Groundwater Flow and Solute Transport Simulations of the VOCs-Contaminated Area in Map Ta Phut Industrial Estate, Rayong Province

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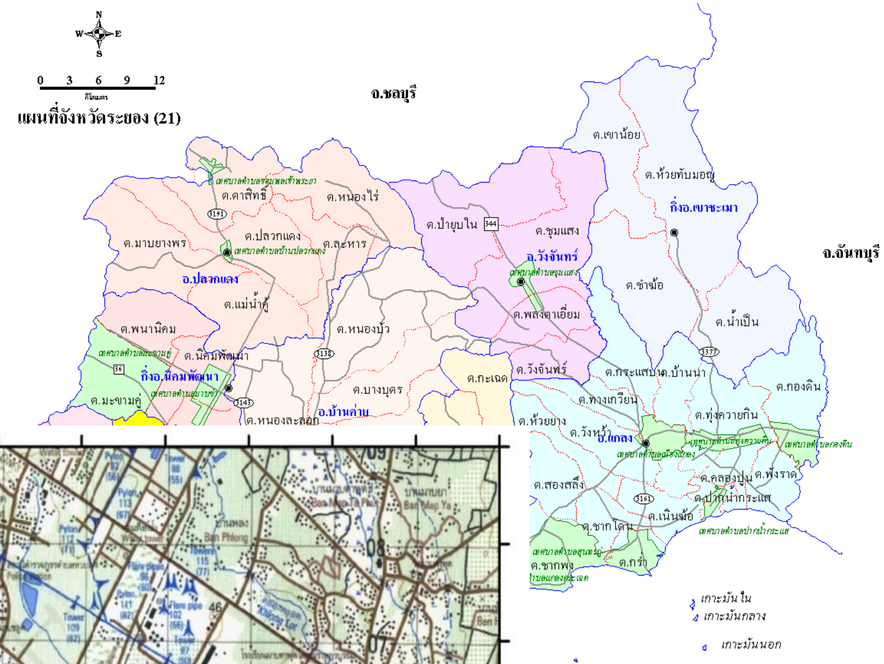
Department of Geological Sciences,
Faculty of Science, Chiang Mai University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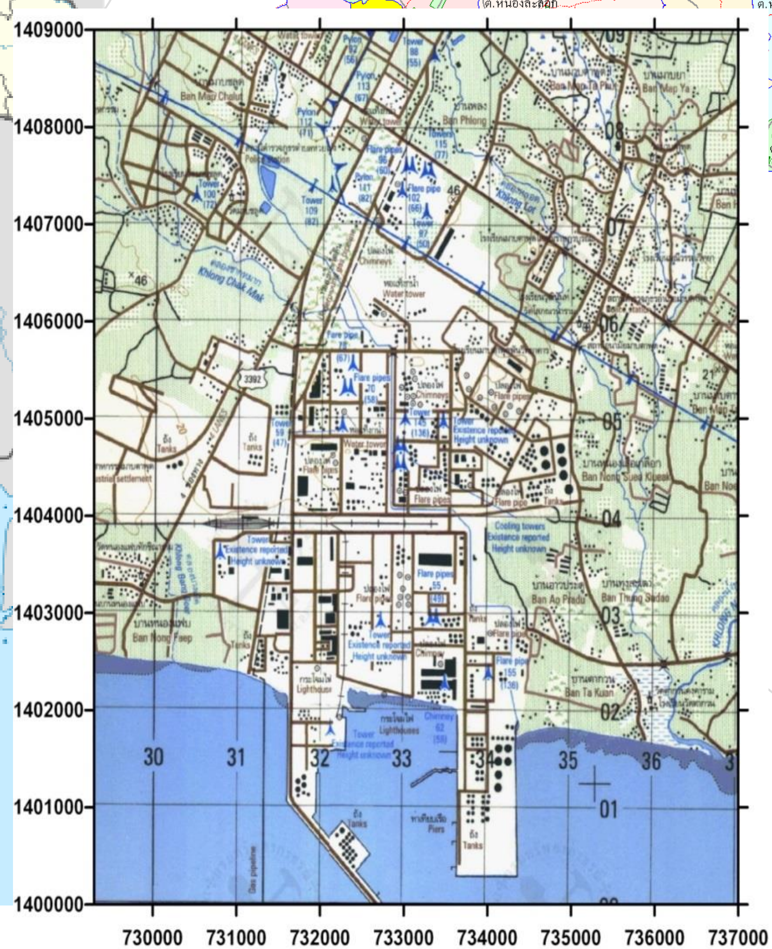
จ.ชลบุรี
จ.จันทบุรี
อ.ปลวกแดง
อ.วังจันทร์
กิ่งอ.เขาชะเมา
กิ่งอ.นิคมพัฒนา
อ.บ้านค่าย
อ.แกลง
เกาะมันใน
เกาะมันกลาง
เกาะมันนอก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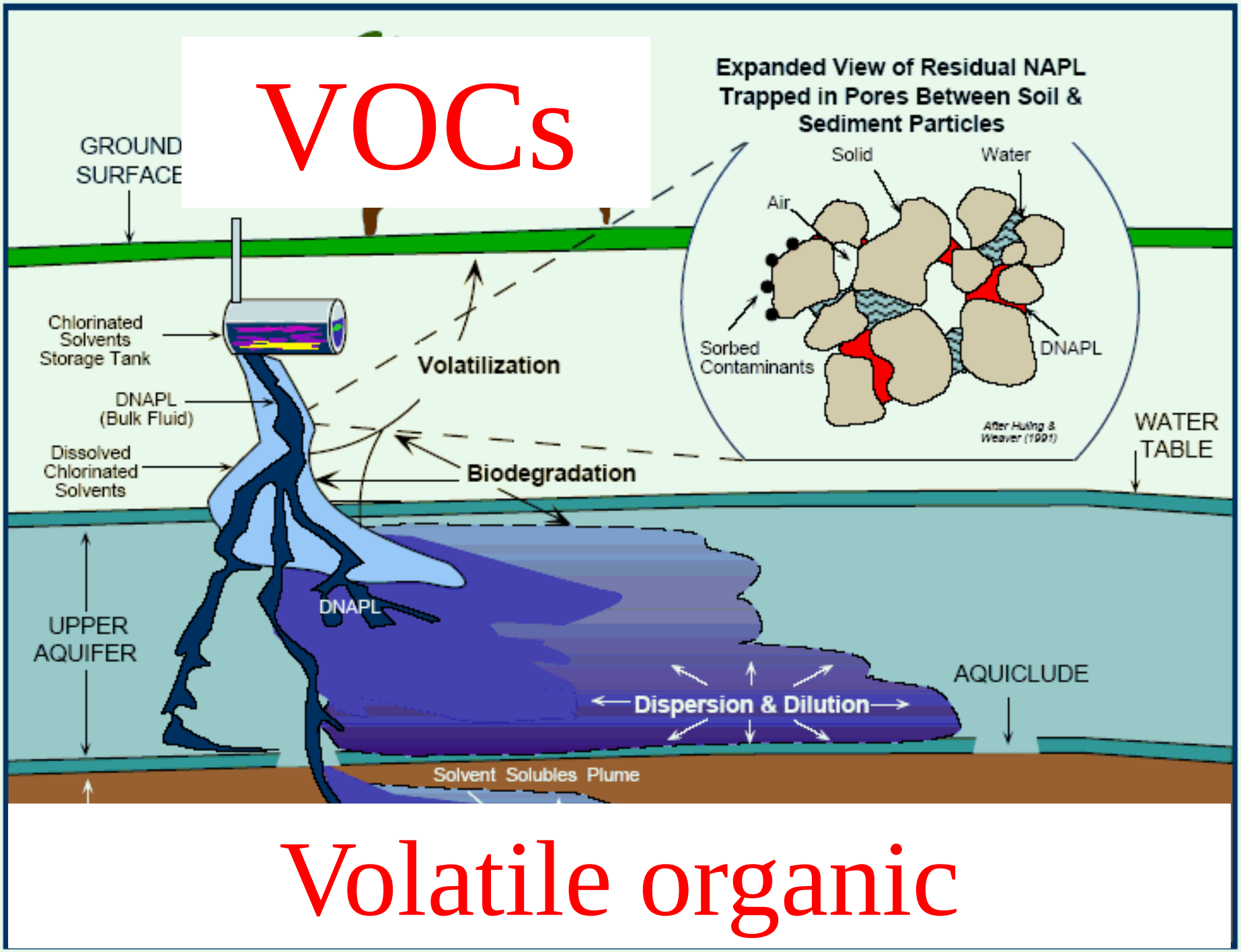
VOCs



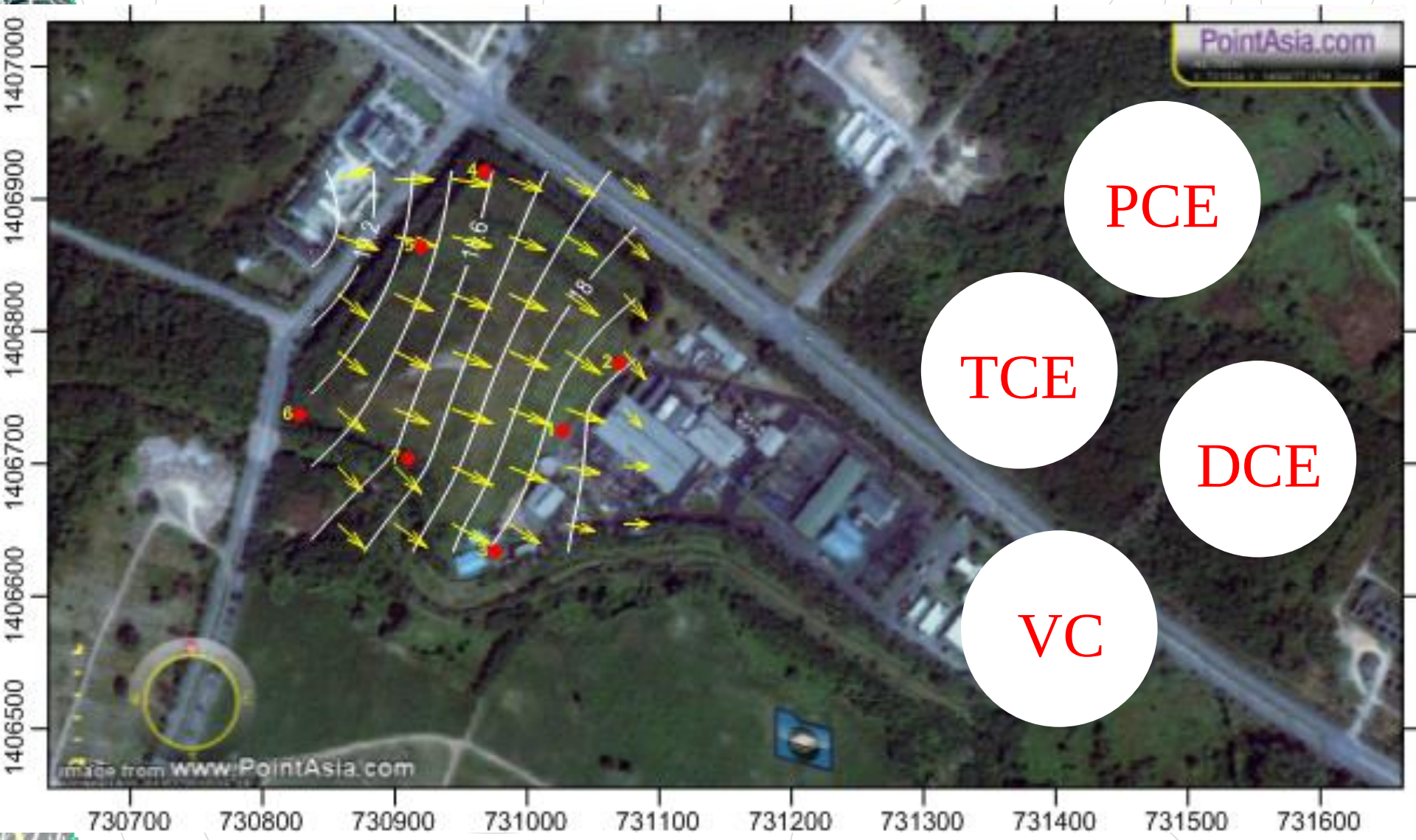
Volatile organic

Objectives

- To conduct detailed site characterization of the selected VOCs-contaminated area in MTPIE.
- To construct comprehensive groundwater flow and solute transport simulations for assessing aquifer contamination.

The developed models that can be used to design appropriate remediation system.

Background Site Information


PointAsia.com
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TCE
DCE
VC
Image from www.PointAsia.com
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731000
731100
731200
731300
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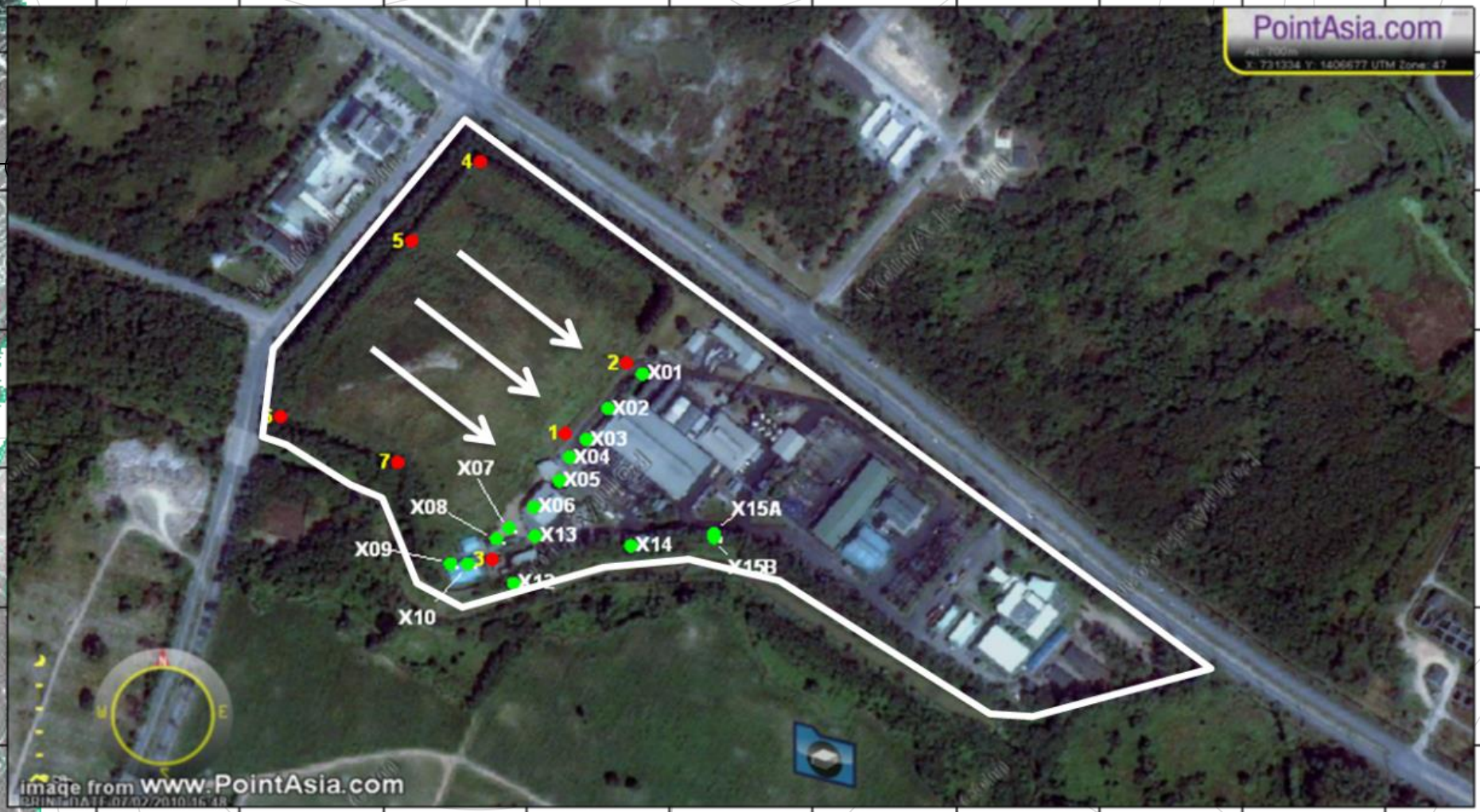
731500
731600

Site Characterization

- **Hydrogeological Characteristics**
  - **Hydrogeologic Settings**
  - **Hydraulic Properties**
- **Hydrogeochemical Characteristics**
  - **Hydrochemical Facies**
  - **VOCs Contamination**


PointAsia.com
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X05
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X07
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X06
X13
X15A
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image from www.PointAsia.com
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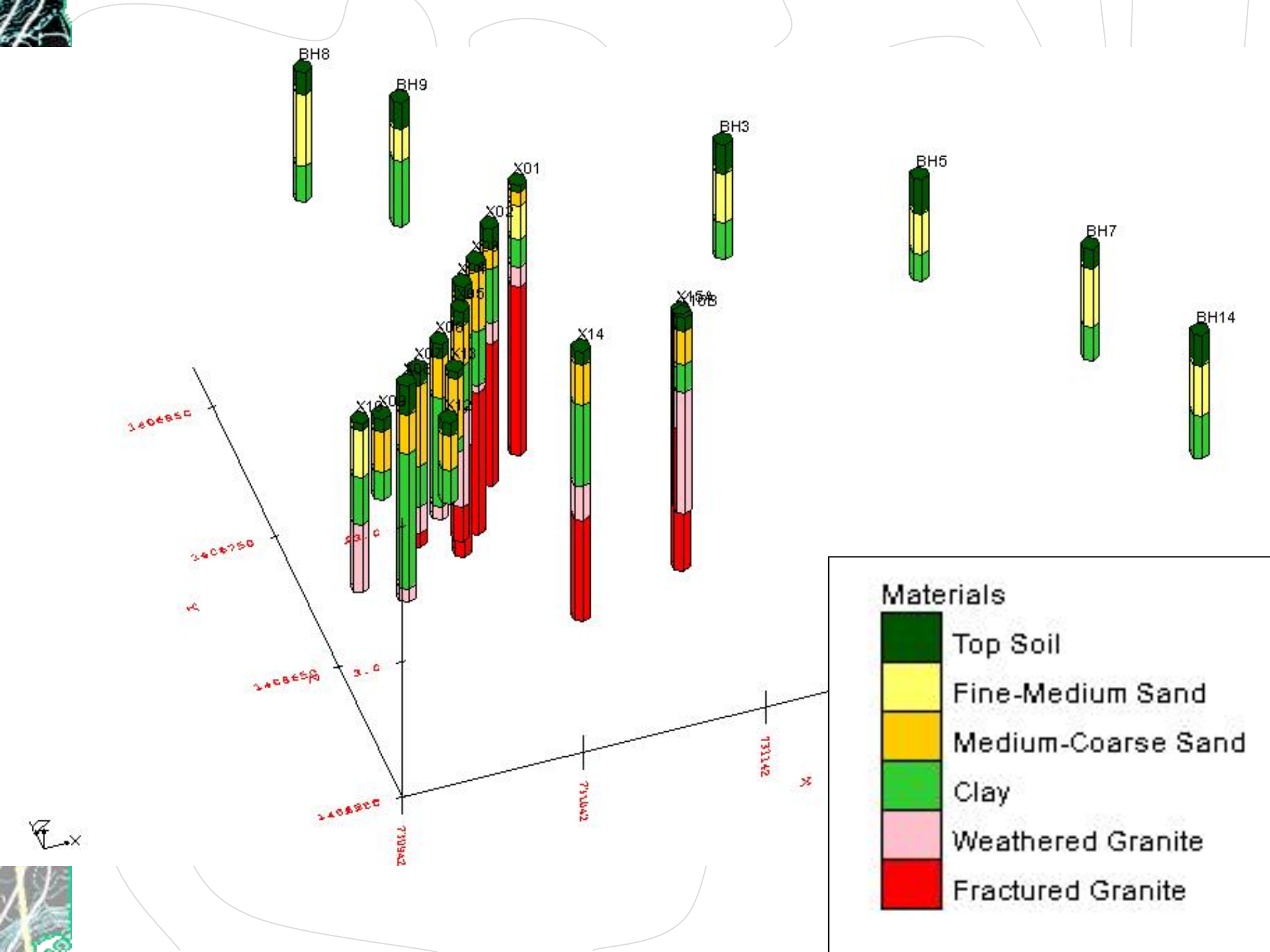
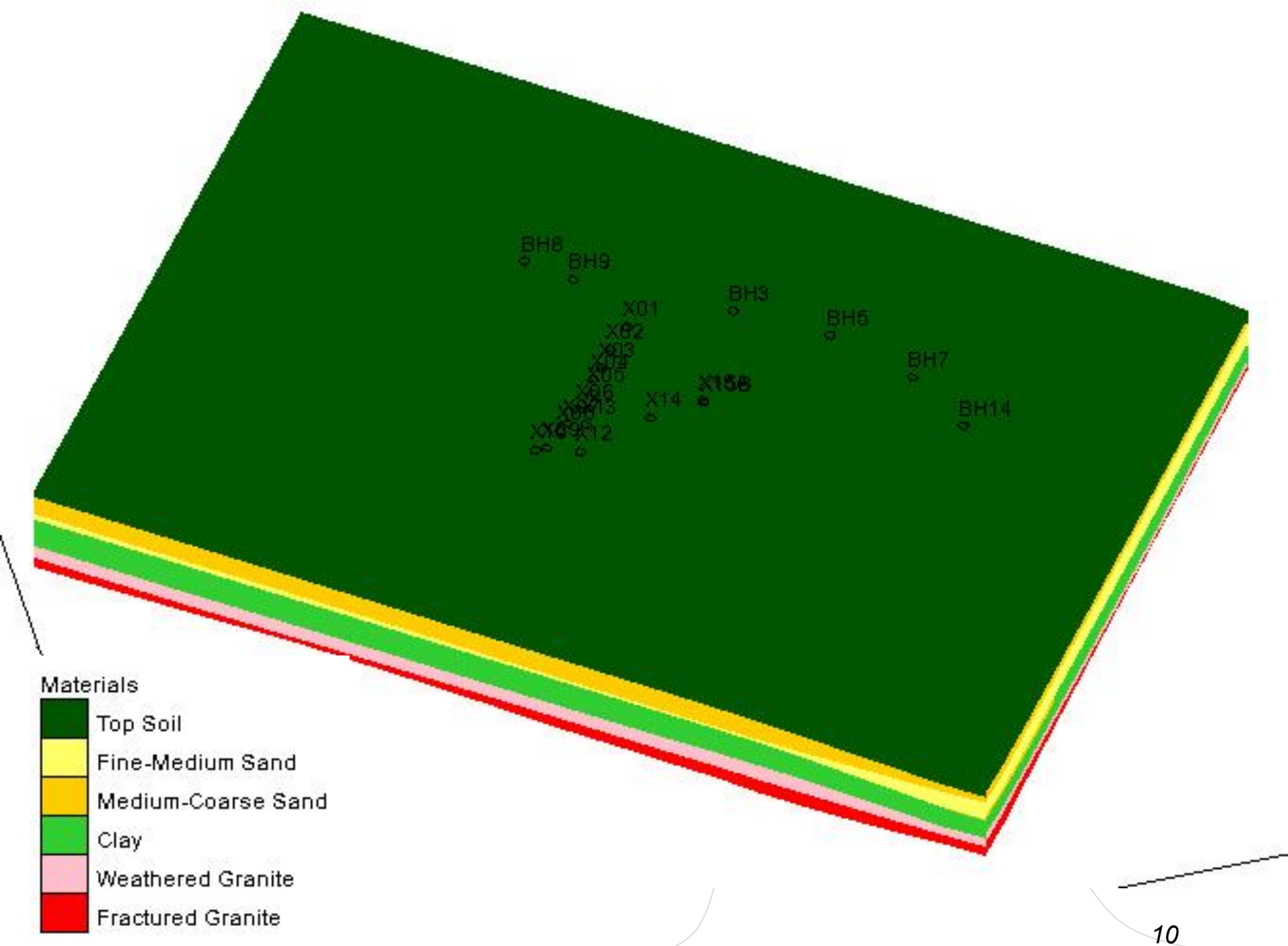

