Overview

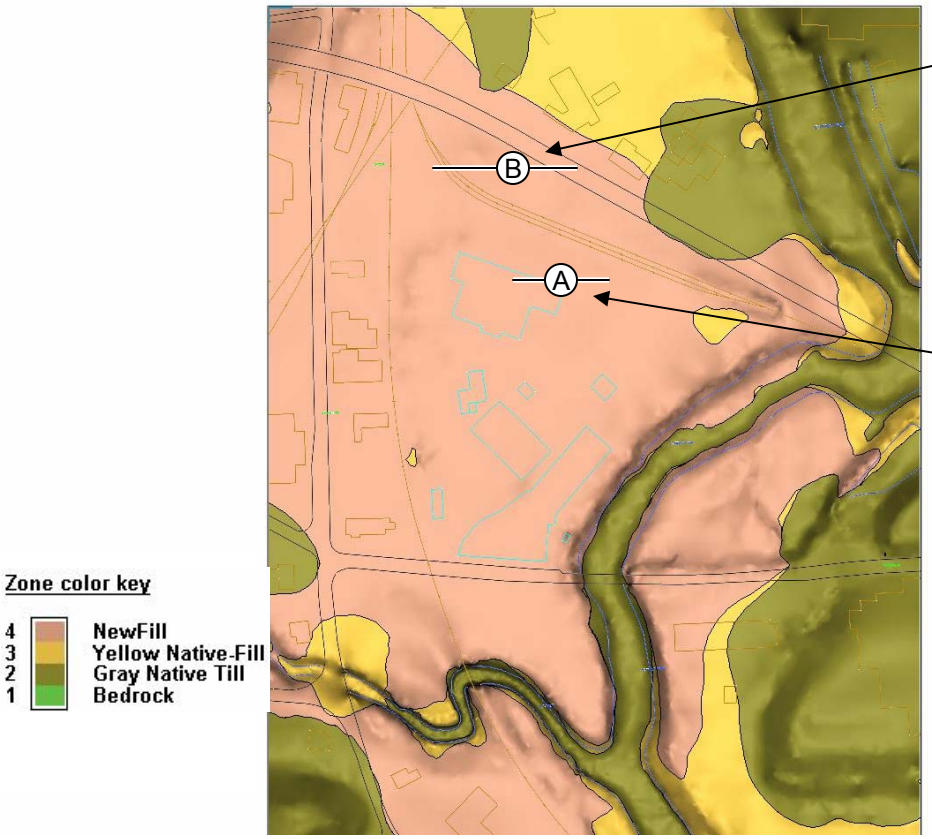
1. Base Map

2. HELP Model for Paved Location A (near Bldg G-1)
   - Soil Column
   - Surface Conditions
   - Subsurface Properties
   - Basecase Model

3. HELP Model for Unpaved Location B (adjacent to railroad tracks)
   - Soil Column
   - Surface Conditions
   - Subsurface Properties
   - Basecase Model

4. Climate Properties

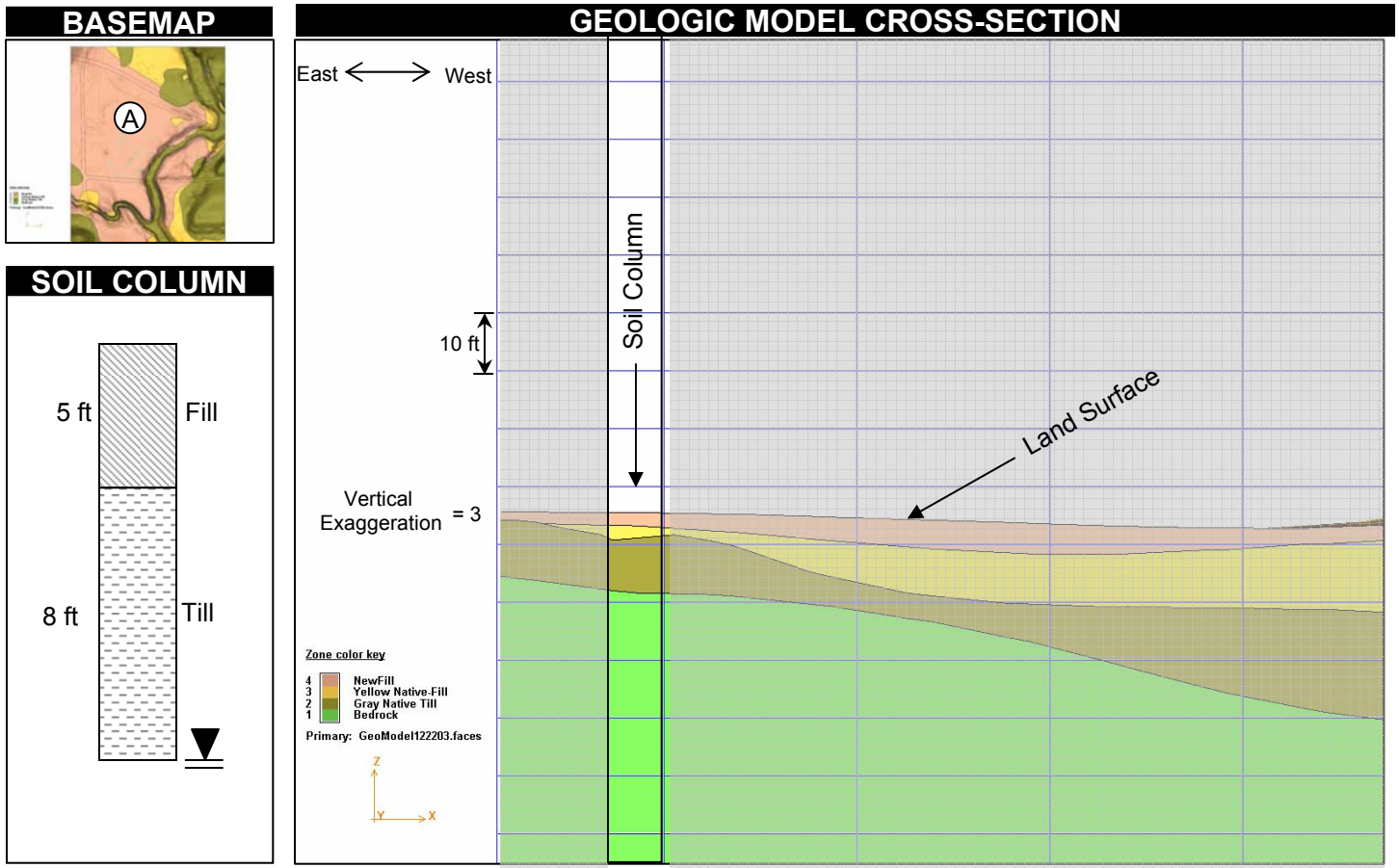
1. Base Map



Unpaved area with vegetation and adjacent to the railroad tracks.

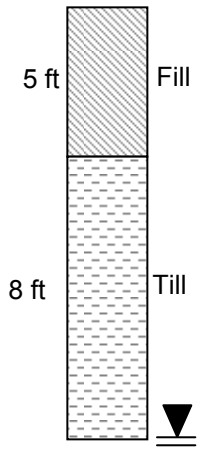
Paved area adjacent to building G-1

2. HELP Model for Paved Location A (near Bldg G-1)



2. HELP Model for Paved Location A (near Bldg G-1)

SOIL COLUMN



SURFACE CONDITIONS

- Fragmented pavement adjacent to building G-1
- Minimal water ponding on pavement presumably due to rapid infiltration through pavement cracks
- Minimal surface slope but runoff does occur

SUBSURFACE PROPERTIES

Soil Layer		USCS	Total Porosity	Field Capacity	Wilting Point	Saturated Hydraulic Conductivity cm/s
Fill	(Help Soil #22)	ML	0.419	0.307	0.18	1.9×10^{-5}
Till	(Help Soil #24)	SC	0.365	0.305	0.202	2.7×10^{-6}

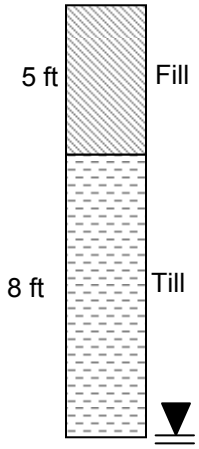
Reference: HELP Ver 3.0 User Manual

Soil layer thickness estimated from geologic model

Water Level estimated from saturation depth in nearby soil borings IA03-SB0131 (12 ft bgs and nearest Location A), IA03-SB0136 (15 ft bgs), IA03-SB0137(12.0 ft bgs).

2. HELP Model for Paved Location A (near Bldg G-1)

SOIL COLUMN



BASELINE MODEL

SELECTED PARAMETERS

Slope:	0.5%
Runoff Area:	50%
Slope Length:	10 ft
Evaporation Depth:	1 in

K_1 = 1.9x10-5 cm/s
K_2 = 2.7x10-6 cm/s

P = Runoff + Evp + I

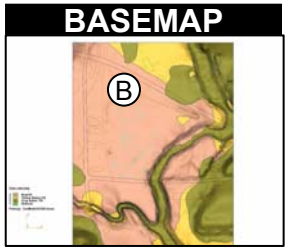
37.4" = 7.6" + 13.3" + 16.6"

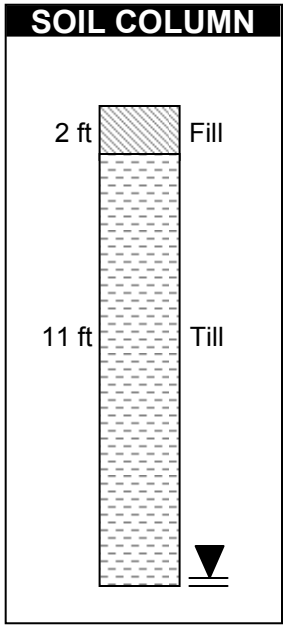
100% = 20% + 35% + 44%

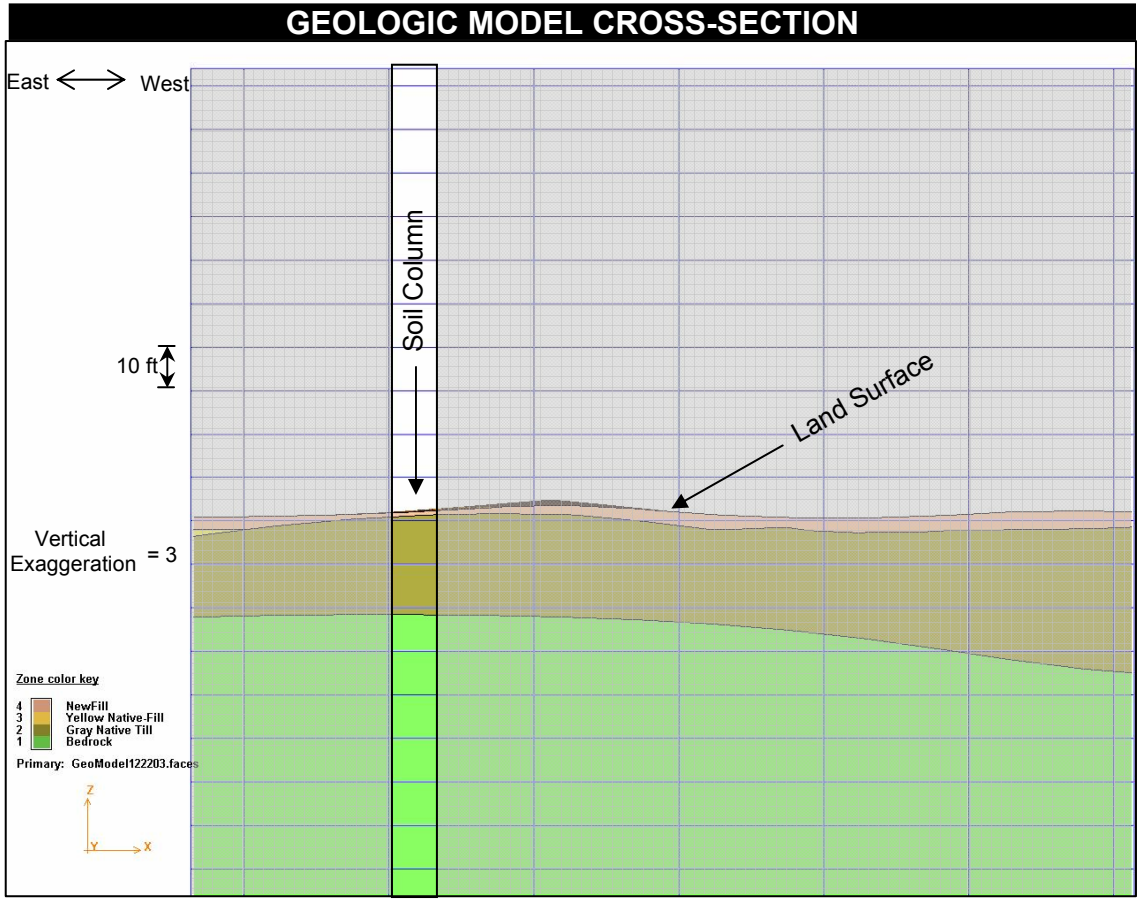
Infiltration = 16.6”

Please see associated Excel file for additional models of Location A

3. HELP Model for Unpaved Location B (adjacent to railroad tracks)

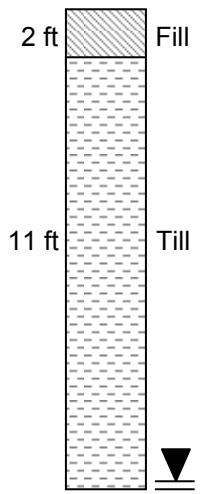






3. HELP Model for Unpaved Location B (adjacent to railroad tracks)

SOIL COLUMN



SURFACE CONDITIONS

- Grassy and lightly vegetated soil cover adjacent to the railroad tracks
- Negligable runoff

SUBSURFACE PROPERTIES

Soil Layer		USCS	Total Porosity	Field Capacity	Wilting Point	Saturated Hydraulic Conductivity cm/s
Fill	(Help Soil #22)	ML	0.419	0.307	0.18	1.9×10^{-5}
Till	(Help Soil #24)	SC	0.365	0.305	0.202	2.7×10^{-6}

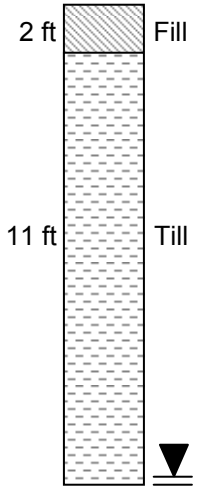
Reference: HELP Ver 3.0 User Manual

Soil layer thickness estimated from geologic model

Water Level estimated from saturation depth in nearby soil boring IA03-SB0078 (11.0 ft bgs) and adjusted for land surface at Location B.

3. HELP Model for Unpaved Location B (adjacent to railroad tracks)

SOIL COLUMN



BASELINE MODEL

SELECTED PARAMETERS

Slope:	-
Runoff Area:	0%
Slope Length:	-
Evaporation Depth:	12 in

K_1 = 1.9x10-5 cm/s
K_2 = 2.7x10-6 cm/s

P = Runoff + Evp + I

37.4" = 0" + 20.3" + 17.2"

100% = 0% + 54% + 46%

Infiltration = 17.2”

Please see associated Excel file for additional model of Location B

4. Climate Properties

PRECIPITATION

	Jan	Feb	Mar	Apr	May	June	July	Aug	Sept	Oct	Nov	Dec
10-yr Average Monthly Temperature (C) 1994-2005	27.6	31.6	37.9	48.5	59.2	68.8	72.3	71.4	64.5	53.6	42.4	31.9

10-yr Average Annual Precipitation (Inches) 1994-2005	37.61	This annual precipitation value is consistent with a value of 36 inches obtained from SESOIL's climate database for the Station "CLEVELAND WSO AP".
10-yr Average Annual Precipitation (Inches) applied in HELP models	37.4	Synthetic daily precipitation is generated in HELP for a period of 10 years based on average monthly precipitation and variability for Cleveland, Ohio. The average annual precipitation based on the daily estimates generated by HELP is 37.4 inches.

4. Climate Properties

AIR TEMPERATURE

	Jan	Feb	Mar	Apr	May	June	July	Aug	Sept	Oct	Nov	Dec
10-yr Average Monthly Temperature (C) 1994-2005	27.6	31.6	37.9	48.5	59.2	68.8	72.3	71.4	64.5	53.6	42.4	31.9

SOLAR RADIATION

Synthetic daily solar radiation data is stochastically generated in the HELP model for a period of 10 years based on precipitation in combination with HELP database parameters for Cleveland, Ohio.

