

# Fate and Transport Modeling of Explosives and Propellants in the Vadose Zone



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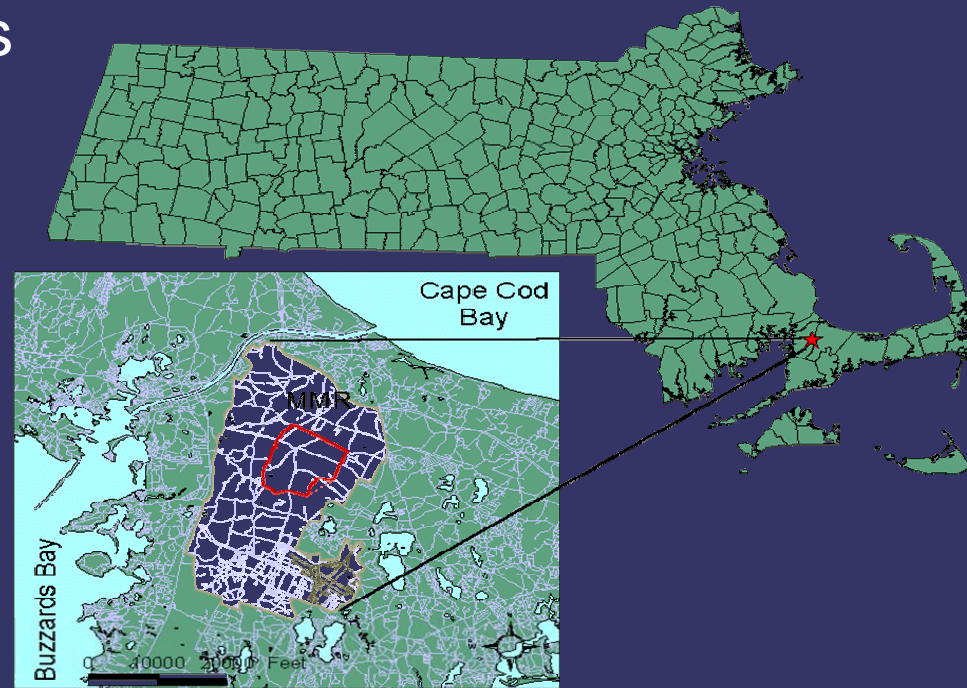
Diane Curry (AMEC)

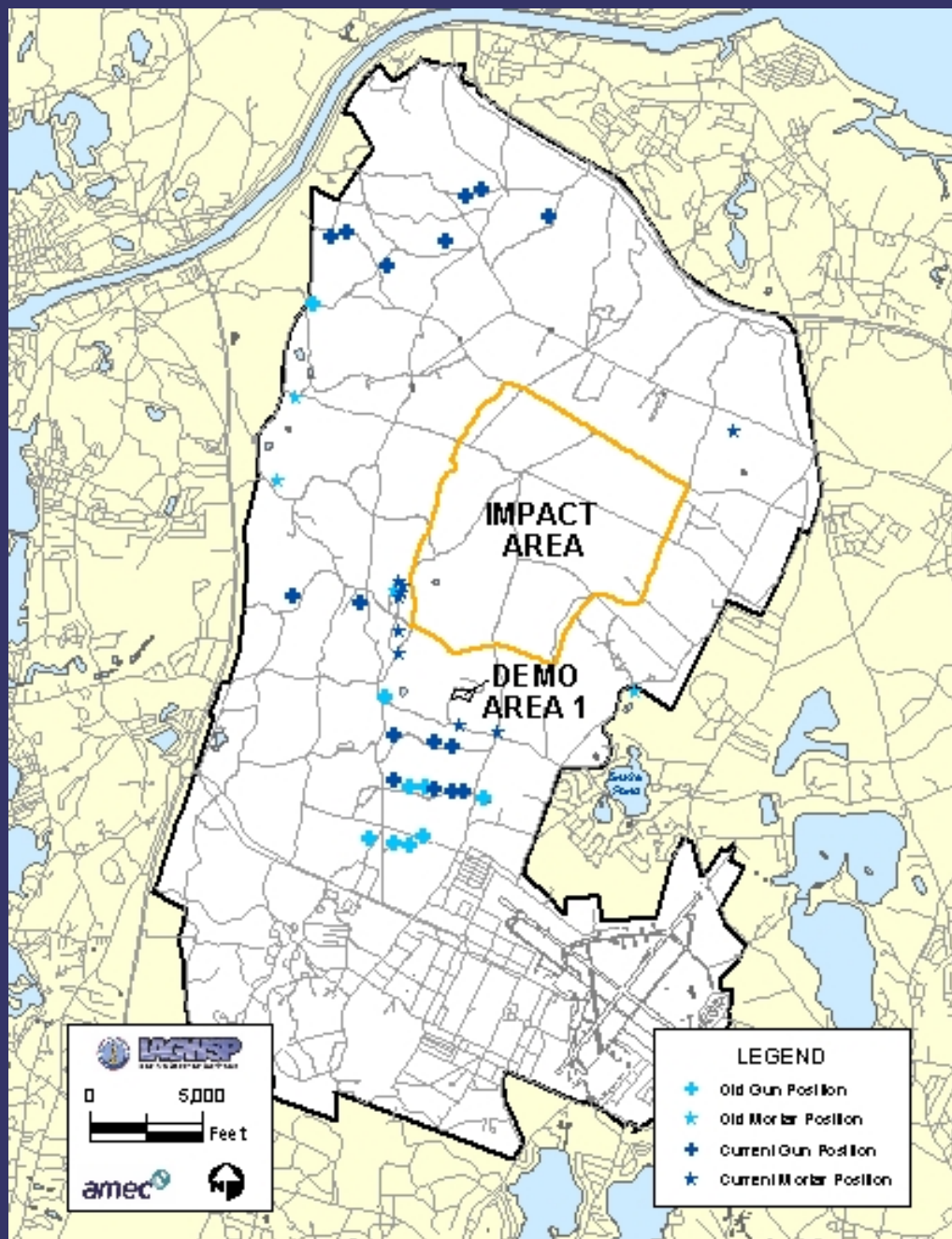
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University of Massachusetts Amherst, October 23 2002**

