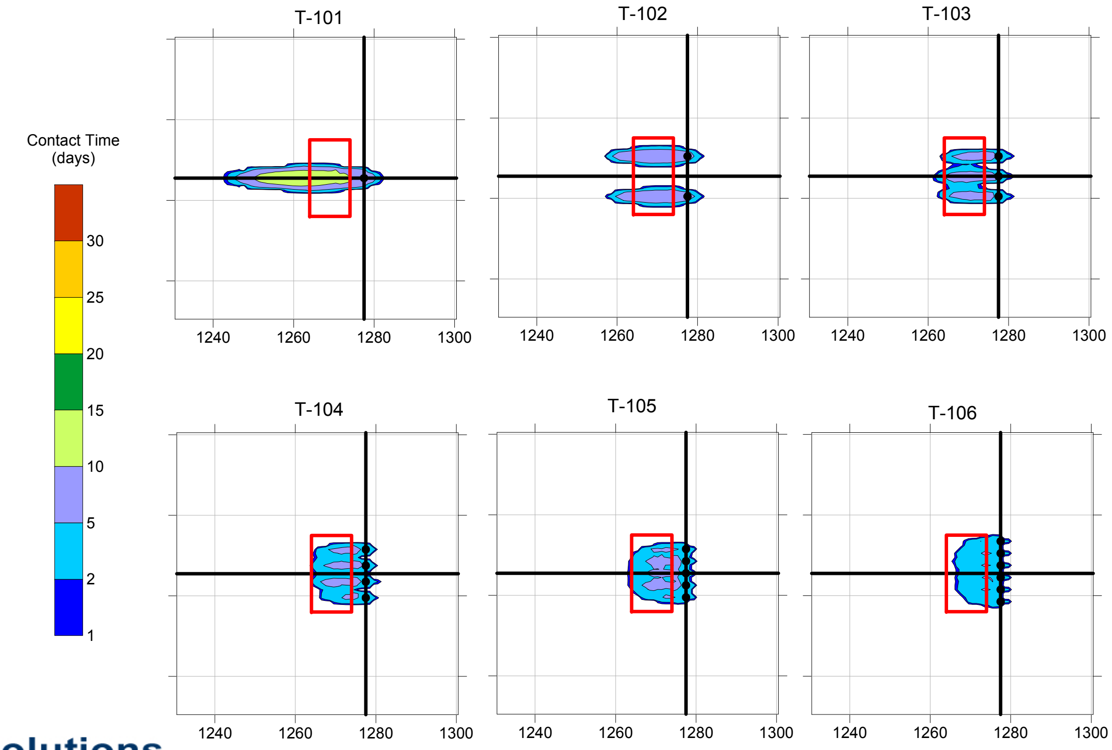
In-Situ Remediation (ISR-MT3DMS^{TM}) Contact Time Distribution



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Introduction

- The success of injection remedies like ISCO depends on maximizing the contact time between the injected reagent, and the contaminant.
- Most models do not calculate contact time as a metric to help with remedy evaluation.
- ISR-MT3DMS™ incorporates a contact time "calculator", which calculates the contact time of an injected reagent in each grid cell, over a specified period of time.
- The distribution of contact time may then be plotted on a figure, to see how this metric is distributed across a source zone. The goal of a remedy may be to balance the distribution of contact time throughout the source zone, so that there is a balanced cleanup of all areas within this zone.

Sample Model Construction

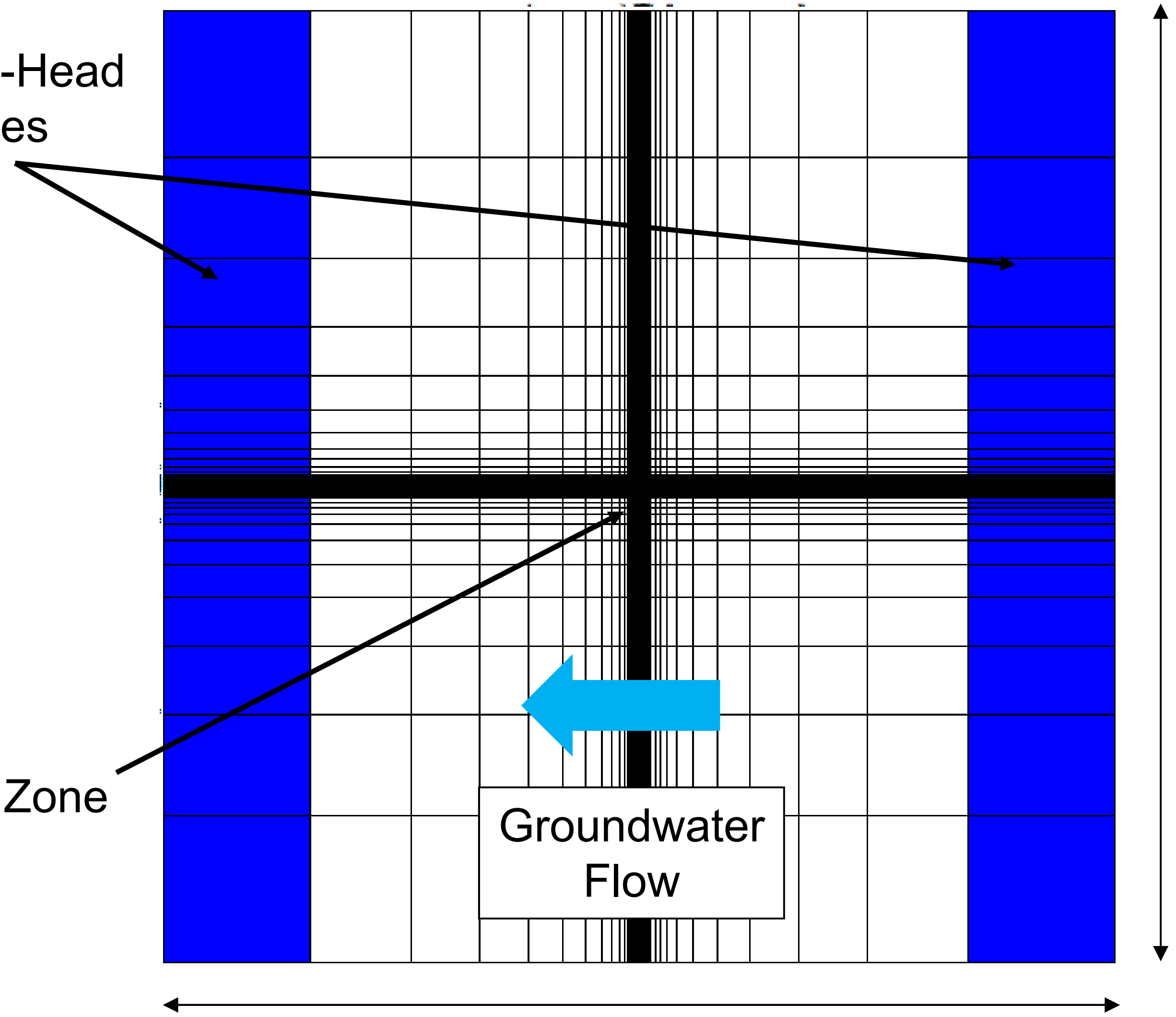
Flow Model Input

- K = 100 m/day
- Gradient = 0.003
- Porosity = 0.2
- Calculated velocity ~ 550 m/year
- Recharge = 8 inches per year

Transport Model Input

- Injected reactant only
  - Did not simulate contaminant in source zone
- Longitudinal dispersivity = 2 m
- No sorption
- Oxidant half-life = 25 days
- Injected concentration = 1 (normalized)

