Headquarters U.S. Air Force

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OT071 Hydrus Model Proposed Setup and Calibration

Former George Air Force Base
September 2017
Sacramento, CA

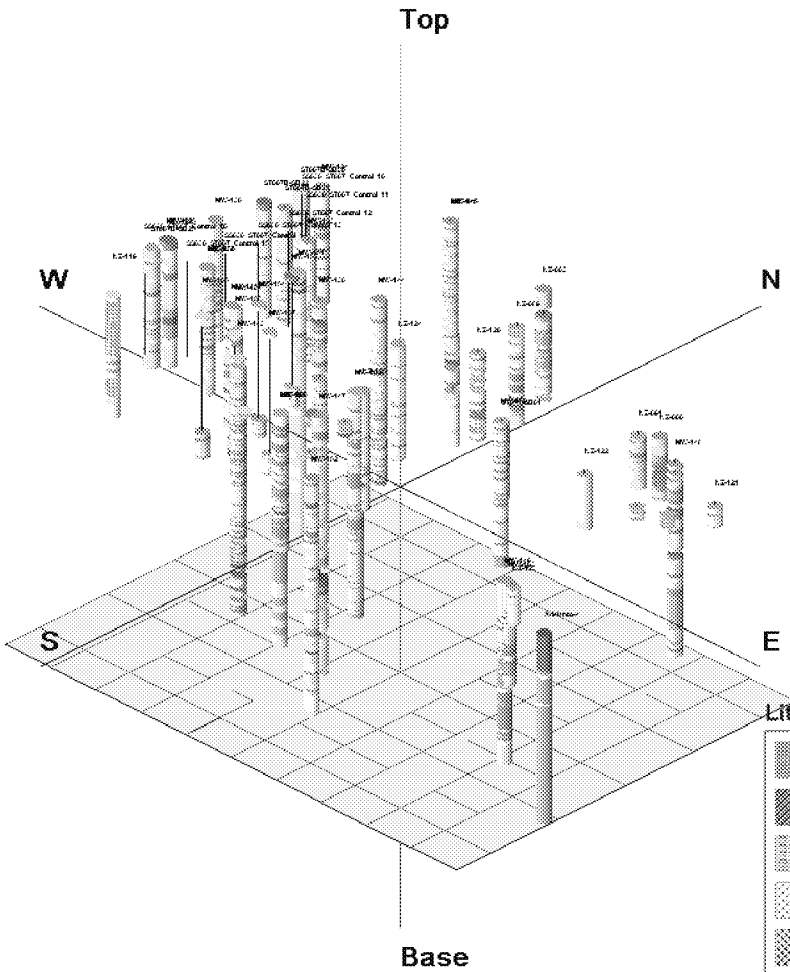
ED_003054_00003448-00001

Overview

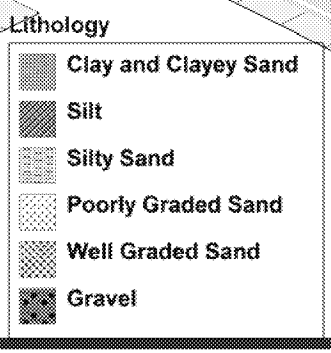
- Purpose of the modeling—Develop concept of how dieldrin migrates and develop tool for remediation analysis
- Key input parameters
  - Lithology
  - Precipitation, evapotranspiration, and artificial recharge
  - Soil geotechnical parameters (previously discussed)
  - Hydraulic conductivity—laboratory and field testing (previously discussed)
- Flow and transport modeling process
  - Stage 1 simple model
    - Define key Dieldrin colloidal transport parameters
    - Recharge from historical irrigation areas—housing, golf course, water tower pond
  - Stage 2 complex model
    - 2D larger area model
    - Incorporate detailed lithology along section line
    - Recharge and colloidal transport parameters from Stage 1 model
    - Calibration goal is to replicate observed Dieldrin plume

