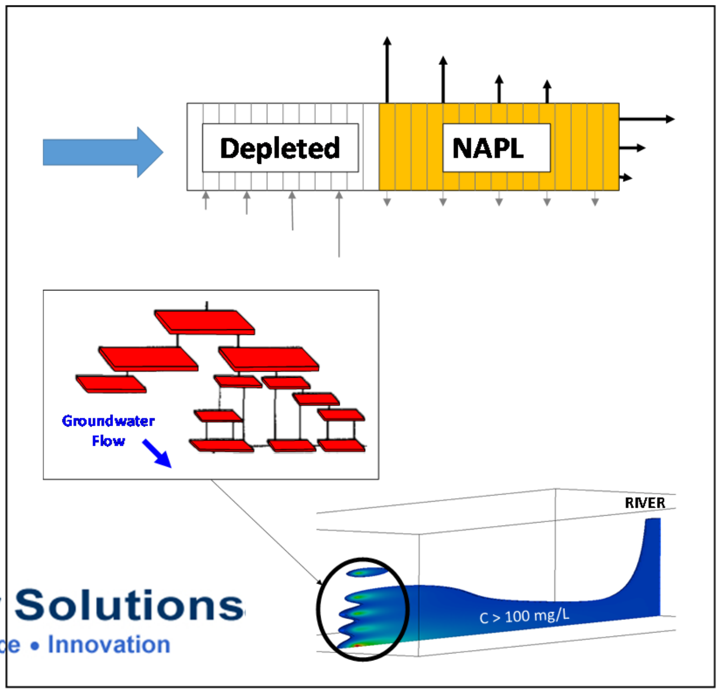
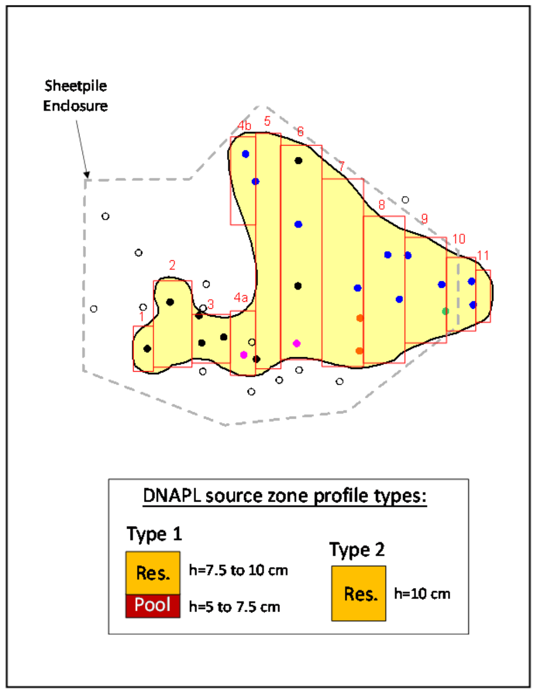
Modeling DNAPL Depletion for a Well-Characterized Source Zone

by Grant R. Carey, Ph.D.

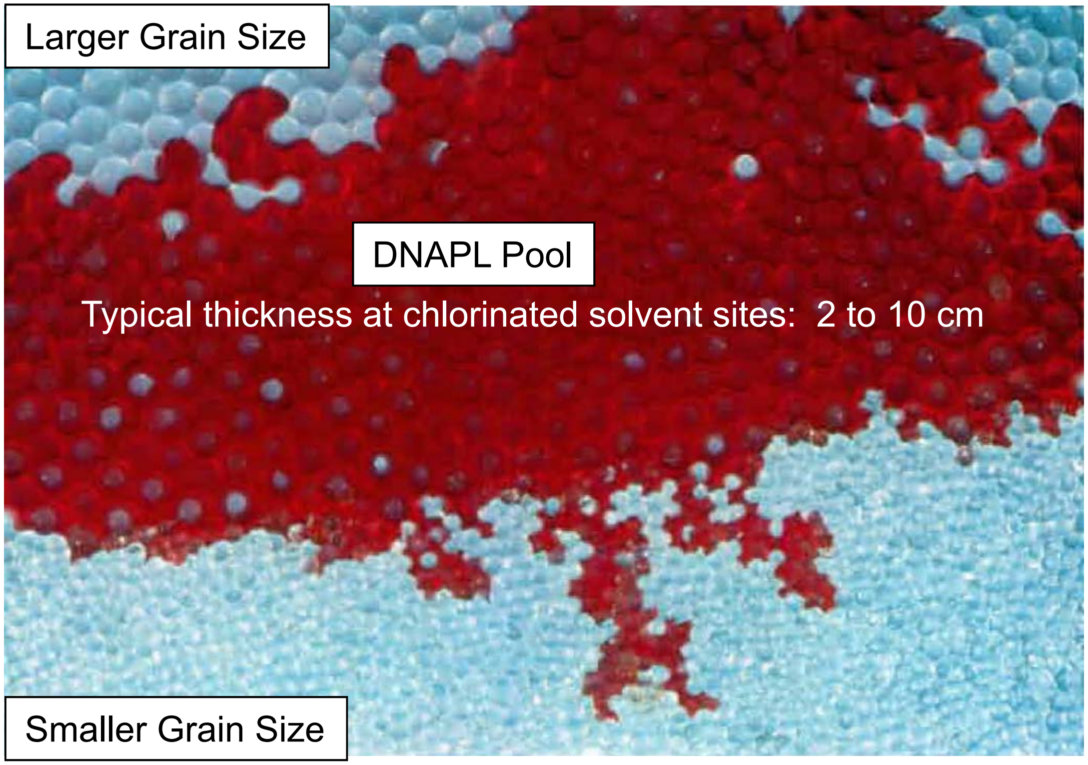
Porewater Solutions, Ottawa, Ontario, Canada





Porewater Solutions
Expertise • Experience • Innovation

NAPL Pool (Free Phase)



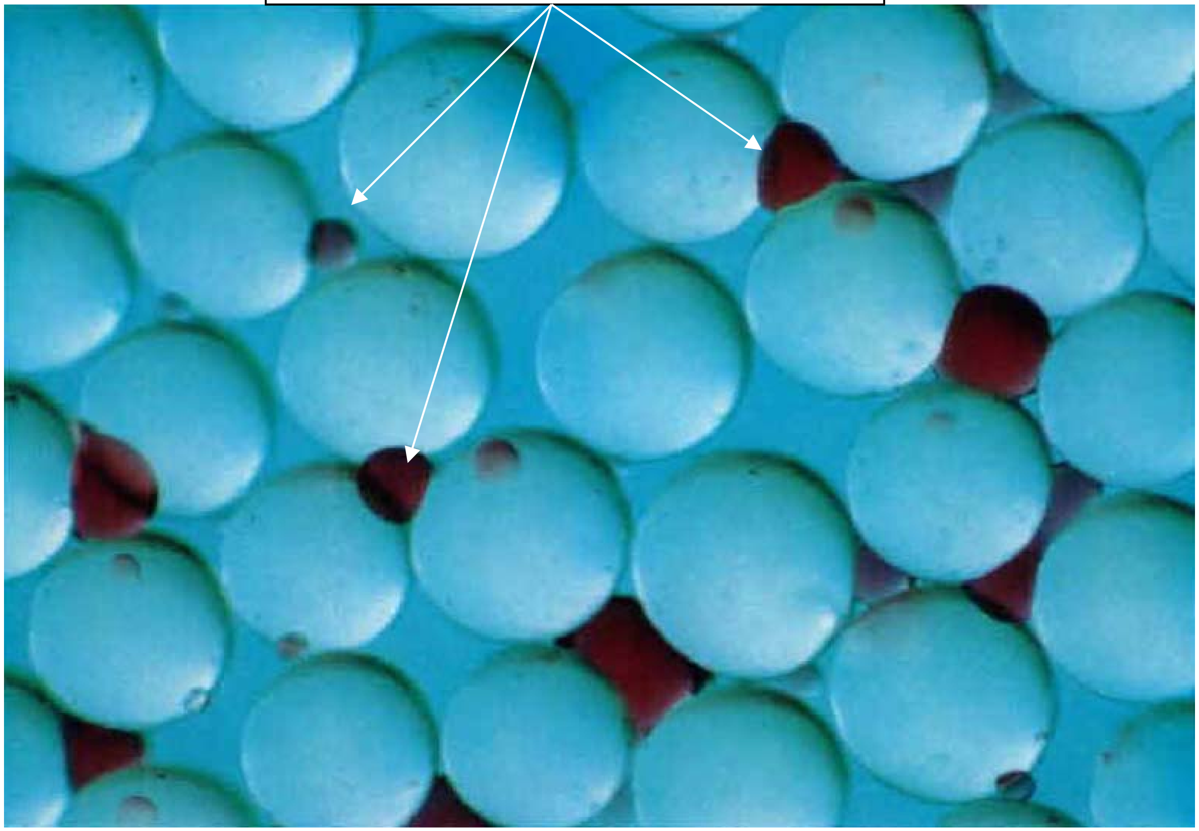
Source: *Schwille, 1988*

NAPL Pools

- Above low-K soil
- Horizontal NAPL layer
- Large mass

Residual NAPL (Ganglia)

DNAPL Ganglia (singlets)



