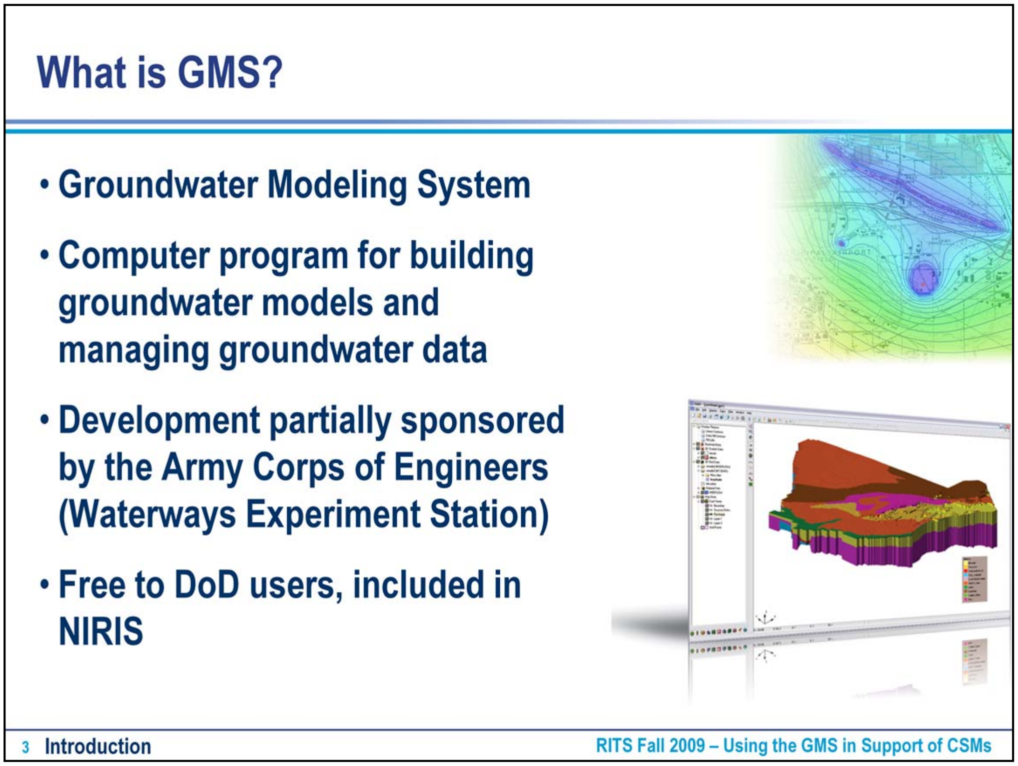
Using the Groundwater Modeling System Tool in NIRIS to Support Conceptual Site Models

RITS Fall 2009

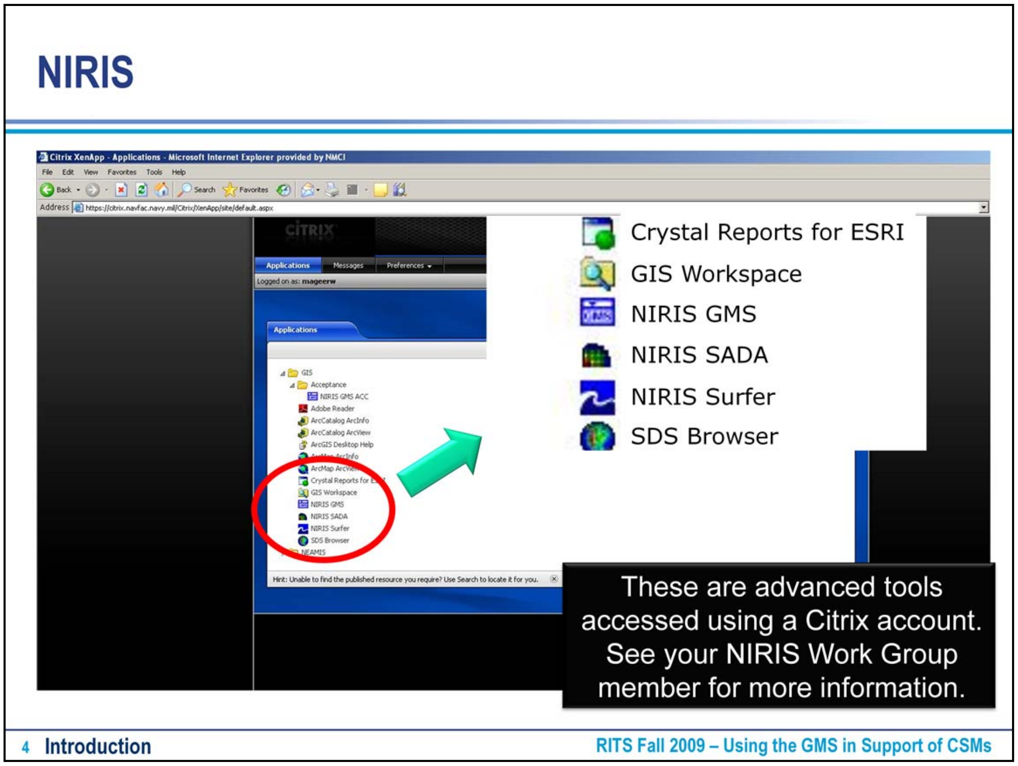
Presentation Overview

- Introduction
  - What is GMS?
  - NIRIS
  - Presentation Objectives
- Contaminant Plume Mapping
- 3D Subsurface Site Characterization
- Groundwater Flow Modeling
- Particle Tracking
- Contaminant Transport Modeling
- Summary/Take-Home Messages

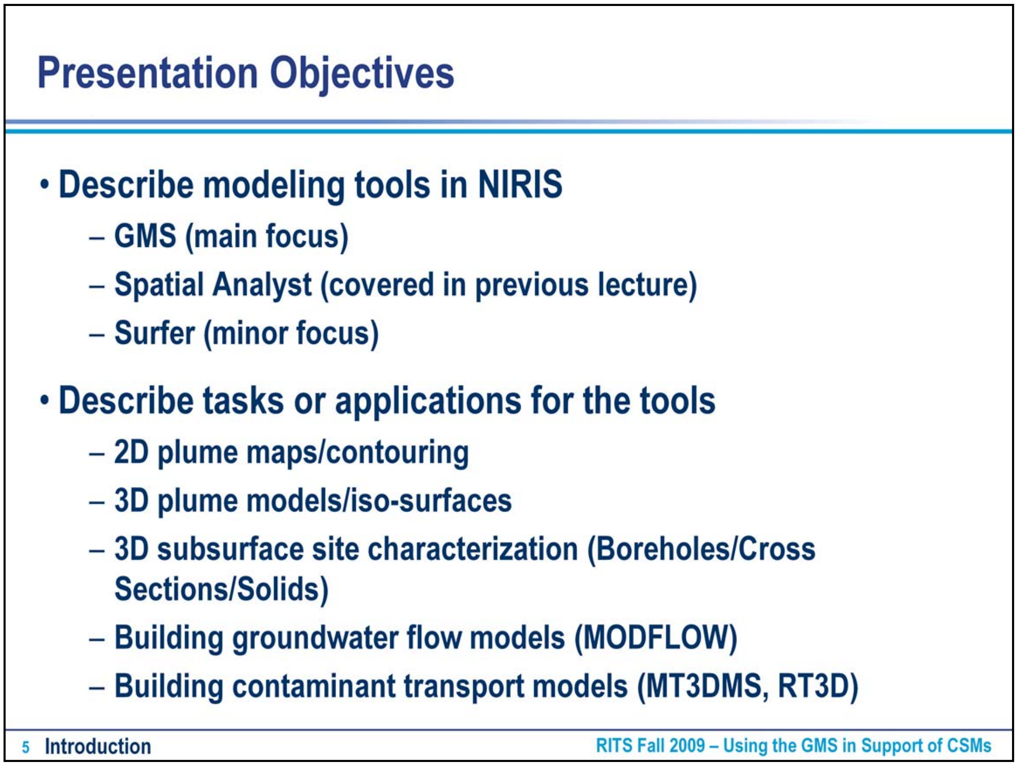


Originally developed at BYU Environmental Modeling Research Laboratory.

GMS does a lot, but there are other software packages outside of GMS that can do similar things to what GMS does (probably would take several separate apps, though). Use what you/your team are familiar with e.g., Surfer.

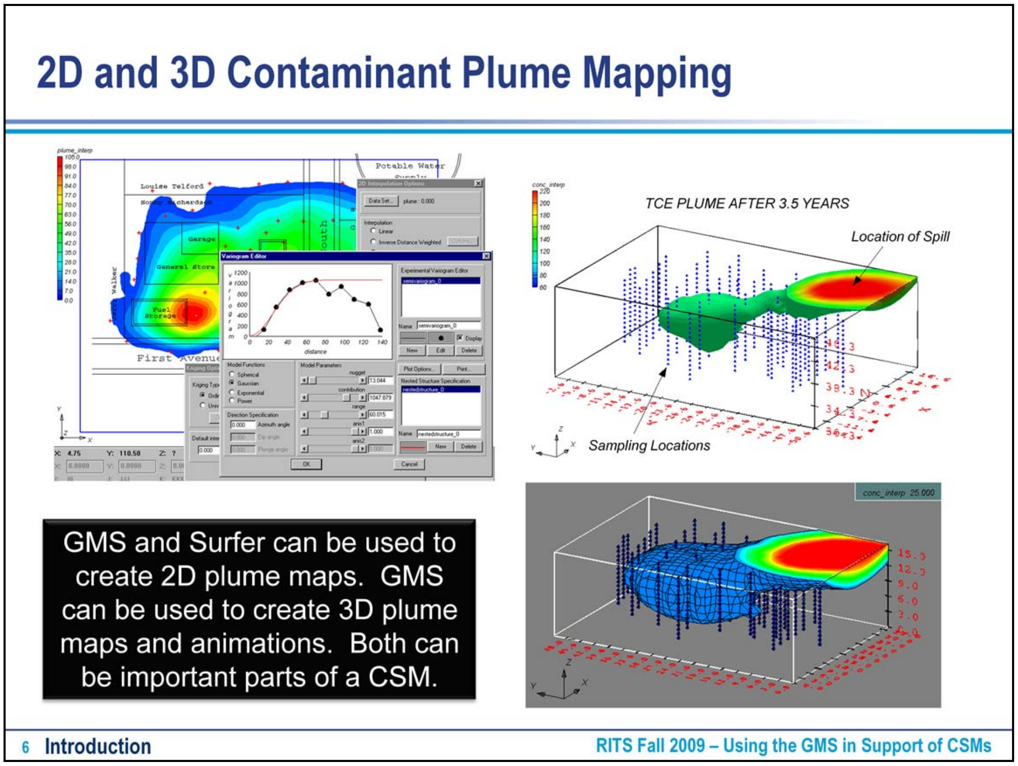


GMS and Surfer are part of the NIRIS system and are available to all Navy RPM's.



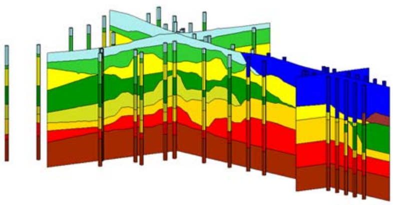
We are focusing on these tools because they are part of NIRIS.

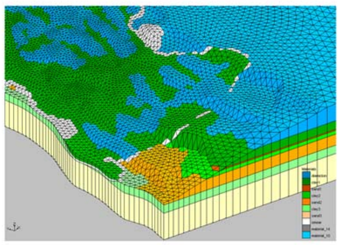
The presentation will be organized based on tasks/applications. We will describe how GMS can be used for these tasks (and Surfer to a smaller degree), but other modeling software could be used for the same purpose.

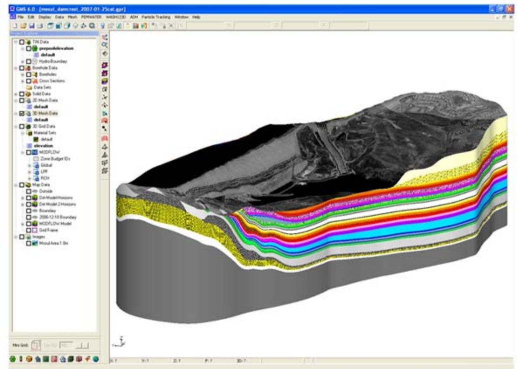


These slides are just an intro into the main topics to be covered. Details will be explained later.

3D Site Characterization and Visualization

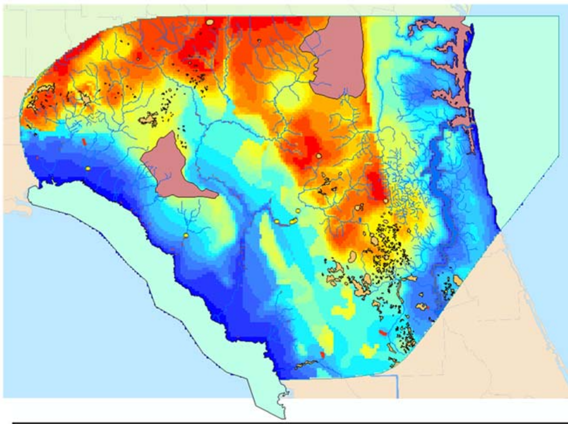


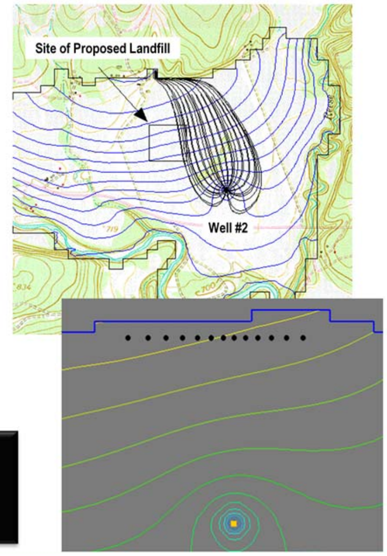




Boreholes, cross sections, and solid models can be built as part of a 3D site characterization process.

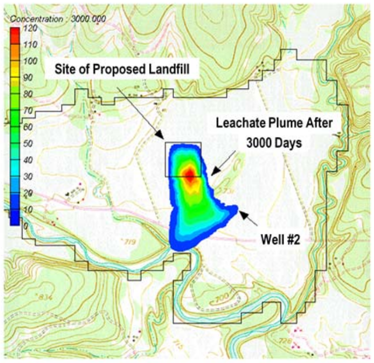
Groundwater Flow Modeling

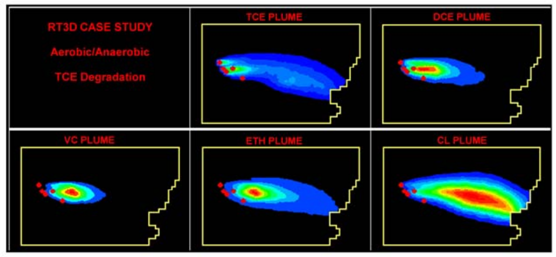


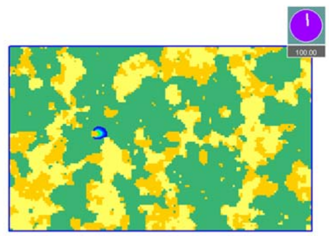


Groundwater flow models can be used to simulate flow conditions and predict travel times using particle tracking analysis.

Contaminant Transport Modeling







Transport models are used to predict the long-term migration of contaminant plumes, including biodegradation.

