

ENVIRONMENTAL FATE AND TRANSPORT MODELING OF EXPLOSIVES IN THE UNSATURATED ZONE



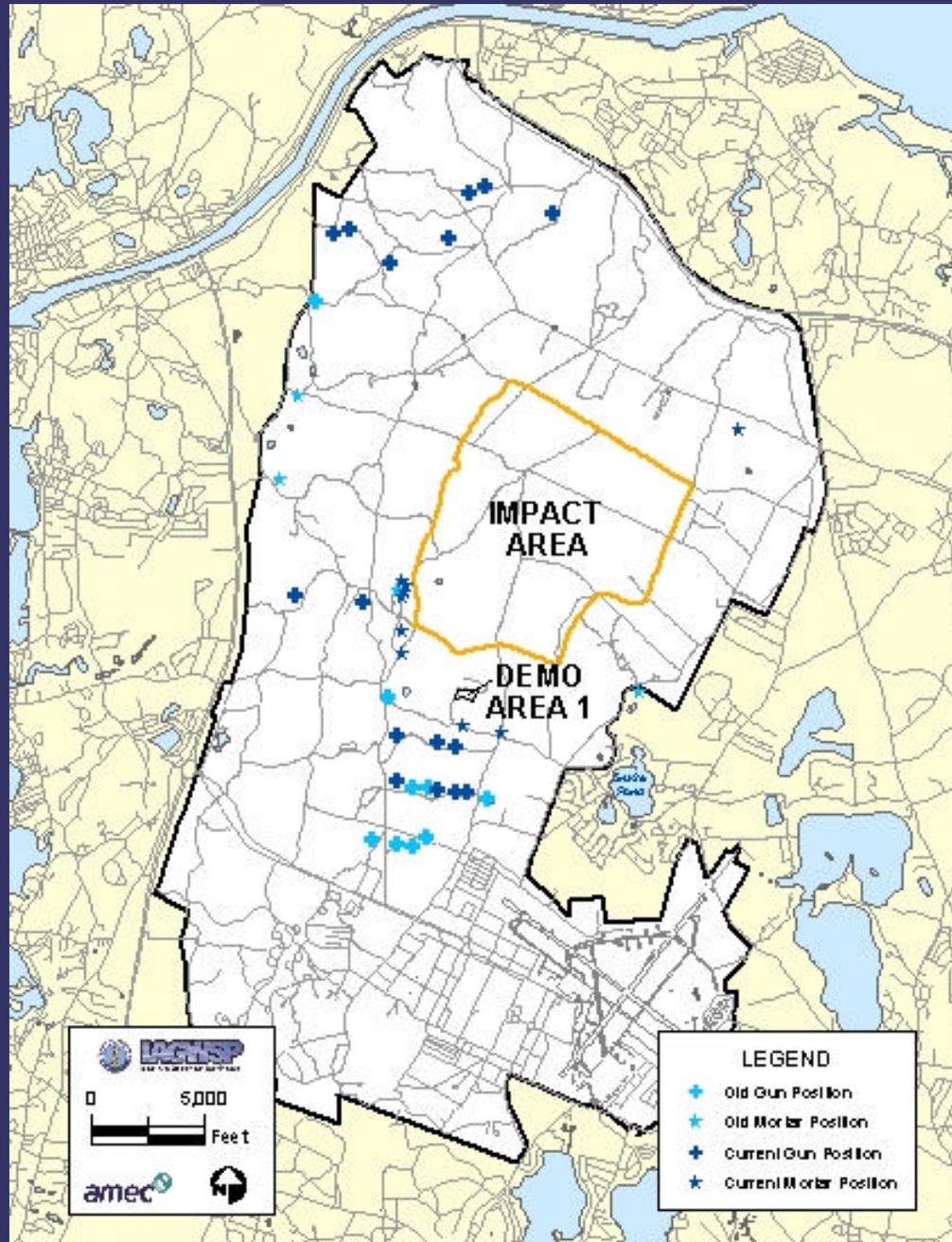
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MODEL OBJECTIVES

- 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.