CLIMATE REFERENCES

Reference: *National Climatic Data Center*
(precipitation and temperature data for Cleveland Hopkins International Airport, Cleveland, Ohio)
http://www.ncdc.noaa.gov/oa/climate/research/cag3/x2.html

Overview

1. SESOIL Description
2. Base Map
3. Soil Column for Paved Location A (near Bldg G-1)
4. Soil Column for Unpaved Location B (adjacent to railroad tracks)
5. SESOIL Vertical Geologic Discretization
6. SESOIL Vertical Initial Contaminant Discretization
7. Geologic Discretization and Initial Contaminant Distribution
8. Other SESOIL Input Parameters
9. SESOIL Results

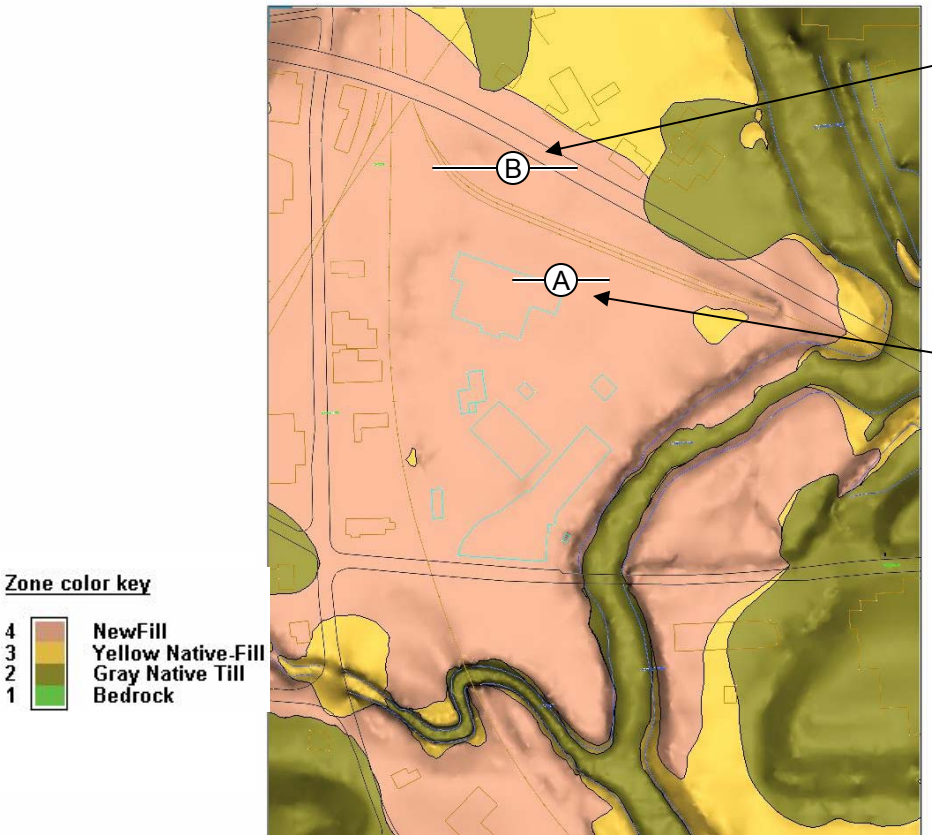
Overview

1. SESOIL DESCRIPTION

- SESOIL is a one-dimensional vertical transport model for the unsaturated soil zone, predicting pollutant concentrations in the soil profile following introduction via direct application and/or interaction with other media.

- Processes simulated in SESOIL are categorized in three cycles
  - **Hydrologic**, which includes
    - Rainfall
    - Surface runoff
    - Infiltration
    - Soil water content
    - Evapotranspiration
    - Groundwater runoff
  - **Sediment** , which includes
    - Sediment washload as a result of rainstorms (i.e., soil erosion that results from surface runoff).
    - Not used in this exercise
  - **Pollutant**, which includes
    - Convective transport
    - Volatilization
    - Adsorption/desorption
    - Degradation/decay.

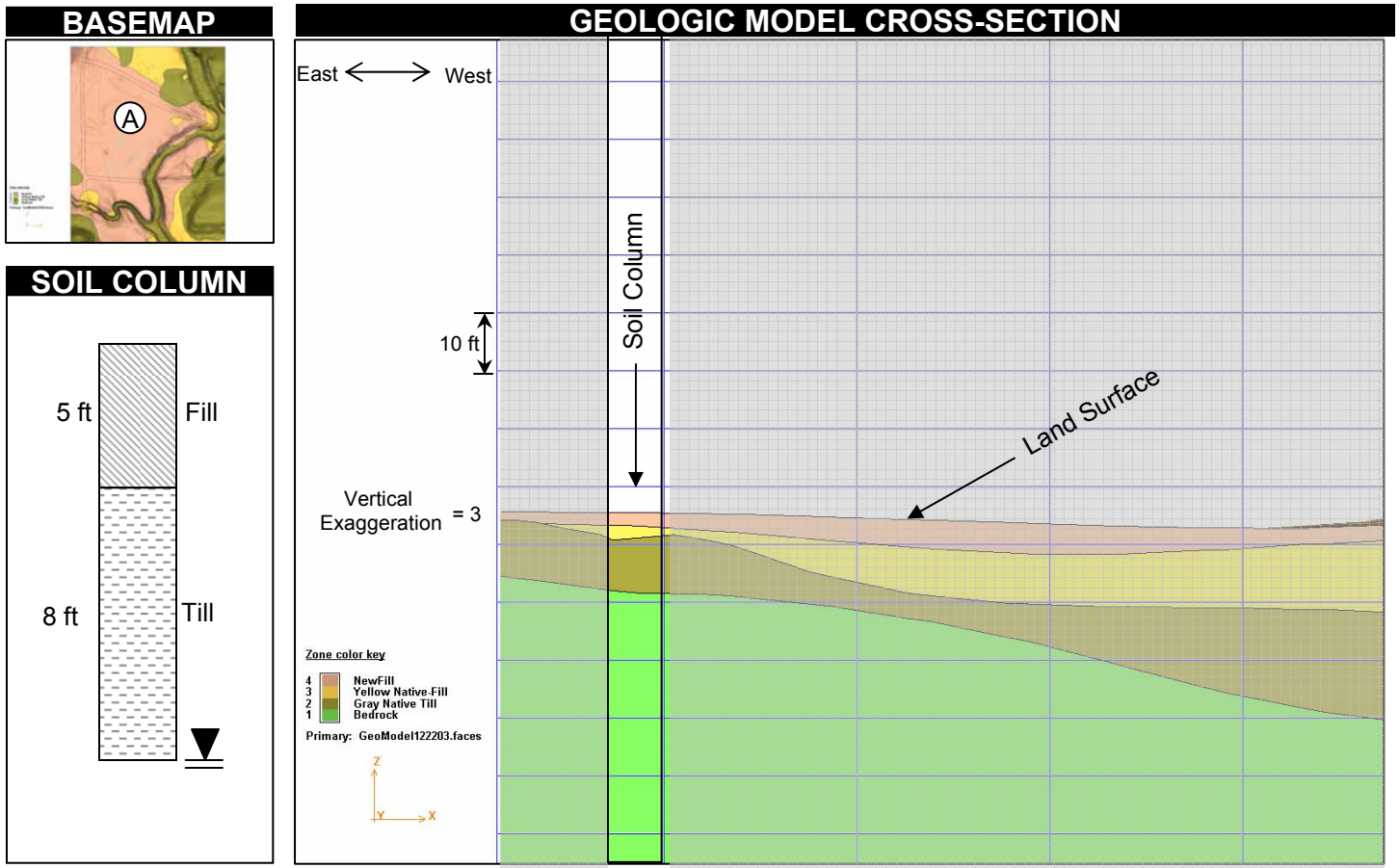
2. Base Map



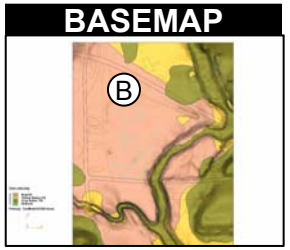
Unpaved area with vegetation and adjacent to the railroad tracks.

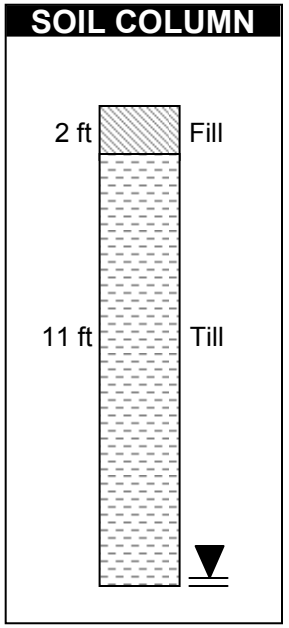
Paved area adjacent to building G-1

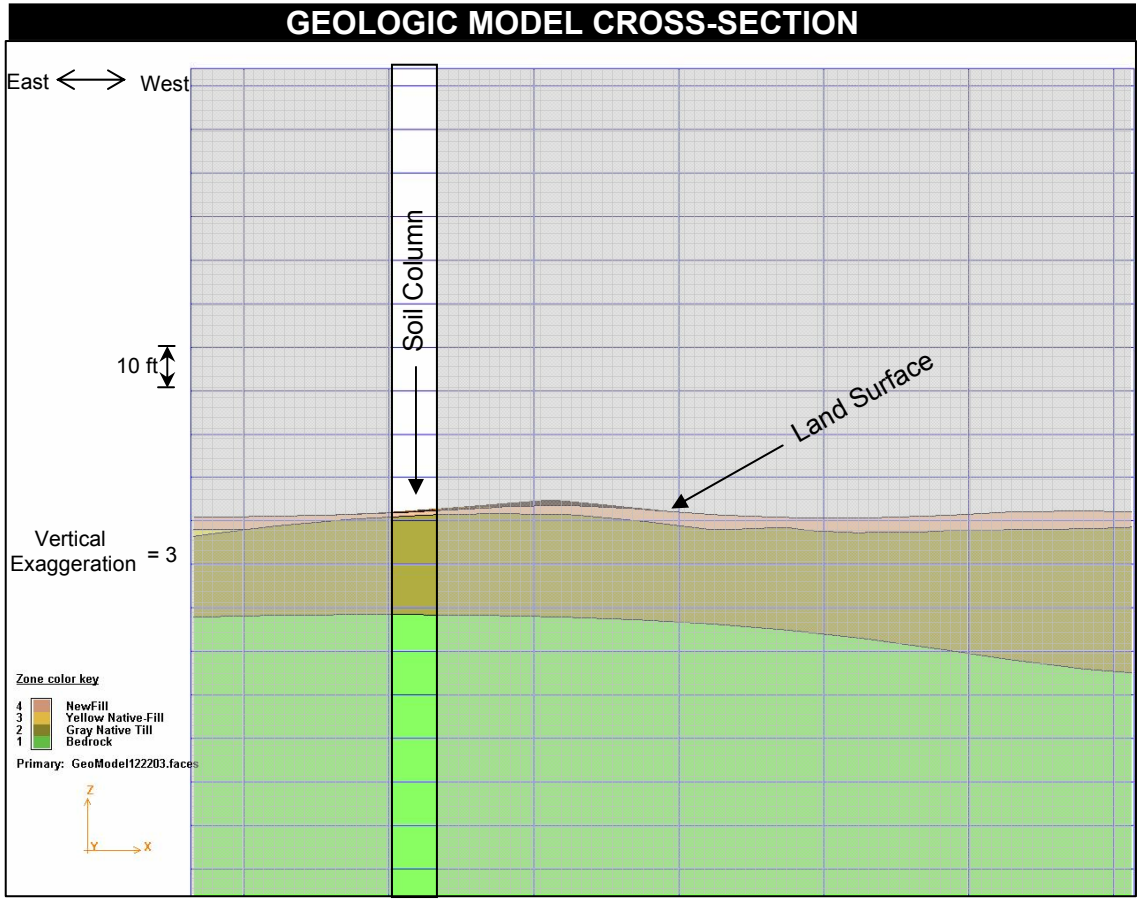
3. Soil Column for Paved Location A (near Bldg G-1)



4. Soil Column for Unpaved Location B (adjacent to railroad tracks)







5. SESOIL Vertical Geologic Discretization

Column A

- 3 Super Layers
  - Super Layer 1
    - 152.5 cm thick
    - 5 Sublayers, each 30.5 cm thick
    - Corresponds to the “Fill” layer at Column A
  - Super Layer 2
    - 244 cm thick
    - 8 Sublayers, each 30.5 cm thick
    - Corresponds to the “Till” Layer at Column A
  - Super Layer 3
    - 10 cm thick
    - Addition to “Till” at Column A

Column B

- 4 Super Layers
  - Super Layer 1
    - 61 cm thick
    - 2 Sublayers, each 30.5 cm thick
    - Corresponds to the “Fill” layer at Column A
  - Super Layer 2
    - 305 cm thick
    - 10 Sublayers, each 30.5 cm thick
    - Corresponds to the “Till” Layer at Column A
  - Super Layer 3
    - 30.5 cm thick
    - Corresponds to the “Till” Layer at Column A
  - Super Layer 4
    - 10 cm thick
    - Addition to “Till” at Column A

6a. SESOIL Vertical Initial Contaminant Discretization

- Average concentrations at each 30.5 cm interval (1 ft interval) in the unconsolidated soil was entered as initial concentrations in soil column
  - Arithmetic average of all reported values of compound concentration from database at the sublayer depth
  - COPC reported at their detection limit with “U” taken into account by including a value equal to ½ of the reported detection limit in the calculation of the averages.
  - The inclusion of ½ the detection limit in calculating averages is the accepted, conservative approach based in Risk Assessment Guidance for Superfund (RAGS) methodology.
  - For sample intervals straddling more than 1 model 30.5 cm sublayer, sample results were applied to each model layer it straddled to calculate the initial concentrations.
  - For sublayer intervals in which a particular COPC was not analyzed, the first nearest vertical soil interval with an averaged initial concentration to be projected to that layer. If such a layer is equidistant from two intervals with values, the higher of the two values is assigned to the layer
- Initial concentration distribution the same for BOTH Column A and Column B

6b. Number of Soil Samples per Layer per COPC Utilized to Assign Initial Concentrations

Layer Top Depth (ft bgs)	Layer Bottom Depth (ft bgs)	Molybdenum	Radium		Thorium		Uranium	
			RA-226	RA-228	Th-230	TH-232	U-235	U-238
0	1	40	192	139	193	140	192	192
1	2	34	147	104	148	105	147	147
2	3	19	50	40	51	40	50	50
3	4	7	20	15	21	15	20	20
4	5	28	128	91	128	91	128	128
5	6	25	125	88	125	88	125	125
6	7		4	1	4	1	4	4
7	8	1	5	2	5	2	5	5
8	9	7	77	56	77	56	77	77
9	10	6	76	55	76	55	76	76
10	11		5		5		5	5
11	12		5		5		5	5
12	13		3	1	3	1	3	3
13	13.3		3	1	3	1	3	3

ft = feet

bgs = below ground surface

RA-226 and RA-228 samples were summed to model total Radium; TH-228, TH-20, TH-232, TH-234 were summed to model total Thorium; U-235, U-238 were summed to model total Uranium

7a. Geologic Discretization and Initial Uranium Distribution for SESOIL Modeling

Column A[1] Layer	Sublayer	Thickness (cm)	Depth (ft bgs)	U[3] (ug/g)
Silt				
1	1	30.5	1.0	1.57E+02
	2	30.5	2.0	1.51E+02
	3	30.5	3.0	2.87E+02
	4	30.5	4.0	1.27E+02
	5	30.5	5.0	1.37E+01
Clayey Sand				
2	1	30.5	6.0	1.37E+01
	2	30.5	7.0	1.52E+01
	3	30.5	8.0	1.30E+01
	4	30.5	9.0	8.90E+00
	5	30.5	10.0	8.96E+00
	6	30.5	11.0	4.98E+01
	7	30.5	12.0	4.98E+01
	8	30.5	13.0	1.15E+01
Clayey Sand				
3	1	10.0	13.3	1.15E+01

Depth to Potentiometric Head of Bedrock Groundwater =13 ft

Column B[2] Layer	Sublayer	Thickness (cm)	Depth (ft bgs)	U[3] (ug/g)
Silt				
1	1	30.5	1.0	1.57E+02
	2	30.5	2.0	1.51E+02
Clayey Sand				
2	1	30.5	3.0	2.87E+02
	2	30.5	4.0	1.27E+02
	3	30.5	5.0	1.37E+01
	4	30.5	6.0	1.37E+01
	5	30.5	7.0	1.52E+01
	6	30.5	8.0	1.30E+01
	7	30.5	9.0	8.90E+00
	8	30.5	10.0	8.96E+00
	9	30.5	11.0	4.98E+01
	10	30.5	12.0	4.98E+01
Clayey Sand				
3	1	30.5	13.0	1.15E+01
Clayey Sand				
4	1	10.0	13.3	1.15E+01

Depth to Potentiometric Head of Bedrock Groundwater =13 ft

Notes:

ft = feet
cm = centimeters
ug = micrograms
g = grams

[1] Column A Water Level estimated from saturation depth in nearby soil borings IA03-SB0131 (12.0 ft bgs and nearest Location A), IA03-SB0136 (15.0 ft bgs), and IA03-SB0137 (12.0 ft bgs).
[2] Column B Water Level estimated from saturation depth in nearby soil borings IA03-SB0078 (11.0 ft bgs) and adjusted for land surface near Location B.
[3] Total elemental Uranium was calculated from the mass-equivalence of activities measured for U-235 and U-238, with specific activities 4.62E-01 ug/pCi and 2.98E+00 ug/pCi, respectively.