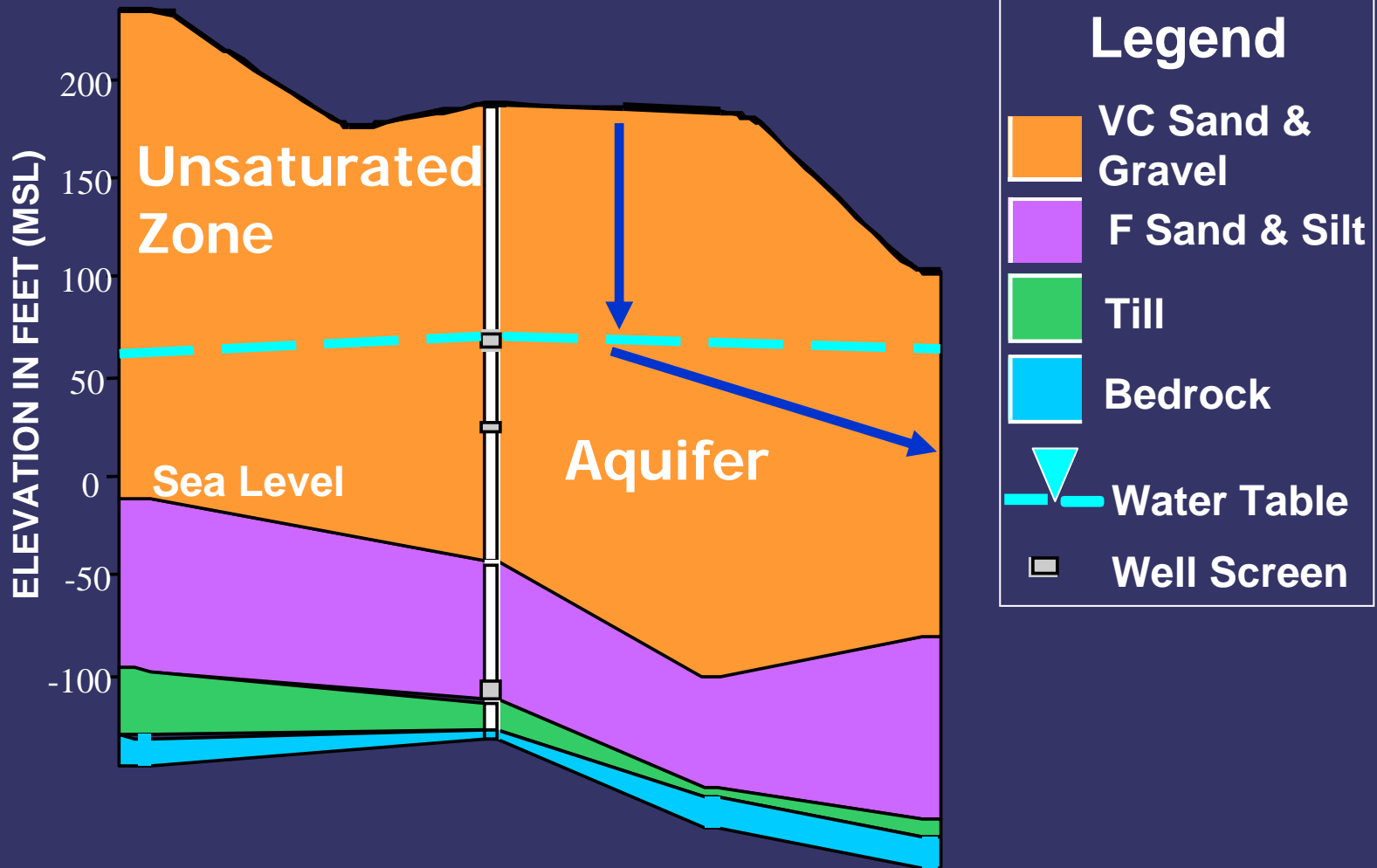
# Massachusetts Military Reservation - Site History

