Application of Transport Optimization Codes to Groundwater Pump and Treat Systems

> Internet Training Seminar September 24, 2003

Today's Presenters

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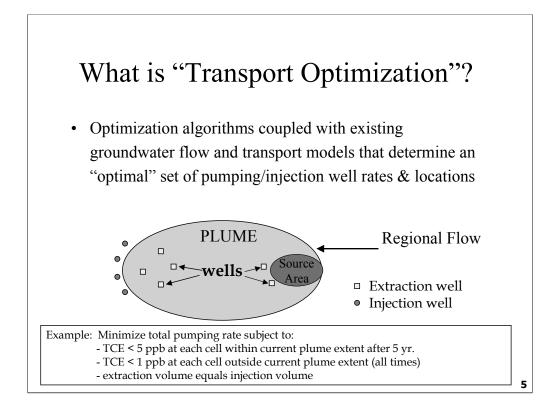
Remedial Optimization For P&T Systems

• Remediation System Evaluation (RSE) or Remedial Process Optimization (RPO) provides a broad assessment of...

- · Goals and exit strategy
- Below-ground performance
- Above-ground performance
- Monitoring and reporting
- Potential for alternate technologies
- Pumpage optimization is a subset or a component of these more general optimization evaluations
 - Trying to determine the "best" extraction/injection strategy assuming P&T is the most appropriate technology

Presentation Outline

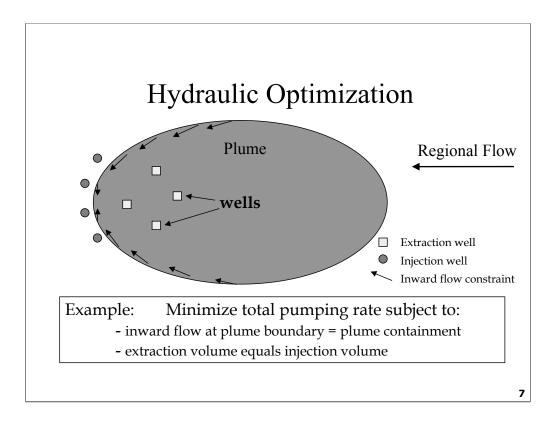
- What is "transport optimization"?
- Why perform transport optimization?
- General optimization process
 - Formulating problems
 - Solving problems
- Recent DOD "ESTCP" groundwater remediation optimization study
 - Project Background
 - Example: Umatilla
 - Example: Blaine
 - Lessons Learned
- Further Information



Why Perform Transport Optimization?

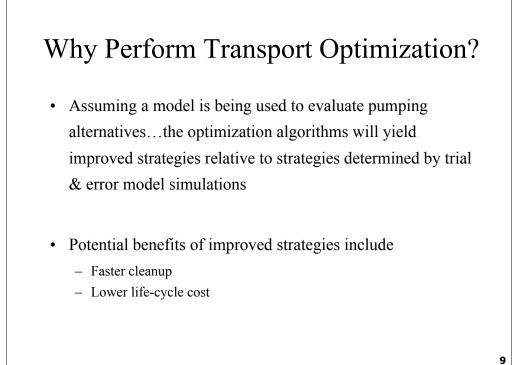
- "Hydraulic Optimization" can be too limiting for many sites (1999 EPA Demonstration project)
 - Optimization based only on ground water FLOW model
 - Focus is on containment, cannot optimize based on concentration or cleanup times

Hydraulic Optimization



Why Perform Transport Optimization?

- "Hydraulic Optimization" can be too limiting for many sites (1999 EPA Demonstration project)
 - Optimization based only on ground water FLOW model
 - Focus is on containment, cannot optimize based on concentration or cleanup times
- Transport Optimization
 - Optimization based on ground water FLOW and TRANSPORT model
 - Not just containment...considers concentrations and cleanup times



The DoD has ~ 200 operating pump-and-treat systems for containment or containment and treatment. The total O&M cost of those sites is about 100M/yr. The optimization codes are expected to be cost effective at 25%-30% of those sites.

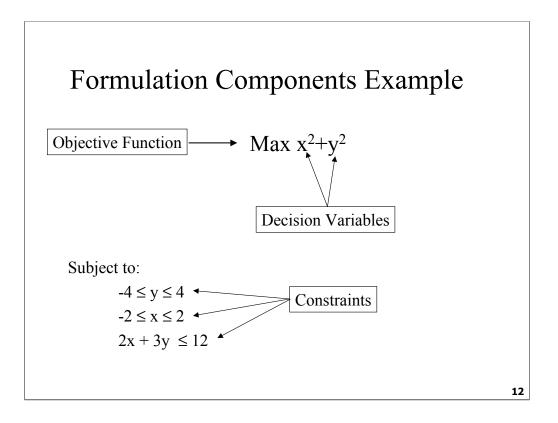
Studies completed by EPA and Navy indicate the majority of the p&t systems are not operating as designed, have unachievable or undefined goals, and have not been optimized since installation.

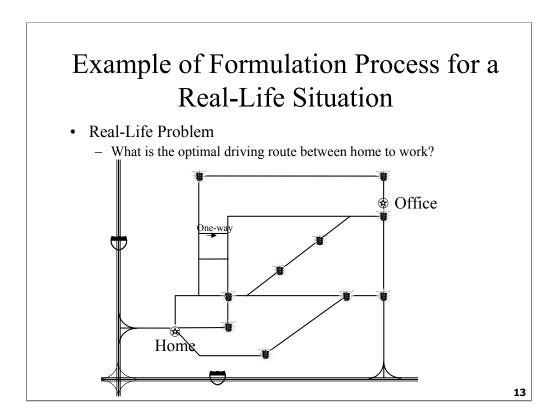
General Optimization Process

- Start with a real-life problem for which you are seeking the "best" or "optimal" solution
- <u>Formulate the Problem</u>. Develop an "optimization formulation" that describes the essential elements of the real world problem *in mathematical terms* to establish...
 - The parameters for which optimal values are to be determined
 - The criteria for determining that one solution is better than another
 - The rules for allowing some solutions and disallowing others
- <u>Solve the Problem</u>. Select and apply an appropriate methodology to search possible and allowable combinations of pumping strategies for an "optimal" solution

Formulation Components (Terminology)

- Decision Variables
 - What we are determining optimal values for
- Objective Function
 - The mathematical equation being minimized or maximized
 - Value can be computed once the value of each decision variable is specified
 - Serves as the basis for comparing one solution to another
- Constraints
 - Limits on values of the decision variables, or limits on other values that can be calculated once the value of each decision variable is specified





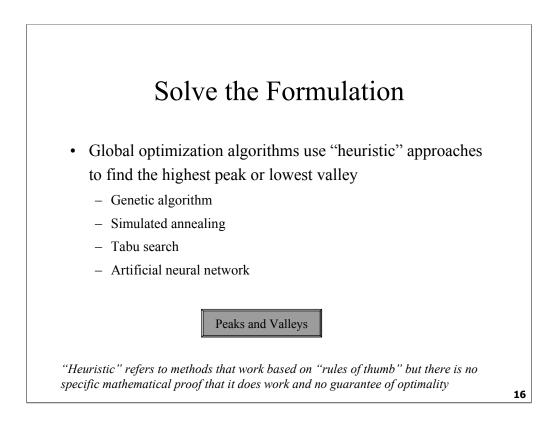
Example of Formulation Process for a Real-Life Situation

