

# Remedial Design Modeling of Explosives and Propellants in Groundwater

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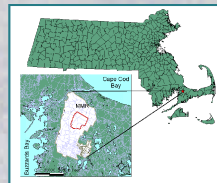
## ABSTRACT

Numerical fate-and-transport modeling of the Cape Cod aquifer is being conducted at the Massachusetts Military Reservation to support remediation of explosive and propellant compounds. Simulations involve nested finite-difference models calibrated to well water levels, stream flows, and plume configurations, which are then applied to design optimization of pump-and-treat systems for multiple constituents-of-concern with different transport properties and multiple cleanup criteria. The modeling methodology incorporates both regional boundary stresses and local scale heterogeneities in a full 3-dimensional steady-state representation of the high permeability unconfined aquifer system.

For each plume, modeling objectives were to: 1) confirm the appropriateness of the underlying conceptual hydrogeologic model, 2) define a source term associated with particulate leaching in soil, 3) assess future plume configuration and its potential to impact local water supply wells, and 4) conduct mass capture analysis to assess various remedial alternatives. Simulation results have: 1) provided a basis for understanding the relative transport characteristics of individual explosive compounds, their breakdown products, and related propellant compounds, 2) demonstrated particle track-based optimization approaches provide a significant computational advantage over conventional trial-and-error modeling for remediation system design, and 3) supported a detailed cost/benefit analysis for selection of an effective flexible long-term cleanup solution to provide for range sustainability and meet regulatory agency priorities. Final implementation of the selected pump-and-treat designs and subsequent collection of system performance data will provide for future model validation. These data may also be used to improve simulation accuracy, so the remediation system can be further optimized during the maintenance and operation phase, and ultimately to support monitoring plan effectiveness and final closure.

## Problem

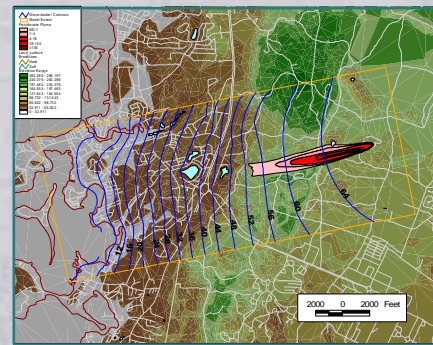
Residual explosive and propellant materials in training range soils have contaminated groundwaters and now require aggressive cleanup to meet regulatory standards in reasonable timeframes. Numerical modeling is a robust and commonly used tool for groundwater pump-and-treat system design. However, typical trial-and-error methods using fate & transport modeling are computationally intensive, subject to significant uncertainty in input parameters, and may not always yield a 'best' solution for the conditions and criteria.



Massachusetts Military Reservation (MMR)



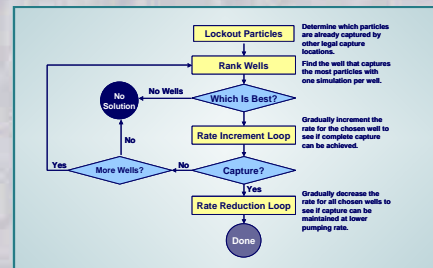
Typical UXO



Subregional Groundwater Model Design

## Methodology

An alternative approach has been developed using Weighted Particle Track Optimization (WPTO), which automates system design using simpler and faster particle track modeling. Weighted particles are assigned to the model domain representing plume mass and the time required for capture to reach a given concentration criteria. Retardation processes are accounted for by adjusting the capture times after Duetsch (1997). The WPTO algorithm then iteratively tries every allowable combination of well locations to best 'capture' the weighted particles within specified time and success criteria.



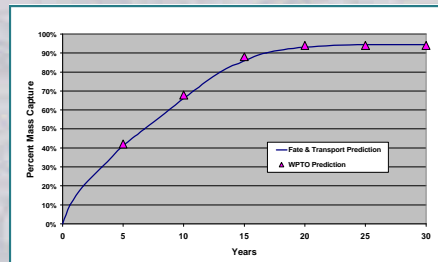
Weighted Particle Track Optimization (WPTO) Algorithm

$$n = \ln(C_0/C_s) / \ln(1-1/R) \quad (\text{Duetsch 1997})$$

where:  
 n = number of pore volumes required removing to achieve standard  
 C<sub>s</sub> = groundwater standard  
 C<sub>0</sub> = initial concentration  
 R = retardation factor

Contaminant	Initial Concentration (log/L)	Groundwater Standard (log/L)	Retardation Factor	Pore Volumes Requiring Removal	Required Days to Remove 1 Pore Volume for 10-Year Cleanup
Perchlorate	500	0.35	1	350	350
RDX	220	0.25	1.2	318	964.6
TNT	5.2	0.25	8.658	24.7	147.6
2,4-DNT	0.52	0.25	2.958	1.8	2058.9

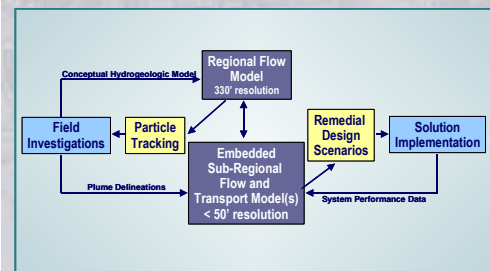
Plume Pore Volume Weighting



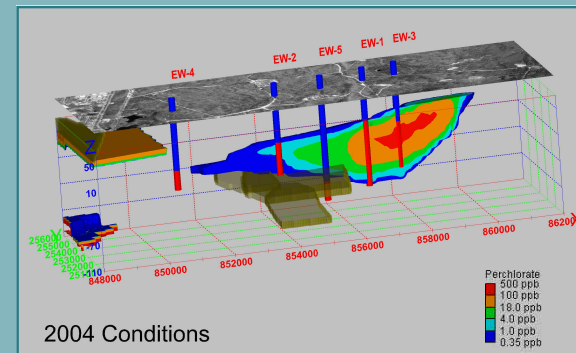
WPTO vs Fate and Transport Model Comparison