- The entire reservation covers nearly 22,000 acres
- Camp Edwards occupies northern 15,000 acres
- Impact Area - 2,200 acres
- Portions used since 1911
- USEPA banned artillery and mortar fire in 1997





# Site Lithology



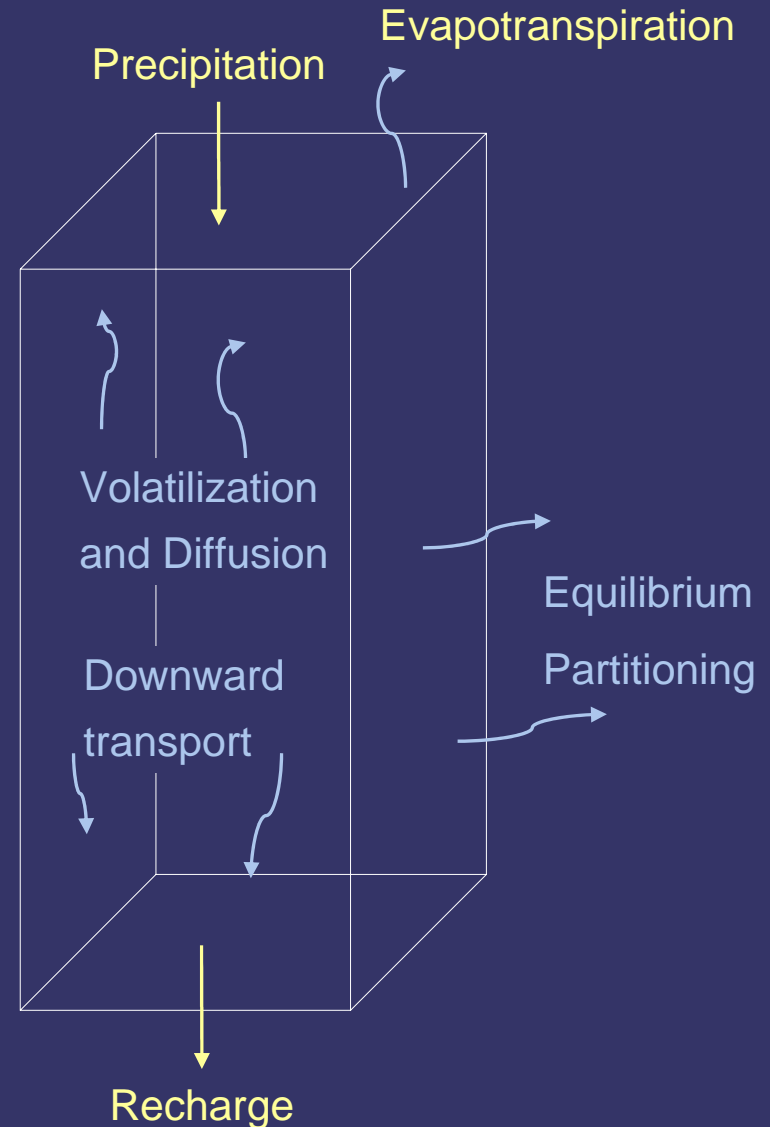
## Model Objectives

- Determine the likelihood that explosives would migrate to the water table
- Determine the appropriate soil action level for explosives that migrate to the water table.