BH8
BH9
BH3
BH5
BH7
BH14
X01
X14
Materials
Top Soil
Fine-Medium Sand
Medium-Coarse Sand
Clay
Weathered Granite
Fractured Granite


BH8
BH9
BH3
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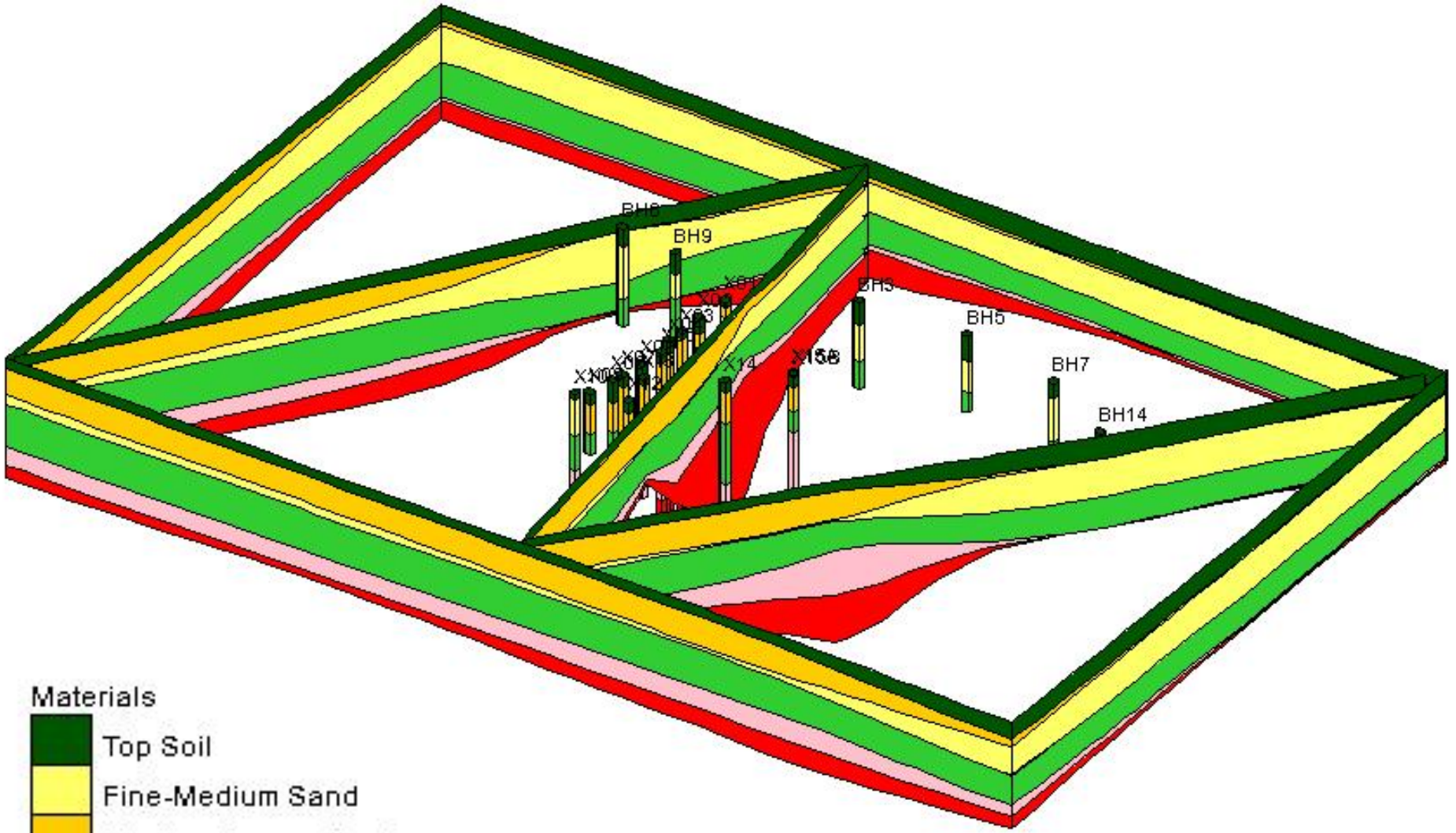
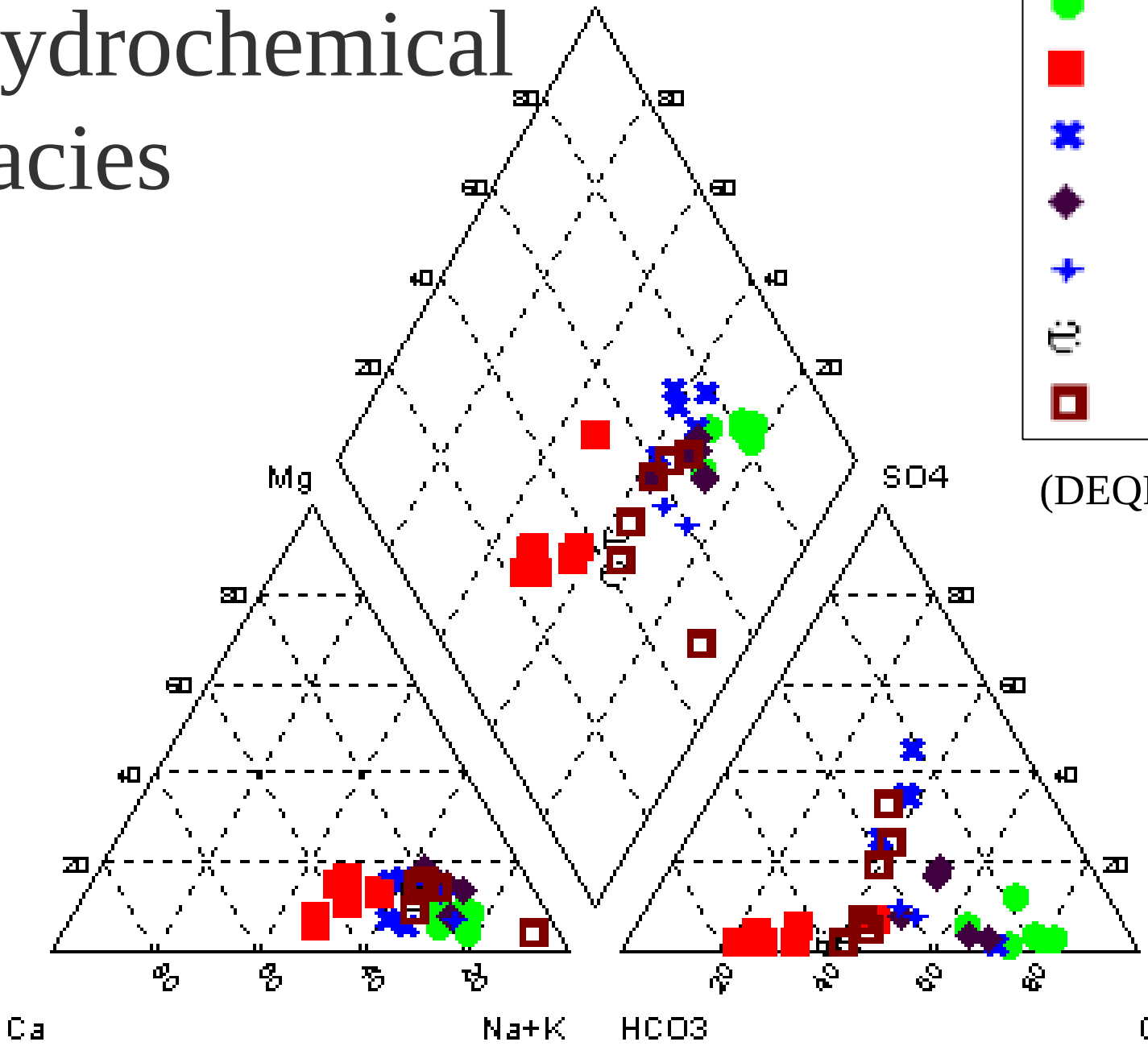
Materials
Top Soil
Fine-Medium Sand
Medium-Coarse Sand
Clay
Weathered Granite
Fractured Granite


BH8
BH9
BH5
BH5
BH7
BH14
Materials
Top Soil
Fine-Medium Sand
Medium-Coarse Sand
Clay
Weathered Granite
Fractured Granite

Hydraulic Properties

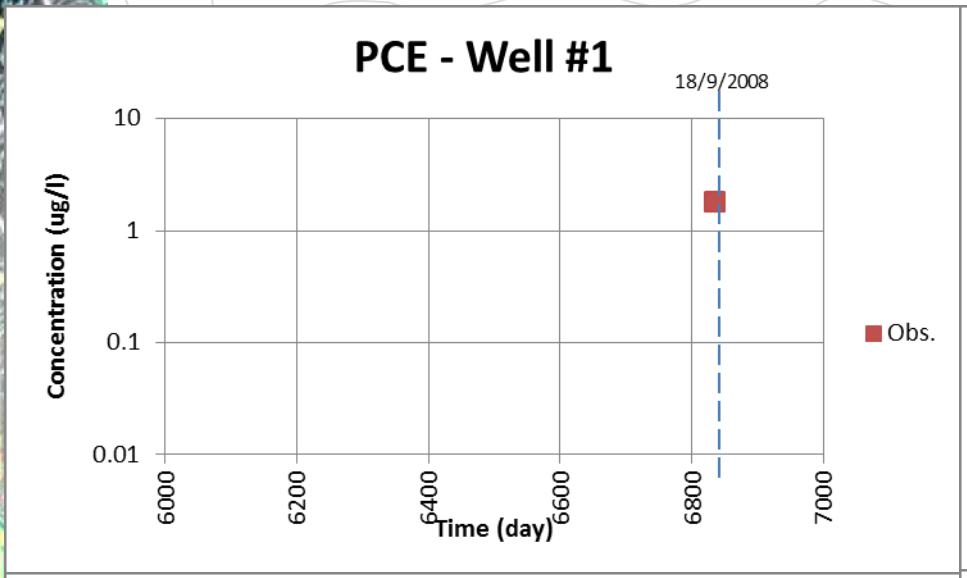
- Hydraulic Conductivity
  - Slug Test
  - 0.03 – 3.55 m/day
- Porosity
  - Gravimetric-Volumetric Method
  - 0.19 - 0.42
- Longitudinal Dispersivity
  - Tracer Test
  - 1.29 – 16.1 m.

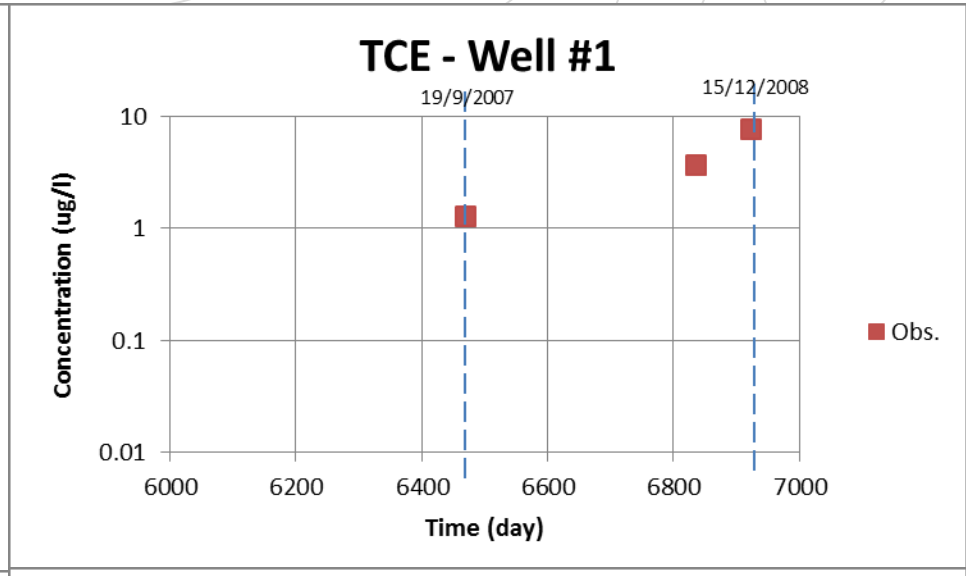
Hydrochemical Facies

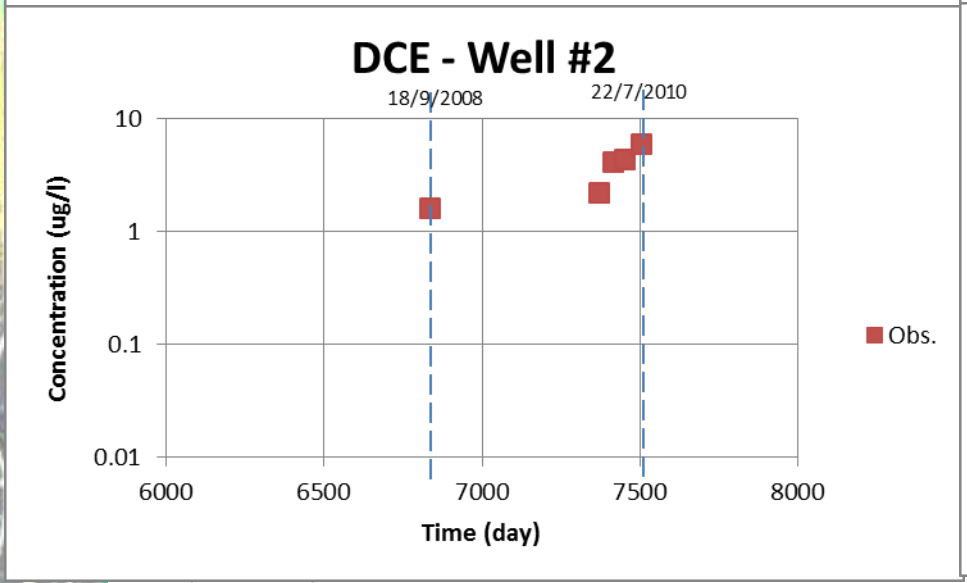


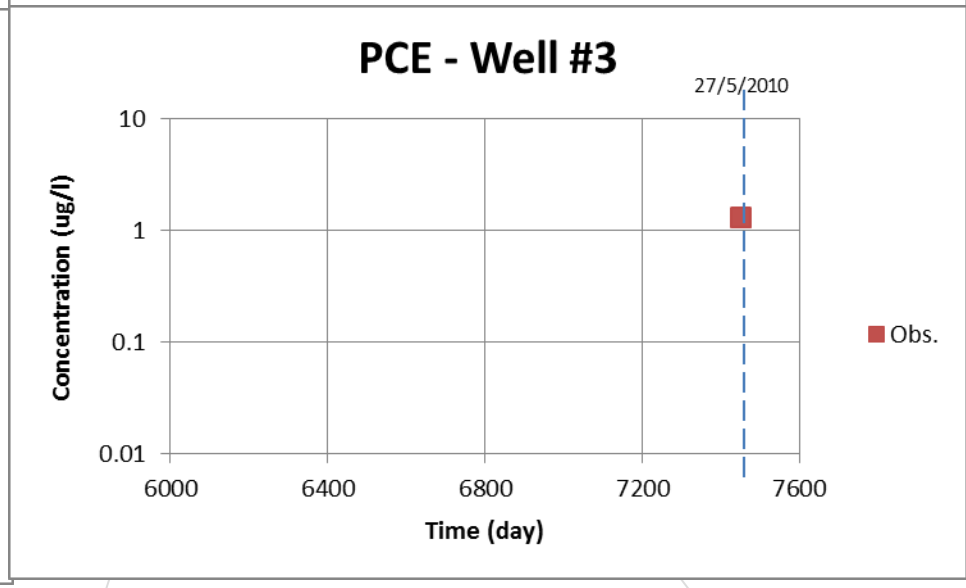
(DEQP, 2010)