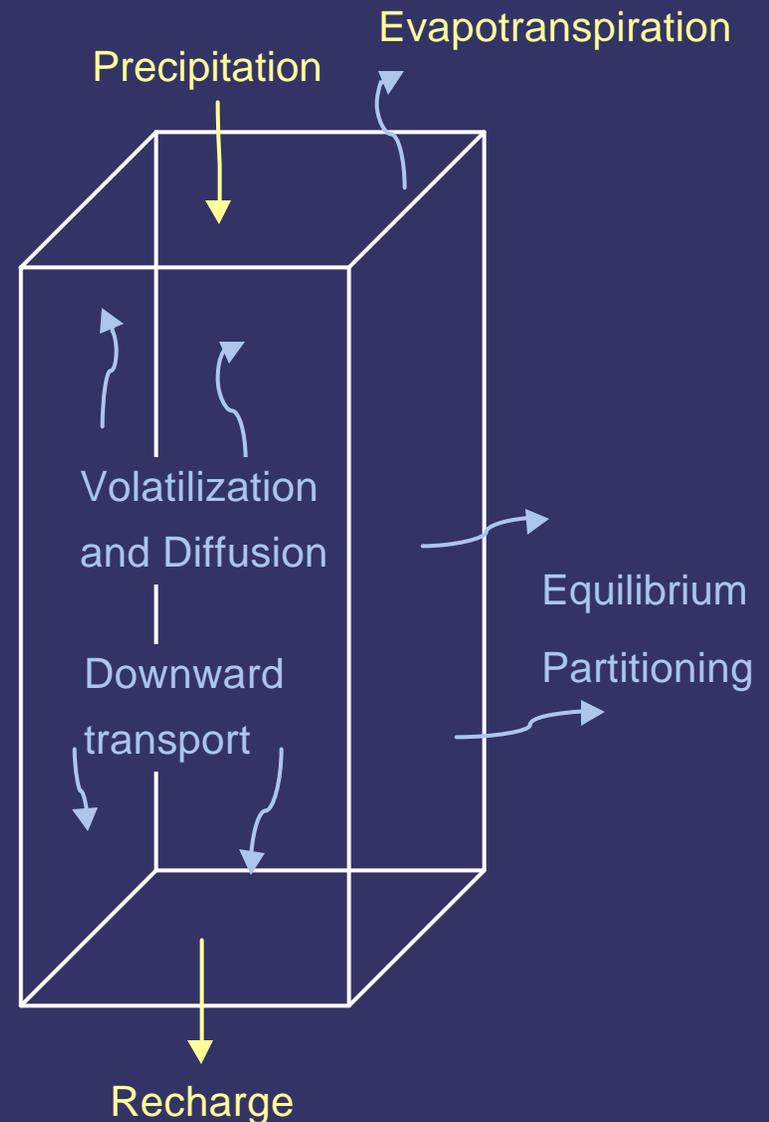




SEASONAL SOIL COMPARTMENT MODEL (SESOIL)



