ENVIRONMENTAL FATE & TRANSPORT MODELING OF EXPLOSIVES & PROPELLANTS IN THE SATURATED ZONE

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UMASS Contaminated Soils, Sediments, and Water Conference

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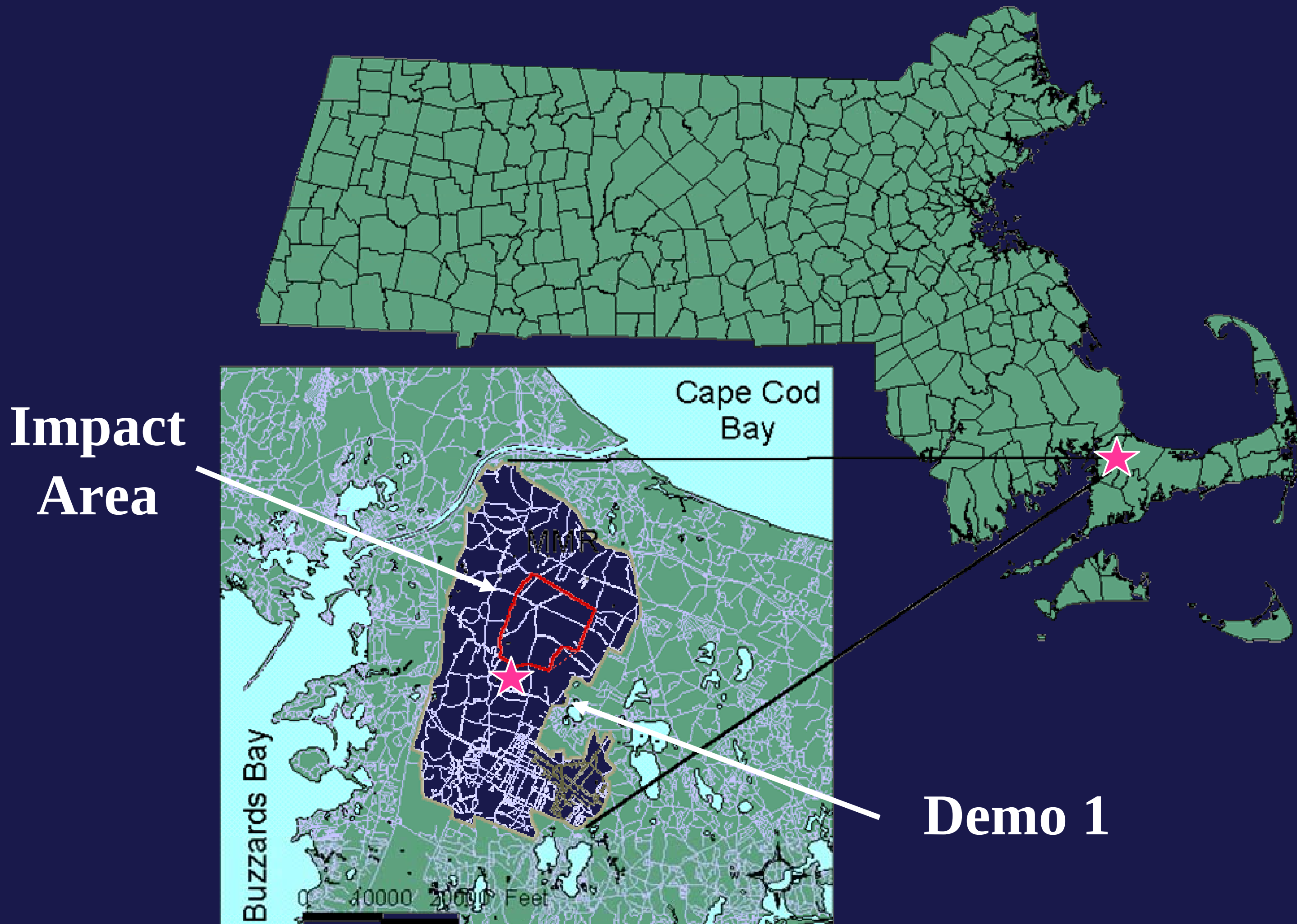
MASSACHUSETTS MILITARY RESERVATION (MMR)



MMR OVERVIEW

- 21,000 acre site for military training activities since 1911 – peaked during WWII
- USEPA banned training in 1997
- Surrounded by coastal resort towns of Bourne, Falmouth, Mashpee and Sandwich, MA

- Lies above recharge area for the Sagamore Lens - the most productive part of Cape Cod Aquifer and sole source of drinking water for surrounding communities

EXPLOSIVE AND PROPELLANT CONSTITUENTS OF CONCERN

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- RDX - Explosive Compound
- TNT - Explosive Compound
- HMX - Impurity of RDX
- 4A-DNT - Degradation Product of TNT
- 2A-DNT - Degradation Product of TNT
- 2,4-DNT - Propellant
- PERCHLORATE - Propellant

*all detected in soils at Demo 1

SCOPE OF MMR/DEMO 1 MODELING PROGRAM

- **Unsaturated Zone** - soil characterization, SESOIL simulation of fate & transport to watertable, HELP simulation of transient recharge
- **Saturated Zone** - aquifer characterization, MODFLOW simulations of steady-state/transient flow, MT3D simulations of fate & transport
  - Regional flow model (Western Cape Cod)
  - Embedded subregional model for Demo 1
  - Fate & transport model of RDX
  - Optimization modeling of remediation scenarios: hydraulic control, aggressive extraction/reinjection to meet time and/ or mass removal criteria for multiple COCs

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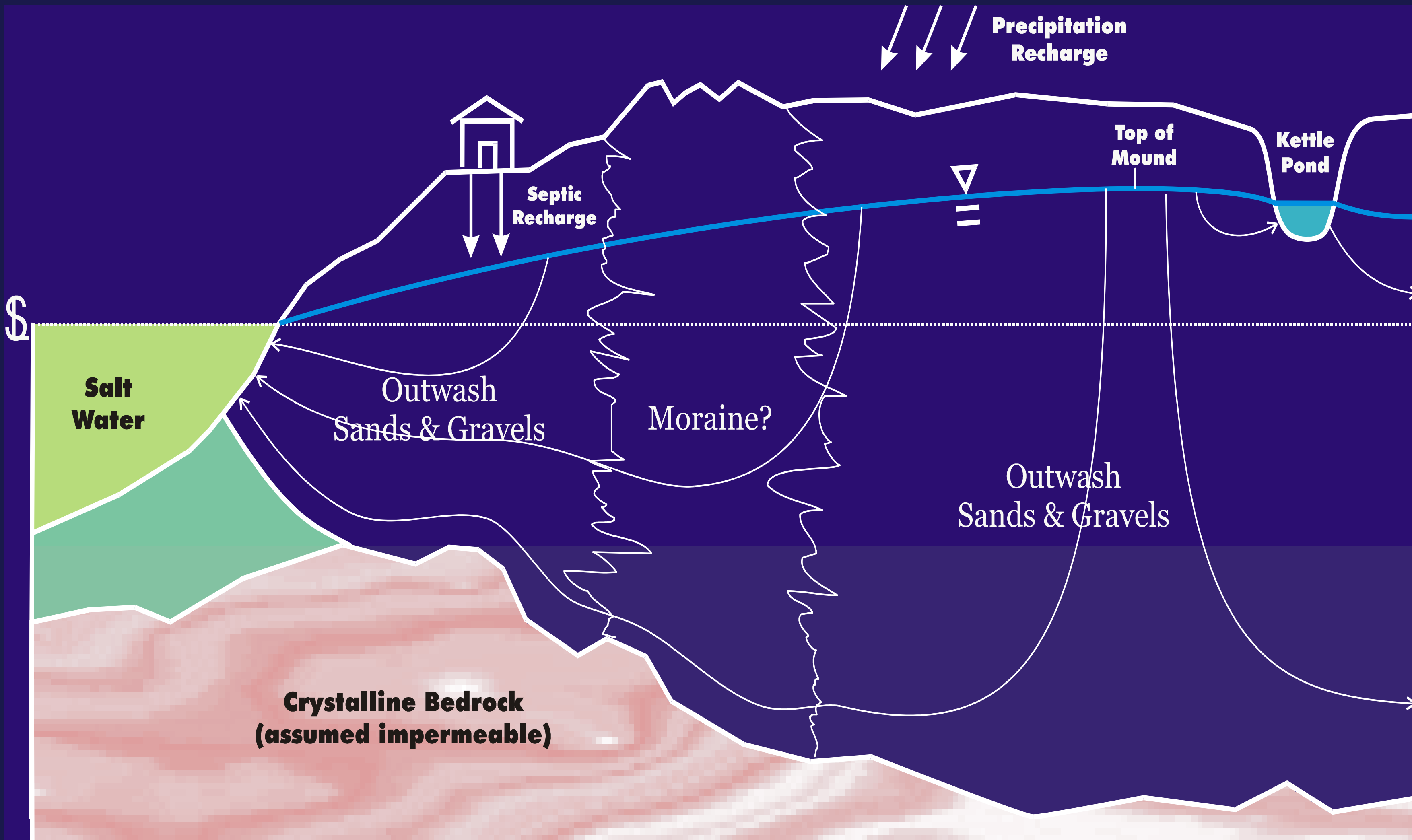
CONCEPTUAL HYDROGEOLOGIC MODEL



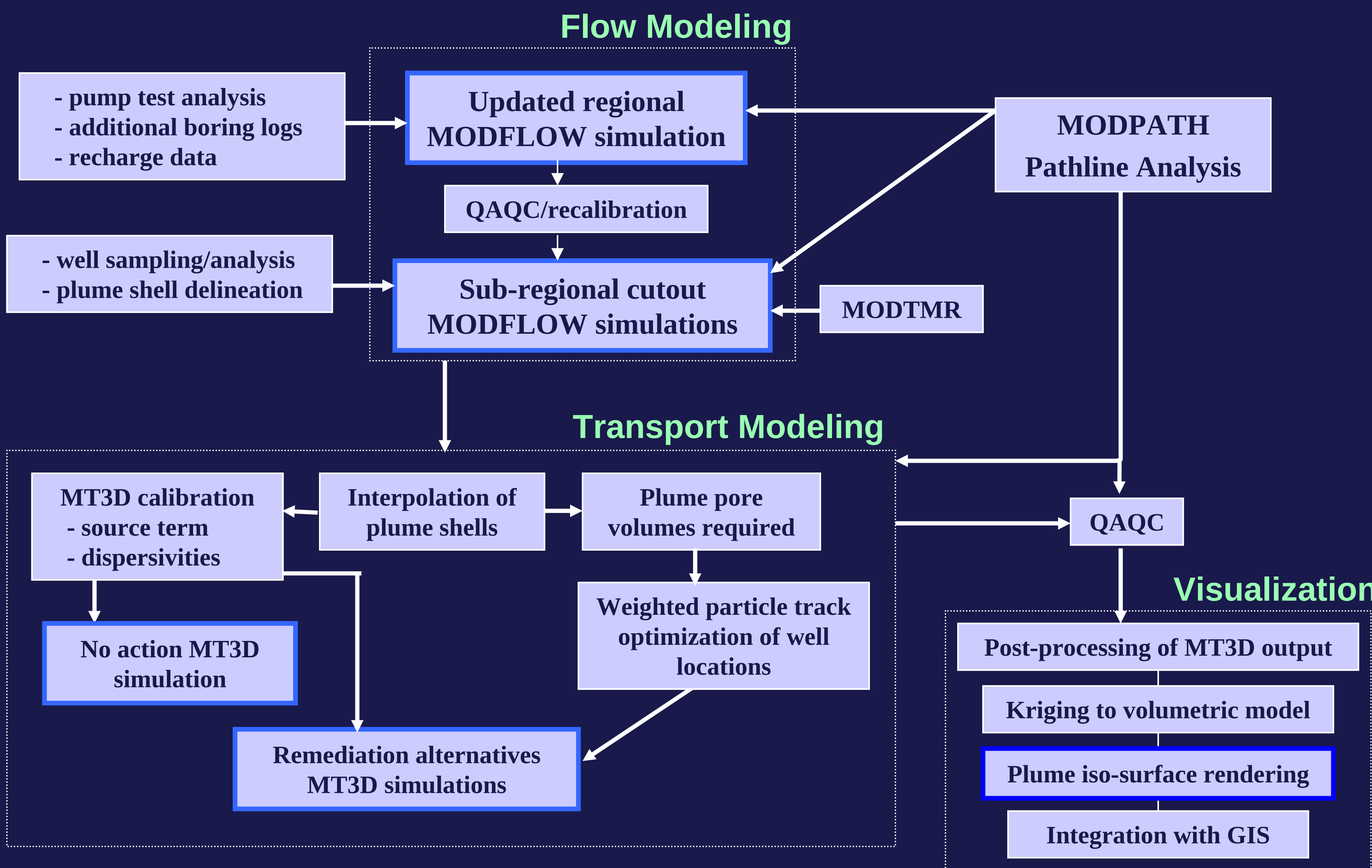
HYDRAULIC CONDUCTIVITY VALUES FOR DEMO 1 IN USGS MODEL

Model Layer	Elevation* (ft ngvd)	Range of K Values (ft/d)	K Values at Demo 1 (ft/d)
1	above 40	125 - 350	290
2	20 to 40	125 - 350	290
3	0 to 20	125 - 300	290
4	-20 to 0	100 - 290	290
5	-40 to -20	70 - 230	230
6	-60 to -40	70 - 230	230
7	-80 to -60	30 – 200	125
8	-100 to -80	10 - 125	70
9	-140 to -100	10 - 70	30
10	bedrock** to -140	10 - 70	30
11	NA	10 - 30	NA

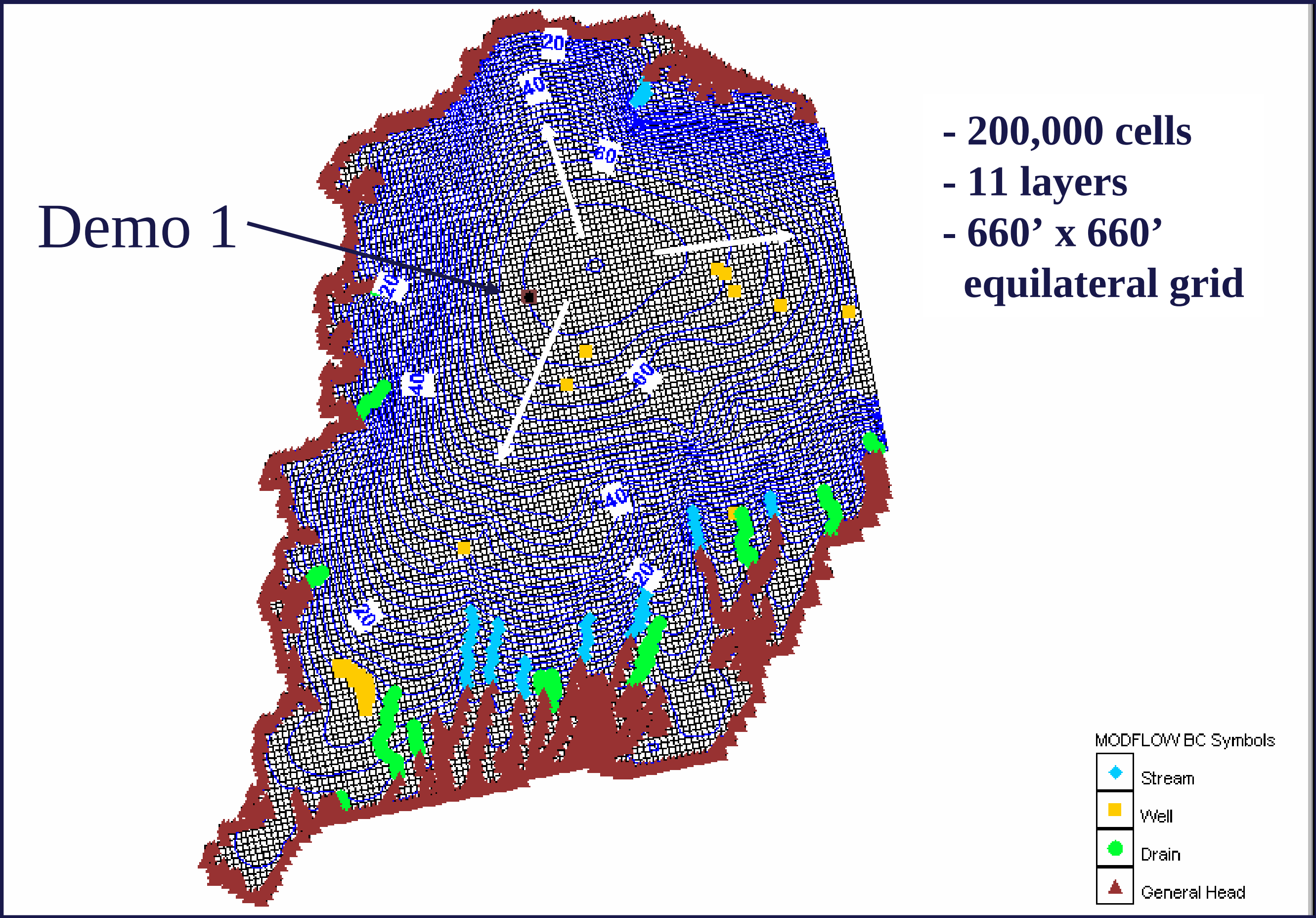
*In the central portion; ** about -200 to -150 ft ngvd