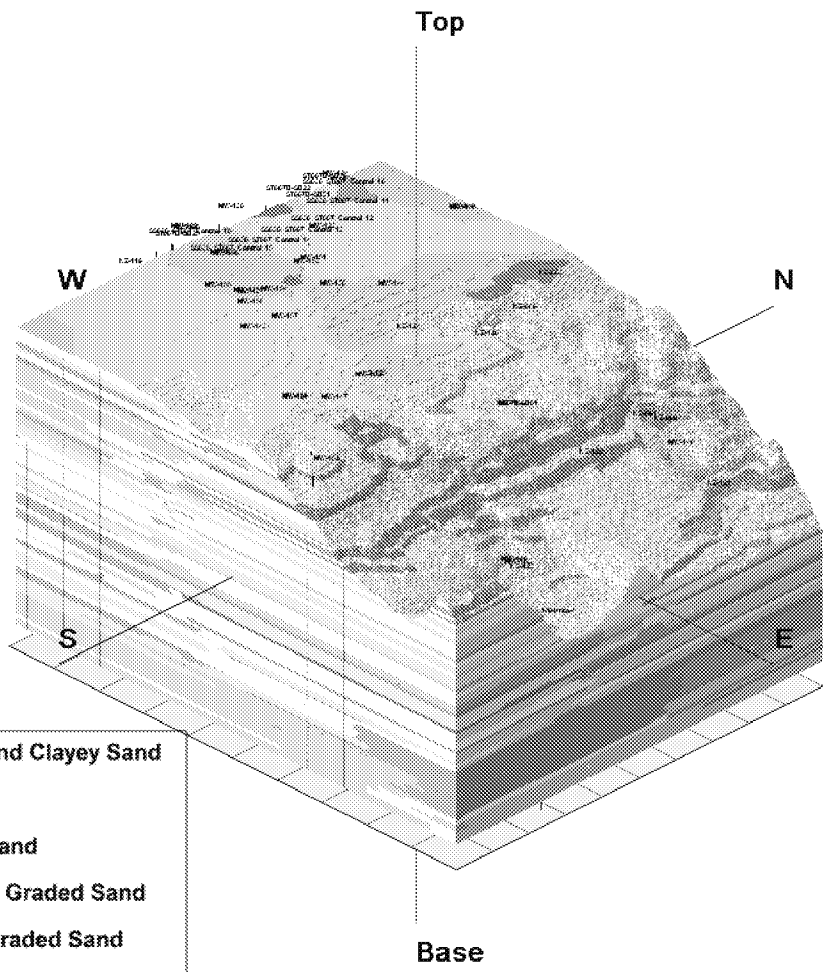
Lithology

OT071 Lithology Model



Input Boring Logs





Resulting Block Model

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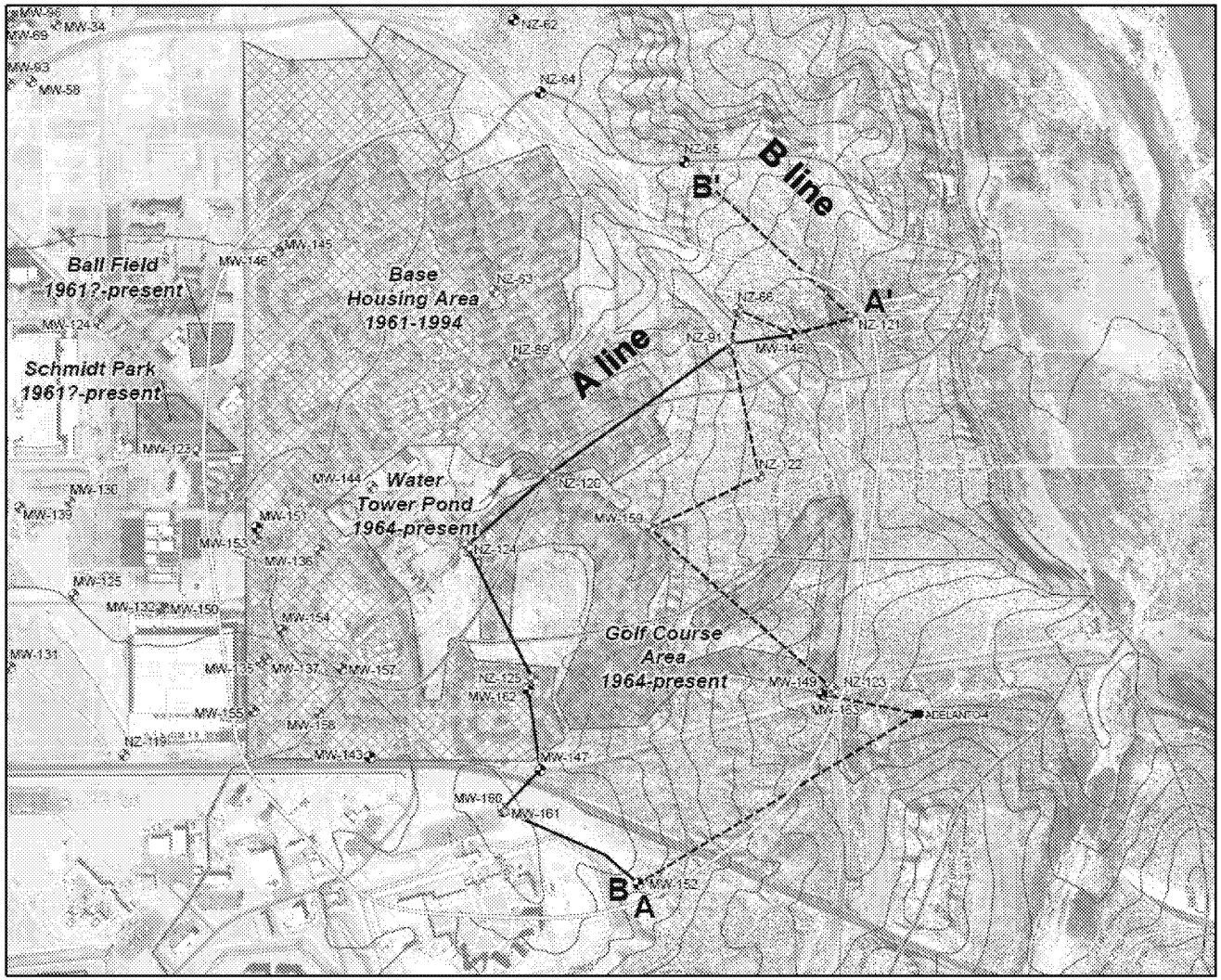
OT071 Cross-section Lines and Artificial Recharge Areas