7b. Geologic Discretization and Initial Radium Distribution for SESOIL Modeling

Column A[1] Layer		Sublayer	Thickness (cm)	Depth (ft bgs)	Ra[3] (ug/g)
Silt					
	1	1	30.5	1.0	1.81E-06
		2	30.5	2.0	1.61E-06
		3	30.5	3.0	1.52E-06
		4	30.5	4.0	1.51E-06
		5	30.5	5.0	1.48E-06
Clayey Sand					
	2	1	30.5	6.0	1.49E-06
		2	30.5	7.0	1.90E-06
		3	30.5	8.0	1.75E-06
		4	30.5	9.0	1.39E-06
		5	30.5	10.0	1.39E-06
		6	30.5	11.0	2.13E-06
		7	30.5	12.0	2.13E-06
		8	30.5	13.0	1.65E-06
Clayey Sand					
	3	1	10.0	13.3	1.65E-06

Depth to Potentiometric Head of Bedrock Groundwater =13 ft

Column B[2] Layer		Sublayer	Thickness (cm)	Depth (ft bgs)	Ra[3] (ug/g)
Silt					
	1	1	30.5	1.0	1.81E-06
		2	30.5	2.0	1.61E-06
Clayey Sand					
	2	1	30.5	3.0	1.52E-06
		2	30.5	4.0	1.51E-06
		3	30.5	5.0	1.48E-06
		4	30.5	6.0	1.49E-06
		5	30.5	7.0	1.90E-06
		6	30.5	8.0	1.75E-06
		7	30.5	9.0	1.39E-06
		8	30.5	10.0	1.39E-06
		9	30.5	11.0	1.39E-06
		10	30.5	12.0	1.39E-06
Clayey Sand					
	3	1	30.5	13.0	1.65E-06
Clayey Sand					
	4	1	10.0	13.3	1.65E-06

Depth to Potentiometric Head of Bedrock Groundwater =13 ft

Notes:

ft = feet
cm = centimeters
ug = micrograms
g = grams
[1] Column A Water Level estimated from saturation depth in nearby soil borings IA03-SB0131 (12.0 ft bgs and nearest Location A), IA03-SB0136 (15.0 ft bgs), and IA03-SB0137 (12.0 ft bgs).
[2] Column B Water Level estimated from saturation depth in nearby soil borings IA03-SB0078 (11.0 ft bgs) and adjusted for land surface near Location B.
[3] Total elemental Radium was calculated from the mass-equivalence of activities measured for Ra-226 and Ra-228, with specific activities 1.01E-06 ug/pCi and 3.66E-09 ug/pCi, respectively.

7c. Geologic Discretization and Initial Thorium Distribution for SESOIL Modeling

Column A[1] Layer	Sublayer	Thickness (cm)	Depth (ft bgs)	Th[3] (ug/g)
Silt				
1	1	30.5	1.0	8.28E+00
	2	30.5	2.0	8.21E+00
	3	30.5	3.0	8.35E+00
	4	30.5	4.0	9.59E+00
	5	30.5	5.0	1.07E+01
Clayey Sand				
2	1	30.5	6.0	1.08E+01
	2	30.5	7.0	1.02E+01
	3	30.5	8.0	1.03E+01
	4	30.5	9.0	1.09E+01
	5	30.5	10.0	1.10E+01
	6	30.5	11.0	1.16E+01
	7	30.5	12.0	1.16E+01
	8	30.5	13.0	1.16E+01
Clayey Sand				
3	1	10.0	13.3	1.16E+01

Depth to Potentiometric Head of Bedrock Groundwater =13 ft

Column B[2] Layer	Sublayer	Thickness (cm)	Depth (ft bgs)	Th[3] (ug/g)
Silt				
1	1	30.5	1.0	8.28E+00
	2	30.5	2.0	8.21E+00
Clayey Sand				
2	1	30.5	3.0	8.35E+00
	2	30.5	4.0	9.59E+00
	3	30.5	5.0	1.07E+01
	4	30.5	6.0	1.08E+01
	5	30.5	7.0	1.02E+01
	6	30.5	8.0	1.03E+01
	7	30.5	9.0	1.09E+01
	8	30.5	10.0	1.10E+01
	9	30.5	11.0	1.10E+01
	10	30.5	12.0	1.10E+01
Clayey Sand				
3	1	30.5	13.0	1.16E+01
Clayey Sand				
4	1	10.0	13.3	1.16E+01

Depth to Potentiometric Head of Bedrock Groundwater =13 ft

Notes:

ft = feet
cm = centimeters
ug = micrograms
g = grams

[1] Column A Water Level estimated from saturation depth in nearby soil borings IA03-SB0131 (12.0 ft bgs and nearest Location A), IA03-SB0136 (15.0 ft bgs), and IA03-SB0137 (12.0 ft bgs).

[2] Column B Water Level estimated from saturation depth in nearby soil borings IA03-SB0078 (11.0 ft bgs) and adjusted for land surface near Location B.

[3] Total elemental Thorium was calculated from the mass-equivalence of activities measured forTh-230 and Th-232, with specific activities 4.95E-05 ug/pCi and 9.13E+00 ug/pCi, respectively.

7d. Geologic Discretization and Initial Molybdenum Distribution for SESOIL Modeling

Column A[1] Layer		Sublayer	Thickness (cm)	Depth (ft bgs)	Mo (ug/g)
Silt					
	1	1	30.5	1.0	5.64E+00
		2	30.5	2.0	4.41E+00
		3	30.5	3.0	3.24E+00
		4	30.5	4.0	3.08E+00
		5	30.5	5.0	5.26E+00
Clayey Sand					
	2	1	30.5	6.0	5.47E+00
		2	30.5	7.0	5.47E+00
		3	30.5	8.0	3.63E+00
		4	30.5	9.0	7.14E+00
		5	30.5	10.0	7.73E+00
		6	30.5	11.0	7.73E+00
		7	30.5	12.0	7.73E+00
		8	30.5	13.0	7.73E+00
Clayey Sand					
	3	1	10.0	13.3	7.73E+00

Depth to Potentiometric Head of Bedrock Groundwater =13 ft

Column B[2] Layer		Sublayer	Thickness (cm)	Depth (ft bgs)	Mo (ug/g)
Silt					
	1	1	30.5	1.0	5.64E+00
		2	30.5	2.0	4.41E+00
Clayey Sand					
	2	1	30.5	3.0	3.24E+00
		2	30.5	4.0	3.08E+00
		3	30.5	5.0	5.26E+00
		4	30.5	6.0	5.47E+00
		5	30.5	7.0	5.47E+00
		6	30.5	8.0	3.63E+00
		7	30.5	9.0	7.14E+00
		8	30.5	10.0	7.73E+00
		9	30.5	11.0	7.73E+00
		10	30.5	12.0	7.73E+00
Clayey Sand					
	3	1	30.5	13.0	7.73E+00
Clayey Sand					
	4	1	10.0	13.3	7.73E+00

Depth to Potentiometric Head of Bedrock Groundwater =13 ft

Notes:

ft = feet
cm = centimeters
ug = micrograms
g = grams
[1] Column A Water Level estimated from saturation depth in nearby soil borings IA03-SB0131 (12.0 ft bgs and nearest Location A), IA03-SB0136 (15.0 ft bgs), and IA03-SB0137 (12.0 ft bgs).
[2] Column B Water Level estimated from saturation depth in nearby soil borings IA03-SB0078 (11.0 ft bgs) and adjusted for land surface near Location B.

8a. Other SESOIL Input Parameters

SOIL Properties				
Soil Type	Bulk Density [1] (gm/cm^3)	Intrinsic Permeability [2] (cm^2)	Effective Porosity [3]	Freundlich Equation Exponent [4]
Silt	1.5	5.00E-11	0.27	1
Clayey Sand	1.5	1.25E-08	0.27	1

Chemical Transport Properties				
COPC	Solubility [5] (mg/l)	Diffusion Coefficient in Air [6] (cm^2/sec)	Kd [7] (ml/g)	Molecular Weight (g/mole)
U	500	0	14.03	238.03
Ra	36	0	253	226.03
Th	650	0	3085	232.04
Mo	1.3	0	20	95.94

Climate
Nearest Weather Data In SESOIL Database to Longitdue = -81.6845 and Latitude 41.44872
Cleveland Weather Station Observatory at Hopkins Airport

Other SESOIL Parameters
Source Loading
Instantaneous

Notes

ft = feet, cm = centimeter, mg = milligram, l = liter, ml = milliliter

1 SESOIL, the Seasonal Soil Compartment Model) help suggests bulk density values (g/cm^3) of 1.18-1.58 for sand, 1.29-1.80 for silt, and 1.40-2.20 for clay. The bulk density value input to sesoil is applied as one value for the entire soil column (average dry soil bulk density (g/cm^3) for the entire soil profile). Soil columns A and B are primarily sand and silt, so value set equal to $5g/cm^3$.

2 Intrinsic permeability for silt was taken from the default SESOIL database. Intrinsic permeability for clayey sand was assigned based upon site knowledge and client-specified professional judgement.

3 Effective Porosity values assigned from SESOIL database for silt and clayey sand.

4 The Freundlich exponent describes with how soil sorption varies with increasing contaminant load. At low concentrations sorption is linear. However, as contaminant load is increased sorption decreases, eventually the soil becomes saturated. Given that most residual contaminant concentrations are significantly below soil saturation limits, sorption is assumed to be linear (i.e. the Freundlich exponent is 1.0).

8b. Other SESOIL Input Parameters (Notes Continued)

[5] Solubility values assigned from experience at other Formerly Utilized Sites Remedial Action Program (FUSRAP) sites and specified from client. Values for U, Ra and Th were modeled using the PHREEQC code for the Luckey site, and the value for Mo was modeled for the Niagara Falls Storage Site (NFSS) site using the MINTEQA2 modeling code. Assigned values were the highest solubilities reported for these COPCs for Lucky and NFSS as transmitted by client.

[6] Simulation of gaseous phase of these COPCs is not appropriate.

[7] U: Lab-estimated values from 3 tests on 3 samples (HARSHAW site groundwater and soil) ranged between 6.81 and 29.51 ml/g, with an arithmetic average of 14.03, geometric average of 12.59, standard deviation of 7.41, median of 11.76, and 95% Confidence Interval of 9.19 to 18.88 mL/g. The recommended single-use value is 14.03 mL/g with a sensitivity range of 9.19 to 18.88 mL/g, since the data are normally distributed.

Th: A pH-sensitive mechanism at HARSHAW, where groundwater has a 95% confidence Interval of 6.25 to 6.66. The Kds for Th may be a little lower than expected (the Kd for Th rises as pH goes through 9). The HGL-based NFSS study showed Kds for GW in the pH=6.5 range to vary between 0.5 and 9.0 mL/g, however this is highly unlikely because we would see it more in the GW (collocated with U maybe). The EPA 402-R-99-004B document* (the 2 volume set) shows several values more coincident with our conditions (soil and GW chem); those data range between 207 and 15,000 mL/g, with a four-number average of 3085 mL/g (and a geometric mean of 3663 mL/g). I tend to agree with the higher EPA value of 3085 mL/g because although we have high Th-230 in the GW below G-1, we do not see it migrating at high values from below G-1, unlike the U. Please add to the discussion if you have additional references.

* U.S. EPA 1999b. Volume II, "Review of Geochemistry and Available Kd Values for Cadmium, Cesium, Chromium, Lead, Plutonium, Radon, Strontium, Thorium, Tritium (3H), and Uranium. Office of Radiation and Indoor Air. Washington, DC. EPA 402-R-99-004B, August 1999.

9a. SESOIL Results – Recharge to Groundwater

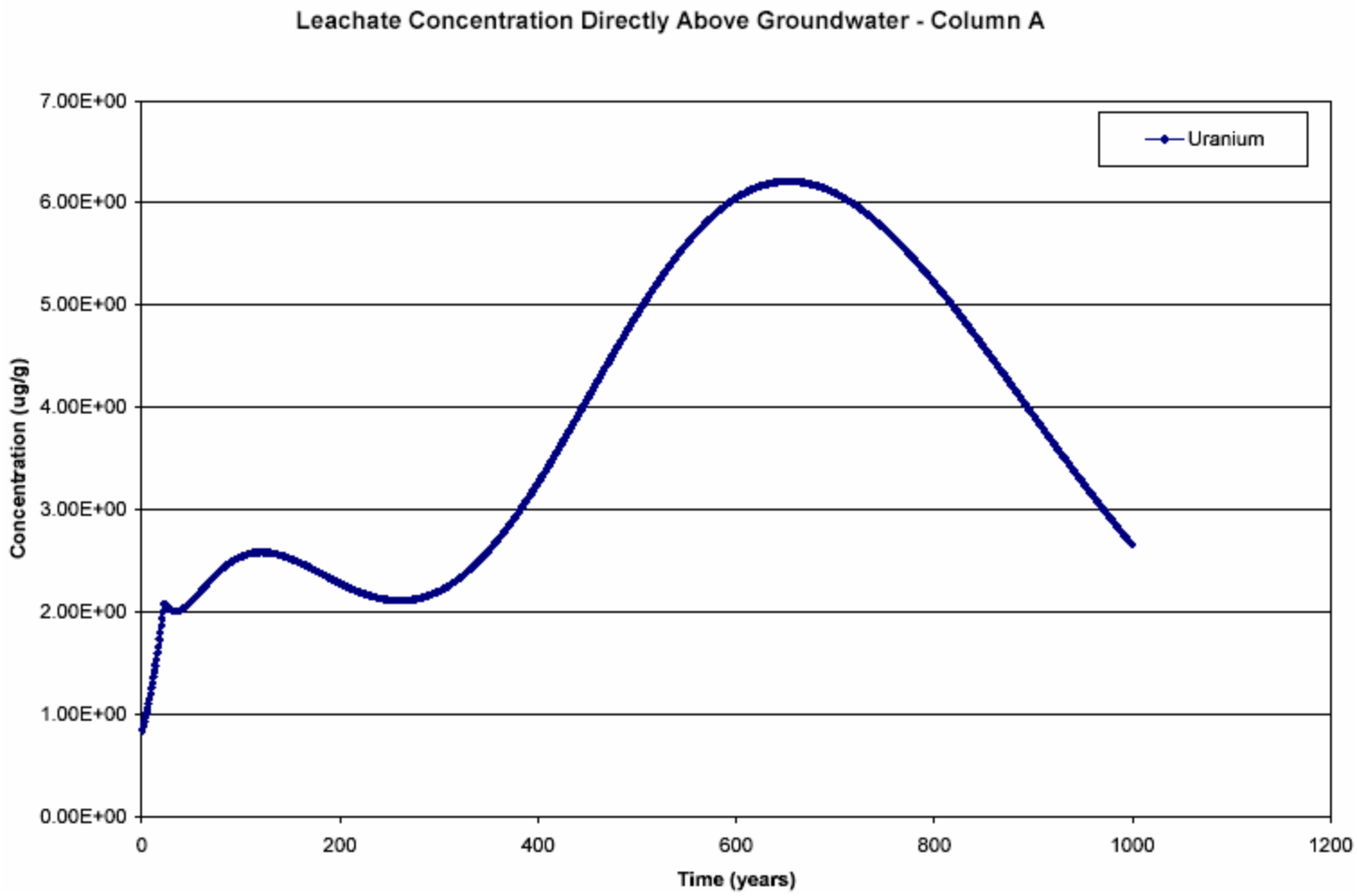
Location A SESOIL Modeled Recharge to Groundwater:

- **3.6 inches per year**

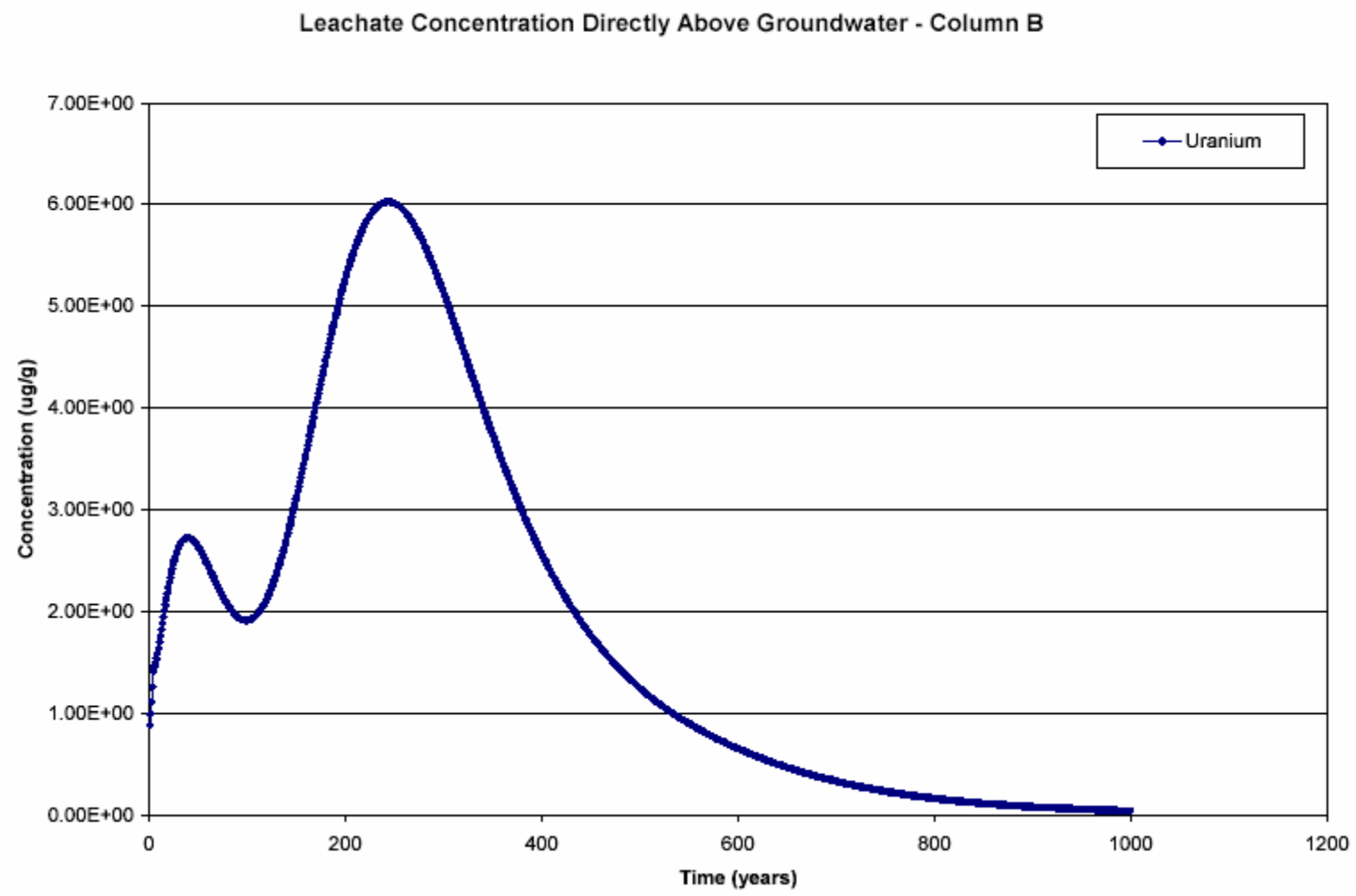
Location B SESOIL Modeled Recharge to Groundwater:

- **8.6 inches per year**

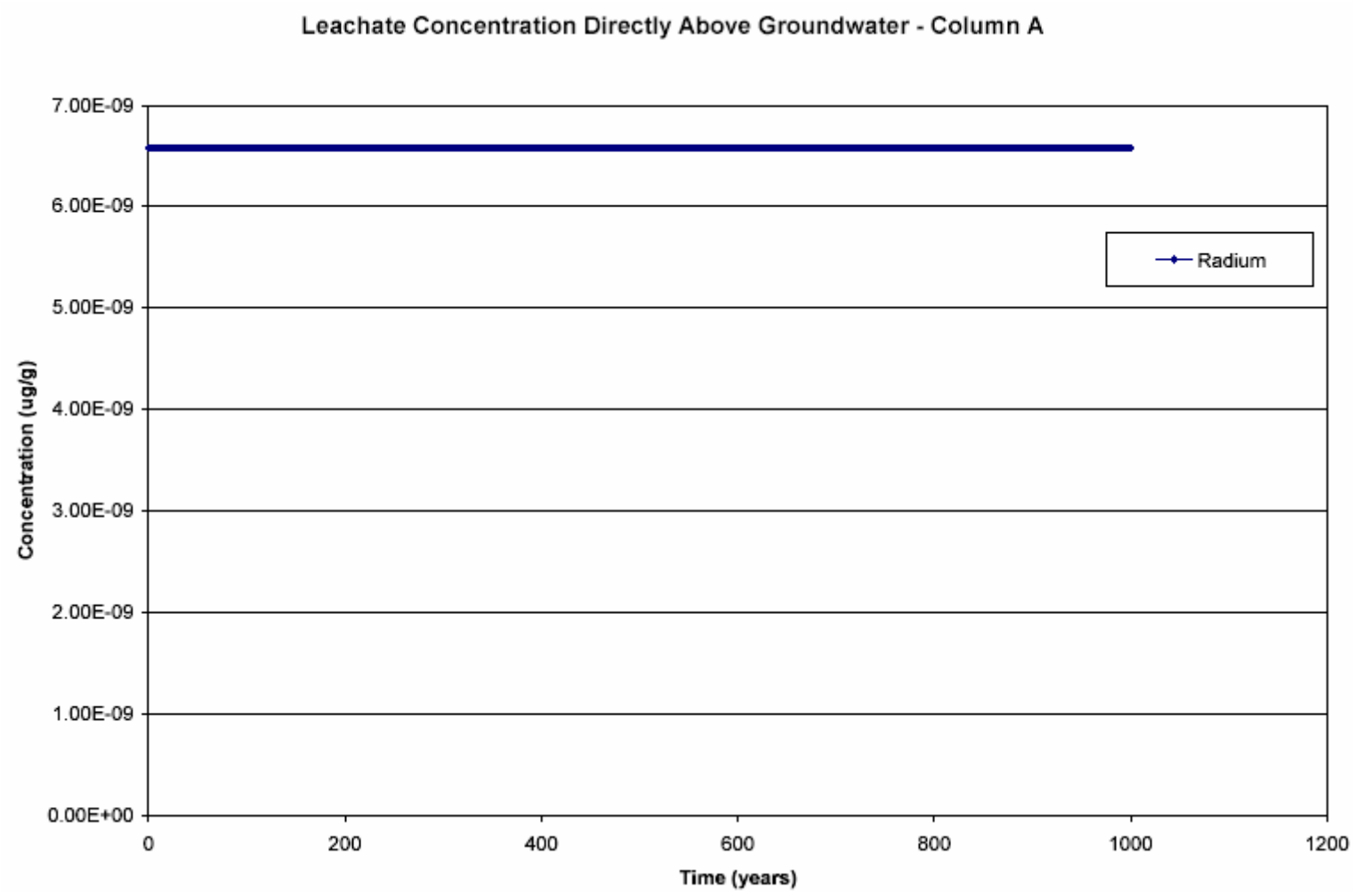
9b. SESOIL Results – Uranium in Column A



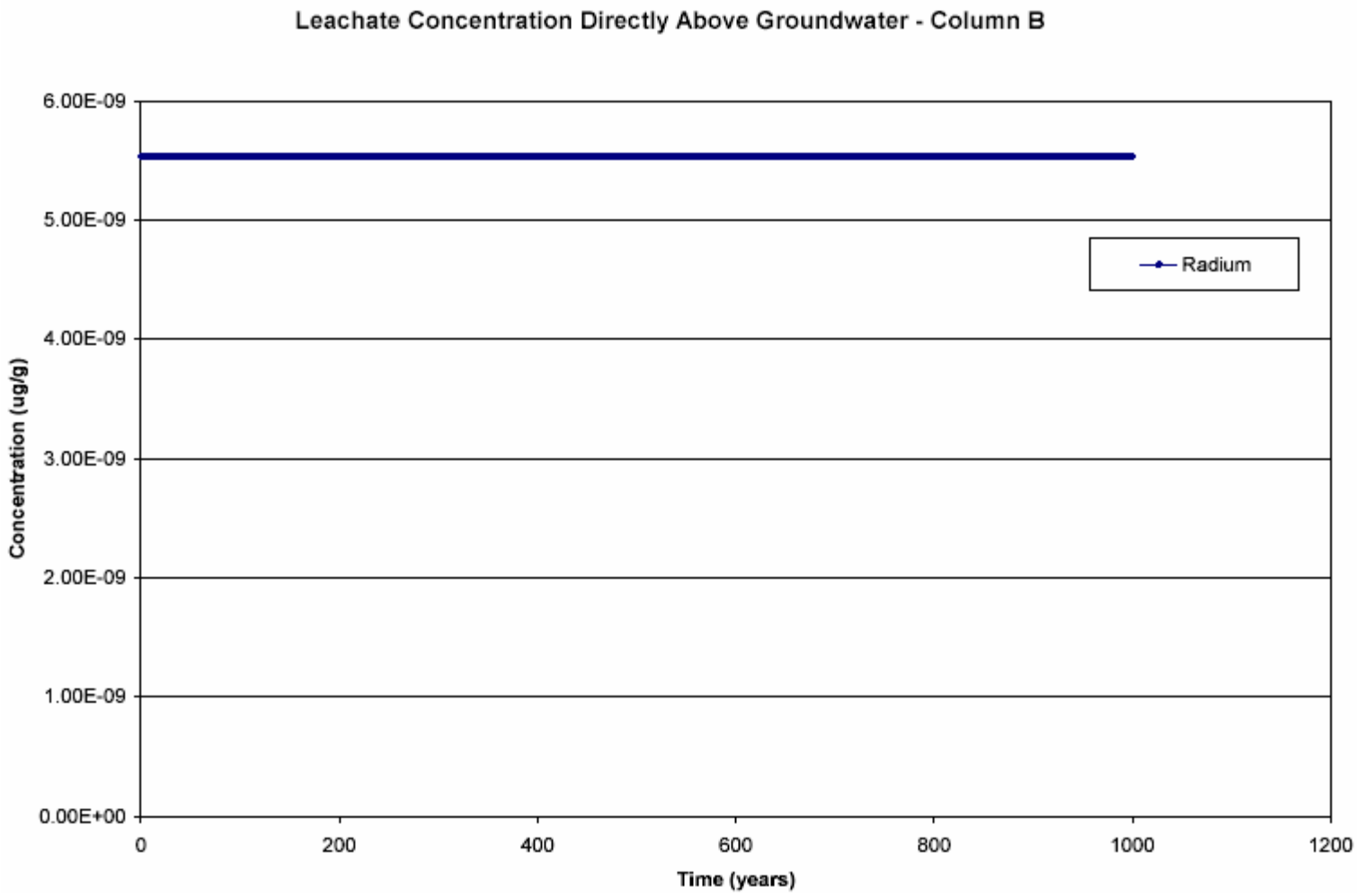
9c. SESOIL Results – Uranium in Column B