VOCs Contamination

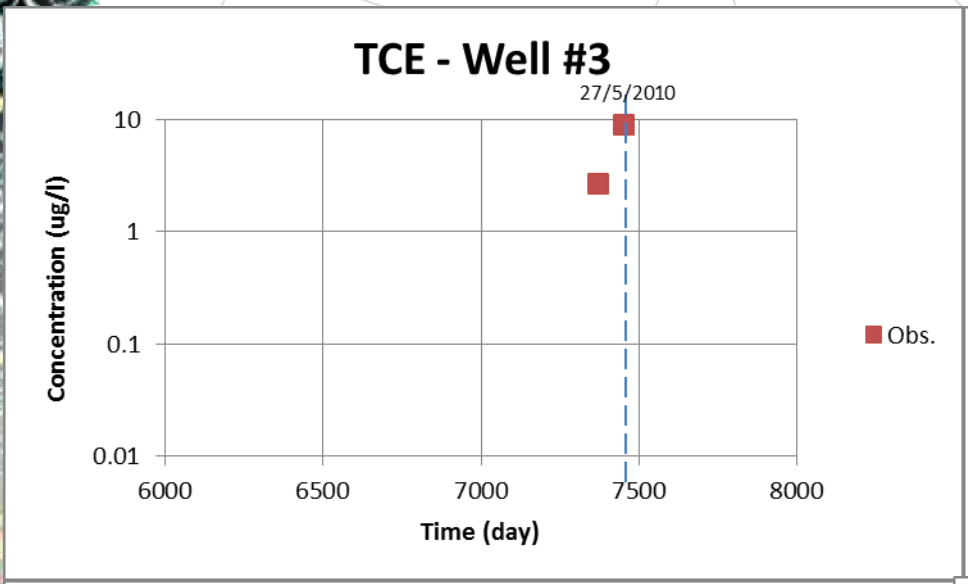








(DEQP, 2010)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0.01
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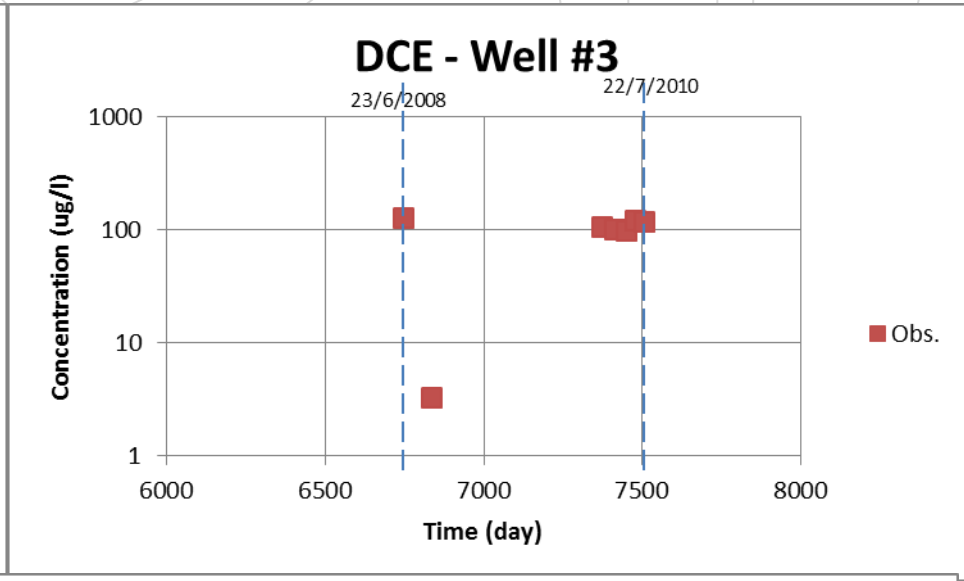
6500
7000
7500
8000
Time (day)
Obs.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23/6/2008
22/7/2010
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100
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Concentration (ug/l)
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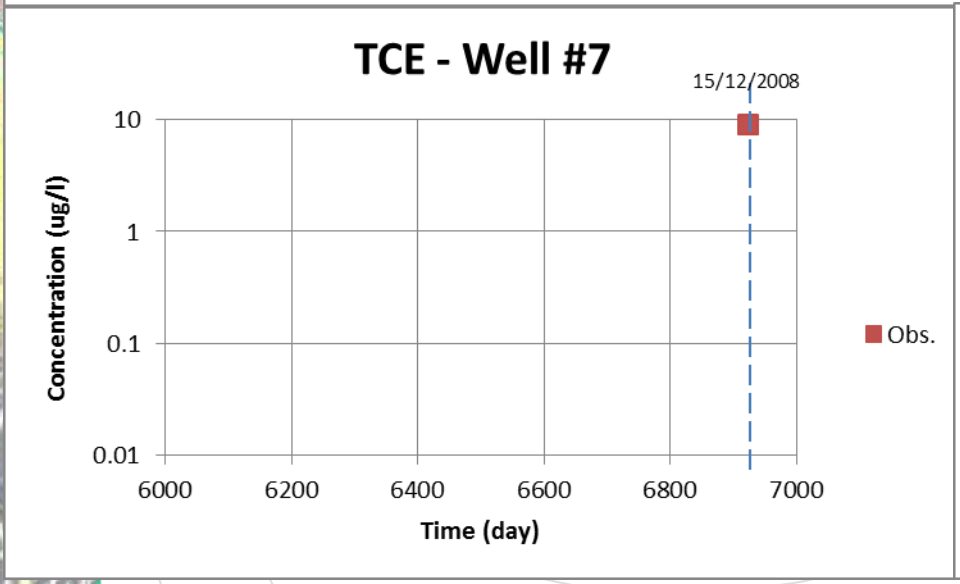
Time (day)
Obs.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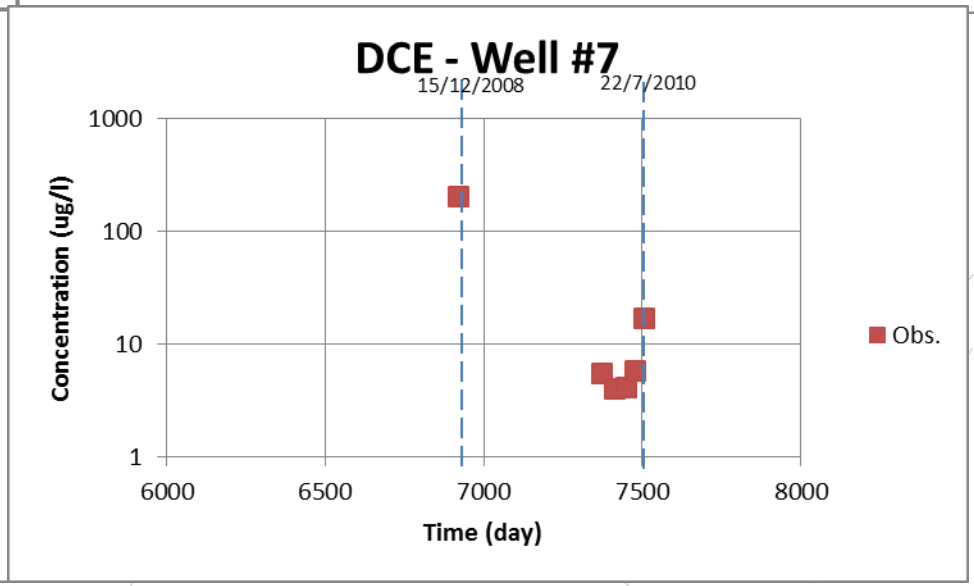
Obs.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22/7/2010
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10
1
Concentration (ug/l)
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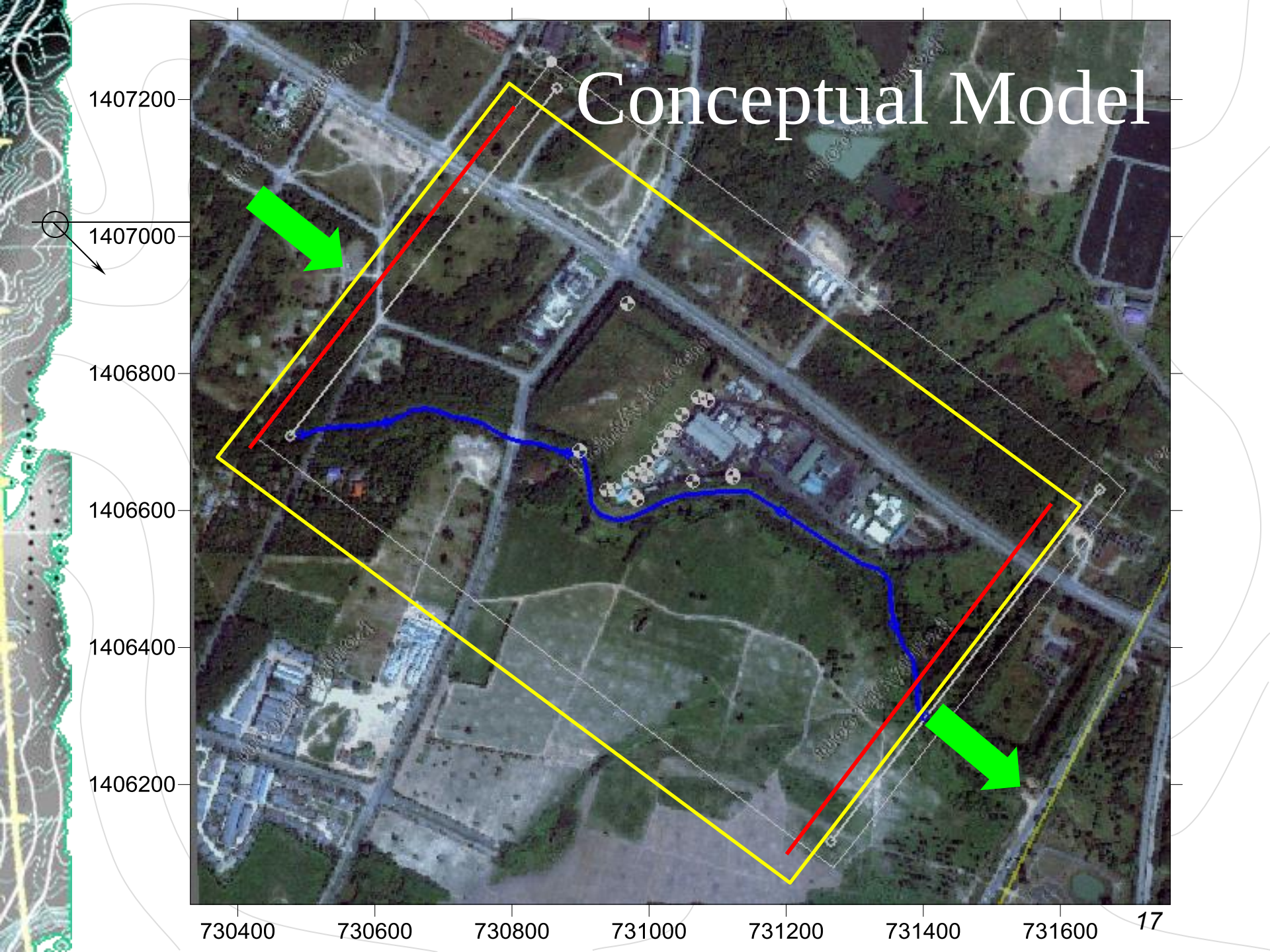
6500
7000
7500
8000
Time (day)
Obs.

(DEQP, 2010)

Groundwater Flow and Solute Transport Simulations

- Conceptual Model
- Model Design
- Groundwater Flow Simulation -> MODFLOW
- Solute Transport Simulation -> RT3D
- Models Calibration -> PEST

Conceptual Model

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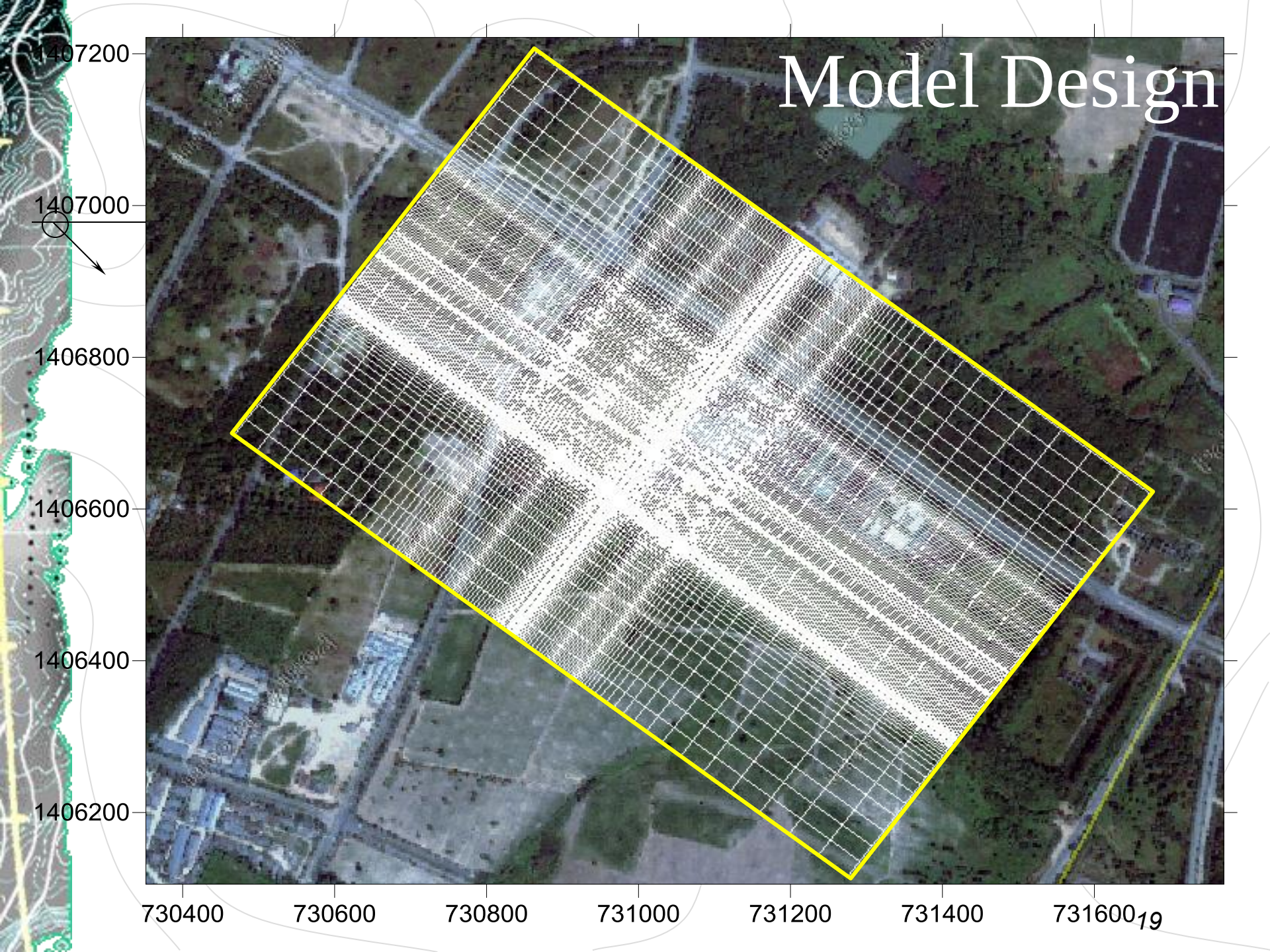
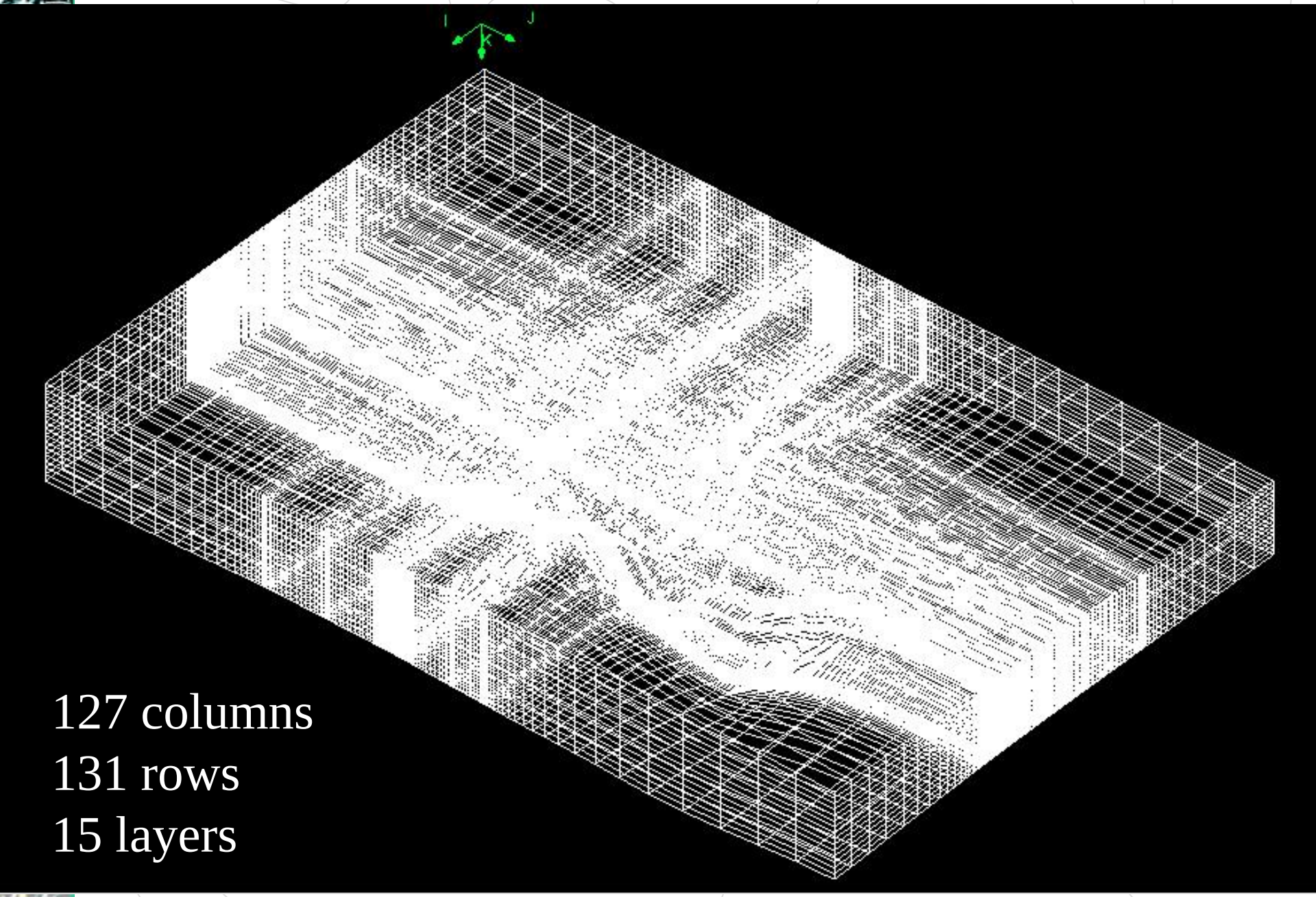
X12
7

Model Design

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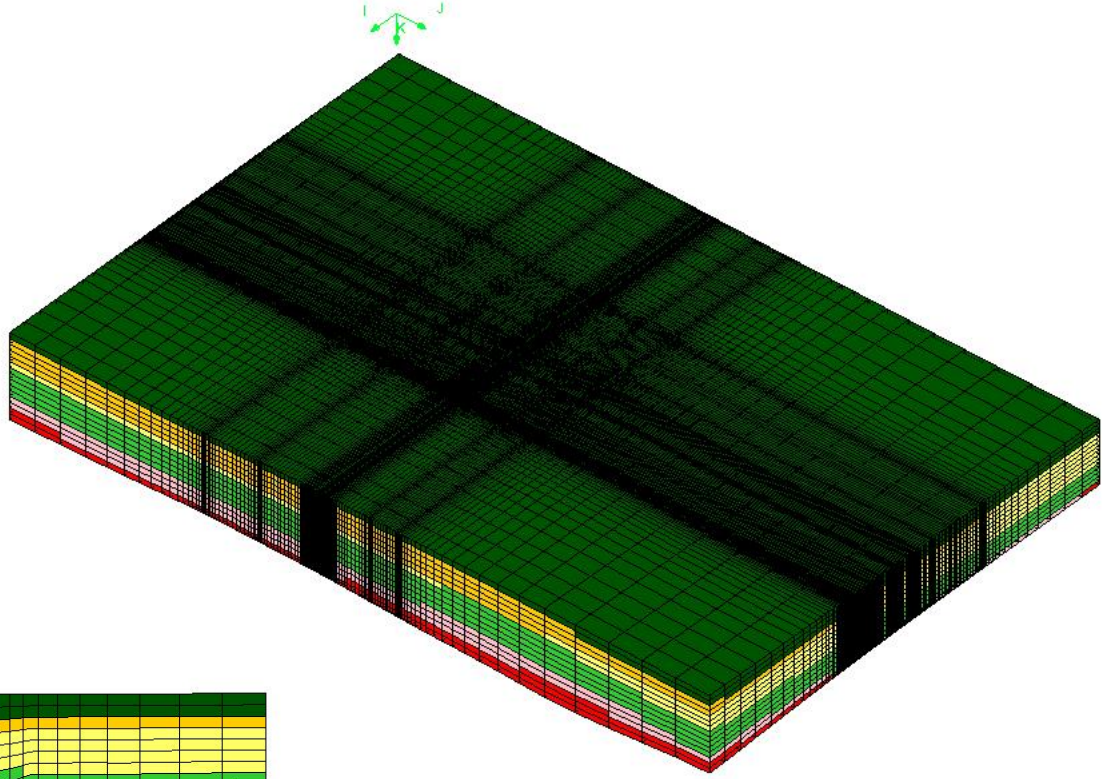
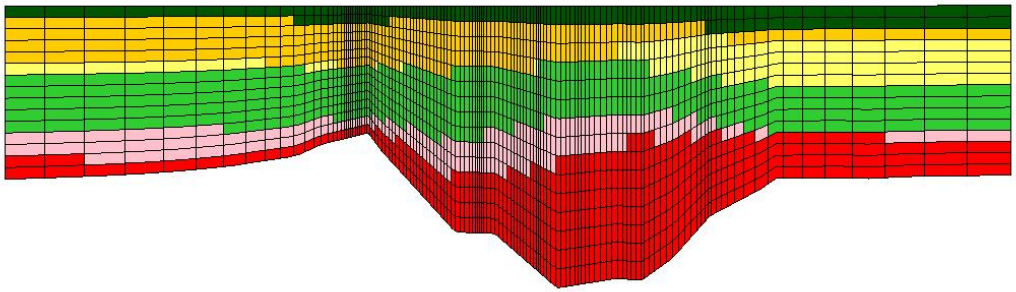
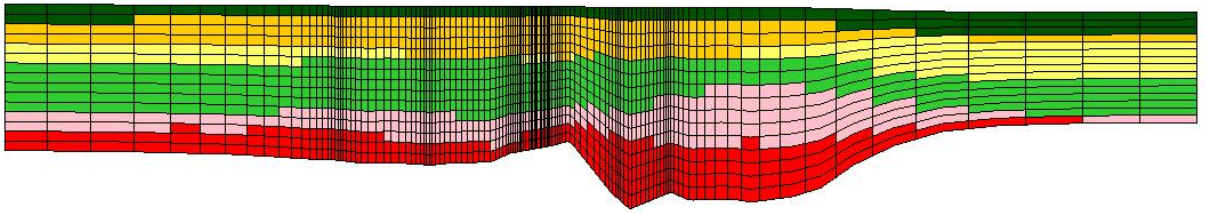