Presentation Overview

- Introduction
- Contaminant Plume Mapping
  - 2D Plume Mapping with GMS
  - 2D Plume Mapping with Surfer
  - 3D Plume Mapping with GMS
- 3D Subsurface Site Characterization
- Groundwater Flow Modeling
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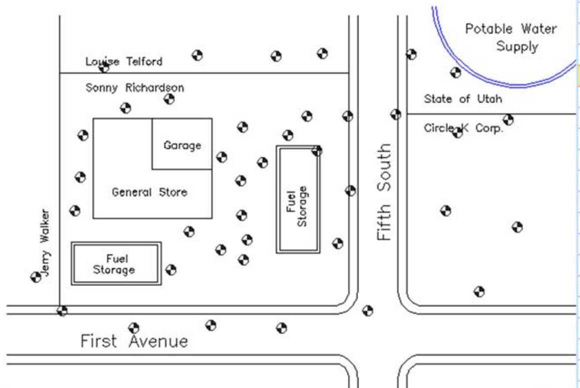
- Contaminant Transport Modeling
- Summary/Take-Home Messages

2D Plume Mapping
Step 1 – Import Field Measurements



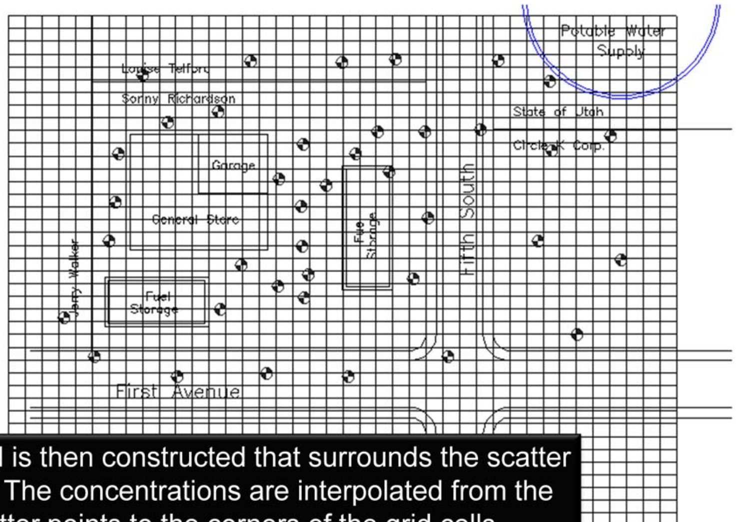
	A	B	C
1	X	Y	plume
2	1.182	-1.637	0.000
3	25.874	-7.629	0.000
4	52.627	-6.744	0.000
5	76.948	-7.629	0.000
6	110.555	-39.688	0.000
7	158.313	27.084	0.000
8	155.090	64.079	0.000
9	121.831	86.560	0.000
10	137.012	80.447	0.000
11	91.098	87.002	0.000
12	75.179	85.897	0.000
13	47.763	86.339	0.000
14	15.596	82.157	0.000
15	-7.857	9.845	0.000
16	8.267	58.704	0.000
17	5.580	32.564	0.000
18	22.925	67.988	10.000
19	7.290	44.291	0.000
20	63.461	61.355	20.000
21	56.386	51.184	50.000

Field measurements of concentration are imported from a simple text file and displayed as 2D scatter points.

11 Contaminant Plume Mapping – 2D GMS   RITS Fall 2009 – Using the GMS in Support of CSMs

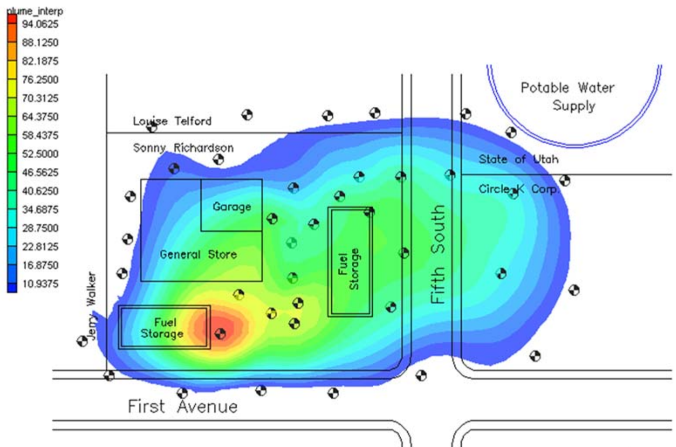
In the NIRIS system, the raw data would have to be imported to the NIRIS database first and then exported into a file on the server before you can import to GMS.

2D Plume Mapping
Step 2 – Construct Grid

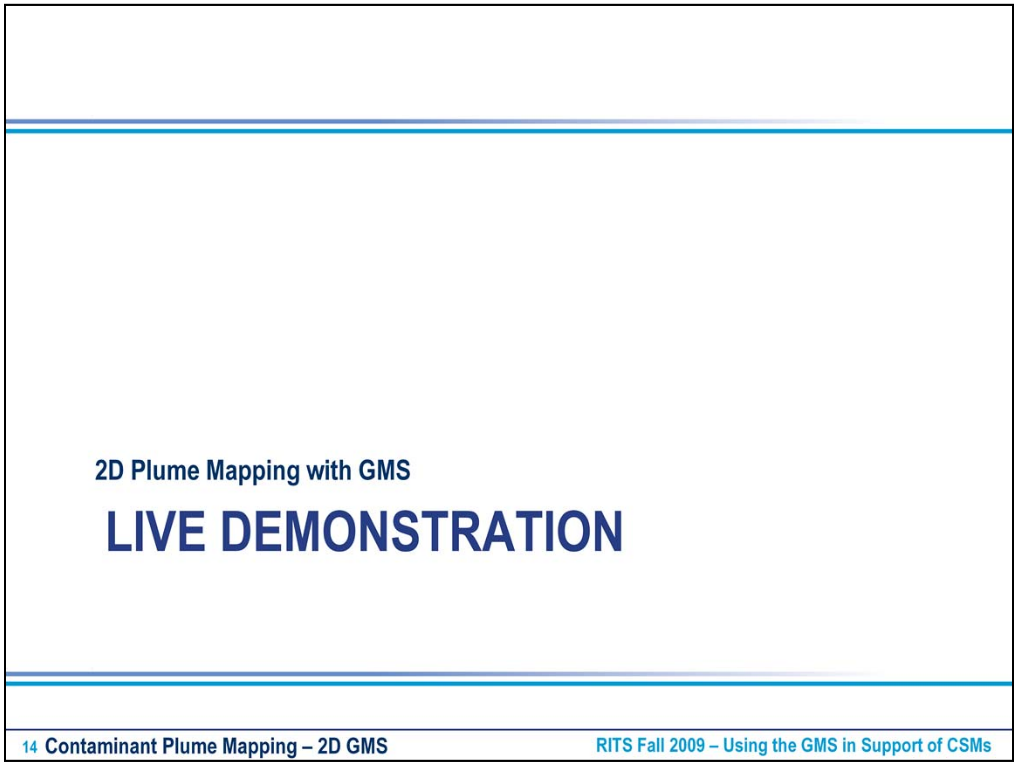


A 2D grid is then constructed that surrounds the scatter points. The concentrations are interpolated from the scatter points to the corners of the grid cells.

2D Plume Mapping
Step 3 – Interpolate and Contour



The interpolated values at the grid corners are then used to generate contour plots showing the distribution of contaminants within the site boundaries.



Import scatter points

Build a grid

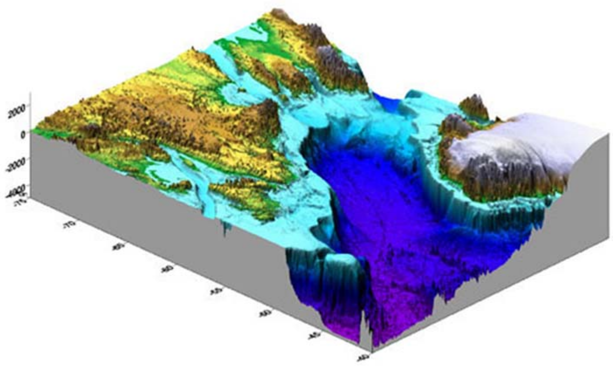
Interpolate

Adjust contouring options

View in oblique view

Surfer

- Contour plots
- 3D surface plots
- Geostatistics
- Shaded relief maps



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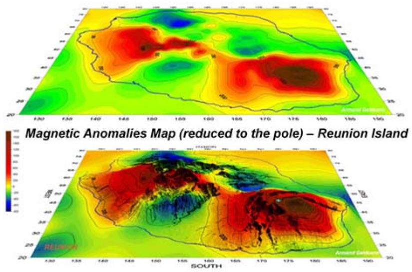
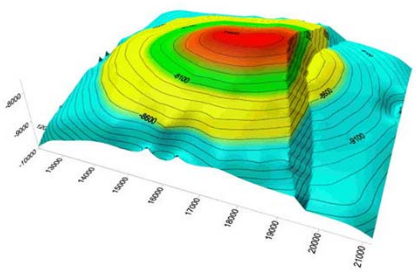
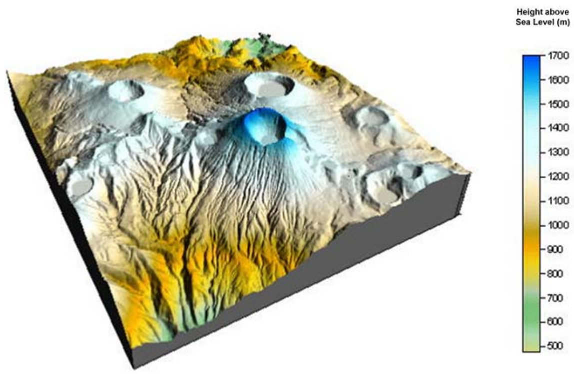
Contour Maps



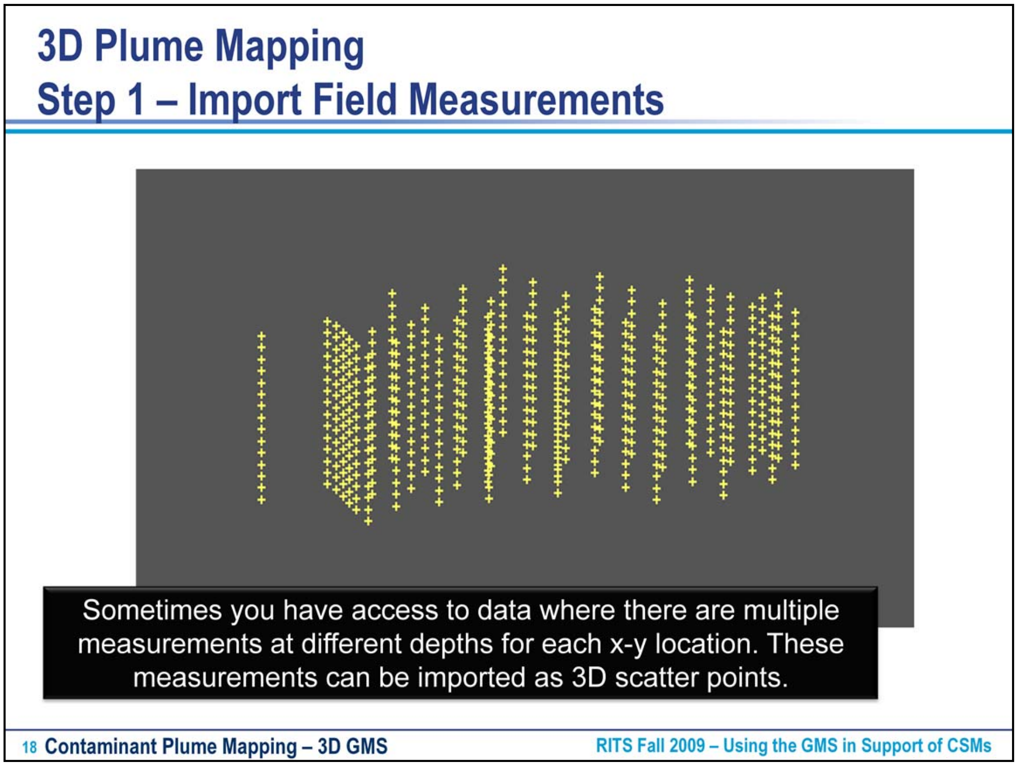


The 2D plume maps shown in previous slides were generated by GMS. Surfer can also be used to generate plume maps showing concentration contours.

3D Surface Maps

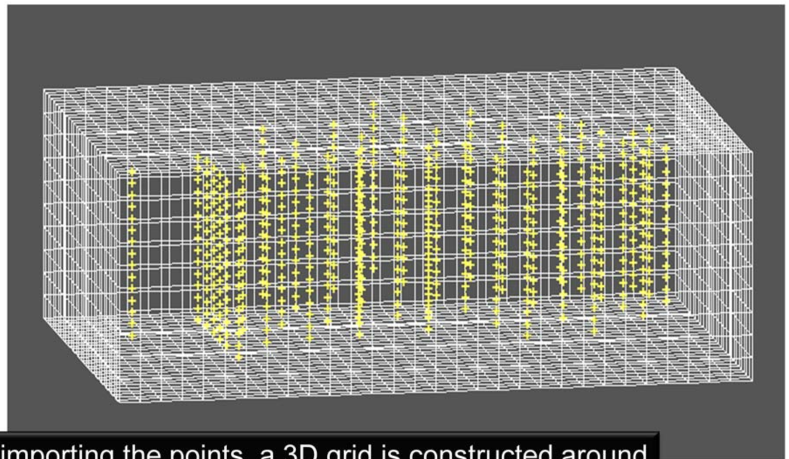


Surfer includes a large variety of 2D and 3D surface plotting options.



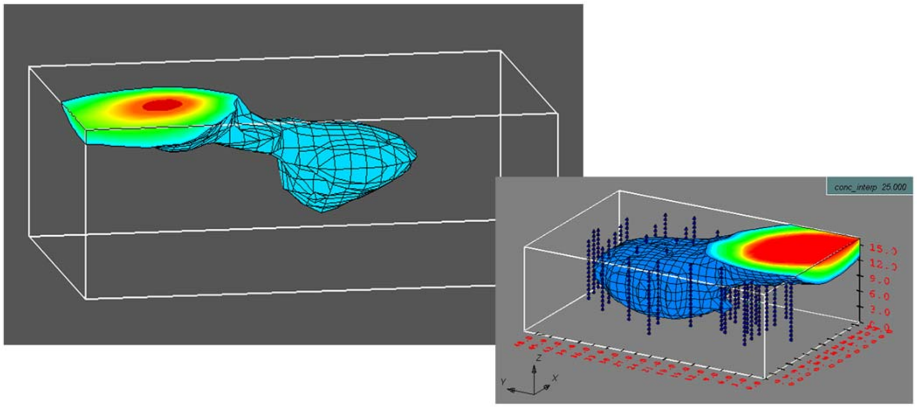
In the NIRIS system, the raw data would have to be imported to the NIRIS database first and then exported into a file on the server before you can import to GMS.

3D Plume Mapping
Step 2 – Generate 3D Grid and Interpolate



After importing the points, a 3D grid is constructed around the points and the concentration measurements are interpolated to the nodes of the 3D grid.

3D Plume Mapping
Step 3 – Iso-Surfaces, 3D Rendering



Selected concentration values are then used to construct iso-surfaces; the 3D equivalent of a 2D contour line. Iso-surfaces illustrate how the concentrations vary spatially.