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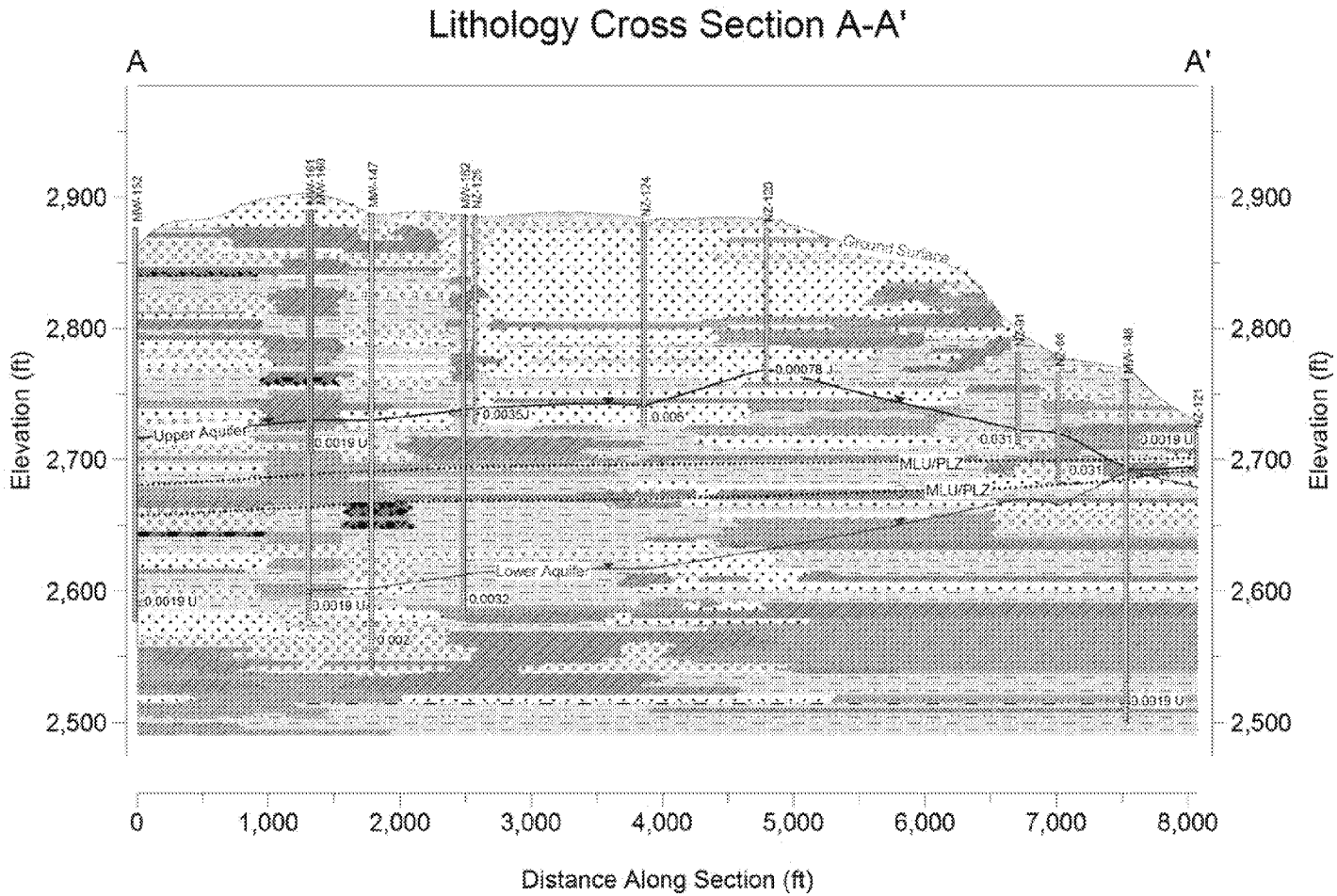
Cross-Section A-A'



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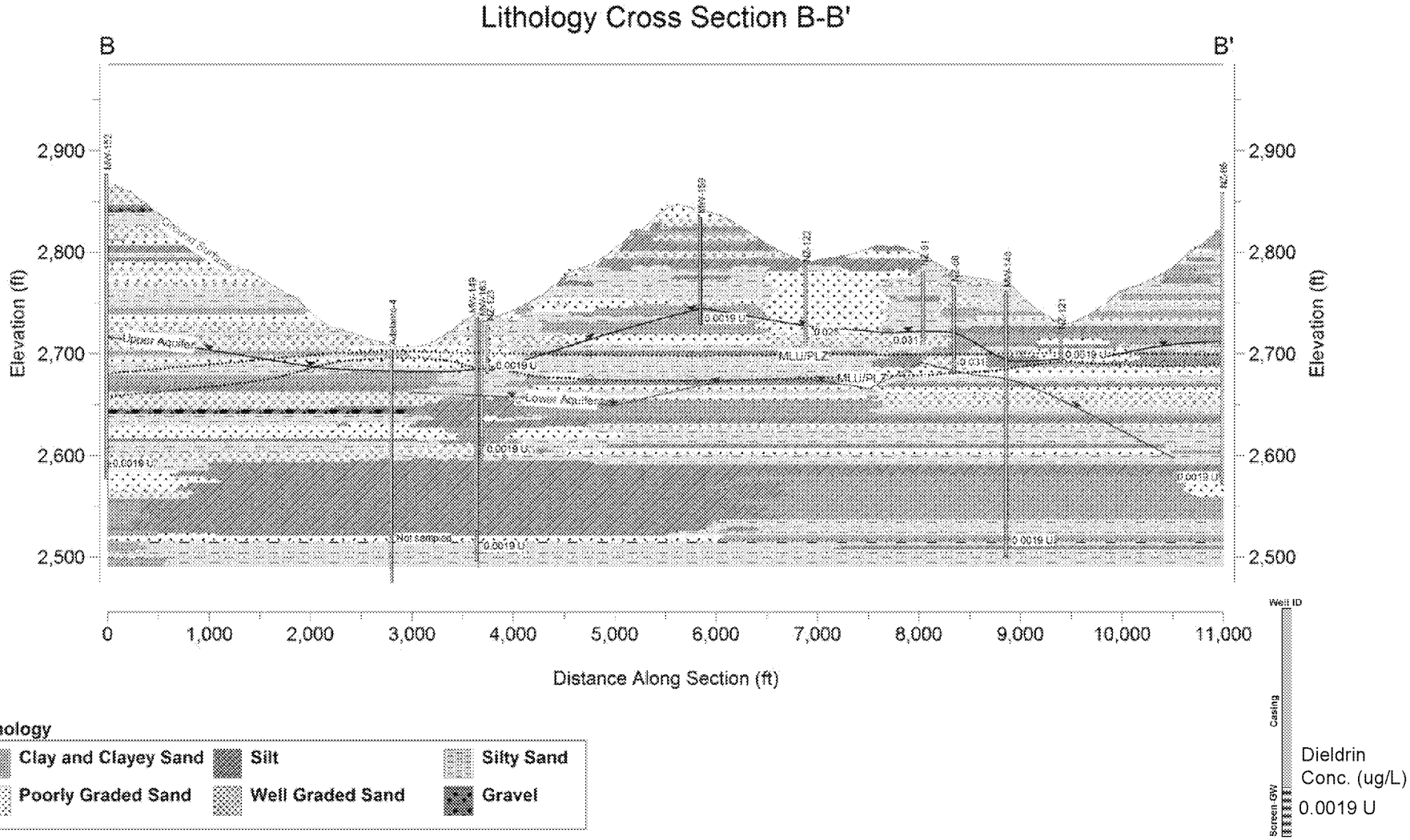
Cross-Section B-B'