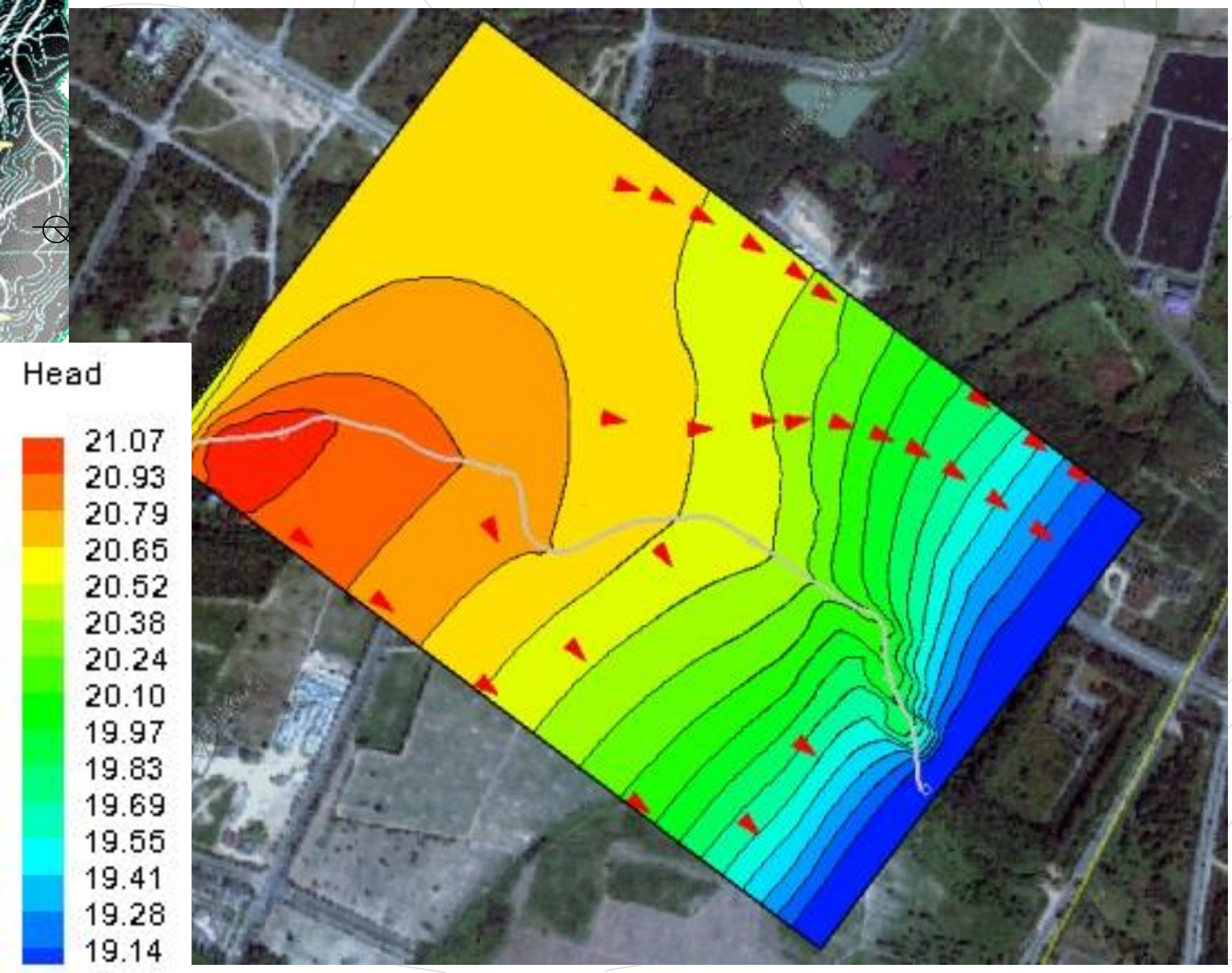




Simulation Results

- Groundwater Flow Simulation Results
- Solute Transport Simulation Results

Parameter		Estimated Value	Relative Sensitivity
Hydraulic Conductivity [m/d]	TopSoil Unit	0.26129	0.5896
	Fine-Medium Sand Unit	1.3303	1.0000
	Medium-Coarse Sand Unit	9.7799	0.0140
	Clay Unit	1.66E-06	0.1229
	Weathered Granite Unit	2.51E-06	0.1568
	Fractured Granite Unit	3.1453	0.0027
Vertical Anisotropy		18.586	0.0789
River Conductance 1 [$(m^2/d)/m$]		218.15	0.0033
River Conductance 2 [$(m^2/d)/m$]		152.05	0.0033
River Conductance 3 [$(m^2/d)/m$]		184.68	0.0037
River Conductance 4 [$(m^2/d)/m$]		71.227	0.0020
River Conductance 5 [$(m^2/d)/m$]		136.19	0.0234
General Head Boundary Conductance NW [$(m^2/d)/m$]		2273.1	0.0034
General Head Boundary Conductance SE [$(m^2/d)/m$]		2538.6	0.0025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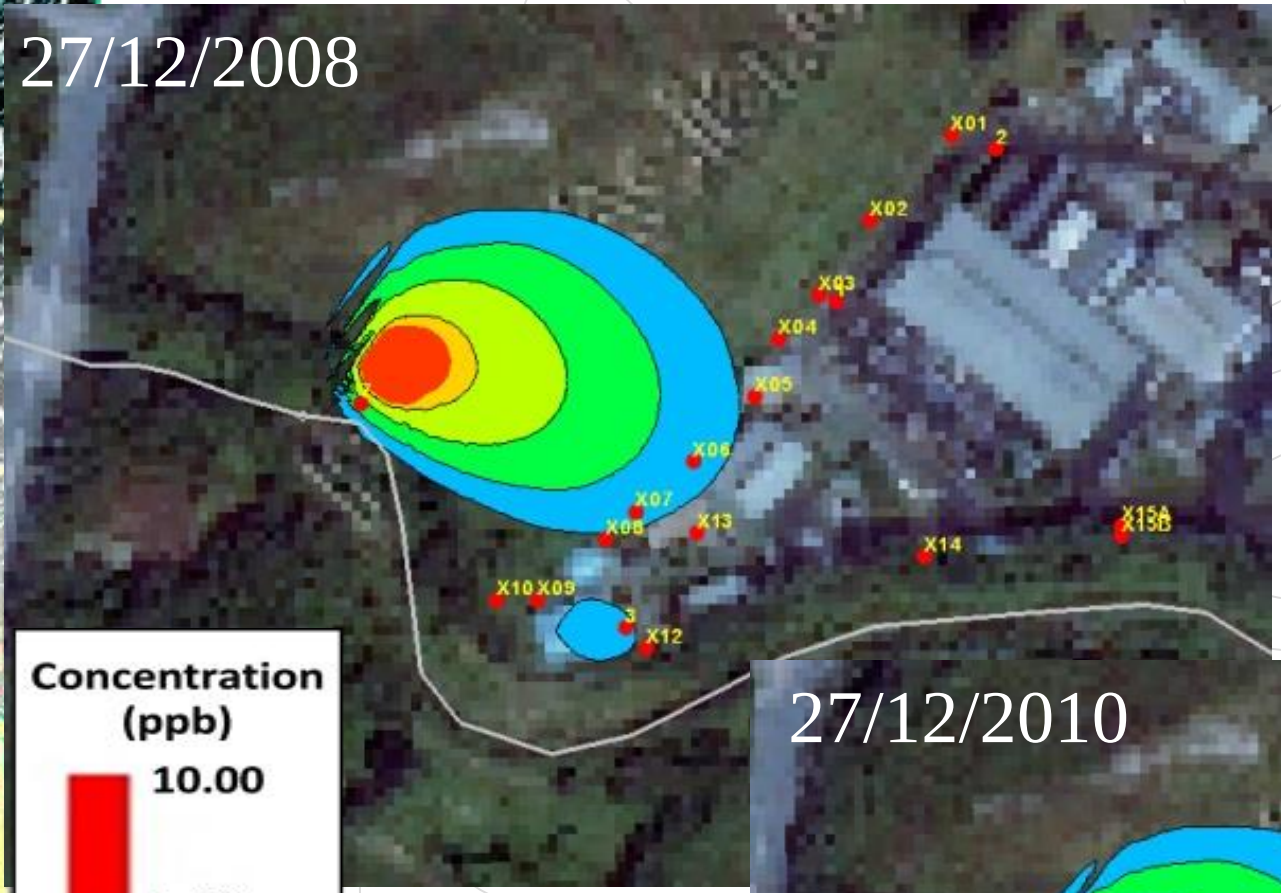
20.79
20.65
20.52
20.38
20.24
20.10
19.97
19.83
19.69
19.55
19.41
19.28
19.14

Parameter			Estimated Value	Relative Sensitivity
	Porosity (n)		0.3000	0.9084
Longitudinal Dispersivity (α_L)			1.0000	0.4366
Degradation Rate (k)	Tetrachloroethene (PCE)		0.0030	1.0000
	Trichloroethene (TCE)		0.0085	0.8096
	1,2 Dichloroethene (DCE)		0.0005	0.9079
	Vinyl Chloride (VC)		0.0030	0.6106
Source Concentration	Source no.1	PCE	6.5000	0.6358
		TCE	15.5000	0.4850
	Source no.2	PCE	0.0070	0.5870
		TCE	0.2500	0.4662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X02
X03
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X05
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X07
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X14
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X15B
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3
X12
Concentration (ppb)
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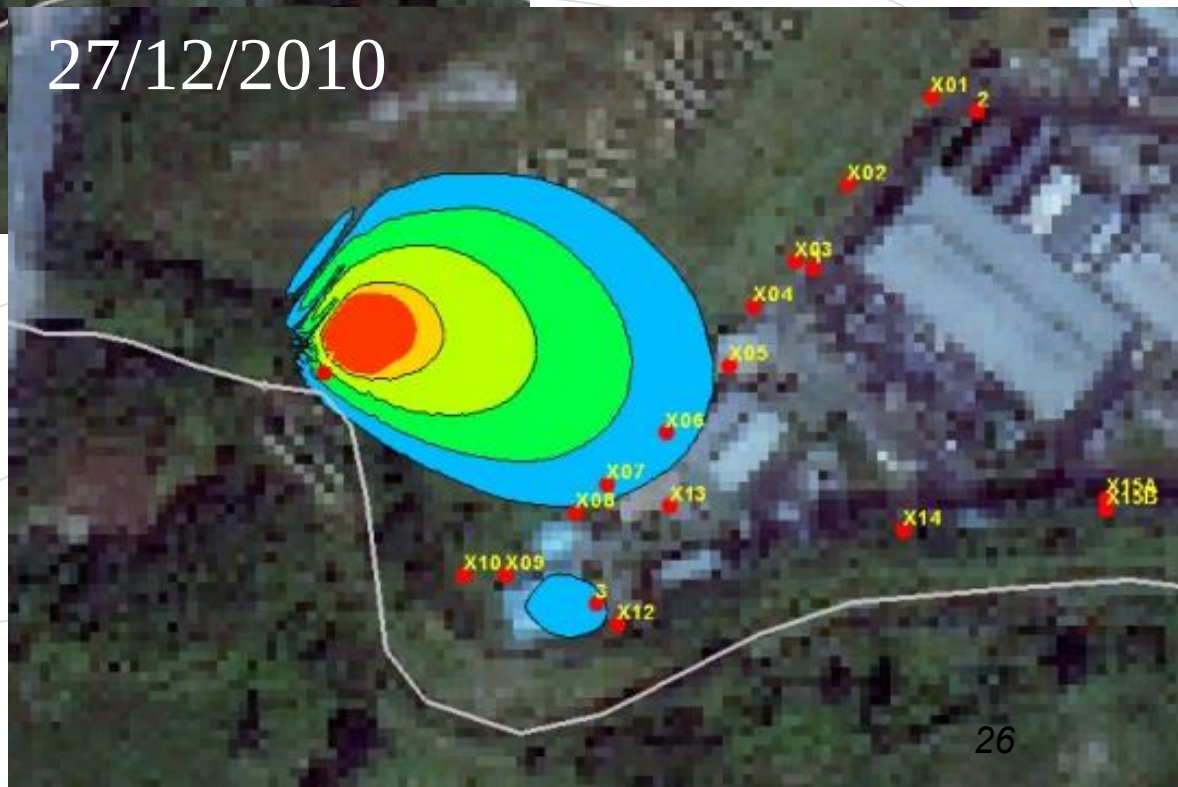
1.00
0.10
0.01
0.00

PCE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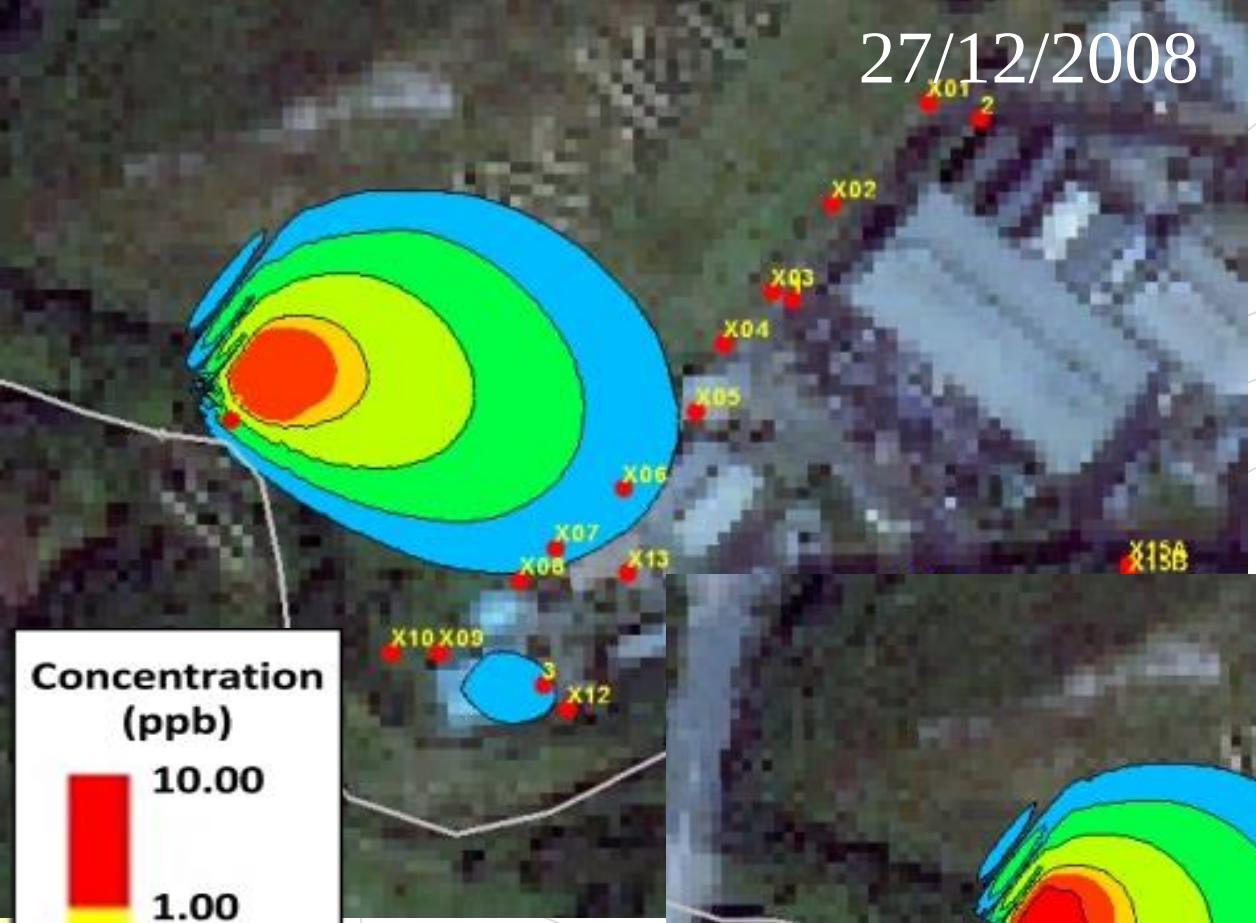
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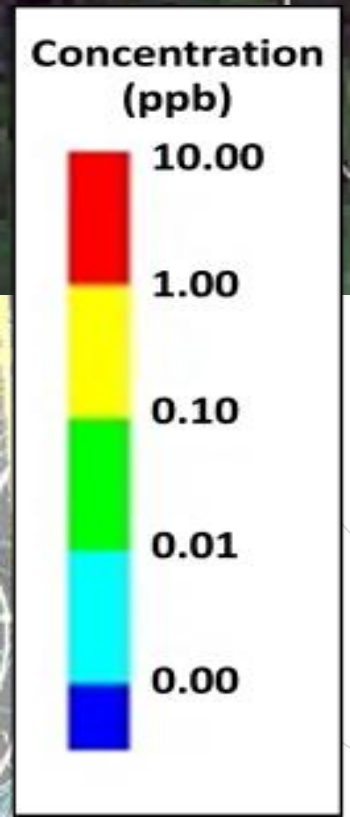
TCE


Concentration (ppb)
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1.00
0.10
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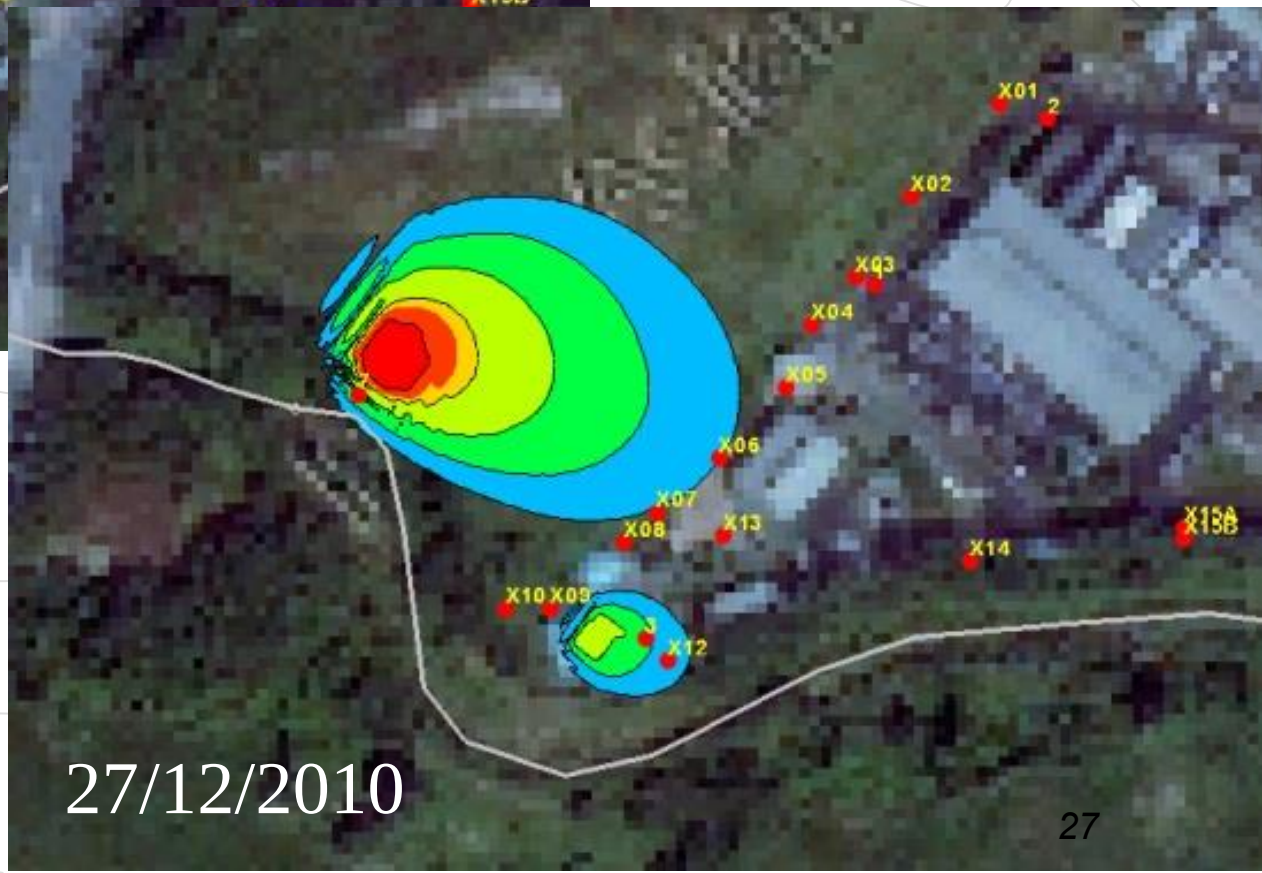
0.00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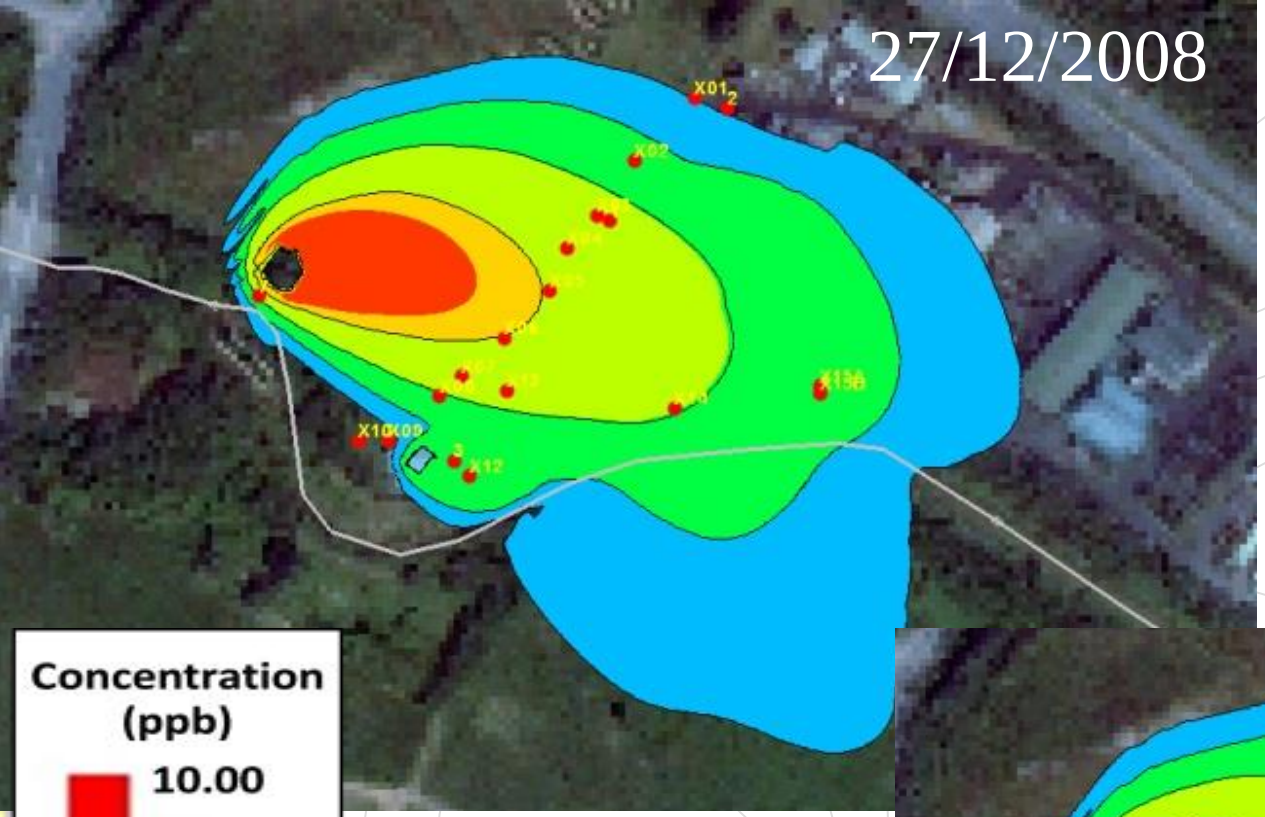
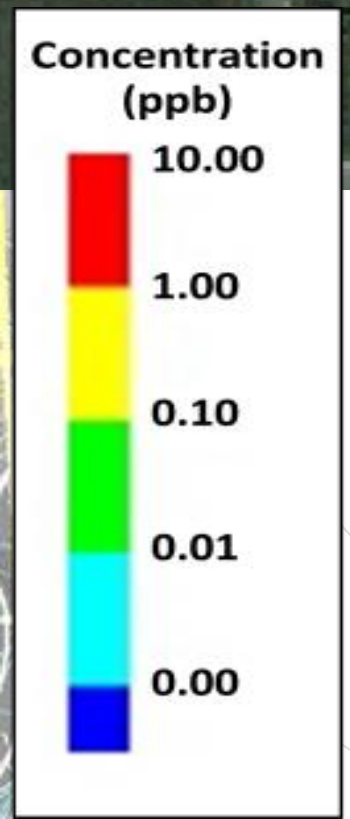
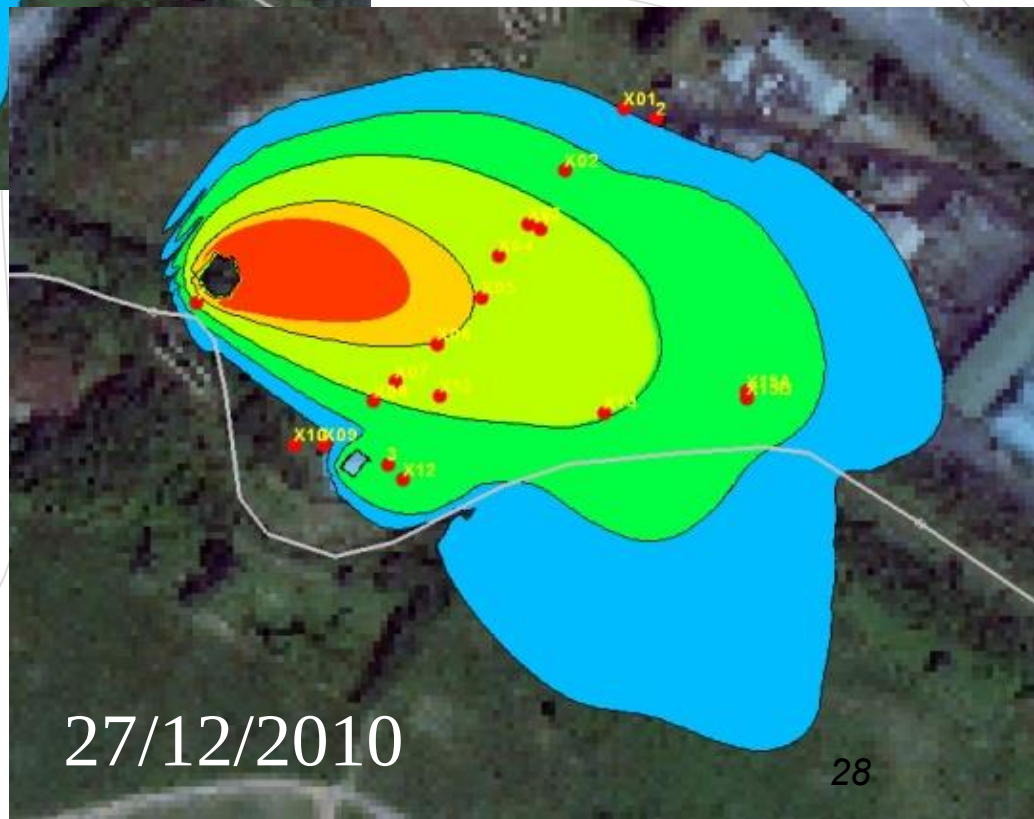