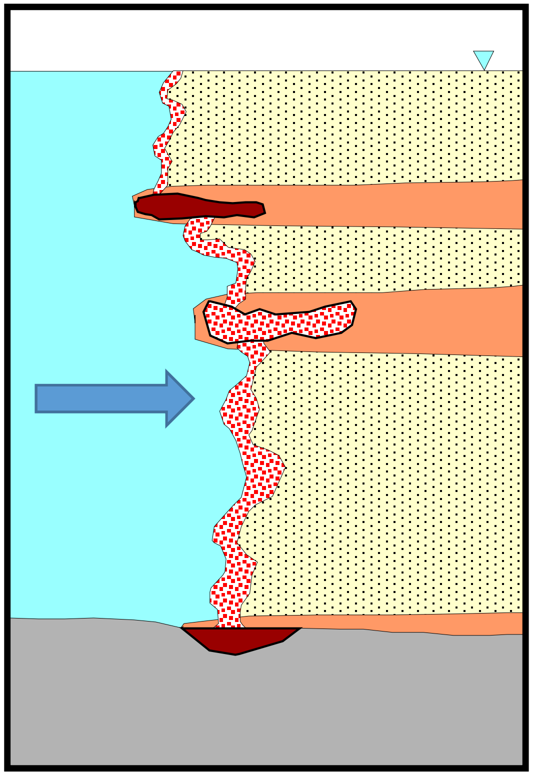
Source: *Schwille, 1988*

Residual NAPL

- Small
- Discontinuous
- Immobile

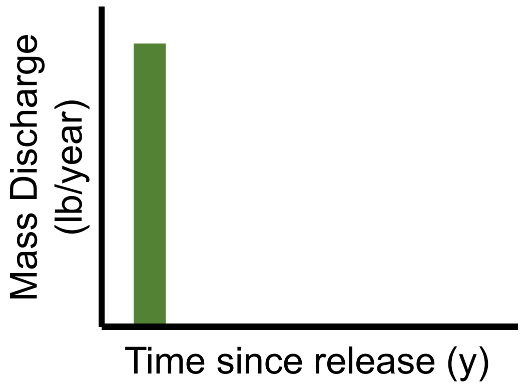
Mass Discharge Trends

Fresh Source



Modified from Parker et al., 2003

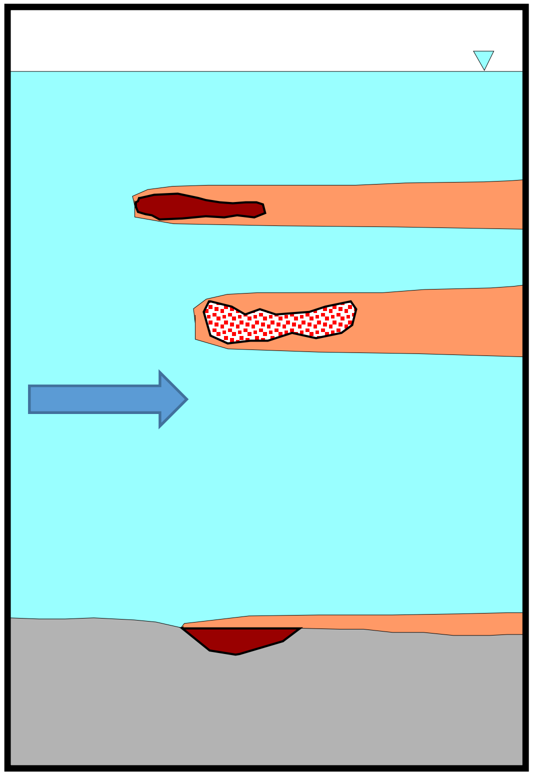
Mass discharge from source zone (kg/y)

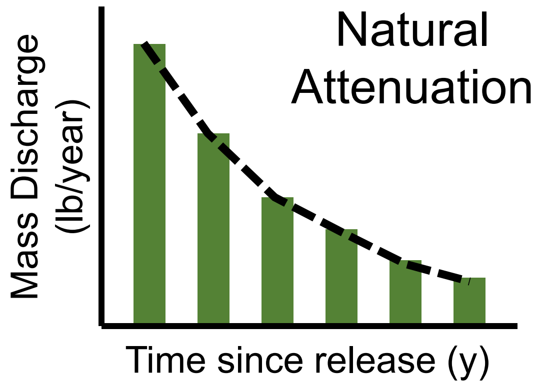


Mass Discharge Trends

Aged Source

Typical source zone mass discharge = 1 to 100 kg/year





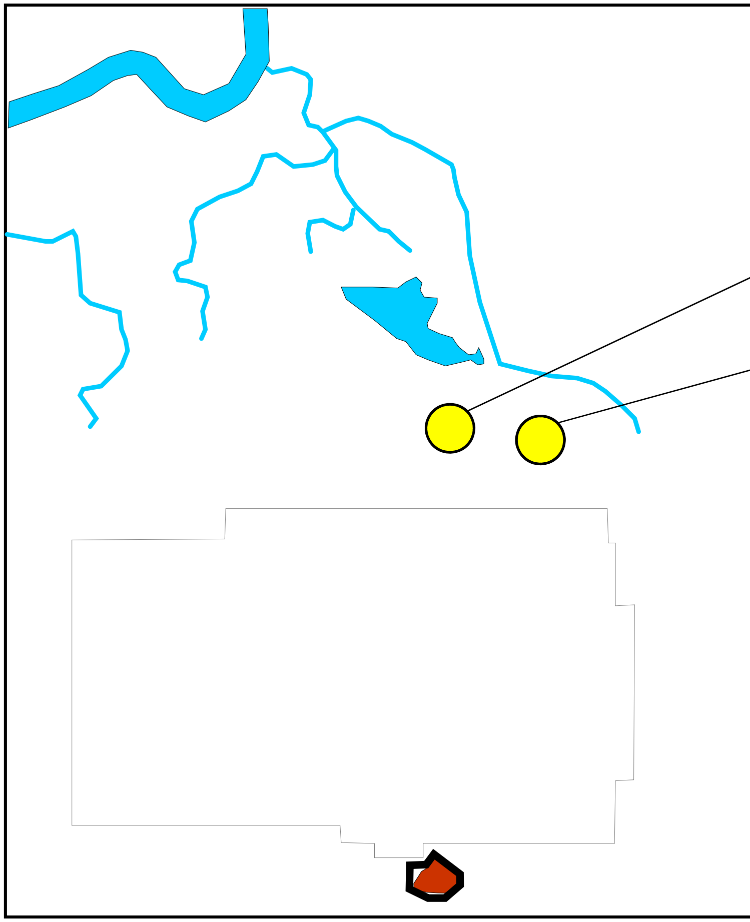
Newell et al., 2006:
Median TCE DNAPL half-life of 6 years

Mass discharge reduction 30x in 30 years

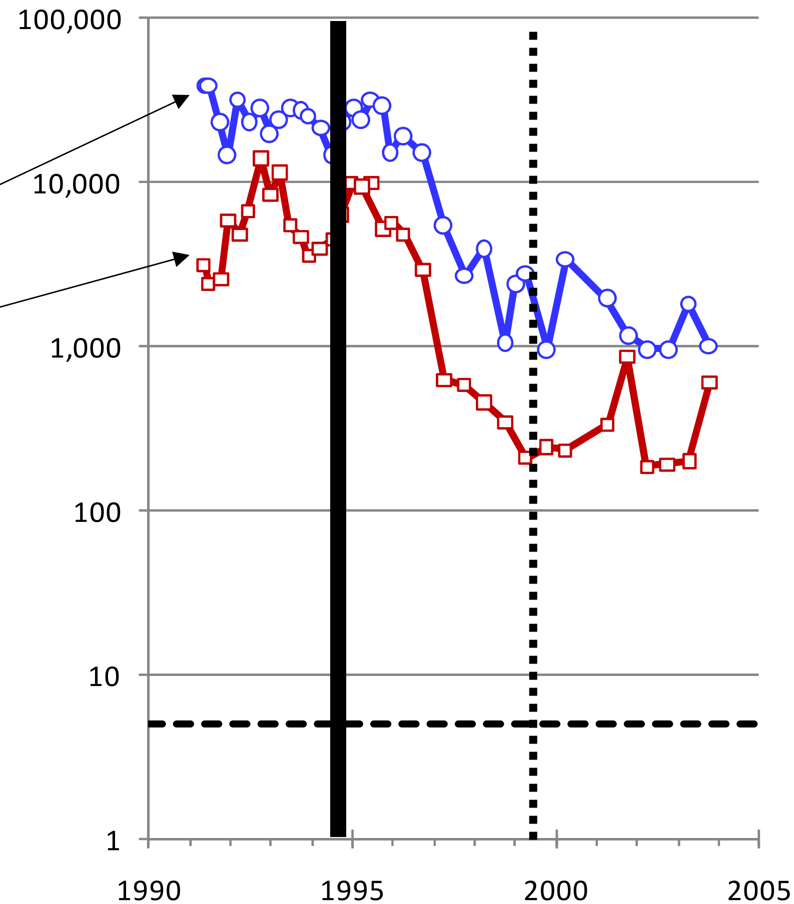
NAPL Depletion Model Uses

- Compare relative timeframes – natural and enhanced NAPL dissolution alternatives
  - Relative benefit of enhanced diss.
- Improved understanding
- Focus site investigation – key data gaps
- Check CSM – forensic evaluation of NAPL architecture
- Input for plume response model (REMCHLOR, MT3DMS)