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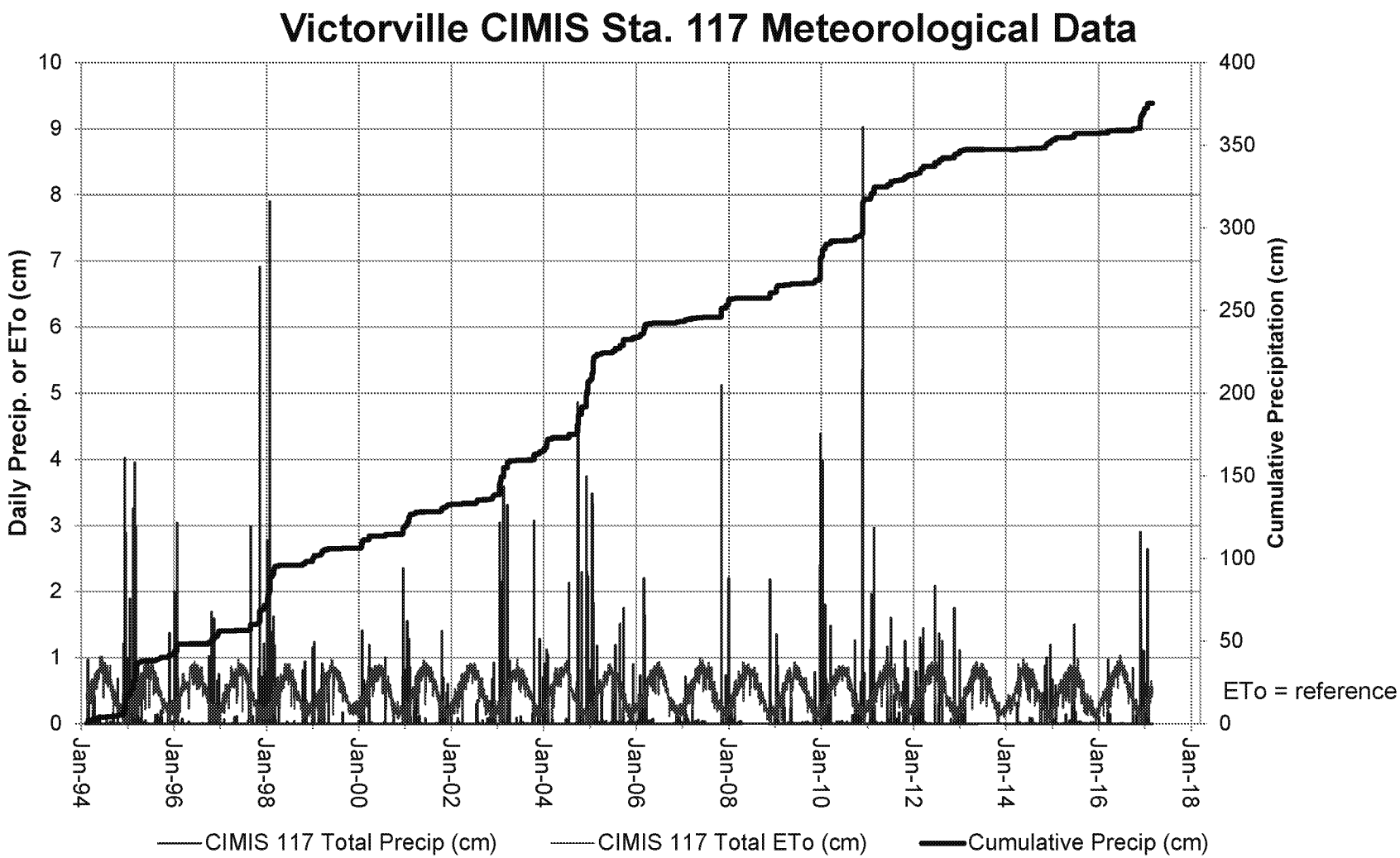
Recharge

Precipitation/Evapotranspiration Model Input)