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



SESOIL MODEL DEVELOPMENT FOR MMR

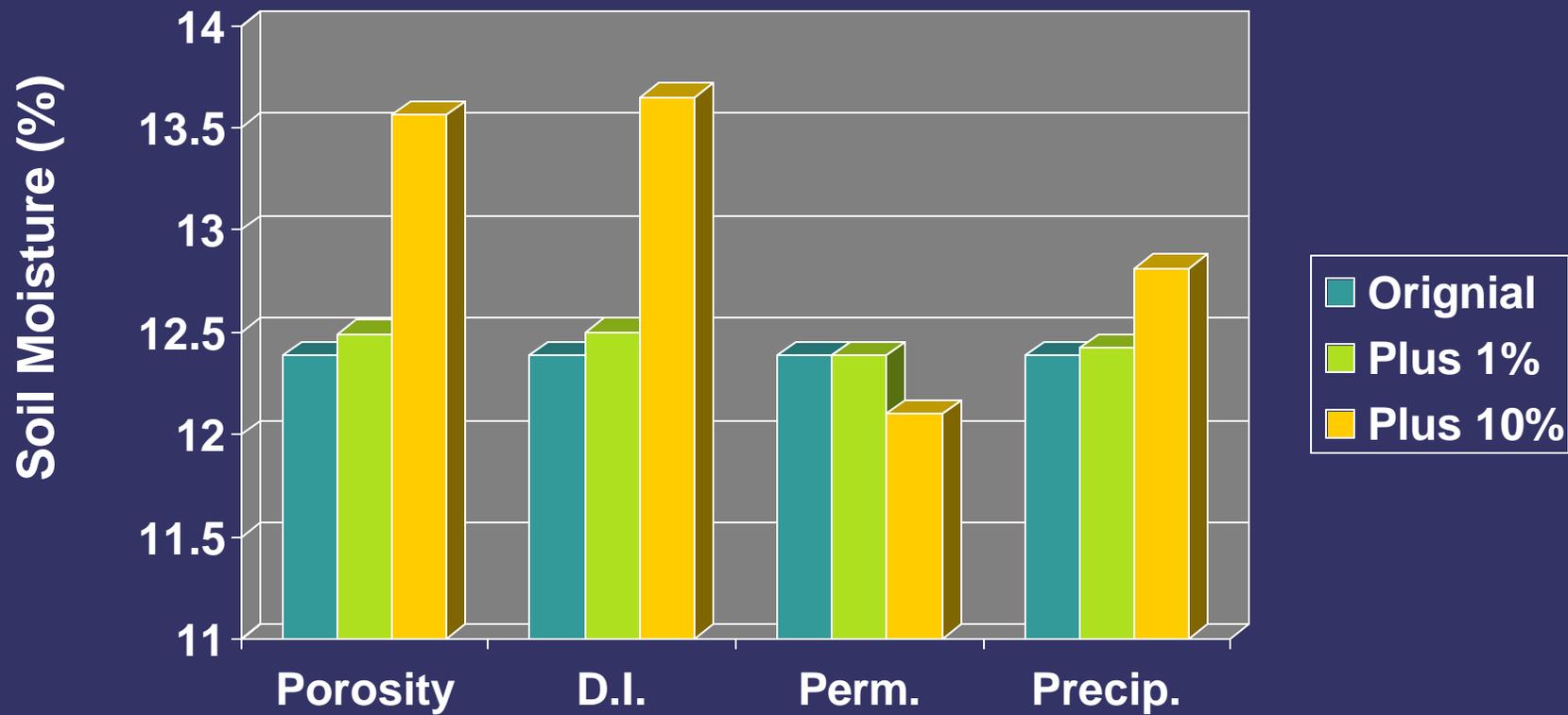
- Model divided into 4 layers with 10 sublayers each
- Meteorological Data from Hatchville, MA Station
- Site-specific soil properties
- Chemical constants