20 Contaminant Plume Mapping – 3D GMS

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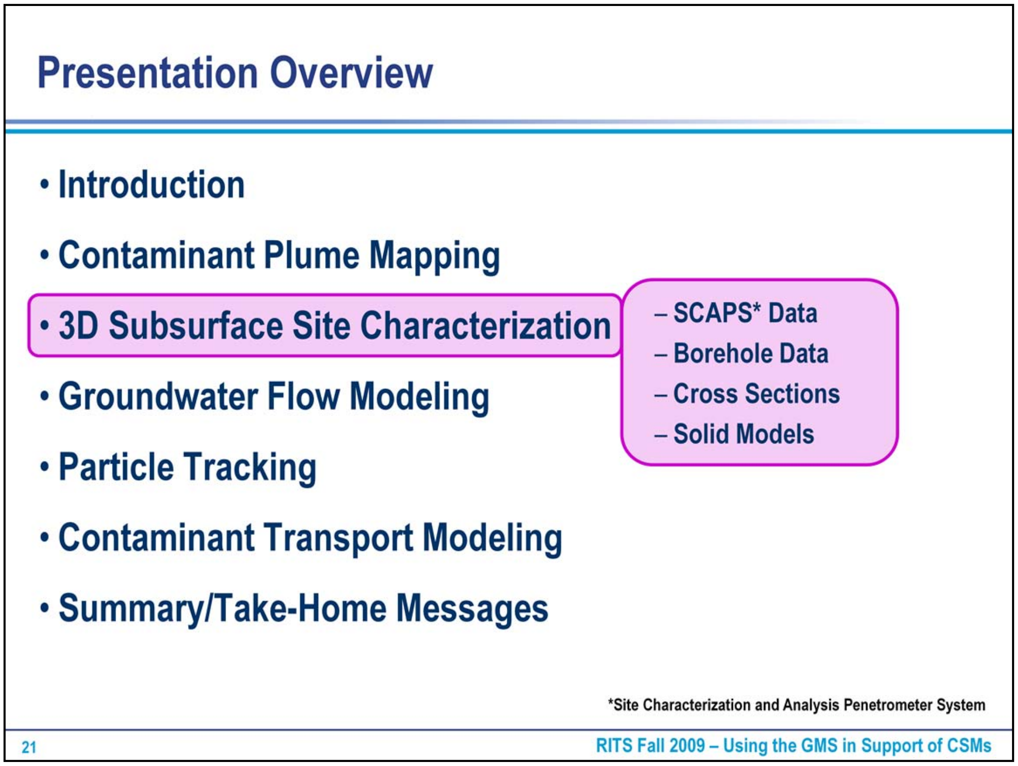
Presentation Overview
• Introduction
• Contaminant Plume Mapping
• 3D Subsurface Site Characterization
– SCAPS* Data
– Borehole Data
– Cross Sections
– Solid Models
• Groundwater Flow Modeling
• Particle Tracking
• Contaminant Transport Modeling
• Summary/Take-Home Messages
*Site Characterization and Analysis Penetrometer System
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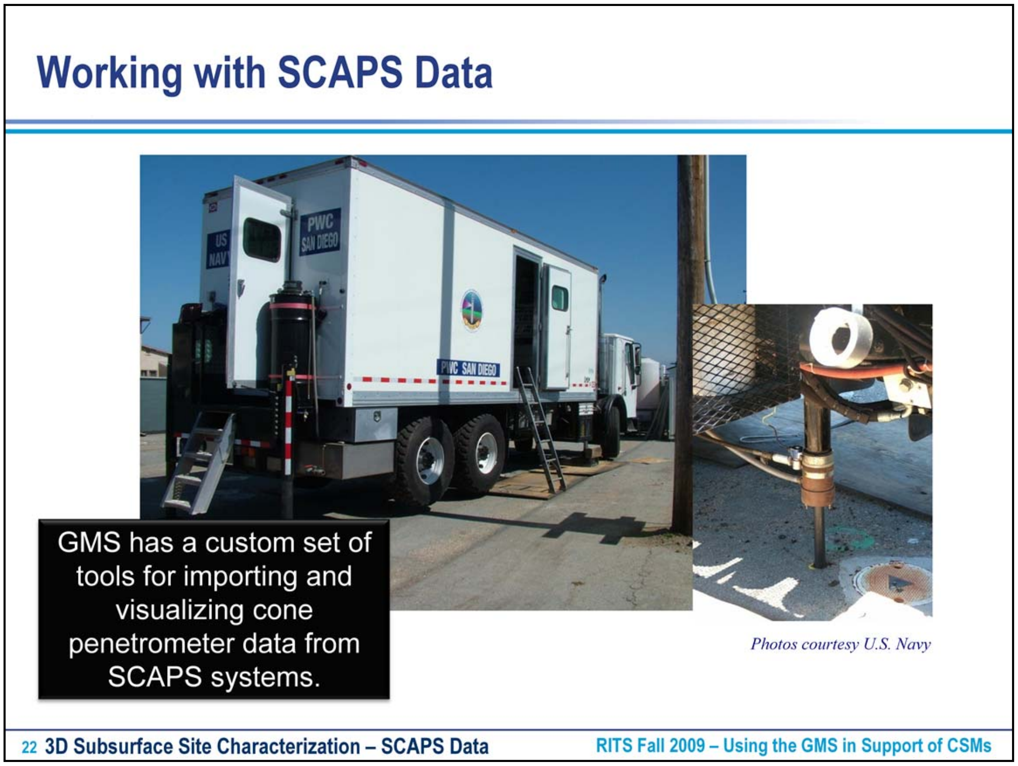
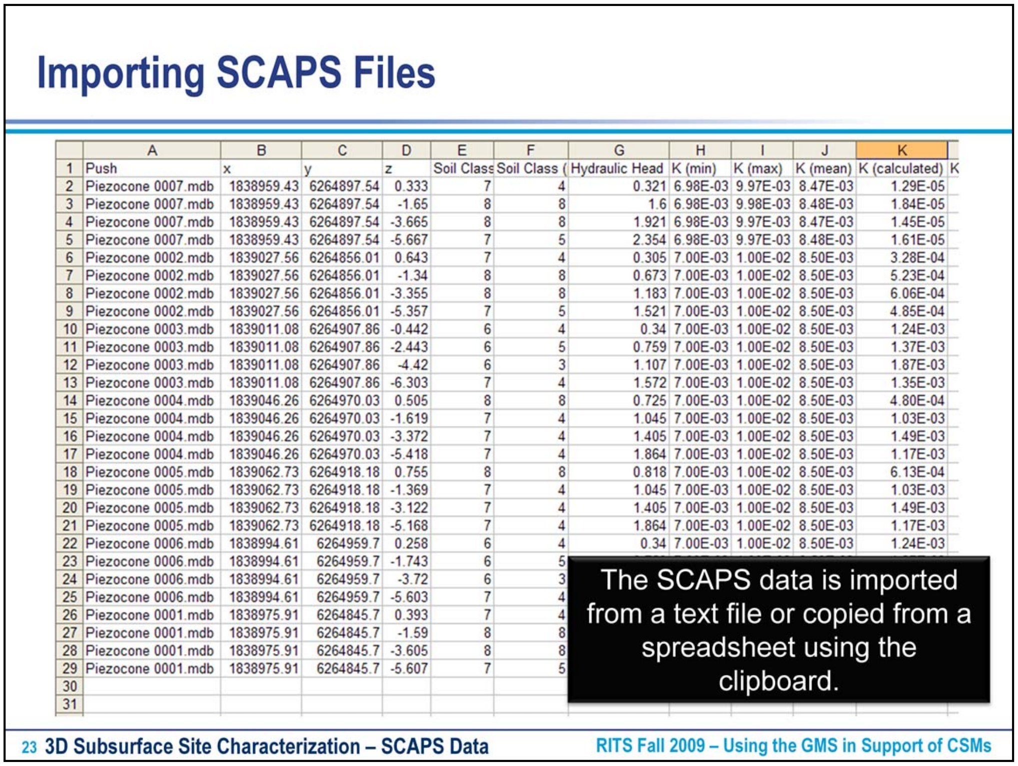


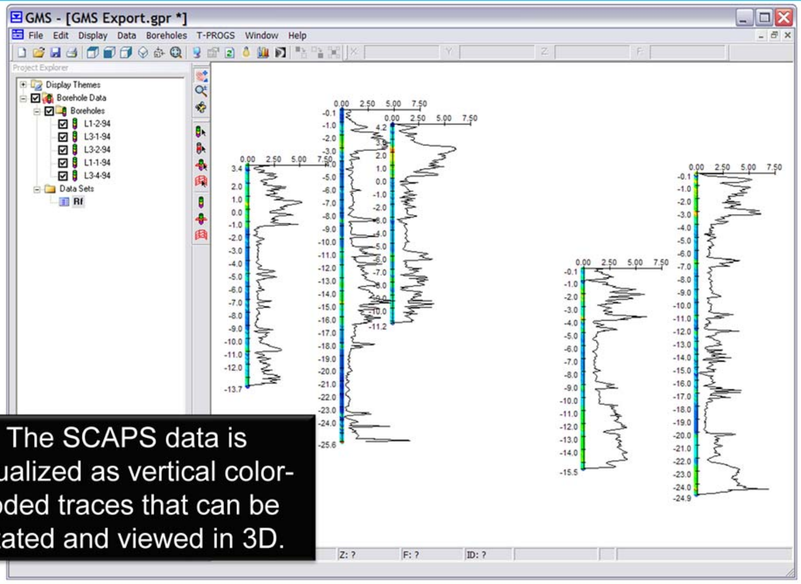
SCAPS = Site Characterization and Analysis Penetrometer System



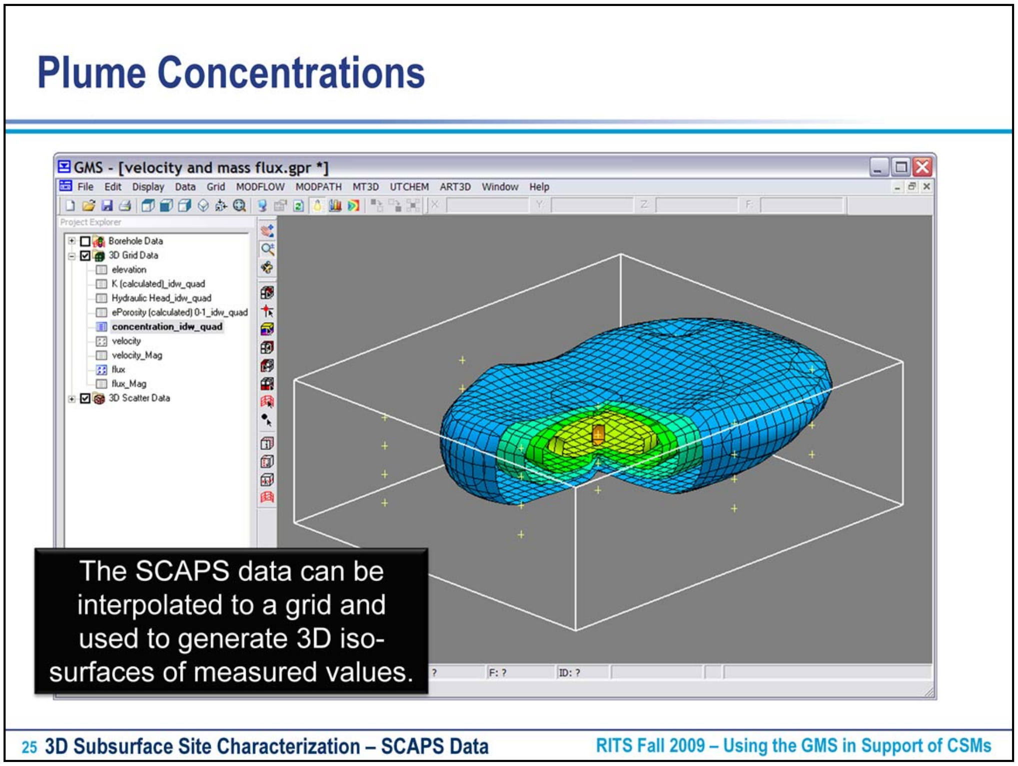
	A	B	C	D	E	F	G	H	I	J	K	
1	Push	x	y	z	Soil Class	Soil Class (	Hydraulic Head	K (min)	K (max)	K (mean)	K (calculated)	K
2	Piezocone 0007.mdb	1838959.43	6264897.54	0.333	7	4	0.321	6.98E-03	9.97E-03	8.47E-03	1.29E-05	
3	Piezocone 0007.mdb	1838959.43	6264897.54	-1.65	8	8	1.6	6.98E-03	9.98E-03	8.48E-03	1.84E-05	
4	Piezocone 0007.mdb	1838959.43	6264897.54	-3.665	8	8	1.921	6.98E-03	9.97E-03	8.47E-03	1.45E-05	
5	Piezocone 0007.mdb	1838959.43	6264897.54	-5.667	7	5	2.354	6.98E-03	9.97E-03	8.48E-03	1.61E-05	
6	Piezocone 0002.mdb	1839027.56	6264856.01	0.643	7	4	0.305	7.00E-03	1.00E-02	8.50E-03	3.28E-04	
7	Piezocone 0002.mdb	1839027.56	6264856.01	-1.34	8	8	0.673	7.00E-03	1.00E-02	8.50E-03	5.23E-04	
8	Piezocone 0002.mdb	1839027.56	6264856.01	-3.355	8	8	1.183	7.00E-03	1.00E-02	8.50E-03	6.06E-04	
9	Piezocone 0002.mdb	1839027.56	6264856.01	-5.357	7	5	1.521	7.00E-03	1.00E-02	8.50E-03	4.85E-04	
10	Piezocone 0003.mdb	1839011.08	6264907.86	-0.442	6	4	0.34	7.00E-03	1.00E-02	8.50E-03	1.24E-03	
11	Piezocone 0003.mdb	1839011.08	6264907.86	-2.443	6	5	0.759	7.00E-03	1.00E-02	8.50E-03	1.37E-03	
12	Piezocone 0003.mdb	1839011.08	6264907.86	-4.42	6	3	1.107	7.00E-03	1.00E-02	8.50E-03	1.87E-03	
13	Piezocone 0003.mdb	1839011.08	6264907.86	-6.303	7	4	1.572	7.00E-03	1.00E-02	8.50E-03	1.35E-03	
14	Piezocone 0004.mdb	1839046.26	6264970.03	0.505	8	8	0.725	7.00E-03	1.00E-02	8.50E-03	4.80E-04	
15	Piezocone 0004.mdb	1839046.26	6264970.03	-1.619	7	4	1.045	7.00E-03	1.00E-02	8.50E-03	1.03E-03	
16	Piezocone 0004.mdb	1839046.26	6264970.03	-3.372	7	4	1.405	7.00E-03	1.00E-02	8.50E-03	1.49E-03	
17	Piezocone 0004.mdb	1839046.26	6264970.03	-5.418	7	4	1.864	7.00E-03	1.00E-02	8.50E-03	1.17E-03	
18	Piezocone 0005.mdb	1839062.73	6264918.18	0.755	8	8	0.818	7.00E-03	1.00E-02	8.50E-03	6.13E-04	
19	Piezocone 0005.mdb	1839062.73	6264918.18	-1.369	7	4	1.045	7.00E-03	1.00E-02	8.50E-03	1.03E-03	
20	Piezocone 0005.mdb	1839062.73	6264918.18	-3.122	7	4	1.405	7.00E-03	1.00E-02	8.50E-03	1.49E-03	
21	Piezocone 0005.mdb	1839062.73	6264918.18	-5.168	7	4	1.864	7.00E-03	1.00E-02	8.50E-03	1.17E-03	
22	Piezocone 0006.mdb	1838994.61	6264959.7	0.258	6	4	0.34	7.00E-03	1.00E-02	8.50E-03	1.24E-03	
23	Piezocone 0006.mdb	1838994.61	6264959.7	-1.743	6	5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
24	Piezocone 0006.mdb	1838994.61	6264959.7	-3.72	6	3	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
25	Piezocone 0006.mdb	1838994.61	6264959.7	-5.603	7	4	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
26	Piezocone 0001.mdb	1838975.91	6264845.7	0.393	7	4	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
27	Piezocone 0001.mdb	1838975.91	6264845.7	-1.59	8	8	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
28	Piezocone 0001.mdb	1838975.91	6264845.7	-3.605	8	8	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
29	Piezocone 0001.mdb	1838975.91	6264845.7	-5.607	7	5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
30												
31												

In the NIRIS system, the raw data would have to be imported to the NIRIS database first and then exported into a file on the server before you can import to GMS.

Viewing SCAPS Data



The SCAPS data is visualized as vertical color-coded traces that can be rotated and viewed in 3D.