# Seasonal Soil Compartment Model (SESOIL)

- One dimensional vertical transport model for unsaturated zone
- Simulates water movement, sediment transport and pollutant fate and transport



## SESOIL Model Development for MMR

- Model divided into 4 layers with 10 sublayers each
- Meteorological Data from Hatchville, MA Station
- Site-specific soil properties
- Chemical constants

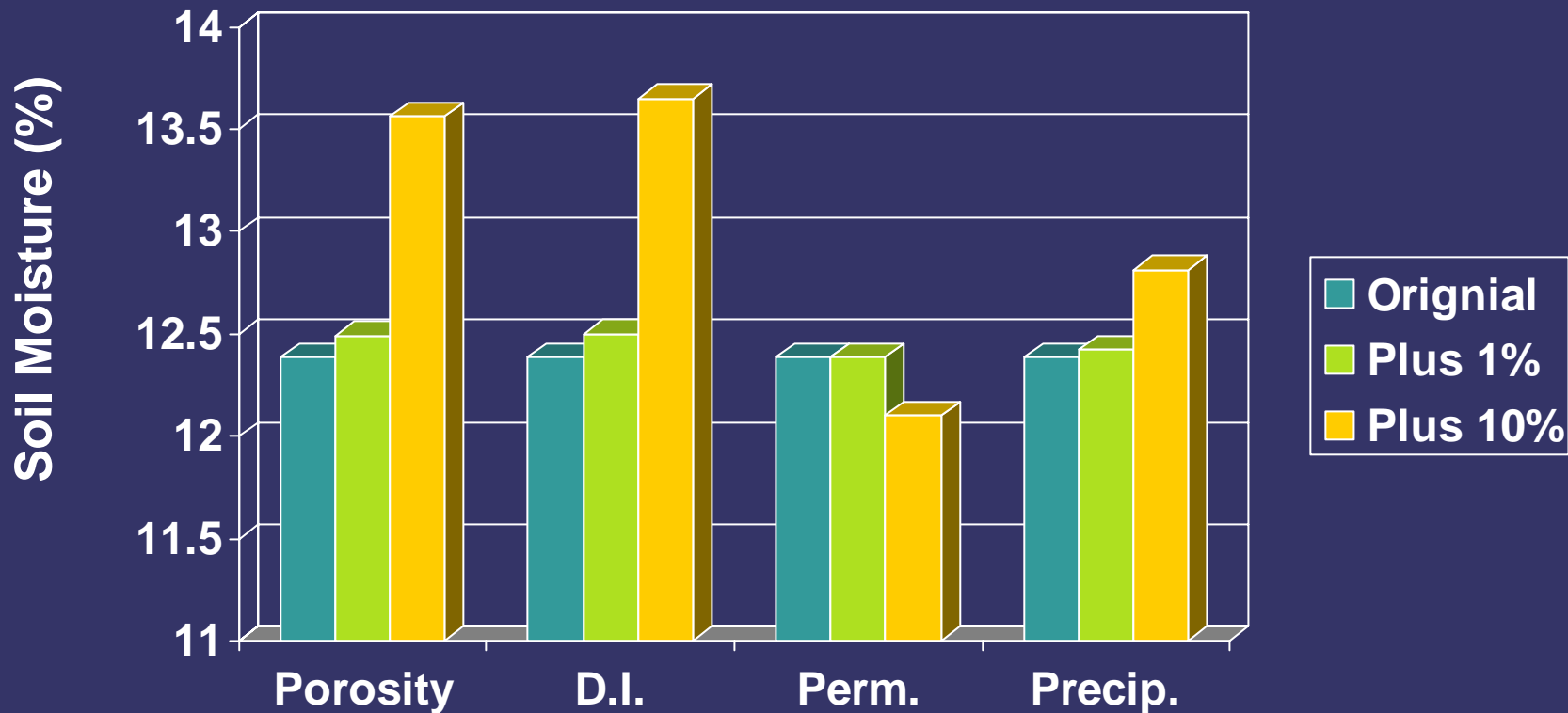