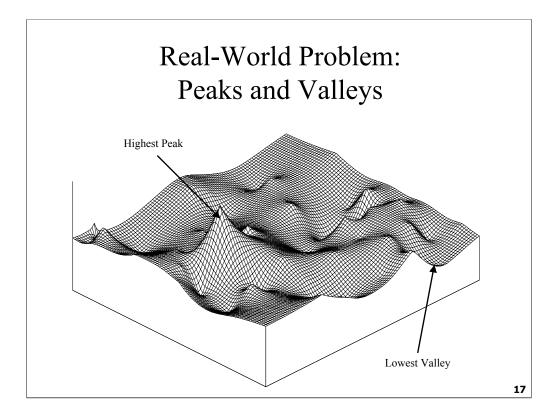
• Formulation must establish...

- The decision variables
 - · Combinations of roads/turns between my house and work
- The objective function (some possibilities)
 - Minimize distance traveled
 - Minimize travel time
 - Minimize number of traffic lights
- The constraints (some examples)
 - Must travel on paved roads
 - No more than four traffic lights allowed
 - · Cannot go wrong way on a one-way street

Mathematical Descriptions are Often Difficult...

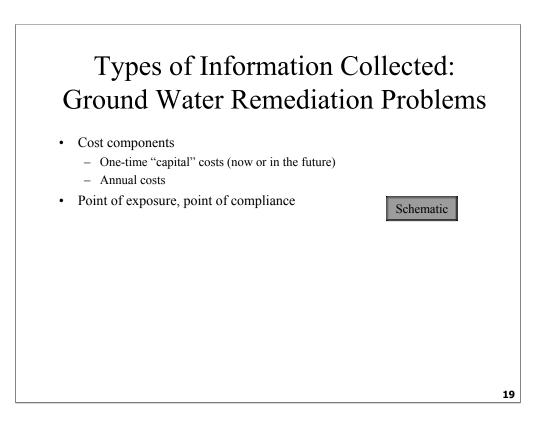
- Example: Minimize Travel Time
 - How do you mathematically account for traffic when calculating time of travel for a selected route of travel?
 - How do you estimate speed on the interstate?
 - Does it depend on time of day?
 - Does it depend on day of the week?
- Simplifications are invariably required in the formulation process
- Many alternative formulations are generally possible, each may have a different optimal solution

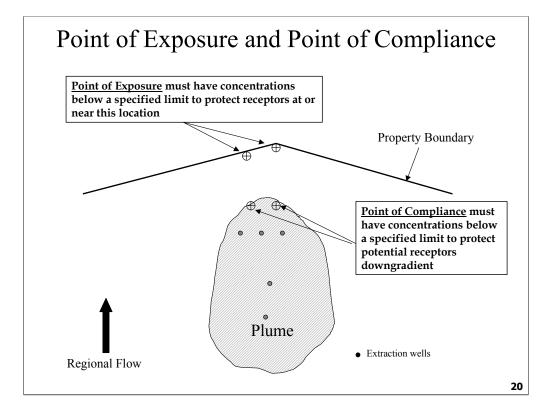




Optimization Process: Ground Water Remediation Problems

- Preliminary Tasks
 - Understand site-specific goals and constraints
 - Verify/update flow & transport model until it is considered valid for design purposes
 - Obtain detailed information required to develop the formulations
- State formulation(s) in mathematical terms
 - Objective function
 - Constraints
- Select optimization codes/algorithms & solve formulations
- Revise formulations and solve as needed

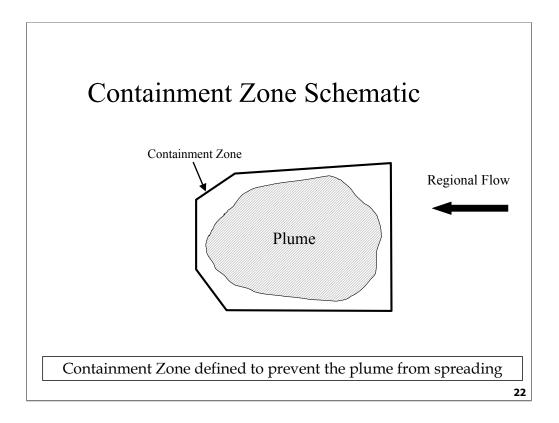


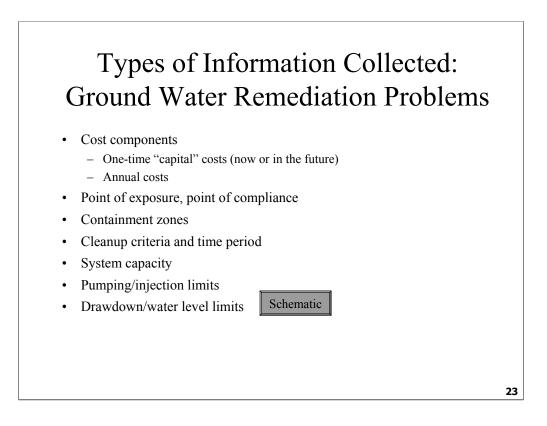


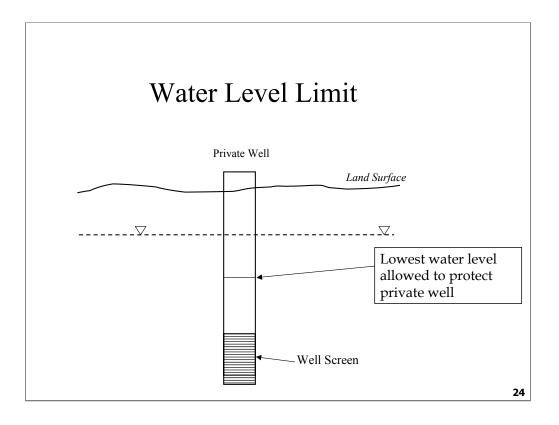
Types of Information Collected: Ground Water Remediation Problems

- Cost components
 - One-time "capital" costs (now or in the future)
 - Annual costs
- Point of exposure, point of compliance

Containment zones Schematic







Types of Information Collected: Ground Water Remediation Problems

- Cost components
 - One-time "capital" costs (now or in the future)
 - Annual costs
- Point of exposure, point of compliance
- Containment zones
- Cleanup criteria and time period
- System capacity
- Pumping/injection limits
- Drawdown/water level limits
- Limit on capital cost, etc.
- Other planned actions (such as source removal) that may impact future remedy performance