27/12/2010

Conclusions

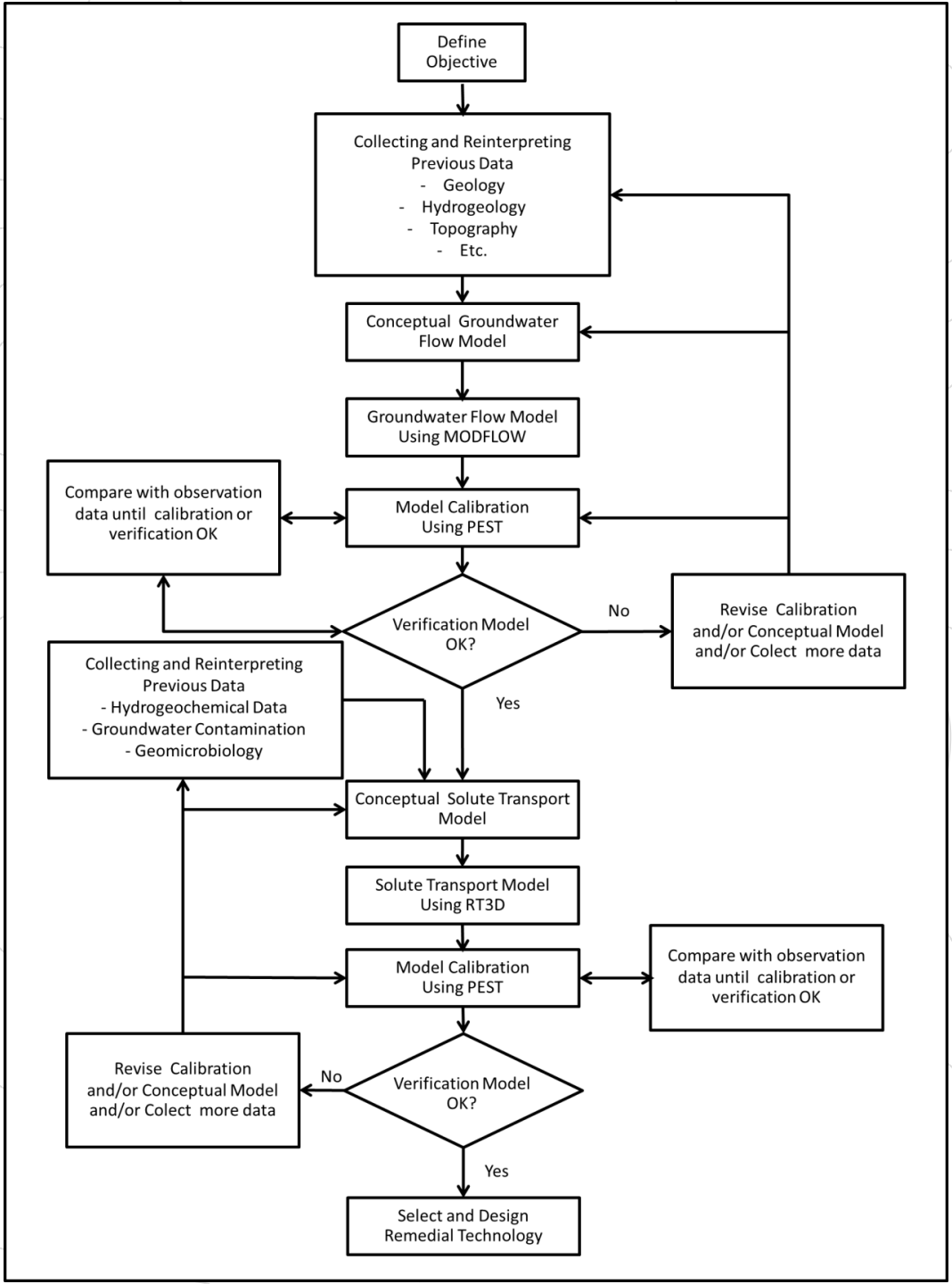
- Site Characterization
  - 6 hydrogeostratigraphic unit (Heterogeneous)
  - PCE TCE DCE contamination
- Groundwater Flow and Solute Transport Simulations
  - Groundwater flow from NW to SE.
  - The plumes show the effect from the groundwater flow direction and degradation of the chemical.

References

Department of Environmental Quality Promotion, 2011, Feasibility Study of In-Situ Bioremediation System Implementation for Treatment of VOCs Contaminated Groundwater and Contaminant Transport Modeling in Saturated and Unsaturated Aquifers (Executive Summary Report), Chiang Mai, Thailand. (In Thai)

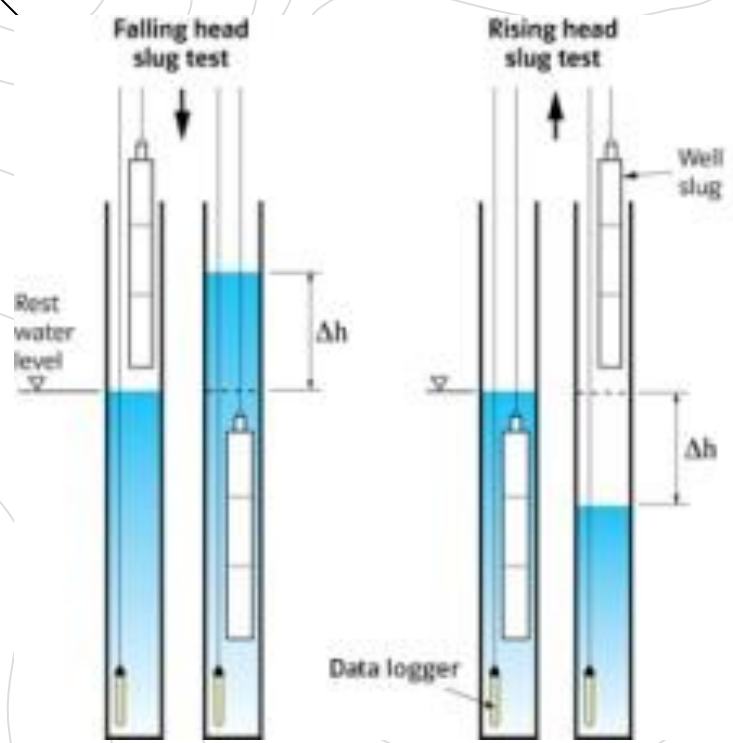
Acknowledgments

- Science Achievement Scholarship of Thailand (SAST), Office of the Higher Education Commission
- Environmental Research and Training Center (ERTC), Department of Environmental Quality Promotion
- Faculty of Science, Chiangmai University


Define Objective
Collecting and Reinterpreting Previous Data
- Geology
- Hydrogeology
- Topography
- Etc.
Conceptual Groundwater Flow Model
Groundwater Flow Model Using MODFLOW
Compare with observation data until calibration or verification OK
Model Calibration Using PEST
Verification Model OK?
No
Revise Calibration and/or Conceptual Model and/or Colect more data
Yes
Collecting and Reinterpreting Previous Data
- Hydrogeochemical Data
- Groundwater Contamination
- Geomicrobiology
Conceptual Solute Transport Model
Solute Transport Model Using RT3D
Model Calibration Using PEST
Compare with observation data until calibration or verification OK
Revise Calibration and/or Conceptual Model and/or Colect more data
No
Verification Model OK?
Yes
Select and Design Remedial Technology

No.	Test Code	UTM-E	UTM-N	Well Name	Longitudinal Dispersivity (m)
1	D1	731094	1406764	2	5.01
2	D4	731047	1406719	1	3.64
3	D5	730985	1406623	3	9.92
4	D6	730970	1406689	7	16.1
5	D7	731131	1406653	X15A	1.29
6	D8	730979	1406649	X08	1.78

Slug Test



0.03 to 3.55 m/day

Department of Geological Sciences
Faculty of Science, Chiang Mai University
Chiang Mai, Thailand 50200
Tel. 0-5394-3417 Fax. 0-5394-3444
http://www.geol.science.cmu.ac.th

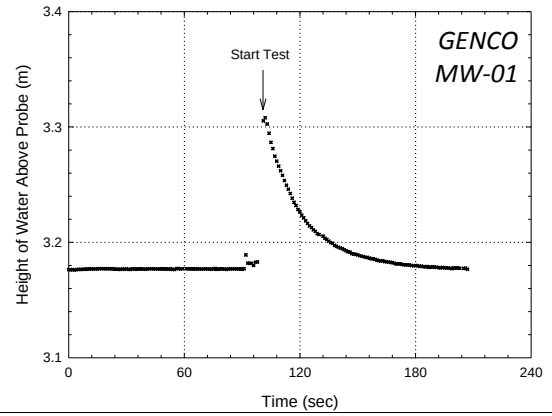
Slug Test Analysis Report

Test Date: 17-21 Sept 08

Tested & Analyzed By *CMU & ERTC*

Test Well Name: GENCO: MW-01			**Location:** บริษัท GENCO	
Well Information	**Depth:**	14 m	**UTM-E:**	731311
	Radius:	0.051 m	**UTM-N:**	1406605
	DTW:	3.76 m	**TOC:**	0.54 m

Test Data



Probe: Solinst Level Logger®

Problems or Comments:
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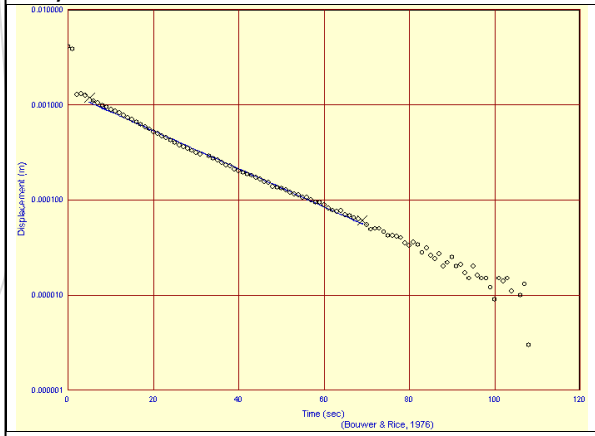
Analysis Results



Hydraulic Conductivity (m/day):	
Hvorslev:	-
Bouwer & Rice:	2.35-2.96

Problems or Comments:
n/a

Tracer Test

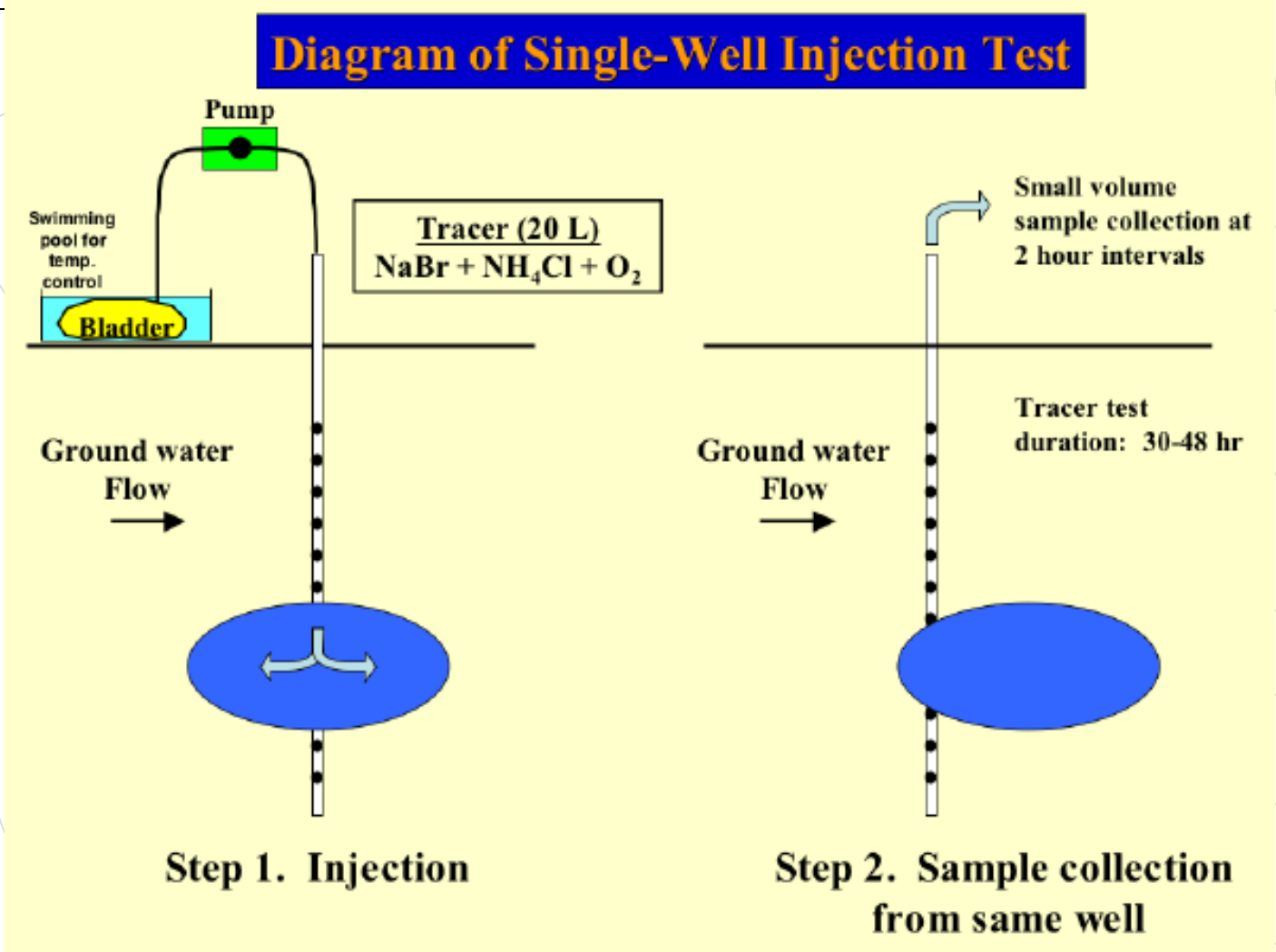
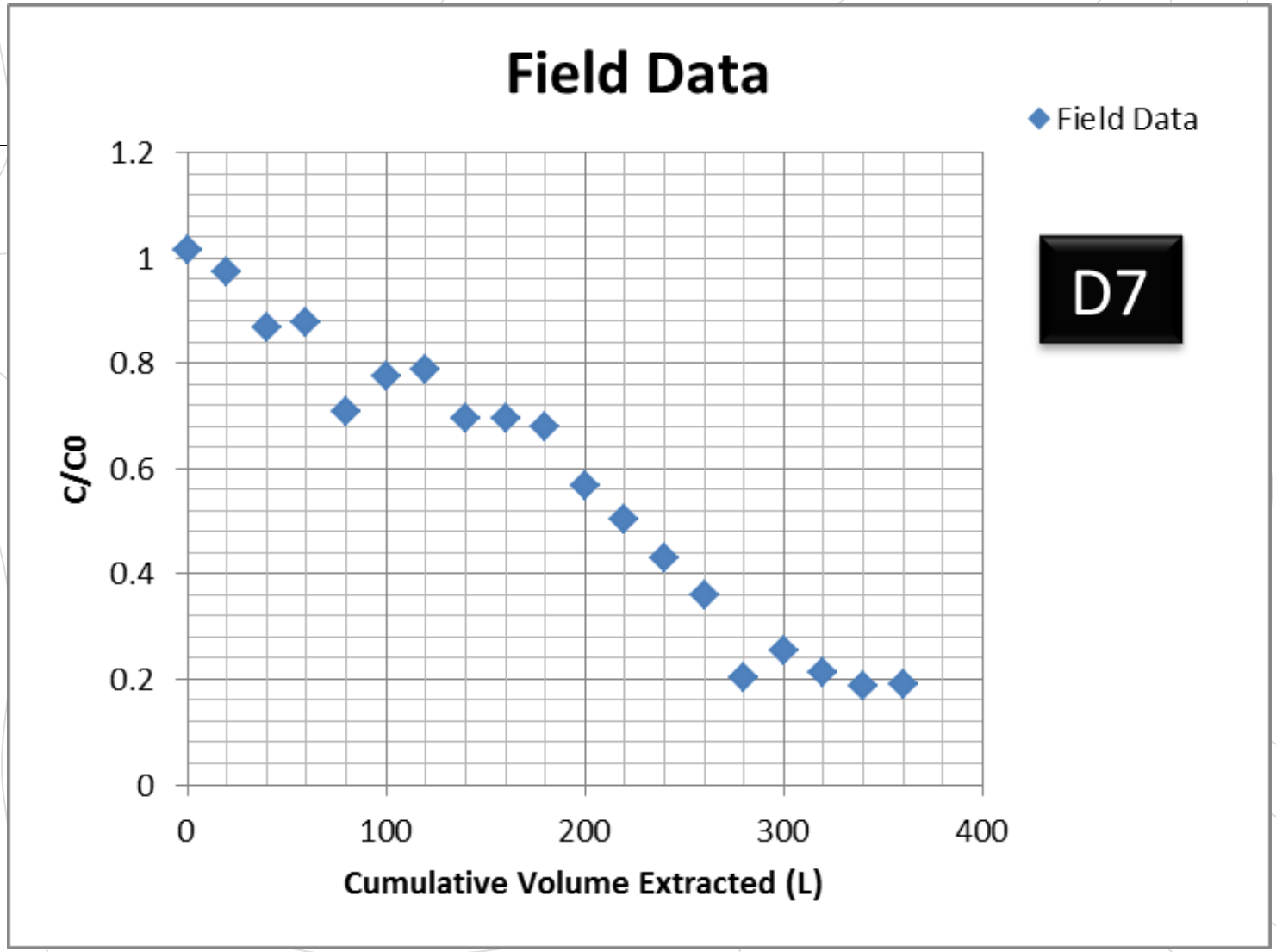
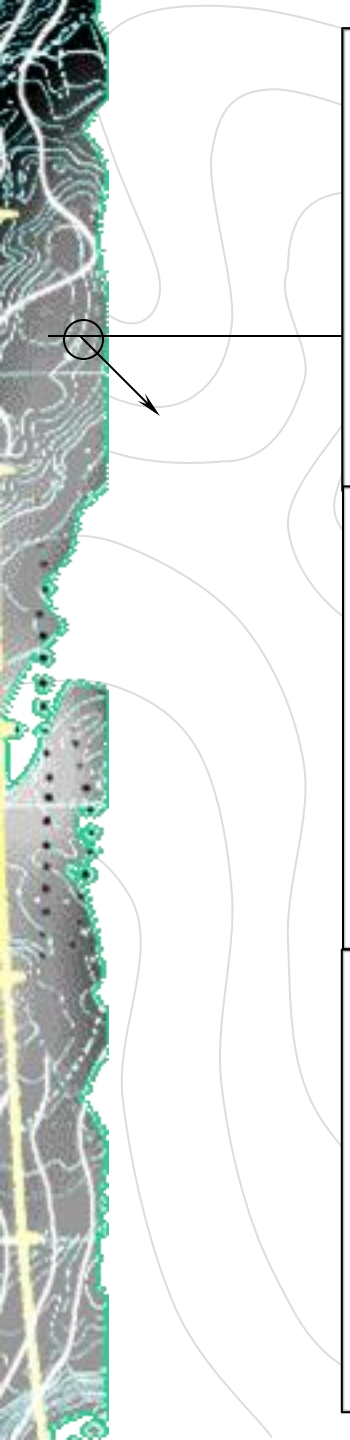