Plume Concentrations
GMS - [velocity and mass flux.gpr *]
File Edit Display Data Grid MODFLOW MODPATH MT3D UTCHEM ART3D Window Help
Borehole Data
3D Grid Data
elevation
K (calculated)_idw_quad
Hydraulic Head_idw_quad
ePorosity (calculated) 0-1_idw_quad
concentration_idw_quad
velocity
velocity_Mag
flux
flux_Mag
3D Scatter Data
The SCAPS data can be interpolated to a grid and used to generate 3D iso-surfaces of measured values.
25 3D Subsurface Site Characterization – SCAPS Data
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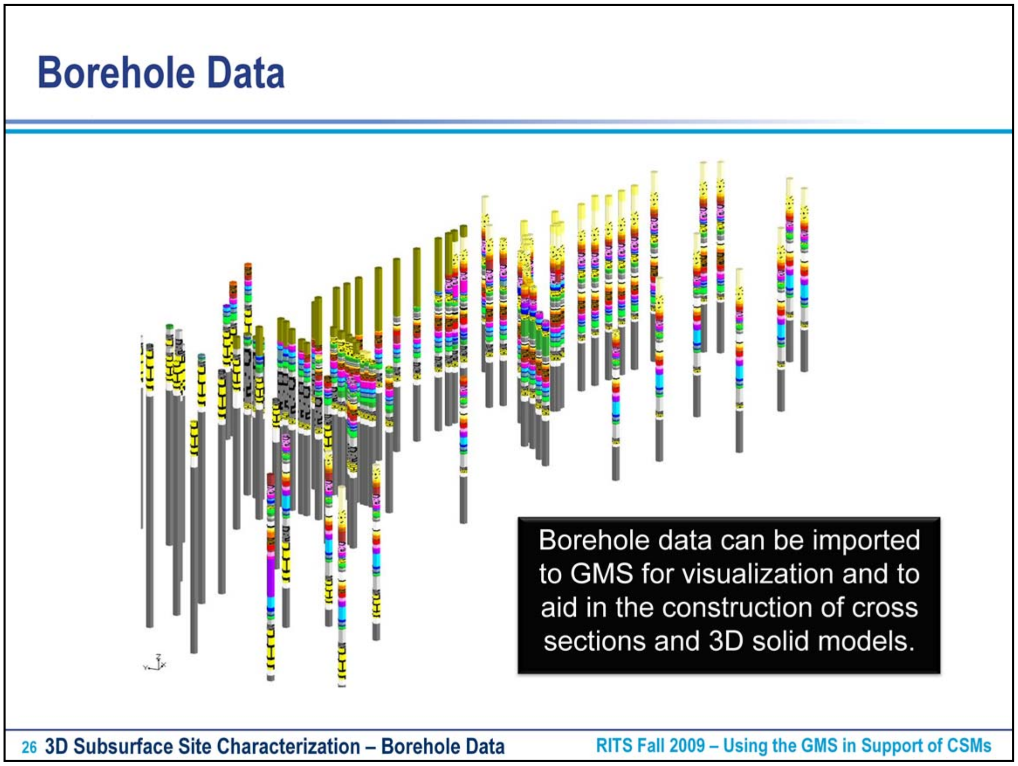


This is an important part of the CSM.

Importing

	A	B	C	D	E	F
1	Name	X	Y	Z	SoilID	HGUID
2	TB-1	217.371	73.017	1221.96	1	1
3	TB-1	217.371	73.017	1207.96	2	2
4	TB-1	217.371	73.017	1200.46	4	4
5	TB-1	217.371	73.017	1185.46	4	4
6	TB-2	141.83	143.775	1208.8	2	2
7	TB-2	141.83	143.775	1200.8	1	1
8	TB-2	141.83	143.775	1196.8	2	2
9	TB-2	141.83	143.775	1185.8	4	4
10	TB-2	141.83	143.775	1177.8	4	4
11	TB-3	72.51	210.764	1204.37	1	1
12	TB-3	72.51	210.764	1189.37	2	2
13	TB-3	72.51	210.764	1183.67	2	2
14	TB-4	329.284	184.959	1218.41	1	1
15	TB-4	329.284	184.959	1199.91	2	2
16	TB-4	329.284	184.959	1186.91	2	2
17	TB-5	250.737	256.704	1208.13	1	1
18	TB-5	250.737	256.704	1197.13	2	2
19	TB-5	250.737	256.704	1160.13	4	4
20	TB-5	250.737	256.704	1158.13	4	4
21	TB-6	182.022	322.498	1207.37	1	1

Borehole 1

Borehole 2

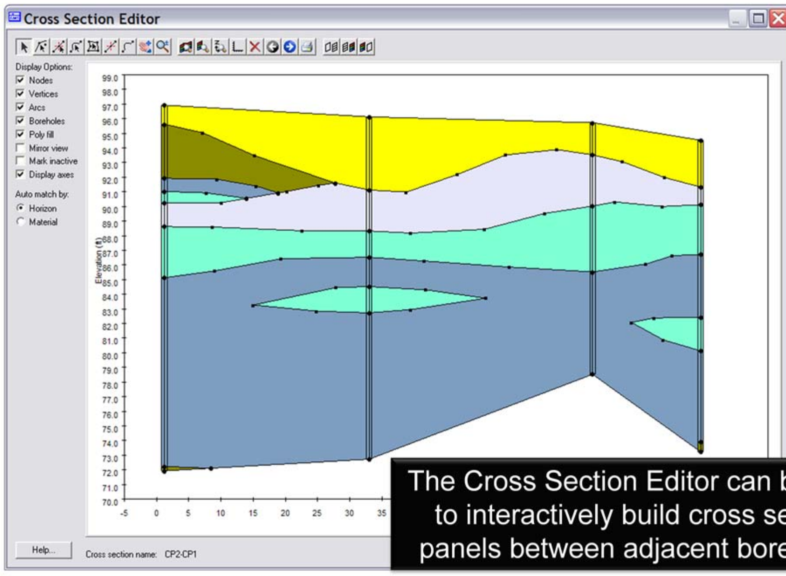
Borehole 3

Borehole 4

Borehole 5

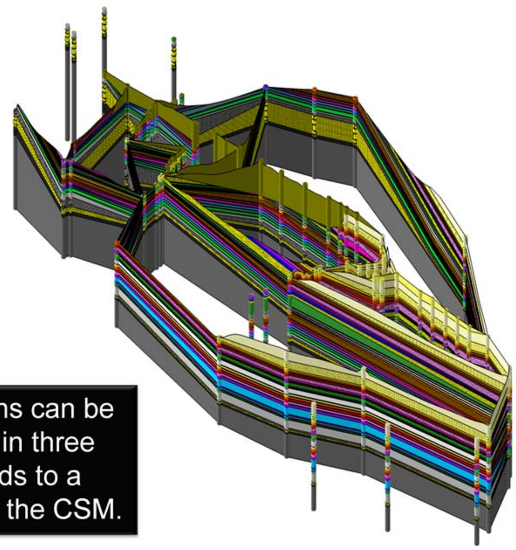
Borehole data is imported using a simple text file or spreadsheet. Each line represents the top of a soil segment on the borehole log.

Cross Section Editor

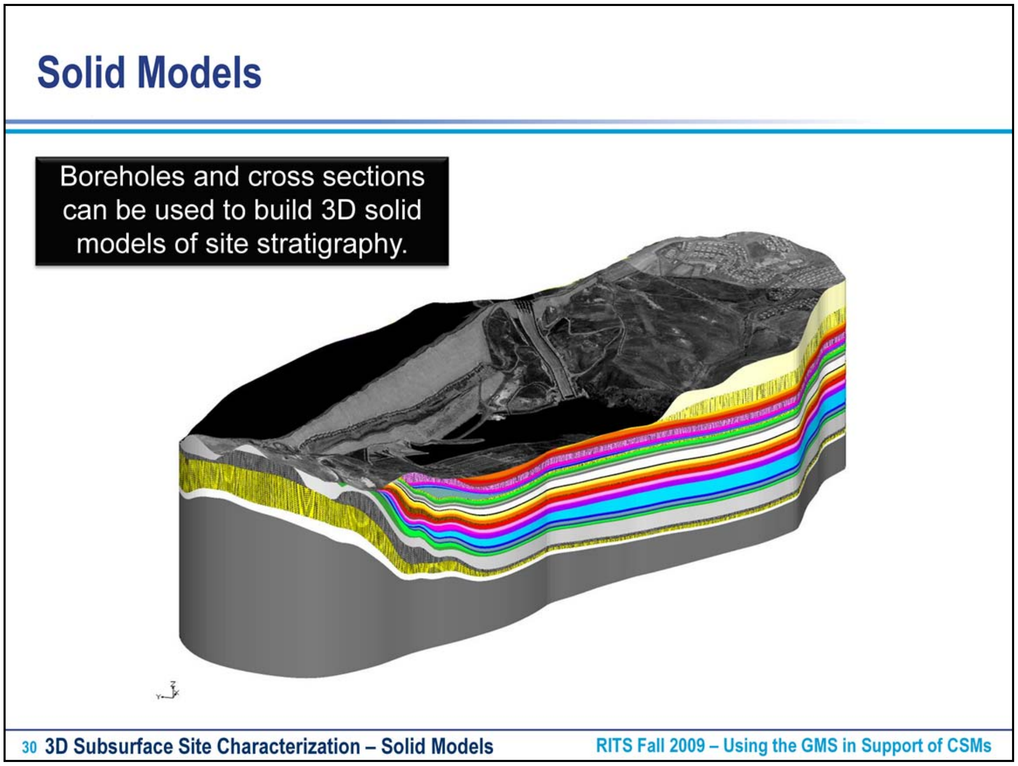


The Cross Section Editor can be used to interactively build cross section panels between adjacent boreholes.

Cross Sections



Completed cross sections can be visualized and rotated in three dimensions. This leads to a greater understanding of the CSM.


Solid Models
Boreholes and cross sections can be used to build 3D solid models of site stratigraphy.
30 3D Subsurface Site Characterization – Solid Models
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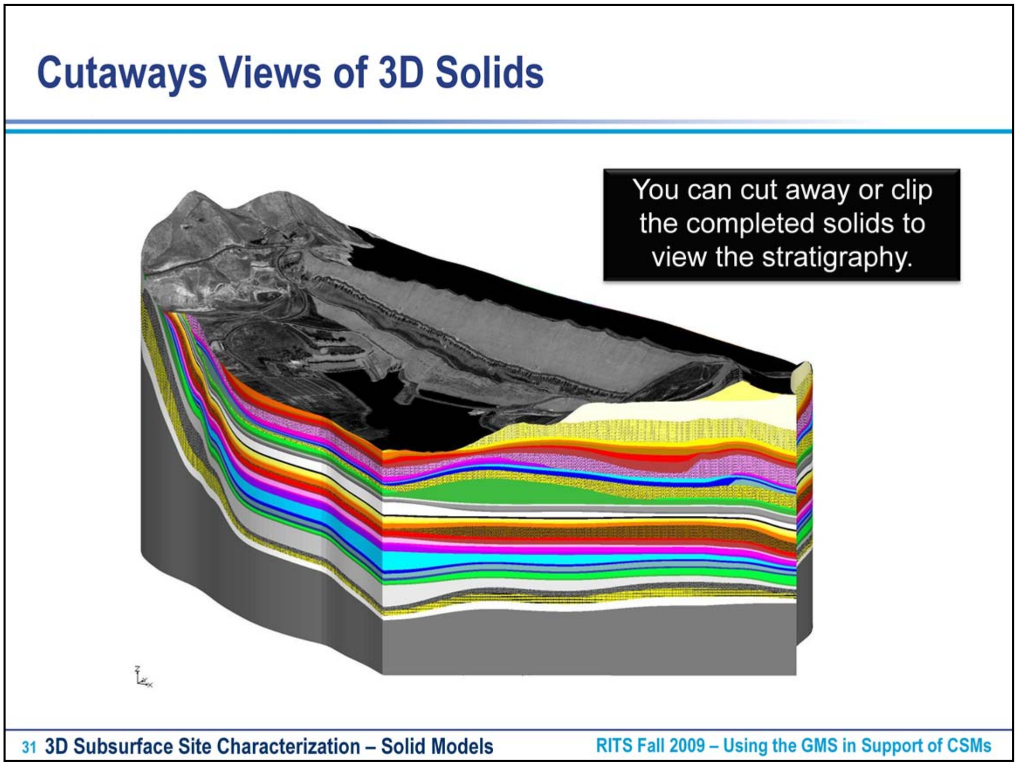
Cutaways Views of 3D Solids
You can cut away or clip the completed solids to view the stratigraphy.
31 3D Subsurface Site Characterization – Solid Models
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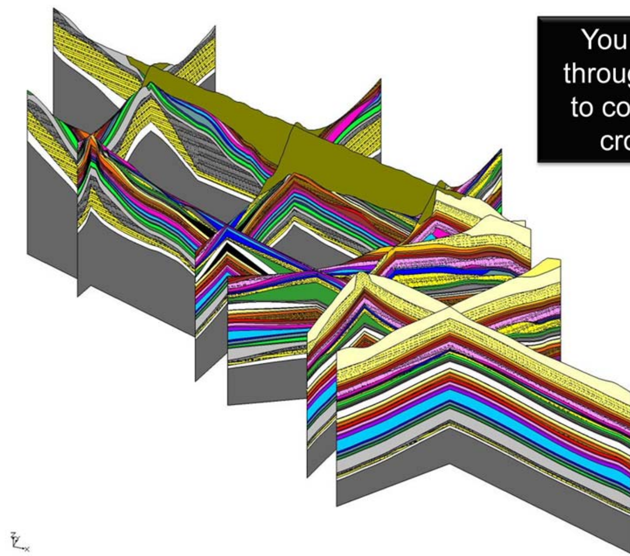
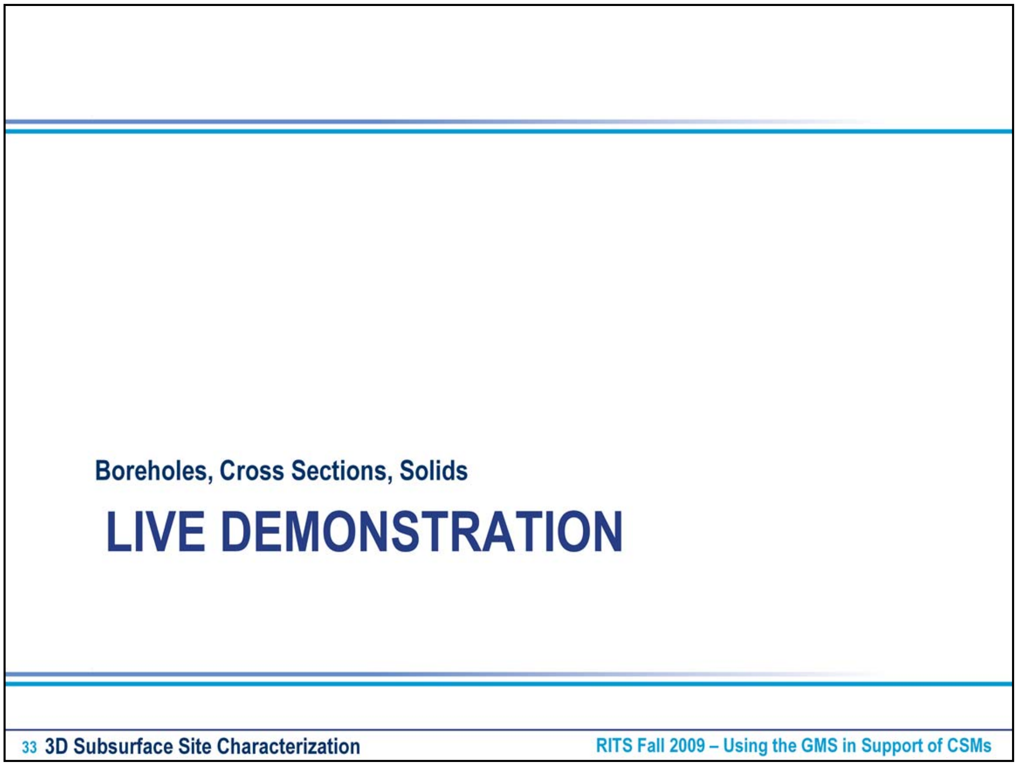
Cutting Slices Through Solids



You can also slice through solid models to construct derived cross sections.