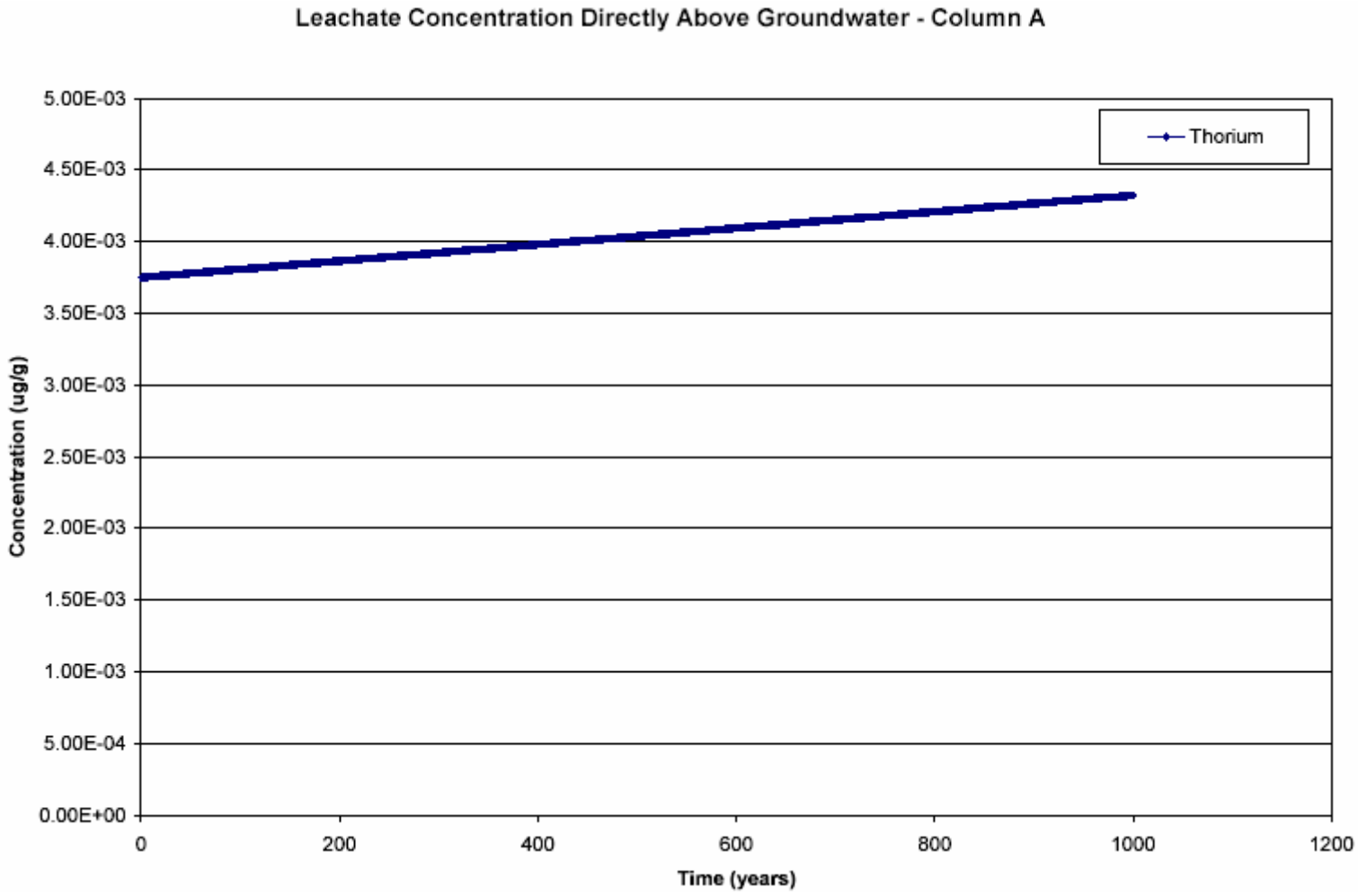
9d. SESOIL Results – Radium in Column A



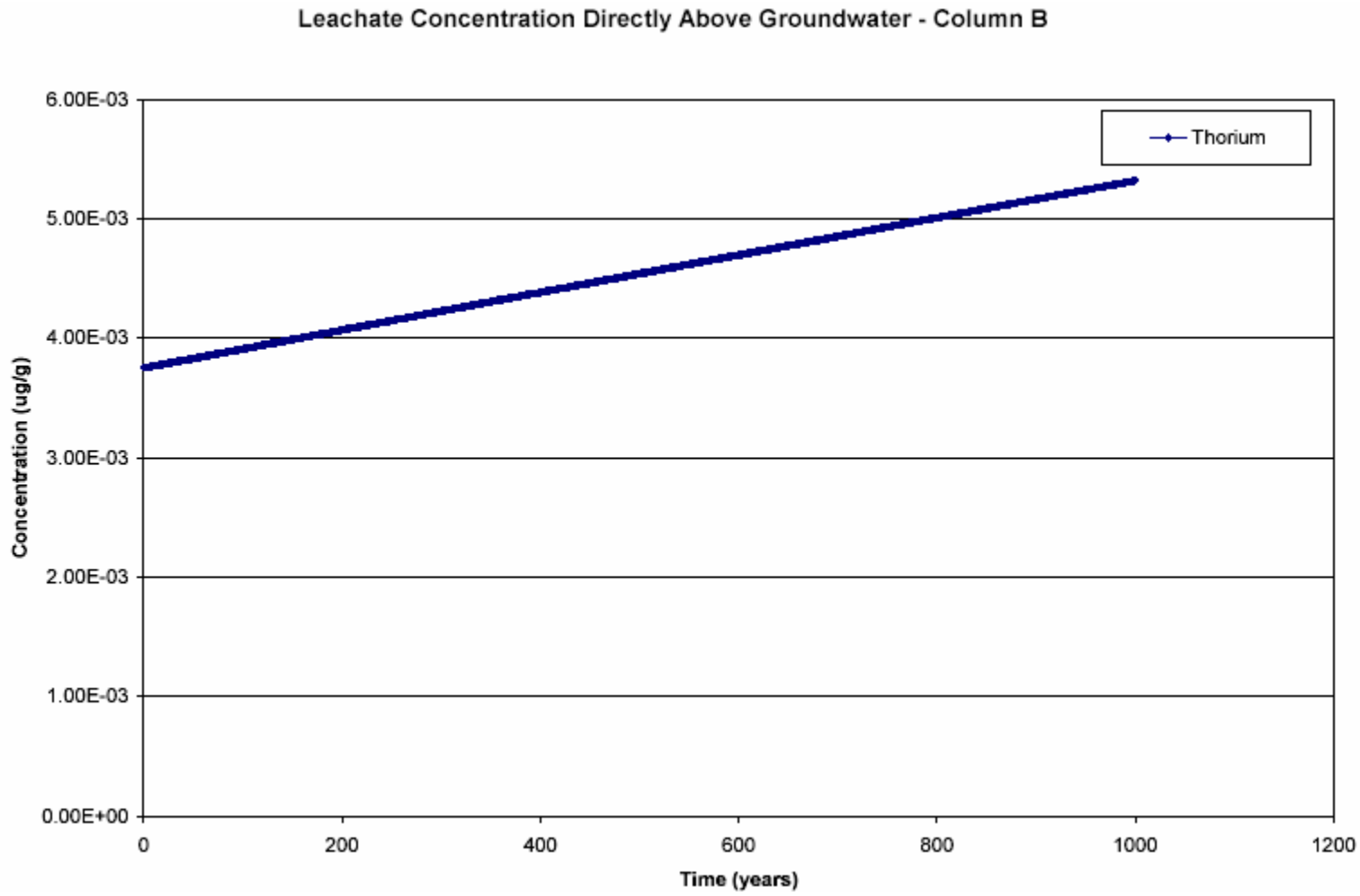
9e. SESOIL Results – Radium in Column B



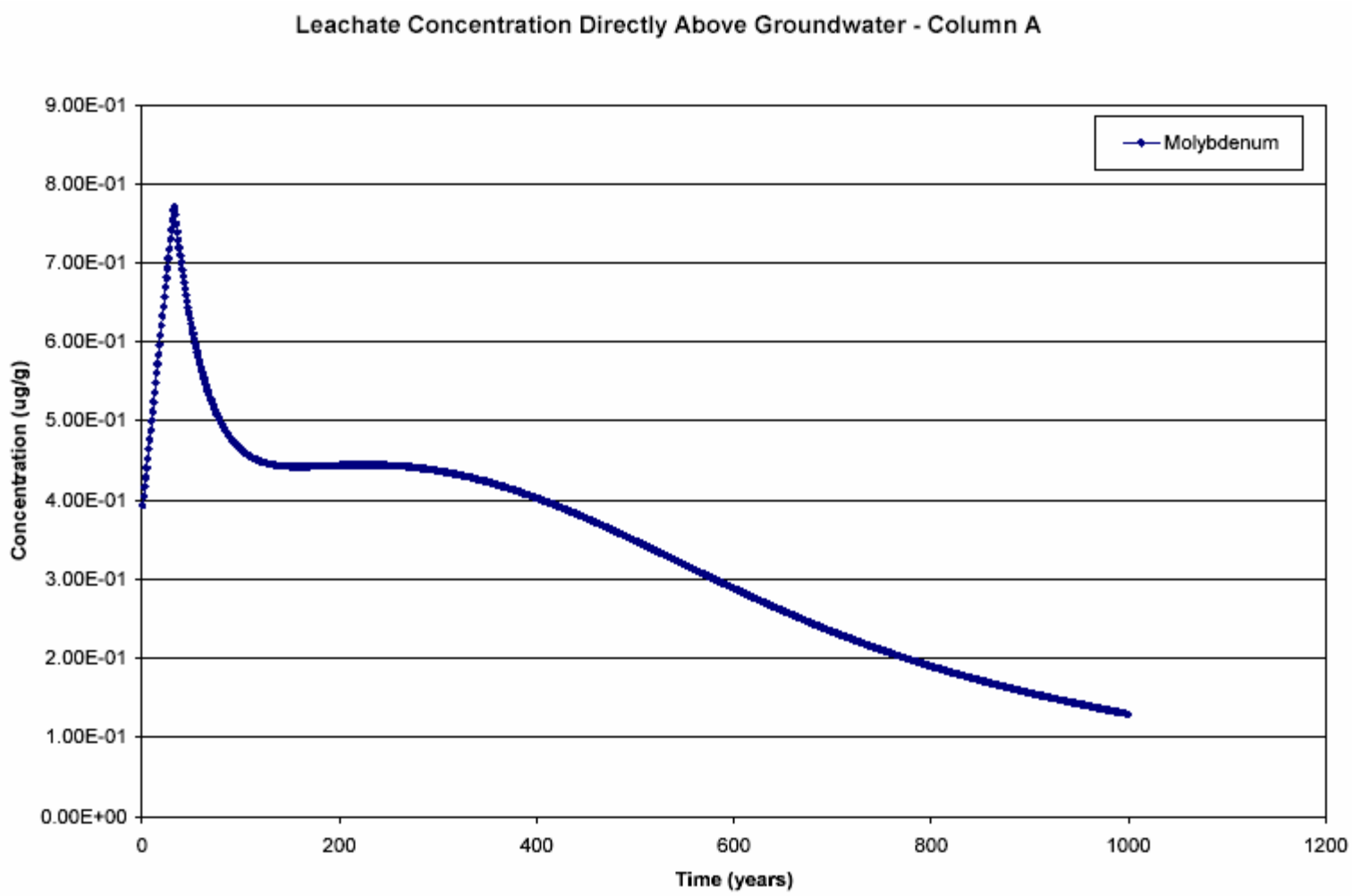
9f. SESOIL Results – Thorium in Column A



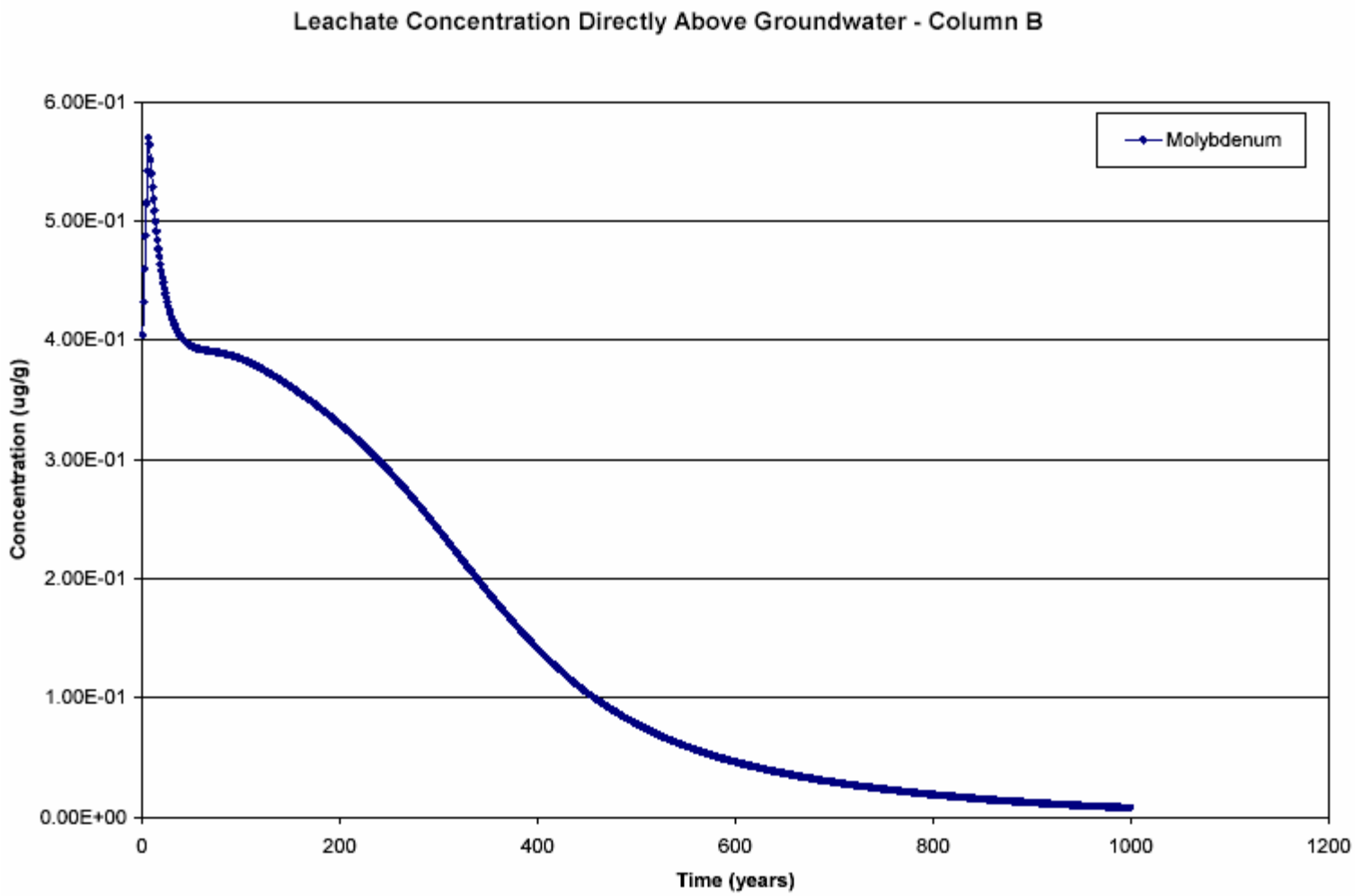
9g. SESOIL Results – Thorium in Column B



9h. SESOIL Results – Molybdenum in Column A



9i. SESOIL Results – Molybdenum in Column B



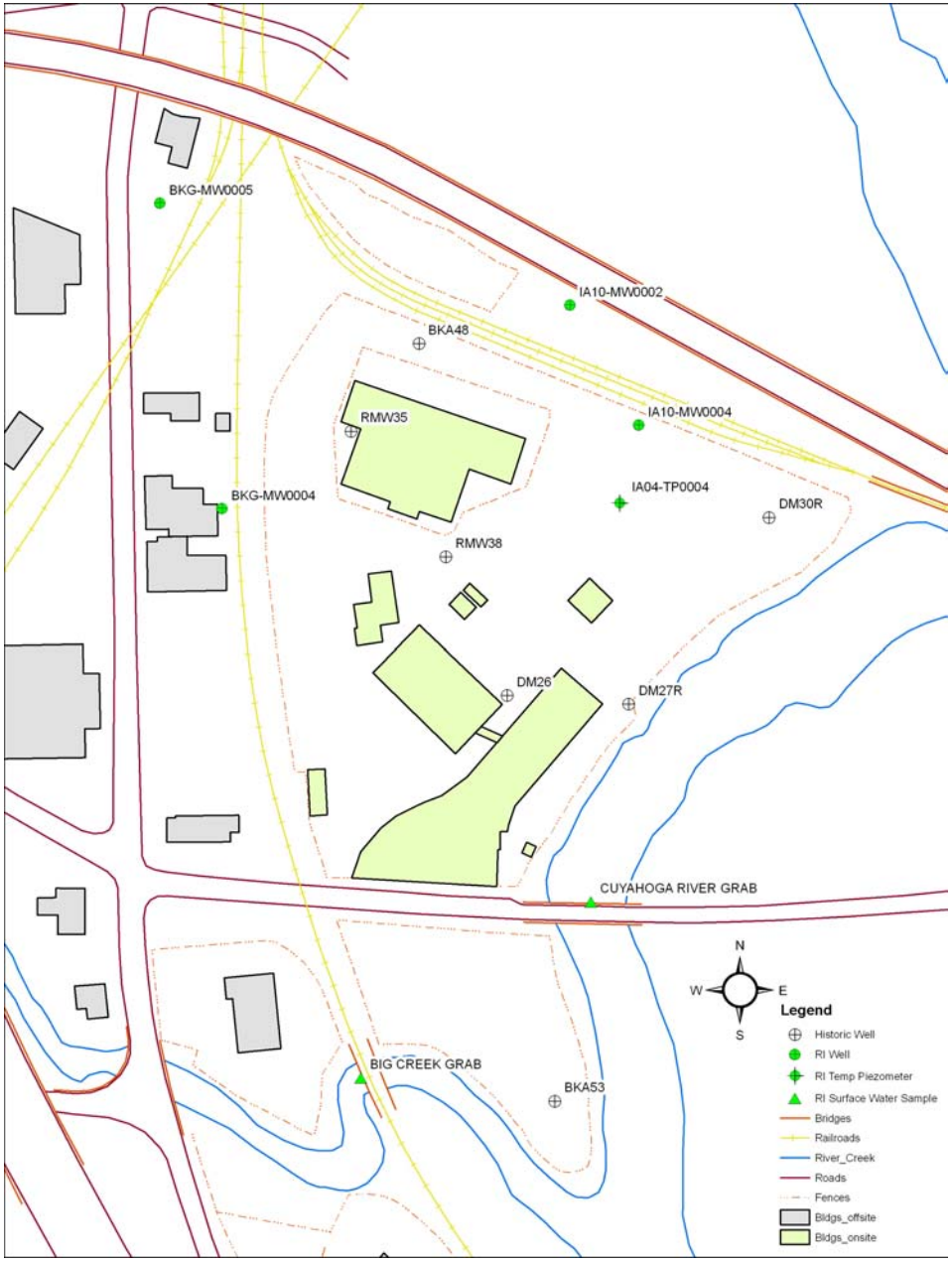
Overview

1. MINTEQ Description
2. Geochemical Model Goals
3. Geochemical Modeling Components
4. Site Groundwater Conceptual Characterization
5. Computer Code
6. MINTEQ Setup Description
7. MINTEQ Results
8. Summary

1. MINTEQ DESCRIPTION

•MINTEQA2 is an equilibrium speciation model that can be used to calculate the equilibrium composition of dilute aqueous solutions in the laboratory or in natural aqueous systems. The model is useful for calculating the equilibrium mass distribution among dissolved species, adsorbed species, and multiple solid phases under a variety of conditions including a gas phase with constant partial pressures. A comprehensive data base is included that is adequate for solving a broad range of problems without need for additional user-supplied equilibrium constants. The model employs a pre-defined set of components that includes free ions such as Na+ and neutral and charged complexes (e.g., H4SiO40, Cr(OH)2+). The data base of reactions is written in terms of these components as reactants.

2. Base Map


BKG-MW0005
IA10-MW0002
BKA48
RMW35
IA10-MW0004
IA04-TP0004
DM30R
BKG-MW0004
RMW38
DM26
DM27R
CUYAHOGA RIVER GRAB
BIG CREEK GRAB
BKA53
N
W
E
S
Legend
Historic Well
RI Well
RI Temp Piezometer
RI Surface Water Sample
Bridges
Railroads
River_Creek
Roads
Fences
Bldgs_offsite
Bldgs_onsite

2. Geochemical Modeling Goals

- Understand Concentration Levels and Trends in Groundwater Composition -- *not the purpose of this effort*
- **Identify Reactive Phases ("Inverse" Modeling)**
- Predictive Application ("Forward" Modeling) -- *not the purpose of this effort*
  - Natural Migration of Contaminants
  - Remediation Design

Geochemical modeling for Harshaw is being conducted to compliment the conceptual model of groundwater geochemistry at the site. USACE has characterized the pH, major anion/cations, contaminant distribution, and conducted Kd studies. This geochemical model effort serves as method of assimilating these parameters to further develop the conceptual model, to understand the controlling reactive mineralogical phases at the site, and to determine the speciation of U in groundwater.