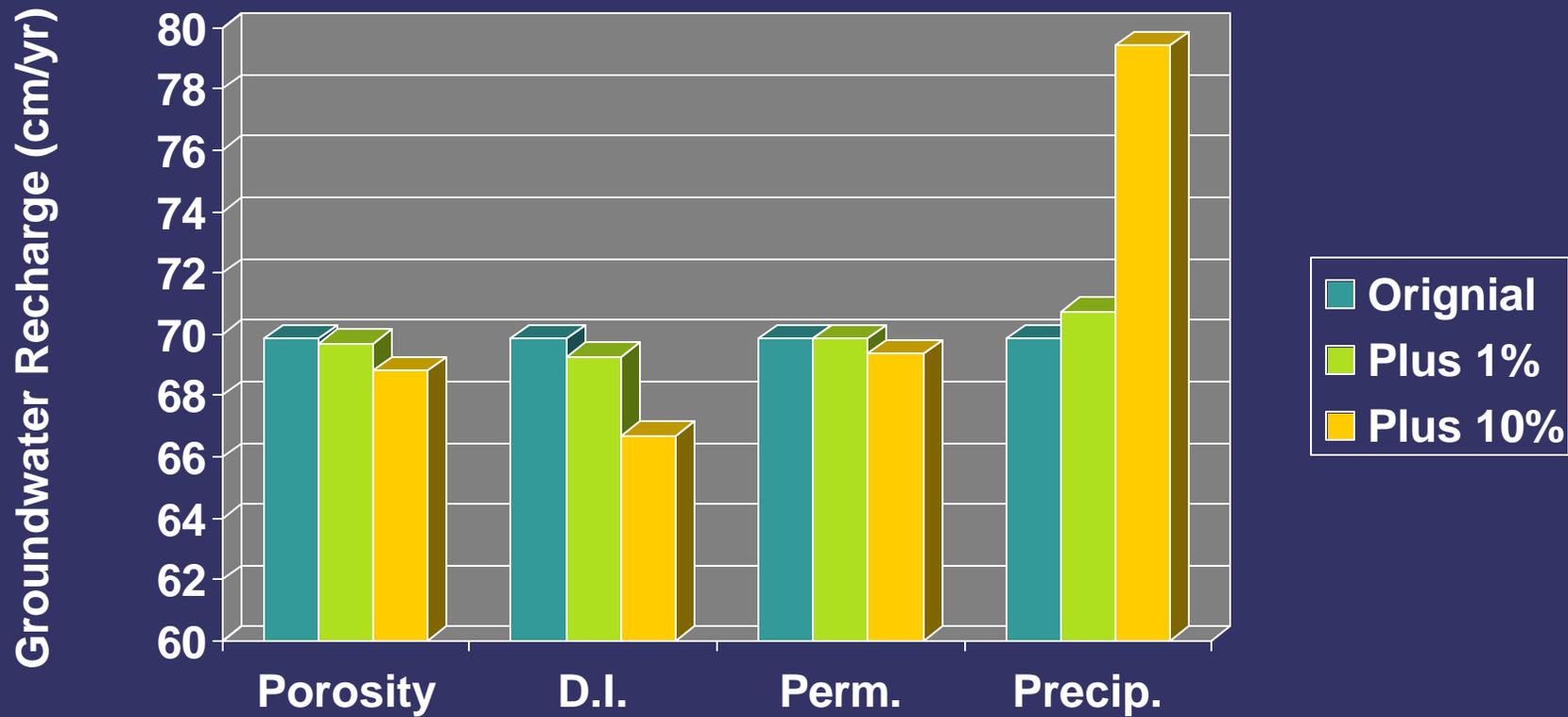
MODEL CALIBRATION

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	2.0E-09 to 1.0E-08 cm ²	3.8E-09 cm ²
Calibration Targets		
Soil Moisture	12.2 to 12.4%	12.3%
Evapotranspiration	45 to 55 cm/yr	46.5 cm/yr
Recharge	60 to 70 cm/yr	69.8 cm/yr
Surface Runoff	0 cm/yr	0.1 cm/yr