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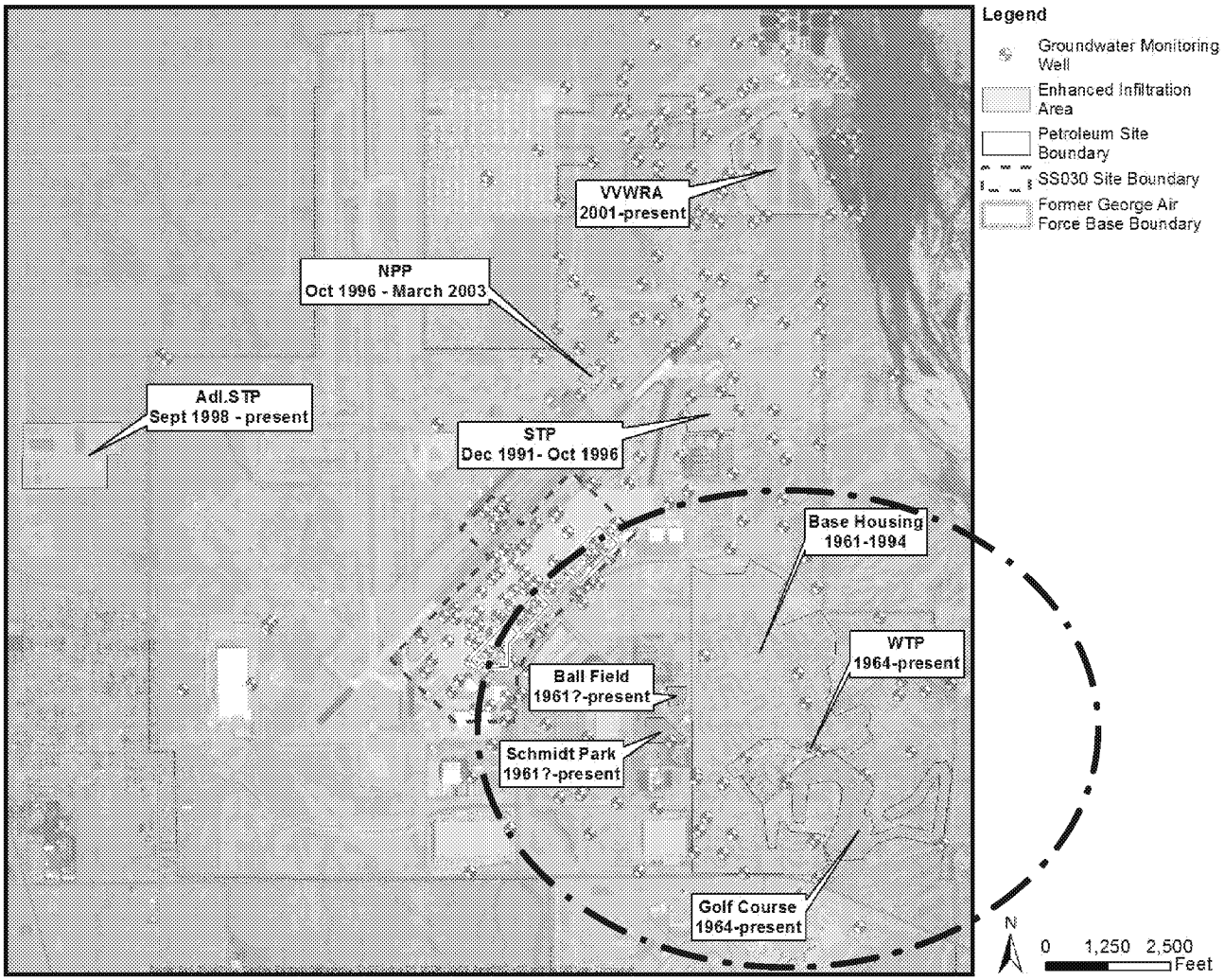
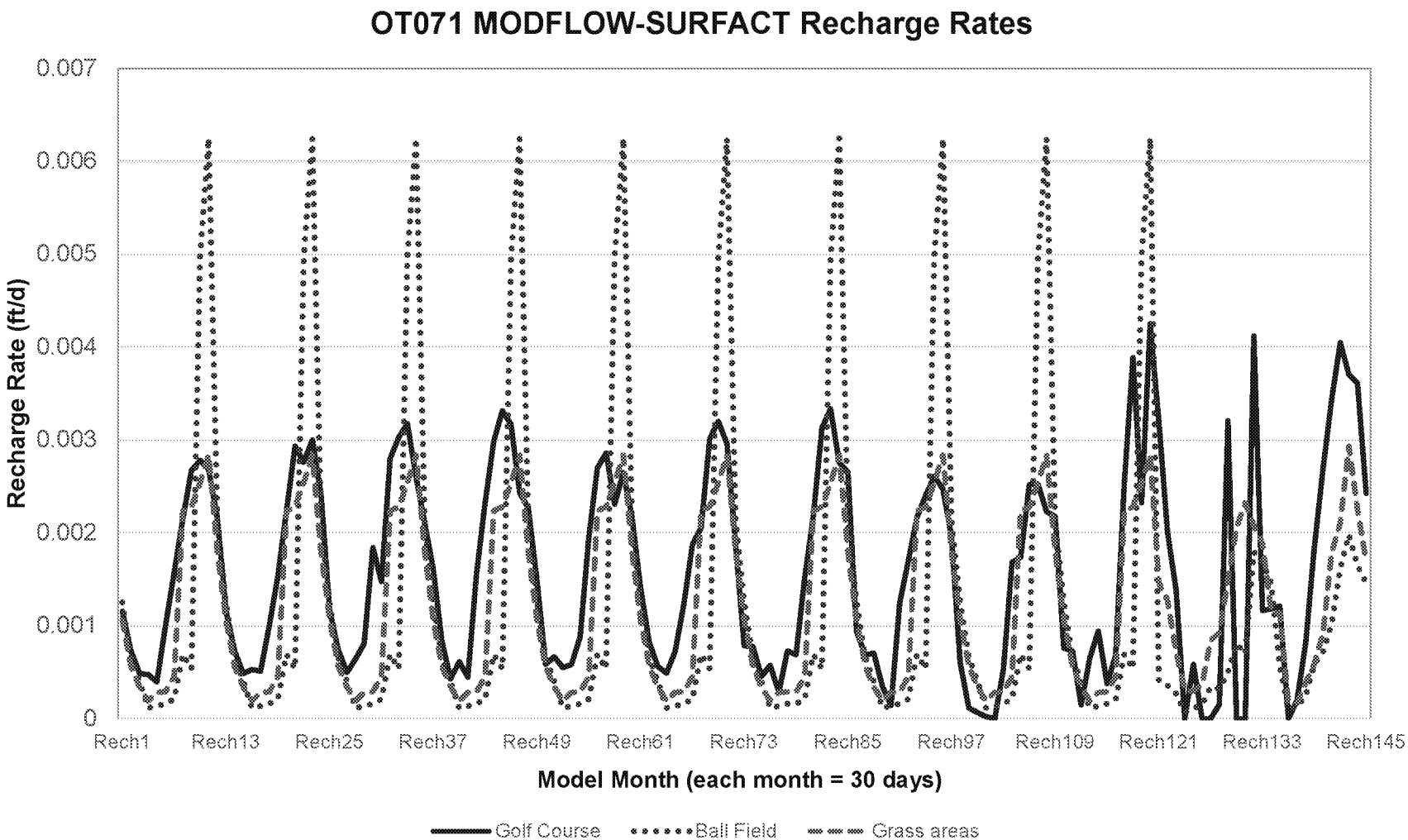
Enhanced Infiltration Areas