Model Domain



Constant-Head Boundaries

Source Zone

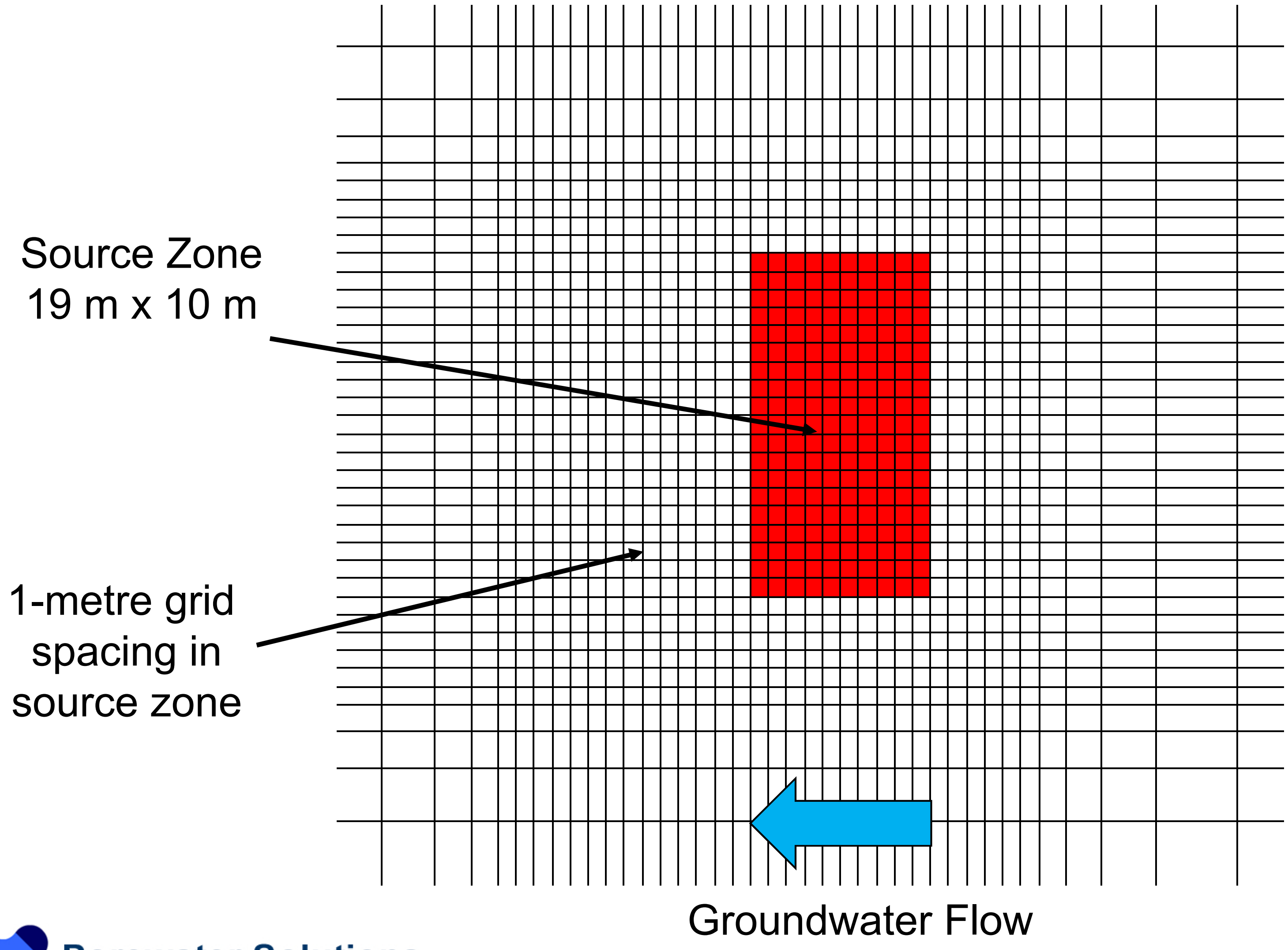
Groundwater Flow

2530 m

2530 m

62 rows and 62 columns

Close-up of source zone



Source Zone
19 m x 10 m

1-metre grid
spacing in
source zone

Groundwater Flow

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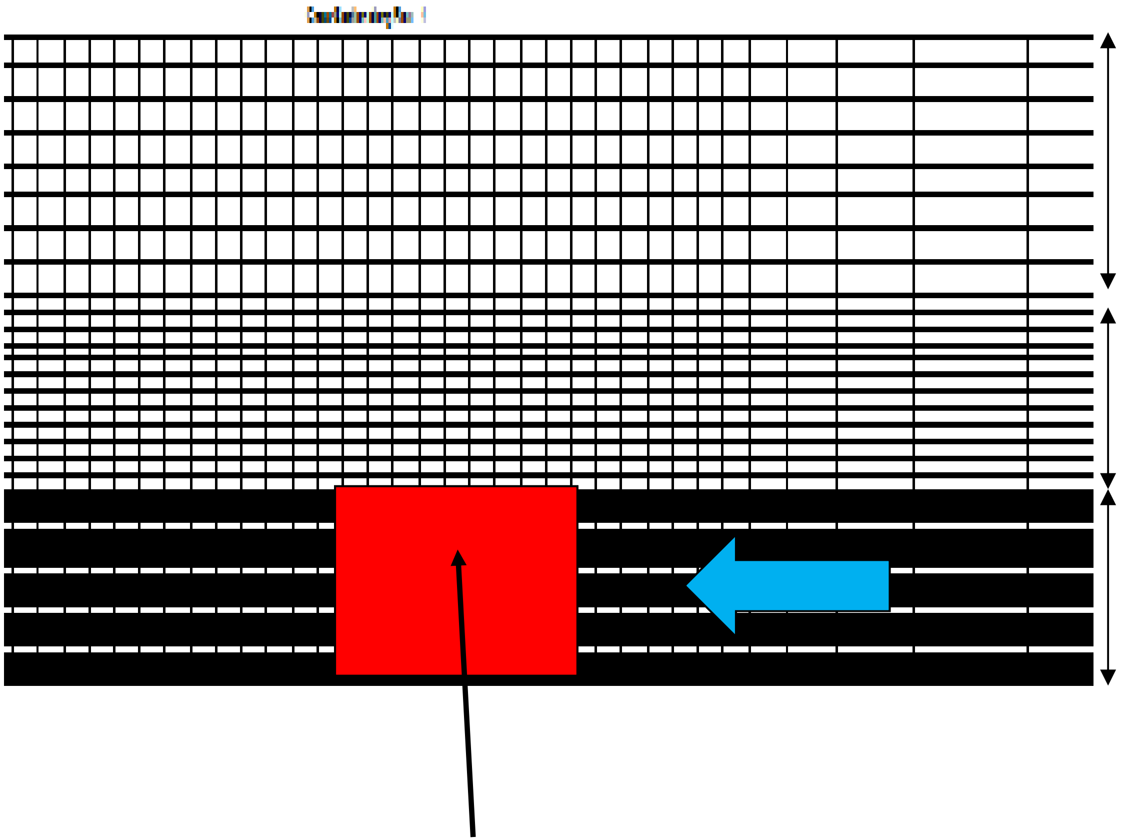
Domain Cross-Section



4 m (0.5 m spacing)

3 m (0.25 m spacing)

3 m (0.1 m spacing)

Source zone

50 model layers

Contact Time Analysis

Contact Time Concept

- Defined several target concentrations for oxidant in source area
  - E.g. 1% or 0.1% of injected concentration
  - If injected solution has permanganate concentration = 20 g/L, then target concentrations are 200 and 20 mg/L of permanganate using 1% and 0.1% thresholds

Contact Time Concept

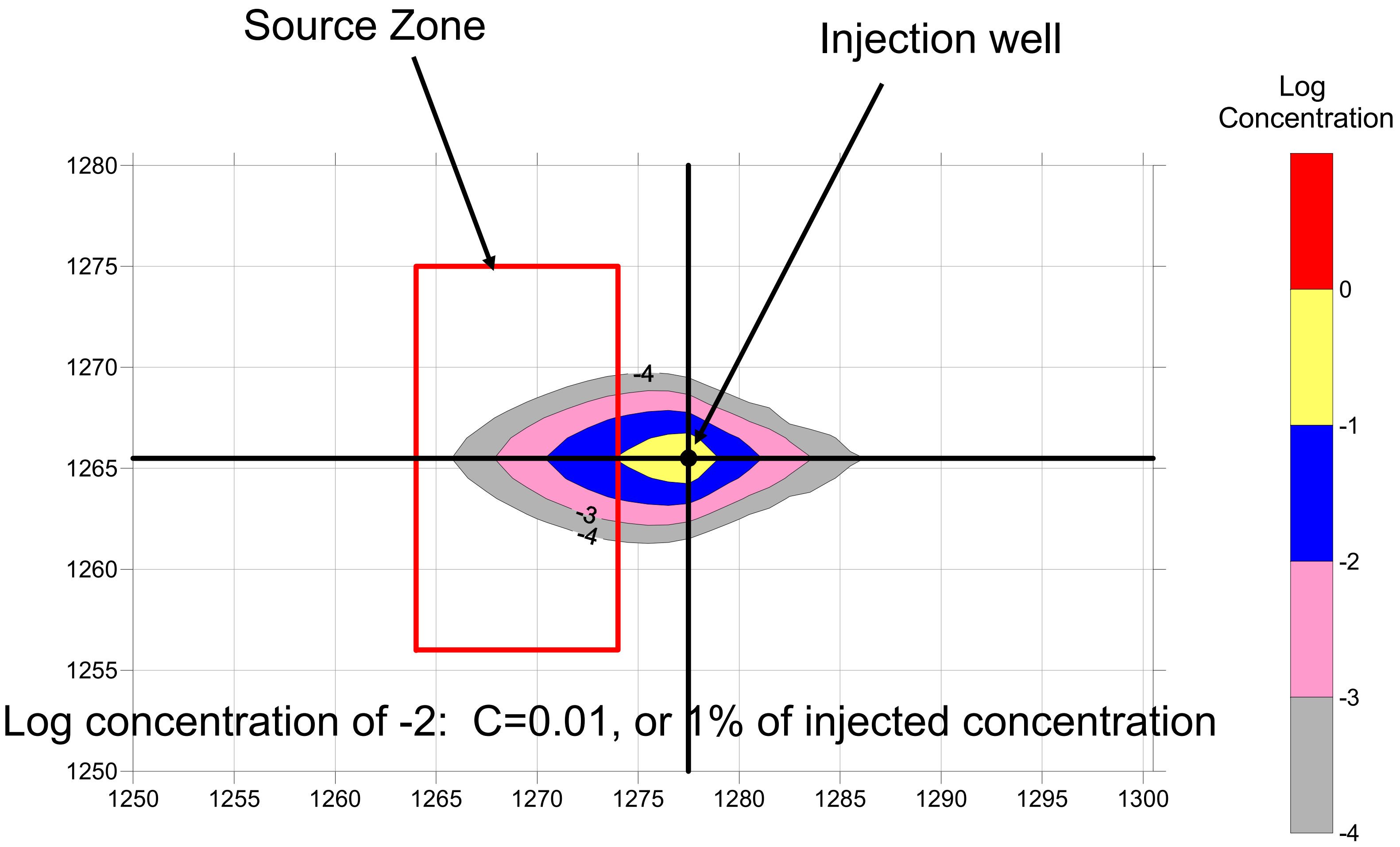
- Contact Time = total time during simulation that permanganate exceeds the target concentration in a model grid cell
- Contouring contact time provides a measure of efficiency in oxidant distribution in the source area over entire simulation
- Evaluating the % of source area with a minimum contact time (e.g. 1 day) is another summary measure of efficiency

Contact Time Distribution

- Next series of slides shows the contact time distribution for a simple one-well scenario
  - Oxidant degradation was not modeled for this simple demonstration
  - Duration of model simulation is 30 days

Step 1. Study PERM concentration

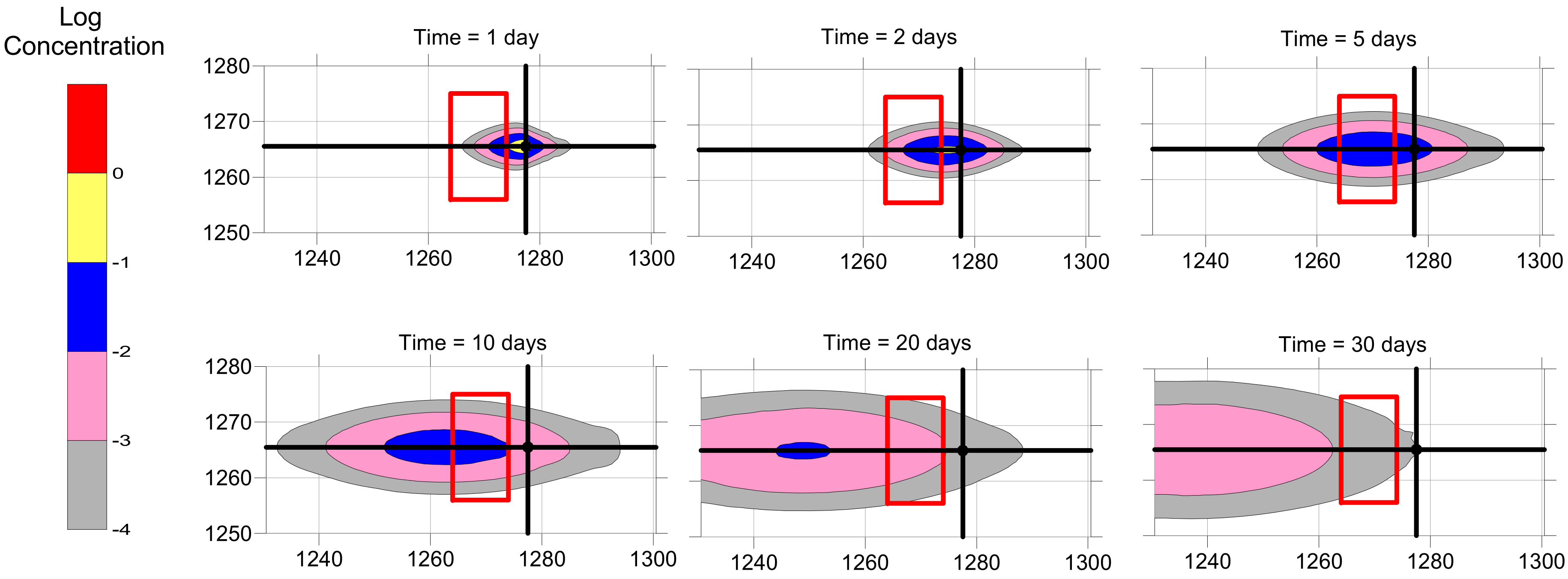
Simulation Time = 1 day



Log concentration of -2: C=0.01, or 1% of injected concentration

PERM conc. over time

Injection duration = 1 day; Volume injected = 2000 L



Log concentration of -2: C=0.01, or 1% of injected concentration

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Findings

- Contaminat degradation, which is based on oxidant concentrations, varies over time and space
- Difficult to get a simple measure of remediation efficiency based on the distribution of reactant concentrations