(based on USGS Regional Model)

Complexity of the Fate & Transport Modeling Process

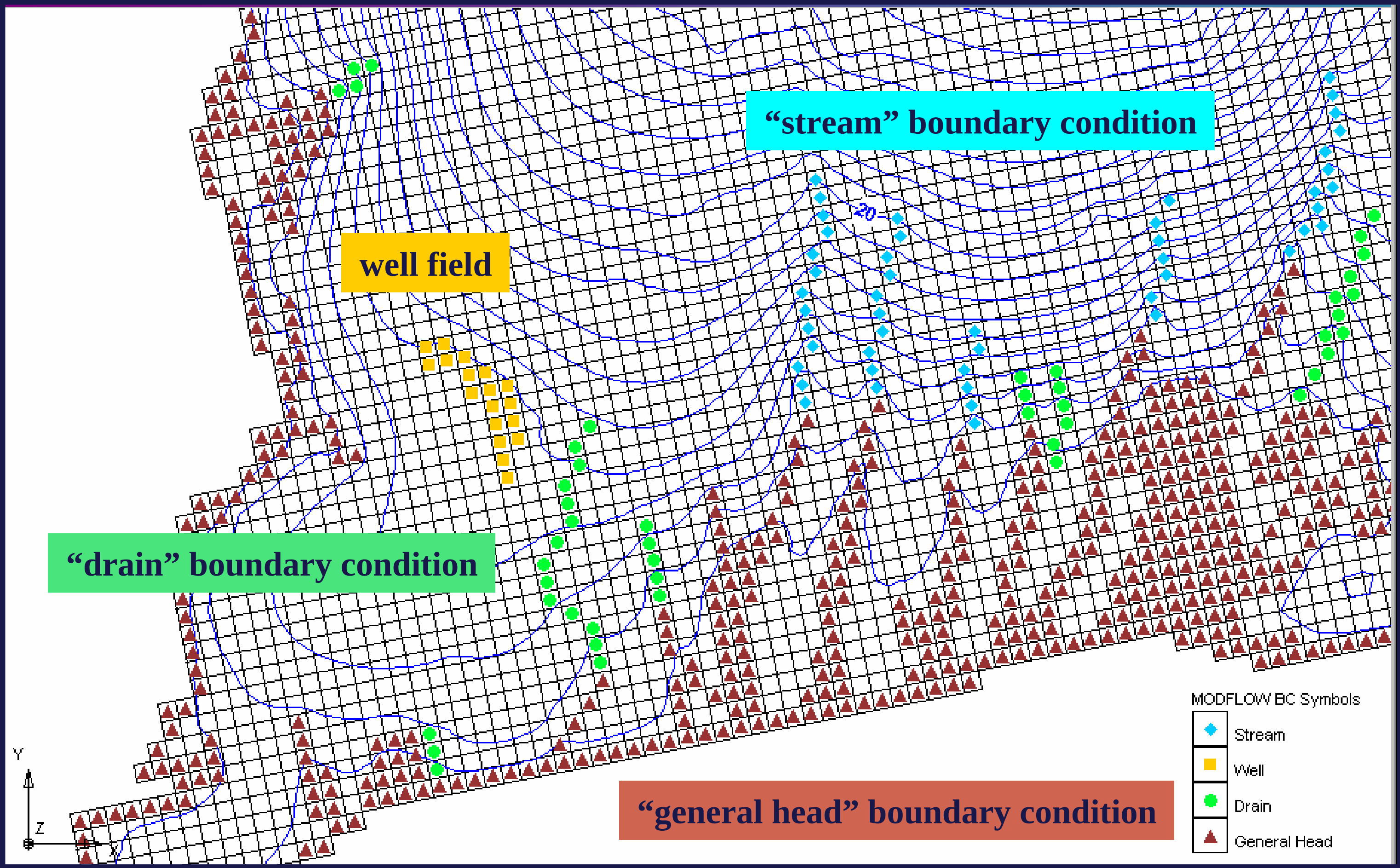


MMR-8 REGIONAL MODFLOW SIMULATION

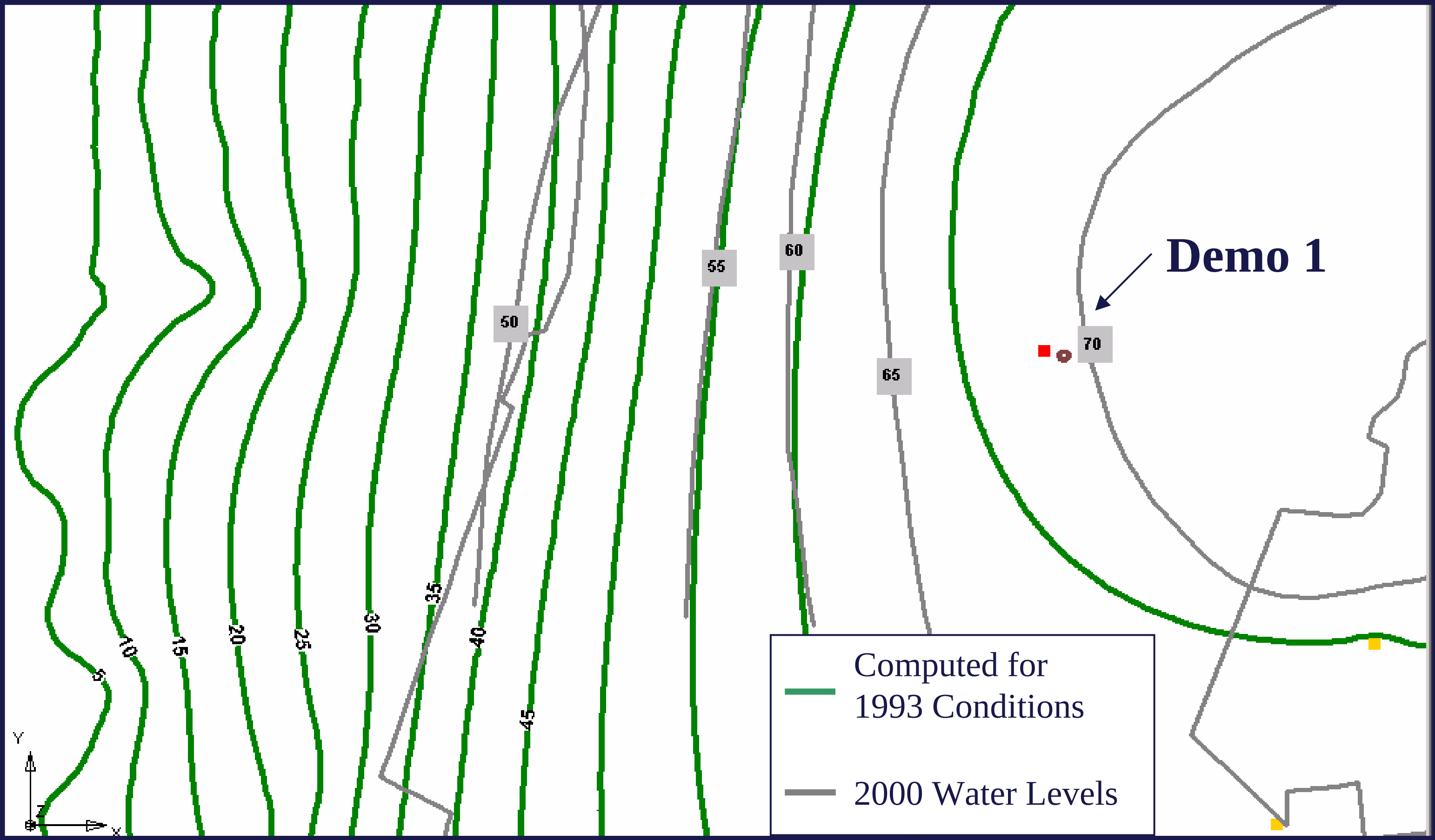


- 200,000 cells
- 11 layers
- 660’ x 660’ equilateral grid

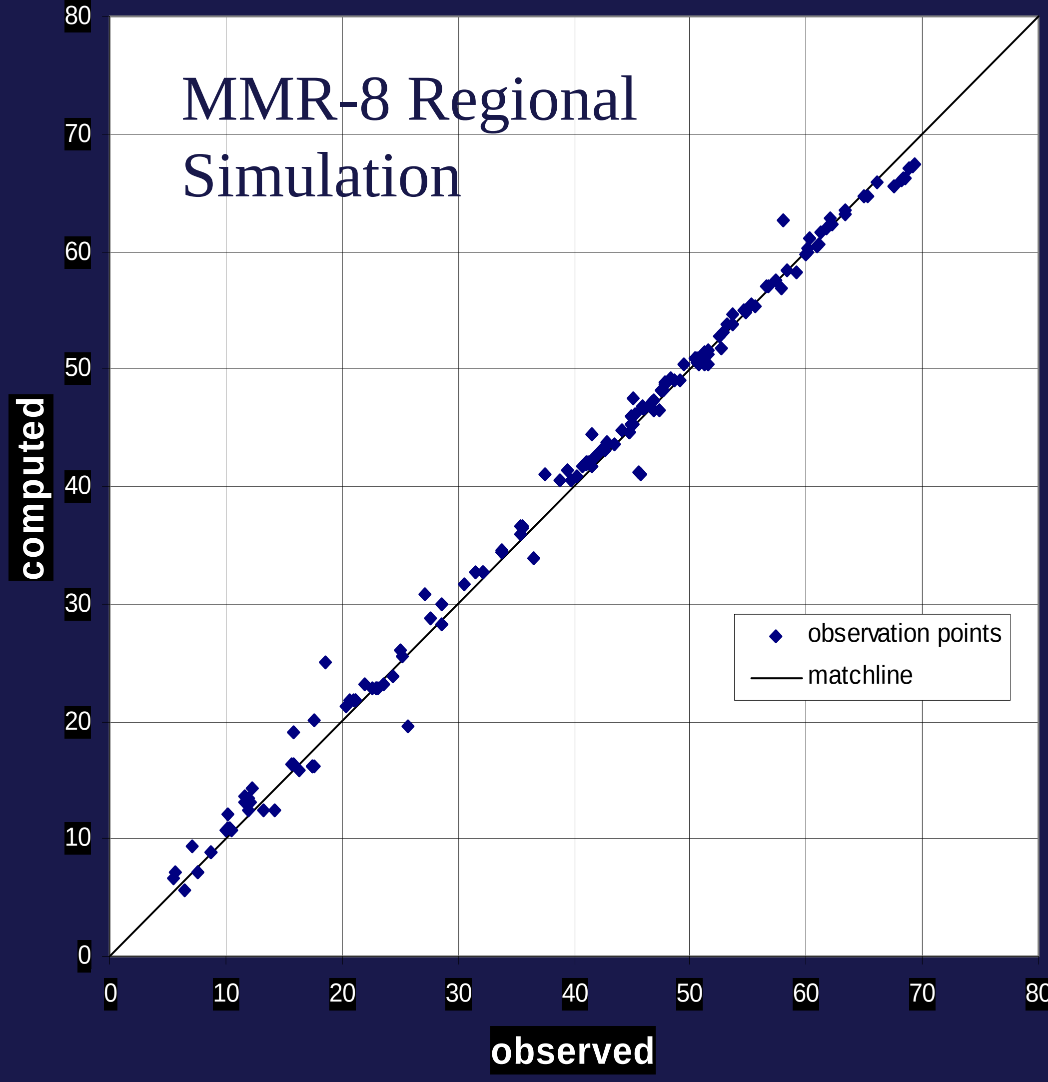
REGIONAL BOUNDARY CONDITIONS



MODELED vs. OBSERVED WATERTABLE



CALIBRATION TO 1993 WATER LEVELS

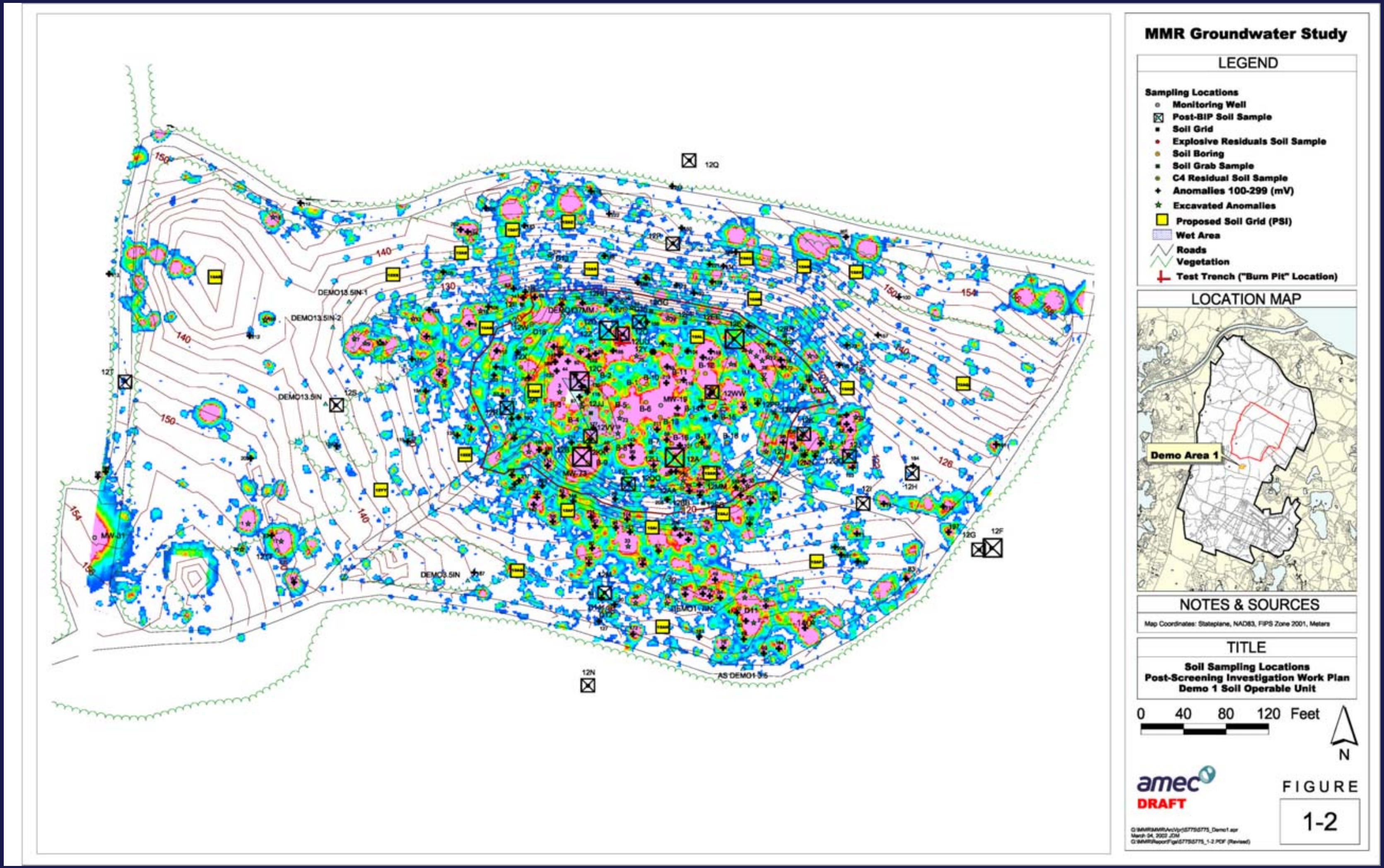


Statistics

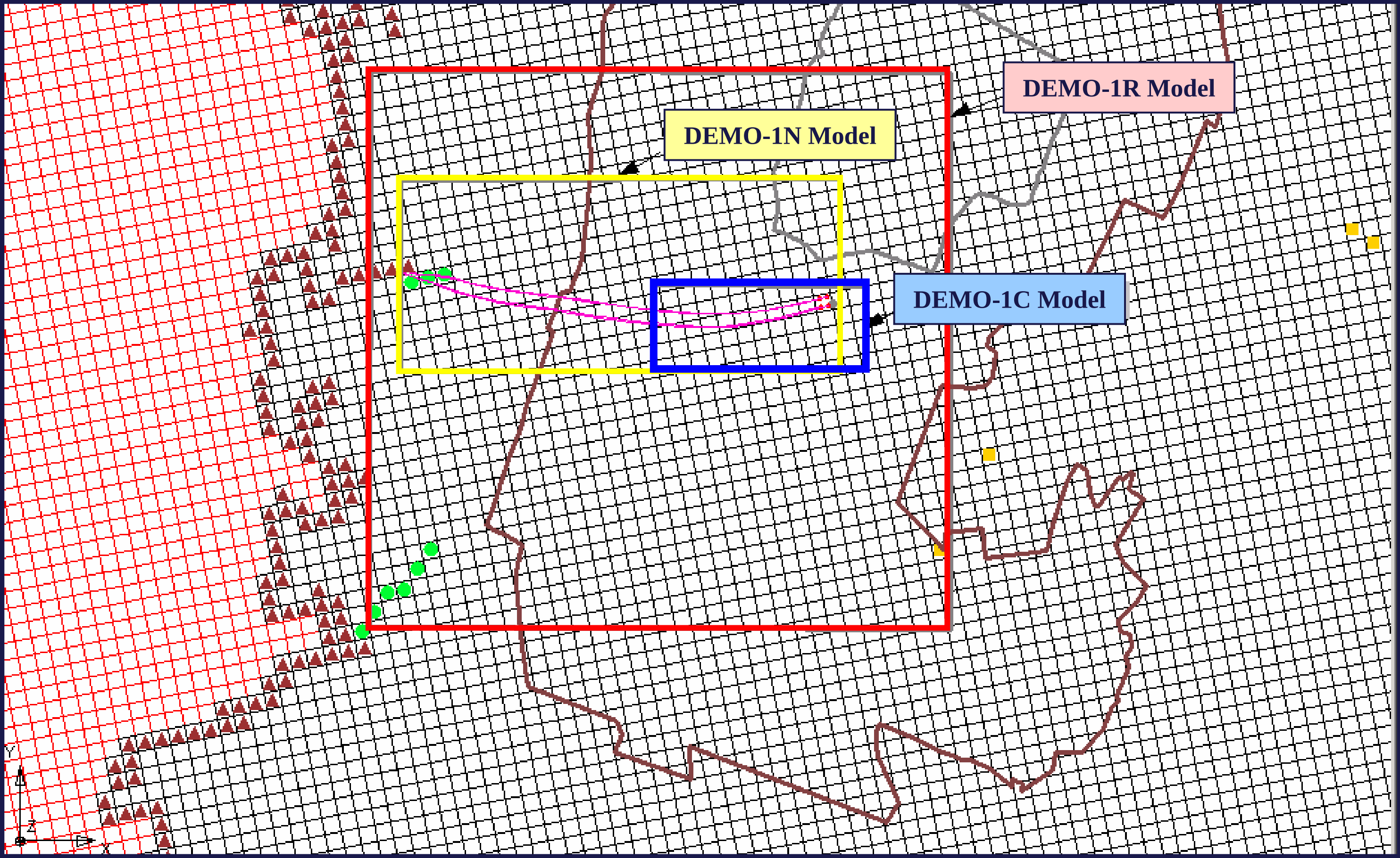
ME = 0.30
MAE = 0.96
RMSE = 1.4
RMSE/Range = 2.08%