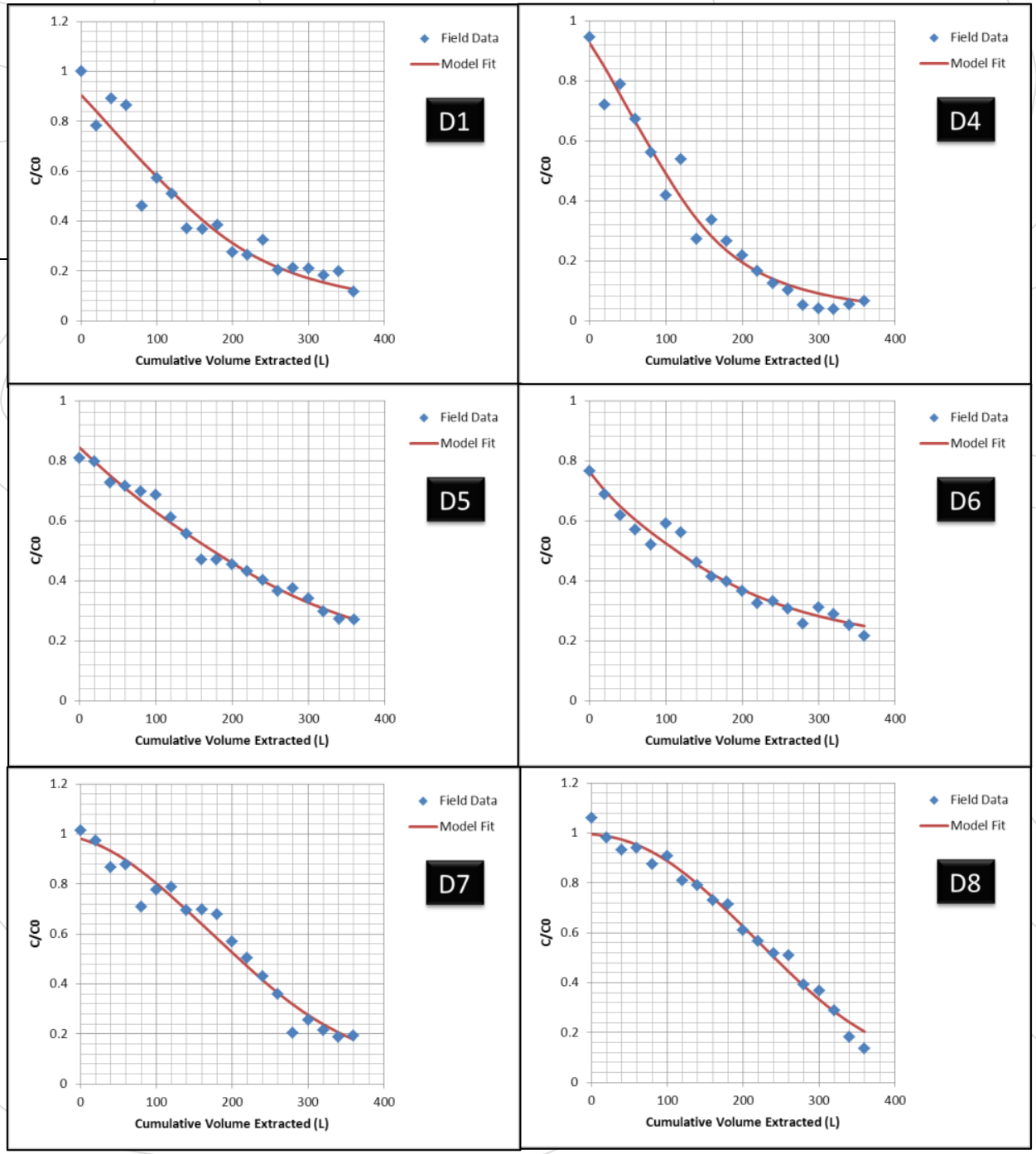
Diagram of Single-Well Injection Test
Pump
Swimming pool for temp. control
Bladder
Tracer (20 L)
NaBr + NH4Cl + O2
Ground water Flow
Step 1. Injection
Small volume sample collection at 2 hour intervals
Tracer test duration: 30-48 hr
Ground water Flow
Step 2. Sample collection from same well


Field Data
Field Data
D7
C/C0
1.2
1
0.8
0.6
0.4
0.2
0
0
100
200
300
400
Cumulative Volume Extracted (L)

$$\frac{C}{C_0} = \frac{1}{2}\,\mathrm{erfc}\left\{ \frac{U_p / U_i - 1}{\sqrt{\frac{16}{3}\frac{\alpha}{R_f}\left[2 - |1 - U_p / U_i|^{0.5}\right]^{0.5}}} \right\}$$

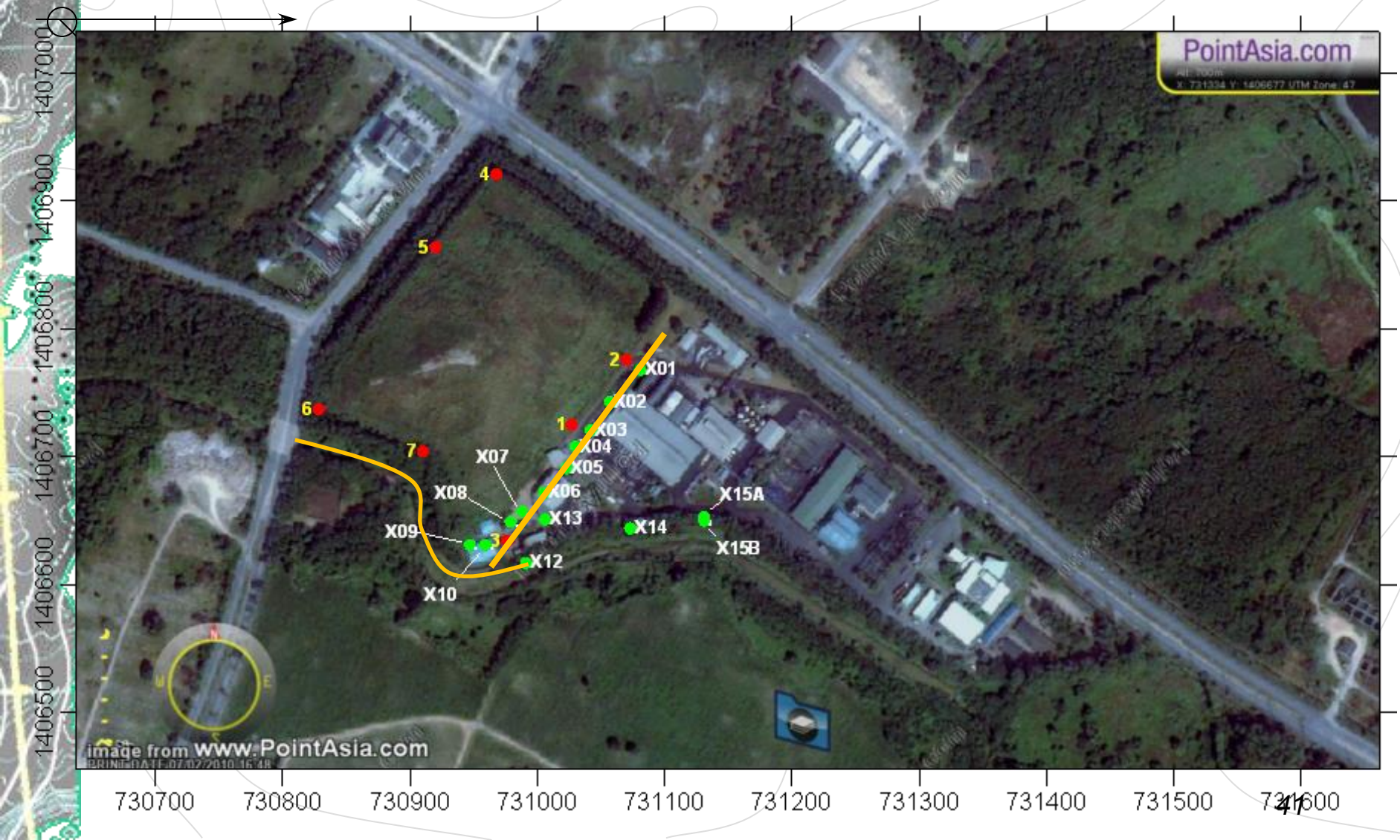
$$R_f = \sqrt{\frac{Qt}{\pi b \phi}}$$




D1
D4
D5
D6
D7
D8
Field Data
Model Fit
C/C0
Cumulative Volume Extracted (L)

No.	Test Code	UTM-E	UTM-N	Well Name	Longitudinal Dispersivity (m)
1	D1	731094	1406764	2	5.01
2	D4	731047	1406719	1	3.64
3	D5	730985	1406623	3	9.92
4	D6	730970	1406689	7	16.1
5	D7	731131	1406653	X15A	1.29
6	D8	730979	1406649	X08	1.78

Geophysical Investigation




GENCO

Geomicrobiology

- *cis*-DCE → biodegradation of PCE/TCE
- Facultative bacteria
  - *Pseudomonas* sp.
  - *Shewanella* sp.
  - *Burkholderia* sp.
  - *Rhodococcus* sp
- Pail Test

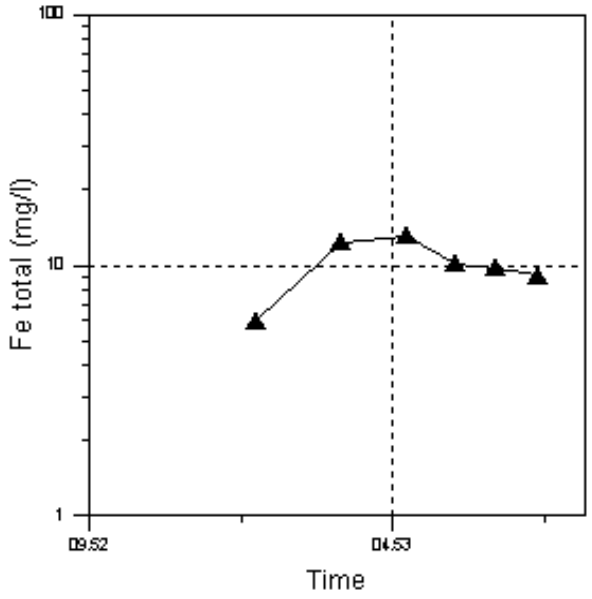

ทำการสูบน้ำจากบ่อทดสอบ
ประมาณ 80-100 ลิตร

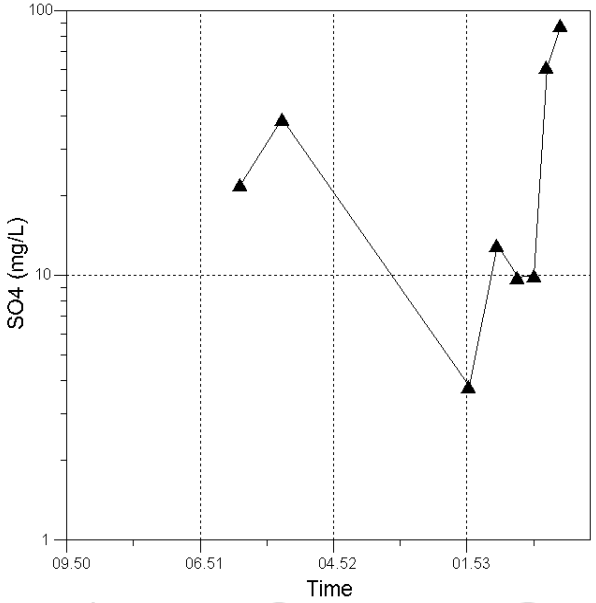

ผสมสารอาหาร

PAIL TEST

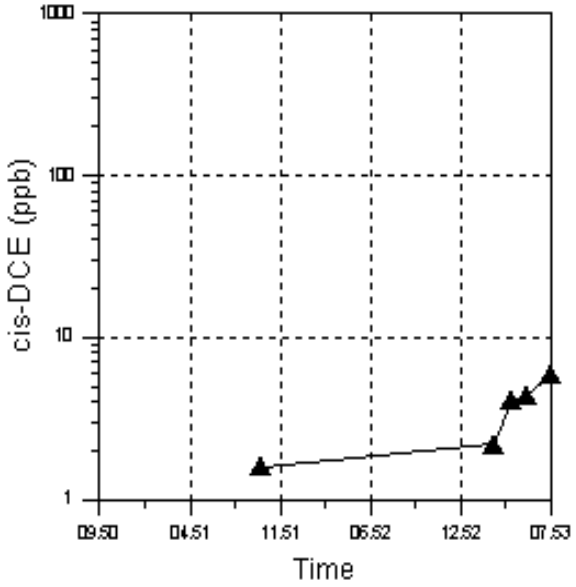

ทำการละลายสารอาหาร
และเพิ่มออกซิเจน

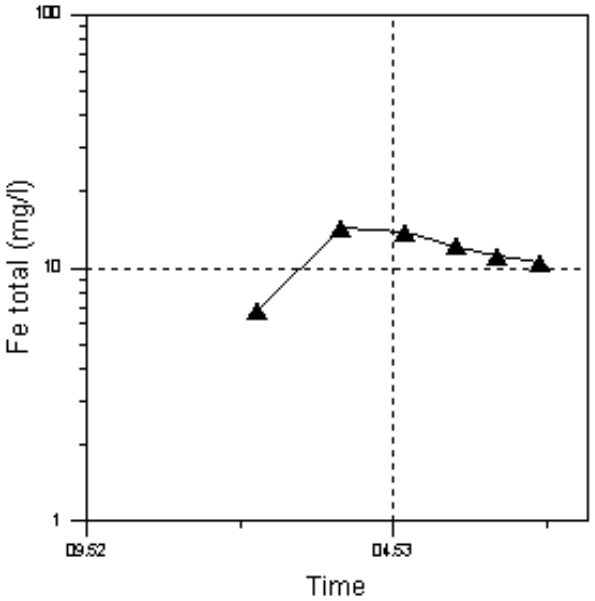

เติมน้ำที่ได้จากการผสม
สารอาหารลงในบ่อทดสอบ

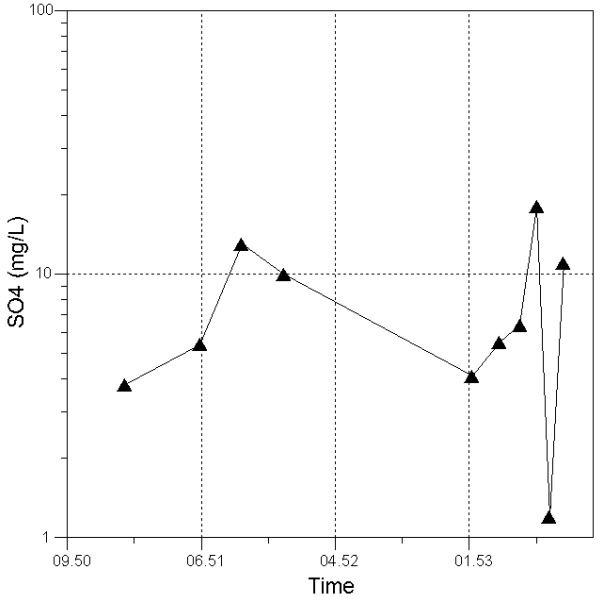




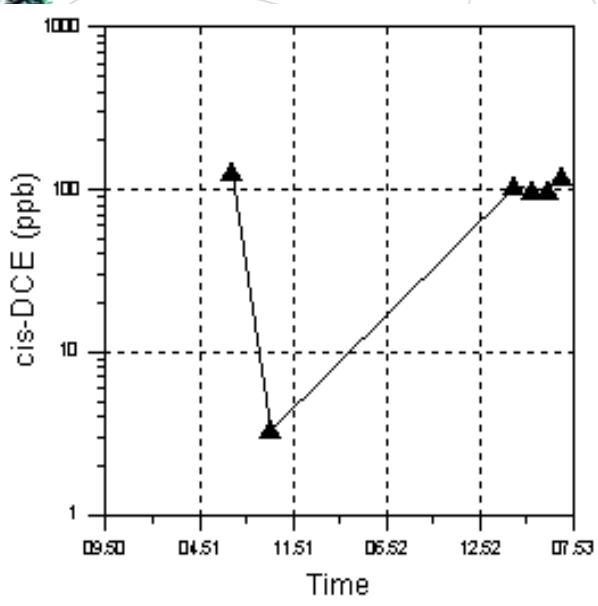
Well no. 1

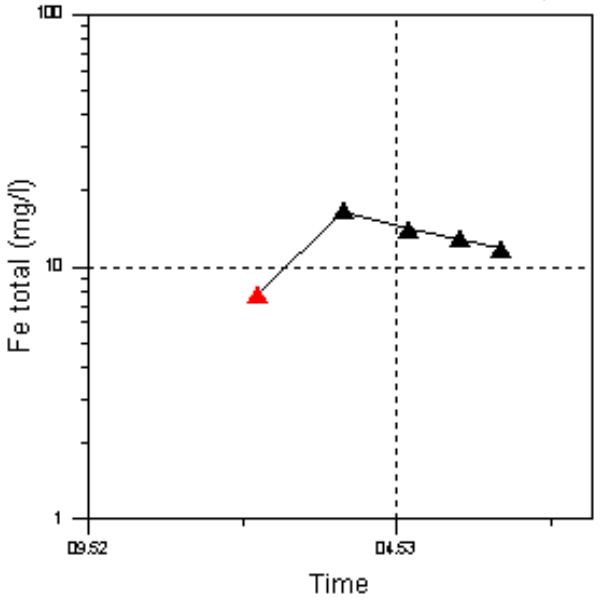


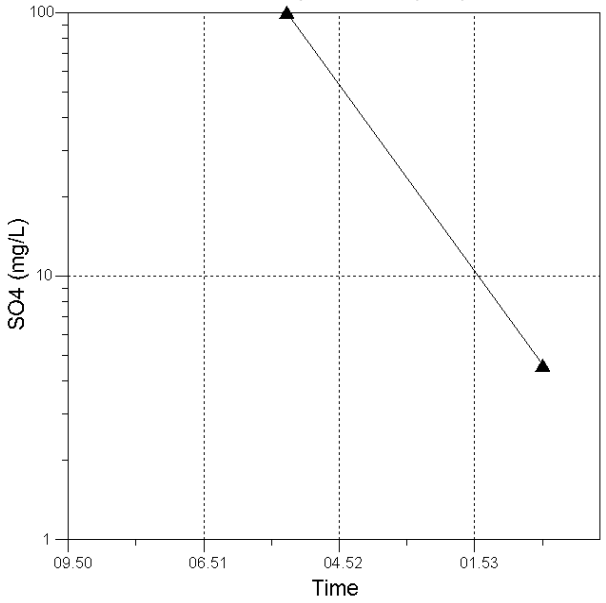




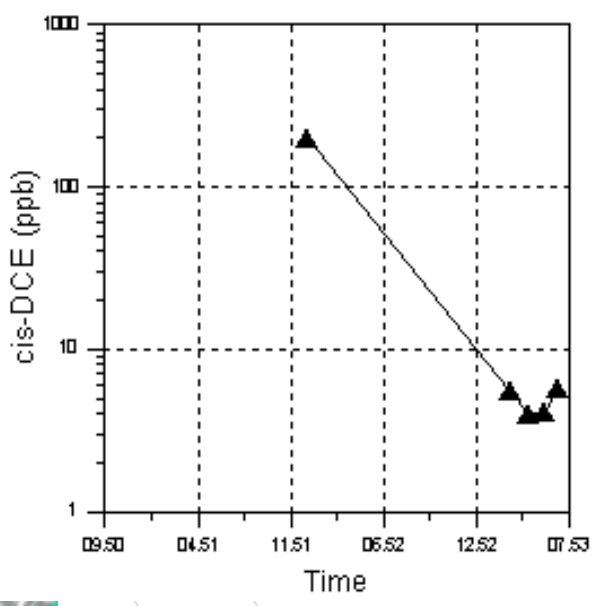
Well no. 2

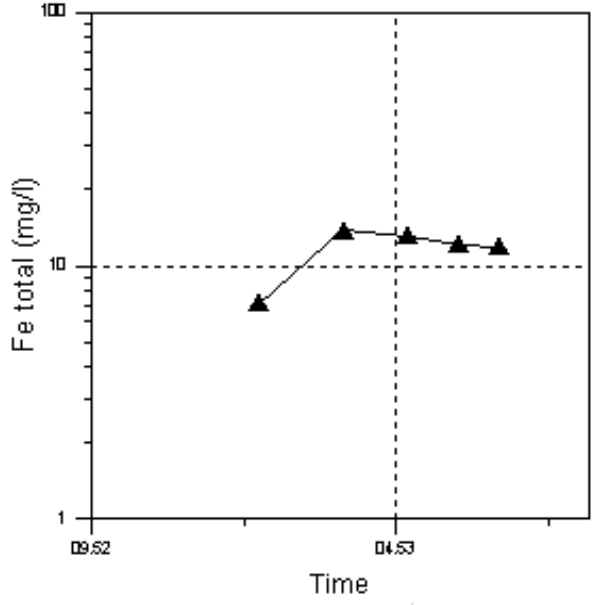


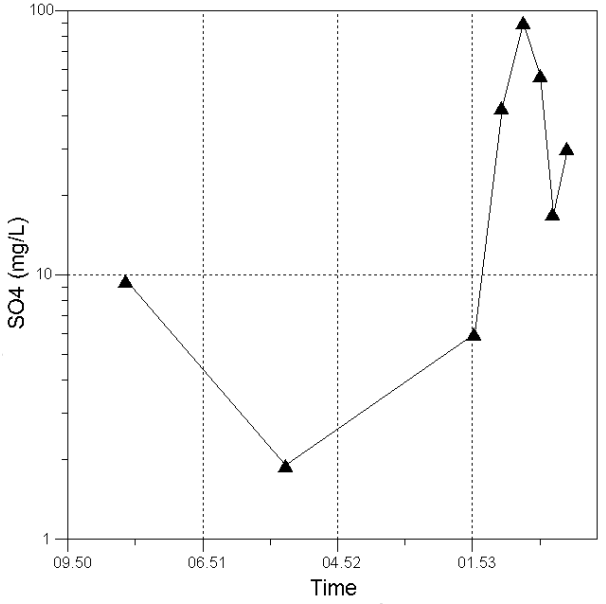




Well no. 3







Well no. 7

Numerical Modeling

Groundwater Flow Model

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right)\pm W=0$$

Solute Transport Model

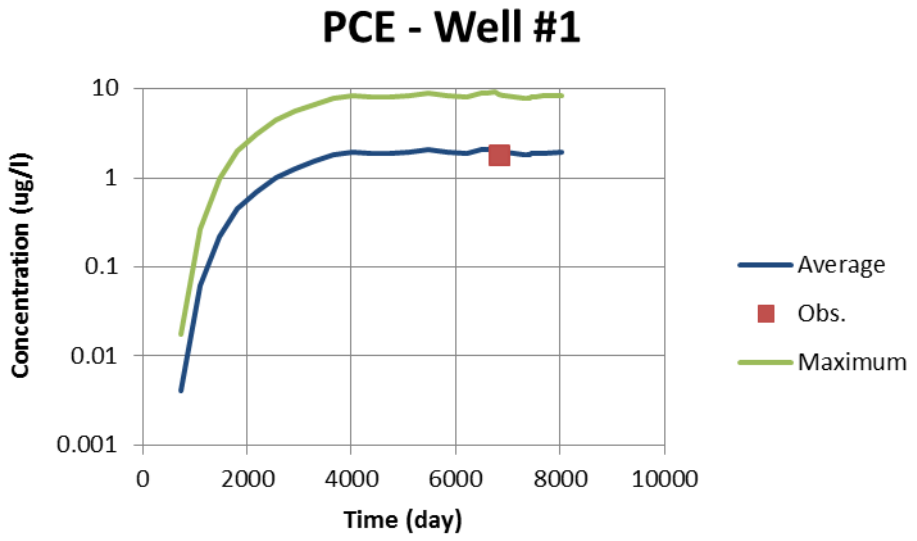
$$\frac{\partial c}{\partial t} = \frac{\partial}{x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i} v_i c + \sum R_n$$