3. Geochemical Modeling Components

Site Geochemical Model

- Site Data
  - **Groundwater**
    Field Parameters
    (Temperature, pH, ORP)
    Lab Measurements
    (Kd, Cw U and anions/cations, alkalinity)
    - **Solid Phase**
      Reactive Minerals
      Adsorbents
      TOC, ANP, CEC, etc.
      (Don't have)
- Computer Code
  MINTEQA2
- Conceptual Model

Overview

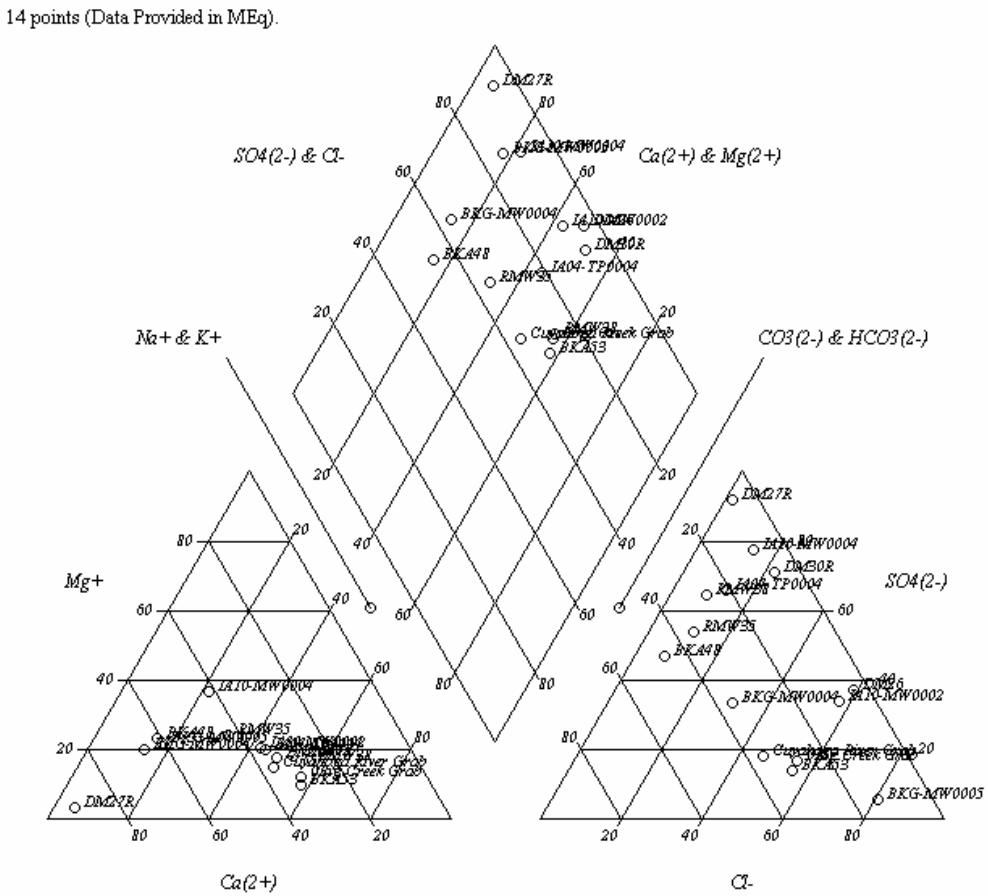
4. Site Groundwater Conceptual Characterization

- Trilinear Diagram from latest groundwater sampling event
  - Trilinear Diagrams used to graphically evaluate spatial changes in groundwater geochemistry. The following cations and anions will be used to construct the diagrams:
  - Ca, Cl, So4, Mg, Na, K, CO3, HCO3
- GW Eh = ranges from -94 to 442 mV; average is 176.35 mV
  - (Eh data corrected to the normal hydrogen electrode for standard half cell potential for the reference electrode) *based on SAIC RFI Phase I and II well development and sampling log sheets and USACE groundwater sampling field data*
- GW Temperature = ranges from 9.80 to 29.97 C; average is 16.10 C
  - *based on SAIC RFI Phase I and II well development and sampling log sheets and USACE groundwater sampling field data*
- GW pH = 6.45
  - *USACE previously indicated via email that pH at the site has a 95% confidence interval of 6.25 to 6.66*

Overview

4. Site Groundwater Conceptual Characterization Trilinear Diagram

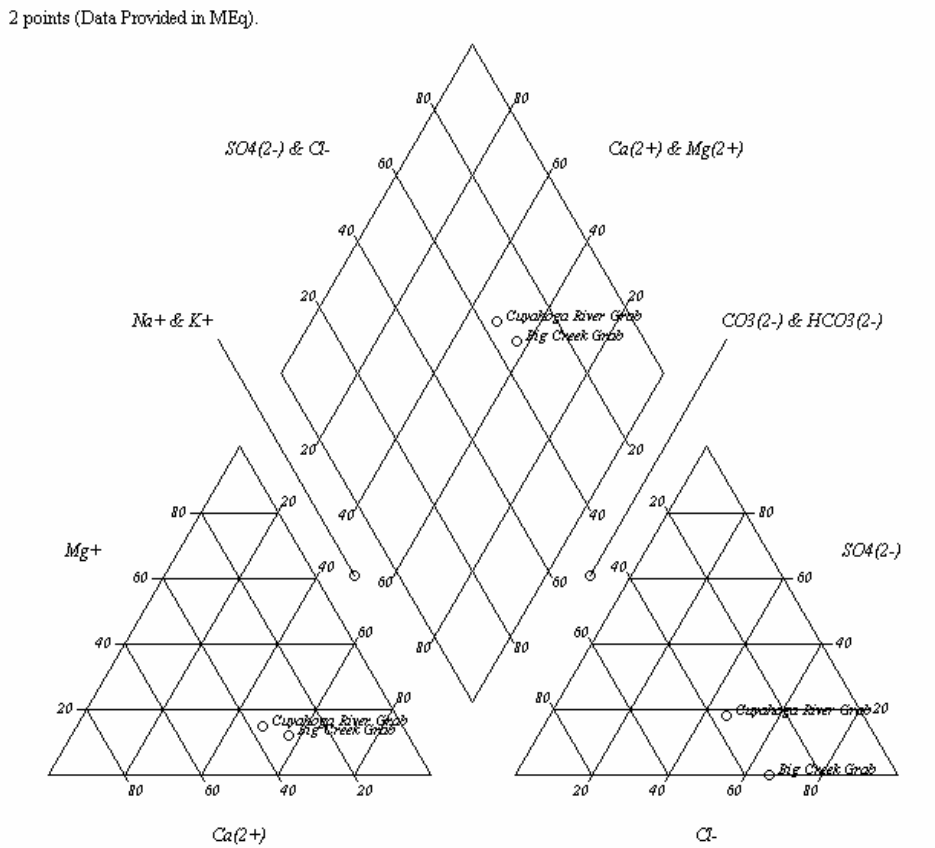
- Includes all monitoring wells (including 2 background locations) and 2 surface water grab sample locations
- Based on August 2004 groundwater sampling data
- *Site groundwater generally plots in the $Ca^{2+}Na^{+}Cl^{-}$ and $Ca^{2+}Cl^{-}$ region*



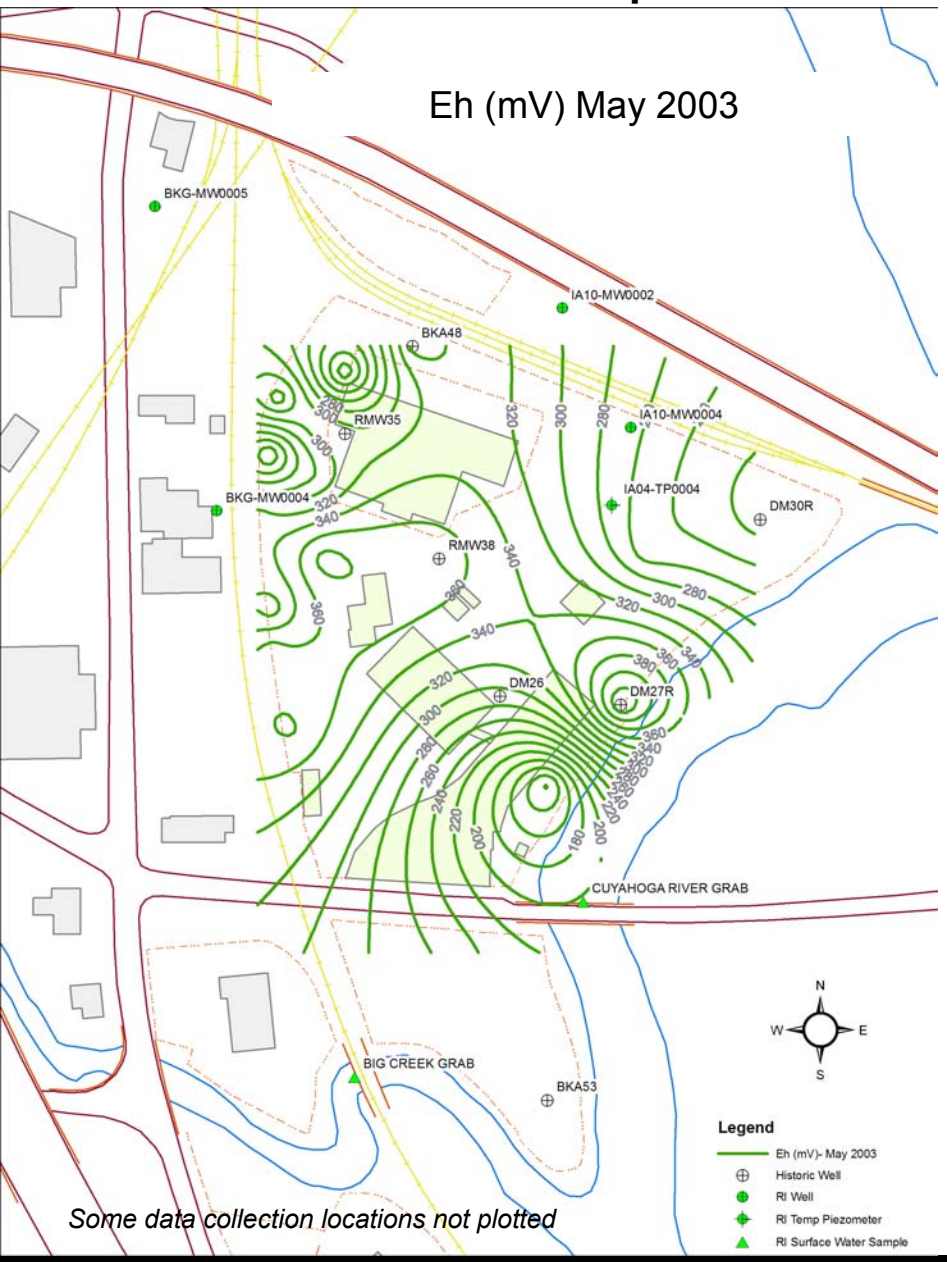
Overview

4. Site Groundwater Conceptual Characterization Trilinear Diagram, cont.

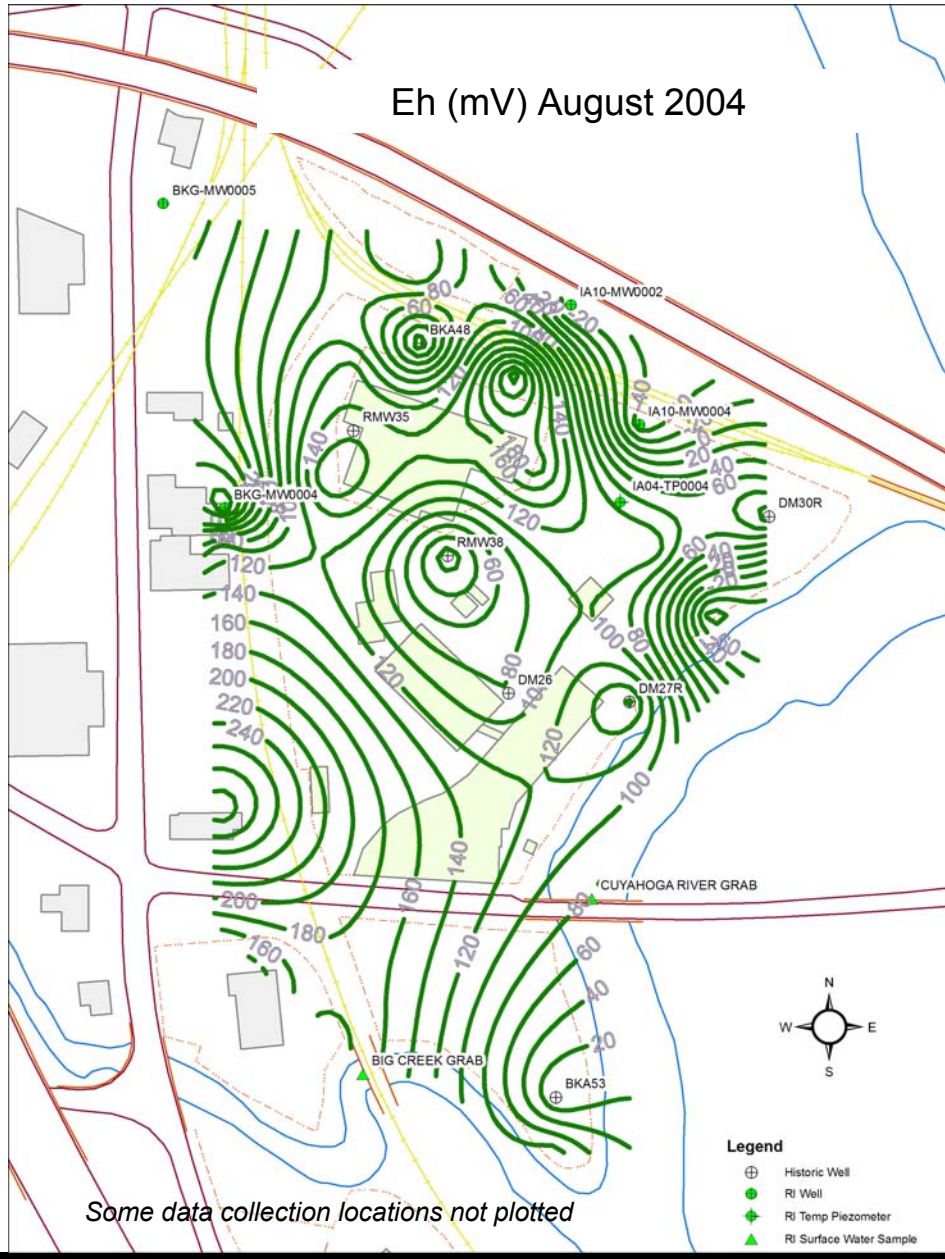
- Includes 2 surface water grab sample locations
- Based on August 2004 sampling data
- *Surface water plots in the $Ca^{2+}Na^{+}HCO_3^{-}Cl^{-}$ region*