Connecticut Site (Chapman & Parker, 2005)



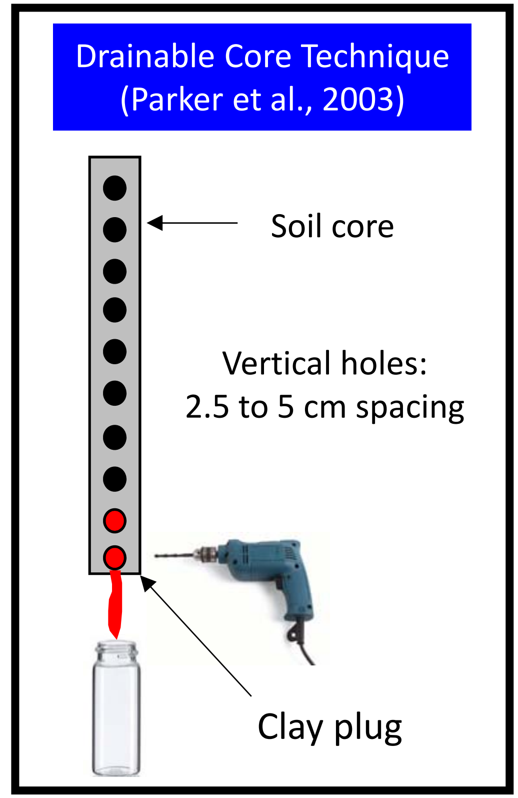
DNAPL Source Zone



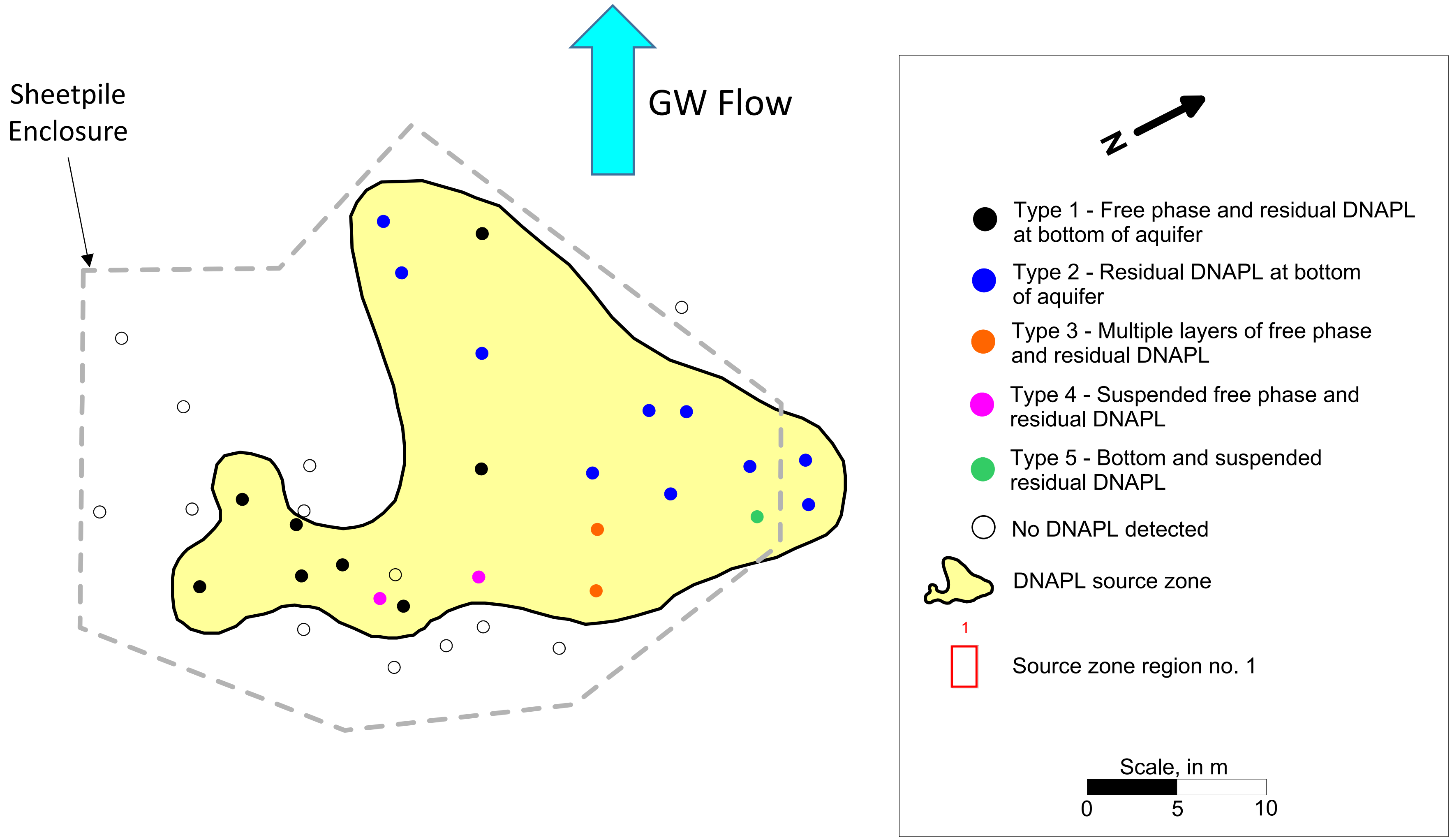
Concentration reduction stalled at 93% (15x)

Case Study: Beth Parker et al. (2003) CT Site

- Connecticut site
- Large DNAPL source zone
  - Bottom of sand aquifer, above aquitard
- Multiple lines of evidence
  - Visual inspection
  - Soil samples – close vertical spacing
    - Partitioning threshold, S_n, & layer thickness
  - Dye tests (Sudan IV)
  - Drainable core technique → Pool thickness