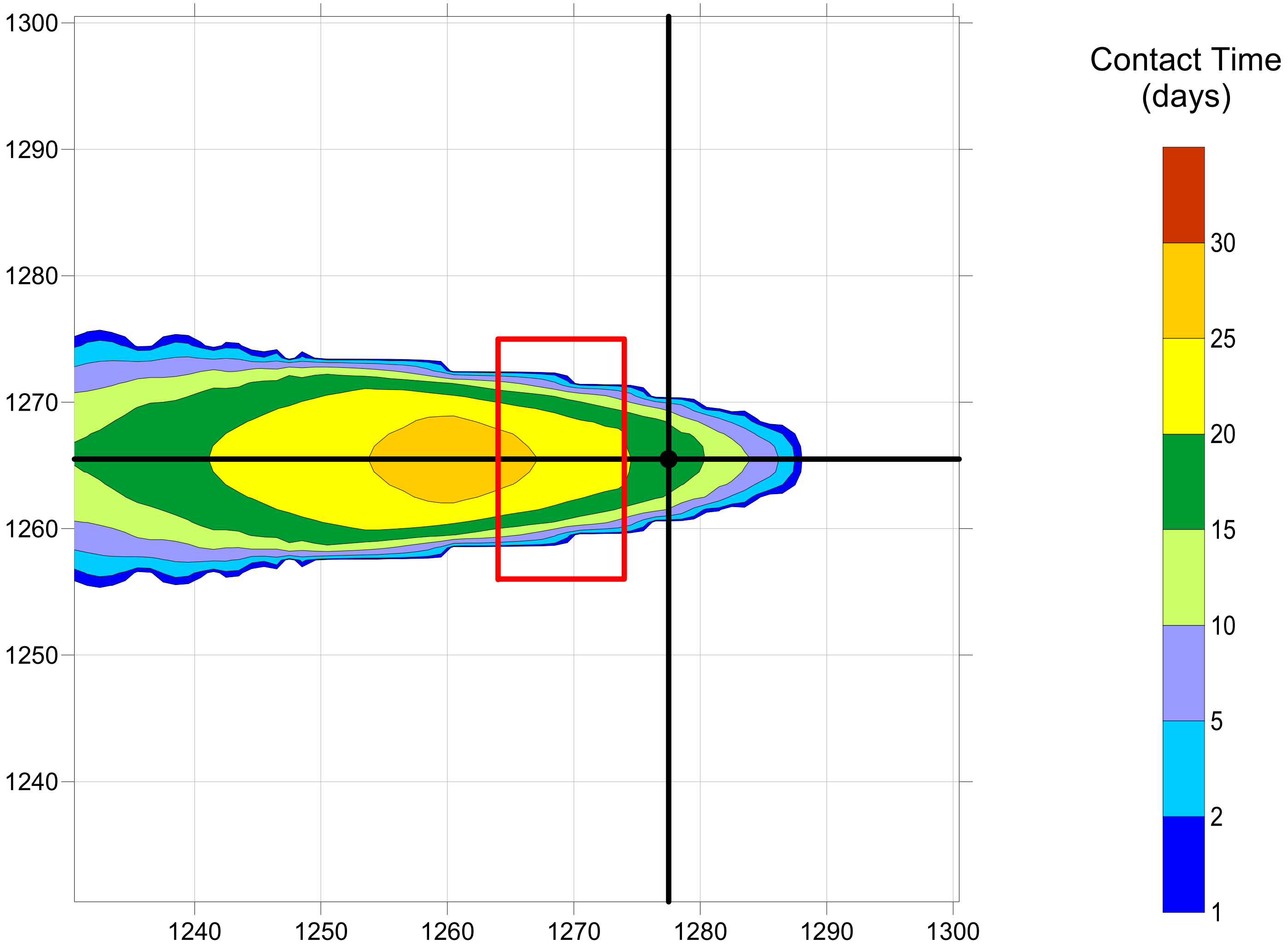
Contact Time Calculation

- Define oxidant concentration "threshold"
  - E.g. one rule-of-thumb is to have at least 1% of injected concentration over entire source zone for a minimum period of time
  - Another reference…need a minimum permanganate concentration to facilitate solvent degradation, based on competition with native organic matter

Contact Time Calculation

- For this simple analysis, several reactant concentration thresholds were defined:
  - C = 10% of injected concentration
  - C = 1% of injected concentration
  - C = 0.1% of injected concentration

Contact Time: Reactant C > 0.1%



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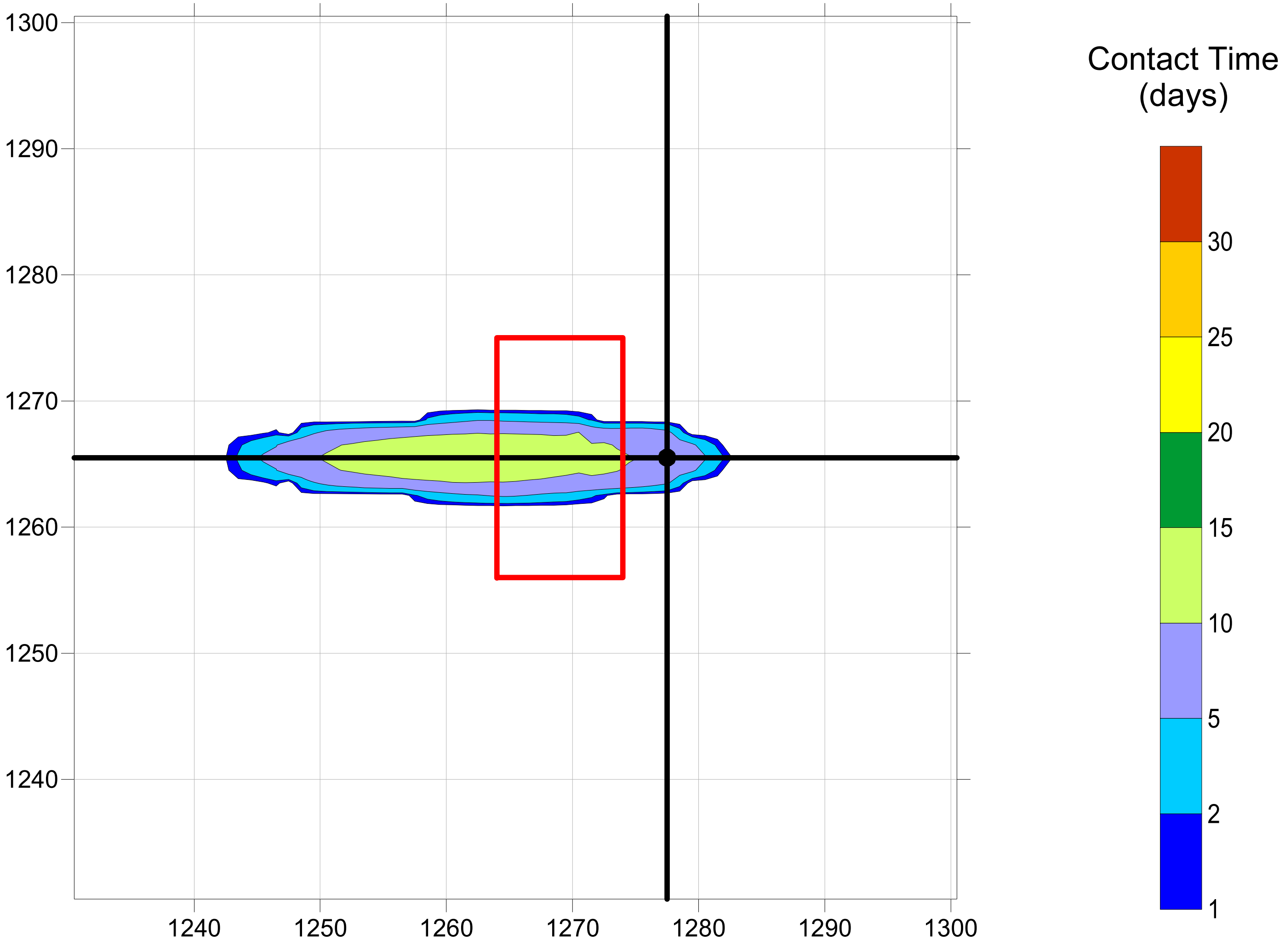
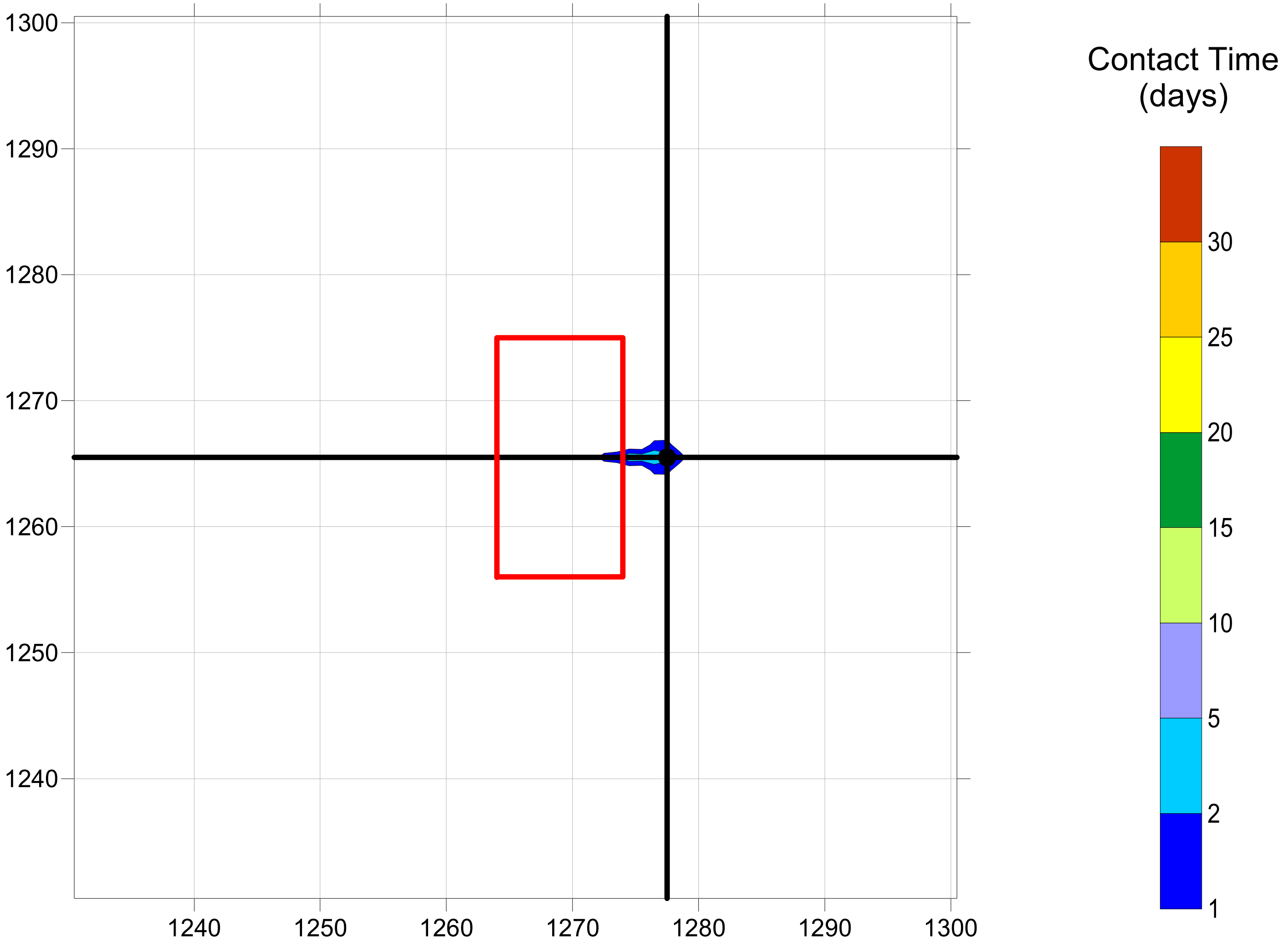
Contact Time: Reactant C > 1%