# Model Calibration

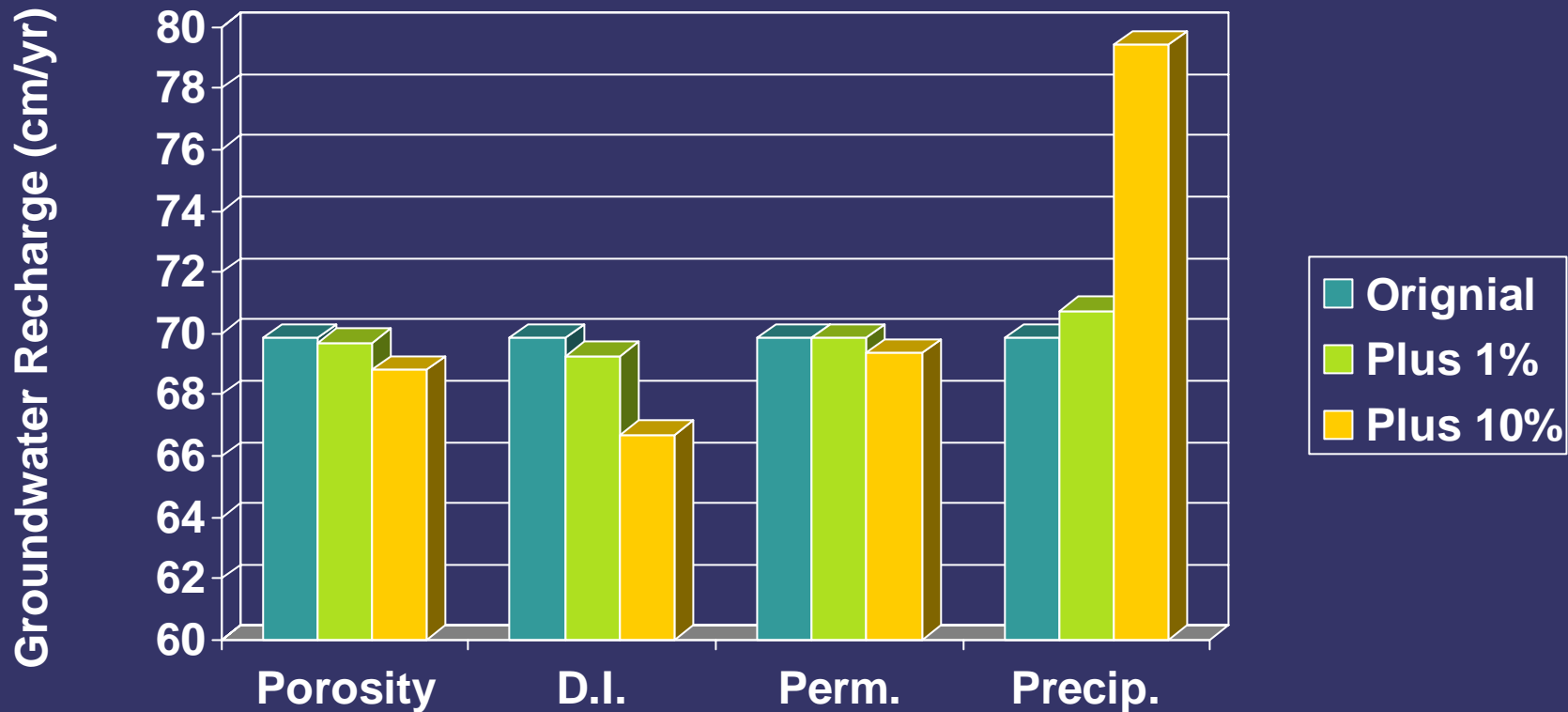
Parameter	Acceptable Range	Calibrated Value
Variables		
Effective Porosity	0.25 to 0.45	0.43
Disconnectedness Index	3.7 to 4.0	3.9
Intrinsic Permeability	1.0E-08 to 2.0E-09 cm <sup>2</sup>	3.8E-09 cm <sup>2</sup>
Calibration Targets		
Soil Moisture	12.2 to 12.4%	12.3%
Evapotranspiration	59 to 73 cm/yr	46.5 cm/yr
Recharge	45 to 55 cm/yr	69.8 cm/yr
Surface Runoff	0 cm/yr	0.1 cm/yr