Formulation Components: Ground Water Remediation Problems

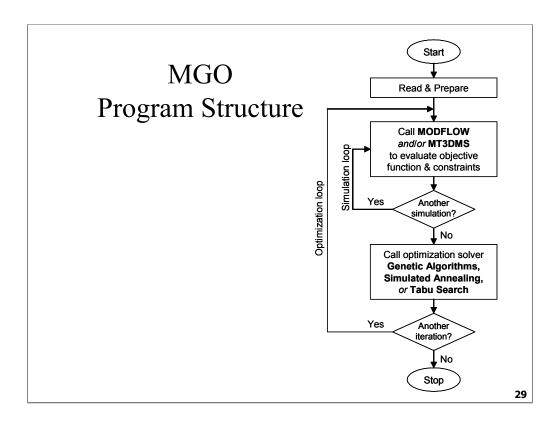
- Decision Variables
 - · Locations of extraction/injection wells
 - · Rates at each extraction/injection well over time
- Potential objective functions (select only one unless using a multiobjective algorithm)
 - Total life-cycle cost {minimize}
 - Cleanup time {minimize}
 - Contaminant mass remaining in aquifer {minimize}
 - Contaminant mass removed from aquifer {maximize}
- Potential constraints (as many as you want...here are some examples)
 - · Limits on pumping rates at specific wells or total pumping rate
 - Limits on concentrations (at specific locations/times)
 - Restrictions on well locations
 - · Limits on aquifer drawdown at specific locations
 - · Financial constraints such as limits on capital costs

Optimization Codes: Ground Water Remediation Problems

- Dr. Chunmiao Zheng (University of Alabama), Modular Groundwater Optimizer (MGO)
 - Genetic algorithms
 - Simulated annealing
 - Tabu search
- Dr. Richard Peralta (Utah State University), Simulation Optimization Modeling Systems (SOMOS)
 - Genetic algorithms
 - Simulated annealing
 - Tabu search
 - Genetic algorithms coupled with artificial neural network

<u>M</u>odular <u>G</u>roundwater <u>O</u>ptimizer (MGO)

- Simulation Components
 - MODFLOW for groundwater flow
 - MT3DMS for multi-species contaminant transport
- Optimization Components
 - Global optimization (heuristic search) techniques
 - Genetic algorithms (GA)
 - Simulated annealing (SA)
 - Tabu search (TS)
 - Integrated techniques
 - Global optimization techniques + response functions for greater computational efficiency

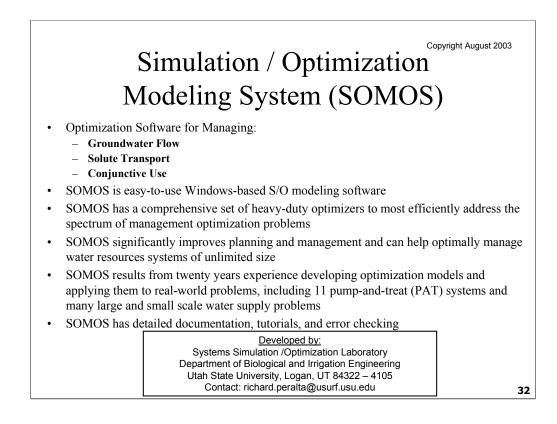


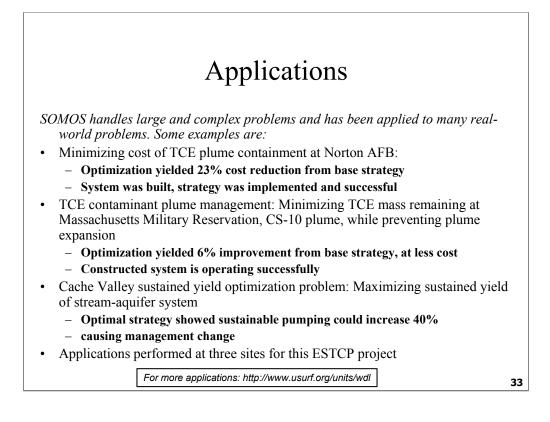
MGO: Setup of Optimization Modeling

- Input files for MODFLOW (no modification)
- Input files for MT3DMS (no modification)
- An optimization input file specifying
 - Optimization Solver (GA, SA, TS)
 - Output options
 - Decision variables (flow rates, well locations)
 - Objective function
 - Constraints

MGO: Additional Information

- Code Compatibility
 - MODFLOW
 - MT3DMS
- Platforms that incorporates MGO
 - Groundwater Vistas