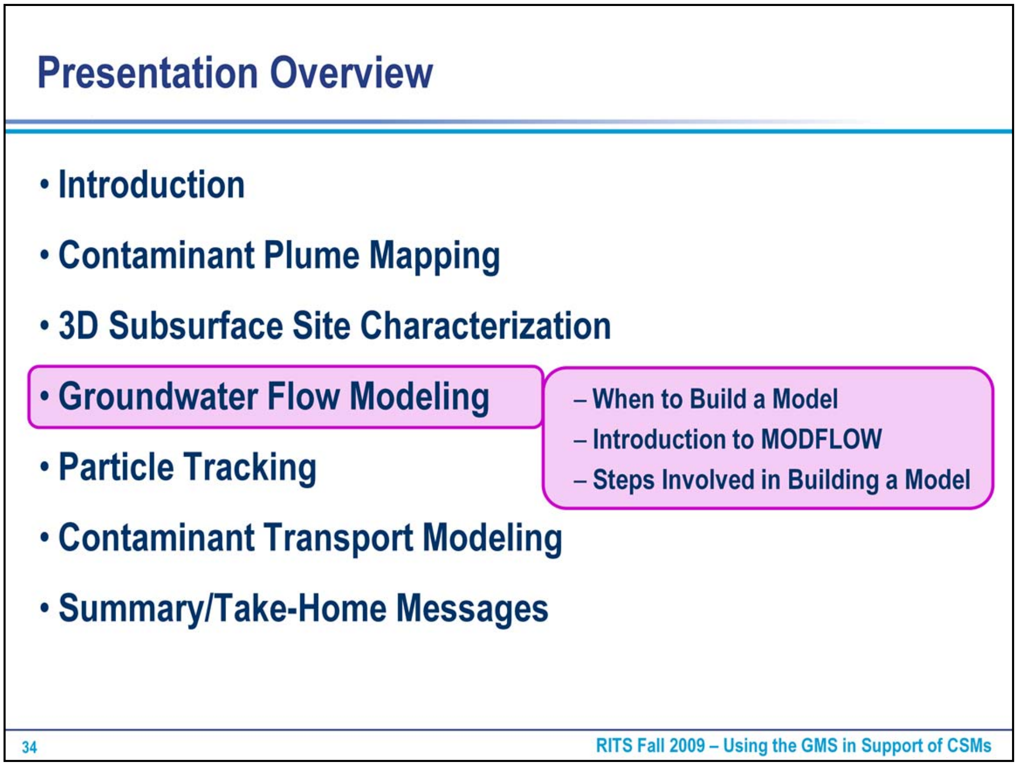


Start with boreholes in 3D

Cross section editor

Turn on existing solids

Slice through solids


Presentation Overview
• Introduction
• Contaminant Plume Mapping
• 3D Subsurface Site Characterization
• Groundwater Flow Modeling
– When to Build a Model
– Introduction to MODFLOW
– Steps Involved in Building a Model
• Particle Tracking
• Contaminant Transport Modeling
• Summary/Take-Home Messages
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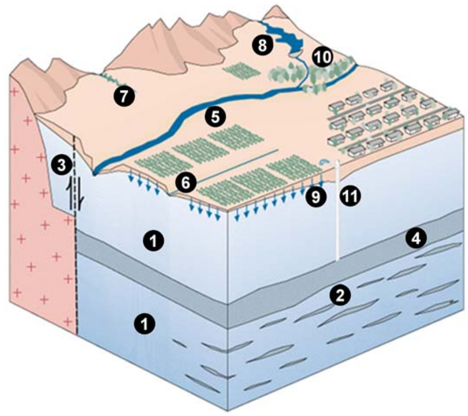
Under What Conditions Should a Flow or Transport Model be Used?

- Travel time questions
  - How long will it take for the plume to reach the river?
- Treatment system design
  - Should we use injection/extraction wells as part of strategy?
  - Should we use barriers? Where should they be located?
- Risk analysis
  - What is the probability that the plume will reach the river in less than 20 years?
- Evaluate remediation alternatives
  - How rapidly will the TCE plume degrade without the addition of a hydrocarbon substrate (electron donor)?

Flow Modeling with MODFLOW

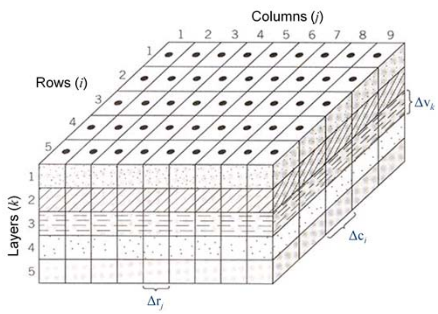
- Developed by McDonald & Harbaugh of the USGS, 1983
- Public Domain
- Most widely used groundwater model
- Steady state or transient saturated flow

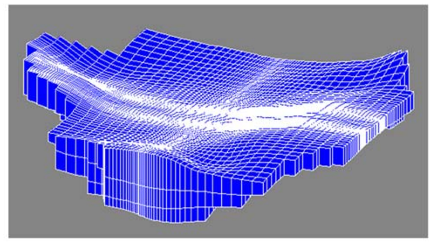


1. Confined/unconfined aquifers
2. Interbeds
3. Faults and barriers
4. Confining units
5. Rivers
6. Drains and springs
7. Streams
8. Reservoirs
9. Recharge
10. Evapotranspiration
11. Wells

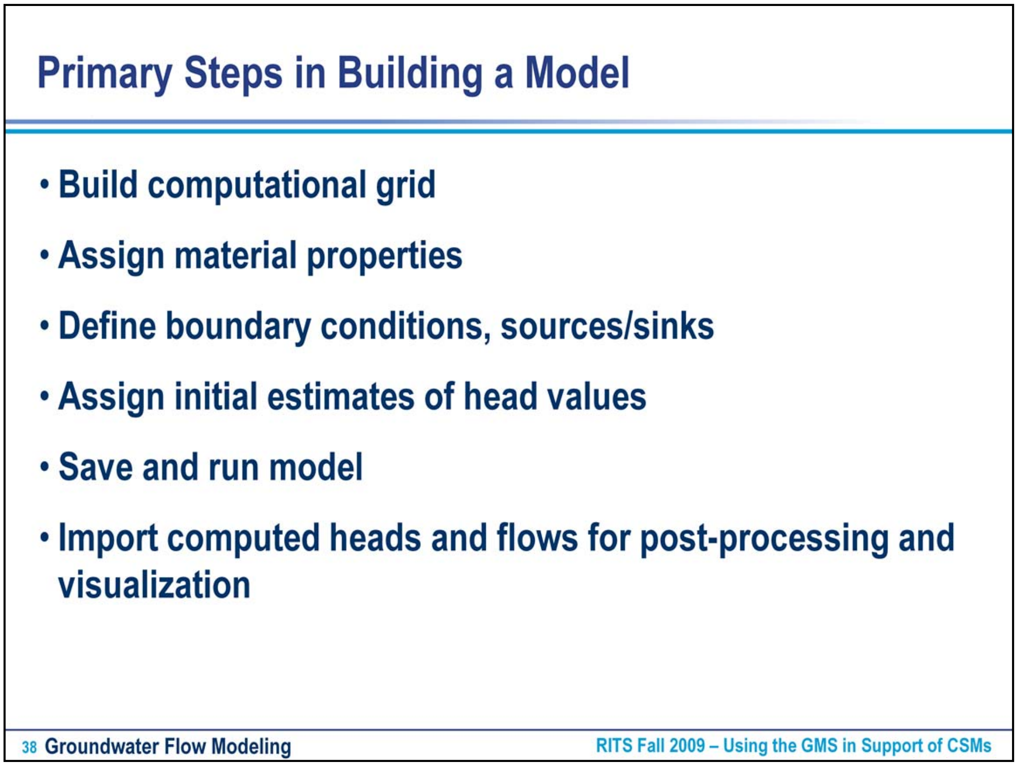
Finite Difference Model

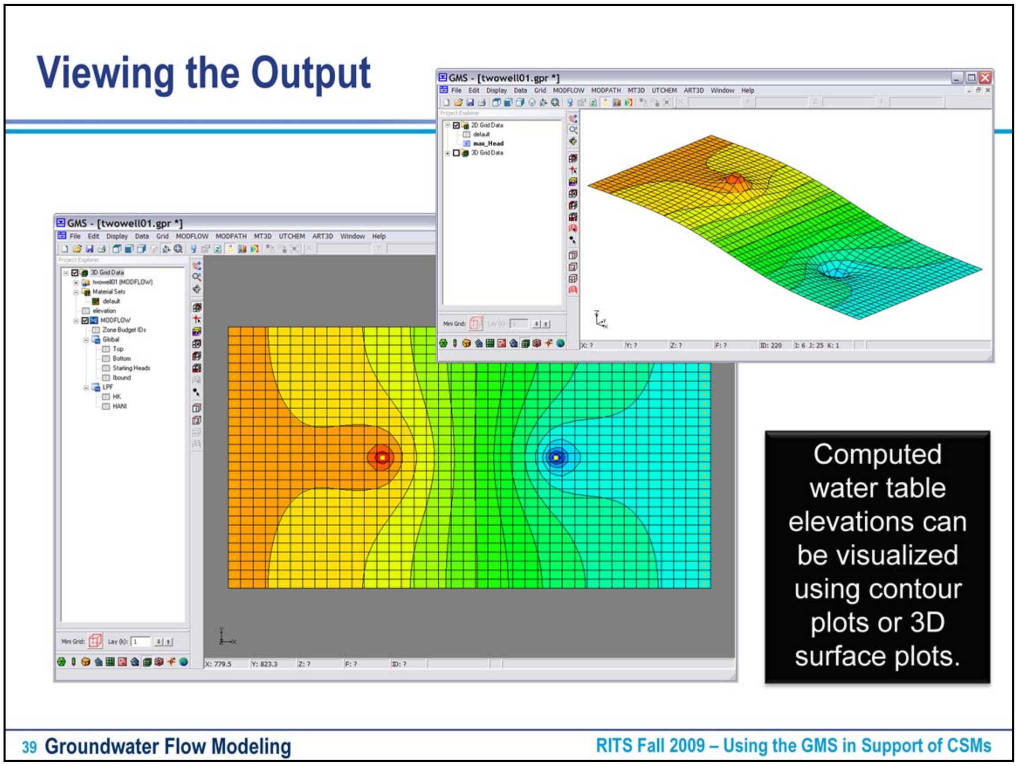
- 3D Cartesian Grid
- Cell-Centered

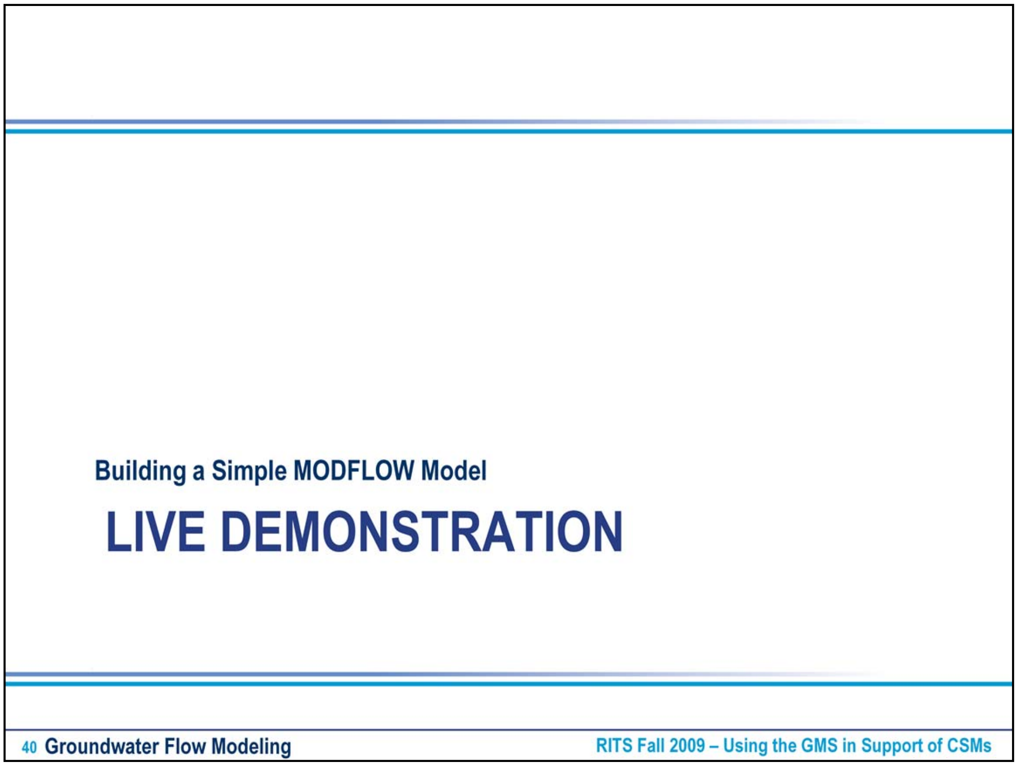




- Orthogonal in XY
- Thickness varies in Z


Primary Steps in Building a Model
• Build computational grid
• Assign material properties
• Define boundary conditions, sources/sinks
• Assign initial estimates of head values
• Save and run model
• Import computed heads and flows for post-processing and visualization
38 Groundwater Flow Modeling
RITS Fall 2009 – Using the GMS in Support of CSMs


Viewing the Output
GMS - [twowell01.gpr *]
GMS - [twowell01.gpr *]
Computed water table elevations can be visualized using contour plots or 3D surface plots.
39 Groundwater Flow Modeling
RITS Fall 2009 – Using the GMS in Support of CSMs



Base example on the injection/extraction well system.

Create grid

Assign basic properties

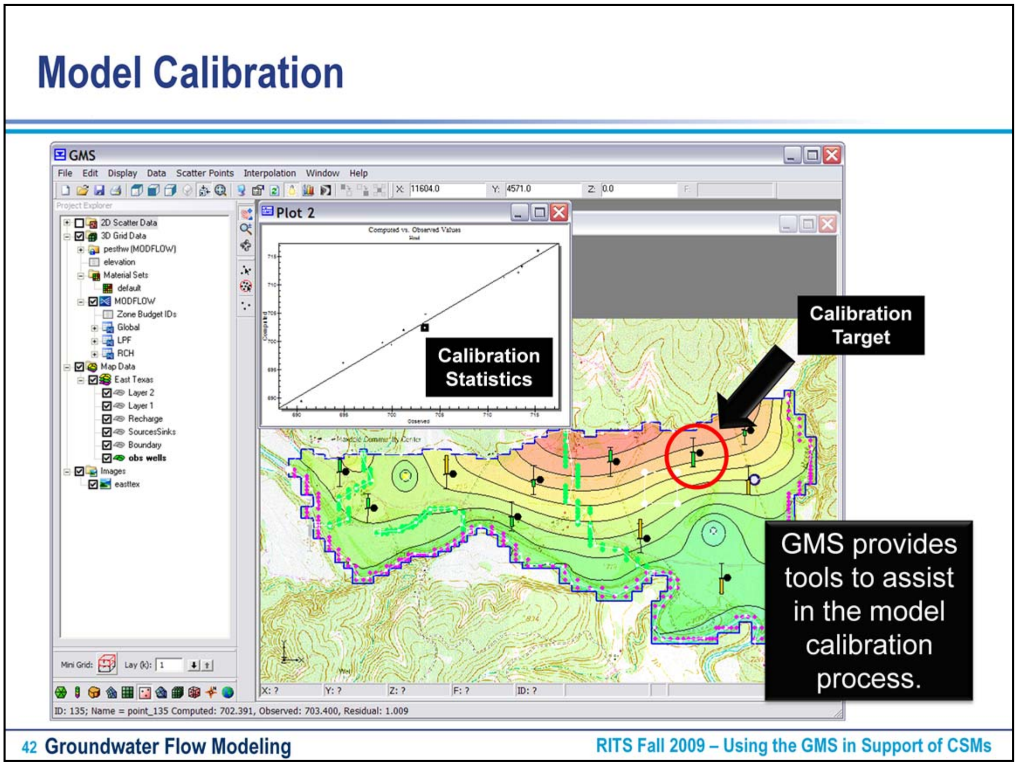
Create two sets of three wells

Save and run the model.