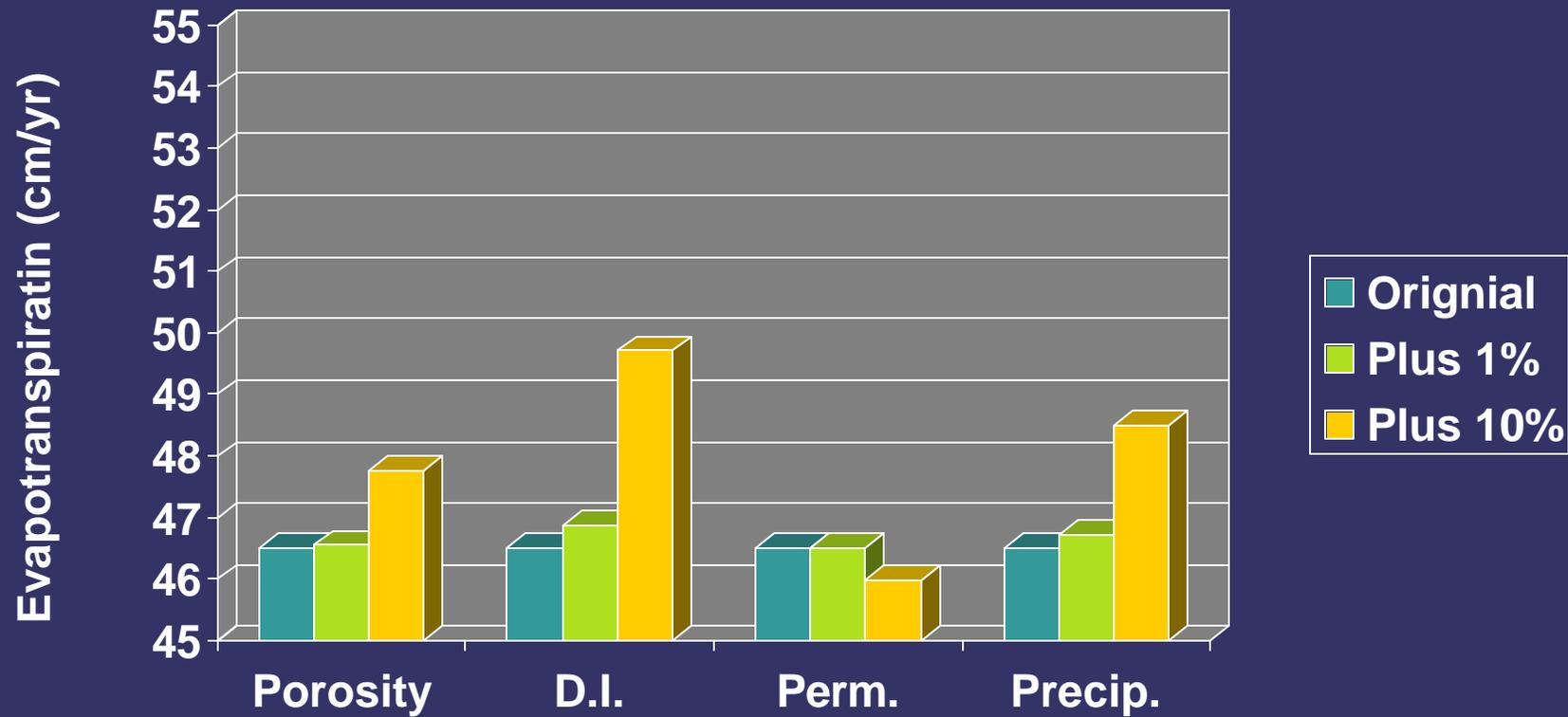
SENSITIVITY ANALYSIS – EFFECT ON SOIL MOISTURE