Contact Time: Reactant C > 10%



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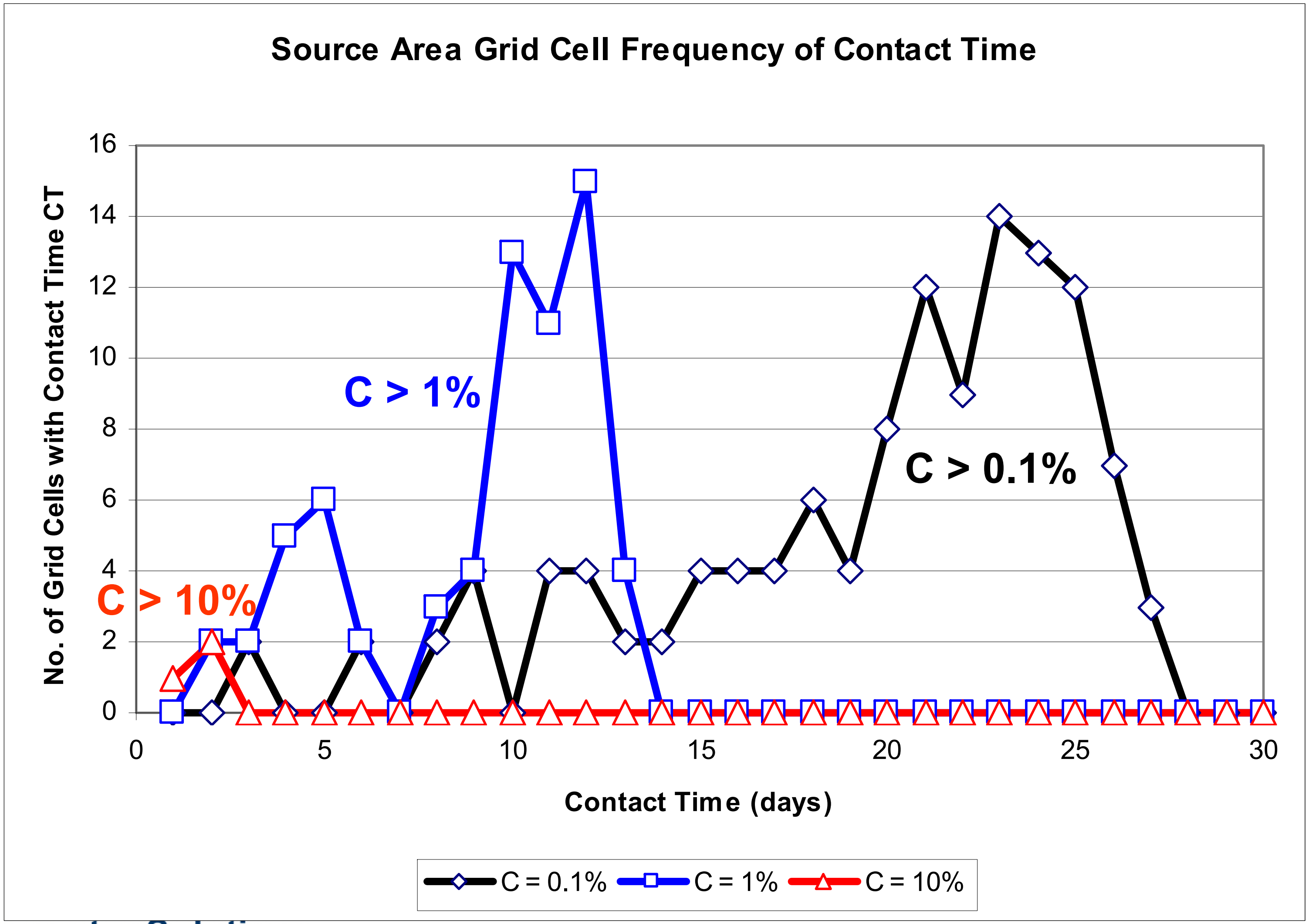
Findings

- Most efficient treatment zone for C>0.1% is downgradient of source zone
- Most efficient treatment zone for C>10% is upgradient of source zone
- Therefore, intensity of the concentration threshold (e.g. 0.1%, 1%, or 10%) for contact time will influence decisions on injection rate and well placement

Findings

- For one injection well, there is a significant difference in remediation efficiency in source zone
    - Greatest efficiency directly downgradient from injection well
    - Decreasing efficiency as move away from centreline of injected reactant plume

Contact Time Frequency for Model Grid Cells in Source Zone



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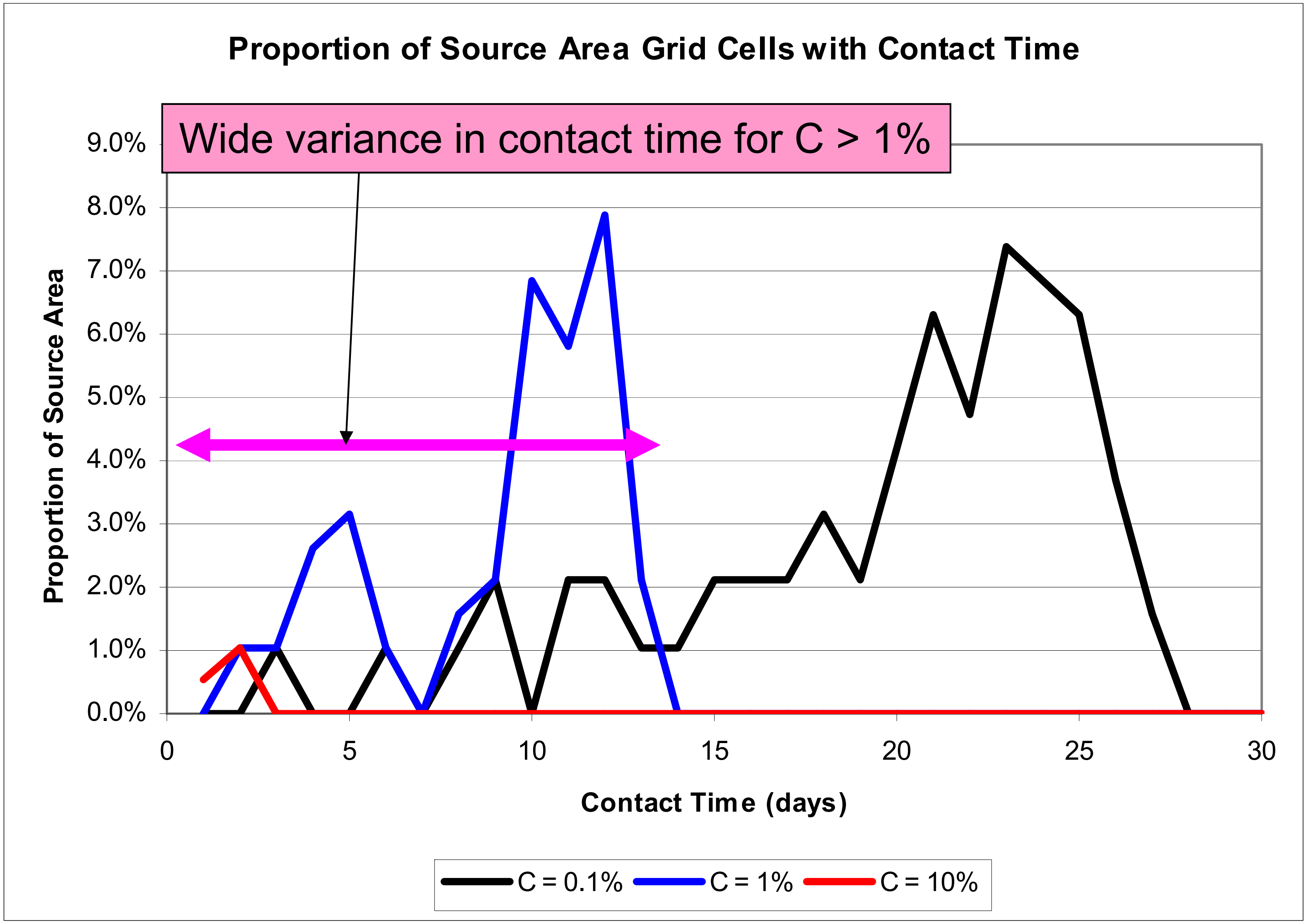
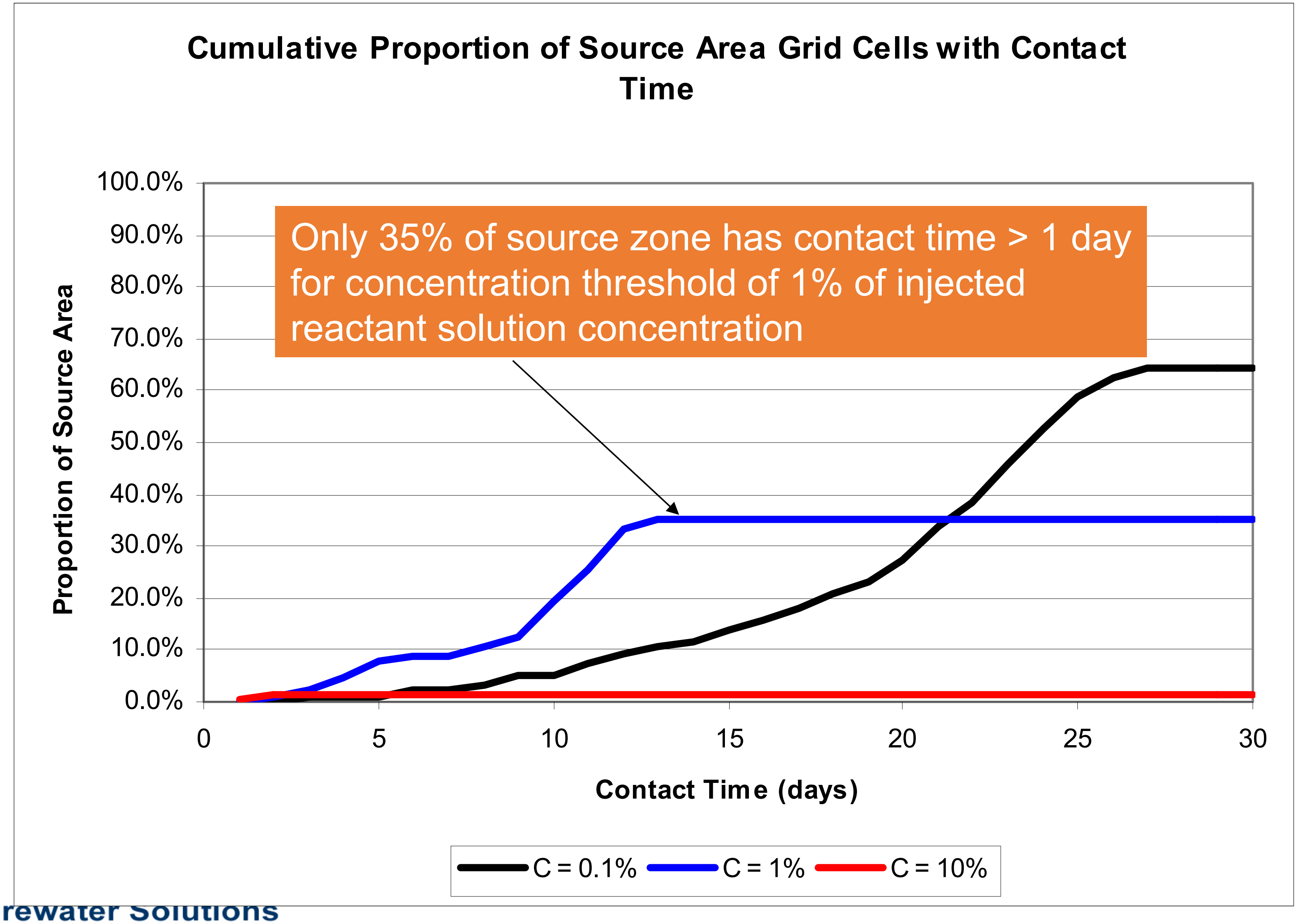
Contact Time Distribution in Source Zone