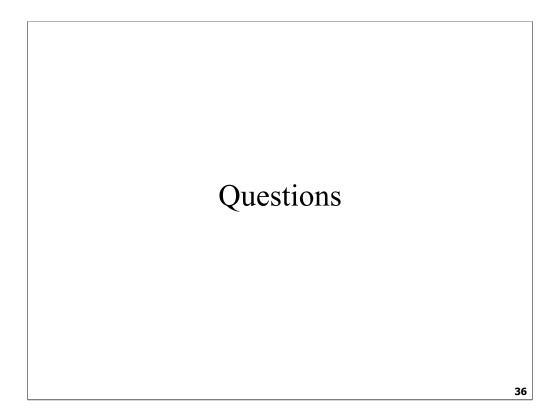


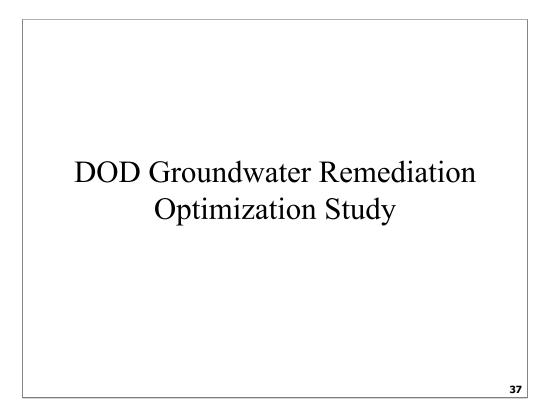
SOMOS Features

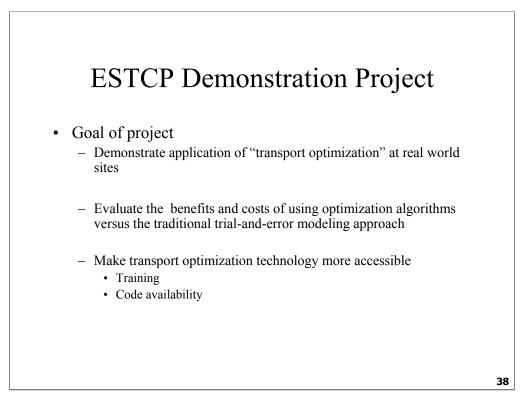
- Windows-based SOMOS runs in background, while user employs other programs.
- SOMOS' spread-sheet based pre-processor, SOMOIN, simplifies input file preparation (availability depends on version).
- SOMOS' professional design has detailed input error-checking and error messages.
- Buttons on SOMOS' user-friendly interface speed accessing/editing I/O files, and optimizations.
- SOMOS' flexibility allows run restarts, result merges, stepwise, sequential, and simultaneous optimization, full control over constraints and bounds in time and space.
- SOMOS' automation allows considering multitudinous candidate wells in a run and speeds sequential running of multiple optimization actions.
- SOMOS includes a 2-D spreadsheet-based tool for mapping layered aquifer parameters, well locations and hypothetical capture zones (availability depends on version).
- SOMOS is being included within groundwater modeling packages such as Visual MODFLOW and Groundwater Vistas
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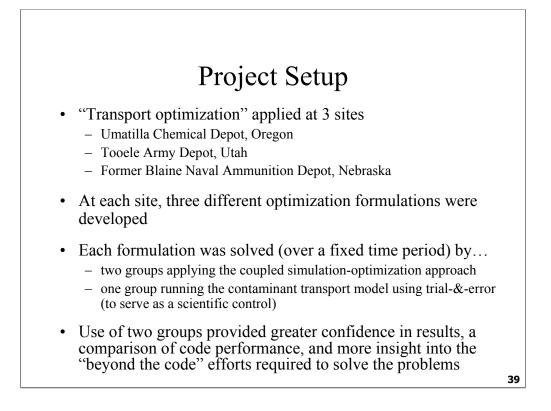
SOMOS Features (vary with version)

- Applicability: Any confined or unconfined aquifer system that can be modeled.
- <u>Simulators:</u> MODFLOW, MT3DMS, SEAWAT, Response Matrix, Response Surface, Artificial Neural Networks, Others.
- <u>12 Optimizers:</u> Including Simplex, Gradient Search, Branch & Bound, Outer Approximation, Genetic Algorithm (GA) linked with Tabu Search (GA-TS) and Simulated Annealing (SA) linked with Tabu Search (SA-TS).
- **Optimization Problem Types:** linear, quadratic, nonlinear, mixed integer, mixed integer nonlinear, multi-objective, stochastic (i.e. under uncertainty).
- <u>Controllable Variables:</u> ground-water pumping, gradient, cell-head, head at well casing; surface water diversion, flow, & head; aquifer/surface body seepage; contaminant concentration, mass remaining & removal; user-definable variables.
- <u>Management Goals</u>: Can optimize for 90+ distinct objective functions plus userdefined objective and multi-objective optimization.









Project Team

- ESTCP and EPA provided funding, USACE also provided support
- Diverse project management team
 - NFESC Karla Harre, Laura Yeh
 - EPA-TIO Kathy Yager
 - USACE Dave Becker
 - GeoTrans, Inc. Rob Greenwald, Yan Zhang
 - University of Illinois Dr. Barbara Minsker

• Transport optimization modelers

- Utah State University Dr. Richard Peralta (SOMOS)
- University of Alabama Dr. Chunmiao Zheng (MGO)

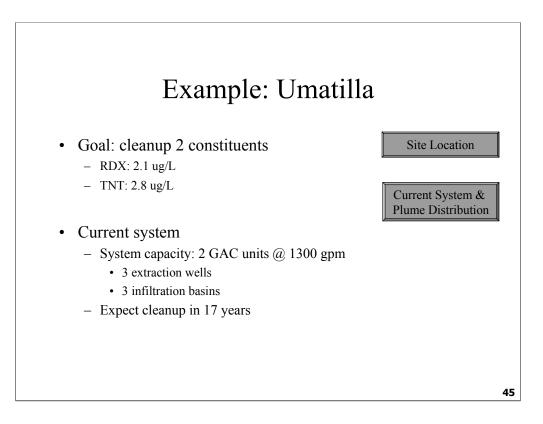
Demonstration Sites						
Site Name	Pump rate (gpm)	# Existing	Contam-	Groundwater		
	and Cost (\$/yr)	Wells	inants	Model Info.		
Umatilla	1300/\$430K	3 ext.	RDX/	5 layers		
Army Depot	(operating)	3 inj.	TNT	10 min runs		
Tooele	5000/\$1M	15 ext.	TCE	4 layers		
Army Depot	(operating)	13 inj.		10 min runs		
Former Blaine NAD	4000/\$2M (in preliminary design)	17 ext. (planned)	TCE*/ TNT	6 layers 2 hr runs		

Formulation Process For Each Site

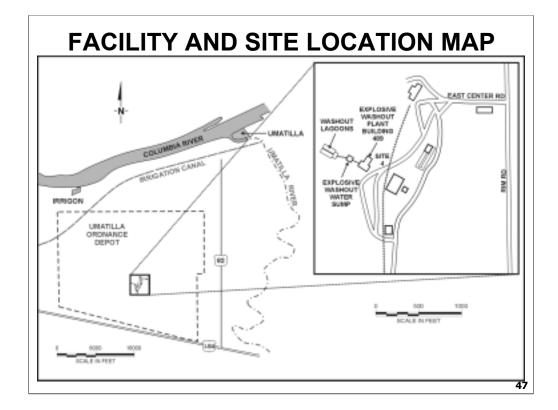
- Perform site visit and review site data
 - Understand the real-life situation
 - Explore real-life objectives and constraints with the installations
 - Initial discussion of how to convert real life situation into mathematical description
- Review site groundwater flow and transport model
 - Receive assurance from installation that they consider the model predictions acceptable for use for remediation design purposes
 - Important because the transport model provides the mathematical relationship between the decision variable values (the pumping locations/rates) and terms in the constraints/objective function

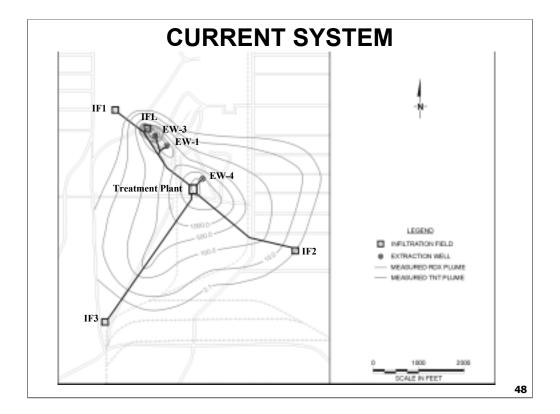
Formulation Process For Each Site Develop 3 "optimization formulations" based on further interaction with the installations Select an "objective function" to be minimized (or maximized) Specify a set of constraints to be satisfied Worked with installation to establish final mathematical representations of key problem components, such as... Cost coefficients (e.g., cost of new well, cost to treat each gpm, etc.) Nature of the relationships between the decision variables and other terms in the objective function and/or constraints (e.g., is the cost to treat each gpm constant, or does it change based on flow rate and/or contaminant concentrations?)