4. Site Groundwater Conceptual Characterization - Site Eh

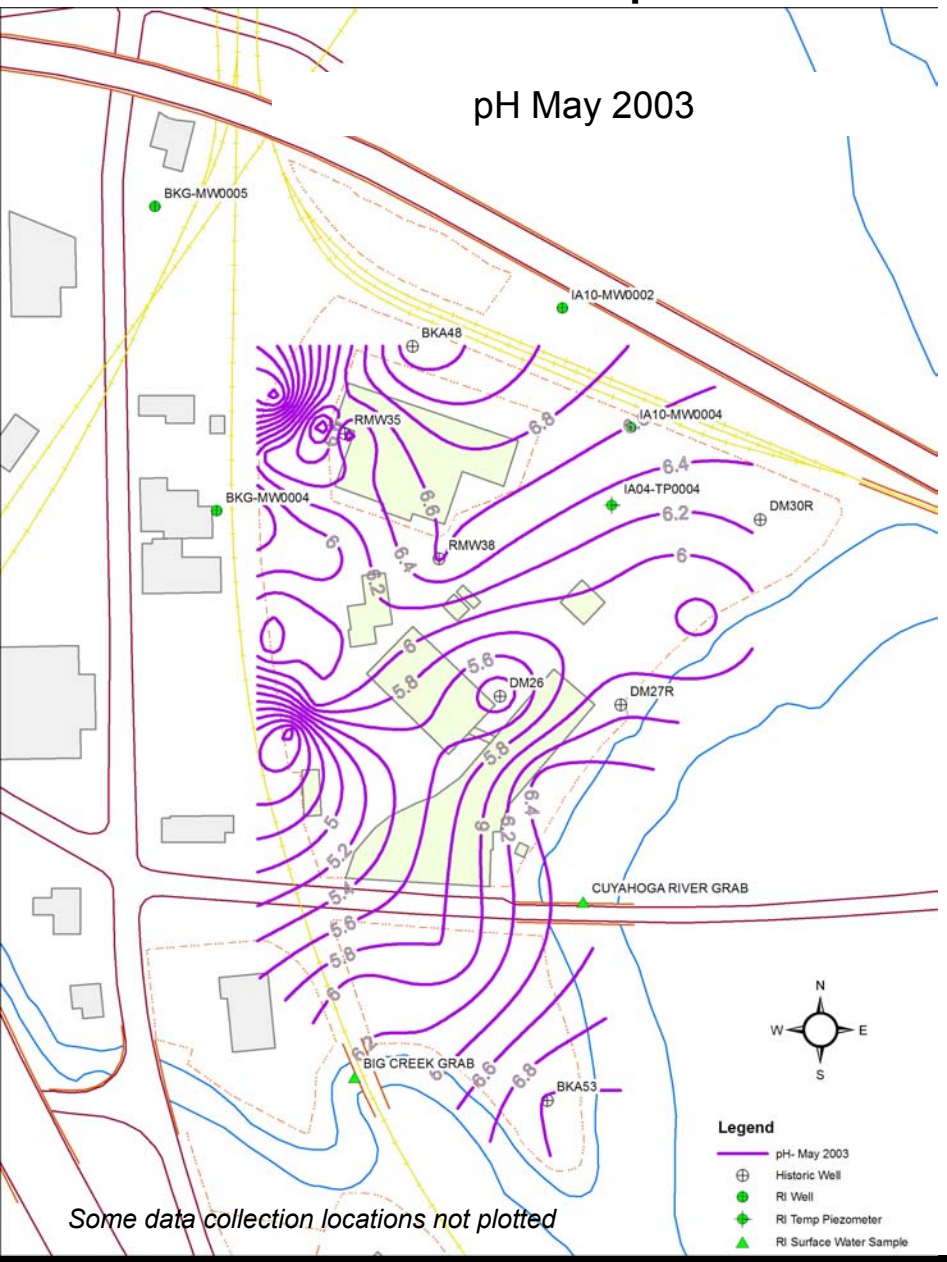


Some data collection locations not plotted

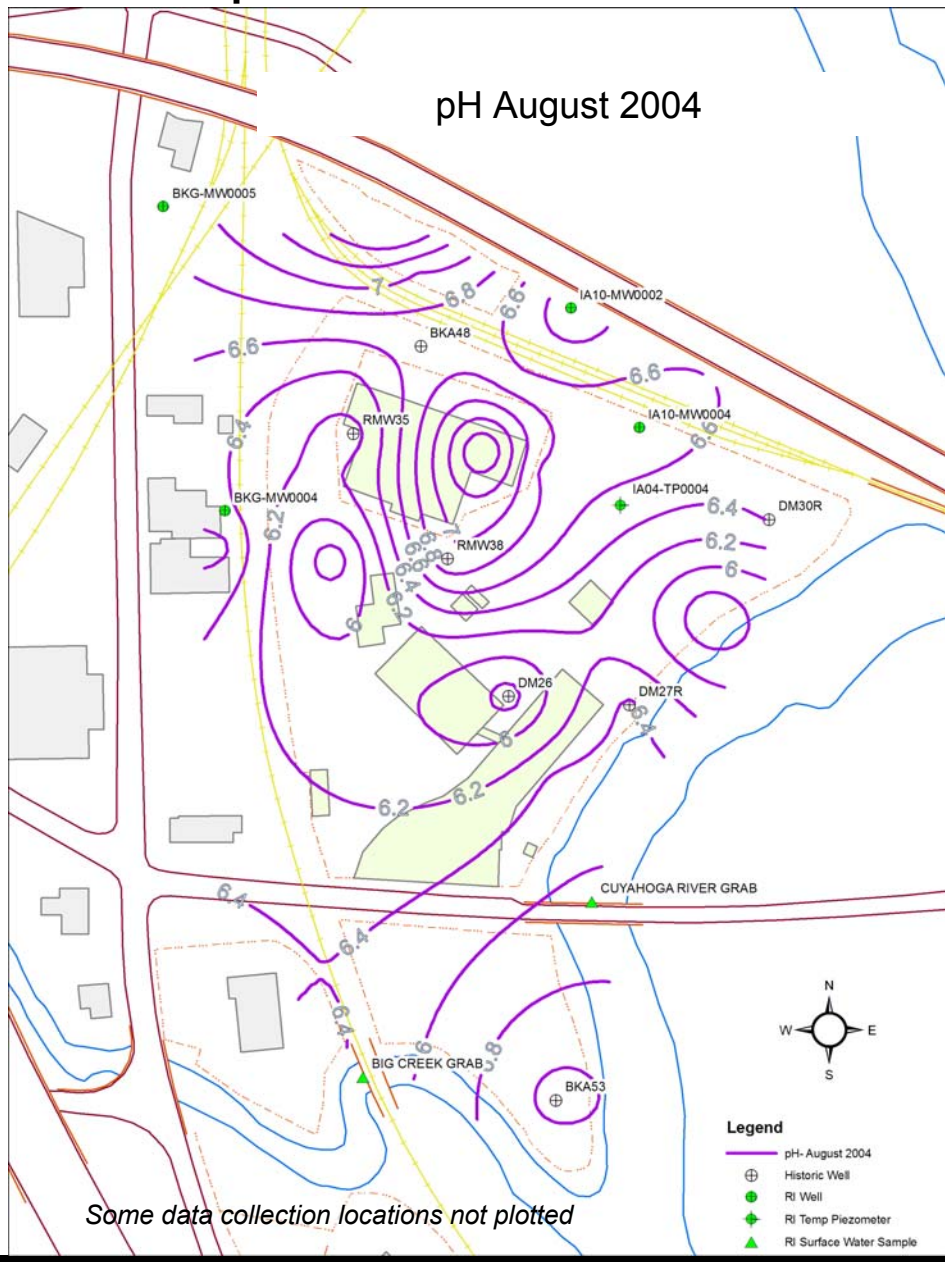


Some data collection locations not plotted

4. Site Groundwater Conceptual Characterization - Site pH

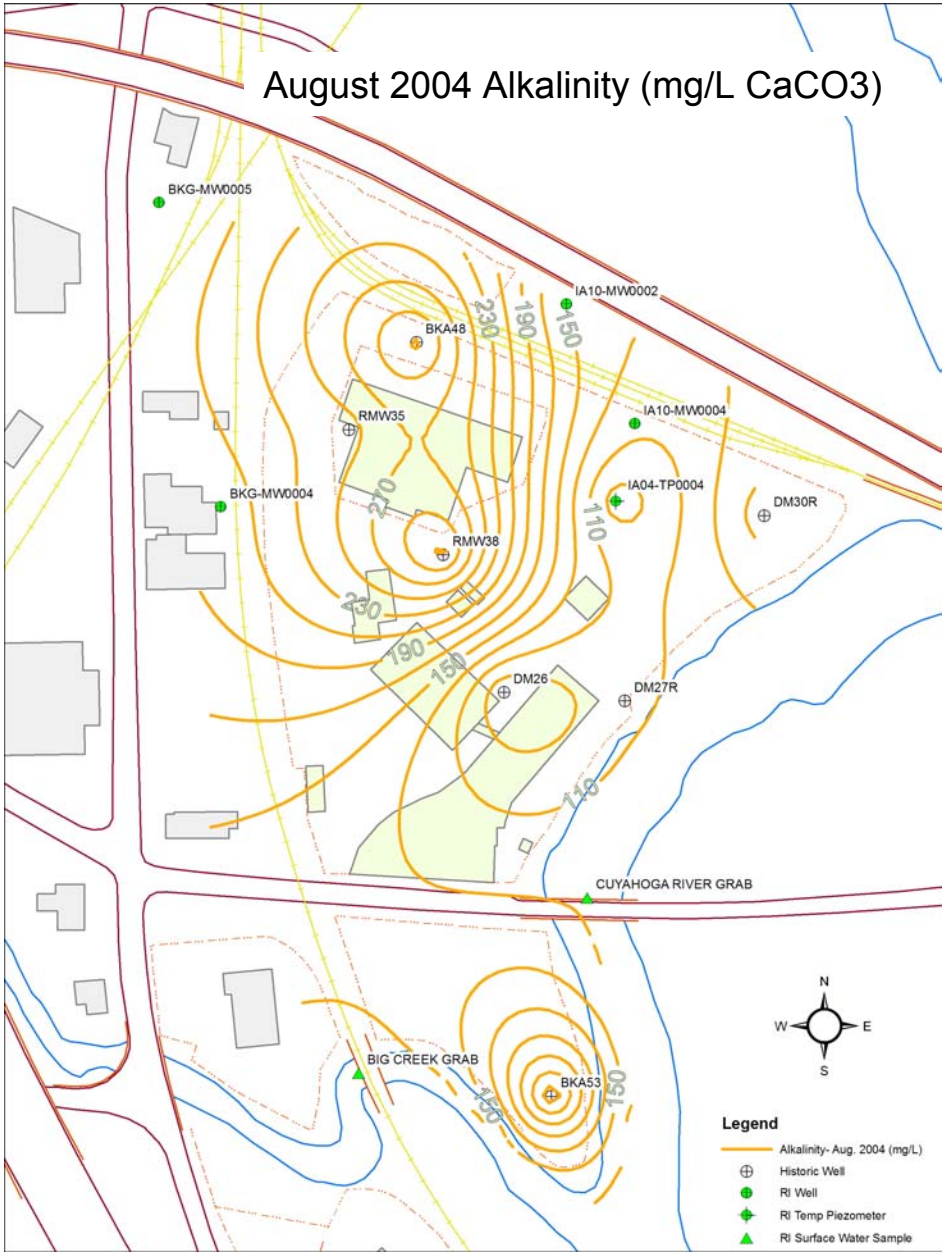


Some data collection locations not plotted



Some data collection locations not plotted

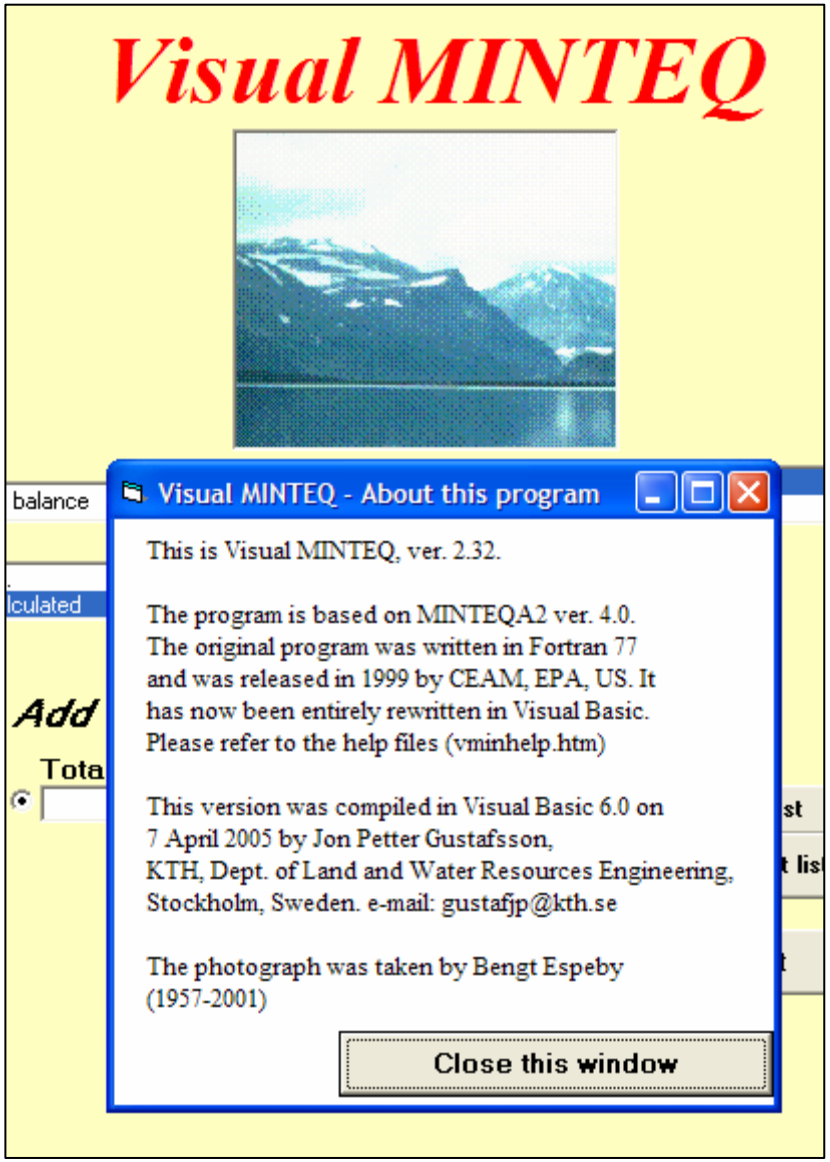
4. Site Groundwater Conceptual Characterization - Site Alkalinity



5. Computer Code

Visual MINTEQ ver 2.32

http://www.lwr.kth.se/English/OurSoftware/vminteq/#download



6. MINTEQ SETUP DESCRIPTION

General specifications for each simulation

Specified

- pH **specified**
- Temperature **specified** and **constant** at 16.10 C
- Eh **specified**
- Alkalinity **specified** per CaC03 concentrations
- Use of MINTEQ database for reactions
- Ionic Strength to be calculated per equilibrium chemistry
- Redox Couples **specified** and **constant** = Fe^{2+}/Fe^{3+}; U^{4+}/UO_2^{2+}
- Components present **specified** and **constant** = sitewide average from August 2004 USACE sampling event, except in individual well simulations

Excluded

- No surface complexation
- No organic constituents
- No DOM
- No U adsorption (not important process for speciation)

Output

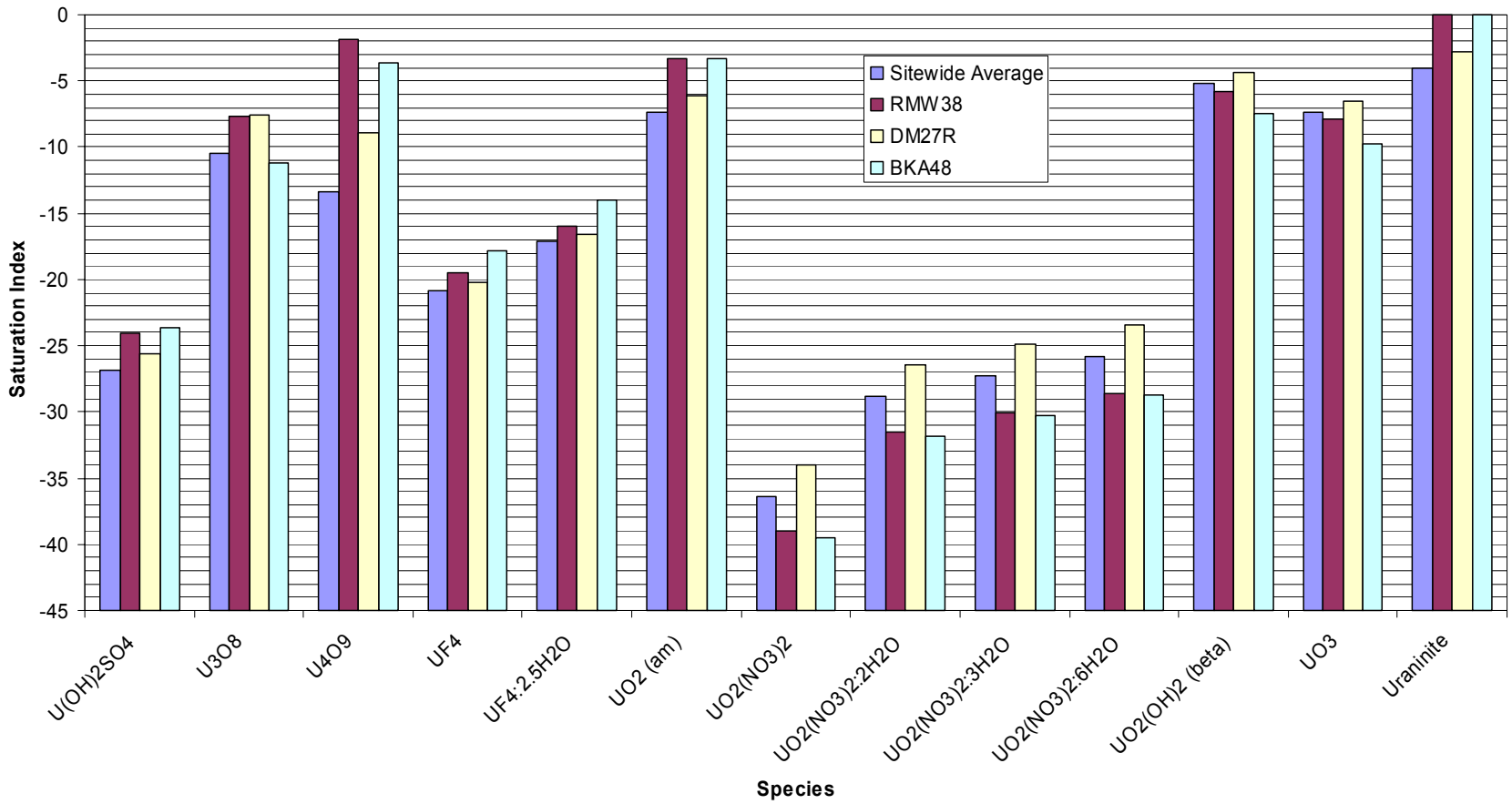
- Saturation Indices
- Dissolved Phase Speciation
- Mass Distribution
- Redox state of Uranium