Cumulative Distribution



Only 35% of source zone has contact time > 1 day for concentration threshold of 1% of injected reactant solution concentration

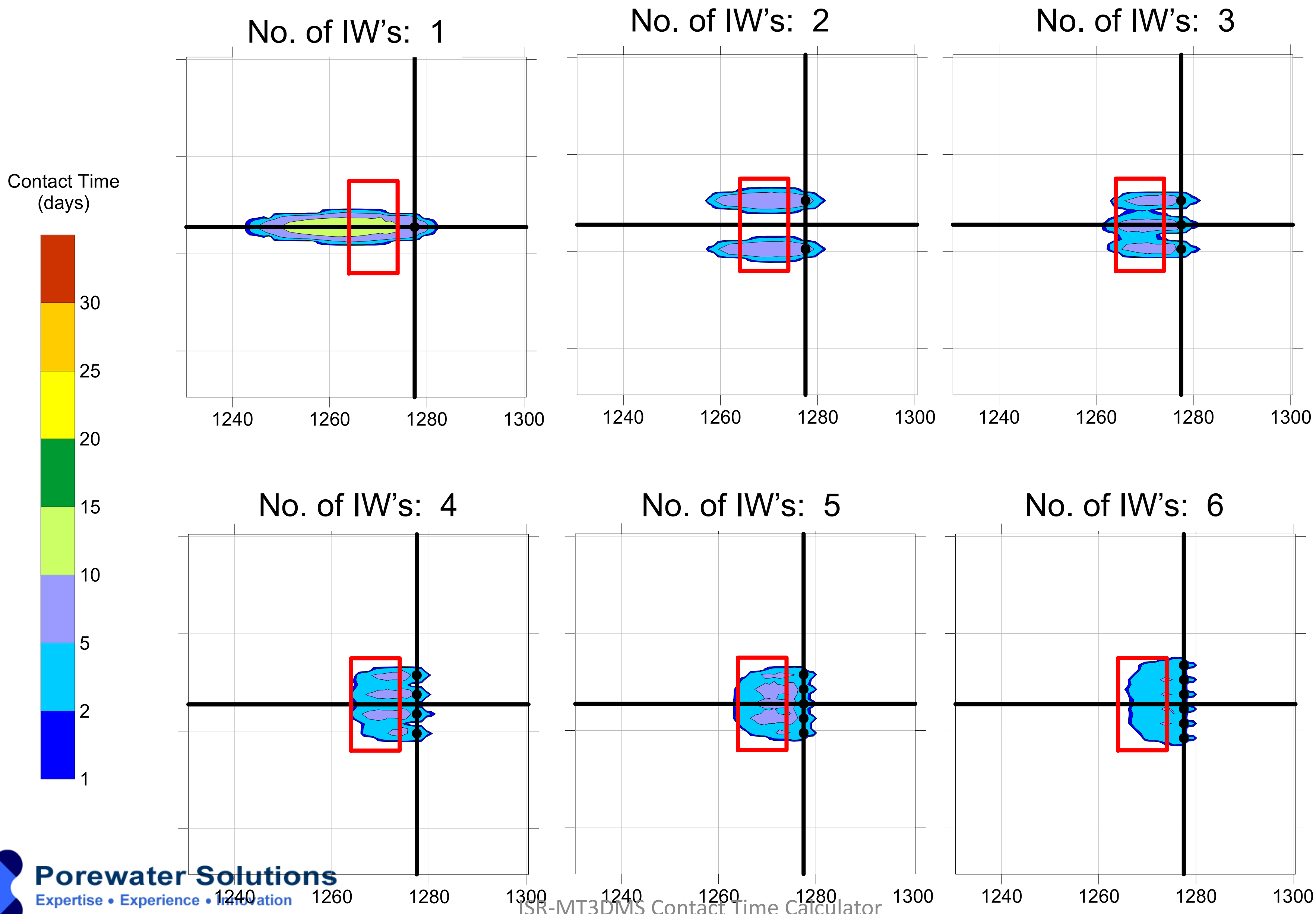
Contact Time Evaluation

Multiple Injection Well Scenarios

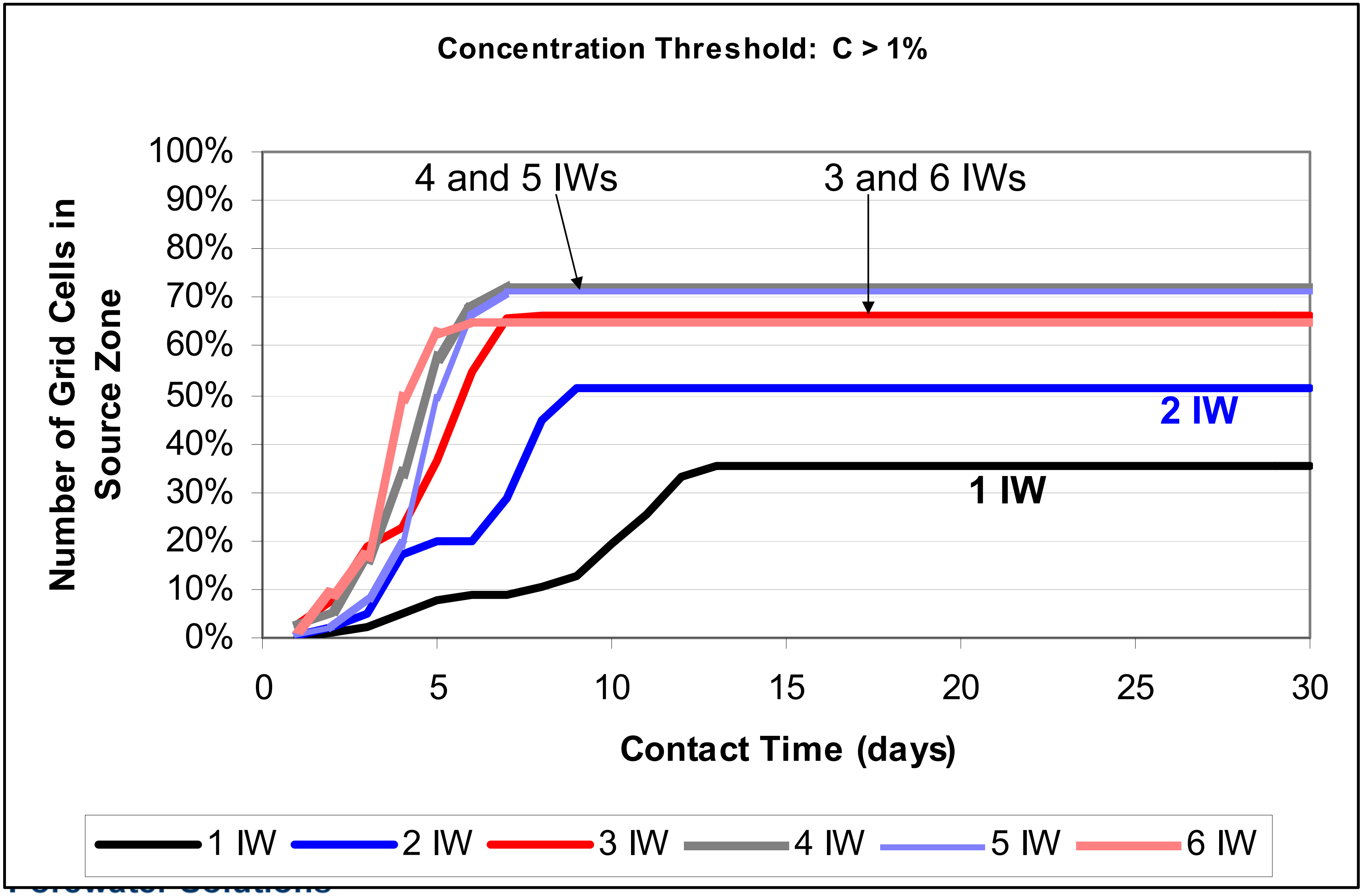
Multiple Well Scenarios

- Fixed Injection Volume: 2000 L
- Injection duration: 1 day
- Contact time calculated at 30 days of simulation
- Number of injection wells (IW) varies
  - From 1 to 6 IW's