OT071 Recharge Rates from 2009 MODFLOW Model



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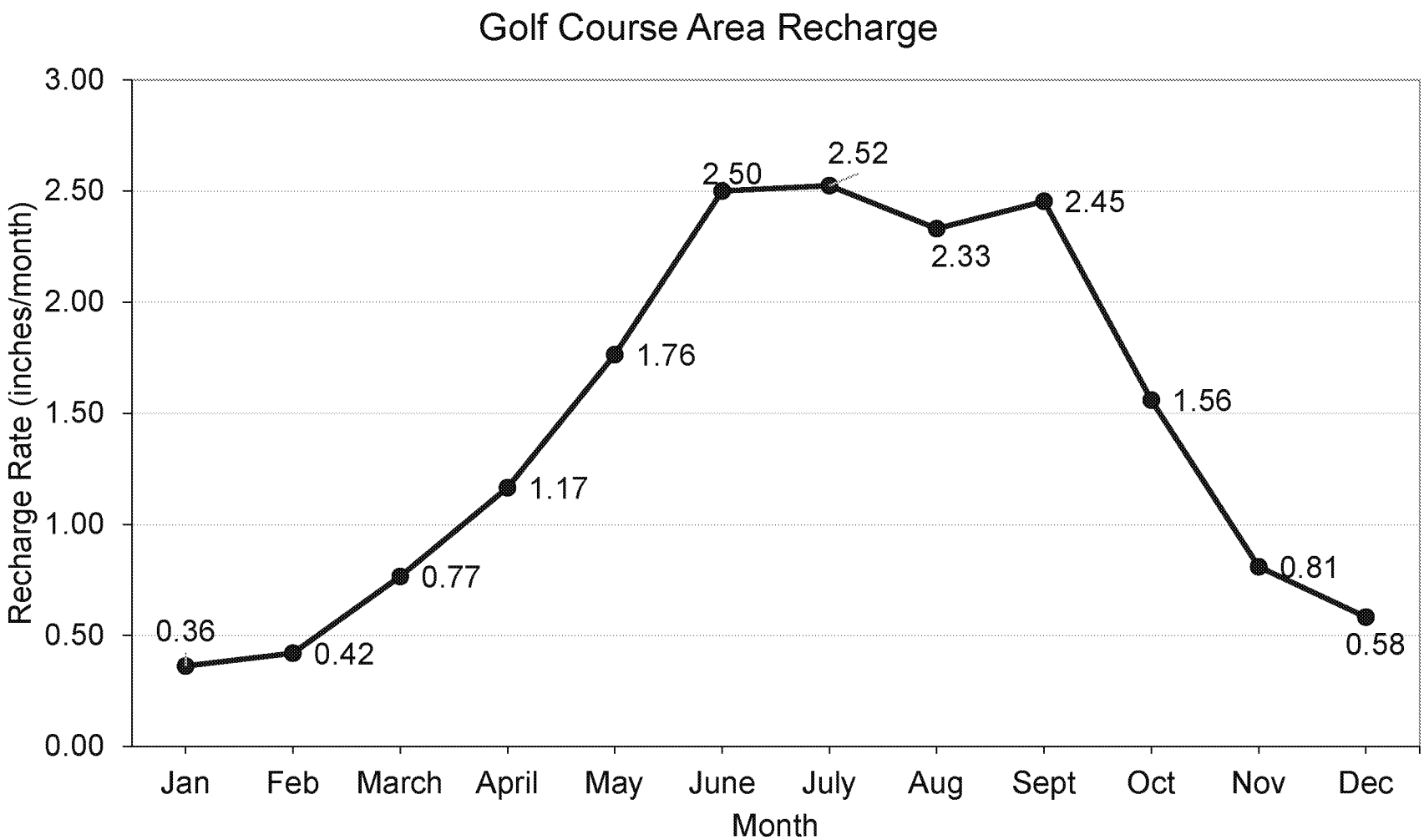
OT071 Model Golf Course Area Average Recharge Rates