SENSITIVITY ANALYSIS – EFFECT ON RECHARGE



SENSITIVITY ANALYSIS – EFFECT ON EVAPOTRANSPIRATION



USE OF SESOIL TO DERIVE SOIL CLEAN-UP STANDARDS

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



OVERALL APPROACH - RDX

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

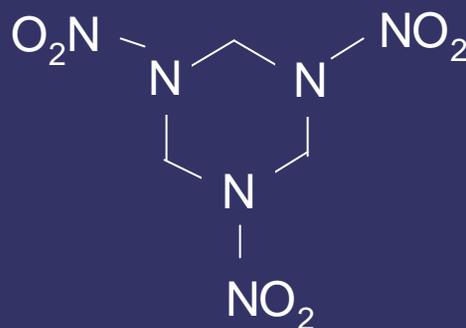
DEMOLITION AREA 1



MODEL SETUP FOR DEMO 1

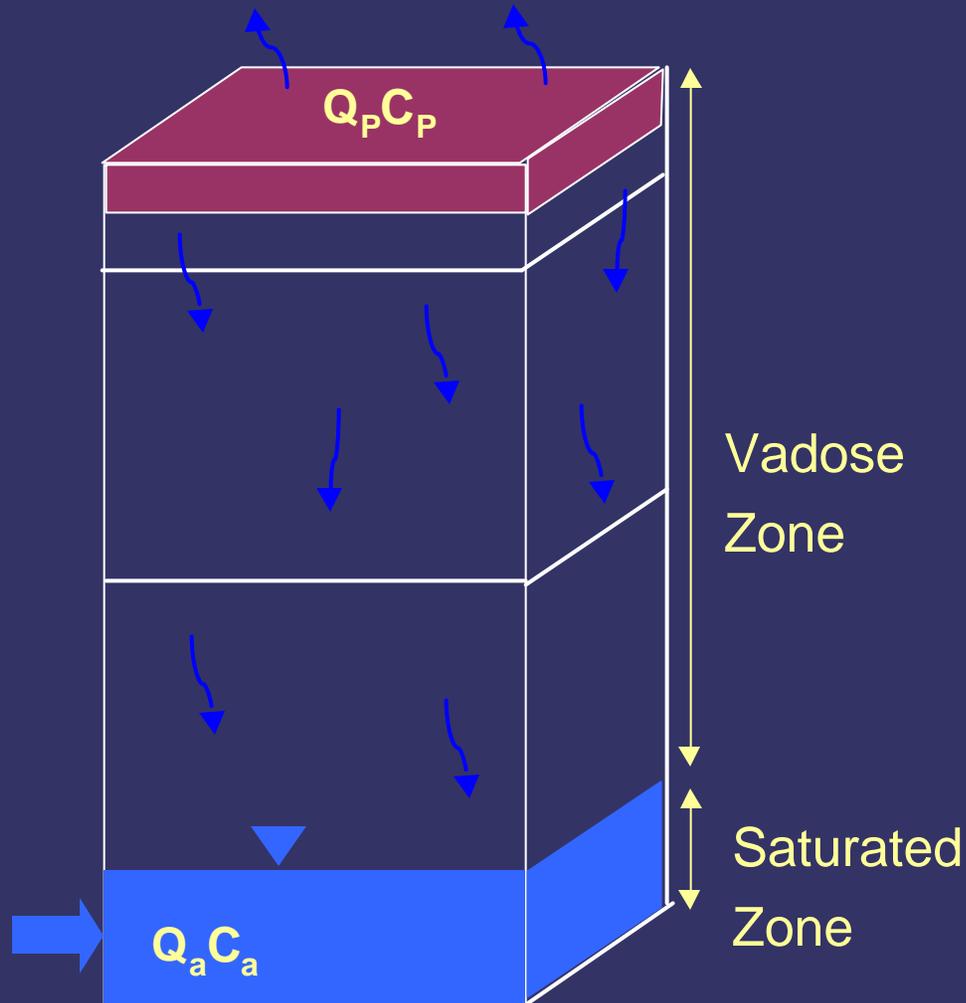
- Depth of Soil Contamination = 1 ft (0.3 m)
- Depth to water table = 40 ft (12.2m)
- Organic carbon = 0.5% (0-12 ft) and 0.01% (12-40 ft)
- Bulk Density = 1.8 g/ml
- Time = 100 years

MODEL INPUT - CHEMICAL PROPERTIES



	RDX
Solubility (mg/L)	38.4
Henry's Law Constant (m ³ -atm/mole)	1E-04
Koc (L/kg)	70.8