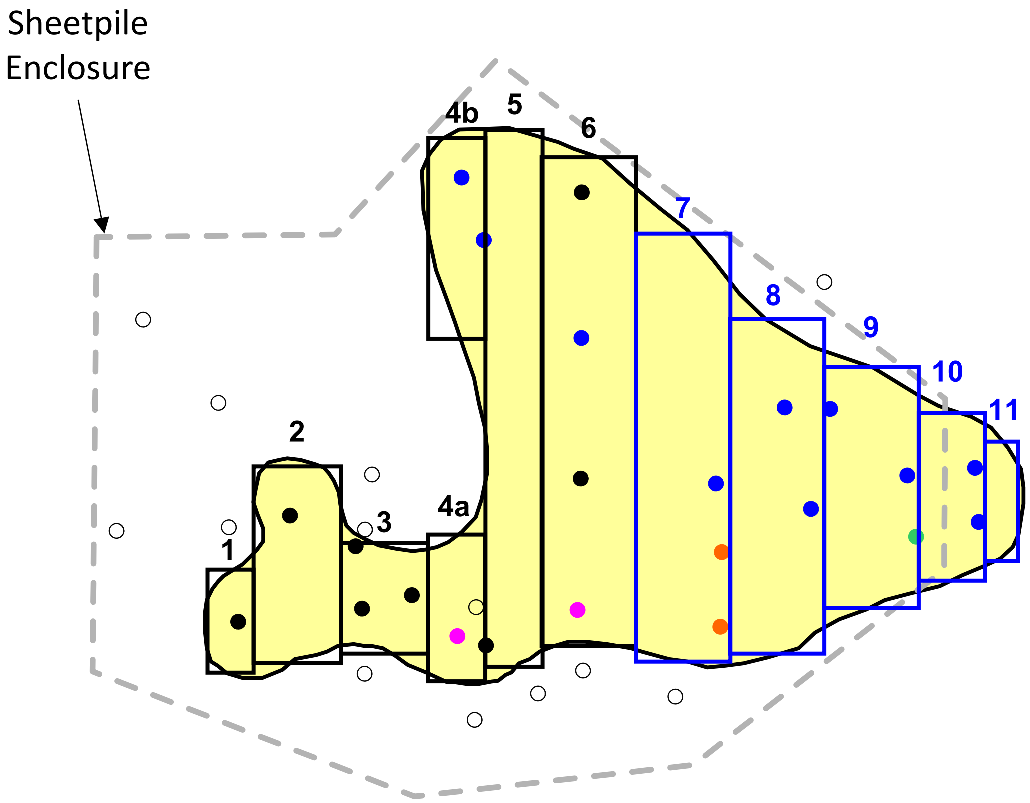


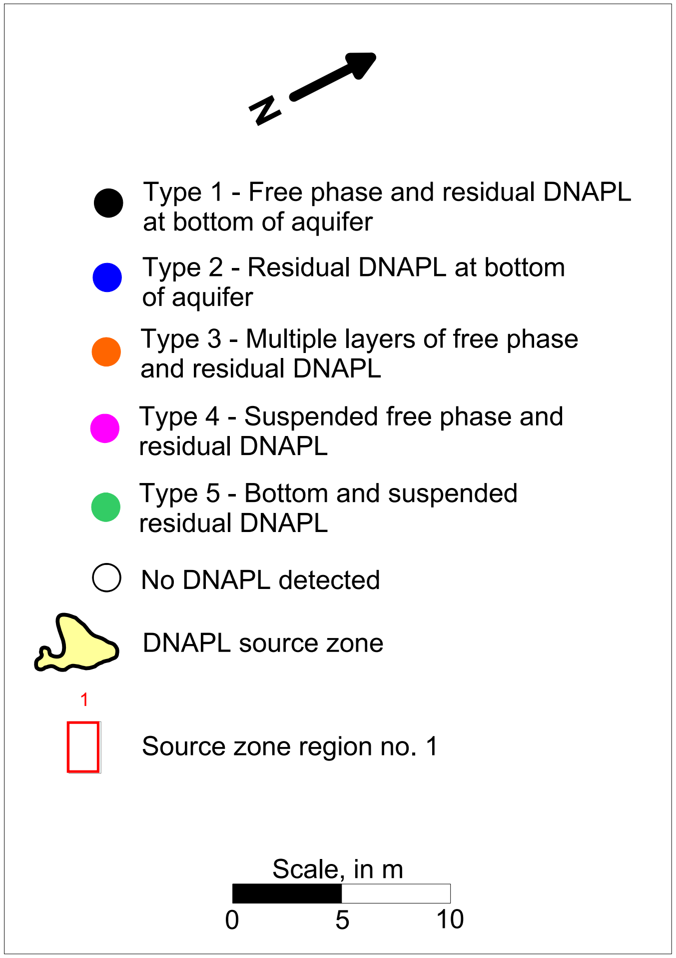
1996/97 Source Zone

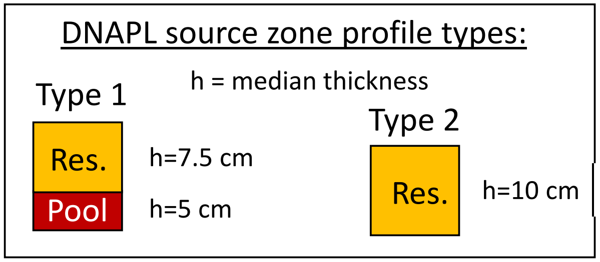


Data summarized in Stewart (2002) and Parker et al. (2003)