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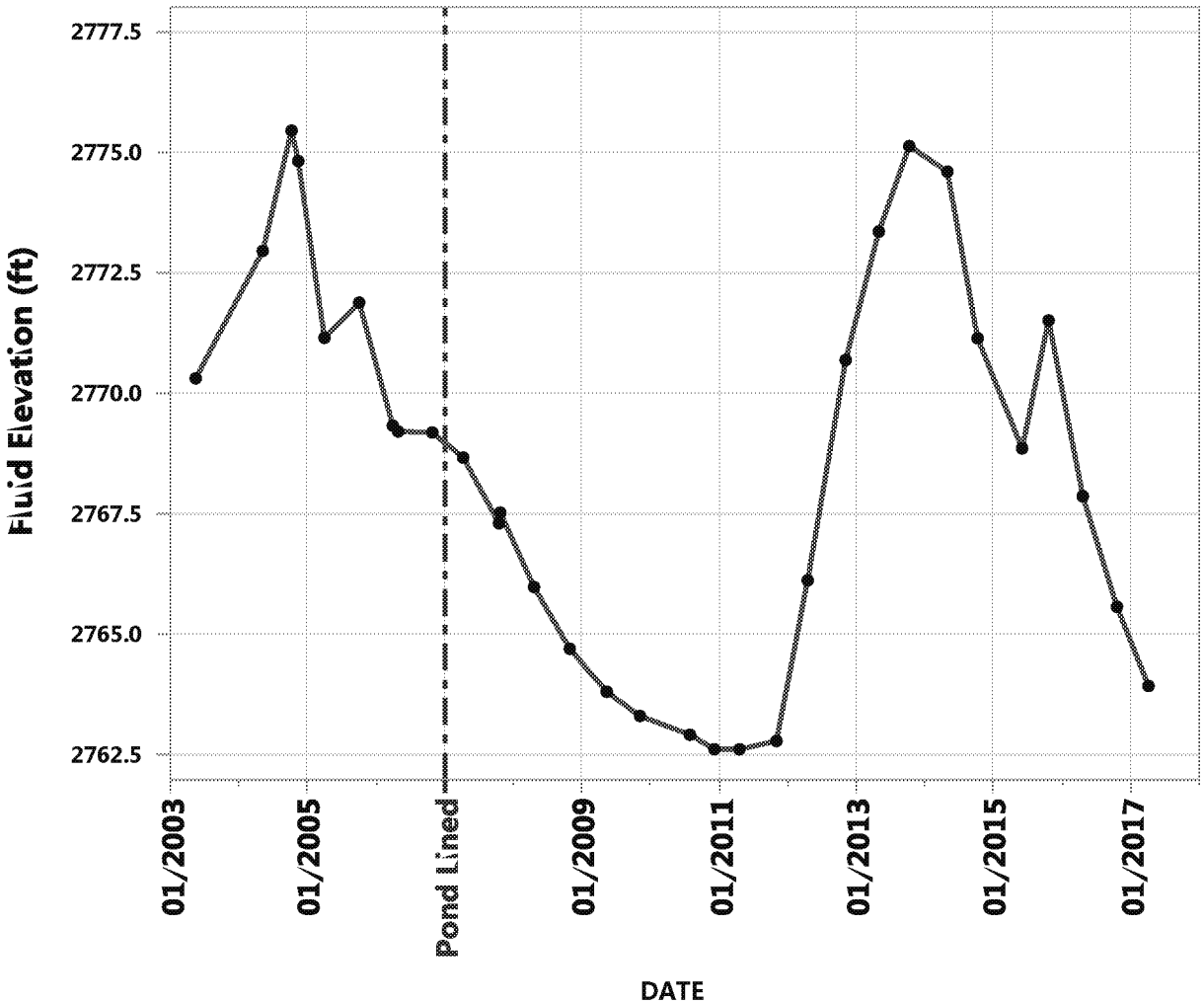
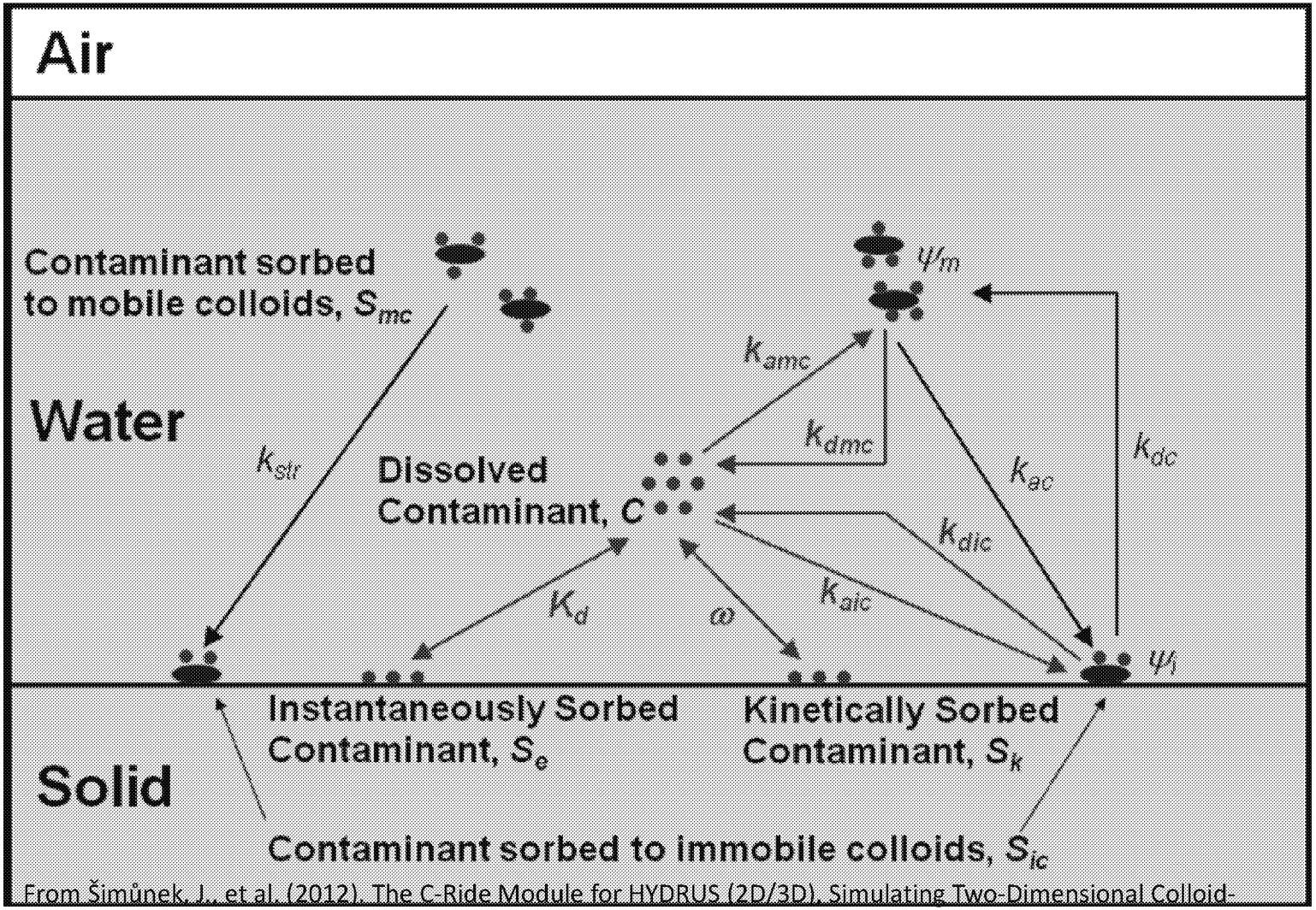
Water Tower (Golf Course) Pond Infiltration: NZ-120 Hydrograph



C-Ride Colloidal Transport Variables



From Šimůnek, J., et al. (2012). The C-Ride Module for HYDRUS (2D/3D), Simulating Two-Dimensional Colloid-Facilitated Solute Transport in Variably-Saturated Porous Media. Prague, Czech Republic, PC-Progress. 45 p., Figure 2.