DEMO 1 SOURCE AREA

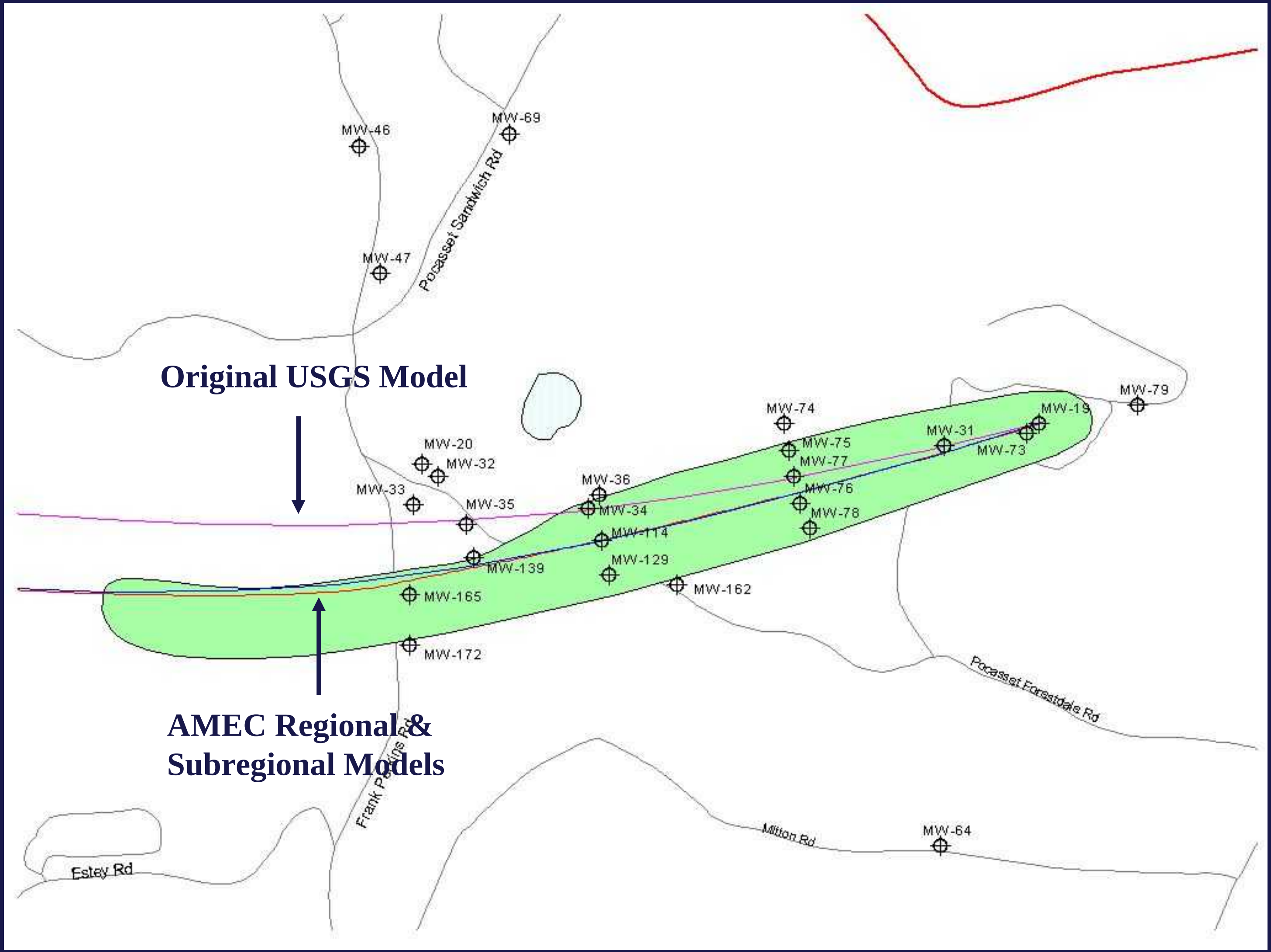
DEMO 1 MAGNETIC ANOMALIES

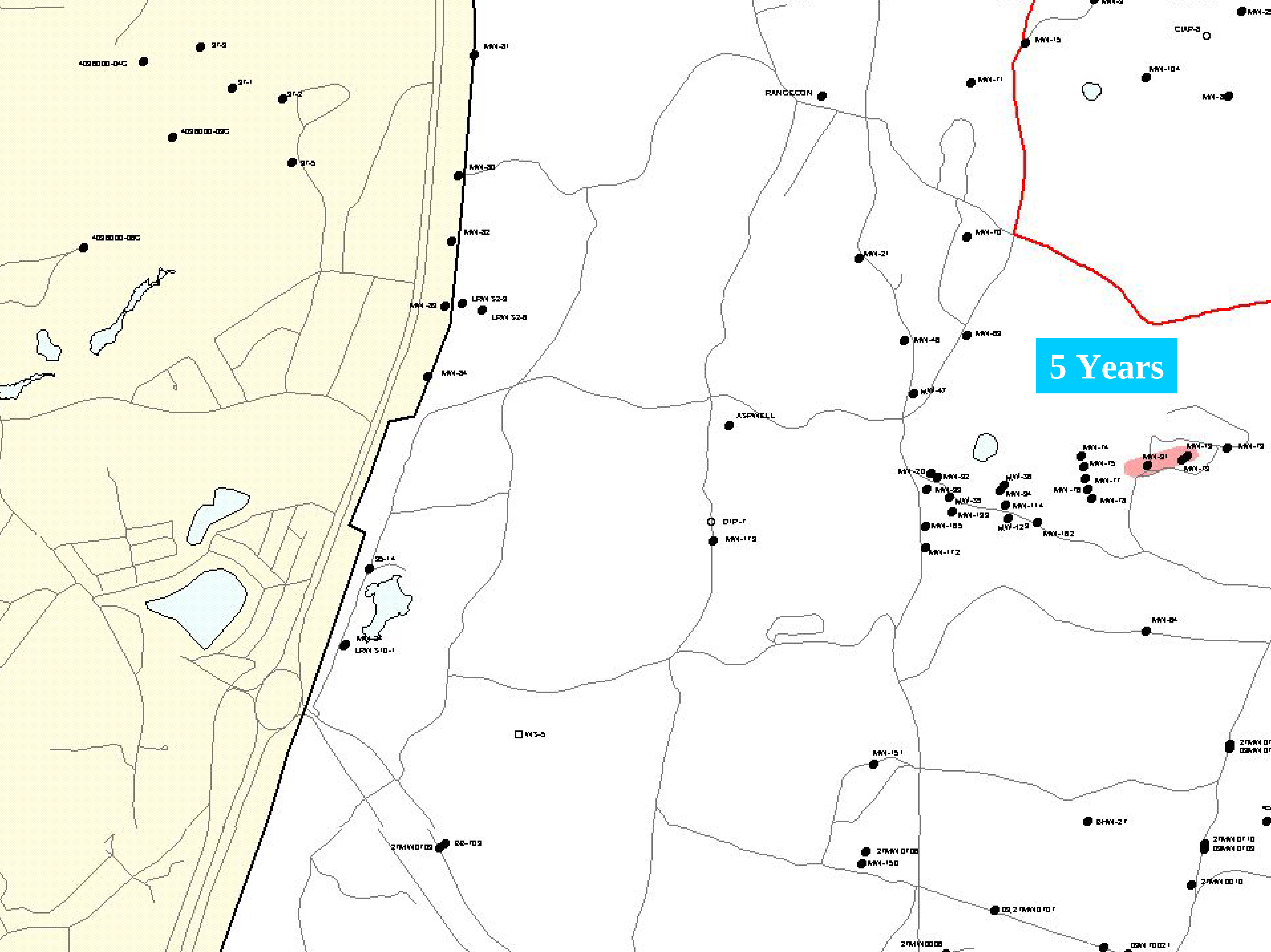


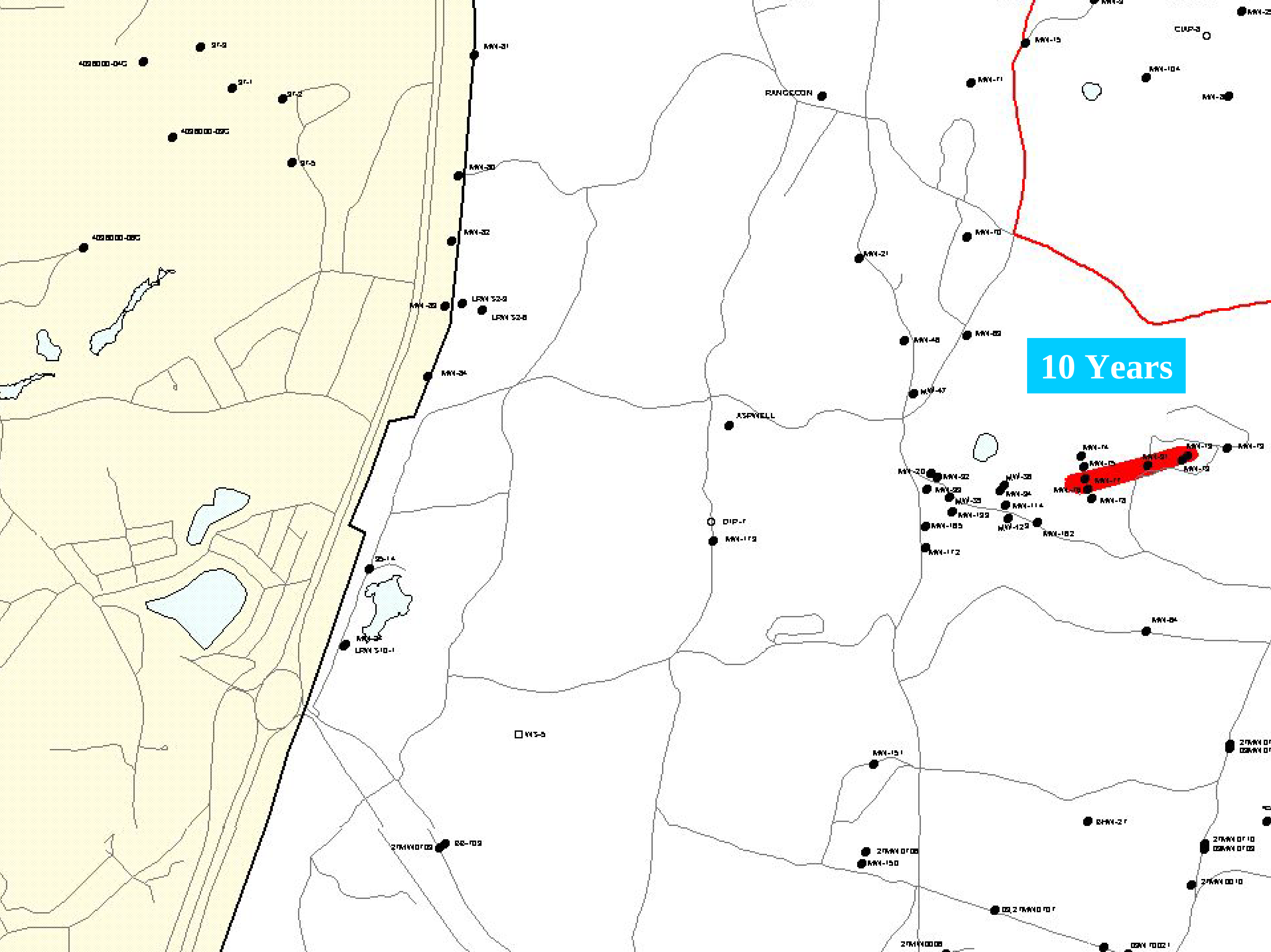
REGIONAL MODEL GRID AND RELATIONSHIP WITH SUB-REGIONAL MODELS