		ptimization For		liations	
Site Name		Objective Function		Major Constraints	
	Form. 1	Min life-cycle cost	1. 2.	Current treatment capacity Cleanup of RDX and TNT	
Umatilla	Form. 2	Min life-cycle cost	 Increased treatment capacity Cleanup of RDX and TNT 		
	Form. 3	Min total mass remaining in layer 1	1.	Cleanup of RDX and TNT	
Tooele	Form. 1	Min total cost	1.	POE concentration limit	
	Form. 2	Min total cost	1.	POE/POC concentration limits	
	Form. 3	Min total cost	1. 2. 3.	POE/POC concentration Limits Declining source term Cleanup (< 50ppb)	
Blaine	Form. 1	Min life-cycle cost	1. 2.	Plume containment Cleanup of TCE and TNT	
	Form. 2	Min life-cycle cost w/ 2400gpm extracted water diversion	1. 2.	Plume containment Cleanup of TCE and TNT	
	Form. 3	Min maximum total pumping	1.	Plume containment	









Umatilla Objective Function: Formulation 1

• Minimize Total Cost Until Cleanup

Total Cost = CCW + CCB + CCG + FCL + FCE + VCE + VCG + VCS

- CCW: Capital Costs of new Wells
- CCB: Capital Costs of new Recharge Basins
- CCG: Capital Costs of new GAC units
- FCL: Fixed Costs of Labor
- FCE: Fixed Costs of Electricity
- VCE: Variable Costs of Electricity
- VCG: Variable Costs of changing GAC units
- VCS: Variable Costs of Sampling

future costs are discounted to yield Net Present Value

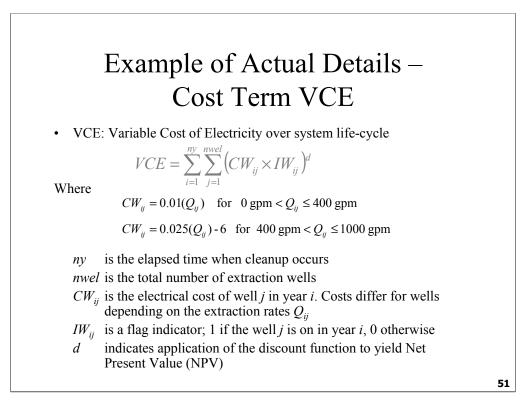
Umatilla: Cost Terms

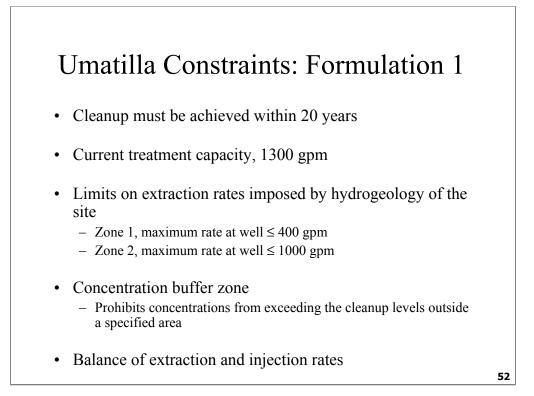
- Up-Front costs
 - New well and piping: \$75K
 - Put EW-2 in service: \$25K
 - New recharge basin: \$25K
 - New GAC unit (325 gpm): \$150K
- Fixed Annual Costs (each year until cleanup)
 - Labor (fixed): \$237K/yr
 - Electric (fixed): \$3.6k/yr

• Variable Costs Depending on Solution (complicated)

- Electric based on pump rate at specific wells
- GAC changeout based on influent concentration
- Sampling costs due to plume area

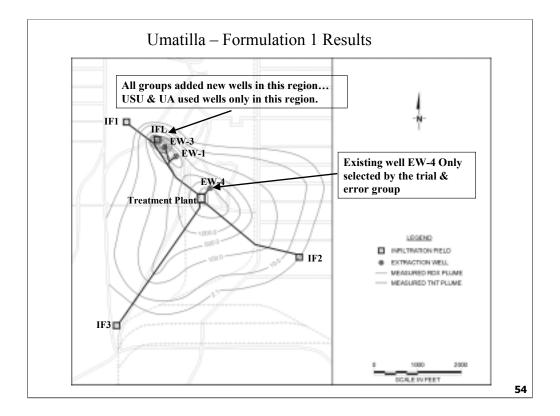
Details: Variable Electric Costs **50**

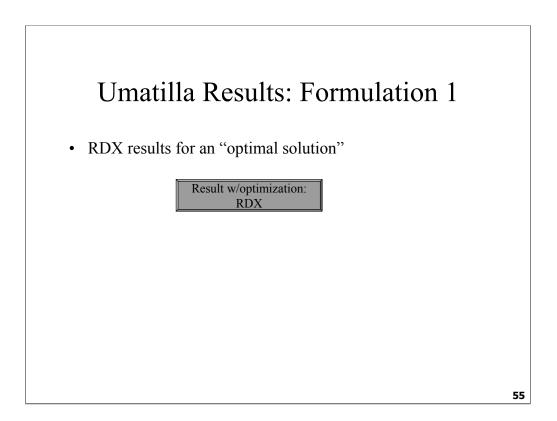


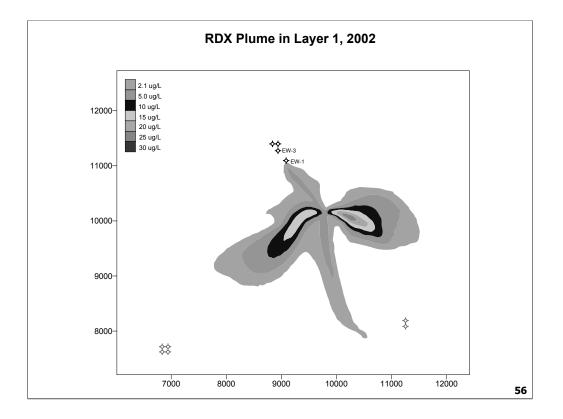


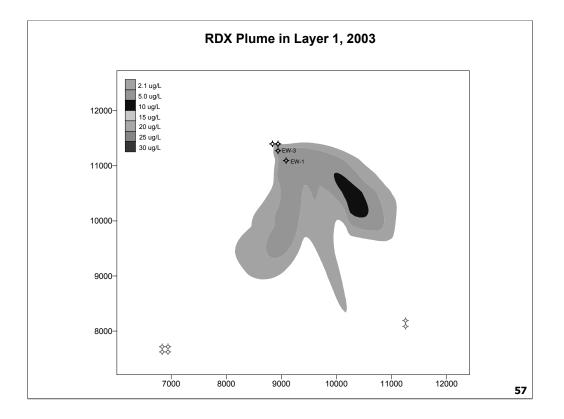
Umatilla Results: Formulation 1

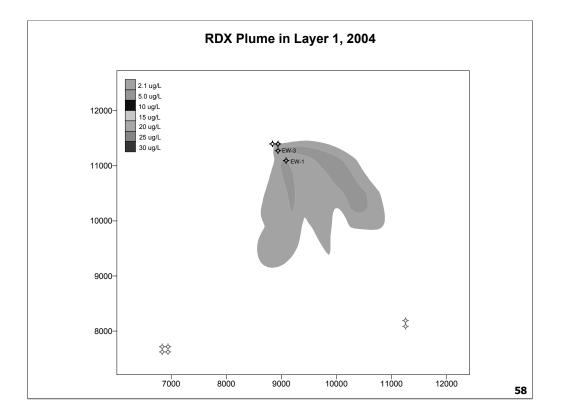
	Transport O Algor	Trial-&-Erro	
Objective Function Value	\$1.66M	\$1.66M	\$2.23M
# new wells	2	2	2
# new recharge basins	0	0	1
# new GAC units	N/A	N/A	N/A
RDX Cleanup (yrs)	4	4	6
TNT cleanup (yrs)	4	4	6
Improvement using	transport	optimizat	tion: ~26%
R	esults Summar	v	