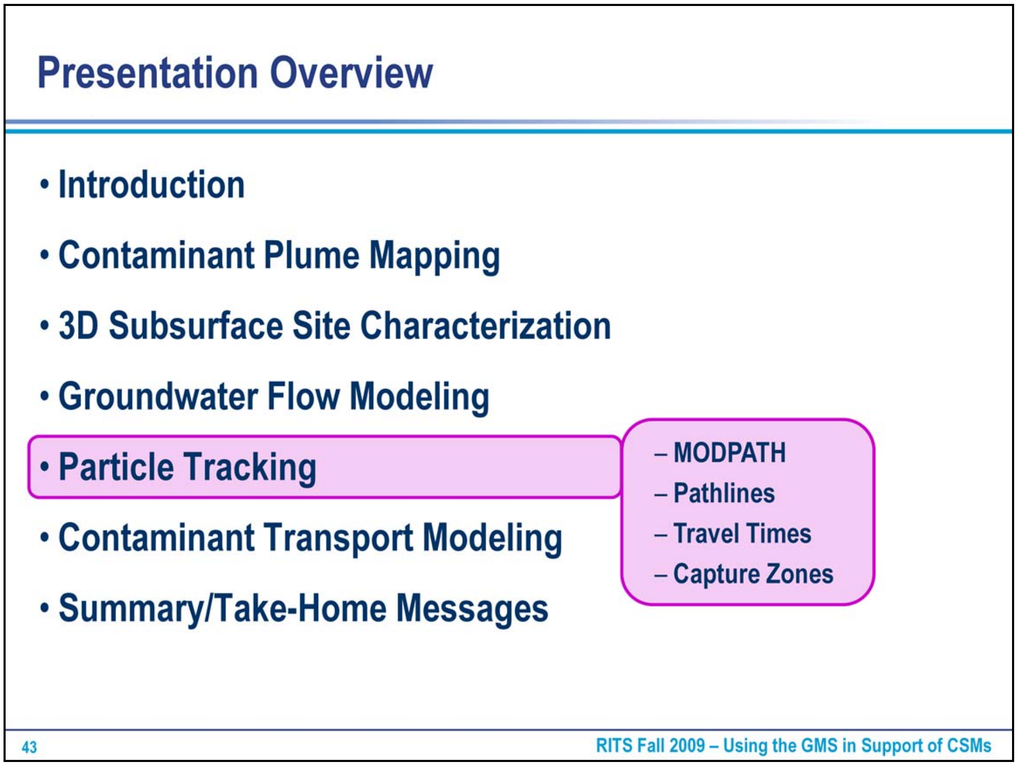
View output.

Model Calibration

- Before a model is used for prediction, it should be calibrated
- Steps
  - Solution is computed by model (MODFLOW, MT3D, etc.)
  - Computed heads/concentrations are compared to field observed values
  - Input parameters (K, recharge, etc.) are adjusted until computed heads match observed heads
  - Sensitivity analysis is performed on each parameter



RITS Fall 2009 – Using the GMS in Support of CSMsRITS Fall 2009 – Conceptual Model Software Tools


Presentation Overview
• Introduction
• Contaminant Plume Mapping
• 3D Subsurface Site Characterization
• Groundwater Flow Modeling
• Particle Tracking
– MODPATH
– Pathlines
– Travel Times
– Capture Zones
• Contaminant Transport Modeling
• Summary/Take-Home Messages
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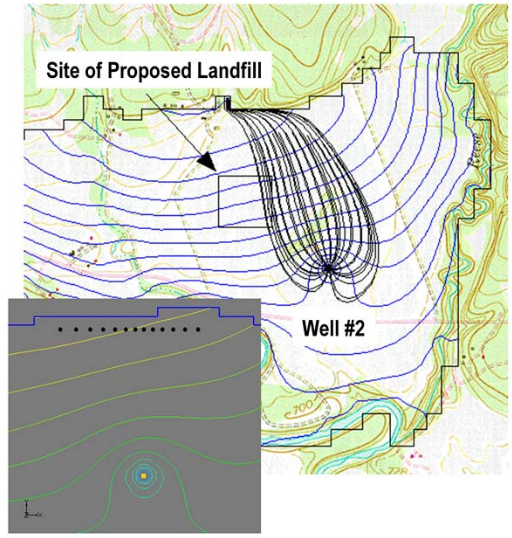
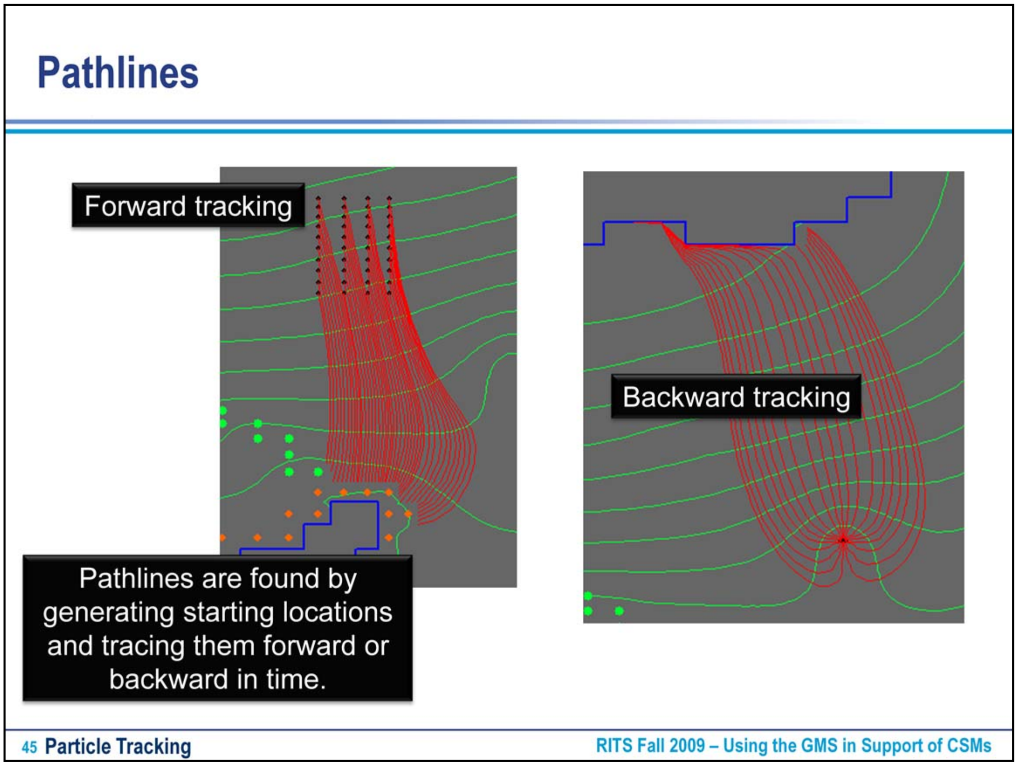
RITS Fall 2009 – Using the GMS in Support of CSMs

Particle Tracking with MODPATH

- Developed by the USGS
- Companion program to MODFLOW
- Applications
  - Particle tracking
  - Travel time analysis
  - Capture zones



Particle Tracking: When would particle tracking be used? To answer what type of questions?


Pathlines
Forward tracking
Backward tracking
Pathlines are found by generating starting locations and tracing them forward or backward in time.
45 Particle Tracking
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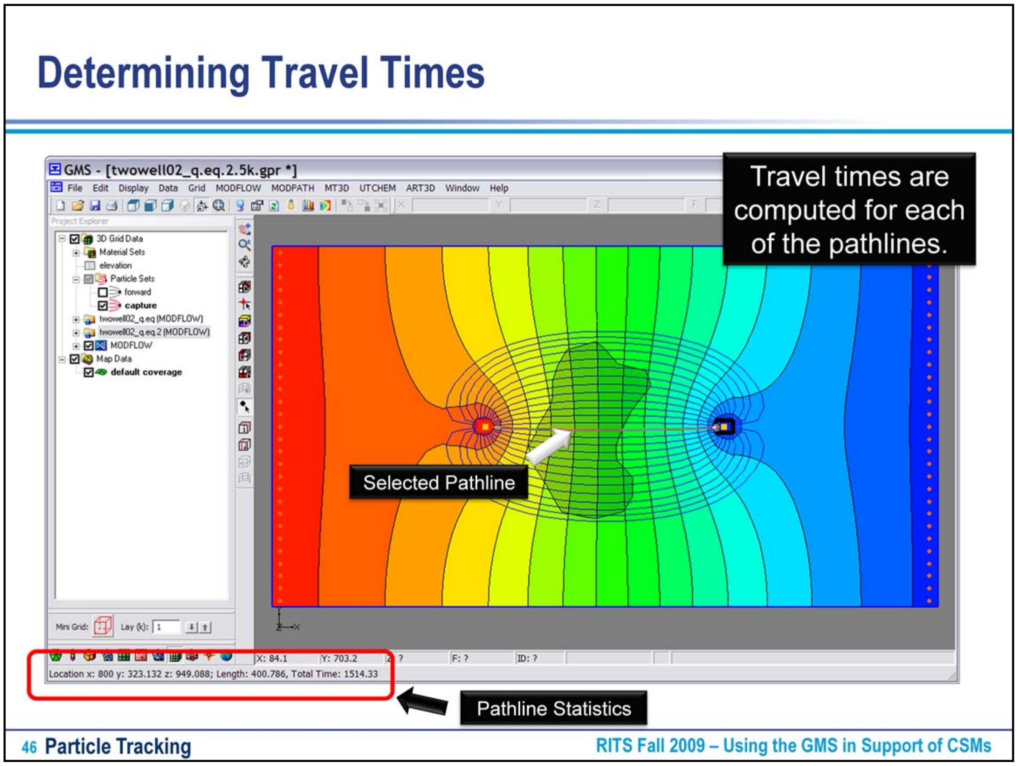
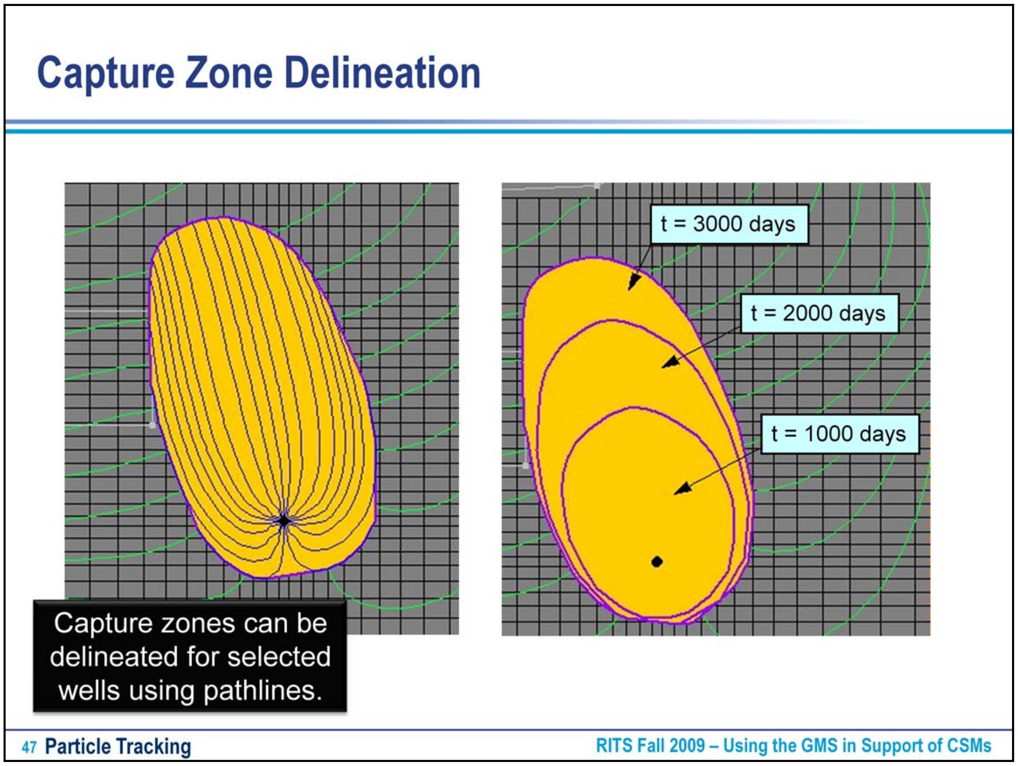
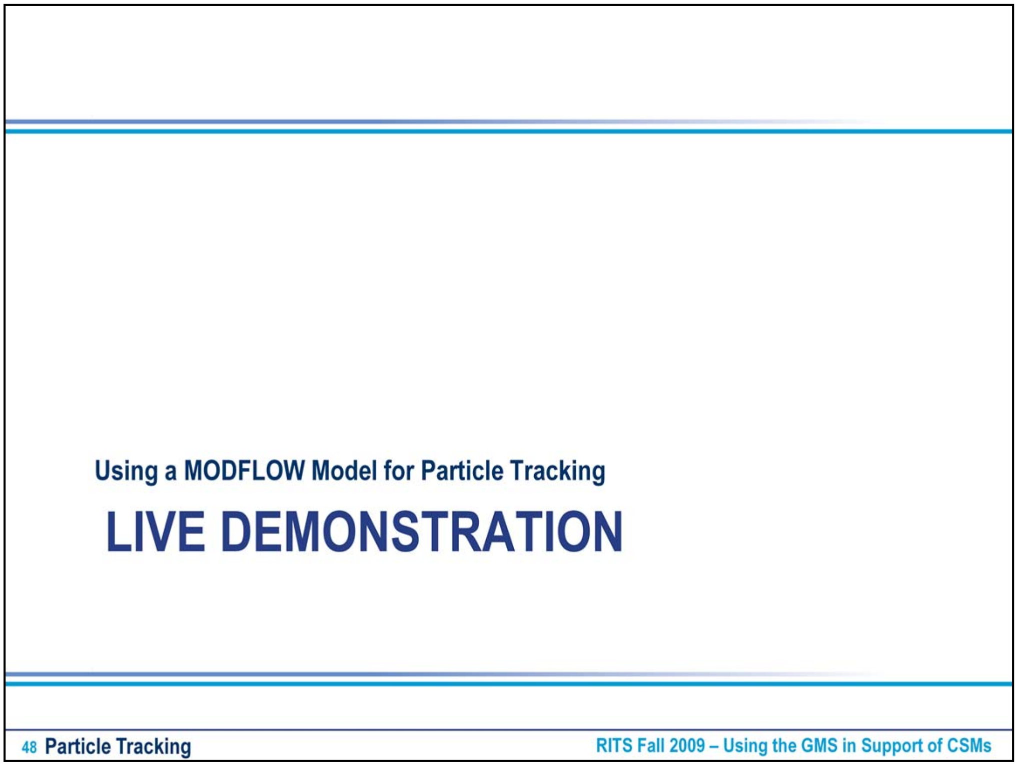


Reason for modeling? Demonstrate complete mixing in an injection/extraction for a substrate like EVO (emulsified veg oil).



Pumping and capturing? To help show capture zones for things like injection of ISCO (if needed by regulators). In pilot tests, regulators might require complete capture of all amendments injected in the ground. This type of modeling should be very beneficial in the work plan outlining.