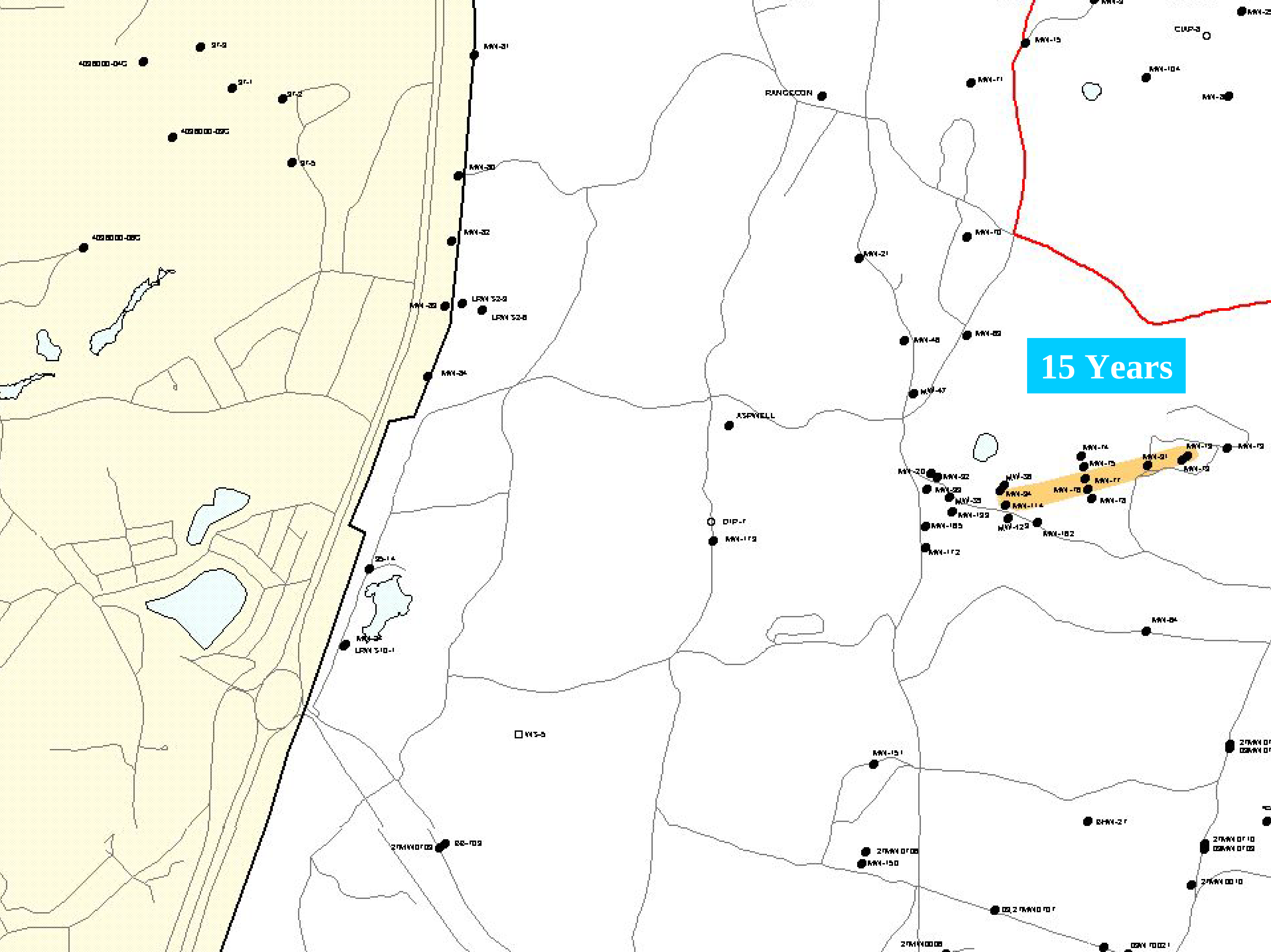


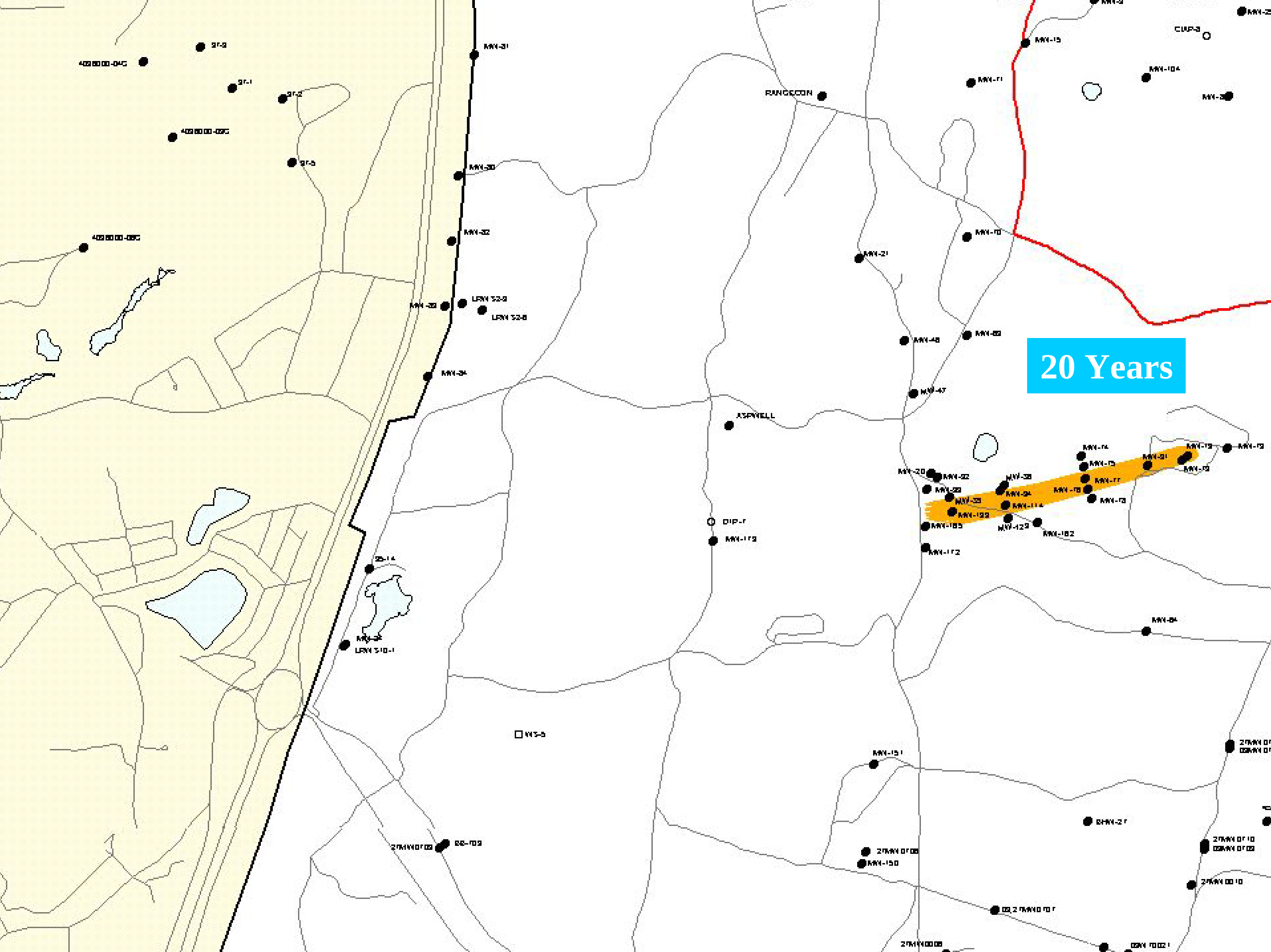
COMPARISON OF PARTICLE TRACKS WITH DEMO 1 RDX PLUME GEOMETRY

