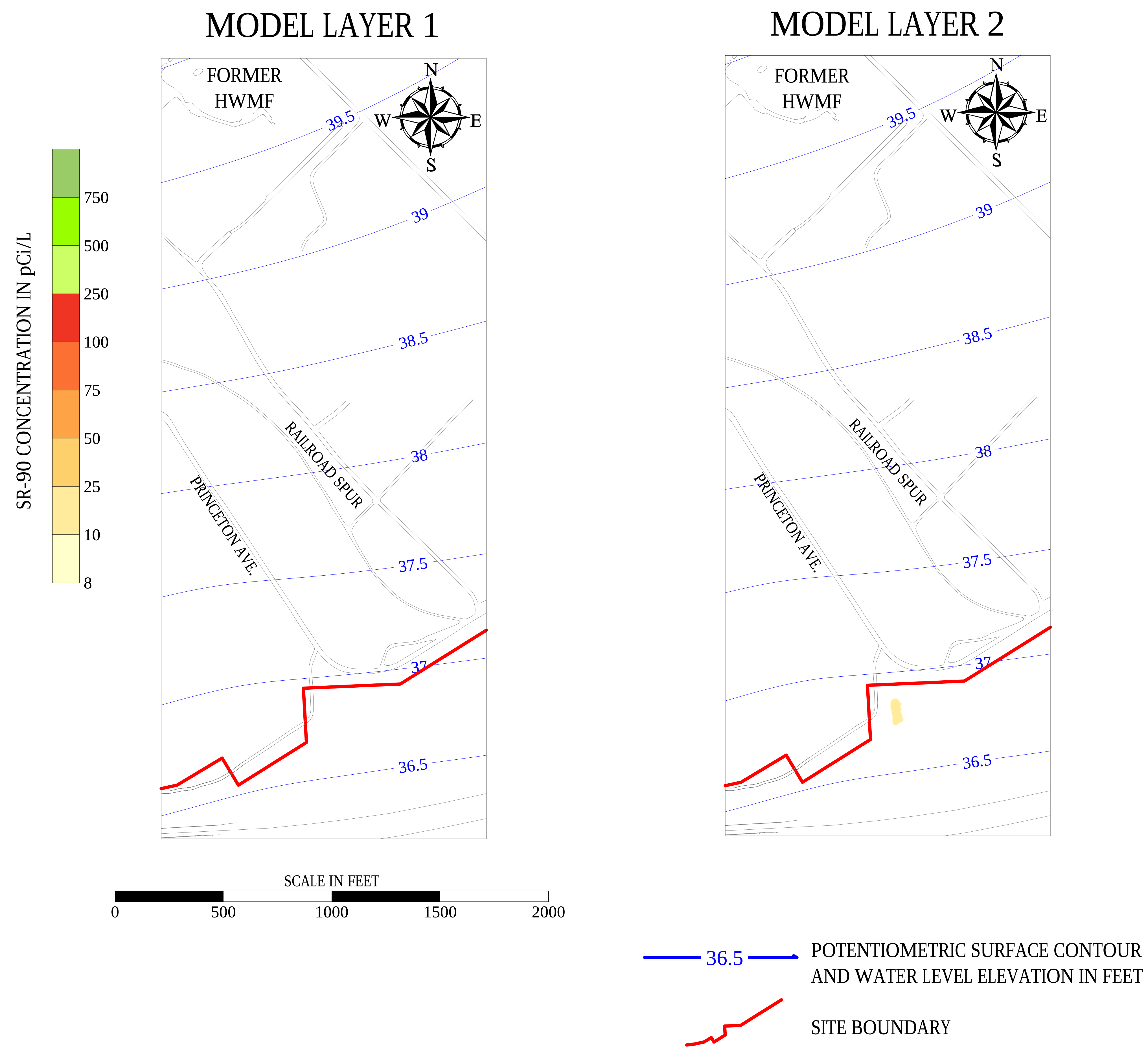
FIGURE 14



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SR-90 TRANSPORT SIMULATION

MODEL PREDICTED SR-90 DISTRIBUTION T=60 YEARS

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FIGURE 15