## Advantages

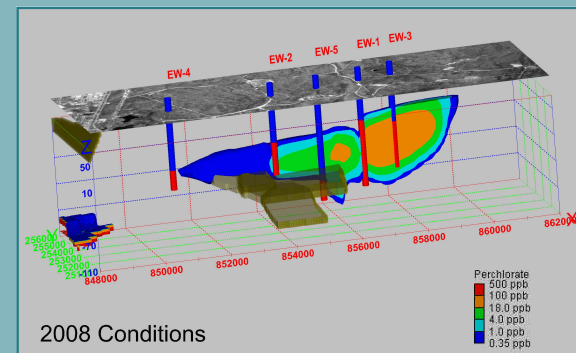
- Yields optimal well configuration and pumping rates for any mass distribution and combination of target concentration and time-to-cleanup criteria.
- A single WPTO design run can be completed in a time equivalent to 2-3 trial-and-error fate & transport simulations.
- Multiple contaminants with different cleanup criteria can be considered simultaneously.
- Drawdown limitations and mass conservative reinjection are dynamically accounted for.
- Particle weighting can also be used to impose a variety of other design constraints and preferences (i.e. exclusion zones, relative cost of well locations)



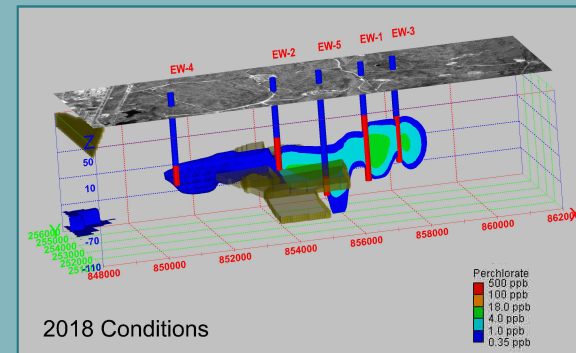
Design Modeling Process



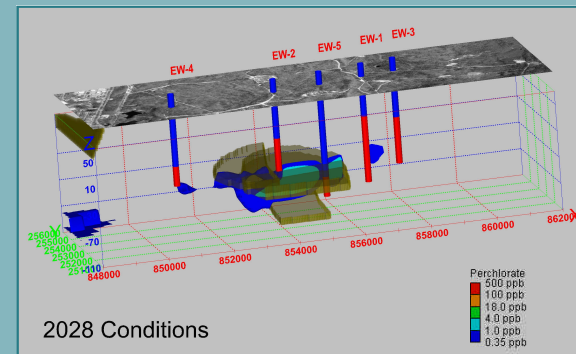
2004 Conditions



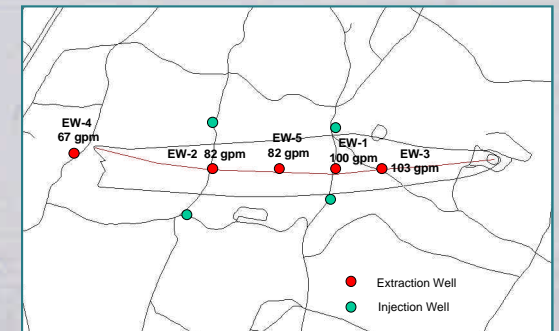
2008 Conditions



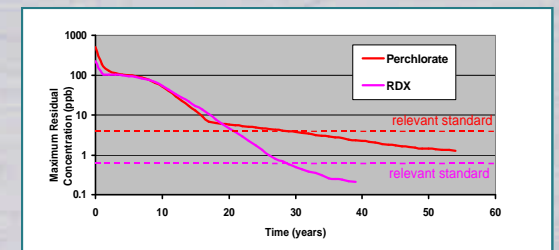
2018 Conditions



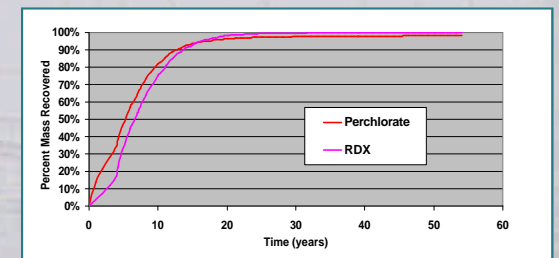
2028 Conditions



Pump and Treat Wellfield Design



Maximum Residual Concentration



Percent Mass Recovered

## Conclusion

Starting with a calibrated flow model, the WPTO method was verified against conventional fate & transport modeling, and then used to develop multiple extraction well network designs to meet mandated cleanup goals. Designs were shown to be highly effective, reaching 90% capture within 15 years followed by a phase of rapidly diminishing returns. Both well number and cumulative pumping rate were effectively minimized, representing the most cost-effective solution for groundwater cleanup. Further validation of the method and proposed design will hopefully be achieved through long-term system performance monitoring of the proposed design.

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