Open the East Texas model.

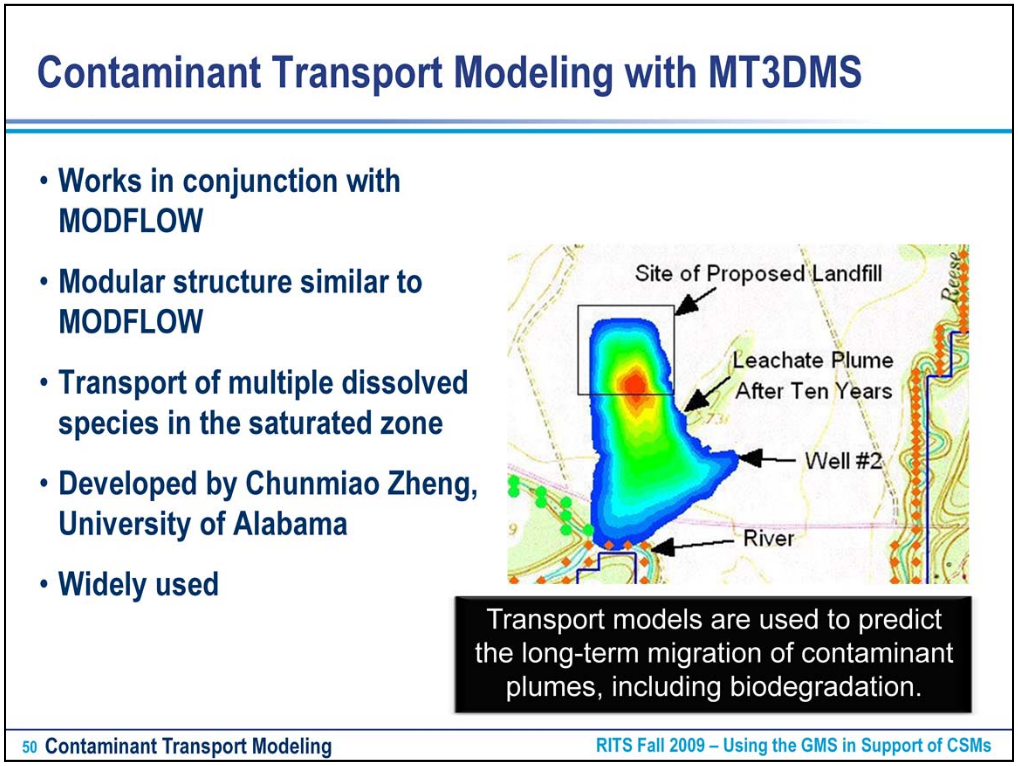
Do backward tracking from the wells

Do forward tracking from the landfill

Put in a barrier between landfill and well and see what happens.

Presentation Overview

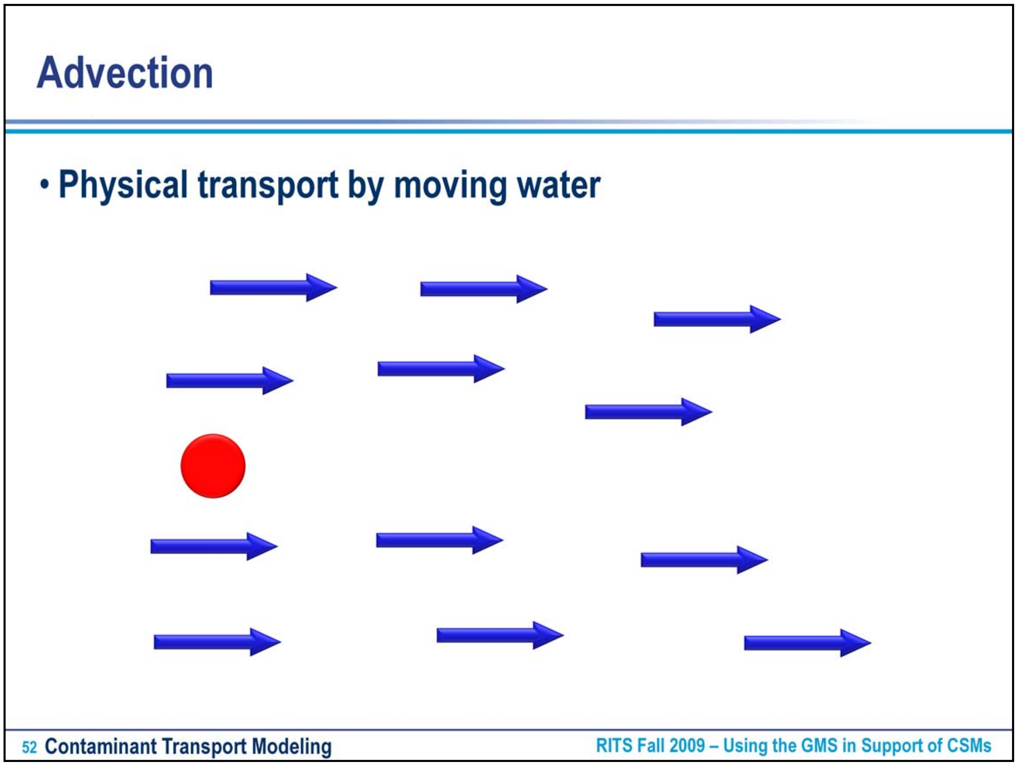
- Introduction
- Contaminant Plume Mapping
- 3D Subsurface Site Characterization
- Groundwater Flow Modeling
- Particle Tracking
- Contaminant Transport Modeling
  - MT3DMS
  - Processes Simulated
  - RT3D
  - Reactive Transport Modeling
  - Dover Case Study
- Summary/Take-Home Messages



The flow model must be completed first. This is different from particle tracking.

Basic Transport Processes

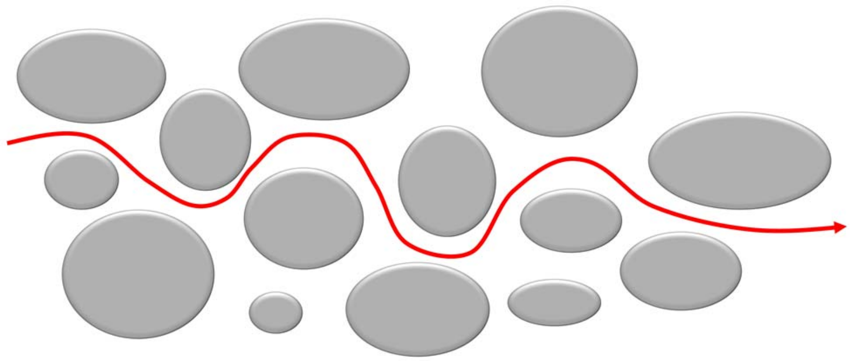
- Advection
- Mechanical Dispersion
- Molecular Diffusion
- Internal Sinks and Sources
- Sorption
- Dual Domain Transport
- Chemical Reactions



MODPATH does advection only.

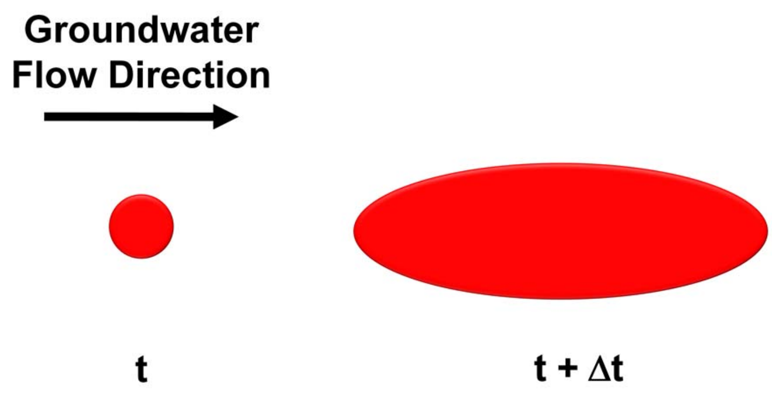
Mechanical Dispersion

- When advective flow is taking place, the pore water is mixed due to the heterogeneity of the soil which causes variations in flow paths and velocities

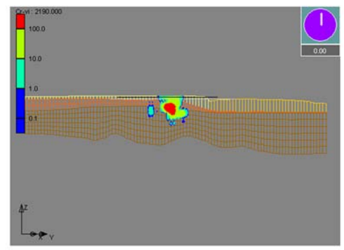


Mechanical Dispersion

- Dispersion causes spreading of plume



Post-Processing, Visualization



20-yr Chromium Transport

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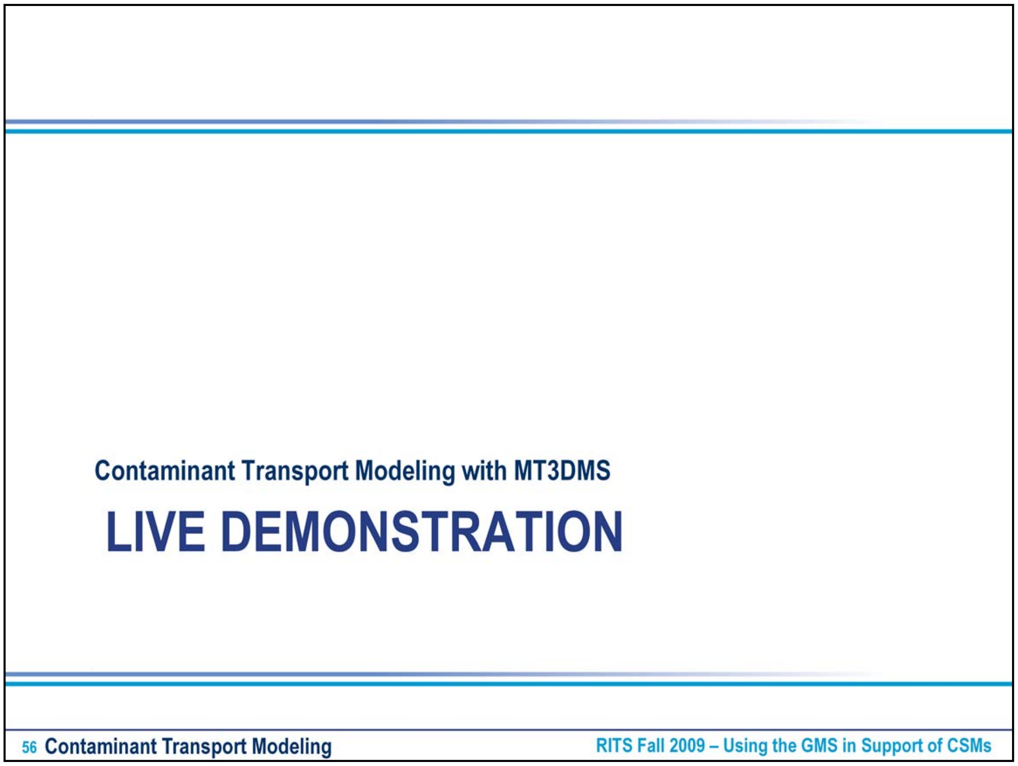
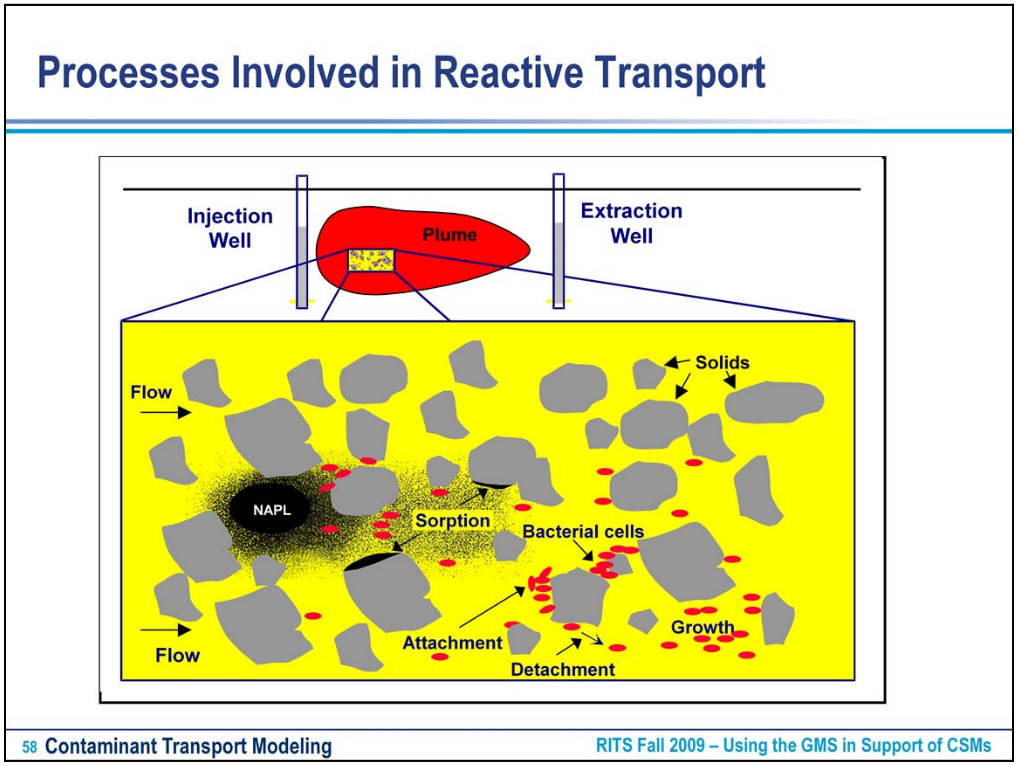


Open the East Texas model.

Review a transport simulation from the landfill

Contaminant Transport Modeling with RT3D

- Modified Version of MT3DMS
- Reactive Transport
  - BTEX degradation
  - Dechlorination
  - User-defined reactions


Processes Involved in Reactive Transport
Injection Well
Plume
Extraction Well
Solids
Flow
NAPL
Sorption
Bacterial cells
Growth
Attachment
Detachment
Flow
58 Contaminant Transport Modeling
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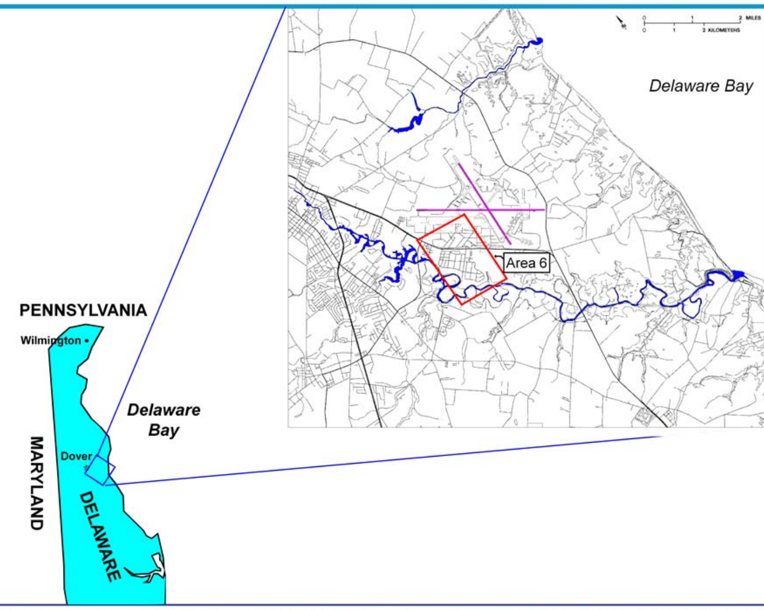
Reaction Packages

- Instantaneous aerobic degradation of BTEX
- BTEX degradation using multiple electron acceptors
- Sequential anaerobic degradation: PCE->TCE->DCE->VC
- User-defined reaction