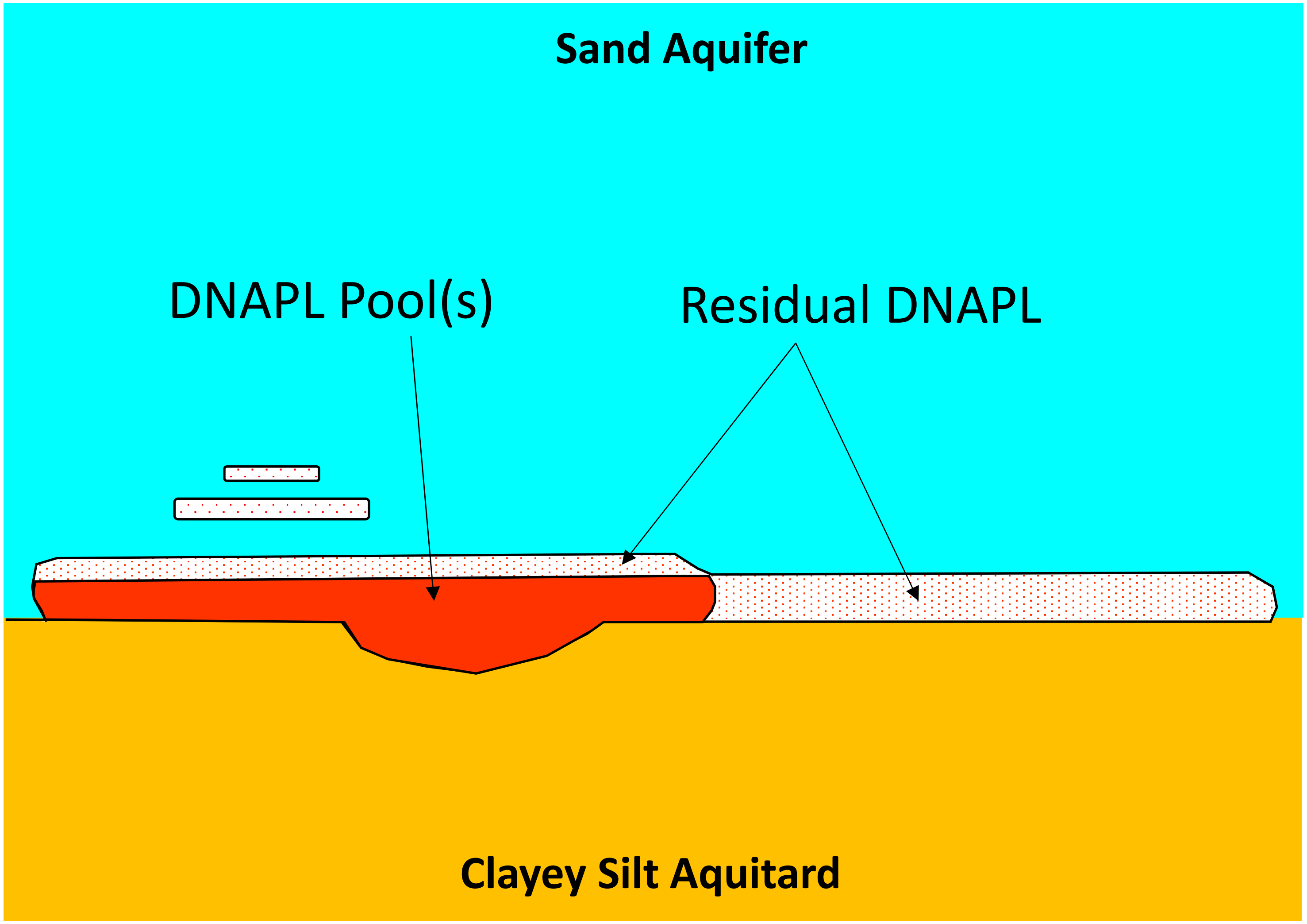
DNAPL Sub-Zones



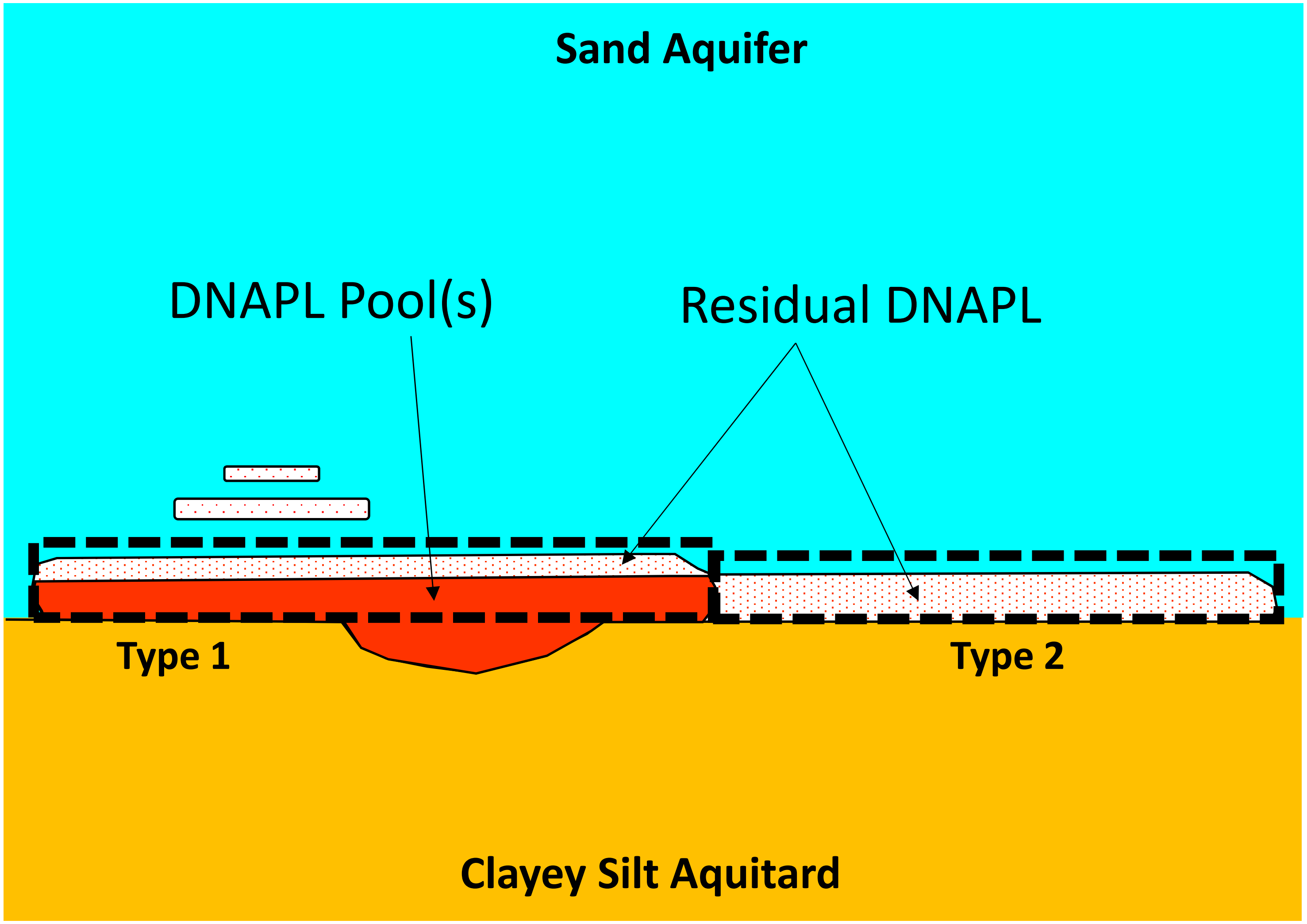




Typical DNAPL Architecture

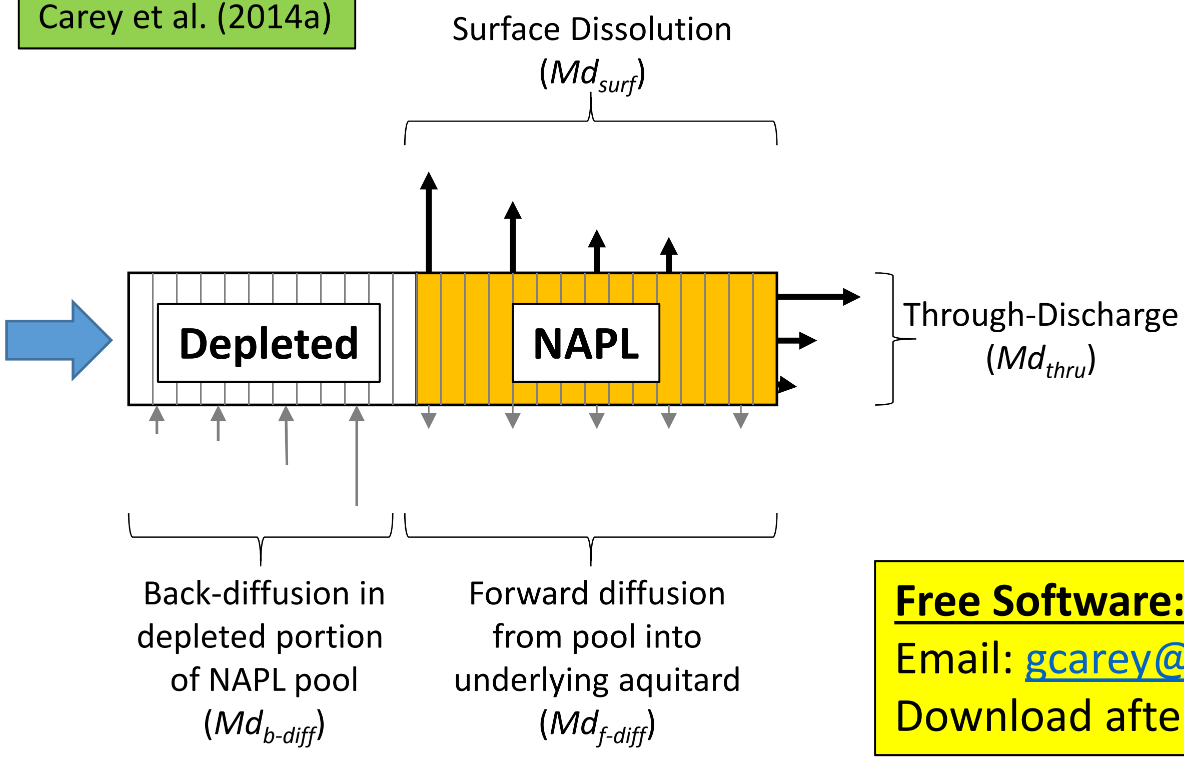


Typical DNAPL Architecture



NAPL Depletion Model (NDM): Mass Discharge-Based

Carey et al. (2014a)



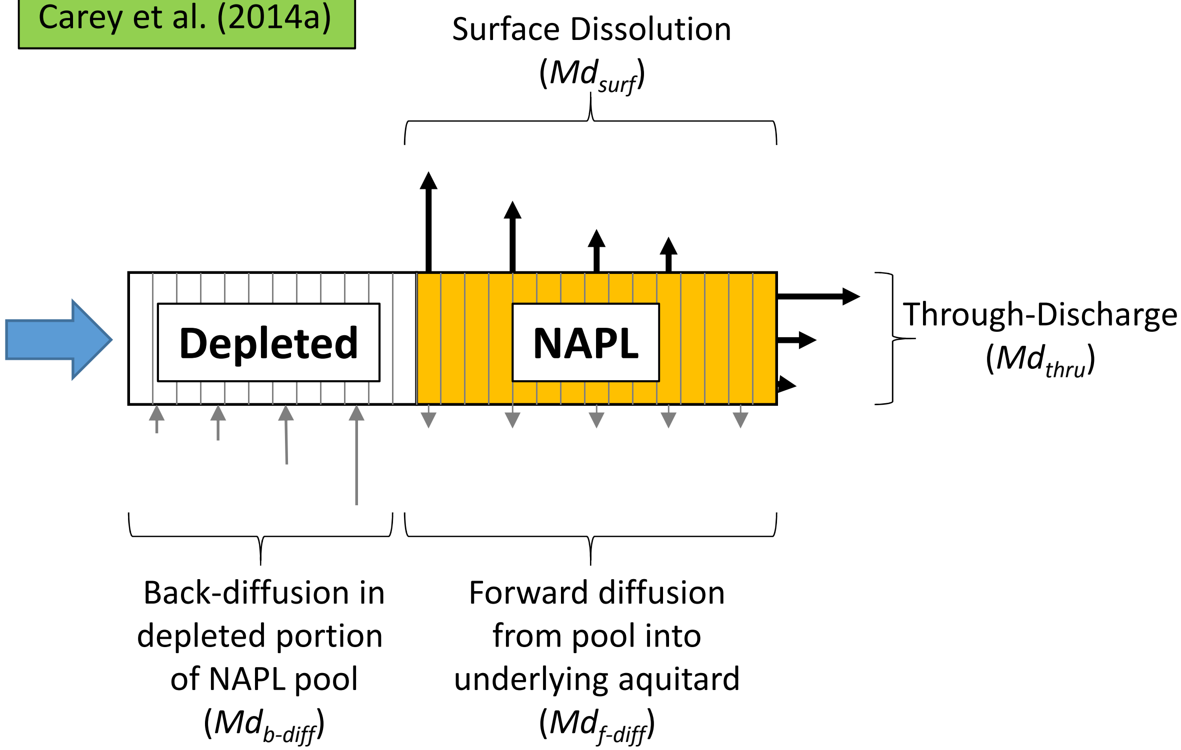
Free Software:

Email: gcarey@porewater.com

Download after Sep. 30th: www.porewater.com

NAPL Depletion Model (NDM): Mass Discharge-Based

Carey et al. (2014a)



Empirical Relationship (*K* in m/s)	
$\tau = 0.60\ K^{0.030}$	(i)
$\theta_t = 0.30\ K^{-0.026}$	(ii)
$\theta_e = 0.41\ K^{0.064}$, $K \le 1\text{x}10^{-2}$ m/s	(iii)
$\theta_e = (0.29\ K^{-0.026}) - 0.03$, $K > 1\text{x}10^{-2}$ m/s	(iv)
$\alpha_{TV} = 0.08\ K^{-0.16}$, $v \le v_c$	(v)
$\alpha_{TV\_NE} = 0.08\ K^{-0.16}\ (v_c/v)^{0.5}$, $v > v_c$	(vi)
$\alpha_{aw} = 0.112\ (100\ K)^{0.211}$	(vii)
$n = 13.14\ (100\ K)^{0.246}$ $K \ge 1\text{x}10\text{-}4$ m/s	(viii)
$S_{wr} = 0.015\ (100\ K)^{-0.218}$	(ix)

Carey et al. (2015a,b,c)

Model Validation Goals

1. DNAPL mass in simplified source zone consistent with Chapman and Parker (2005).

2. Initial (1994) Mass discharge – estimated to be 360 to 720 kg/y.

3. Mass discharge decline half-life – estimated to be about 10 years (Chapman and Parker, 2005).

NDM Simulation Results

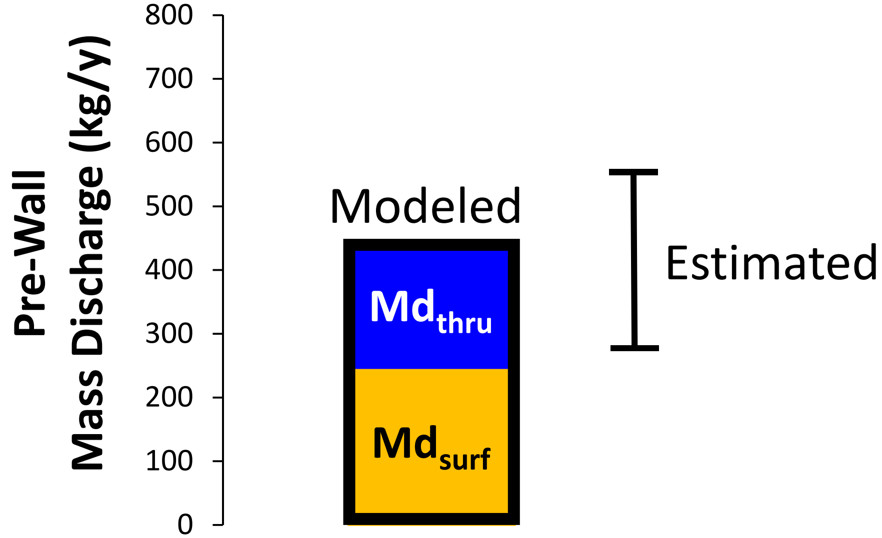
- Simulated DNAPL mass = 4,250 kg
  - Chapman and Parker (2005) estimated 5,000 to 20,000 kg
  - Our simplified source zone ignored several large areas with thicker DNAPL
    - Limited contribution to overall mass discharge
    - Simulated DNAPL mass consistent with observed on that basis