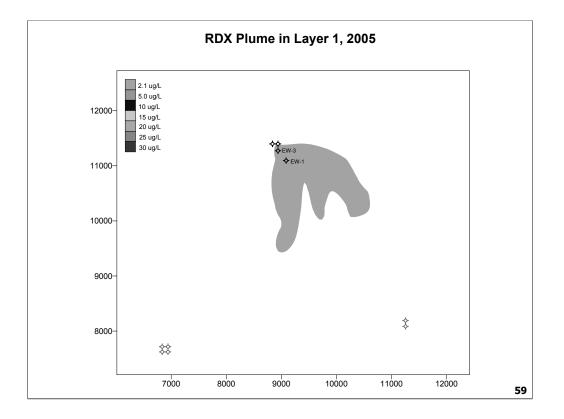


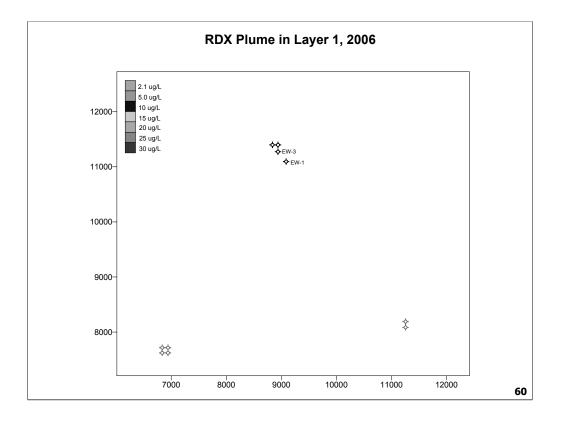


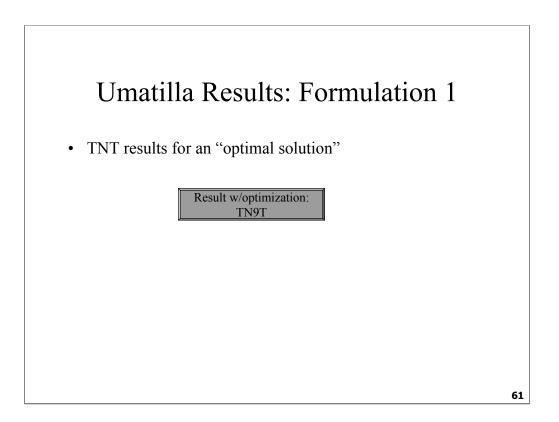


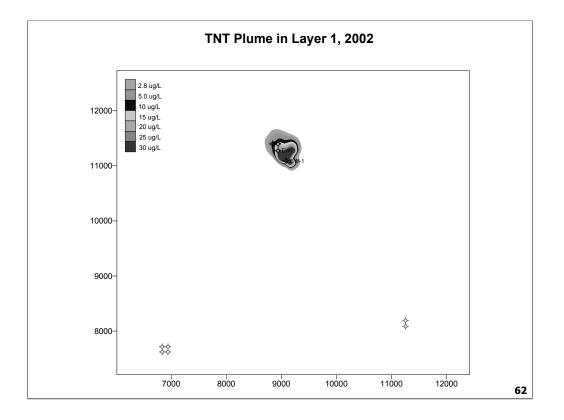


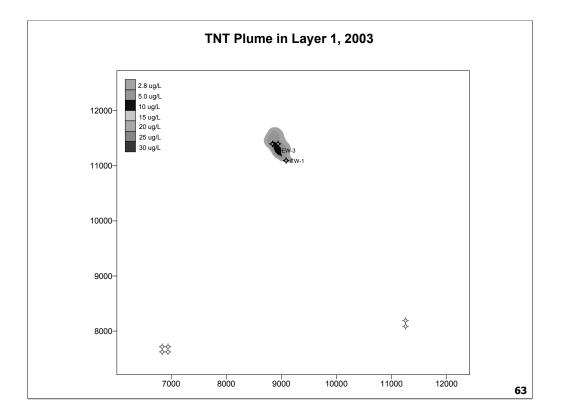


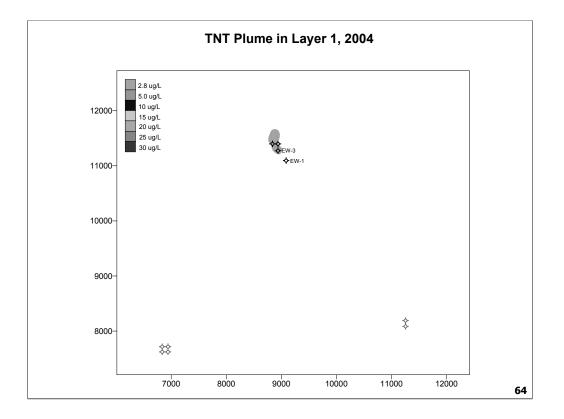


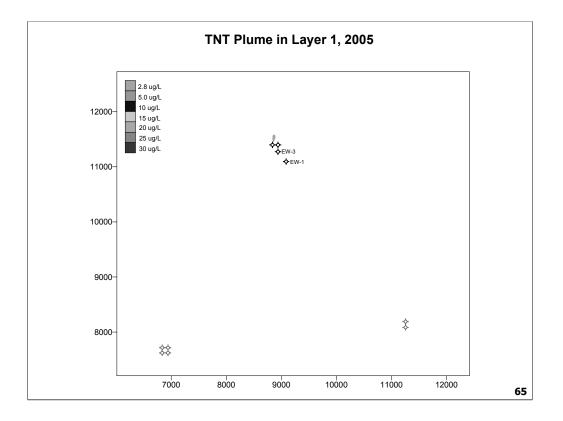


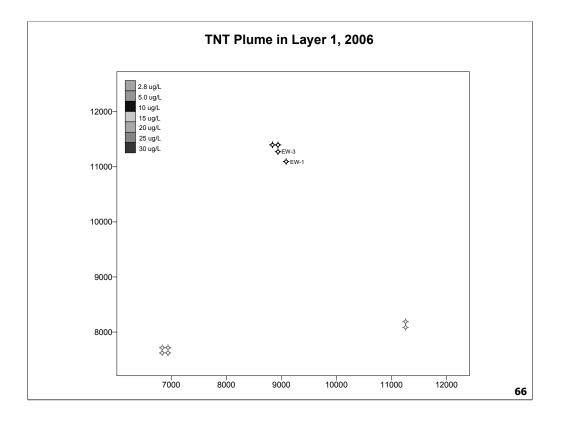


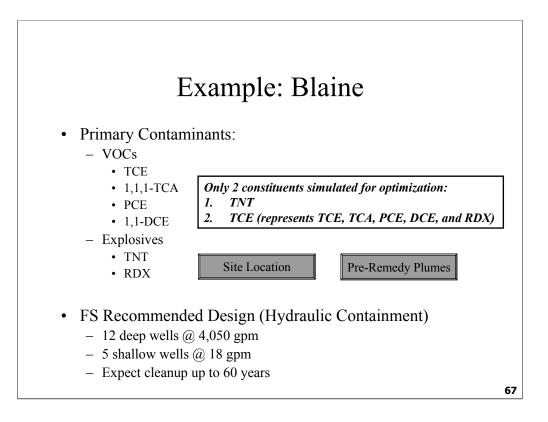


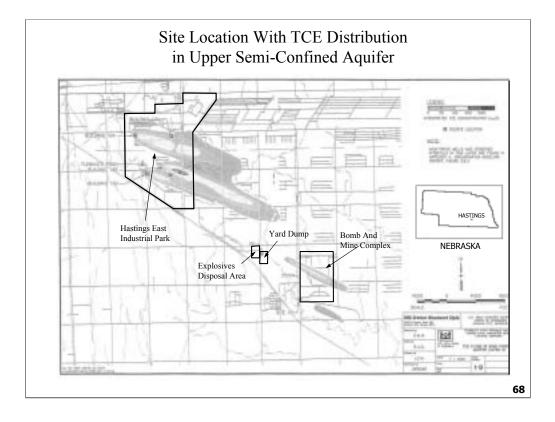


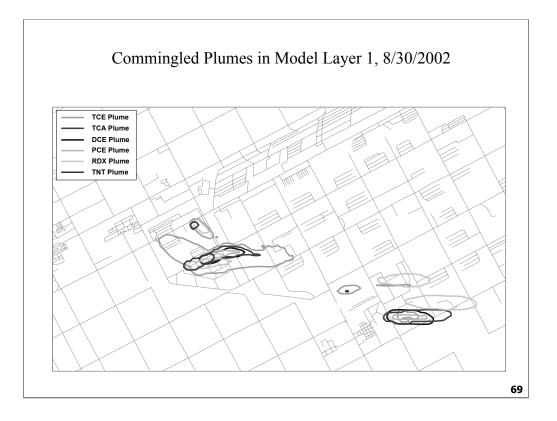


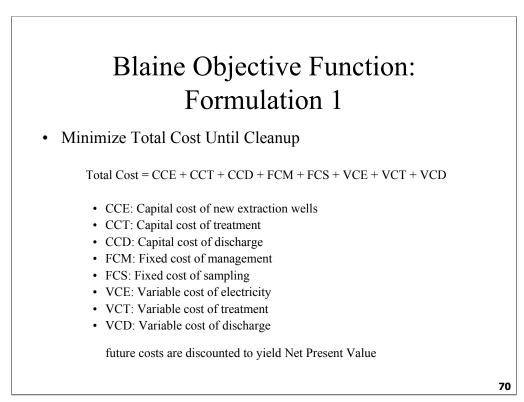












Blaine: Cost Terms

- Up-Front Costs
 - New extraction well: \$400K
 - Capital Treatment: \$1.0K/gpm
 - Capital Discharge: \$1.5K/gpm
- Fixed Annual Costs (each year until cleanup)
 - Fixed O&M: \$115K/yr
 - Sampling: \$300K/yr

• Variable Costs

- Electric: \$0.046K/gpm/yr
- Treatment: \$0.283K/gpm/yr
- Discharge: \$0.066K/gpm/yr

Blaine Constraints: Formulation 1

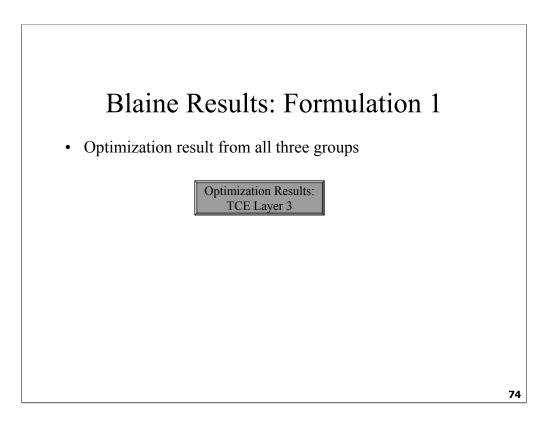