Injected Volume: 2000 L



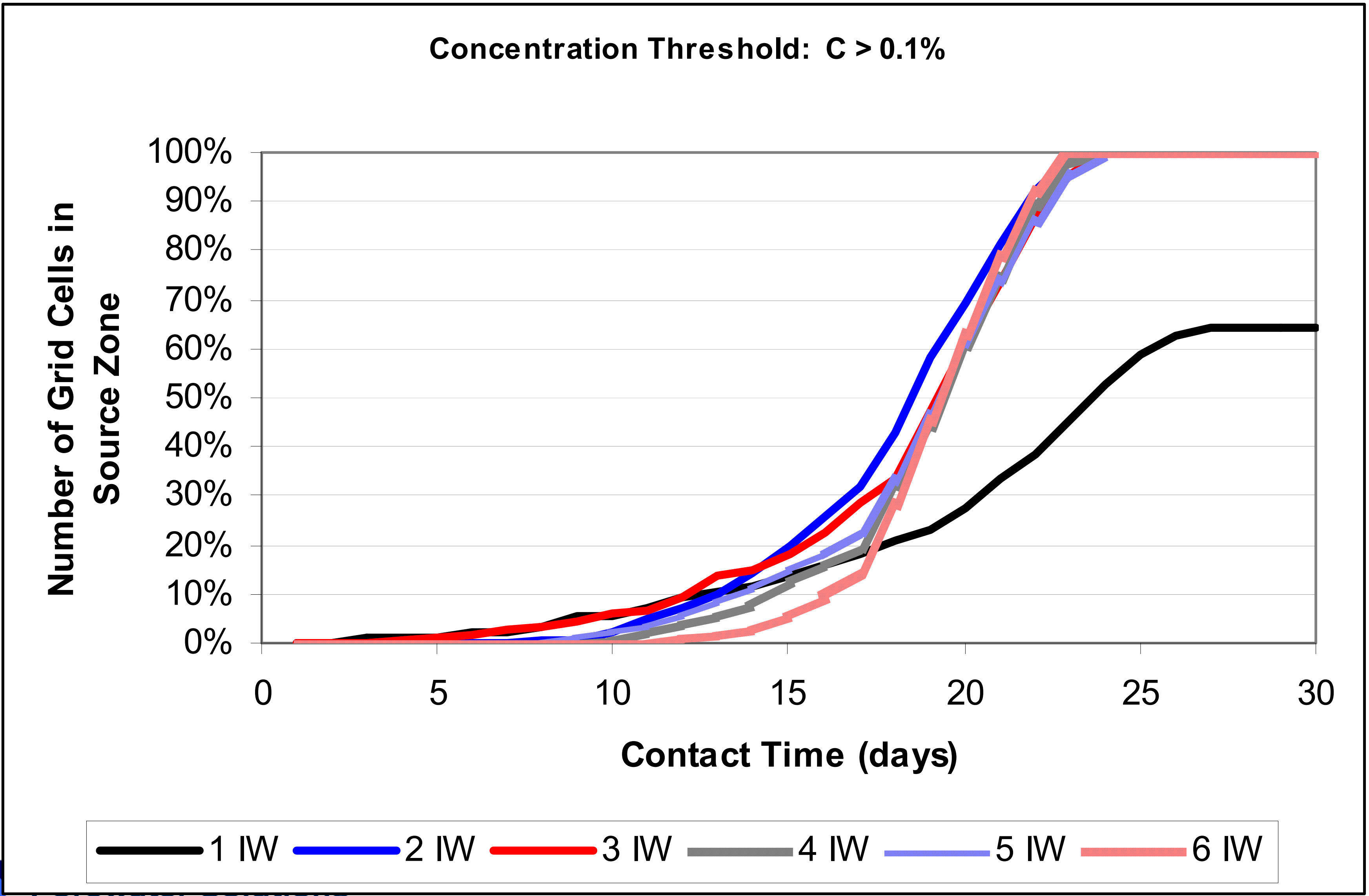
Cumulative Frequency: Reactant C > 1%



Cumulative Frequency: Reactant C > 1%

- FINDINGS:
  - 1 well and 2 well have significantly reduced performance based on contact time and fixed solution volume injected
  - 4 and 5 wells had similar/best performance when trying to achieve the high threshold of C>1% of reactant solution concentration
  - 6 wells results in less efficient performance than 4 or 5 wells assuming fixed solution volume because of dispersion

Cumulative Frequency: Reactant C > 0.1%



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Cumulative Frequency: Reactant C > 0.1%

- FINDINGS:
  - If target threshold concentration is lower intensity (0.1%), then 2 or 3 injection wells would suffice for the fixed solution volume

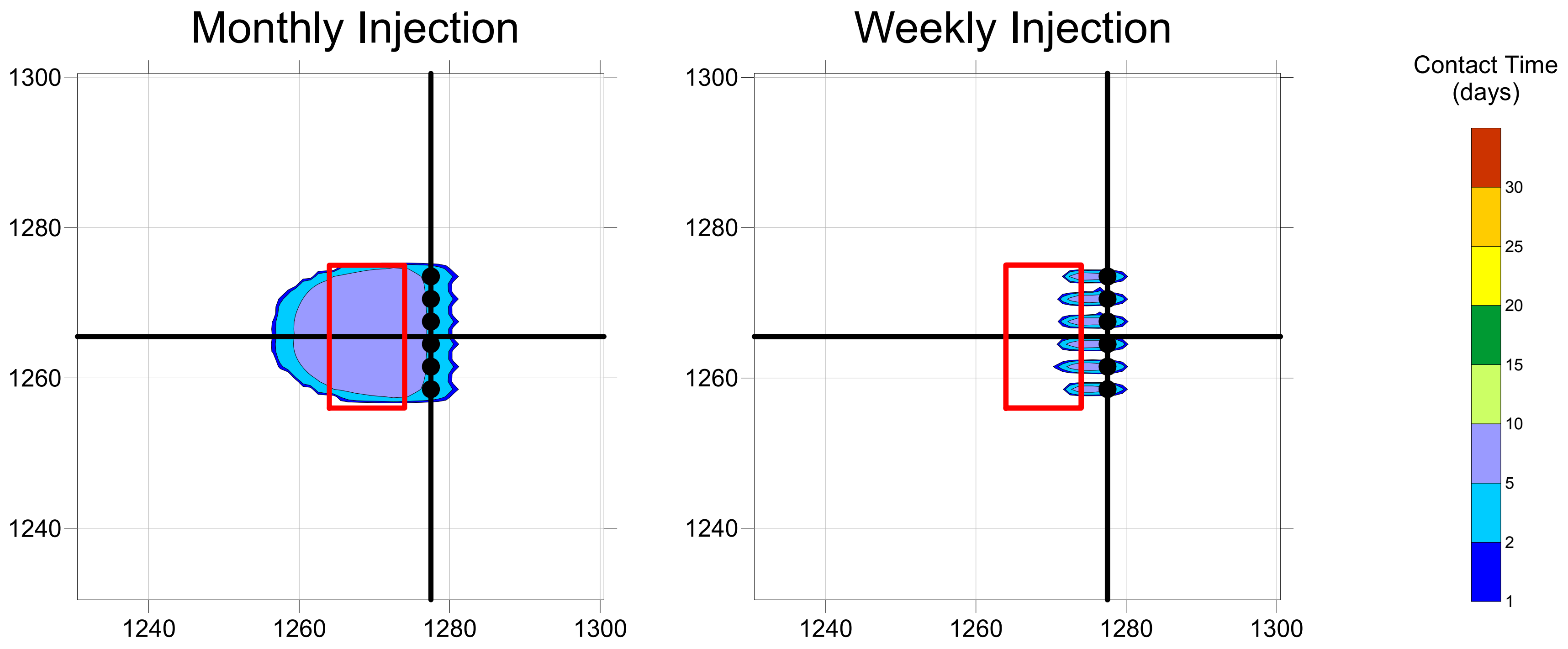
Goal

- Compare the contact time distribution for two alternatives – injection of fixed solution volume:
  - One event per month; or
  - One event per week.

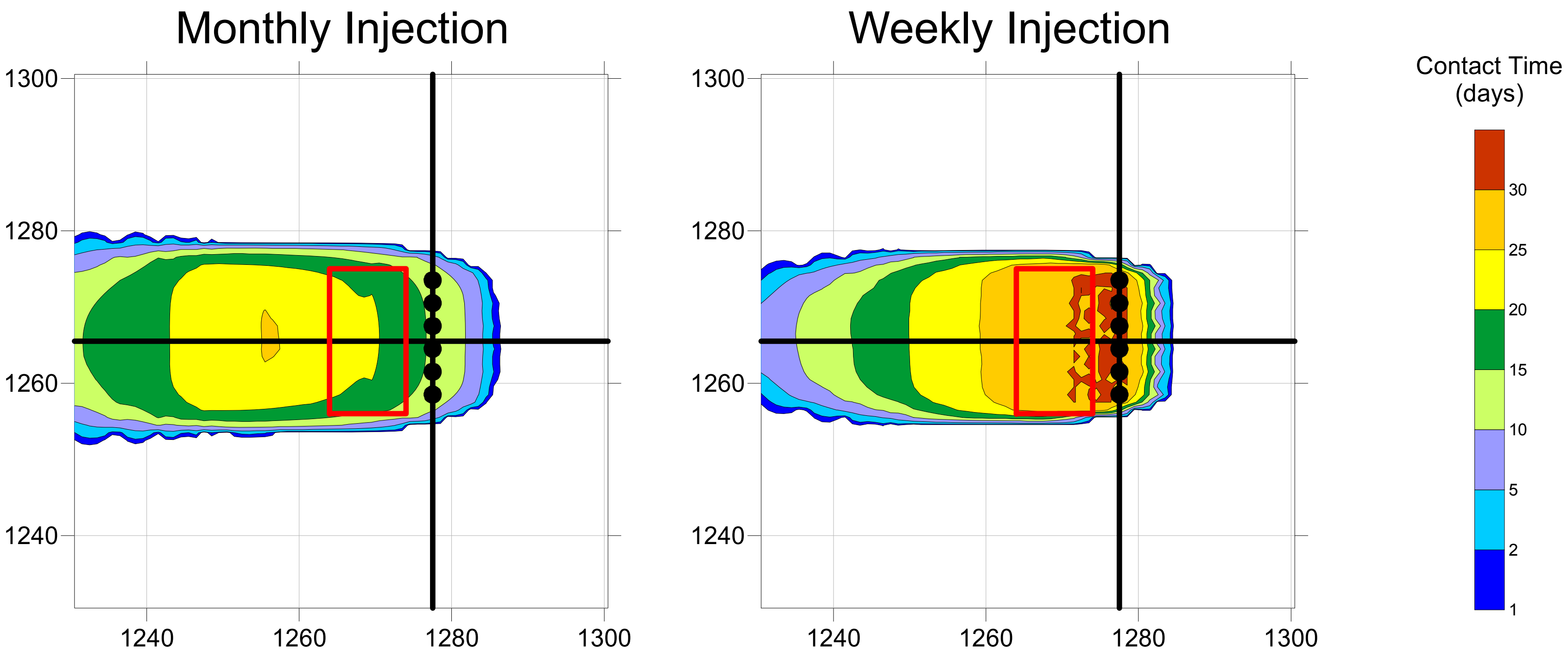
Injection Scenarios

- Run T-121:
  - Injection of 4000 L in 6 hours at start of month
- Run T-122:
  - Injection of 1000 L in 6 hours on weekly basis
  - Same total volume injected as Run T-121
- Both simulations conducted for 30-day period