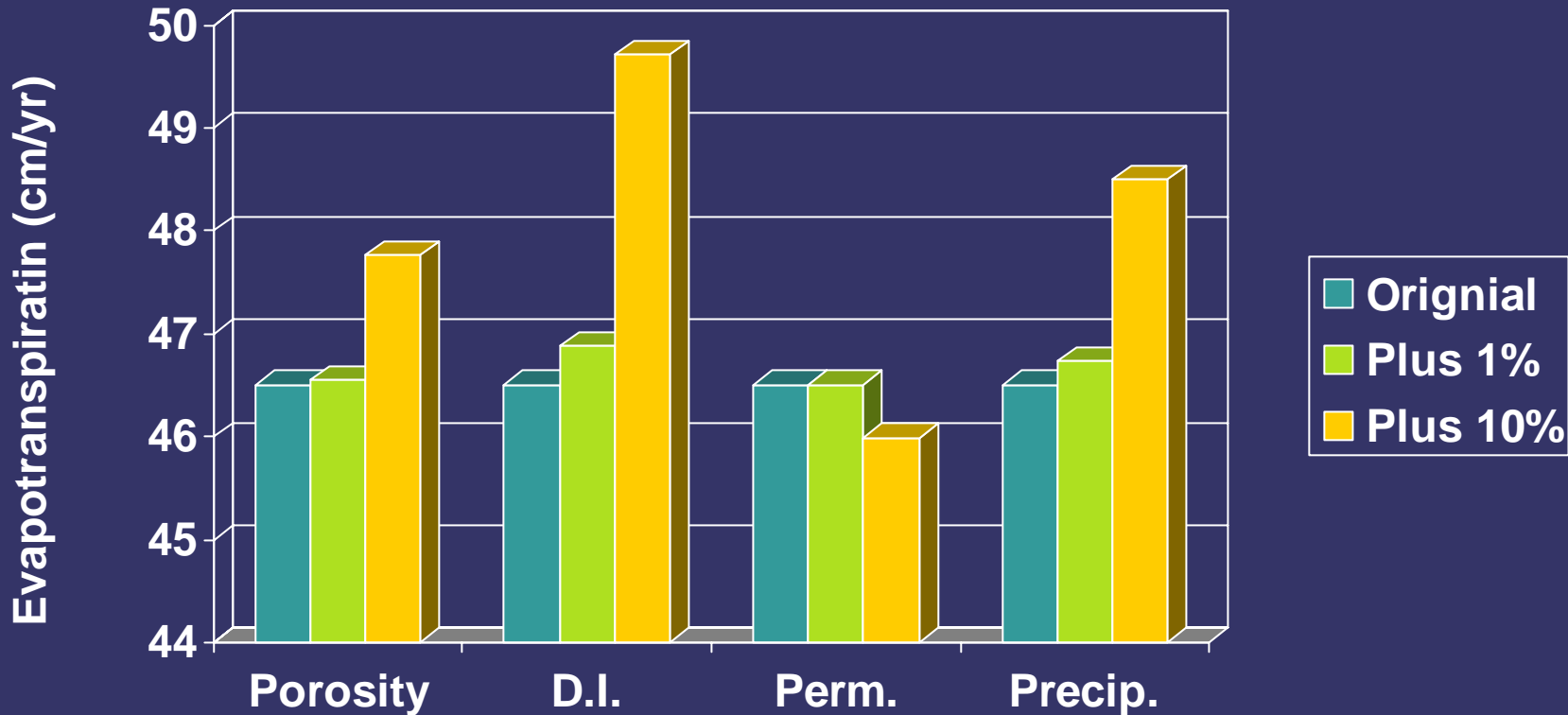
# Sensitivity Analysis – Effect on Soil Moisture