SESOIL + SUMMERS MODEL



Q_p = Flow through vadose zone

C_p = Soil concentration

Q_a = Flow through aquifer

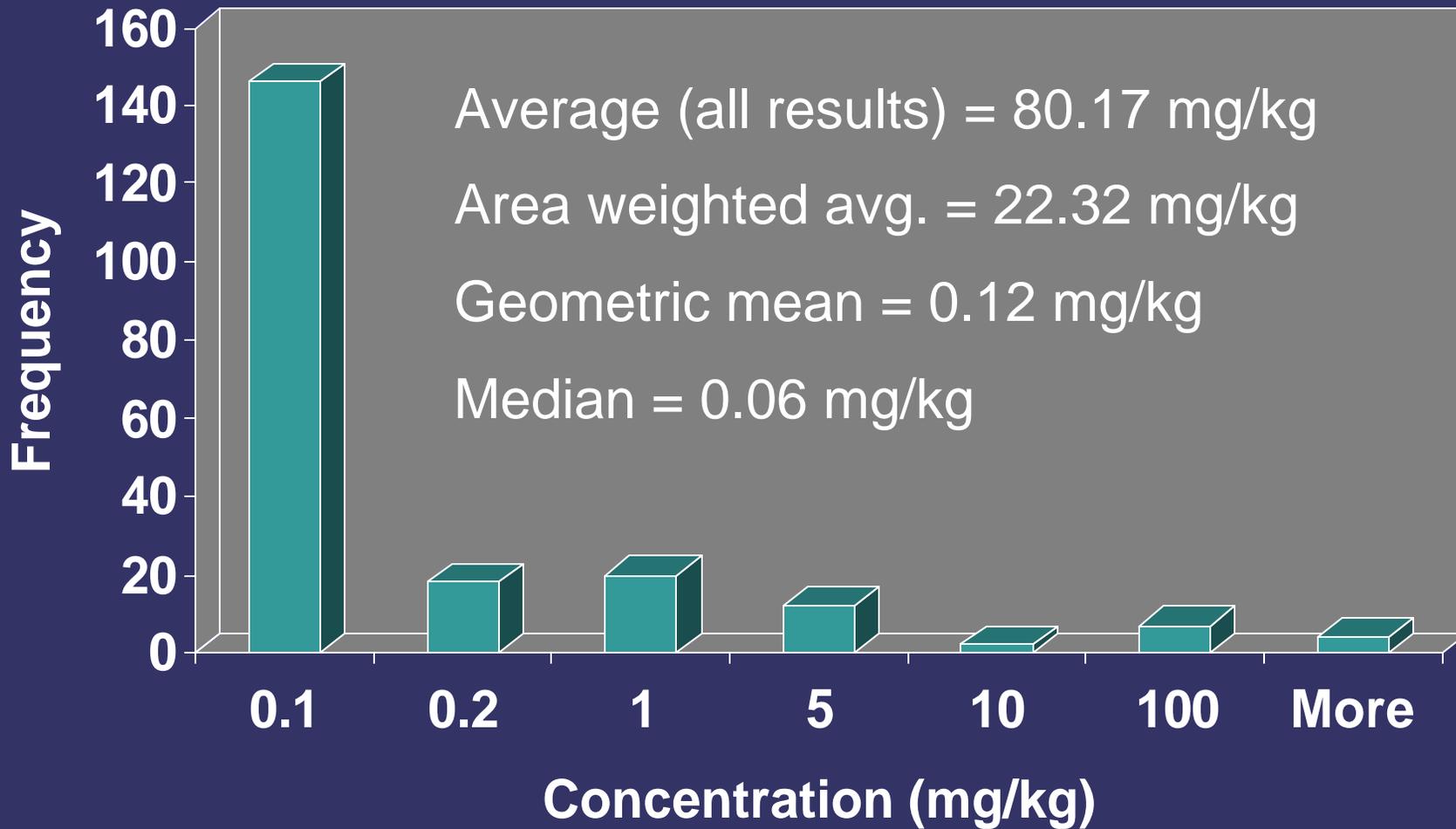
C_a = Groundwater concentration

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

TRANSPORT CALIBRATION

- Estimate soil concentration (average, area weighted average, geometric mean, median)
- Vary source size to match observed mass flux (0.4 – 0.5 kg/yr)
- Vary mixing zone size to match average groundwater concentration (115 ug/L RDX)

DEMO 1 RDX IN SOIL



TRANSPORT CALIBRATION RESULTS

	Soil Concentration (mg/kg)	Source Size* (cm ²)	Predicted Mass Flux (kg/yr)	Predicted GW Concentration (ug/L)
Average (all results)	80.17	2 x 10 ⁵ (220 ft ²)	0.5	115
Area weighted average	22.32	6.5 x 10 ⁵ (700 ft ²)	0.5	115
Geometric mean	0.12	1.1 x 10 ⁸ (2.7 acres)	0.5	49
Median	0.06	1.6 x 10 ⁸ (4 acres)	0.35	2.6

PRELIMINARY RDX SOIL CLEANUP STANDARDS

Source Size (cm ²)	Source Concentration (mg/kg)	Predicted GW Concentration (ug/L)
2 x 10 ⁵ (220 ft ²) (based on average calibration)	1.2	2
6.5 x 10 ⁵ (700 ft ²) (based on area weighted average calibration)	0.4	2

COMPARISON OF RESULTS

- AMEC: 0.4 to 1.2 mg/kg
 - Preliminary value
 - Currently under EPA review
- AFCEE for CS-19 Site: 5.5 mg/kg
- INEEL: 0.2 to 2.0 mg/kg (currently under review)



SENSITIVITY ANALYSIS

- High Sensitivity
 - Estimate of initial soil concentration
 - Estimate of average groundwater concentration
- Moderate Sensitivity
 - Source thickness
 - Mixing zone thickness
 - Mixing zone length
- Low Sensitivity
 - Number of sublayers per layer
 - Literature Koc vs. Laboratory Measured Kd values

POTENTIAL NEXT STEPS

- Install Lysimeters to measure RDX in vadose zone pore water
- Refine SESOIL model based on observations

THANKS

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