6. MINTEQ SETUP DESCRIPTION, cont.

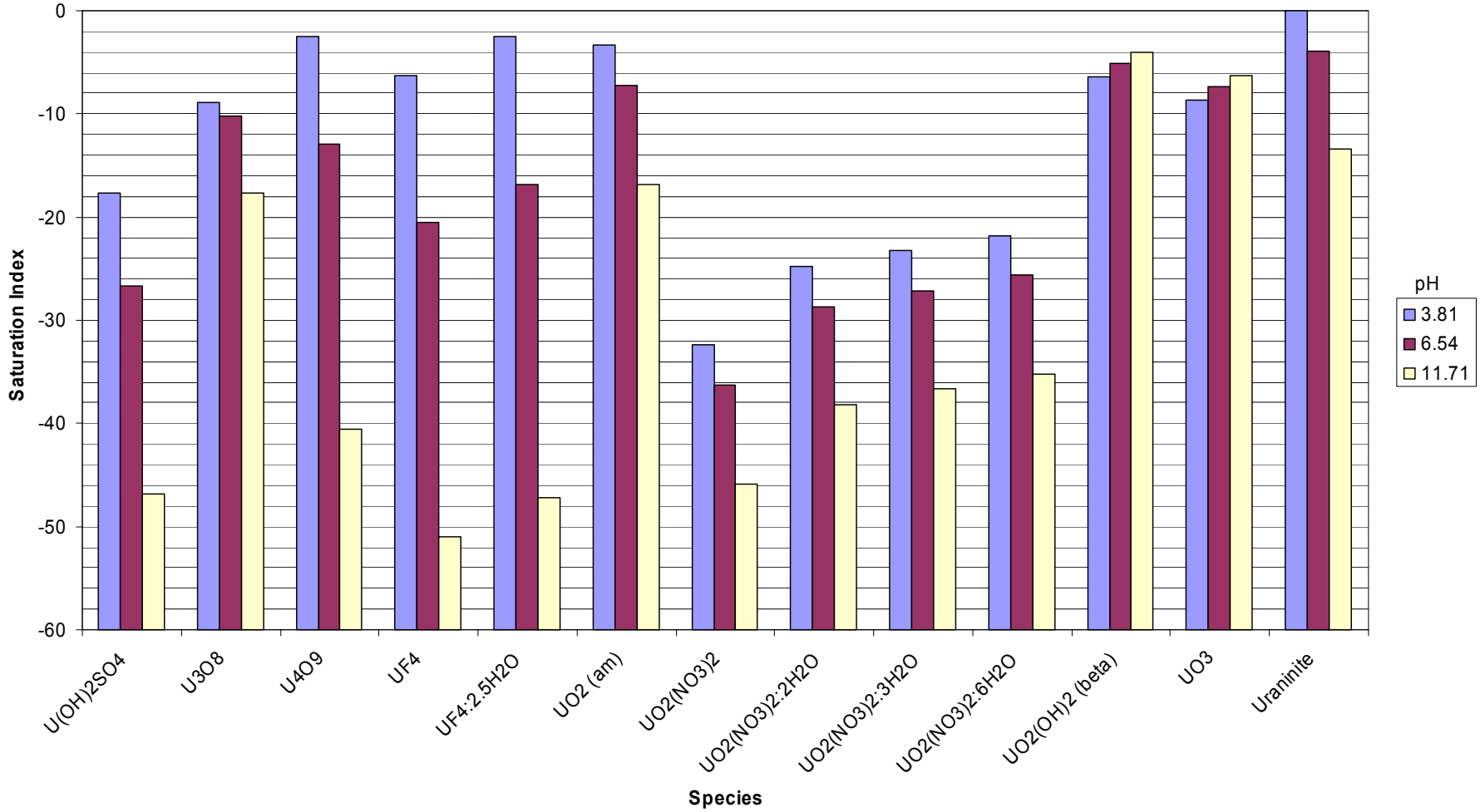
Simulation accounting

- Sitewide Average Groundwater Composition (Baseline)
  - *pH = 6.45; Eh = 176.35 mV; $CaCO_3$ = 182 mg/L;*
- Eh Sweep
  - *pH = 6.45; Eh = -94 to 56 mV and 135 to 442 mV; $CaCO_3$ = 182 mg/L;*
- pH Sweep with Li
  - *pH = 3.81 to 11.71; Eh = 176.35 mV; $CaCO_3$ = 182 mg/L;*
- pH Sweep without Li
  - *pH = 3.81 to 11.71; Eh = 176.35 mV; $CaCO_3$ = 182 mg/L;*
- Alkalinity Sweep with Li
  - *pH = 6.45; Eh = 176.35 mV; $CaCO_3$ = 79 to 316 mg/L;*
- Alkalinity Sweep without Li
  - *pH = 6.45; Eh = 176.35 mV; $CaCO_3$ = 79 to 316 mg/L;*
- Individual Well Composition (August 2004 sampling data)
  - BMW38
    - *pH = 6.98; Eh = 5 mV; $CaCO_3$ = 316 mg/L;*
  - DM27R
    - *pH = 6.44; Eh = 163 mV; $CaCO_3$ = 99 mg/L;*
  - BKA48
    - *pH = 6.69; Eh = -19 mV; $CaCO_3$ = 315 mg/L;*

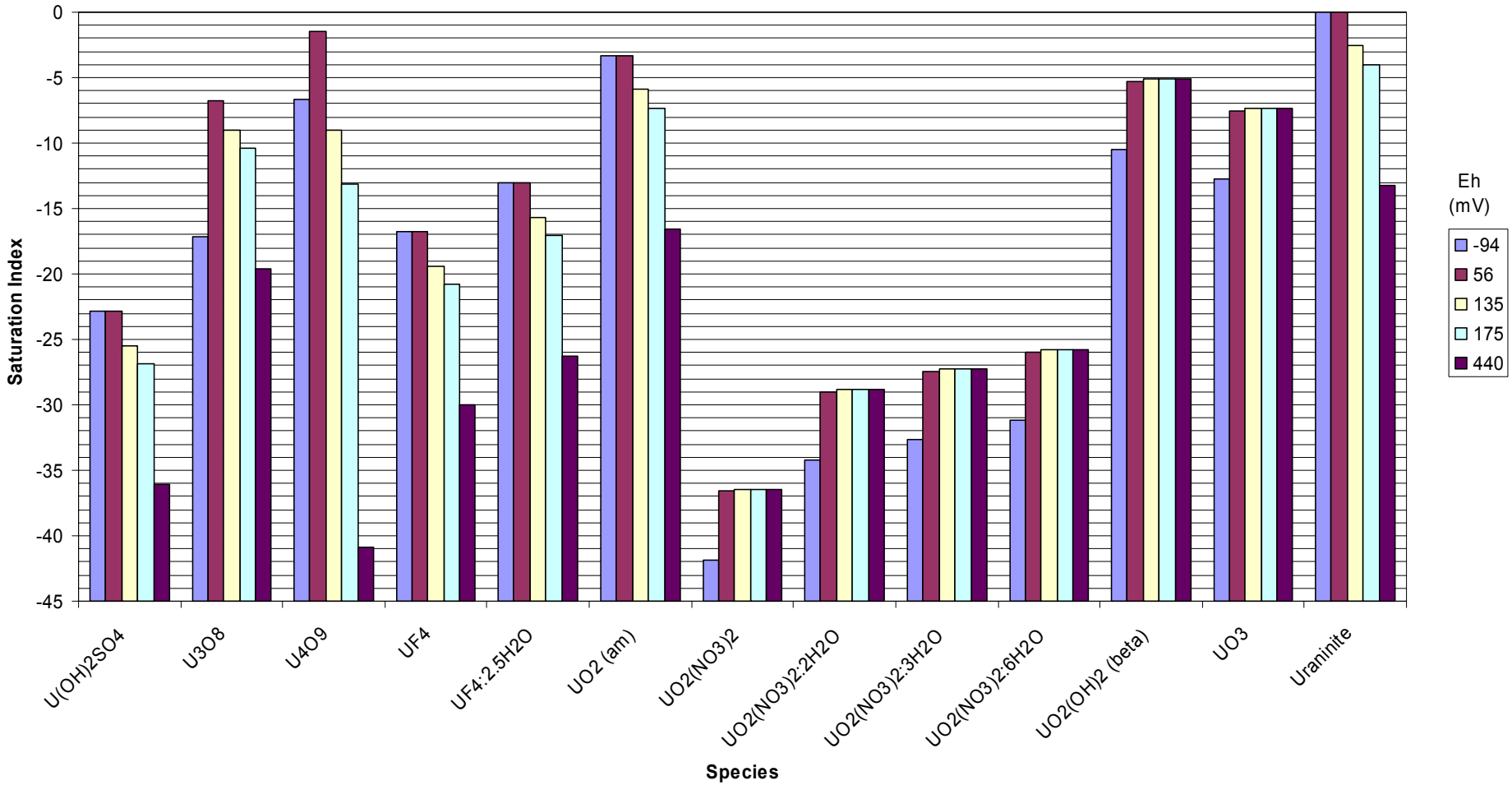
7. MINTEQ Results
Saturation Indices for Uranium-containing Species in Representative Wells



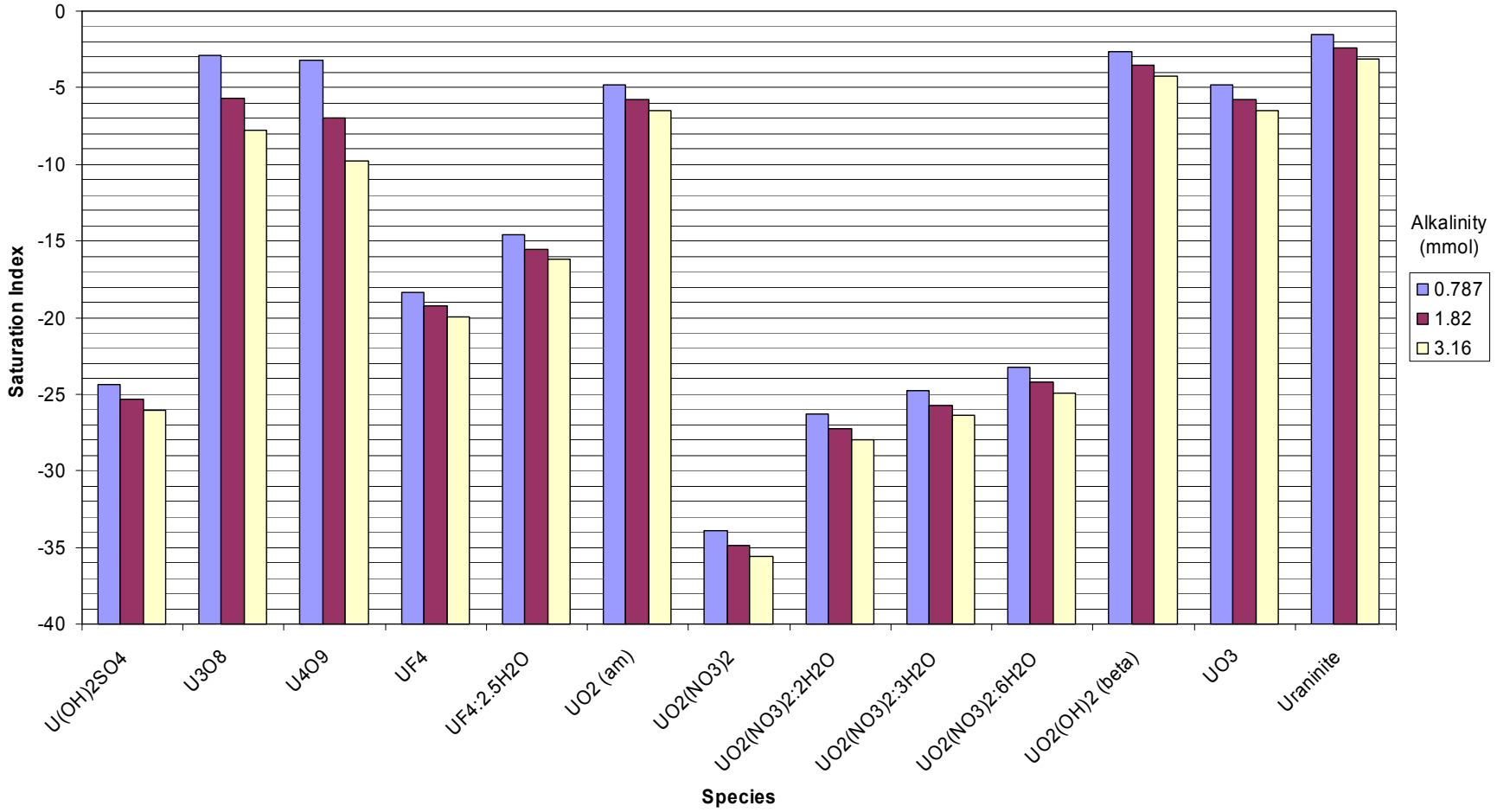
7. MINTEQ Results
Saturation Indices for Uranium-containing Species at Varying pH, based on Sitewide Average Component Concentrations



7. MINTEQ Results
Saturation Indices for Uranium-containing Species at Varying Eh, based on Sitewide Average Component Concentrations



7. MINTEQ Results
Saturation Indices for Uranium-containing Species at Varying Alkalinity, based on Sitewide Average Component Concentrations

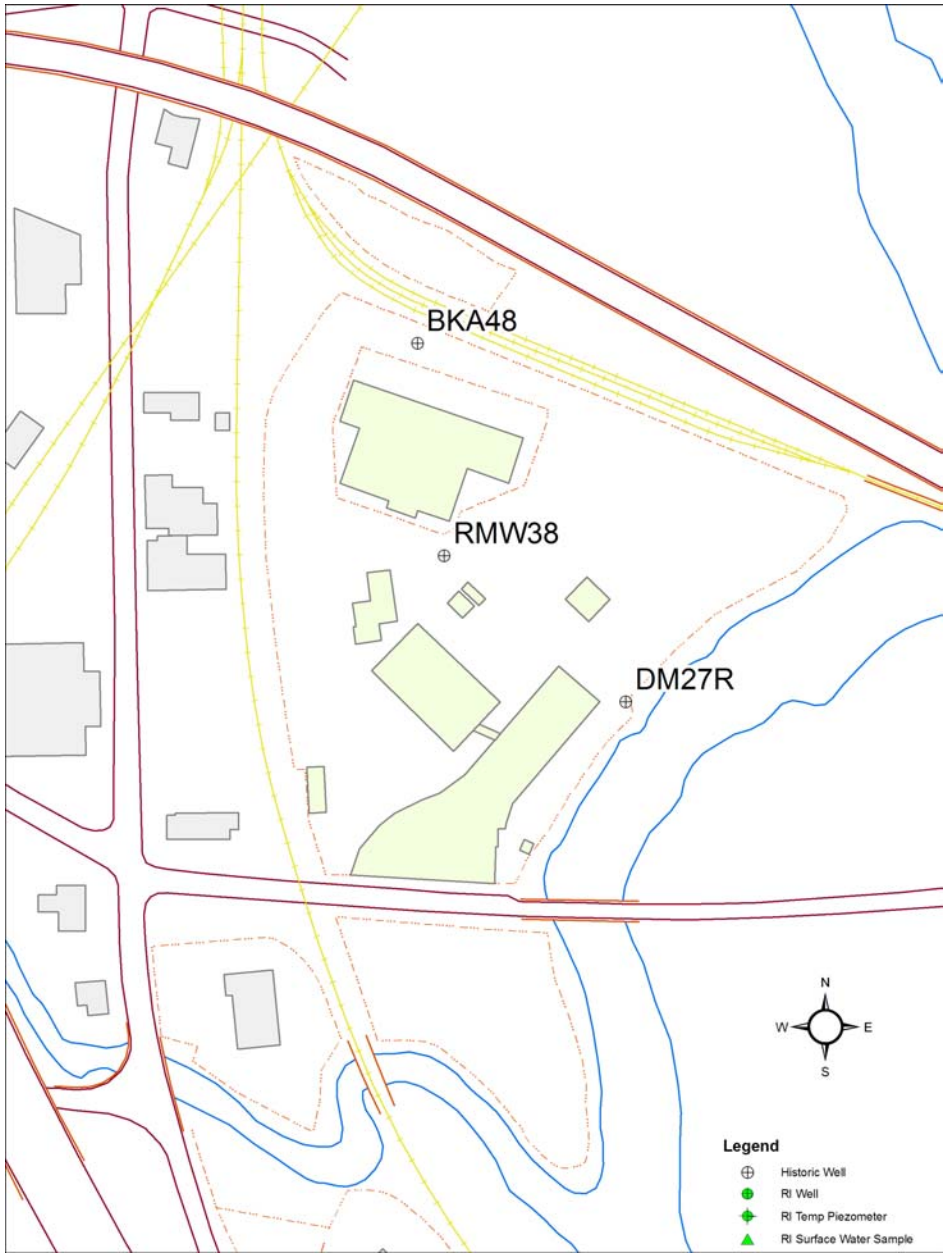


7. MINTEQ Results
Concentration (molal) of U+4 and U+6 in Representative Wells

Valence State	Sitewide Average		RMW38		DM27R		BKA48	
U+4	5.2974E-19	0.00%	7.1408E-07	52.13%	6.6122E-18	0.00%	1.6873E-05	99.90%
U+6	4.0708E-07	100.00%	6.5567E-07	47.87%	1.6597E-06	100.00%	1.7709E-08	0.10%

Eh	176	5	163	-19
pH	6.45	6.98	6.44	6.69

7. MINTEQ Results Locations of Representative Wells



7. MINTEQ Results
Concentration (molal) of U+4 and U+6 at Varying pH, Eh, and Alkalinity using Component Concentrations from Sitewide Averages

	Varying pH			Varying Eh (mV)					Varying Alkalinity (mmol)		
	3.18	**6.41**	**11.71**	**-94**	**56**	**135**	**175**	**440**	**0.787**	**1.82**	**3.16**
U+4	9.8881E-08	6.7E-19	1.96E-28	4.07E-07	1.33E-07	1.46E-17	5.9E-19	3.44E-28	1.76E-16	2.01E-17	4.06E-18
% of total	24%	0%	0%	100%	33%	0%	0%	0%	0%	0%	0%
U+6	3.082E-07	4.07E-07	4.07E-07	1.62E-12	2.74E-07	4.07E-07	4.07E-07	4.07E-07	4.07E-07	4.07E-07	4.07E-07
% of total	76%	100%	100%	0%	67%	100%	100%	100%	100%	100%	100%

8. Summary

- Evaluated groundwater geochemistry by producing trilinear diagrams and mapping field parameters

- Used MINTEQ to evaluate uranium speciation using average component measurements

- Examined cation/anion balance
  - Error generally less than 1% under pH and Eh values representative of site conditions

- Results of MINTEQ simulations indicate:
  - Eh and pH are major controlling factors of Uranium speciation at the site
  - Eh speciation breakpoint determined to be between 56 and 135 mV
  - In some areas where the groundwater has low pH and Eh, uraninite precipitation will occur
  - At high pH (e.g. 11.71), uranium hydroxals are the only complex.