# Sensitivity Analysis – Effect on Recharge



# Sensitivity Analysis – Effect on Evapotranspiration



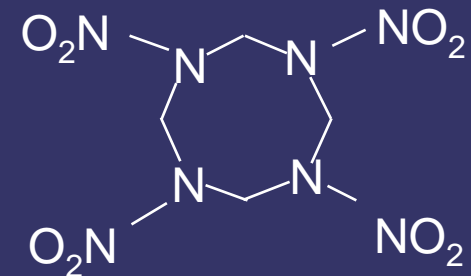
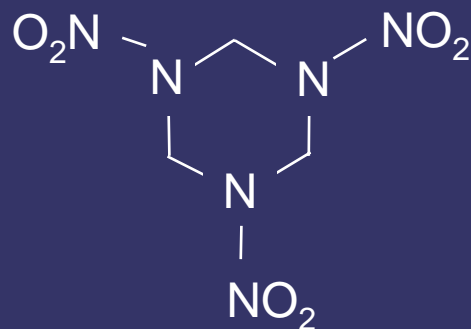
# Demo 1



## Model Setup for Demolition Area 1 (Demo 1)

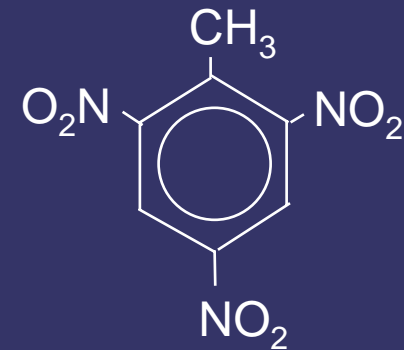
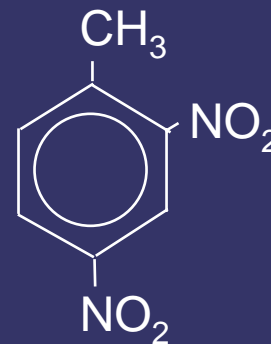
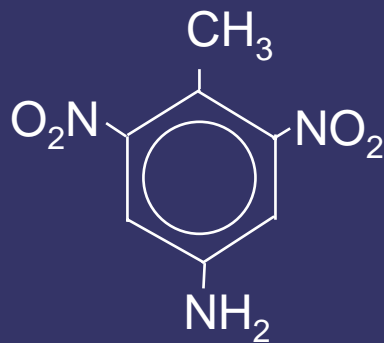
- Depth of Soil Contamination = 1 ft (0.3 m)
- Area of Soil Contamination = 4 acre (1.62 Ha)
- Depth to water table = 40 ft (12.2m)
- Organic carbon = 0.5% (0-12 ft) and 0.01% (12-40 ft)
- Bulk Density = 1.8 g/ml
- Time = 100 years

# Model Input - Chemical Properties



	<b>RDX</b>	<b>HMX</b>
Solubility (mg/L)	38.4	6.6
Henry's Law Constant (m <sup>3</sup> -atm/mole)	1E-04	1E-04
Koc (L/kg)	70.8	631

# Model Input - Chemical Properties



	<b>4-Amino-2,6-DNT</b>	<b>2,4-DNT</b>	<b>TNT</b>
Solubility (mg/L)	2,800	270	124
Henry's Law Constant (m <sup>3</sup> -atm/mole)	3.71E-09	9.26E-08	4.9E-09
Koc (L/kg)	59.2	94.6	1,585

## Results

Compound	Time to Reach Groundwater (years)	K <sub>oc</sub> (L/kg)
TNT	50	1,585
HMX	17	631
2,4-DNT	5	94.6
RDX	4	70.8
2,6-DNT	4	68.9
4-Amino-2,6-DNT	4	59.2
2-Amino-4,6-DNT	4	59.2