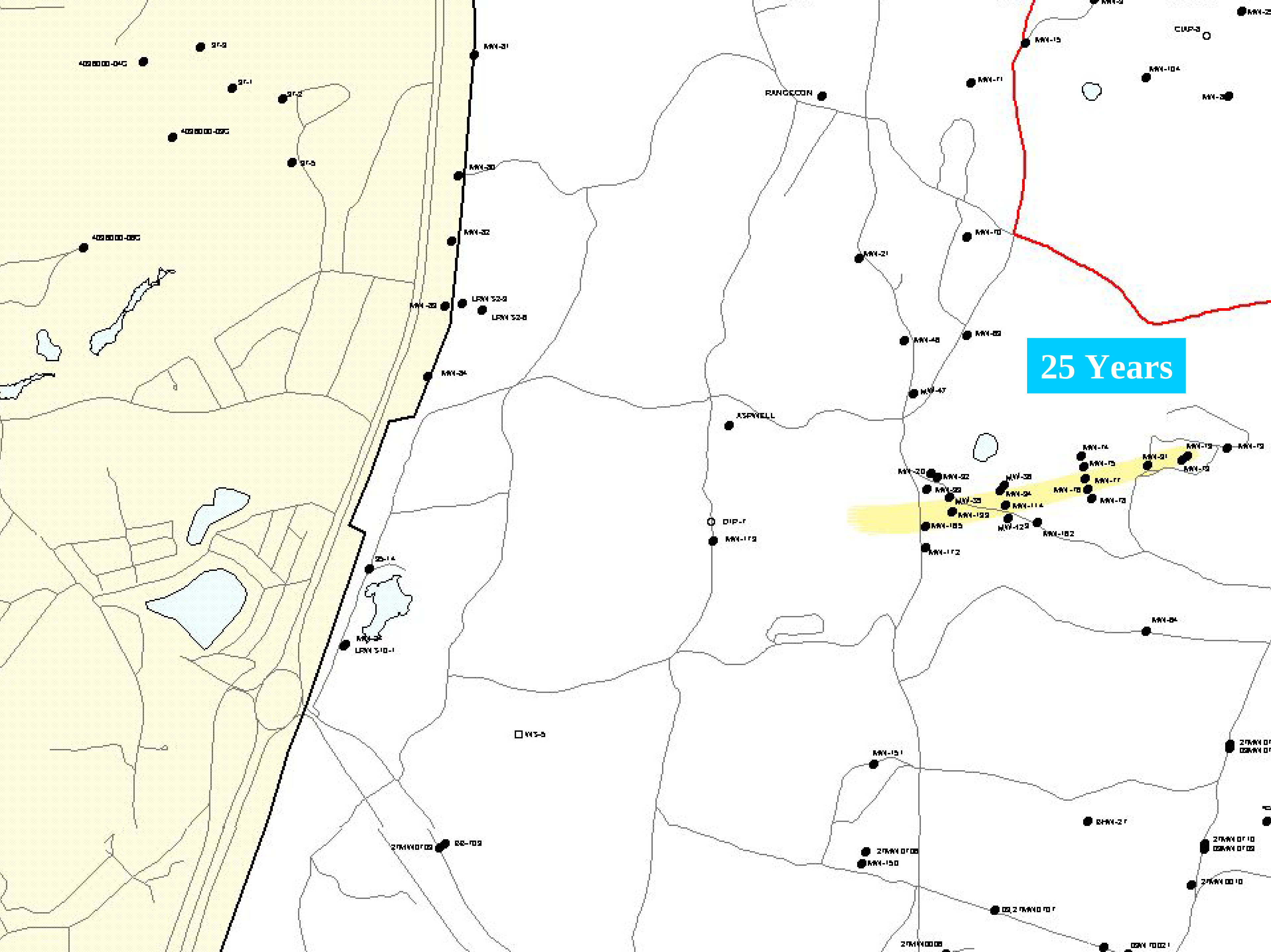



5 Years
RANGECON
ASPWELL

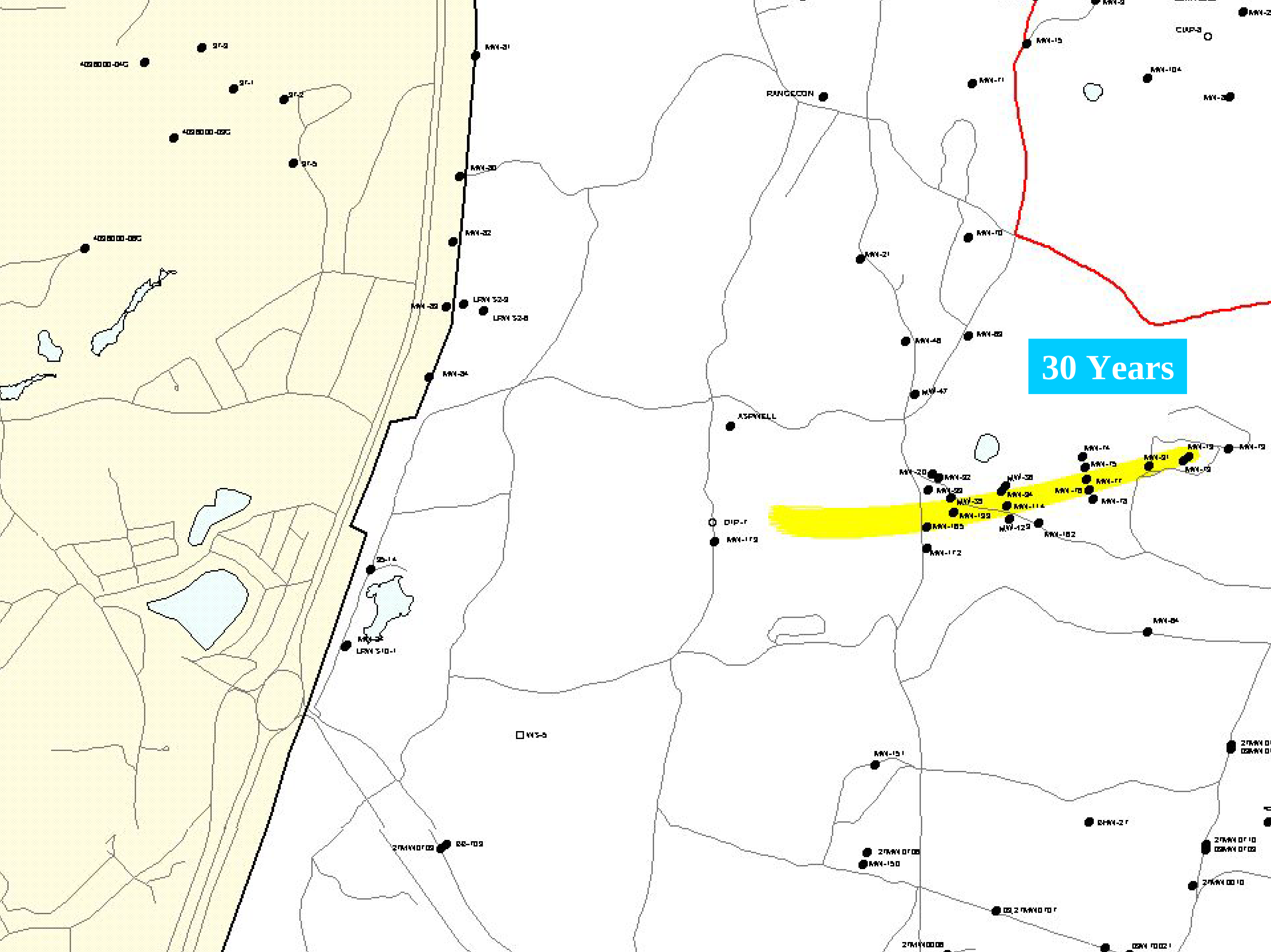

10 Years
RANGECON
ASPWELL

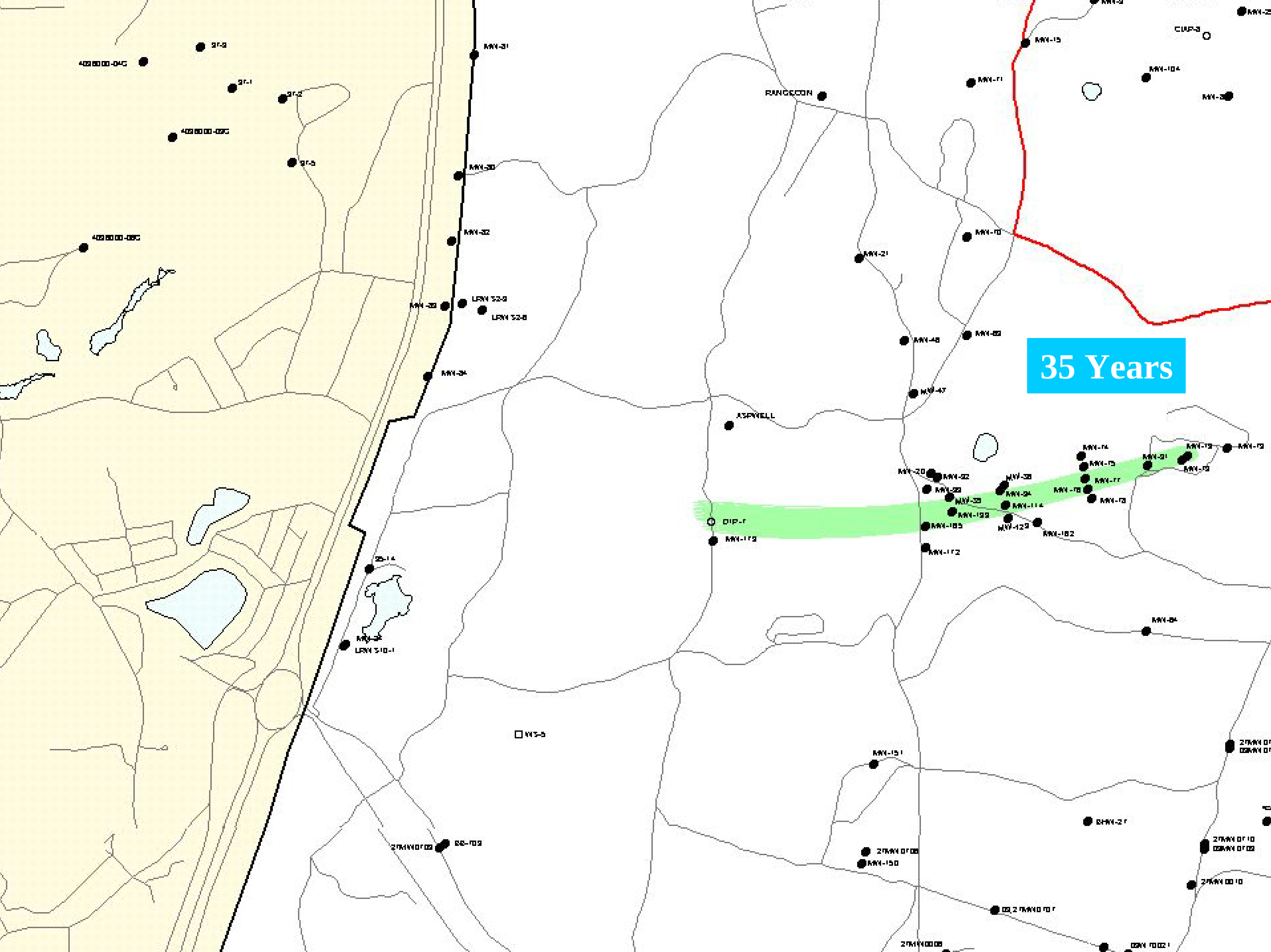

15 Years

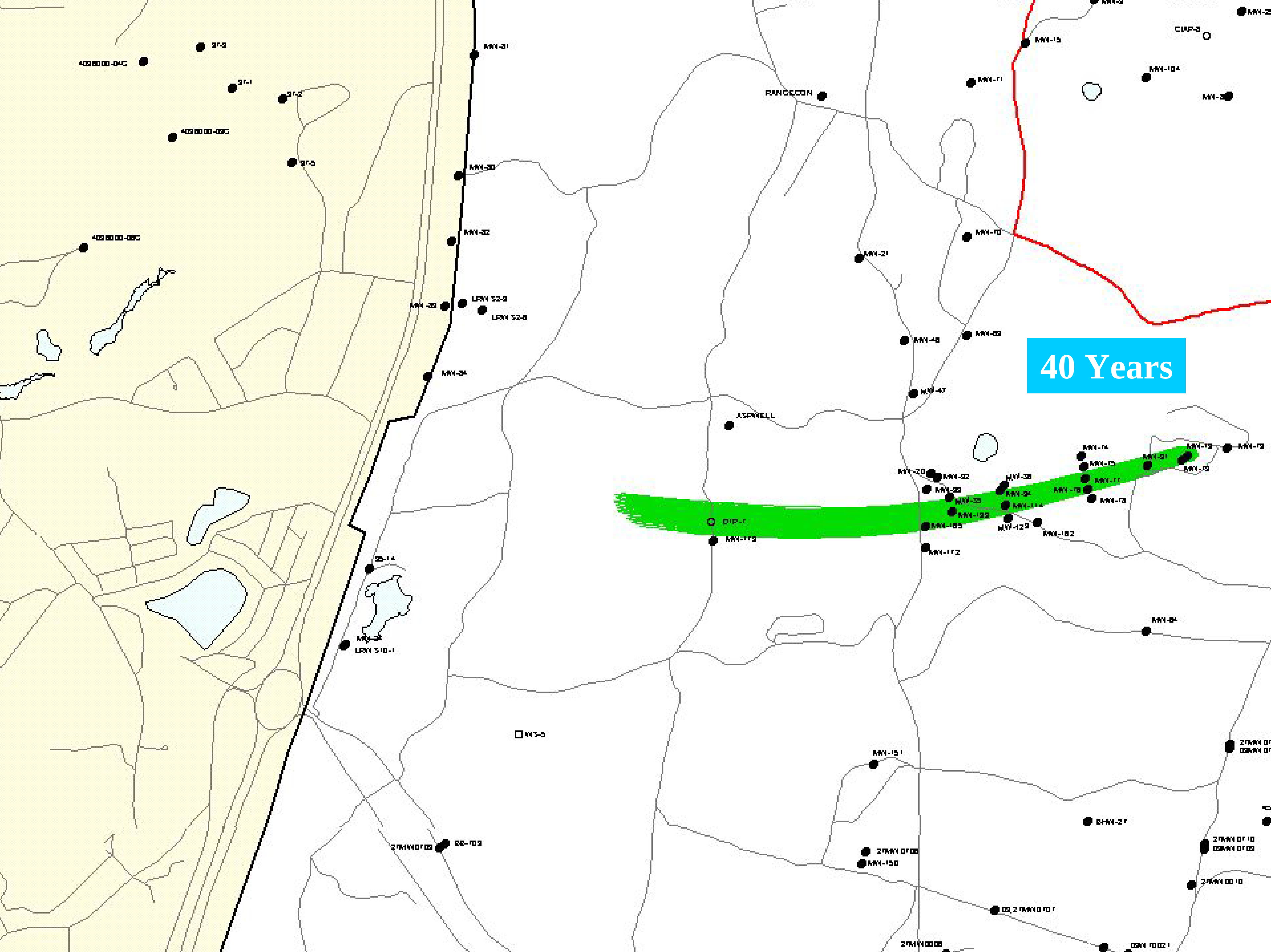

20 Years

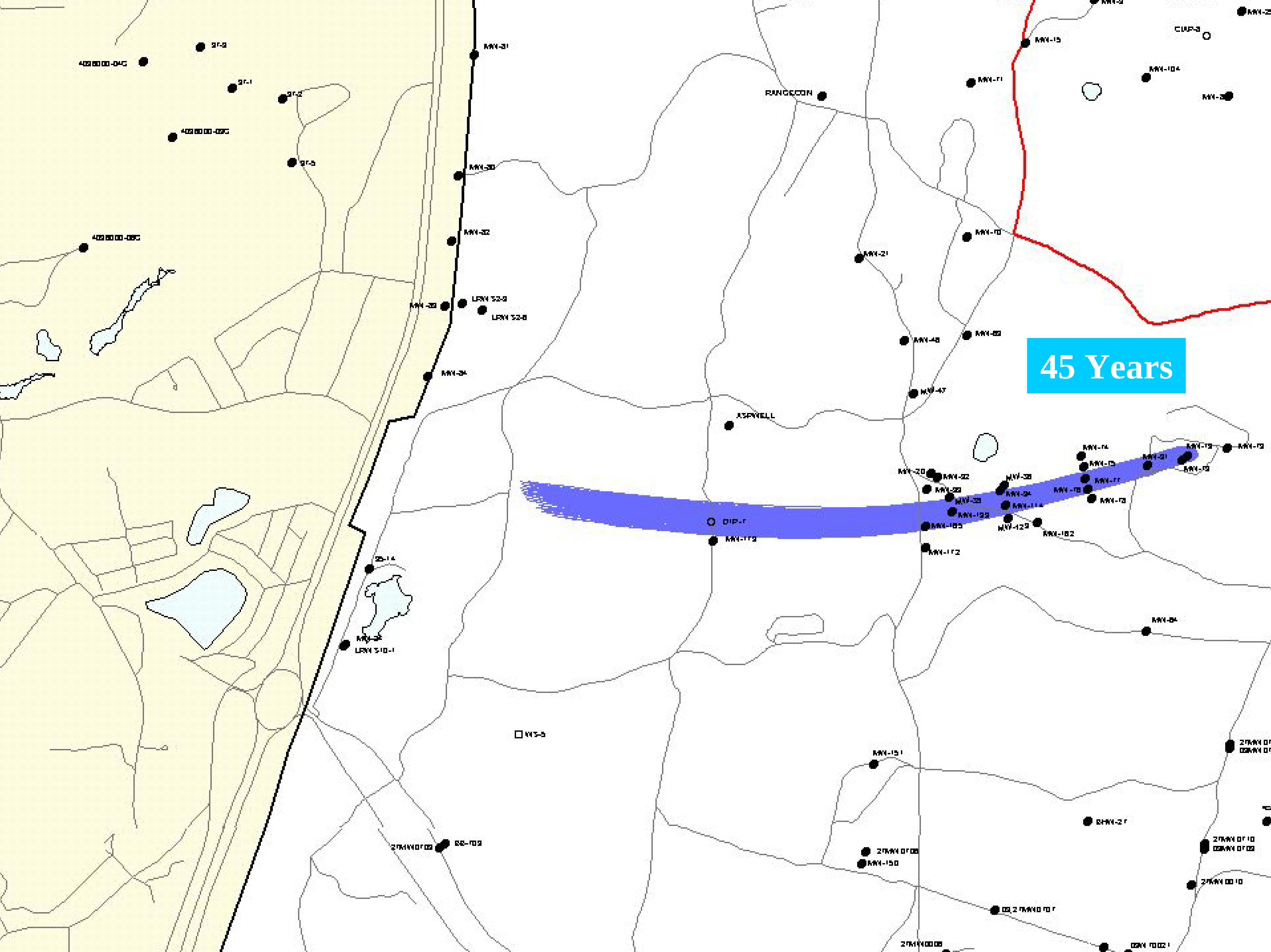


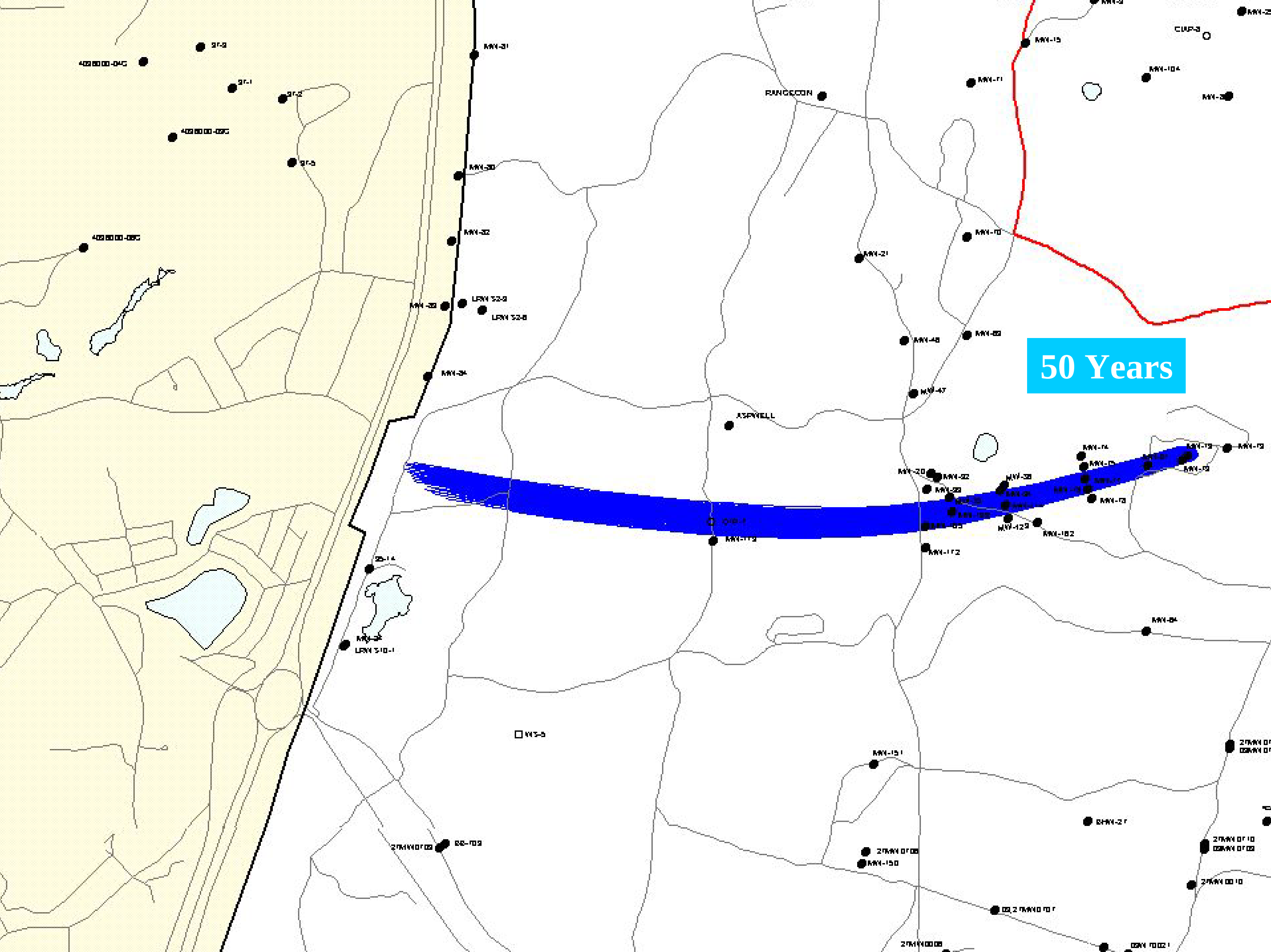
25 Years
RANGECON
ASPWELL

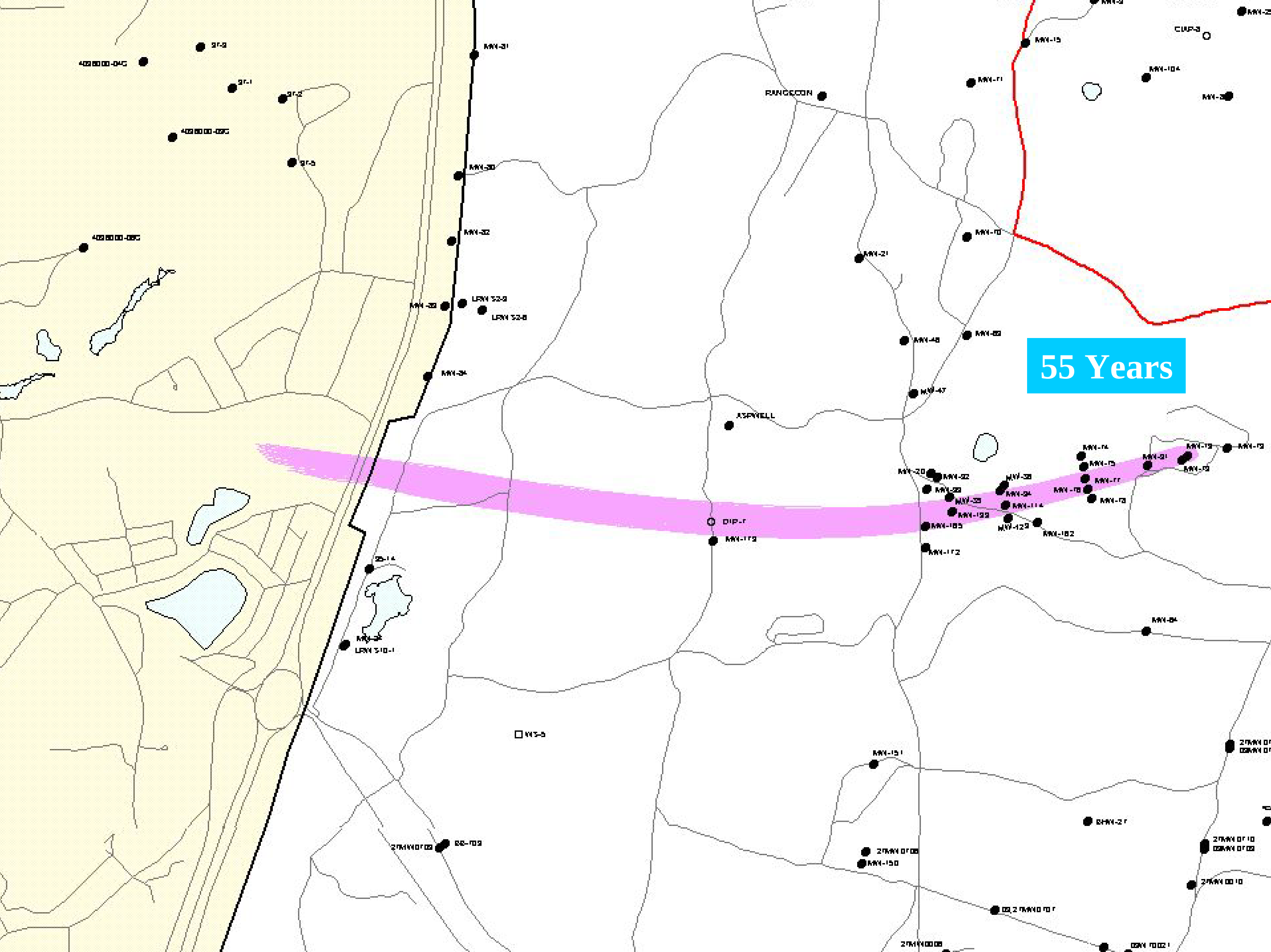

30 Years

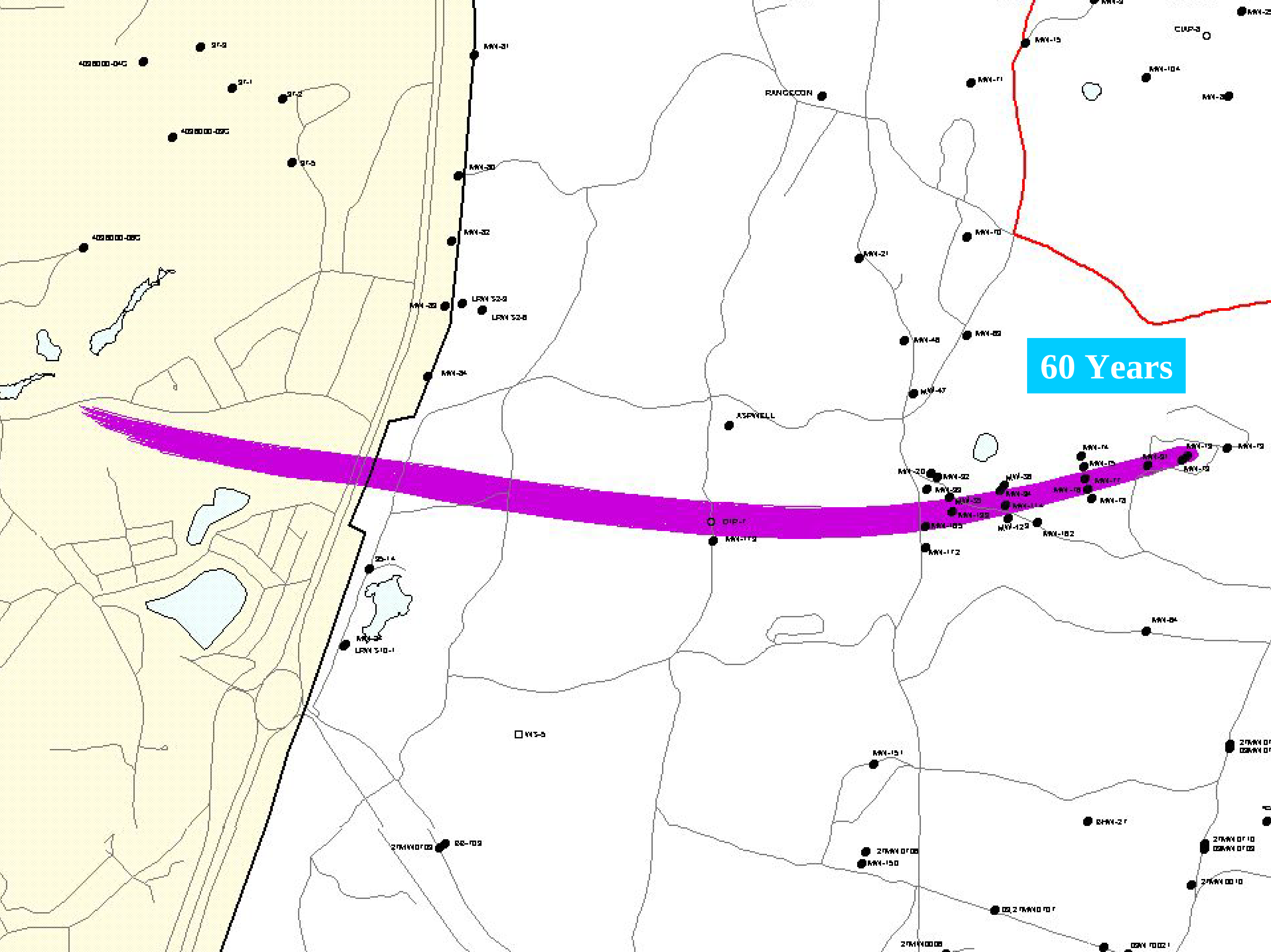

35 Years


40 Years
RANGECON
ASPWELL


45 Years


50 Years


55 Years


60 Years

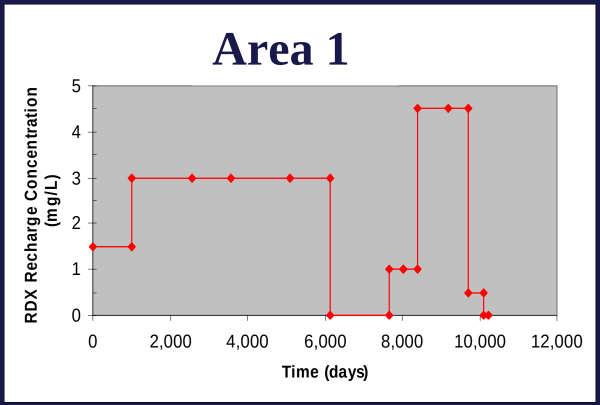
MODEL PREDICTED PARTICLE PATHS VS CURRENT PLUME CONFIGURATION