Contact Time for C > 1%

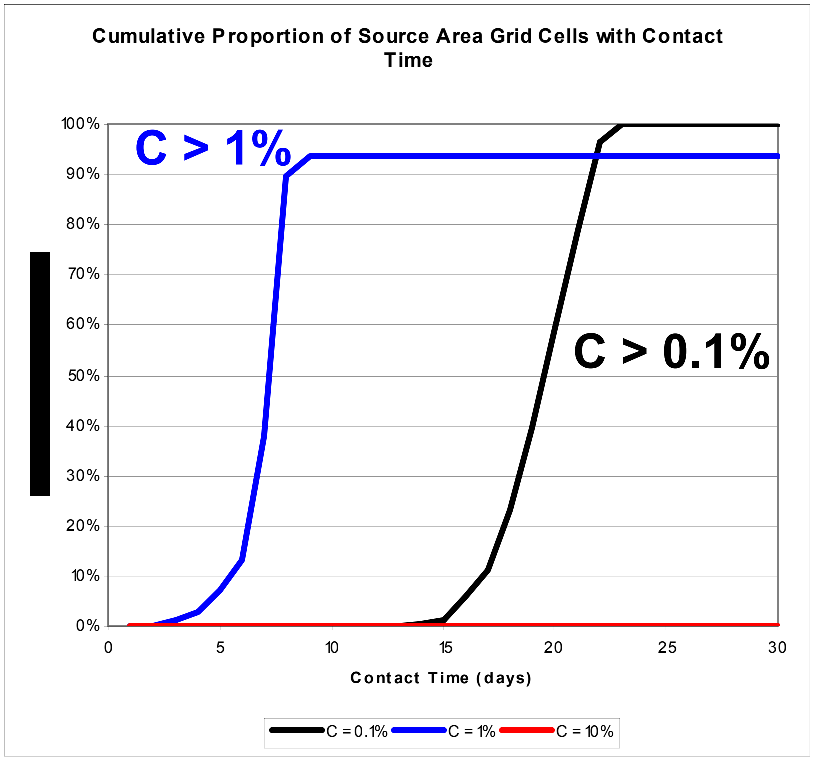


Contact Time for C > 0.1%

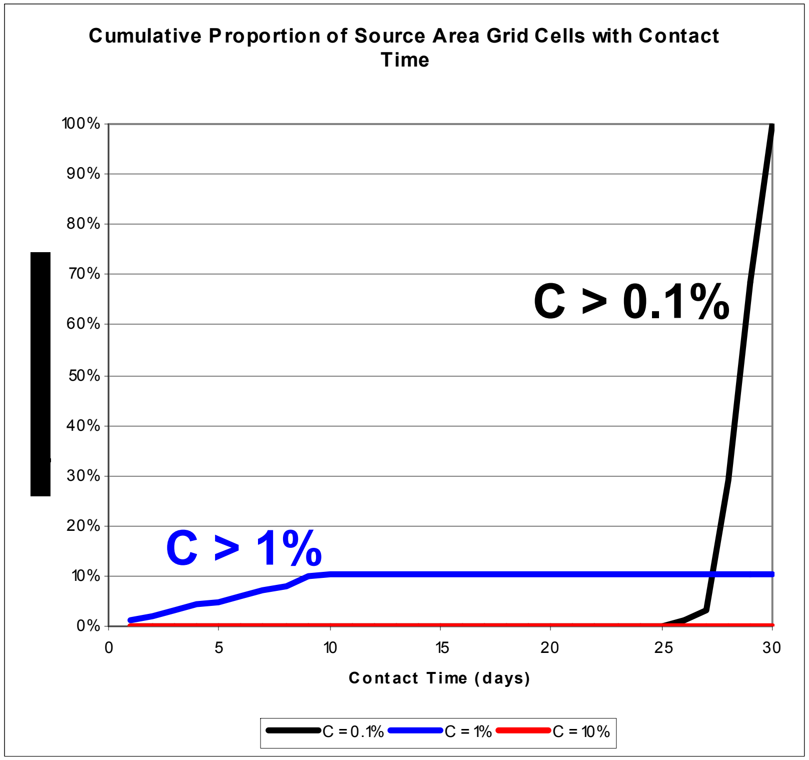


Contact Time Distribution

Monthly Injection



Weekly Injection



Findings

- % of source zone with more than 1 day contact time at threshold concentration:
  - C > 1%:
    - Monthly Injections: 94% of source zone
    - Weekly Injections: 11% of source zone
  - C > 0.1%:
    - Monthly and weekly injections: 100%
    - Average contact time for monthly injection is 10 days less than weekly injection

Findings

- If target is higher threshold concentration:
  - Less frequent injections are better than more frequent (assuming same monthly solution volume)
- If target is lower threshold concentration:
  - More frequent injections result in higher contact times, but need to weigh benefit vs additional labor cost

Flux Analysis

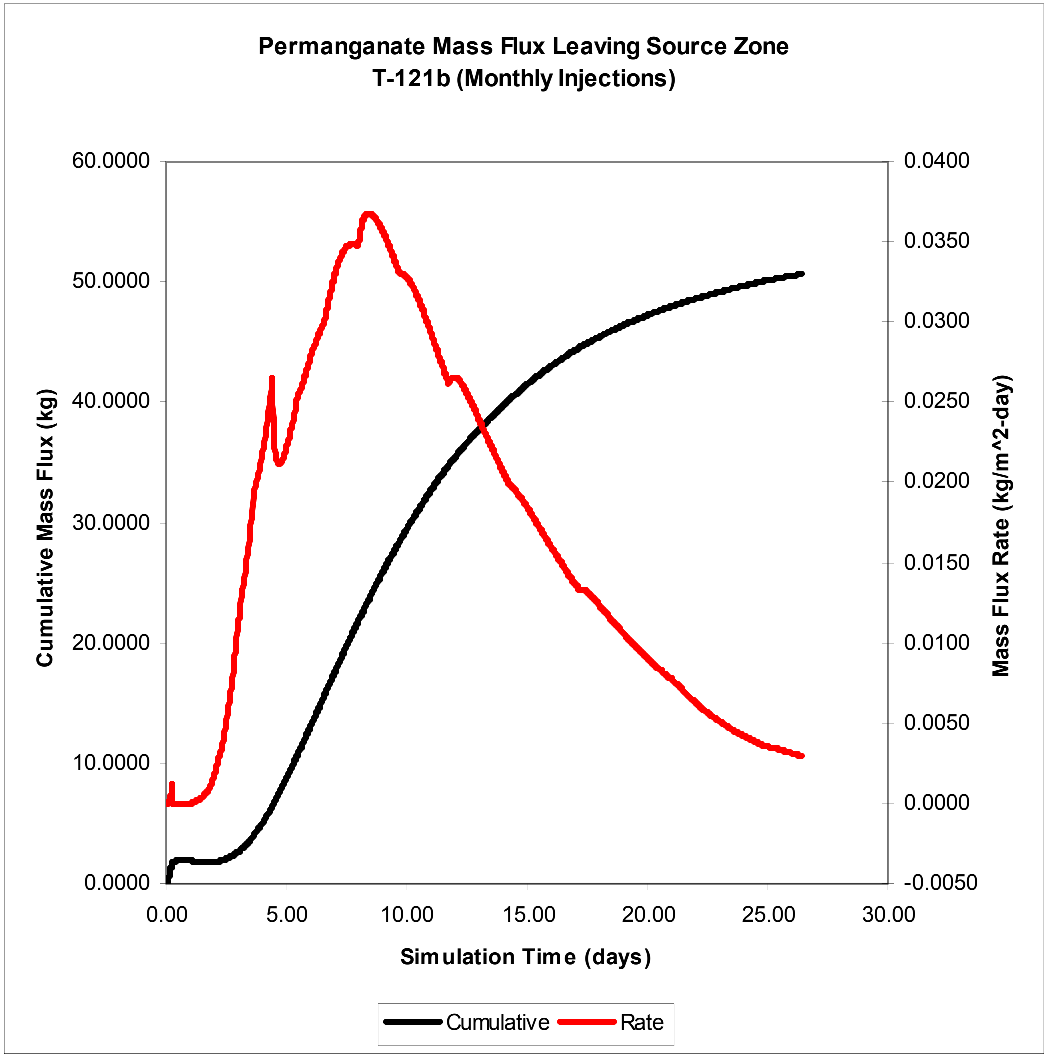
Flux Analysis

- Modified MT3DMS to calculate flux across user-defined region (e.g. source area)
    - Advective, dispersive, and total flux
    - Oxidant flux out of source area – measure of efficiency
    - Contaminant flux – evaluate contaminant flux reduction over time for different design alternatives