- Cleanup within 30 years
- Containment limits to prevent plume spreading
- Limits on extraction well rates
 - Well screens one model layer: 350 gpm
 - Well screens two model layers: 700 gpm
 - Well screens three model layers: 1050 gpm
- Restricted areas where no wells allowed
- Remediation wells not allowed in same cells as irrigation wells
- No dry cells allowed

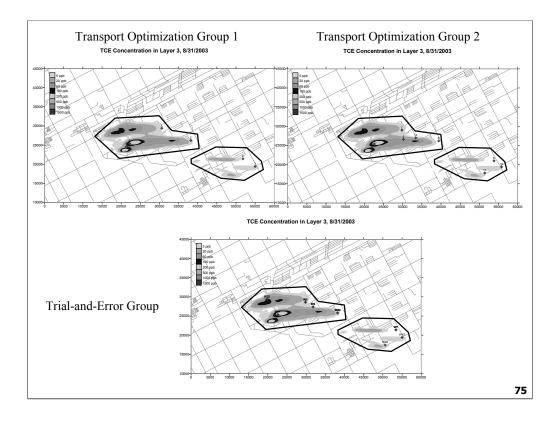
Blaine Results: Formulation 1

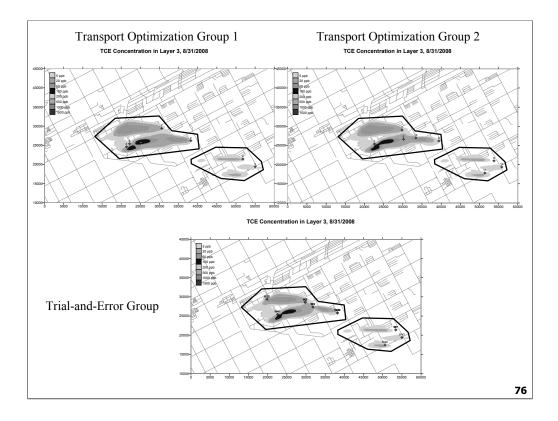
Objective Function Value	Transport Optimization Algorithms		Trial-&-Error	
	\$45.28M	\$40.82M	\$50.34M	
# New Extraction Wells	15	10	8	
Pumping Rate by Management Period	1968 gpm 3104 gpm 3356 gpm 3700 gpm 3750 gpm 3750 gpm	2486 gpm 2632 gpm 2644 gpm 2752 gpm 3306 gpm 3378 gpm	3995 gpm 3975 gpm 3995 gpm 3995 gpm 3925 gpm 3105 gpm	
Elapsed Years Until Cleanup for TCE	30	30	30	
Elapsed Years Until Cleanup for TNT	30	29	25	