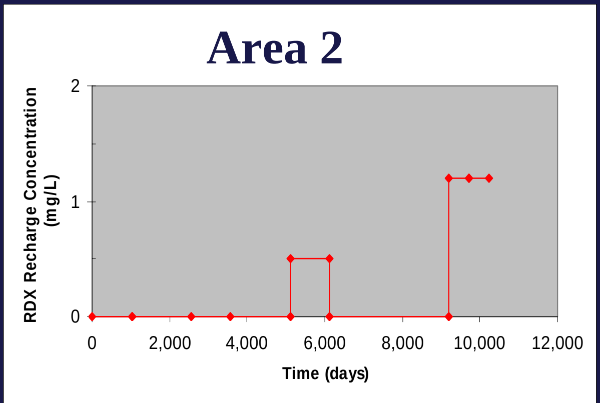
CALIBRATED F&T MODEL PARAMETERS

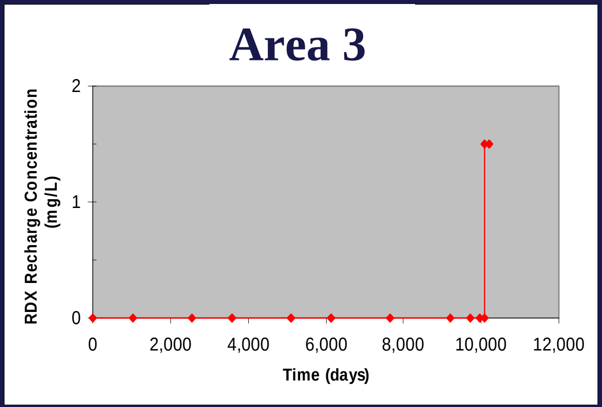
Parameter	Initial Value/Location	Calibrated Value/ Location	Reference/Comment
Porosity	0.39	0.39	
Soil Bulk Density (kg/L)	1.609	1.609	
Water-Soil Distribution Coefficient (L/kg)	0.056	0.056	Average of the Kd values for deep soil obtained by UTX (2001).
Dispersivity (ft)			Garabedian et al., WWR, May 1991
Longitudinal	3	3	
Transverse Horizontal	0.06	0.06	
Transverse Vertical	0.0015	0.0015	
First-Order Degradation Rate (day^{-1})	0	0	Negligible degradation of RDX (McGrath, 1994; JE Inc., June 2000).
Source Location(s)	Kettle Hole	Kettle Hole, southwest and northeast of Kettle Hole	Figure 5 shows calibrated location of RDX sources within Demo Area 1
Source Strength/ Concentration (µg/L)	120	0 – 4,500	Initial source concentration was calculated based on the estimated current RDX dissolved mass of 18 kg and the assumed release time of 30 years

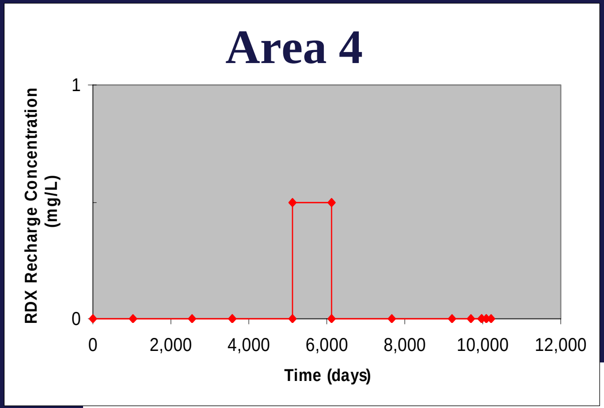
Note: Utilized porosity, soil bulk density and water-soil distribution coefficient values resulted in the retardation factor of 1.23.

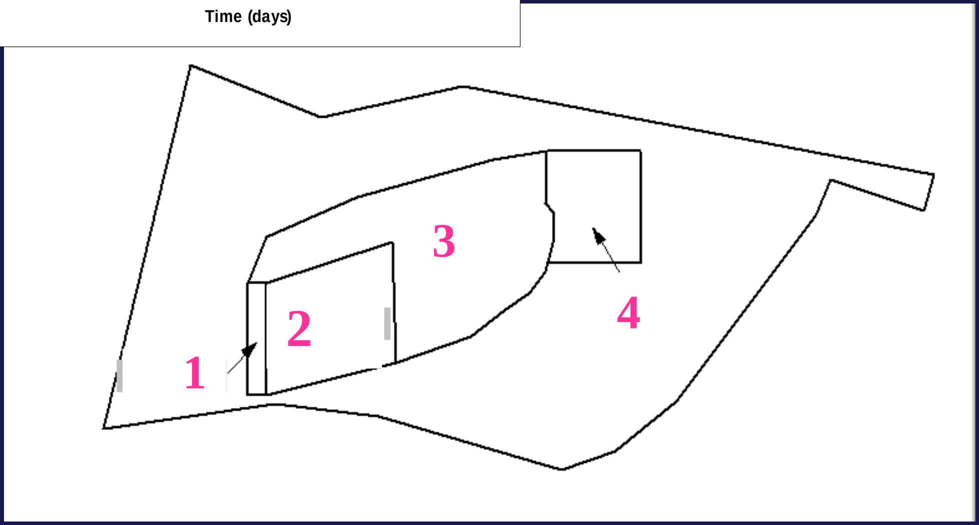
RECHARGE SOURCE TERMS







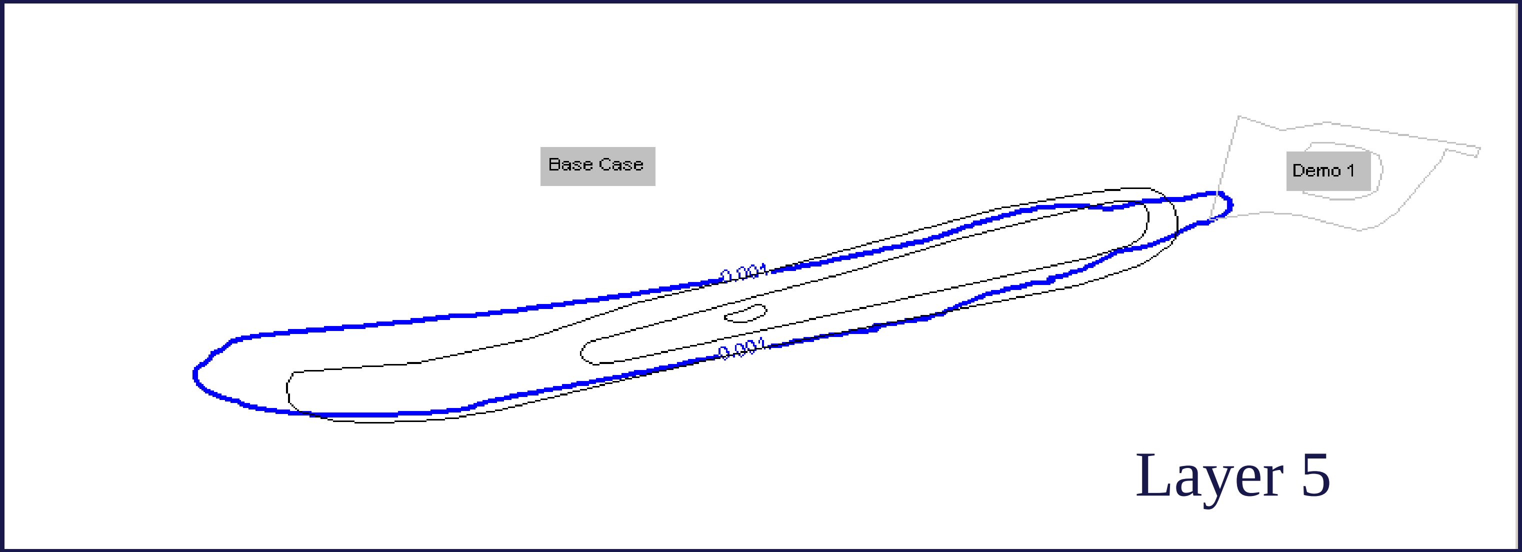




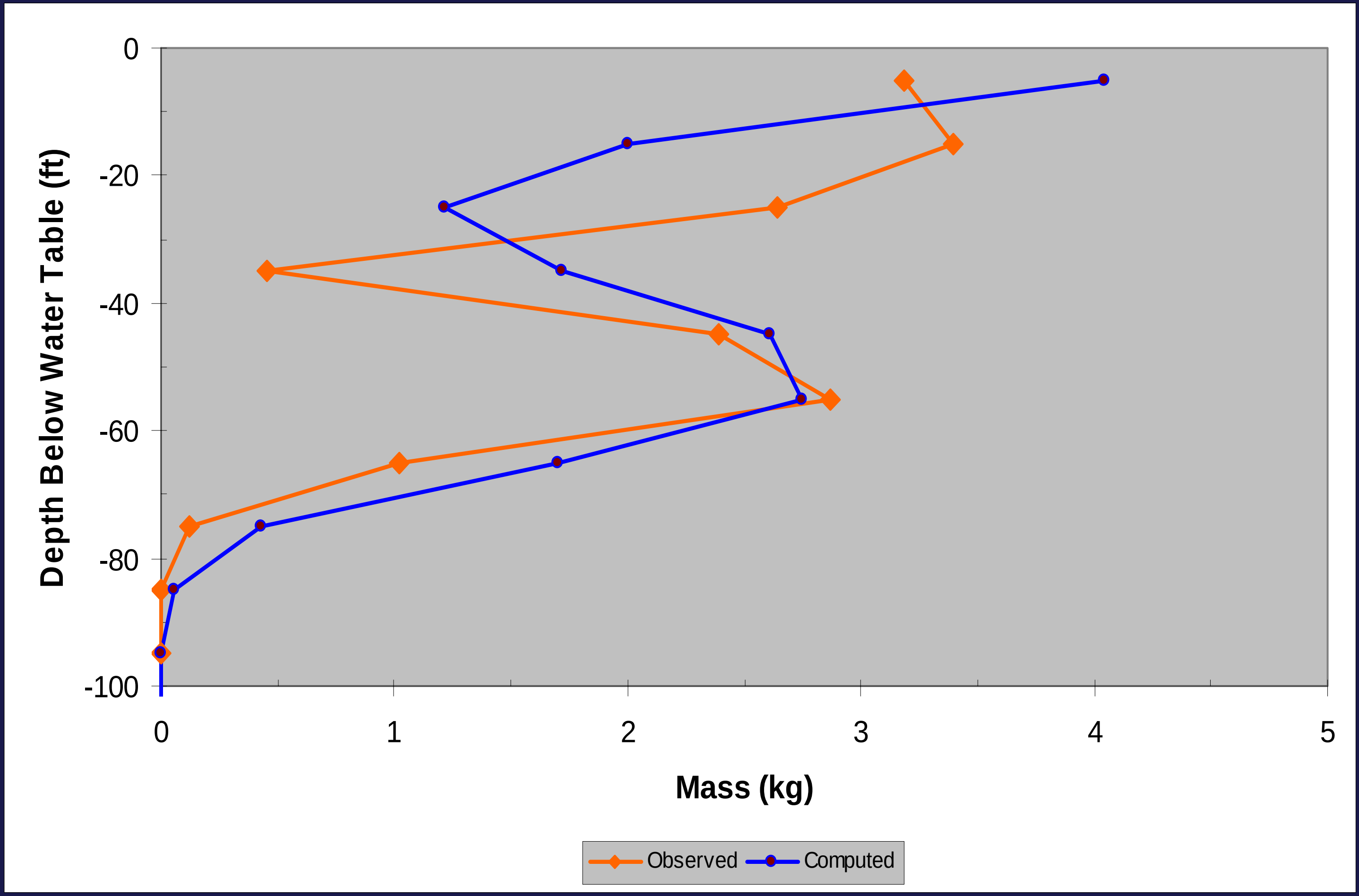
TRANSPORT CALIBRATION SUMMARY

PARAMETER	MODEL PREDICTED	OBSERVED/ ESTIMATED
Total Mass of Dissolved RDX (kg)	14	16
Width of RDX Plume (ft)	450	500
Length of RDX Plume (ft)	5,600	5,500
Depth of RDX Plume (ft bwt)	90	80
Maximum Concentration of RDX within Demo 1 (ug/L)	420	390

TRANSPORT CALIBRATION: PLUME GEOMETRY



SIMULATED RDX MASS WITH DEPTH

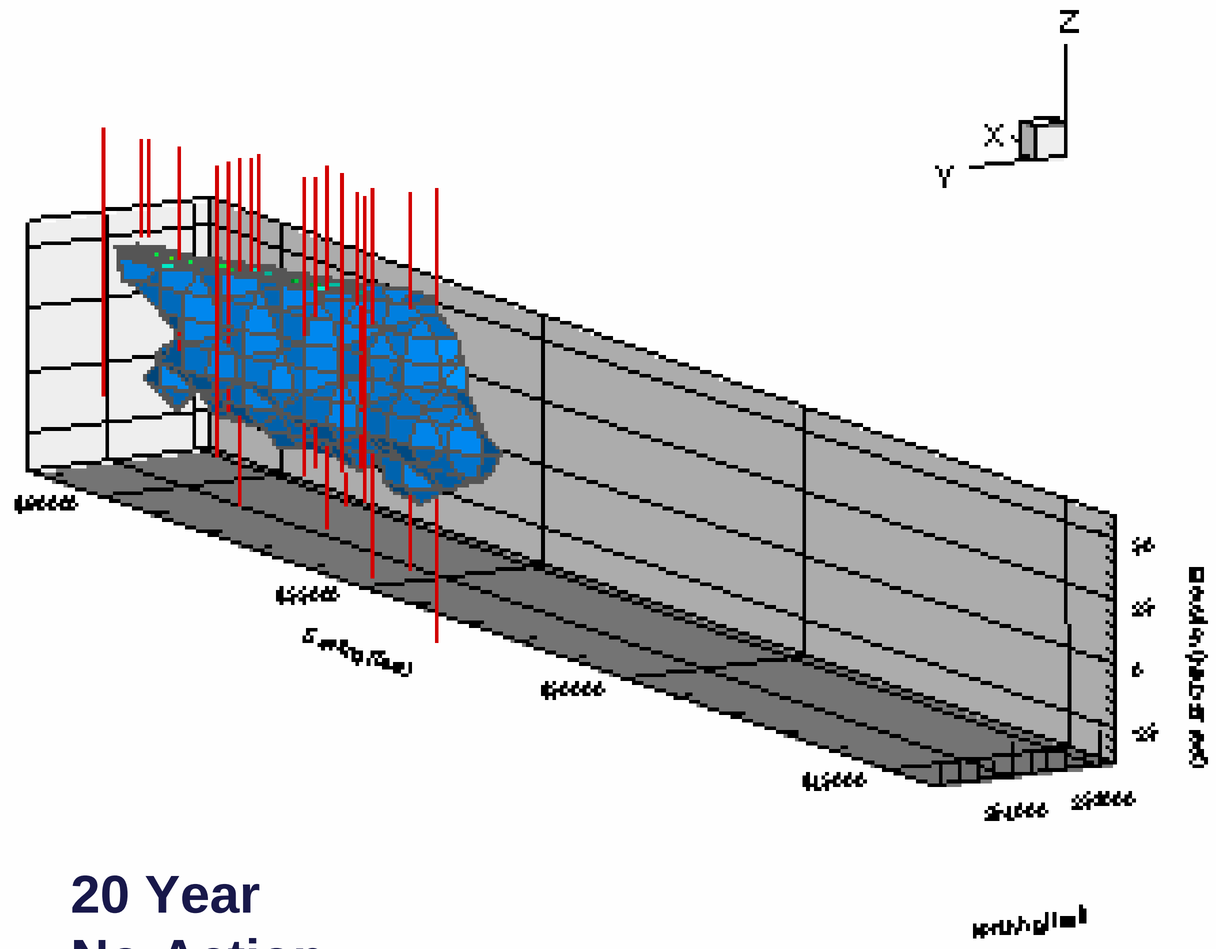


TRANSPORT SENSITIVITY ANALYSIS

Varied Parameter(s)	Interpreted RDX Mass (kg)	Simulated RDX Mass (kg)
Base Case (no variation)*	16.1	16.5
Water-Soil Distribution Coefficient (Kd)		
Kd=0.070 L/kg (increased by 25%)	16.1	15.7
Kd=0.042 L/kg (decreased by 25%)	16.1	17.4
Porosity (ϕ)		
ϕ=0.32	13.2	16.0
ϕ=0.42	17.3	16.7
Porosity and Water-Soil Distribution Coefficient		
ϕ=0.32, Kd=0.1 L/kg**	13.2	13.5
Dispersivity (λ_L)		
λ_L = 6 ft (increased by a factor of 2 in all layers)	16.1	16.5
λ_L = 30 ft in Layer 1, λ_L = 3 ft elsewhere (increased by a factor of 10 in Layer 1)	16.1	16.5

*Base Case combination of input parameters is shown in Table 1; **Same retardation factor as in the Base Case scenario.