# Use of SESOIL to Derive Soil Clean-Up Standards

- SESOIL developed for EPA in 1981
- Used by NJDEP, ORDEQ, HDOH, MADEP, WIDNR



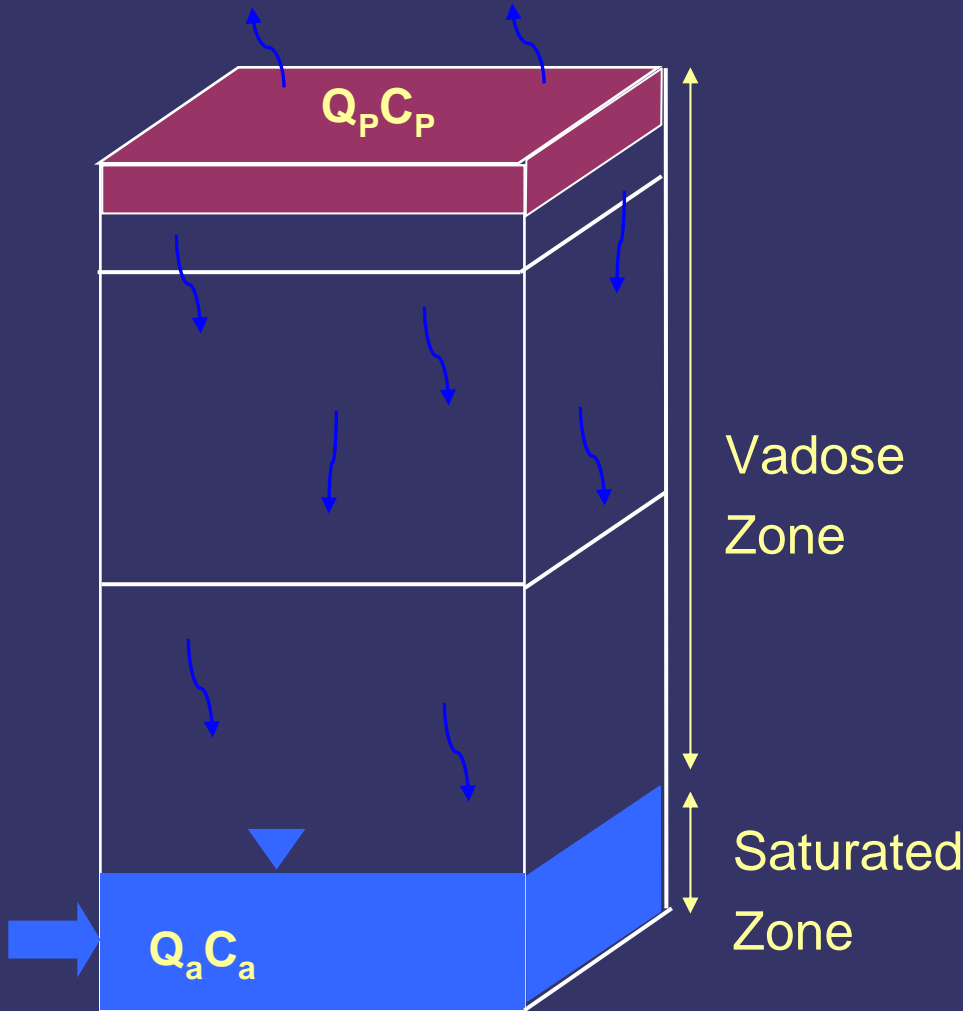
# RDX Leaching Based Soil Standards

	RDX (ug/kg)
MMR Soil Screening Level (EPA, 2001)	0.11
Draft S-1/GW-1 Standard (MADEP, 2001)	700

## Approach for RDX

- Utilize SESOIL and Summers Groundwater Mixing Zone models
- Perform transport calibration so model predicts average observed groundwater concentration
- Use calibrated model to calculate soil concentration that results in 2 ug/L RDX in groundwater (EPA Lifetime Health Advisory)

# SESOIL + Summers Model



$Q_p$  = Flow through vadose zone

$C_p$  = Soil concentration

$Q_a$  = Flow through aquifer

$C_a$  = Groundwater concentration

$$C_{GW} = \frac{[(Q_p C_p) + (Q_a C_a)]}{(Q_a + Q_p)}$$

## Calibration Approaches

- Vary source size to match average groundwater concentration
- Vary initial soil concentration to match average groundwater concentration
- Vary source size until mass flux predicted by SESOIL = mass flux predicted by saturated zone model
- Vary source size until mass flux predicted by SESOIL = observed mass flux, based on plume mass, age

## Results

- AFCEE for CS-19 Site: 5.5 mg/kg
- INEEL: 0.2 to 2.0 mg/kg (currently under review)
- AMEC: 0.84 to 1.75 mg/kg
  - Preliminary value
  - Not reviewed by EPA
  - Sensitivity analysis required



## Sensitivity Analysis

- Not yet completed; model sensitive to assumptions of:
  - Source size
  - Number of sublayers
  - Source thickness
  - Mixing zone thickness
  - Mixing zone length
  - Initial soil concentration

## Thanks

- Impact Area Groundwater Study Program
- US Army Corp of Engineers – New England District
- Air Force Center for Environmental Excellence