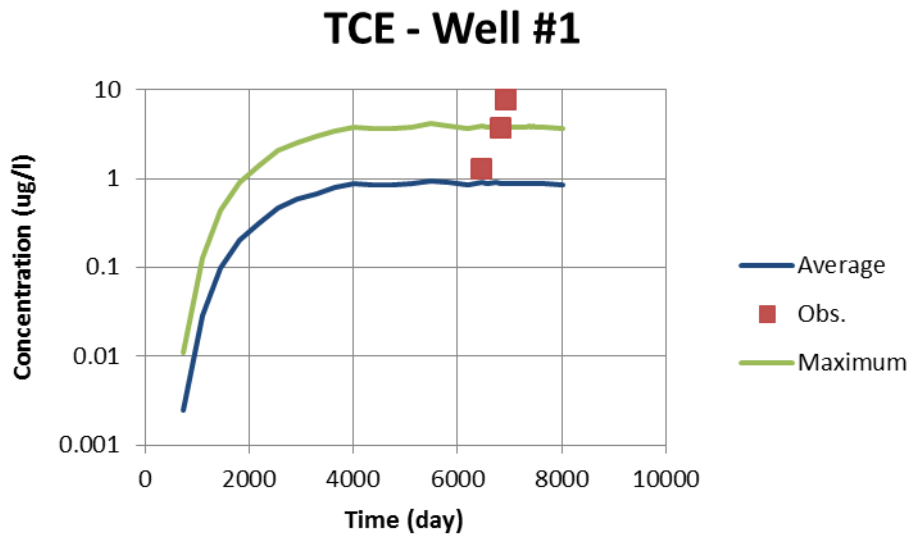
Dispersion

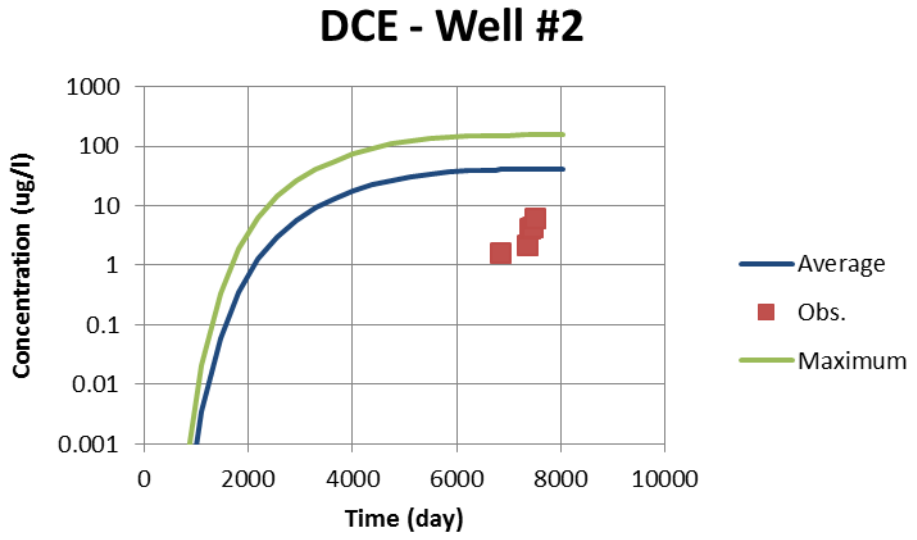
Advection

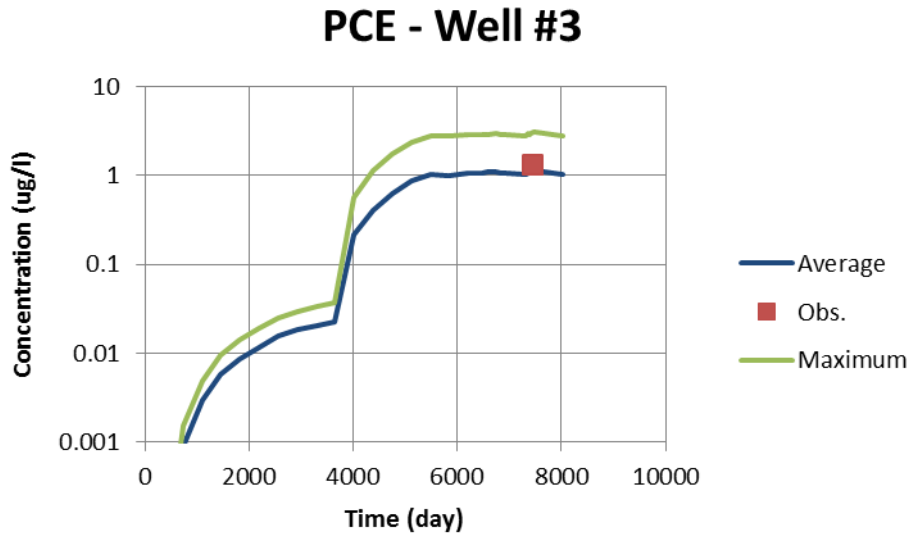
Chemical reaction

Result of Source Concentration Calibration

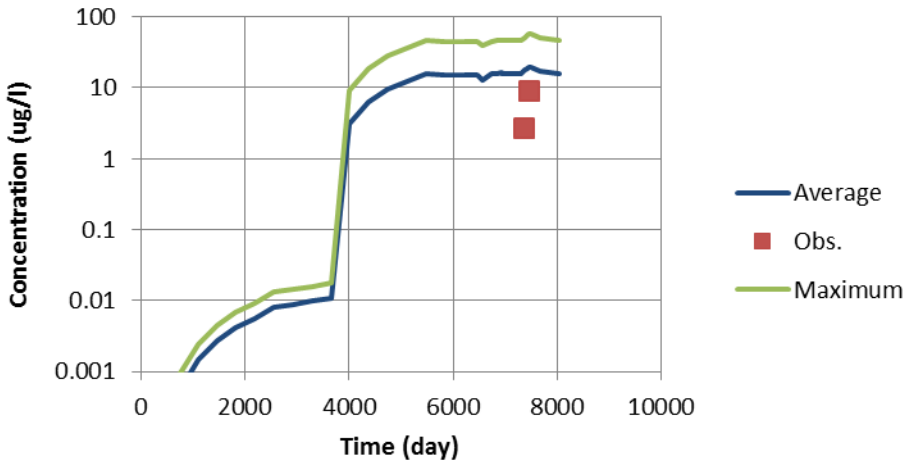




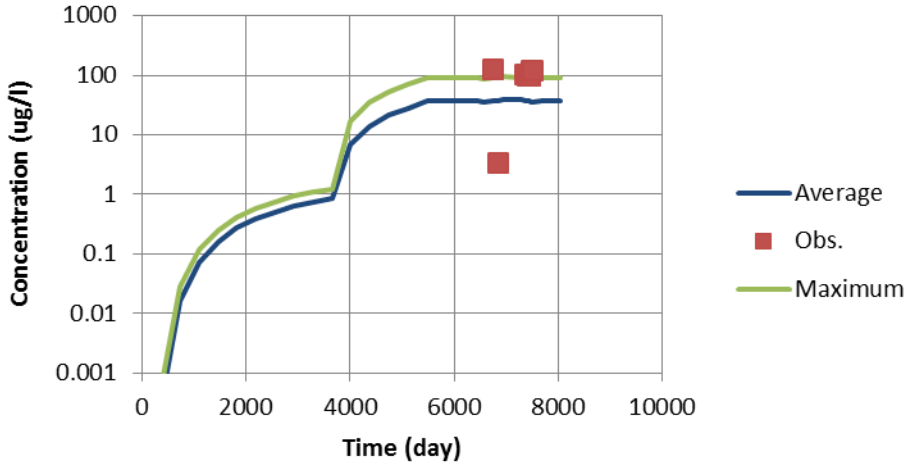




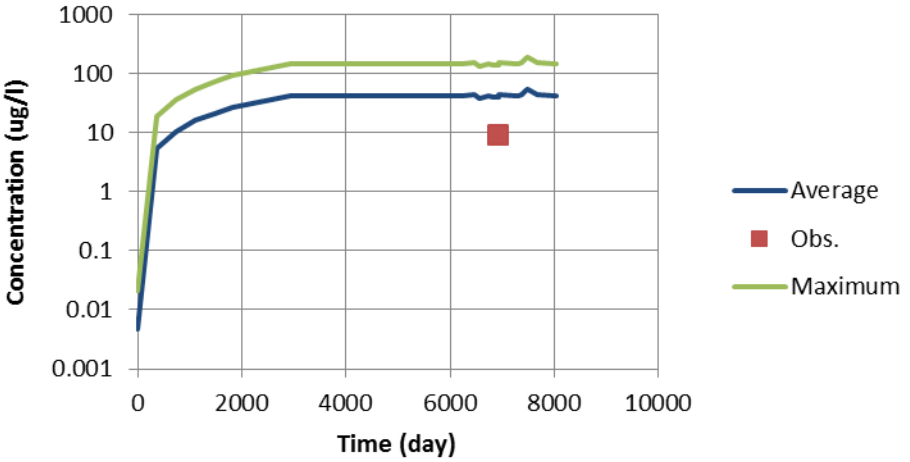
TCE - Well #3



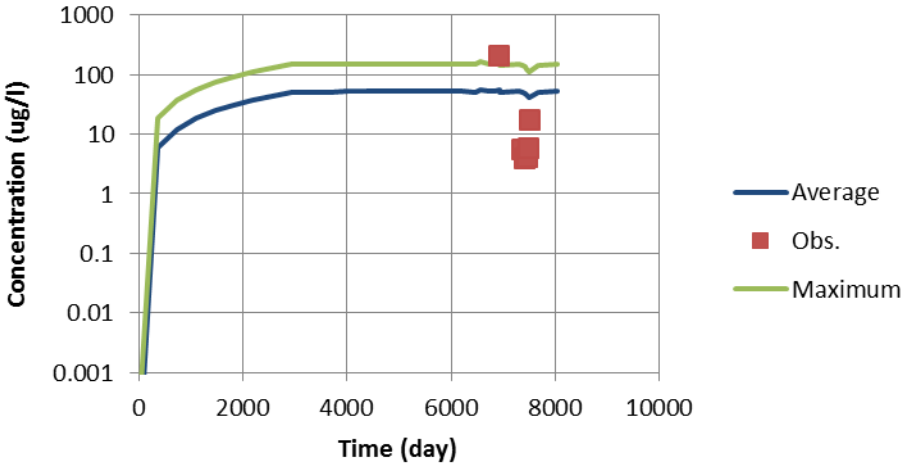
DCE - Well #3



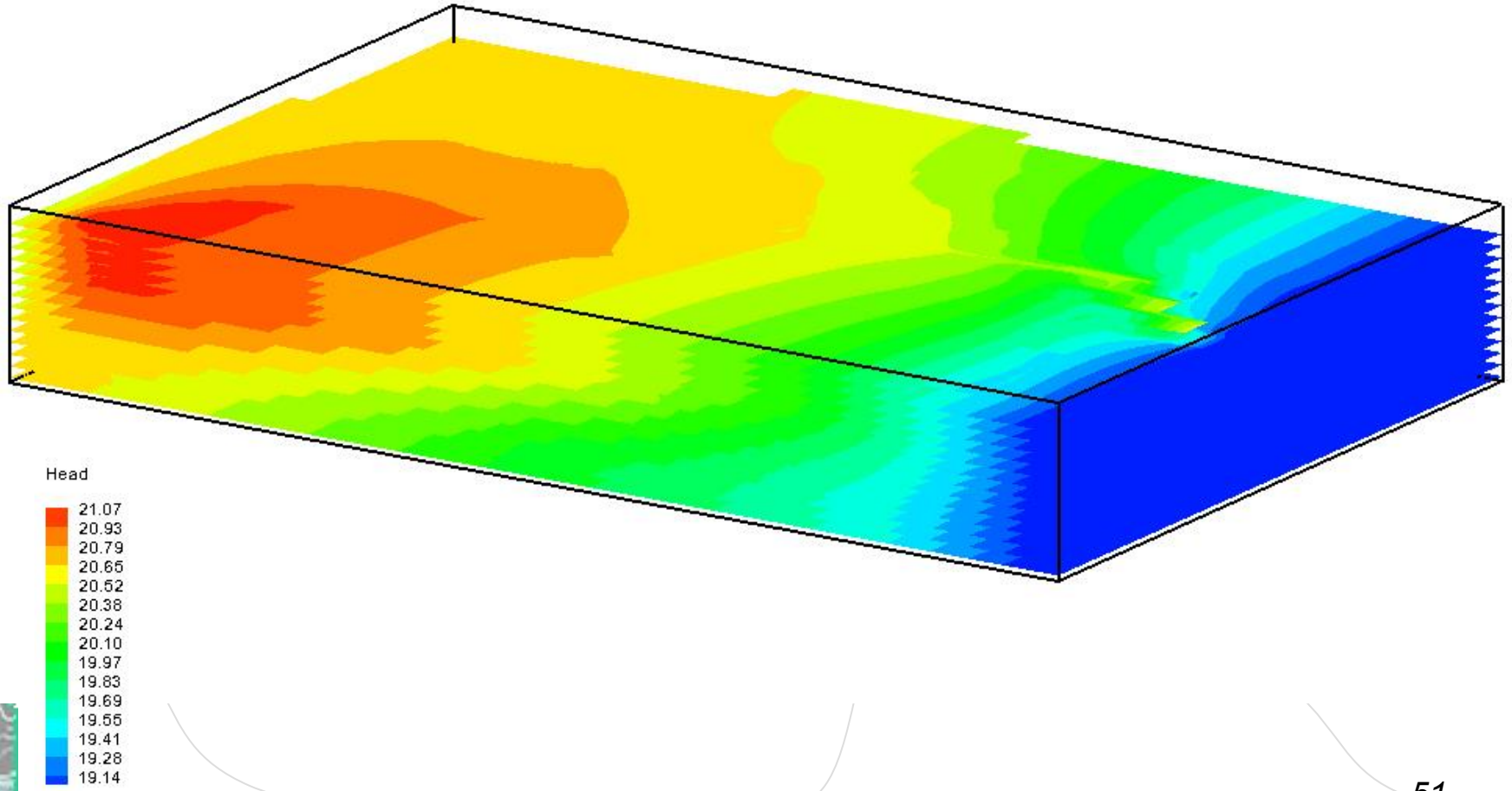
TCE - Well #7

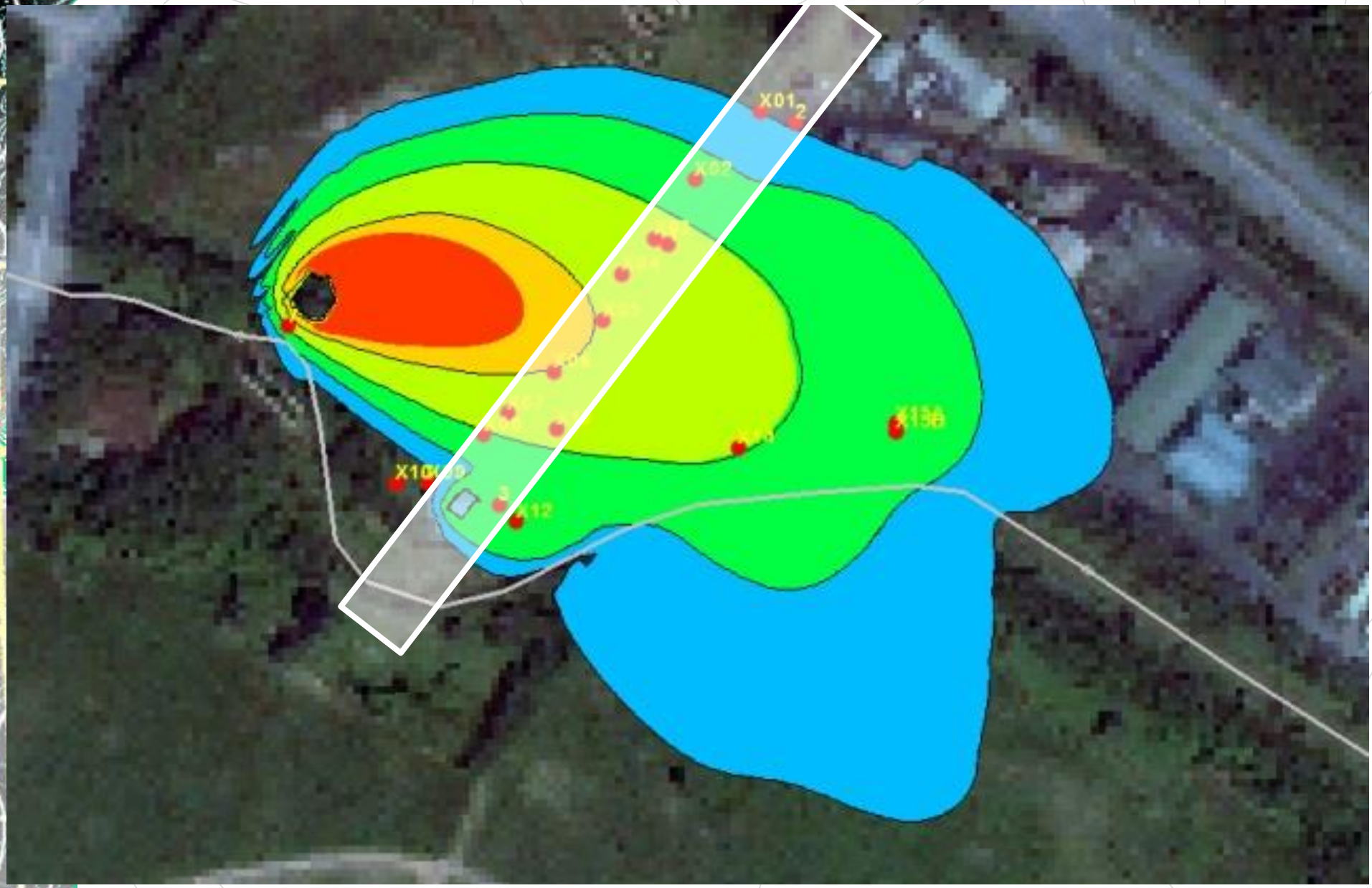


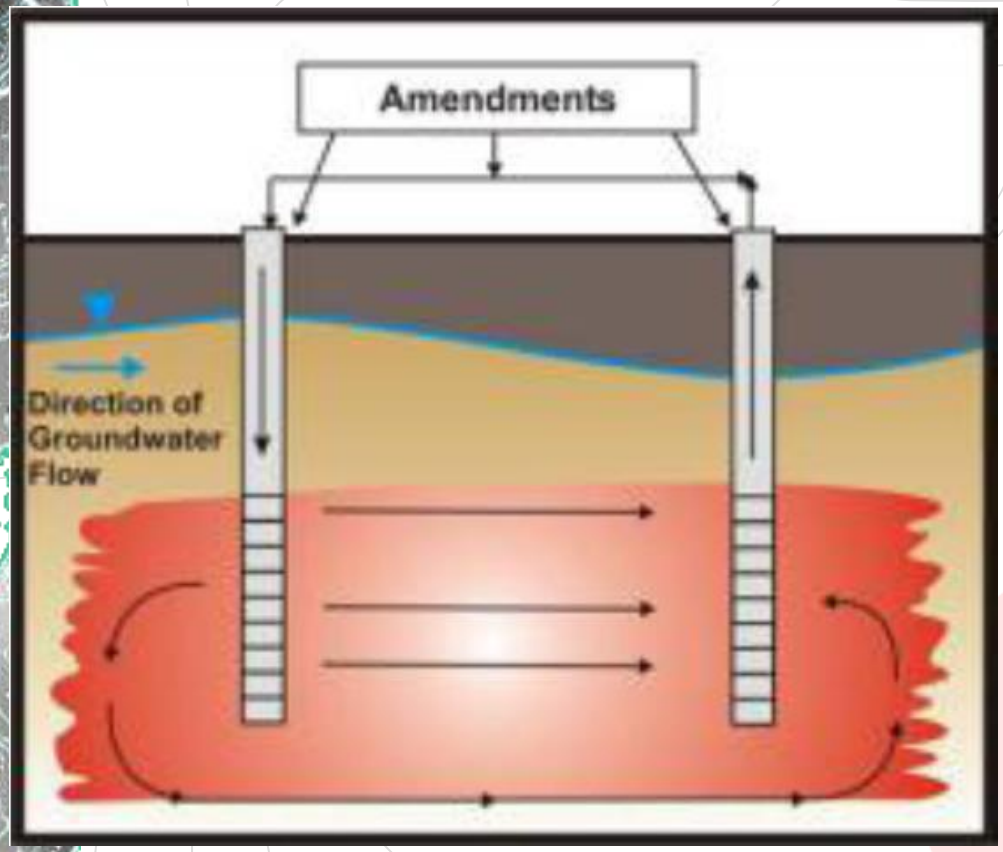
DCE - Well #7

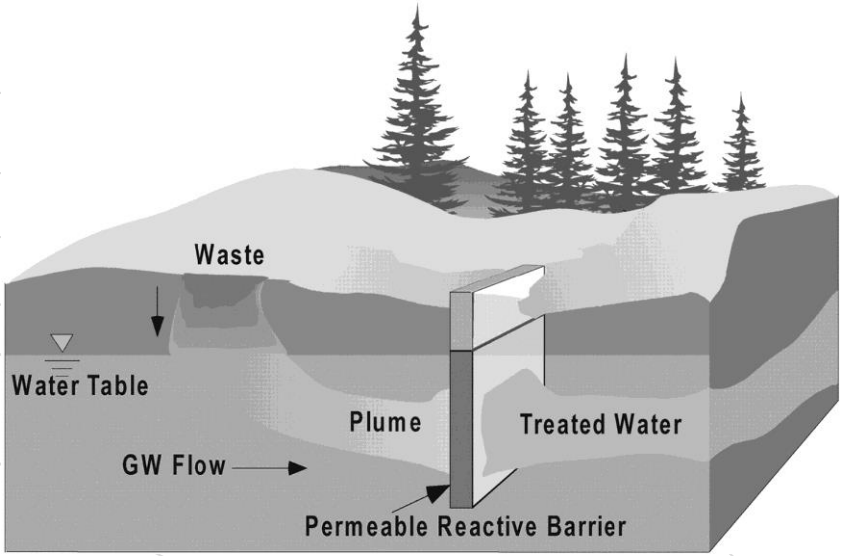


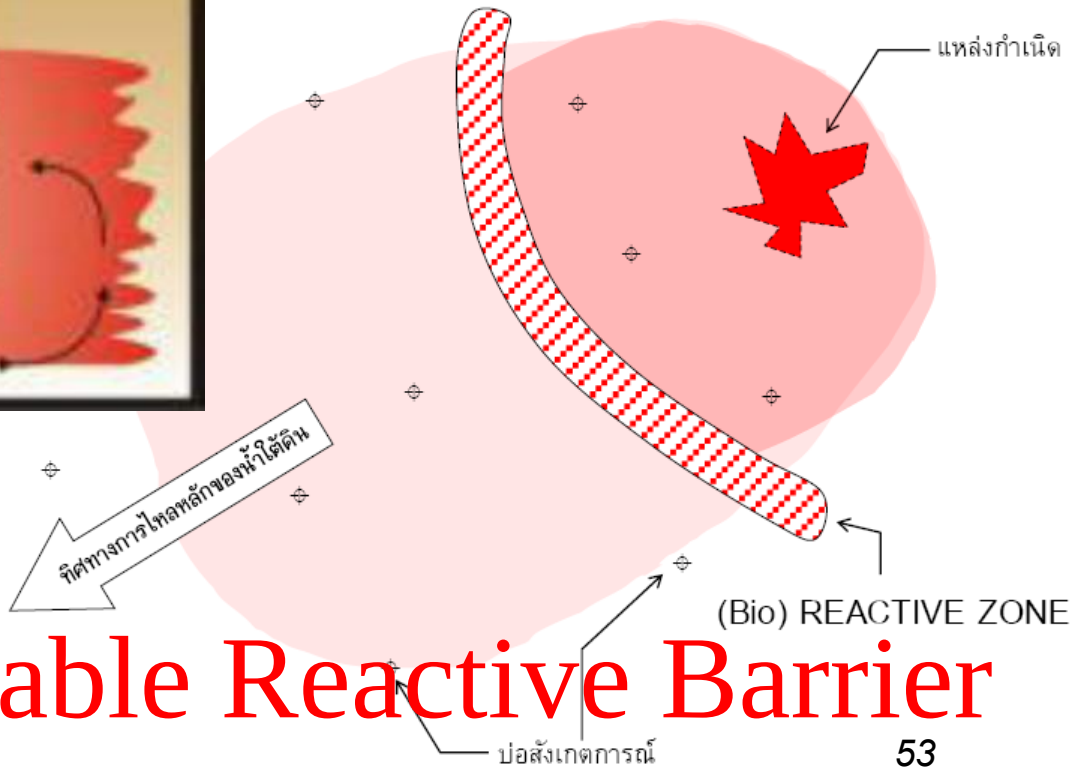
Result of Groundwater Flow Model




X01
X02
X12



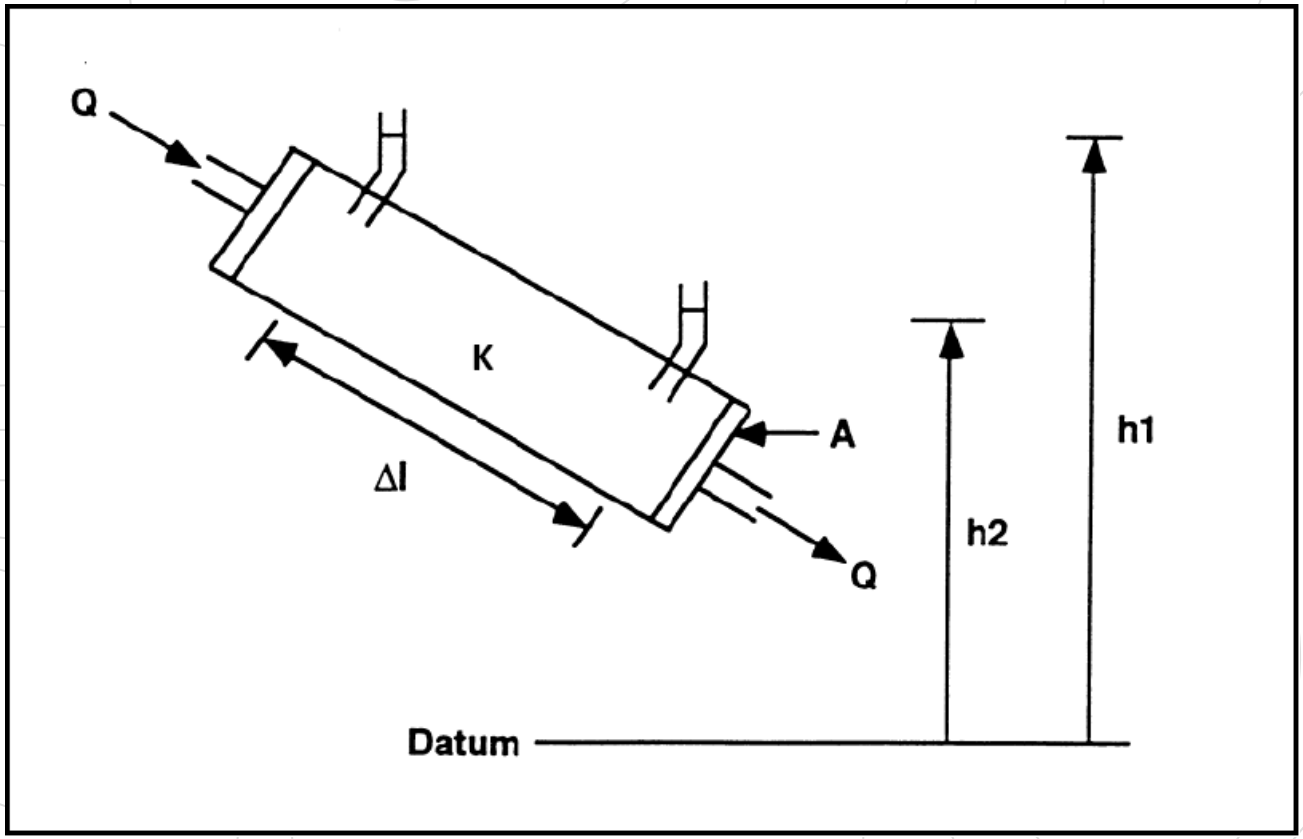




Bio-Permeable Reactive Barrier

$$Q = KA\frac{\Delta h}{L}$$

$$Q = -KA\frac{dh}{dl}$$



$$v = \frac{Q}{A} = -K\frac{dh}{dl} \qquad \bar{v} = \frac{Q}{n_e A} = \frac{-K}{n_e}\frac{dh}{dl}$$

Confined aquifer: $S = S_s b$,

Unconfined aquifer: $S = S_y + S_s b$.

$$D^* = \omega D_d$$

$$D_L = \alpha_L v_i + D^*$$

$$D_T = \alpha_T v_i + D^*$$

$$D_{ij} = \begin{bmatrix} D_L & 0 & 0 \\ 0 & D_{T,h} & 0 \\ 0 & 0 & D_{T,v} \end{bmatrix}$$

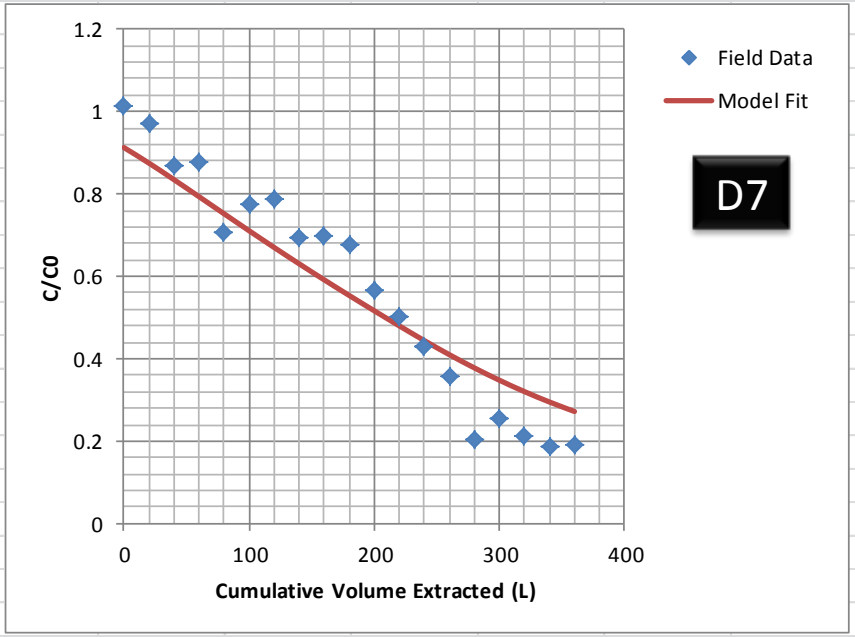
$$D_{ij} = \begin{bmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{bmatrix}$$

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right)\pm W = S_s \frac{\partial h}{\partial t}$$

Q*t	208.9906	L
b	32	m
n	0.3	
α	0.03	m
R_f	0.147546	m
Ui	208.9906	L
C0	15.38246	

$$\frac{C}{C_0} = \frac{1}{2}\operatorname{erfc}\left[\frac{U_p/U_i - 1}{\sqrt{\frac{16}{3}\frac{\alpha}{R_f}\left[2 - \left|1 - U_p/U_i\right|^{0.5}\left(1 - U_p/U_i\right)\right]^{0.5}}}\right]$$

Up	[Bromide]	Up/Ui	C/C0		model C/C0	0.153055
0	15.59737	0	1.013971	-0.96029	0.912778	0.01024
20	14.95181	0.095698	0.972004	-0.81331	0.874967	0.009416
40	13.33718	0.191396	0.867039	-0.68825	0.834805	0.001039
60	13.50468	0.287094	0.877927	-0.57899	0.793555	0.007119
80	10.87527	0.382792	0.706992	-0.48152	0.752055	0.002031
100	11.93721	0.47849	0.776027	-0.39306	0.710849	0.004248
120	12.11406	0.574189	0.787525	-0.31159	0.67027	0.013749
140	10.67608	0.669887	0.694042	-0.23561	0.630508	0.004037
160	10.71886	0.765585	0.696824	-0.16389	0.591646	0.011062
180	10.44558	0.861283	0.679058	-0.09543	0.55368	0.01572
200	8.729906	0.956981	0.567524	-0.02928	0.516513	0.002602
220	7.726426	1.052679	0.502288	0.035663	0.479888	0.000502
240	6.601465	1.148377	0.429155	0.099343	0.444136	0.000224
260	5.528267	1.244075	0.359388	0.160953	0.40997	0.002559