NDM Simulation Results

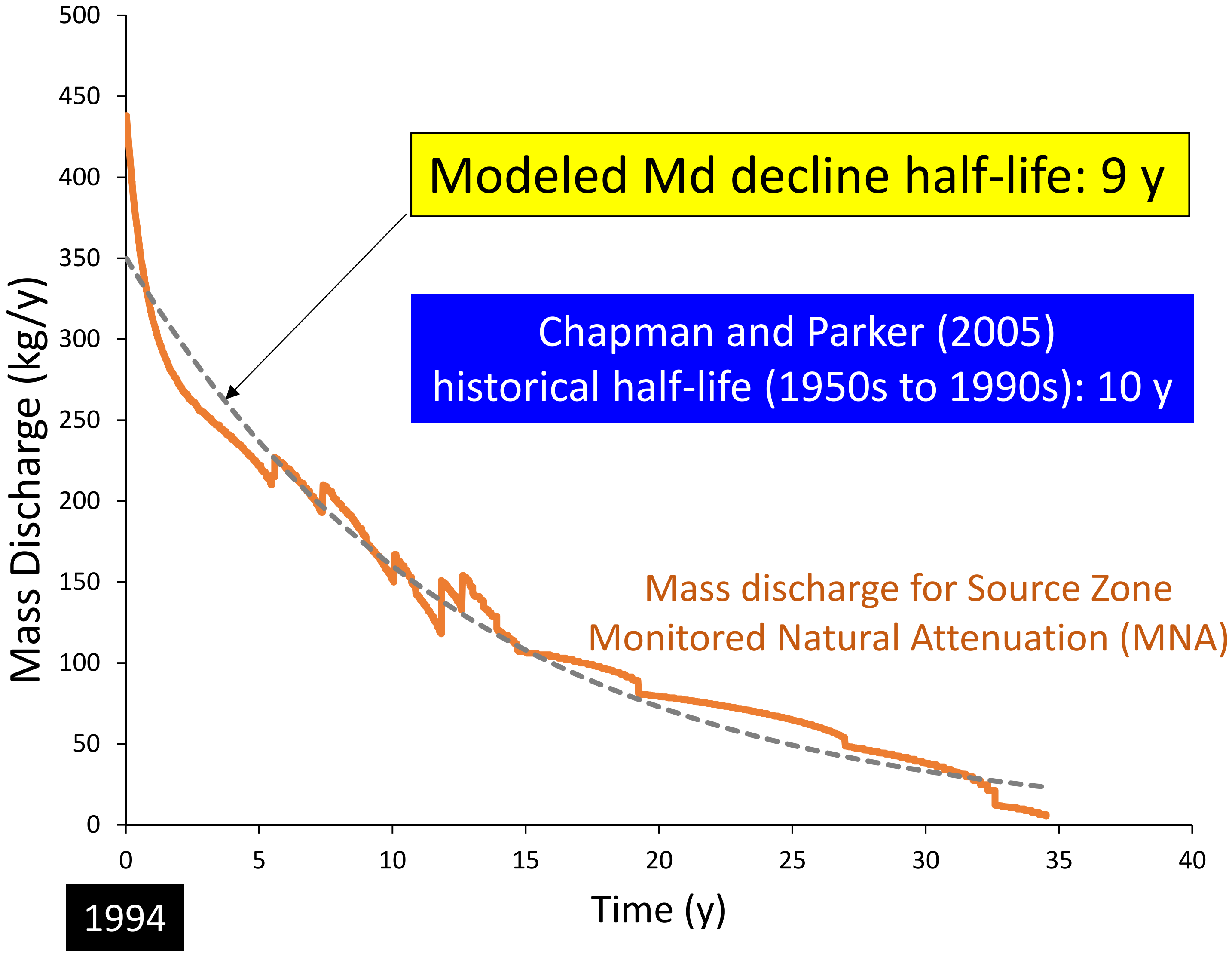
- Simulated DNAPL mass = 4,250 kg
  - Chapman and Parker (2005) estimated 5,000 to 20,000 kg
  - Our simplified source zone ignored several large areas with thicker DNAPL
    - Limited contribution to overall mass discharge
    - Simulated DNAPL mass consistent with observed on that basis

---

- Simulated 1994 Mass Discharge

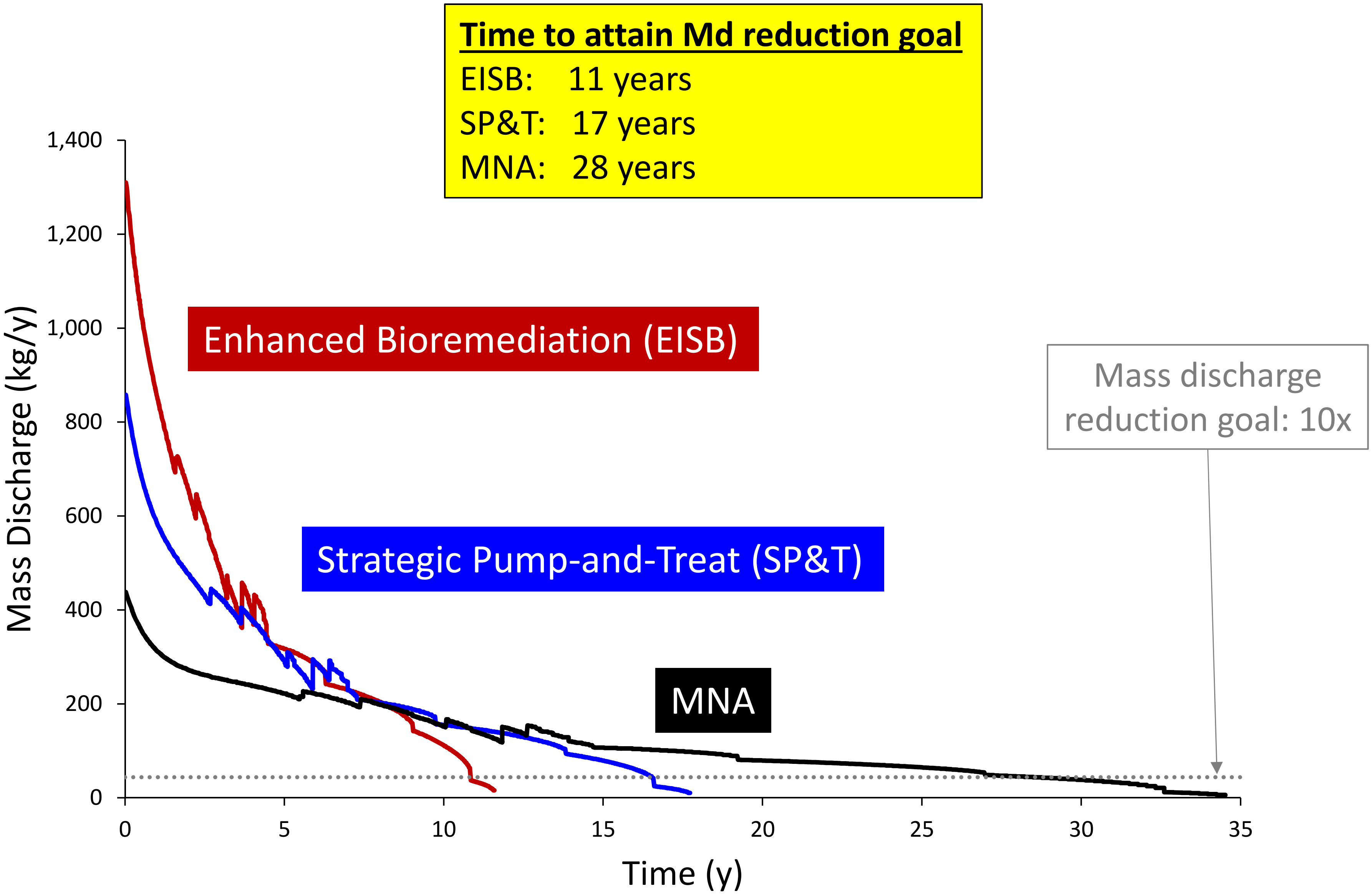


Modeled vs. Estimated Md Half-Life



Md = Mass discharge

Relative Depletion Timeframes



DNAPL Architecture Sensitivity Analysis

- Varied NAPL architecture and re-ran model – any other scenarios that match **1994 Md** and **half-life**?
  - Length / 2
  - Width / 2
  - Uniform thickness of 4”, 8”, or 1 ft
    - a) All pooled DNAPL; or
    - b) All residual DNAPL
  - Zero flux through all DNAPL sub-zones
  - Type 1 – residual zone is suspended above pool.
- No other scenarios matched **both** observations.
  - Half-life criteria: 10 years +/- 25%