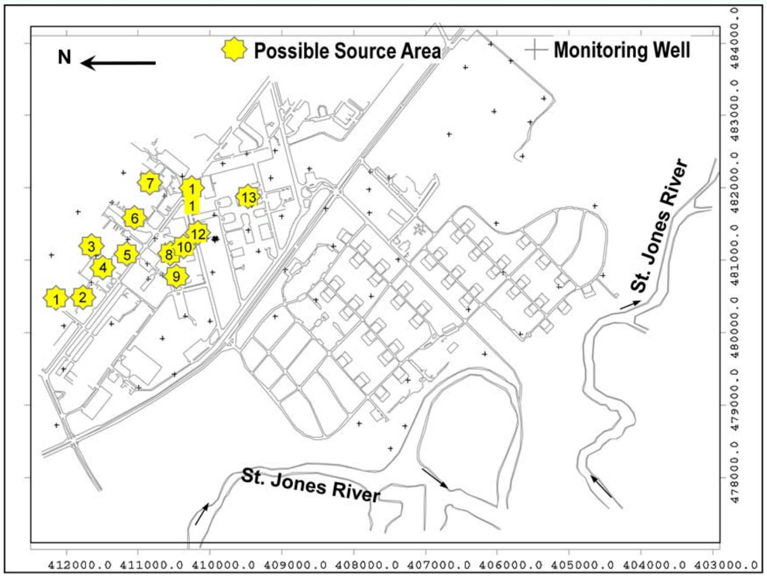
Case Study

DOVER AIR FORCE BASE DECHLORINATION

Location of Dover Air Force Base



Area 6 Map



62 Contaminant Transport Modeling – Case Study – Dover

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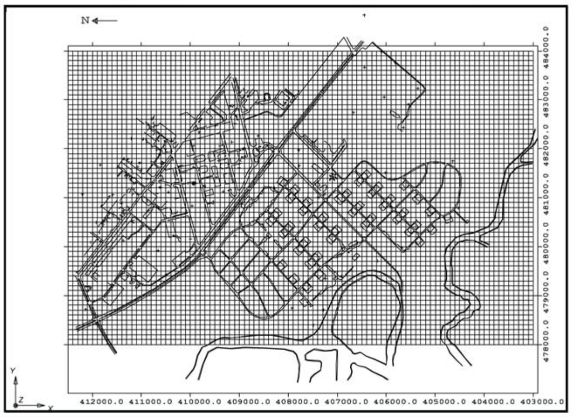
Simulation Grid Configuration

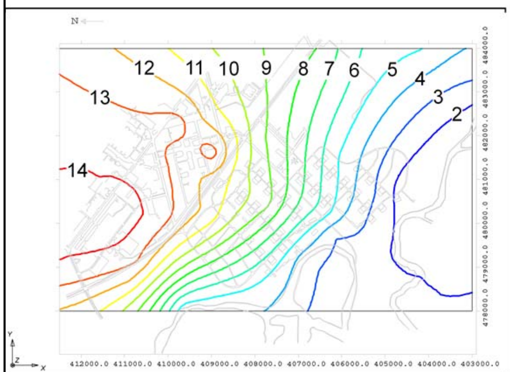
	x	y	z	Units
Number of Cells	95	60	1	—
Total Length	9,500	6,000	10	ft.
Cell Size	100	100	12	ft.
Origin Coordinates*	412500.0	47800.0	0.00	ft.



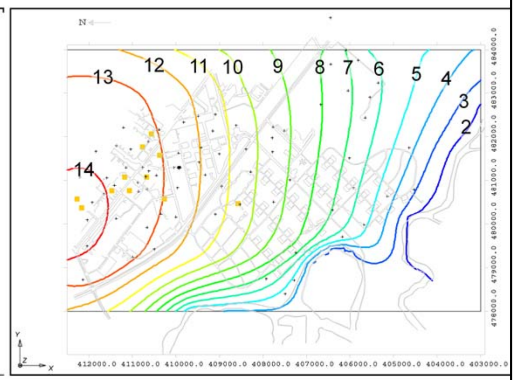
*Coordinates are in State Plane (NAD 83). The simulation software refers to coordinates in the x-direction as increasing from left to right from the origin, which is the opposite direction of the state plane coordinates that are shown in the picture.

Flow Calibration

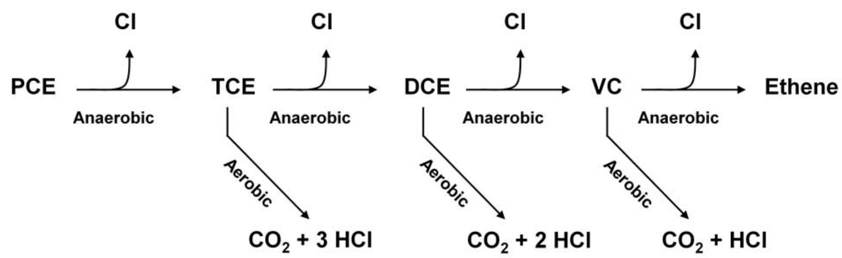
Head contours from 1997 field data (ft MSL)



Head contours from model data (ft MSL)

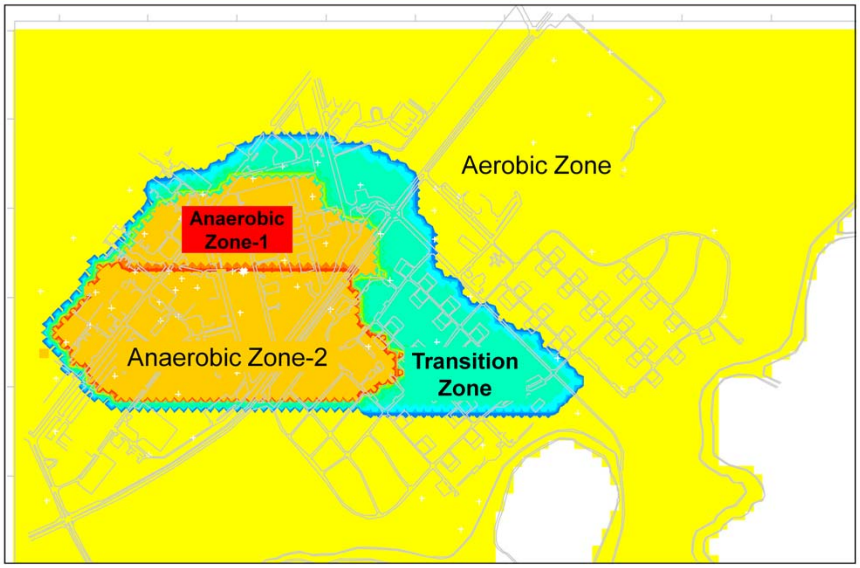


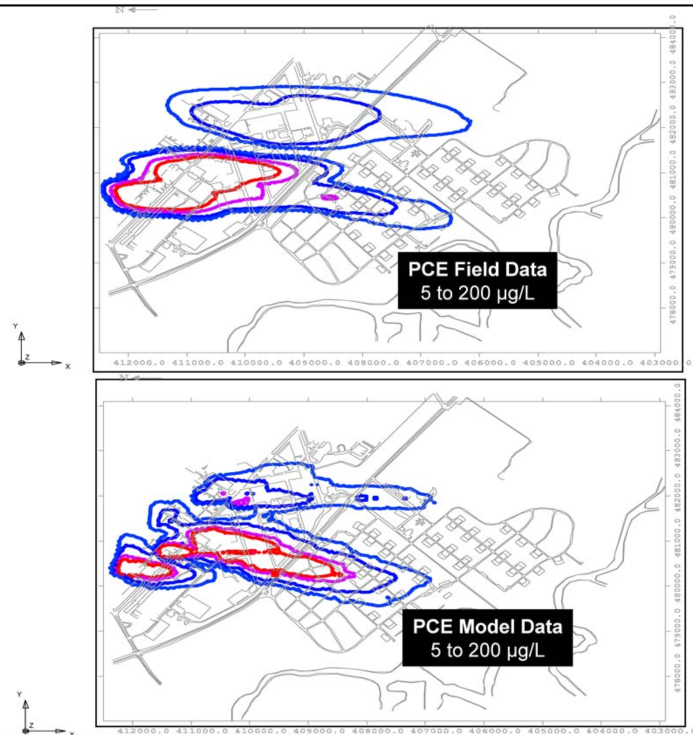
Dechlorination



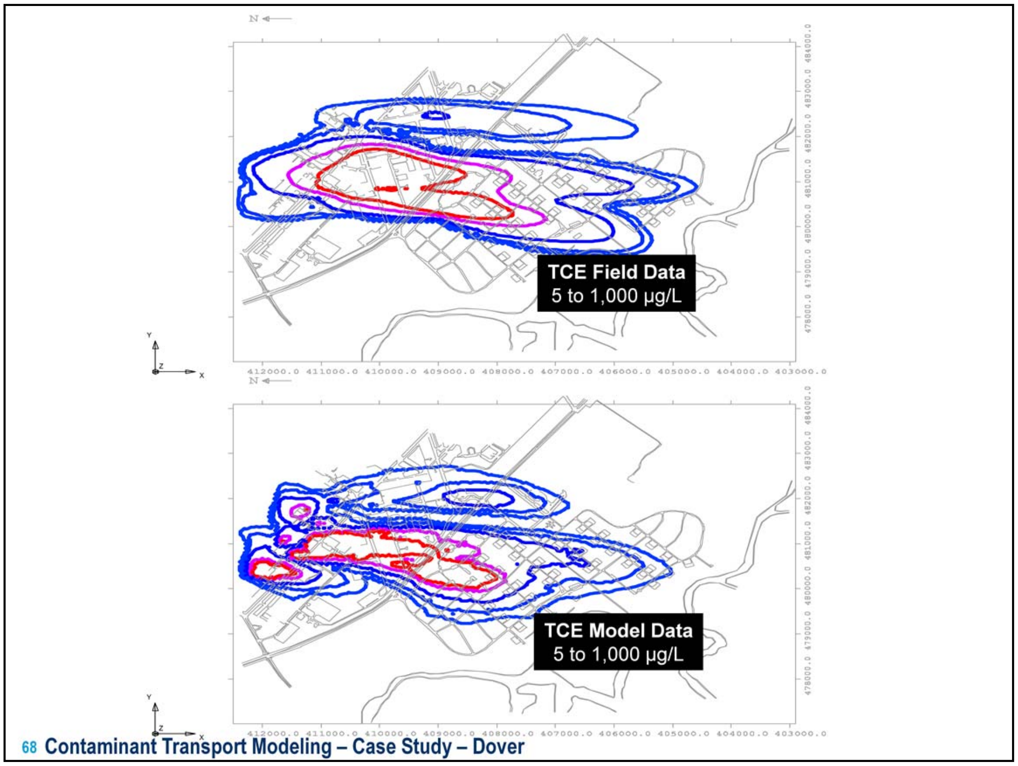
- **Reaction Model**
  - Transport of PCE, TCE, DCE, VC, and Ethene are considered
  - Kinetics of all the reactions are assumed to be first-order
  - Both anaerobic and aerobic rates are used
  - Anaerobic and aerobic zones are delineated using spatially variable reaction parameter values

Anaerobic and Aerobic Zones





67 **Contaminant Transport Modeling – Case Study – Dover**


TCE Field Data
5 to 1,000 µg/L
TCE Model Data
5 to 1,000 µg/L
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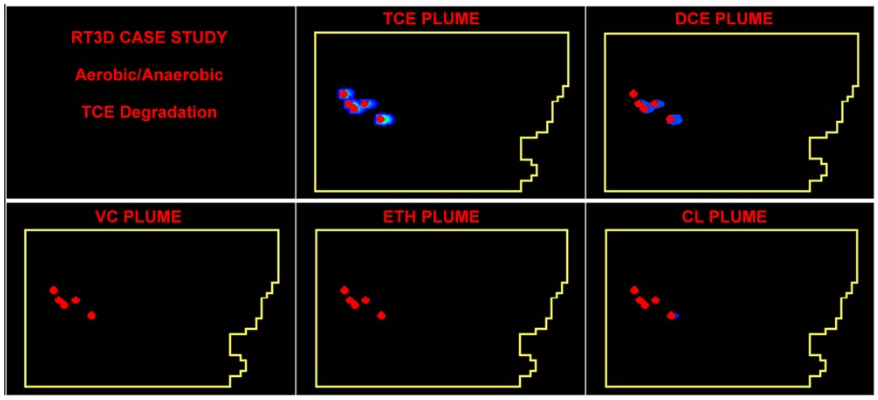
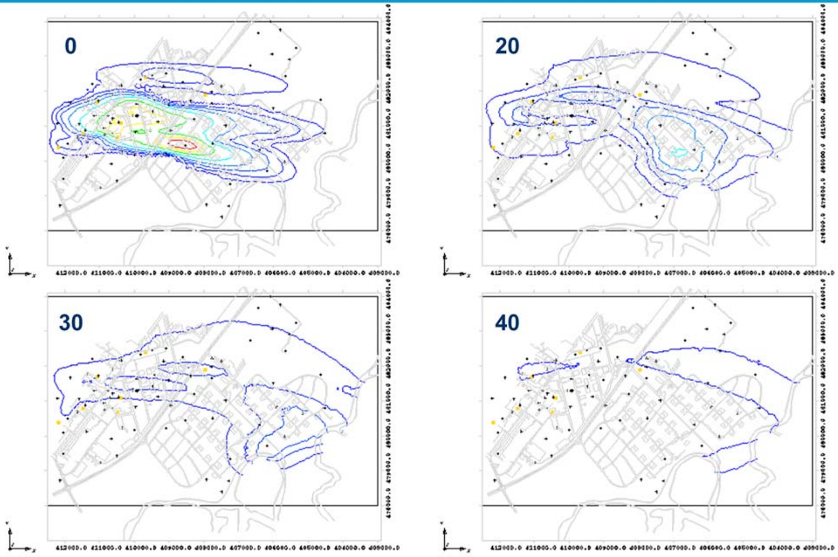
Combined Animation



Model Forecasting Results (no source) – TCE Transport 0, 20, 30, and 40 Years



Contour levels (5 to 2,000 µg/L)

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- **Summary/Take-Home Messages**
  - Summary of Applications
  - Level of Difficulty
  - Take Home Messages
  - NAVFAC Point of Contact

Summary of Applications

Application	GMS	ArcGIS/Spatial Analyst	Surfer
Geostatistics/interpolation	X	X	X
Contouring/mapping	X	X	X
3D plume models/iso-surfaces	X		
SCAPS data import/visualization	X		
Boreholes	X		
Cross sections	X		
Solids (3D geologic volumes)	X		
Flow models (MODFLOW)	X		
Particle tracking	X		
Transport modeling	X		
Database management		X	

Learning Curve, Level of Effort

Application	GMS	ArcGIS/Spatial Analyst	Surfer
Geostatistics/interpolation	Easy	Moderate	Easy
Contouring/mapping	Easy	Moderate	Easy
3D plume models/iso-surfaces	Moderate		
SCAPS data import/visualization	Moderate		
Boreholes	Easy		
Cross sections	Moderate		
Solids (3D geologic volumes)	Moderate		
Flow models (MODFLOW)	Difficult		
Particle tracking	Difficult		
Transport modeling	Difficult		
Database management		Difficult	

● **Easy** ◉ **Moderate** ○ **Difficult**

73 **Summary/Take Home Messages** RITS Fall 2009 – Using the GMS in Support of CSMs

Learning GMS

- Tutorials
  - Hands-on tutorial are provided for self learning
  - Each tutorial includes sample data and step-by-step instructions
- Training courses
  - GMS training courses are offered at regular intervals in various US locations
  - Custom on-site training can be arranged

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Take-Home Messages

- GMS and Surfer are part of NIRIS and both can be used effectively to develop CSMs
- 2D and 3D plume maps help document the results of a site investigation in a simple and intuitive fashion
- Borehole data can be used to build 3D cross sections and volumetric model of site stratigraphy
- Flow models and particle tracking can be used to perform travel time analysis and as a design aid
- Transport models can be used to perform long-term predictions and risk analysis

75 Summary/Take Home Messages RITS Fall 2009 – Using the GMS in Support of CSMs