DEMO 1: RDX 3-d PLUME ANIMATION

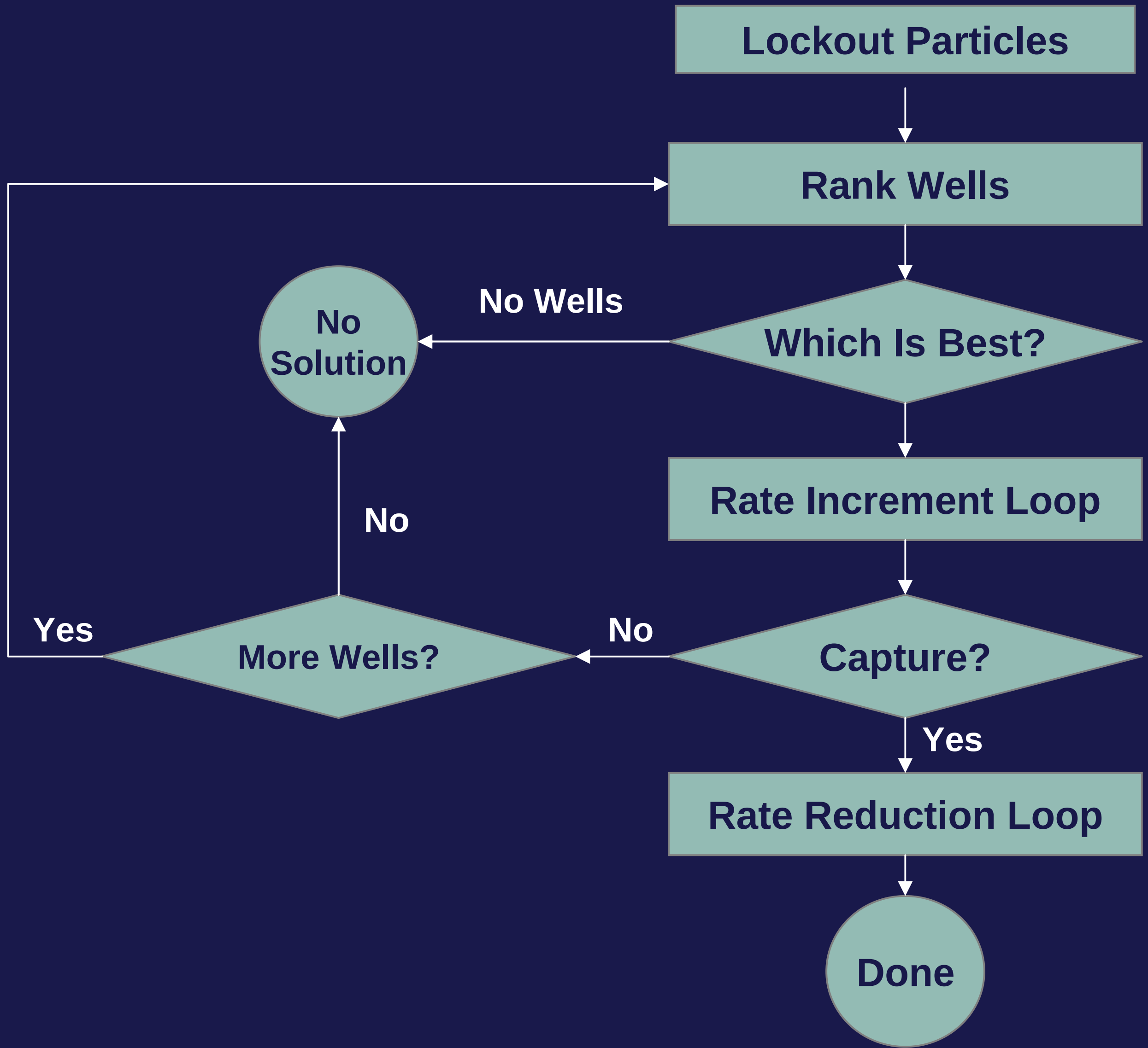


**20 Year
No-Action
Scenario**

OPTIMIZATION MODELING APPROACH

- Optimize extraction system design through iterative evaluation of capture at <u>all potential</u> well locations
  - every model cell or only “allowable” locations
- Plume represented by particles, capture success and time evaluated through standard forward particle tracking
- Weighting particles by mass density constitutes a proxy for more computationally intensive transport modeling and allows approximation of mass recovery
- Weighting particles by “pore volumes required for cleanup” provides a means of simultaneously evaluating multiple COCs

PARTICLE TRACKING OPTIMIZATION ALGORITHM



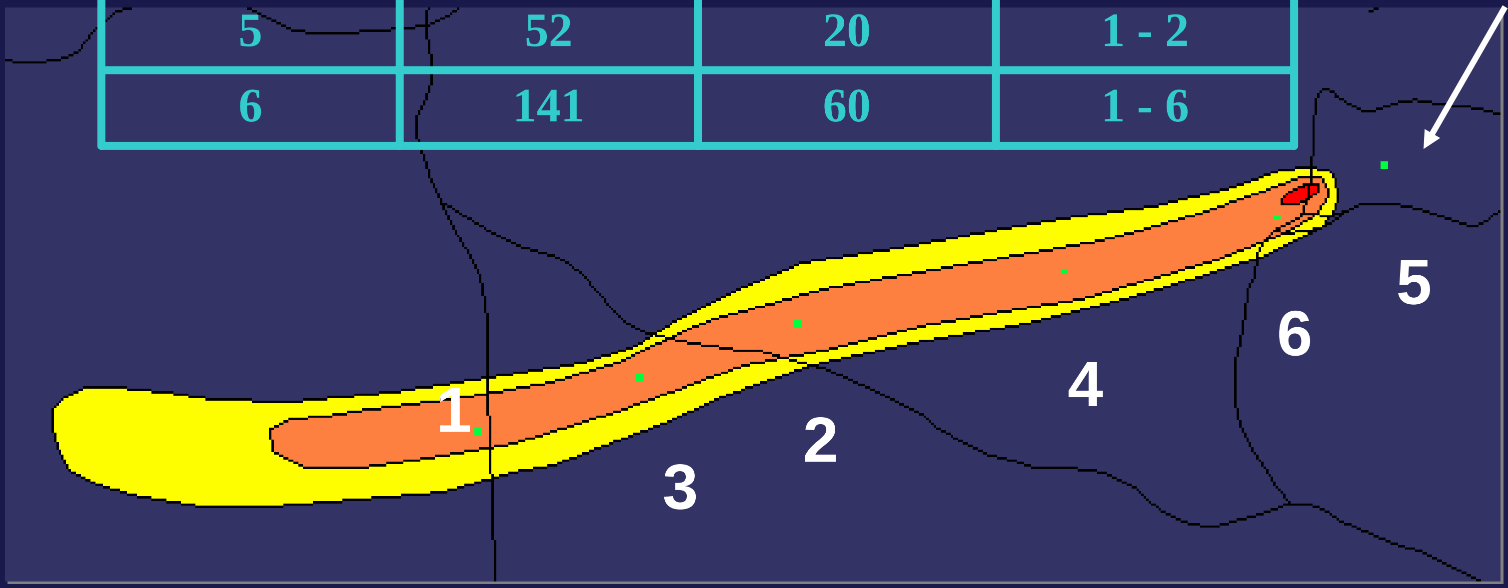
Find the well that captures the most particles with one simulation per well.

Gradually increment the rate for the chosen well to see if complete capture can be achieved.

Gradually decrease the rate for all chosen wells to see if capture can be maintained at lower pumping rates.

DEMO 1:PRELIMINARY 10-YEAR REMOVAL DESIGN OPTIMUM WELL LOCATIONS AND PUMPING RATES

Well	Q, gpm	Screen Length	Model Layers
1	189	90	4 - 11
2	189	90	4 - 11
3	189	90	4 - 11
4	182	70	2 - 8
5	52	20	1 - 2
6	141	60	1 - 6



COMPUTING PORE VOLUMES REQUIRED FOR CLEANUP

$n = \ln(C_s/C_i)/\ln(1-1/R)$ (Duetsch 1997)

where:

n = number of pore volumes required removing to achieve standard

C_s = groundwater standard

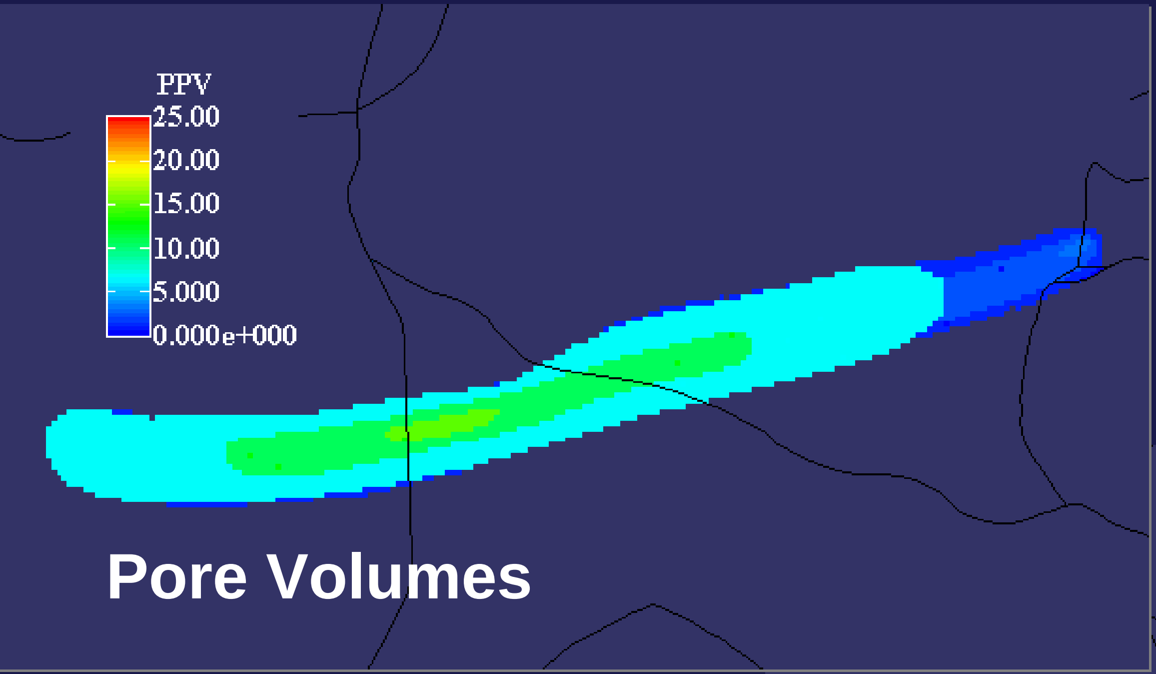
C_i = initial concentration

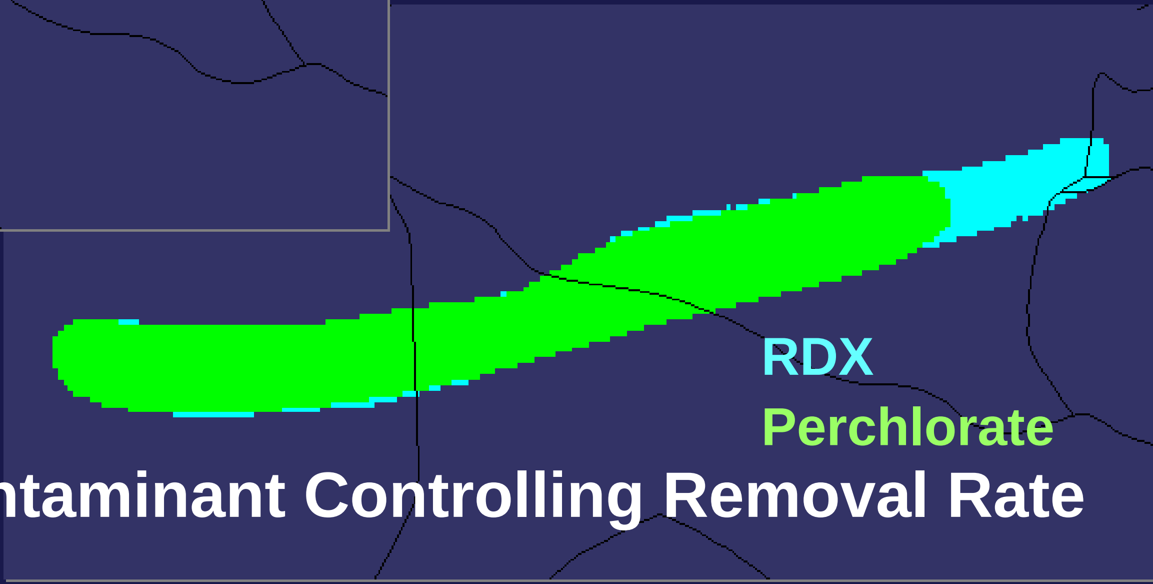
R = retardation factor

COMPARISON OF PORE VOLUMES REQUIRING REMOVAL TO ACHIEVE STANDARD

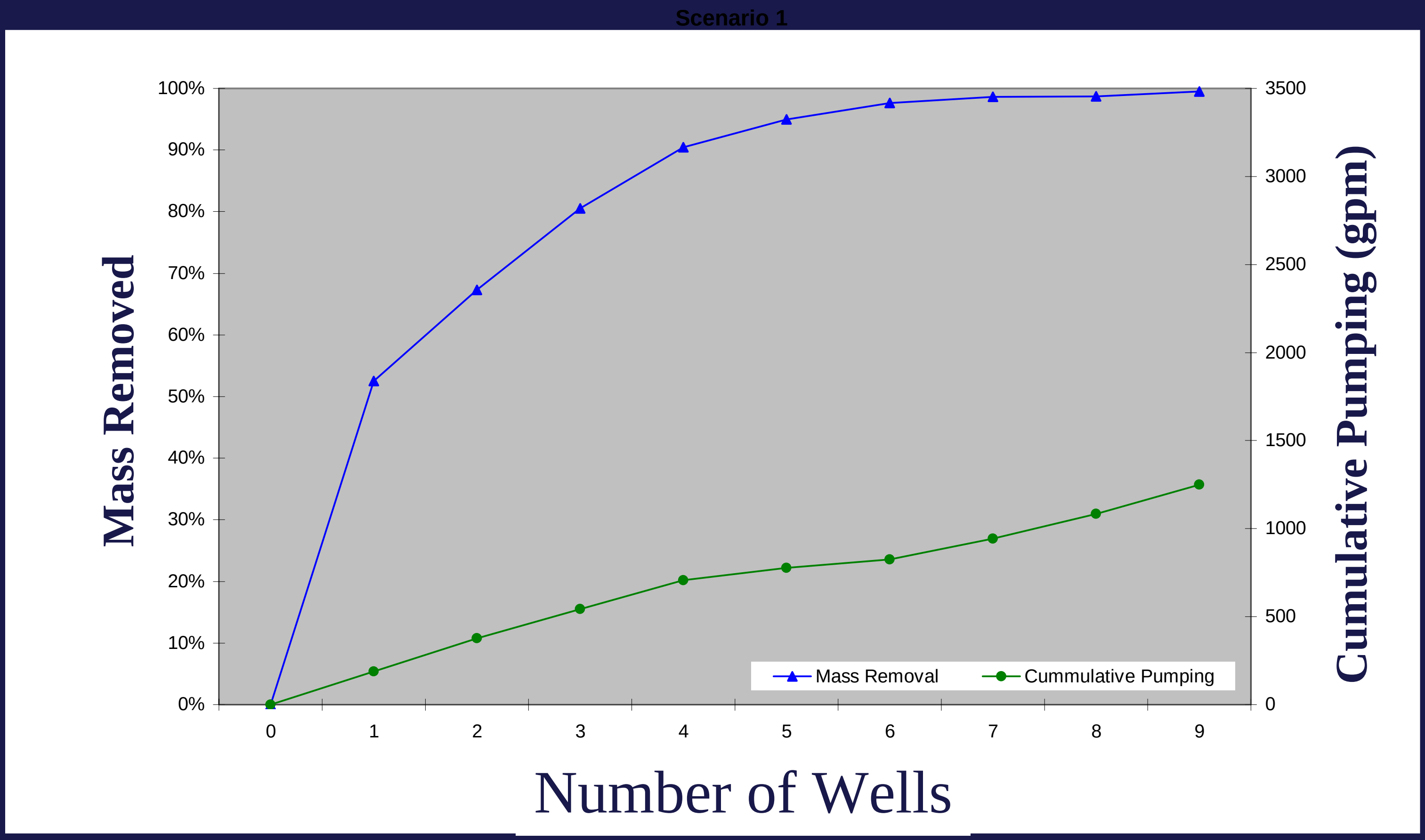
Contaminant	Initial Concentration ug/L	Groundwater Standard, ug/L	Retardation Factor	Pore Volumes Requiring Removal to Achieve Standard	Required Days to Remove 1 Pore Volume for 10-Year Cleanup
RDX	100	0.20	1.17	3.22	1133
TNT	100	0.20	2.07	9.42	388
Perchlorate	100	0.35	3.14	14.75	247
2,4-DNT	100	0.20	16.51	99.46	37