Colloidal Transport Variables

Species description	Variable	Units
Colloid species		
Mobile colloids	C_c	nL^{-3}
Colloids attached to the solid phase	S_c^{att}, S_{c1}	nM^{-1}
Strained colloids	S_c^{str}, S_{c2}	nM^{-1}
Solute (contaminant) species		
Dissolved contaminant	C	ML^{-3}
Contaminant instantaneously sorbed to the solid phase	S_e	MM^{-1}
Contaminant kinetically sorbed to the solid phase	S_k	MM^{-1}
Contaminant sorbed to mobile colloids	S_{mc}	Mn^{-1}
Contaminant sorbed to immobile colloids (attached)	S_{ic1}	Mn^{-1}
Contaminant sorbed to immobile colloids (strained)	S_{ic2}	Mn^{-1}

L is the length unit, M is the mass unit, and n is the number of colloids

Initial values will be from literature values from column tests

Reaction Parameters for First Component (Colloids)

No.	Parameter	Symbol	Description	Example Value
1	Kd	K_d	Should be equal to 0, not used with colloid transport [L3/M]	0
2	Nu	η	Should be equal to 0 (used for Langmuir η [L3/M]).	0
3	Beta	β	Should be equal to 1 (used for Freundlich exponent β).	1
4	Henry	K_H	Should be equal to 0 (used for the Henry's law constant K_H, which is not used with colloid transport).	0
5	SinkL1	μ_{cw}	Should be equal to 0 (used for colloid immobilization in the liquid phase μ_{cw}). Parameter not be used when the colloid-facilitated solute transport is considered.	0
6	SinkS1	μ_{cs}	Should be equal to 0 (used for colloid immobilization in the solid phase μ_{cs}).	0
7	iPsi2	–	Type of blocking on the second sorption sites (=0; no blocking; =1: Langmuirian dynamics; =3: random sequential adsorption model; =4: depth dependent blocking coefficient).	0
8	iPsi1	–	The same for the first sorption sites.	0
9	SMax2	S_{max}	Parameter in the blocking function for the second sorption sites.	0
10	AttachS2	k_{ac}	First-order deposition (attachment) coefficient, k_{ac} (or k_{str}) [T-1], for second sorption sites.	0
11	DetachS2	k_{dc}	First-order entrainment (detachment) coefficient, k_{dc} [T-1], for second sorption sites.	0
12	SMax1	S_{max}	Parameter in the blocking (straining) function for first sorption sites.	0.01
13	AttachS1	k_{ac}	First-order deposition (attachment) coefficient, k_{ac} (or k_{str}) [T-1], for first sorption sites.	0.01/min
14	DetachS1	k_{dc}	First-order entrainment (detachment) coefficient, k_{dc} [T-1], for first sorption sites.	0.005/min

Reaction Parameters for Second Component (Dieldrin on Colloids)

No .	Parameter	Symbol	Description	Example Value
1	Kd	K_d	Should be equal to 0. This parameter is usually reserved for the sorption parameter Kd, which is not used with colloid transport [L3/M].	0
2	Nu	η	Should be equal to 0 (used for Langmuir η [L3/M]).	0
3	Beta	β	Should be equal to 1 (used for Freundlich exponent β).	1
4	Henry	K_H	Should be equal to 0 (used for the Henry's law constant KH, which is not used with colloid transport).	0
5	SinkL1	μ_{cw}	Should be equal to 0 (used for colloid immobilization in the liquid phase μcw). This parameter should not be used when the colloid-facilitated solute transport is considered.	0
6	SinkS1	μ_{cs}	Should be equal to 0 (commonly used for colloid immobilization in the solid phase μcs).	0
7	Not used			
8	Not used			
9	RefImCol	ψ_i	Parameter adjusting the sorption rate to the number of immobile colloids present	0
10	AttImCol	k_{aic}	Solute adsorption rate to immobile colloids [T-1]	0.05/min
11	DetImCol	k_{dic}	Solute desorption rate from immobile colloids [T-1]	0.02/min
12	RefMobCol	ψ_m	Parameter adjusting the sorption rate to the number of colloids present	1
13	AttMobCol	k_{amc}	Solute adsorption rate to mobile colloids [T-1]	0.05/min
14	DetMobCol	k_{dmc}	Solute desorption rate from mobile colloids [T-1]	0.02/min

Reaction Parameters for Third Component (Dieldrin in Water)

No .	Parameter	Symbol	Description	Example Value
1	Kd	K_d	Should be equal to 0. This parameter is usually reserved for the sorption parameter Kd, which is not used with colloid transport [L3/M]	0
2	Nu	η	Should be equal to 0 (commonly used for Langmuir η [L3/M])	0
3	Beta	β	Should be equal to 1 (commonly used for Freundlich exponent β)	1
4	Henry	K_H	Should be equal to 0 (commonly used for the Henry's law constant KH, which is not used with colloid transport).	0
5	SinkL1	μ_w	Degradation rate for contaminant dissolved in the liquid phase [T-1]	
6	SinkS1	μ_s	Degradation rate for contaminant sorbed to the solid phase [T-1]	
7	Not used			
8	Not used			
9	Not used			
10	Not used			
11	Not used			
12	Not used			
13	Not used			
14	Alpha	ω	First-order rate coefficient for one-site or two-site nonequilibrium adsorption [T-1]	0/min

OT071 Calibration

- Flow calibration
  - Include natural and artificial recharge over time
  - Match observed water level fluctuations
  - Gradients in Upper and Lower Aquifers and changes over time
- Transport calibration
  - Simulate dieldrin migration from 1961 to 2016
  - Compare results to observed dieldrin concentrations over time
  - Because this is a 2D profile model and dieldrin concentrations are dispersed, observed results may come from wells across the plume

Questions / Comments