Summary

1. We can use process-oriented NAPL depletion models when architecture well defined
    - Predict relative timeframes for natural and enhanced dissolution
    - Interpretive tool – improve our understanding
2. When architecture has higher uncertainty but still relatively well understood – may be able to use model as forensic tool
    - Evaluate range of potential architectures
    - Identify data gaps
3. Multiple goals needed to calibrate a NAPL depletion model

Supplemental Slides

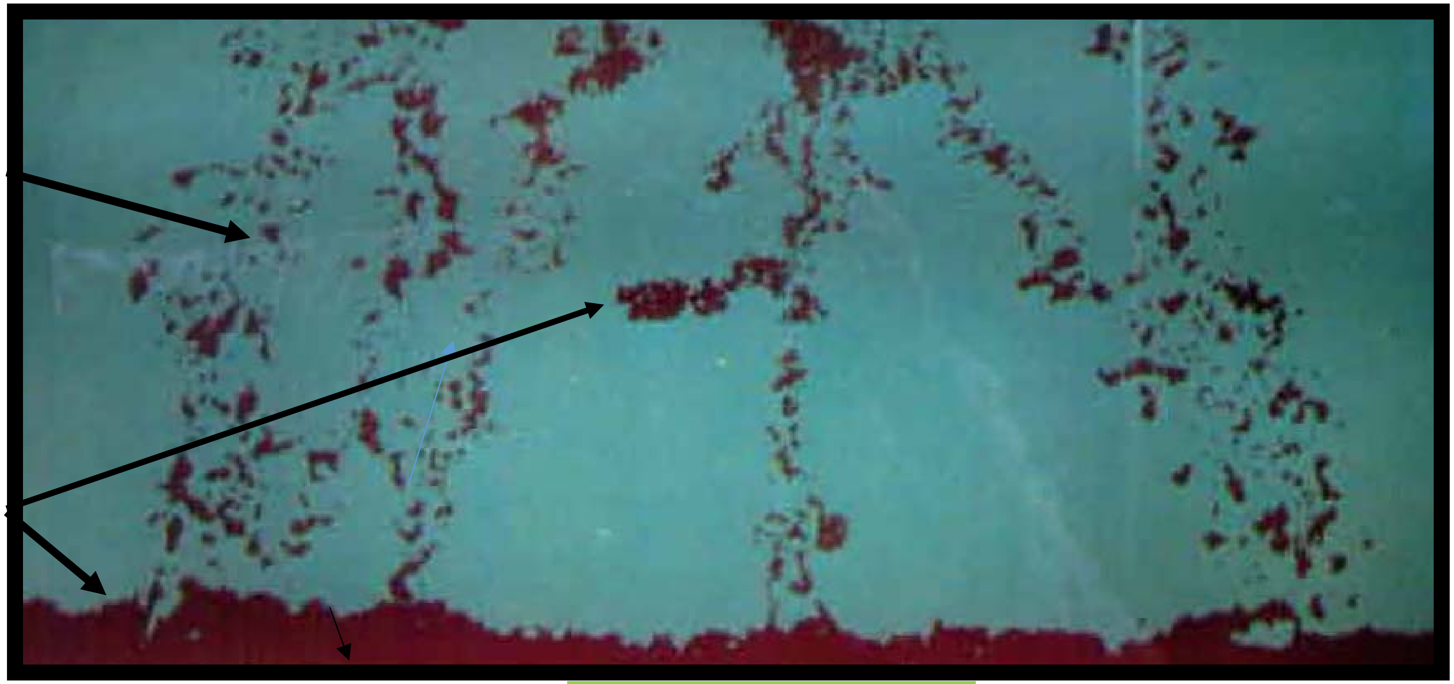
Fresh DNAPL Source Zone

Ganglia (residual NAPL)

Timeframe: Years

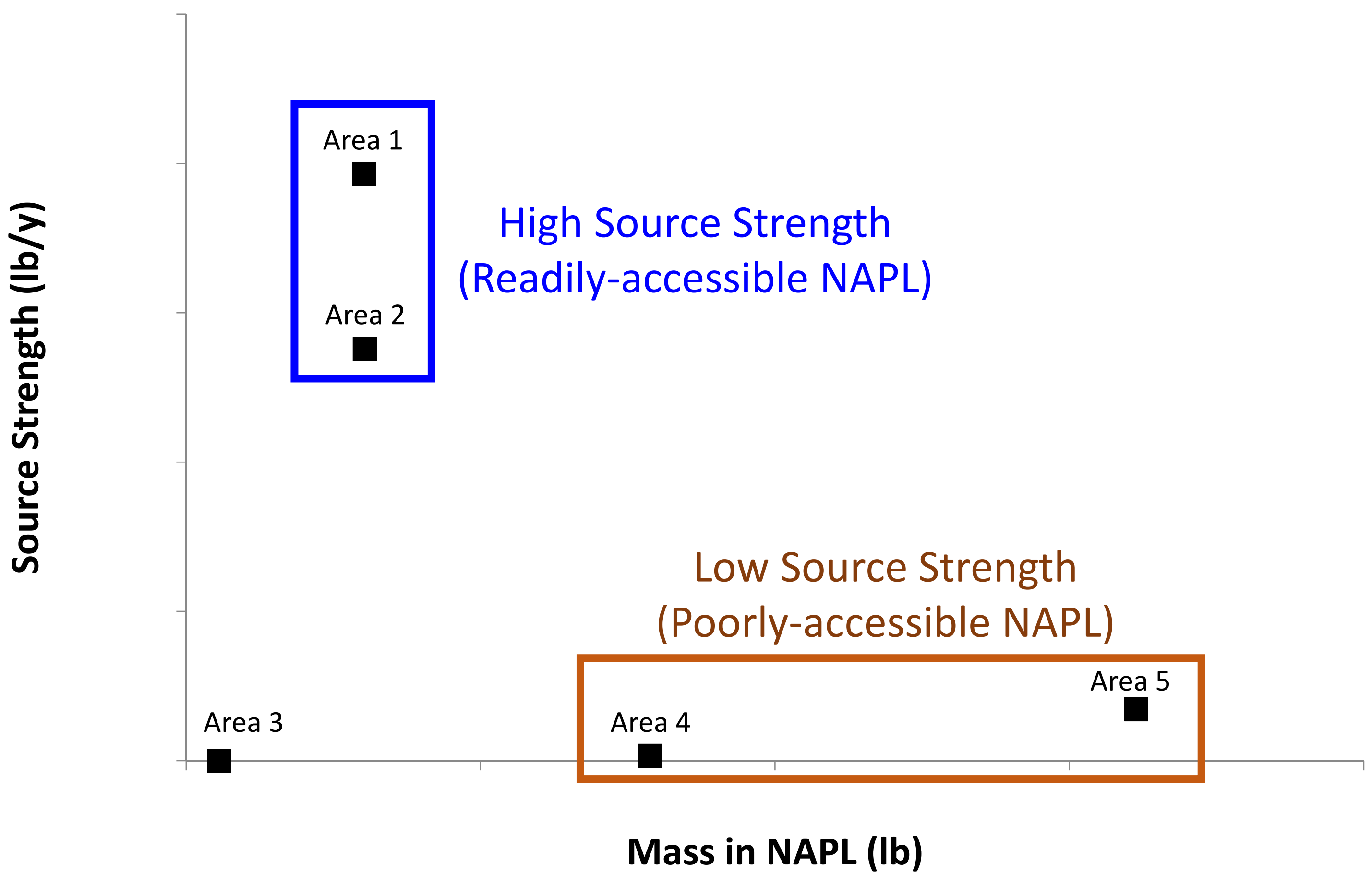
Pools (free phase NAPL)