LAYER 6 – PORE VOLUMES REQUIRING REMOVAL TO ACHIEVE STANDARD

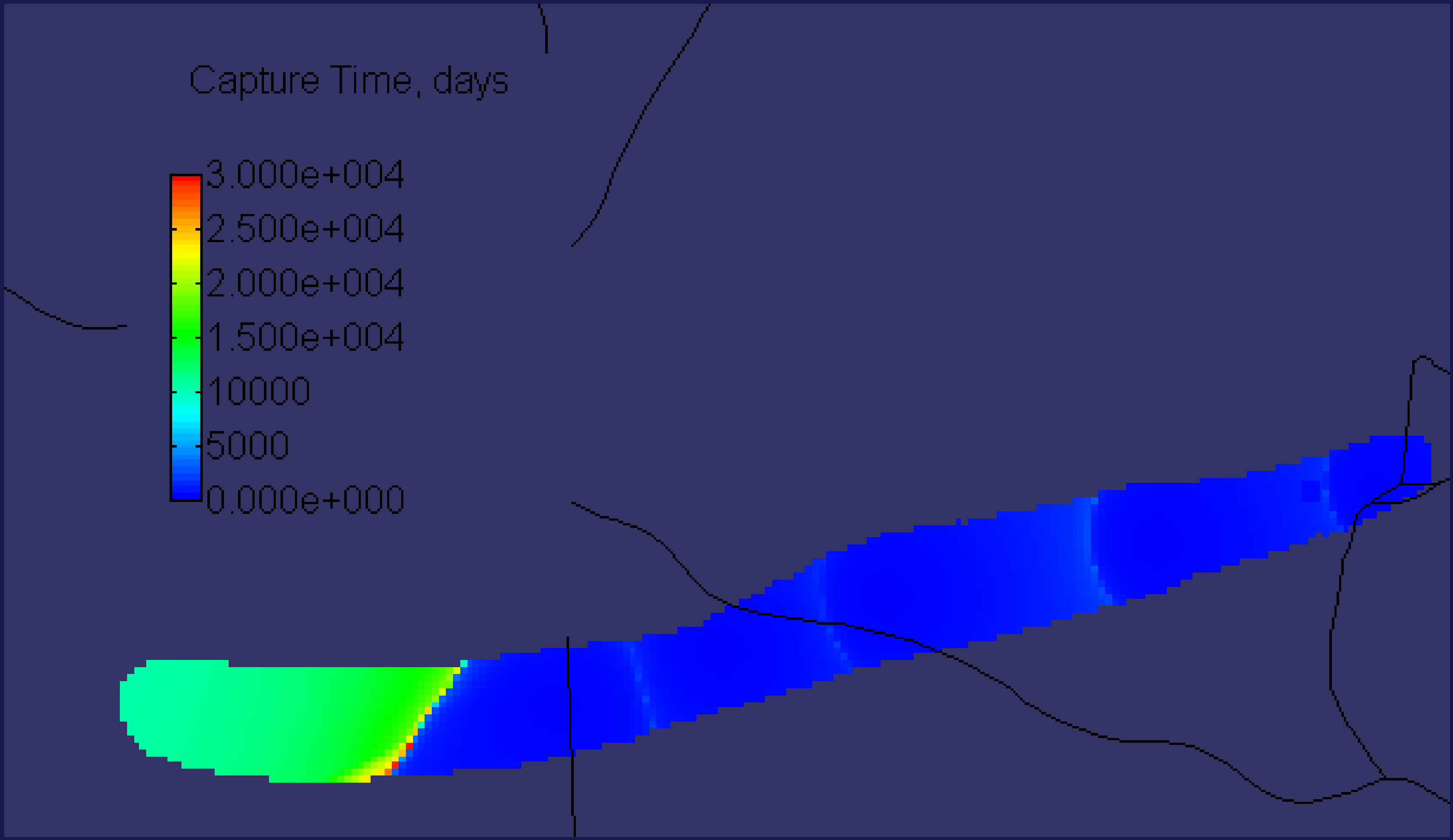




DEMO 1: PRELIMINARY 10-YEAR REMOVAL DESIGN MASS REMOVAL



DEMO 1:PRELIMINARY 10-YEAR REMOVAL DESIGN LAYER 6 CAPTURE TIMES

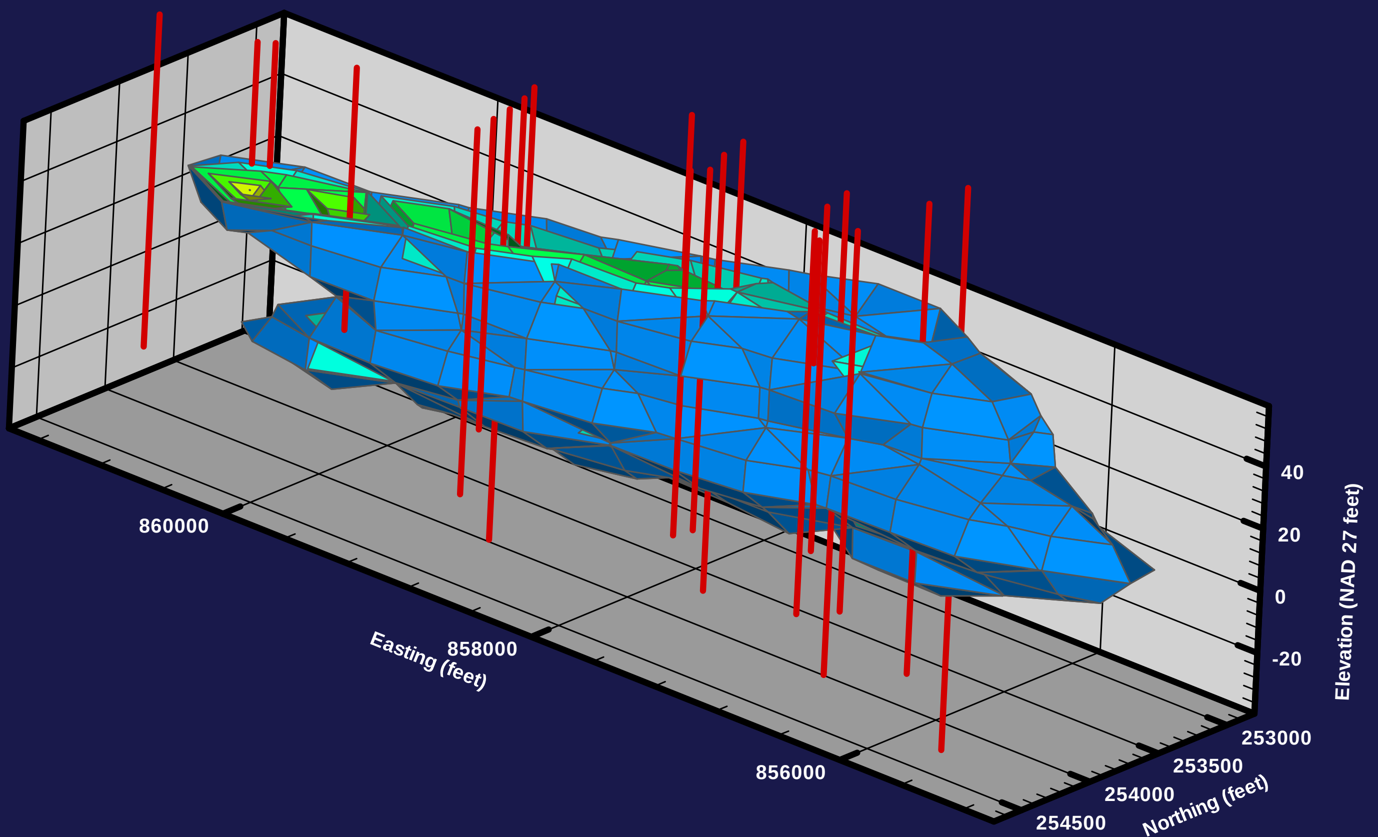


…. IN CONCLUSION

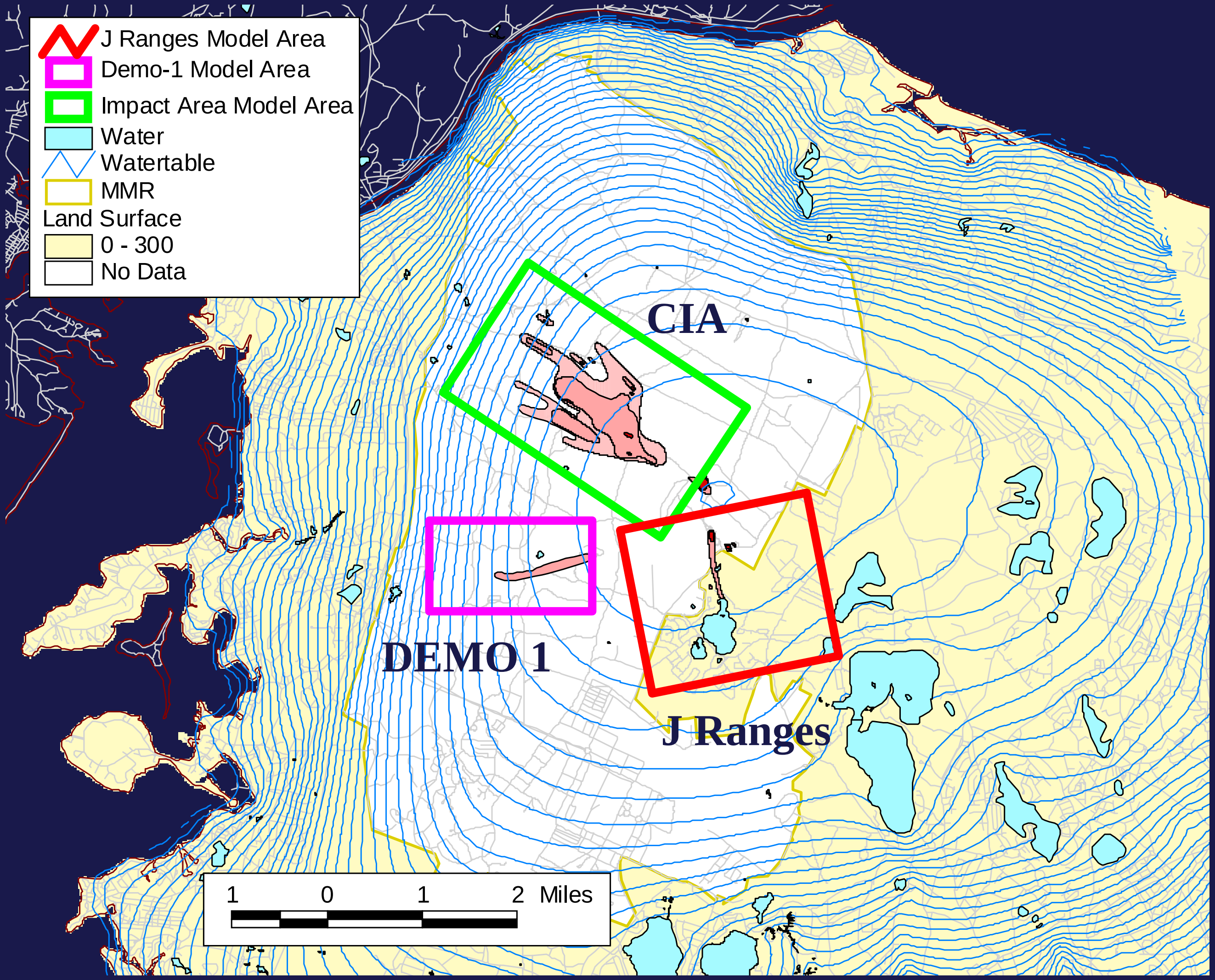
- **Regional and Subregional Flow Modeling**
  - ideal geology for Darcian assumptions and finite difference approach, public domain codes adequate
- **Transport Modeling**
  - literature values of major transport parameters appear reasonable
  - computationally intensive
- **Optimization Modeling**
  - replaces conventional trial & error approaches and speeds design
  - in conjunction with pore volume removal calculations provides a proxy for transport modeling (to be verified)
  - makes use of parallel computing (Brute Force)

Thanks!

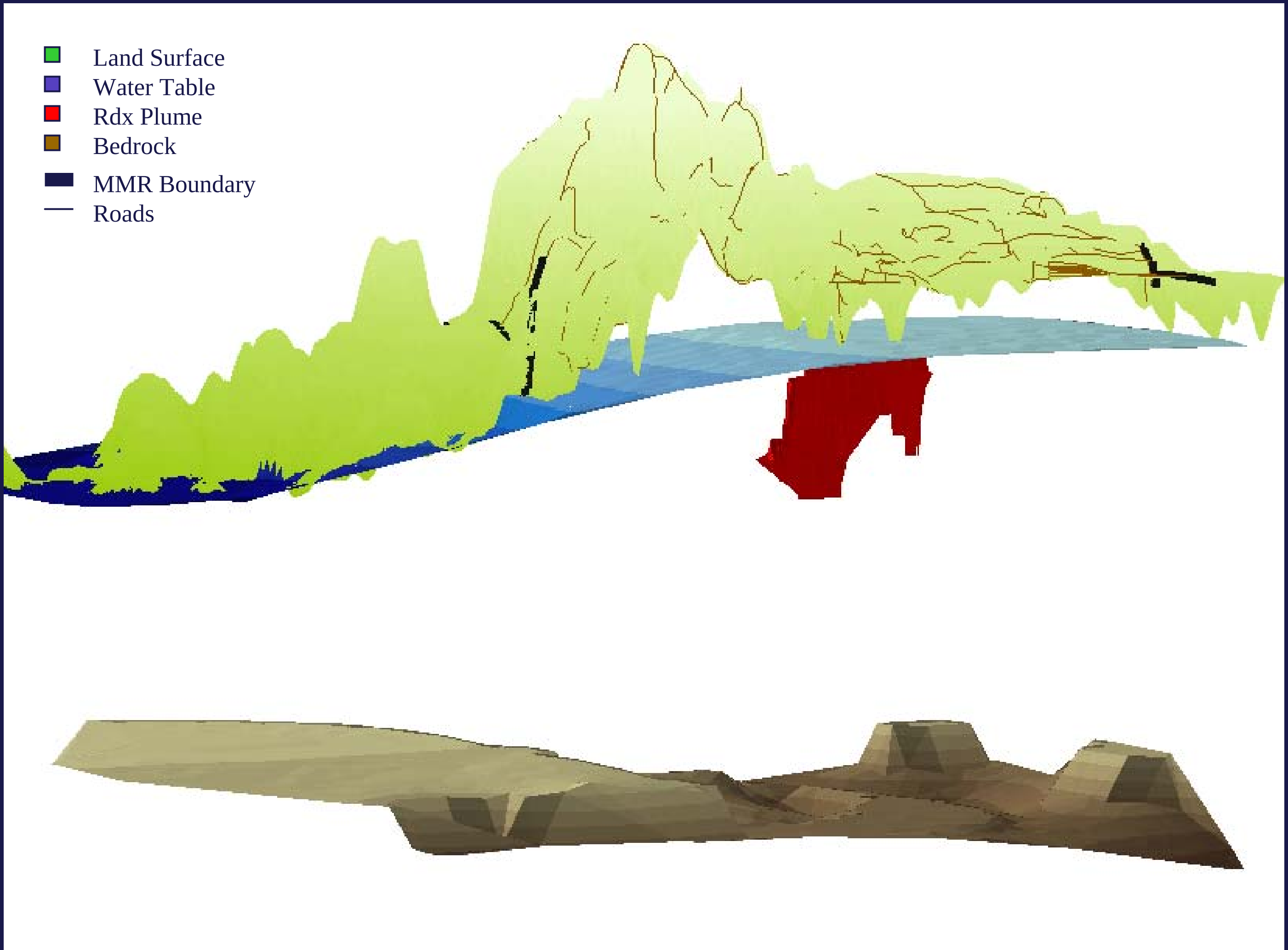
DEMO 1: RDX PLUME ISOSURFACES



SUB-REGIONAL MODEL GRIDS



DEMO 1 CONCEPTUALIZATION



RELATED TASKS

- **Particle tracking**

  1) assist monitoring well location and design and

  2) locate source areas related to groundwater detections

- **Zones of Contribution** (ZOCs)

  Updated for existing and proposed municipal water supply wells (42 total on Western Cape).

DEMO 1 LOCATION