280	3.117801	1.339773	0.202685	0.220077	0.377811	0.030669
300	3.928603	1.435471	0.255395	0.2765	0.347887	0.008555
320	3.295218	1.531169	0.214219	0.330141	0.320289	0.011251
340	2.884721	1.626868	0.187533	0.381004	0.295005	0.01155
360	2.944815	1.722566	0.19144	0.429152	0.271955	0.006483



U_p คือปริมาตรน้ำใต้ดินที่สูบออกมา ณ เวลาต่างๆ

U_i คือปริมาตรสารละลายโบรไมด์ที่เติมลงไป

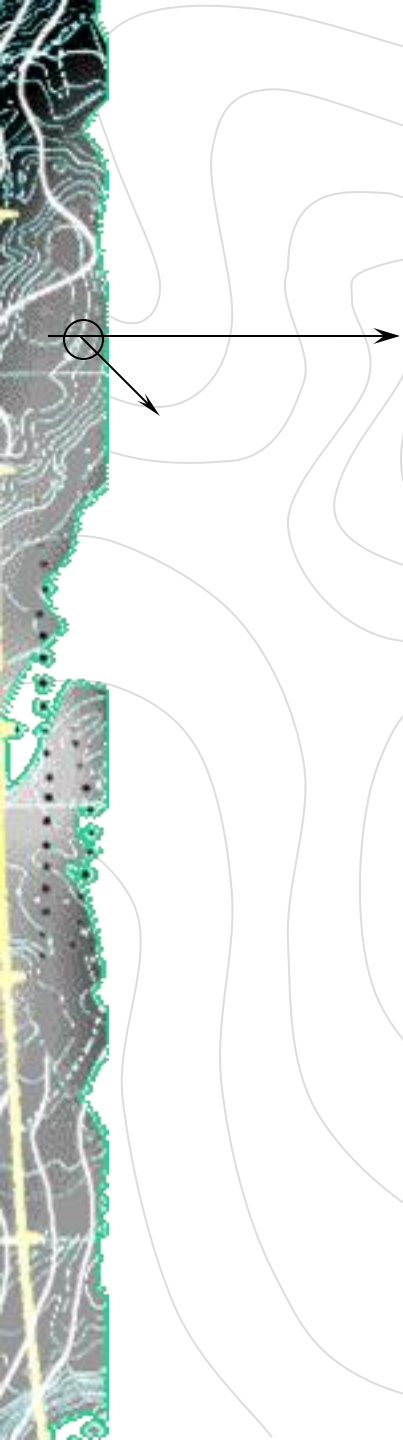
R_f รัศมีเฉลี่ยที่สารละลายโบรไมด์ไหลออกไปจากบ่อทดสอบ ซึ่งคำนวณได้จากสมการ

Q คืออัตราการเติมสารละลายลงไปในบ่อ

t คือเวลาที่ใช้ในการเติมสารละลายลงไปในบ่อ (ตั้งแต่เริ่มเติมจนกระทั่งระดับน้ำคืนตัว)

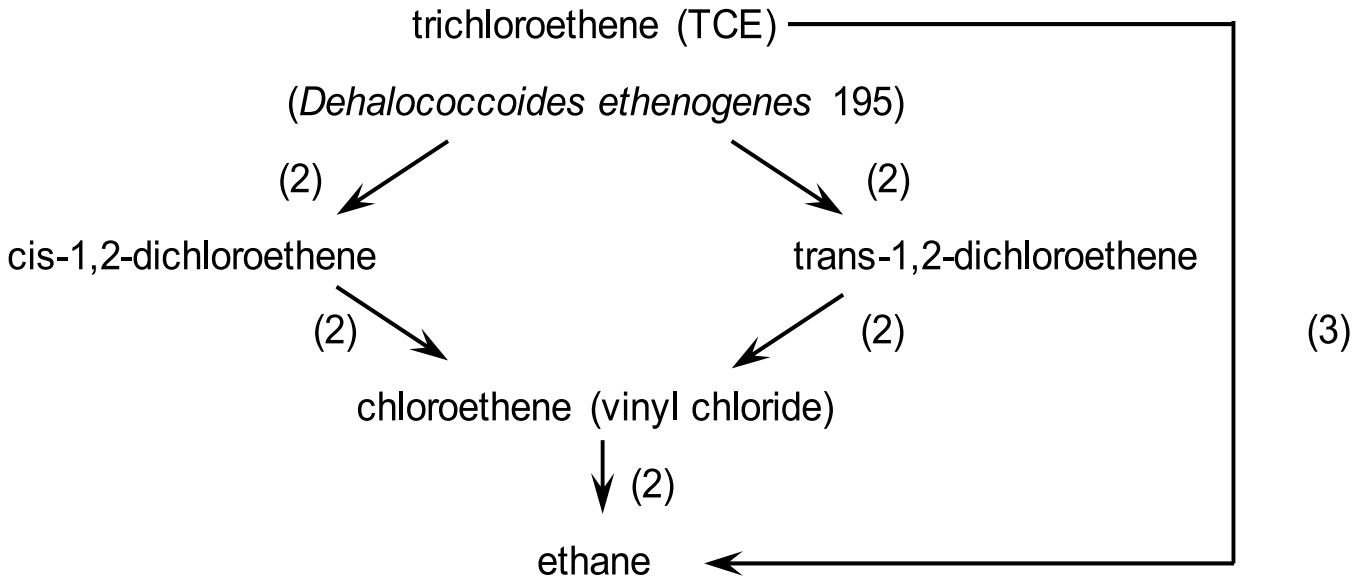
b คือความหนาของช่วงท่อกรอง

n คือความพรุนของตัวกลาง



Observation wells	Measured Value	Calculated Value	%Error
4	20.66	20.626	0.16
7	20.36	20.594	1.14
1	20	20.434	2.12
3	20.23	20.5079	1.36
2	20.07	20.3488	1.37
X01	20.23	20.3505	0.59
X02	19.96	20.3957	2.14
X03	20.07	20.4388	1.80
X04	21.34	20.4648	4.28
X05	20.33	20.4742	0.70
X06	20.58	20.486	0.46
X07	20.21	20.4796	1.32
X08	20.39	20.5017	0.54
X09	20.34	20.5779	1.16
X10	20.54	20.5891	0.24
X12	20.28	20.4882	1.02
X13	19.98	20.4348	2.23
X14	20.51	20.4644	0.22
X15B	20.55	20.3909	0.78
X15A	20.89	20.3941	2.43
Average %Error			1.30

มาตรฐานคุณภาพน้ำใต้ดิน			
ดัชนีคุณภาพน้ำ	หน่วย	ค่ามาตรฐาน	วิธีการตรวจวัด
1.สารอินทรีย์ระเหยง่าย (Volatile Organic Compound)			
1) เบนซิน (Benzene)	ไมโครกรัม /ลิตร	ต้องไม่เกิน 5	วิธี Purge and Trap Gas Chromatography หรือวิธี Purge and Trap Gas Chromatography/Mass Spectrometry หรือวิธีอื่นที่กรมควบคุมมลพิษเห็นชอบ
2) คาร์บอนเตตระคลอไรด์ (Carbon Tetrachloride)	"	ต้องไม่เกิน 5	"
3) 1,2 - คลอโรอิเทน (1,2-Dichloroethane)	"	ต้องไม่เกิน 5	"
4) 1,1-ไดคลอโรเอทธิลีน (1,1-Dichloroethylene)	"	ต้องไม่เกิน 7	"
5) ซิส -1,2 - ไดคลอโรเอทธิลีน (cis-1,2-Dichloroethylene)	"	ต้องไม่เกิน 70	"
6) ทรานส์ -1,2-ไดคลอโรเอทธิลีน (trans-1,2-Dichloroethylene)	"	ต้องไม่เกิน 100	"
7) ไดคลอโรมีเทน (Dichloromethane)	"	ต้องไม่เกิน 5	"
8) เอทธิลเบนซิน (Ethylbenzene)	"	ต้องไม่เกิน 700	"
9) สไตริน (Styrene)	"	ต้องไม่เกิน 100	"
10) เตตระคลอโรเอทธิลีน (Tetrachoroethylene)	"	ต้องไม่เกิน 5	"
11) โทลูอิน (Toluene)	"	ต้องไม่เกิน 1,000	"
12) ไตรคลอโรเอทธิลีน (Trichloroethylene)	"	ต้องไม่เกิน 5	"
13) 1,1,1-ไตรคลอโรอิเทน (1,1,1-Trichloroethane)	"	ต้องไม่เกิน 200	"
14) 1,1,2-ไตรคลอโรอิเทน (1,1,2-Trichloroethane)	"	ต้องไม่เกิน 5	"
15) ไซลีนทั้งหมด (Total Xylenes)	"	ต้องไม่เกิน 10,000	"



Reaction pathway

→ Co-methabolism

Literature

(1) Neumann *et al*., 1996

(2) Maymo-Gatell *et al*., 1997

(3) Magnuson *et al*., 1998