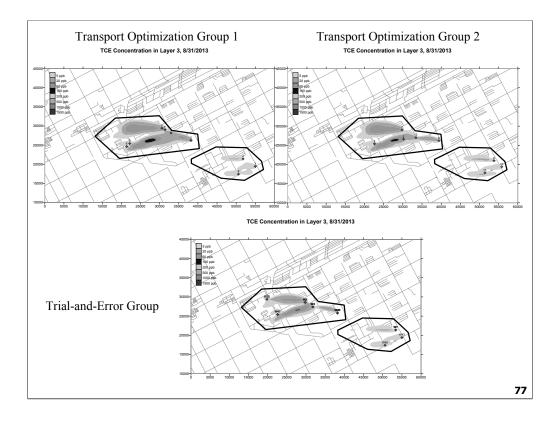
Improvement using transport optimization: ~10 - 20%

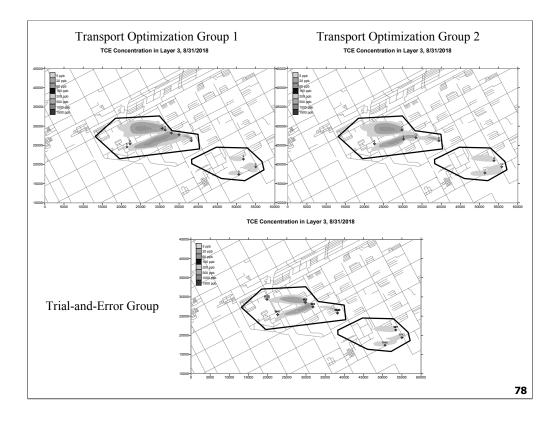
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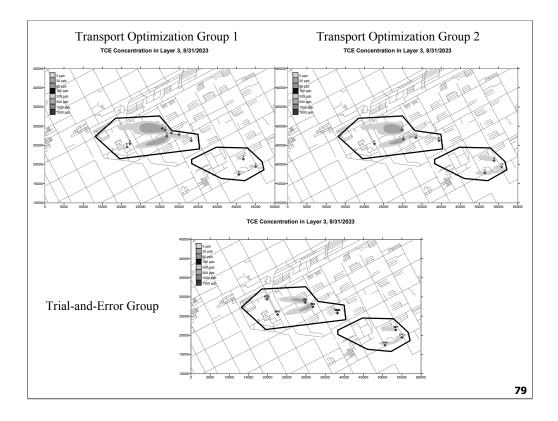


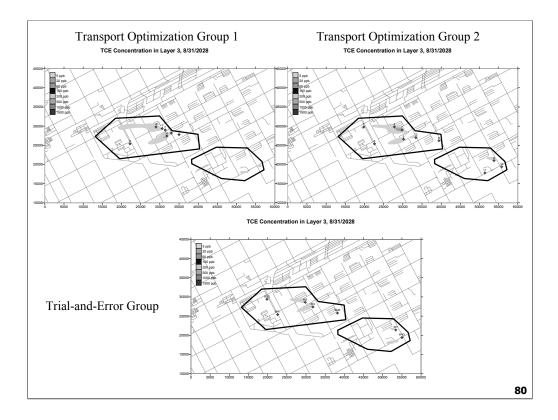


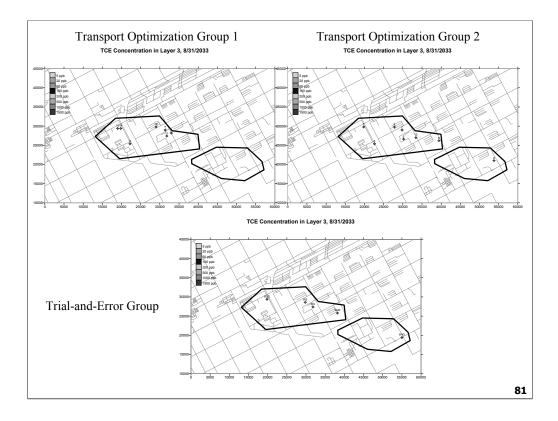


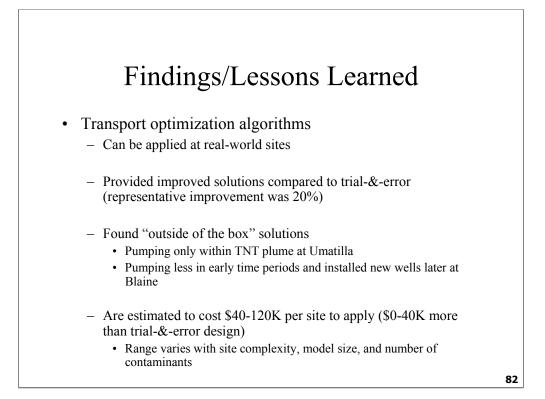






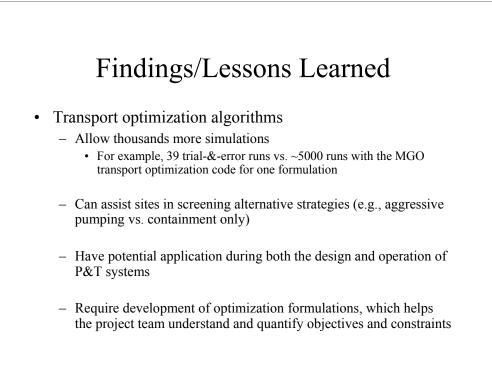






Typical Costs Estimated for A Transport Optimization Analysis

Costs Associated With Basic Items*				
	Low Cost	Typical Cost	High Cost	Expected Duration
Site visit and/or transfer information	\$2,500	\$5,000	\$10,000	1-2 months
Develop 3 optimization formulations	\$5,000	\$10,000	\$15,000	1-2 months
Solve optimization formulations	\$25,000	\$40,000	\$60,000	2-4 months
Prepare report and/or present results	\$5,000	\$15,000	\$25,000	1 month
Project management	\$2,500	\$5,000	\$10,000	NA
Total	\$40,000	\$75,000	\$120,000	5-9 months
Costs Assoc	iated With Op	tional Items		•
	Low Cost	Typical Cost	High Cost	Expected Duration
Update and improve simulation models	0	\$20,000	\$50,000	Add 1-3 months
Up to 3 additional formulations	\$15,000	\$25,000	\$40,000	Add 2-3 months
		620.000	\$30,000	Add 1-2 months
Additional constituent simulated	\$10,000	\$20,000	\$50,000	Add 1-2 monuis



Technology Transfer Activities

• Project Website

(http://www.frtr.gov/optimization/simulation/transport/general.html)

- Optimization codes and documentations
- Final project report
- Modeling files for each demonstration site
- Sample optimization code input and output files for Blaine
- Powerpoint animations illustrating results for Each group

• Training

- 2-day workshop 2004
- Case Study / Site Follow-Up
 - Through summer 2004

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