Timeframe: Decades +

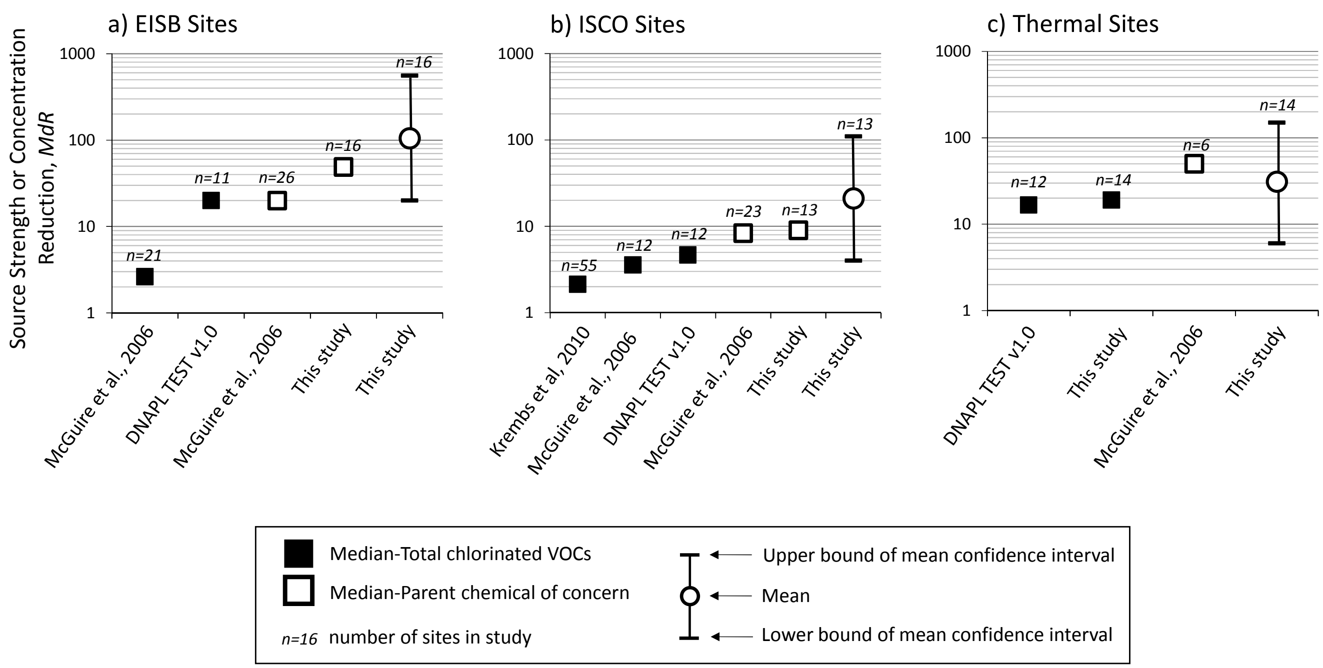


Source: *Schwille, 1988*

Prioritizing Treatment Based on Mass Discharge



Q: What is ATTAINABLE Source Strength Reduction?



Mean Mass Discharge Reduction

	Mean	Conf. Int.
EISB:	105x	(20x to 556x)
ISCO:	21x	(4x to 110x)
Thermal:	31x	(6x to 150x)

Simple Site → Mean

Complex Site → Conf. Int.

REMEDIATION Autumn 2014

Source: *Carey et al., 2014*

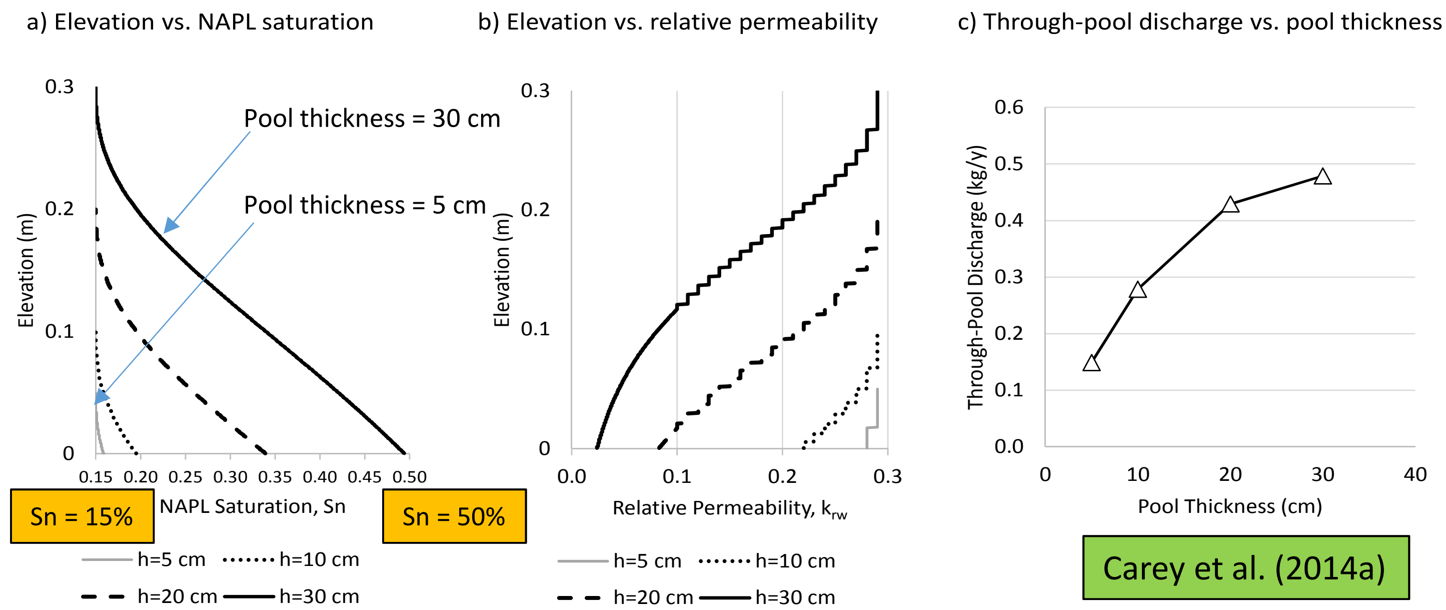
Grant R. Carey

Edward A. McBean

Stan Feenstra

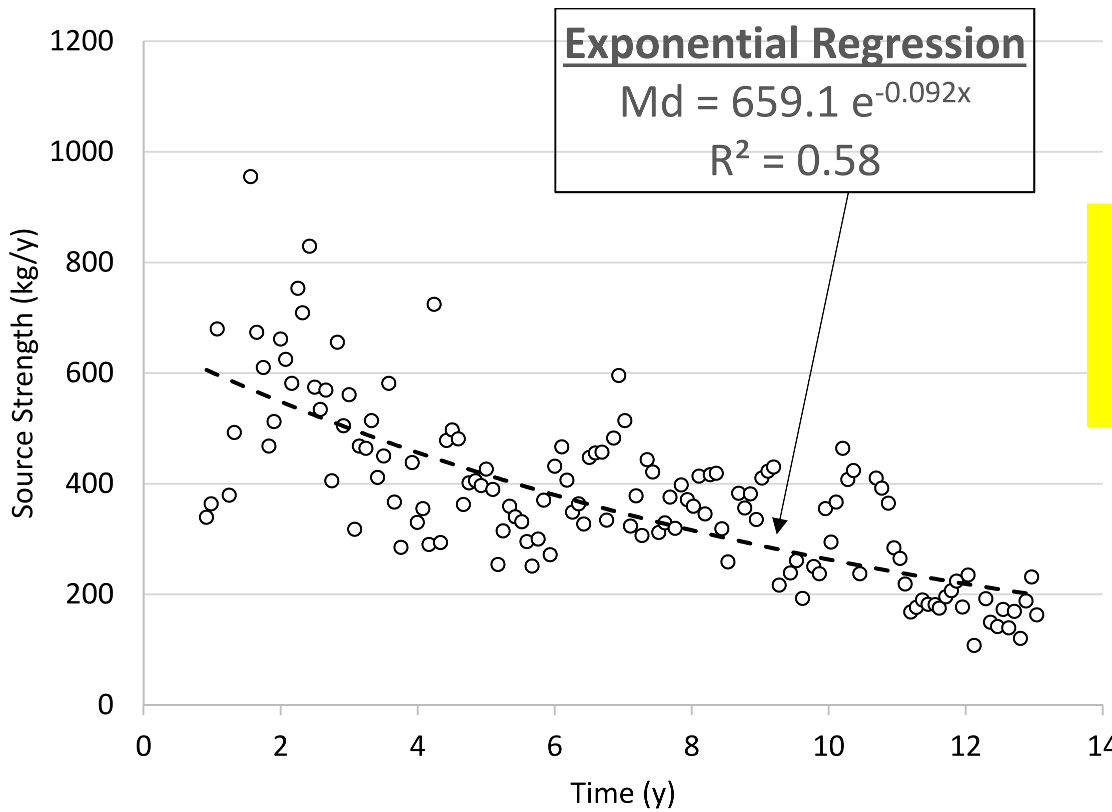
DNAPL Source Depletion: 2. Attainable Goals and Cost–Benefit Analyses

NAPL Saturation vs. Depth in a DNAPL Pool ($K_{sat}=10^{-2}$ cm/s)



Vertical distribution of DNAPL in pool – above calculations based on Eq. 3.18 in McWhorter and Kueper (1996), and assume P_c=0 at the top of the pool.

Estimating Mass: Mass Discharge Method



Initial Md (Md_o) = 660 kg/y
Decline rate (λ_{Md}) = 0.092 y^{-1}
Decline half-life = 7.5 y

Graph modified from Brusseau et al. (2011)

Estimating Mass: Mass Discharge Method

Estimating initial mass (M_o) in source zone (based on Newell et al., 2005):

$$M_o = Md_o / \lambda_{Md}$$

[M_o in kilograms, Md_o in kg/y, and λ_{Md} in y^{-1}.]

Example calculation for Tuscon Airport Site:

$$M_o = (660\ kg/y) / (0.092\ y^{-1})$$

$$= 7{,}164 \text{ kg}$$ ~ **Minimum NAPL mass in subsurface**

Calculation assumes uniform decline rate, and
based on readily-accessible NAPL mass.

May underestimate mass in pool-dominated source zones.