Flux Analysis – Monthly Injection

Total Mass Injected = 80 kg

63% leaving Source area

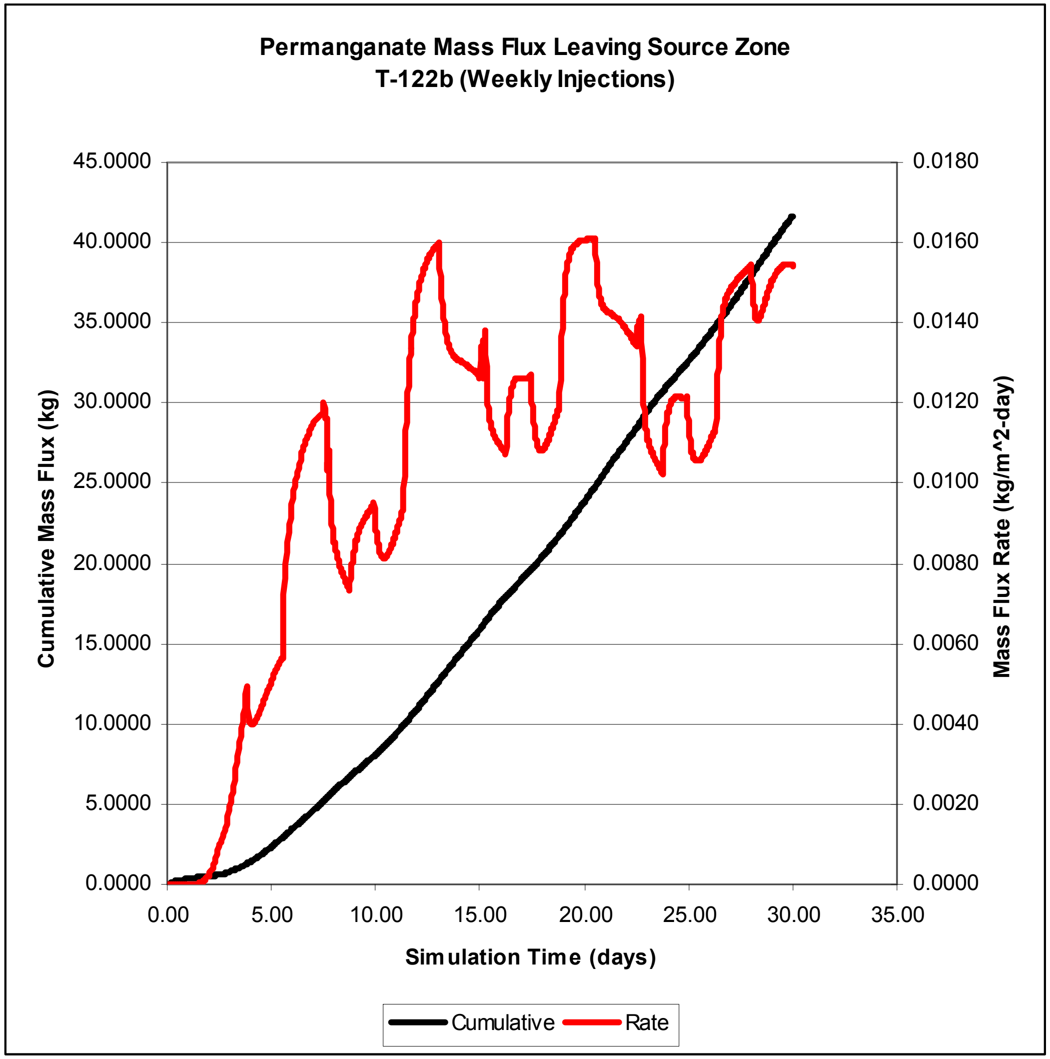


Advective flux

Flux Analysis – Weekly Injection

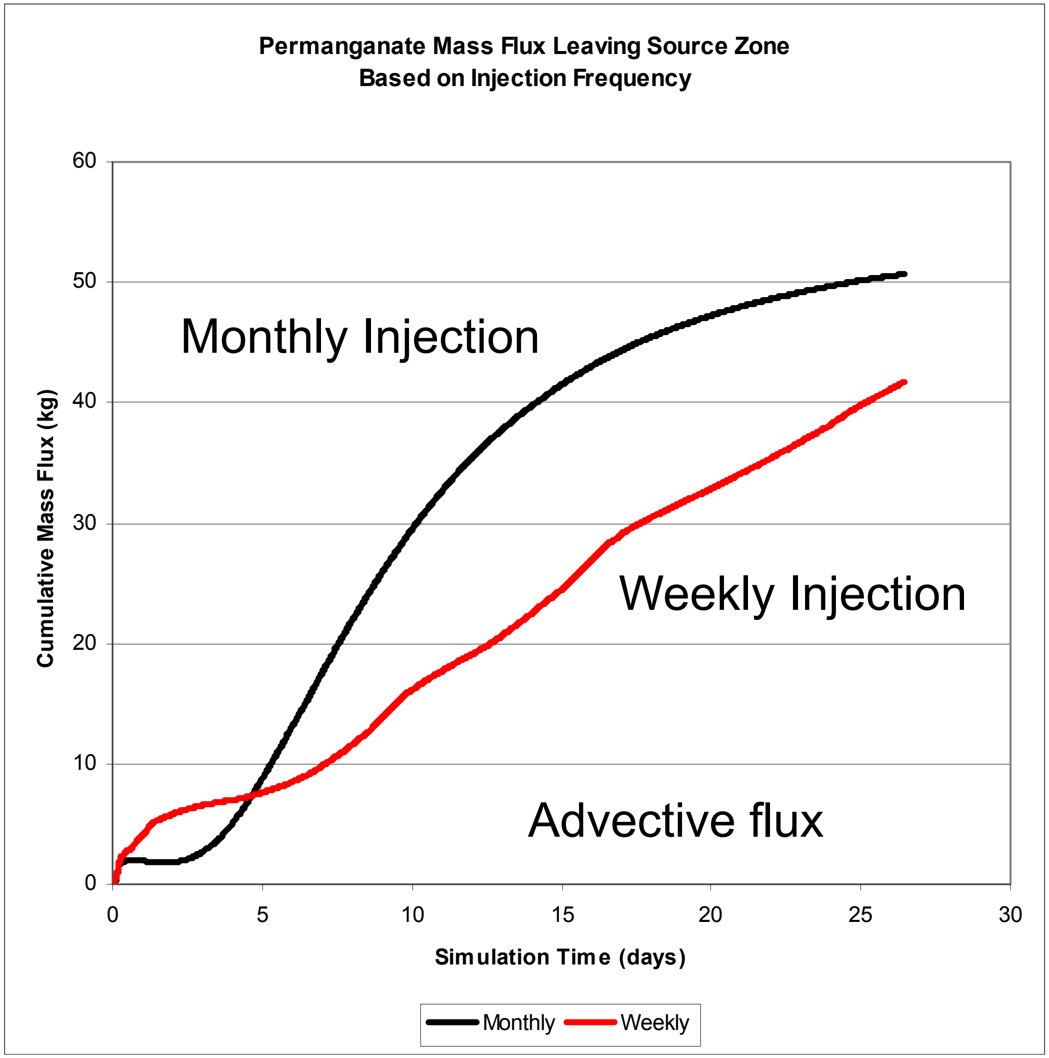
Total Mass Injected = 80 kg

50% leaving Source area



Advective flux

Permanganate Mass Leaving Source Area



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Correlation Between Contact Time and NAPL Depletion

Goal

- To demonstrate that contact time of injected reagant is proportional to the mass of DNAPL that will be depleted for a remedy
  - i.e. as contact time increases for a remedy, the corresponding depletion of DNAPL mass will also increase
- If proven, we don't have to simulate contaminants/DNAPL dissolution (higher uncertainty)

Approach

- Simplified model for now to assess degree of correlation
  - Permanganate injection
  - Rate-limited TCE DNAPL dissolution
  - TCE degradation rate based on permangate concentration

Approach

- Calculate average contact time of oxidant in source zone when changing:
  - Number of injection wells
  - Permanganate (KMnO4) degradation rate
  - Injected solution concentration of KMnO4
  - TCE degradation rate (which should not change contact time but will increase DNAPL dissolution rate)

Approach

- Calculated average contact time in source zone over 30 day period between injections
- Two concentration thresholds:
    - 20 and 200 mg/L KMnO4

NAPL Mass Depletion

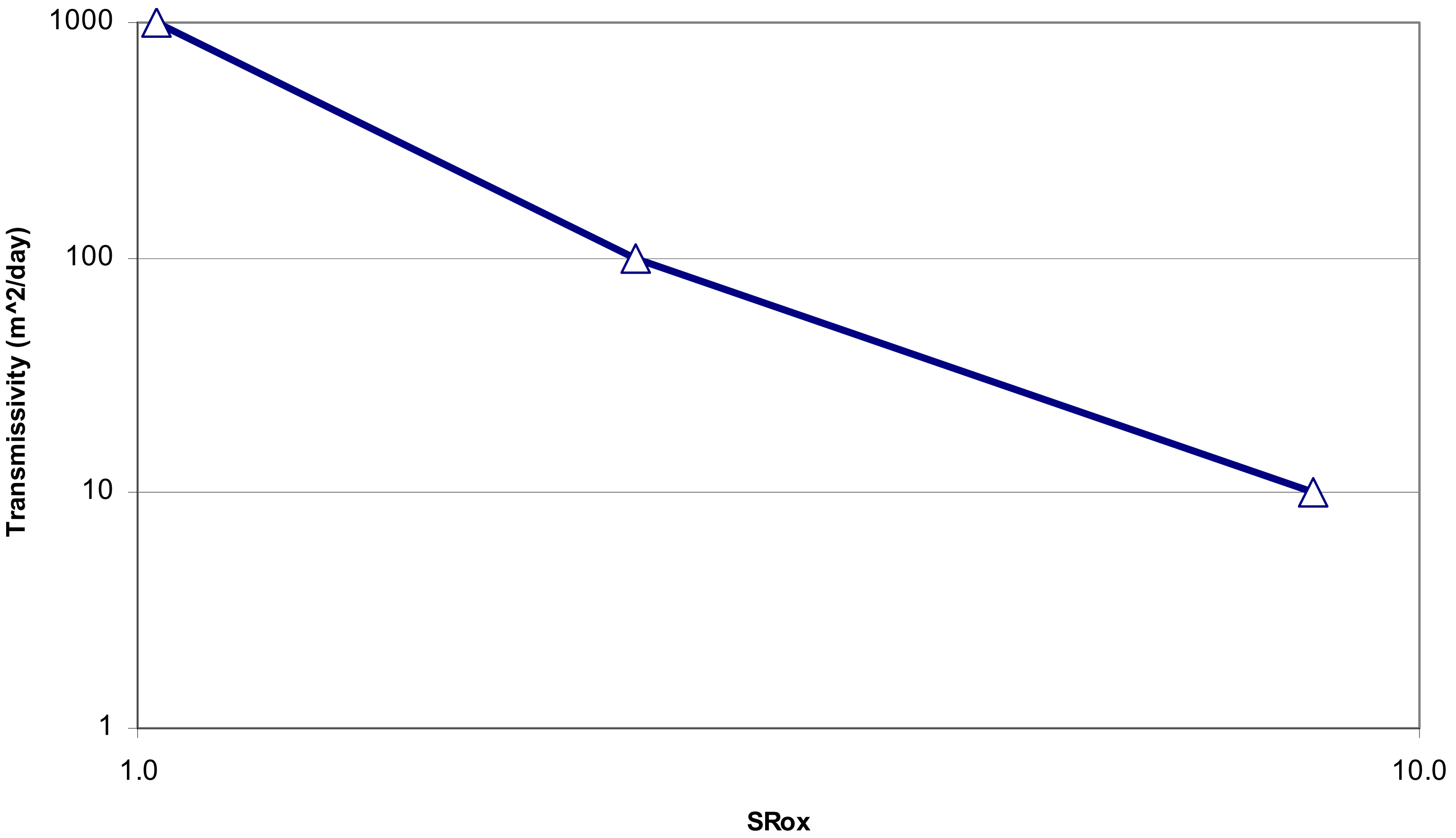
- Compare mass depleted for remedy to mass depleted under no action scenario (i.e. natural dissolution)
  - SRox = remedy mass depletion

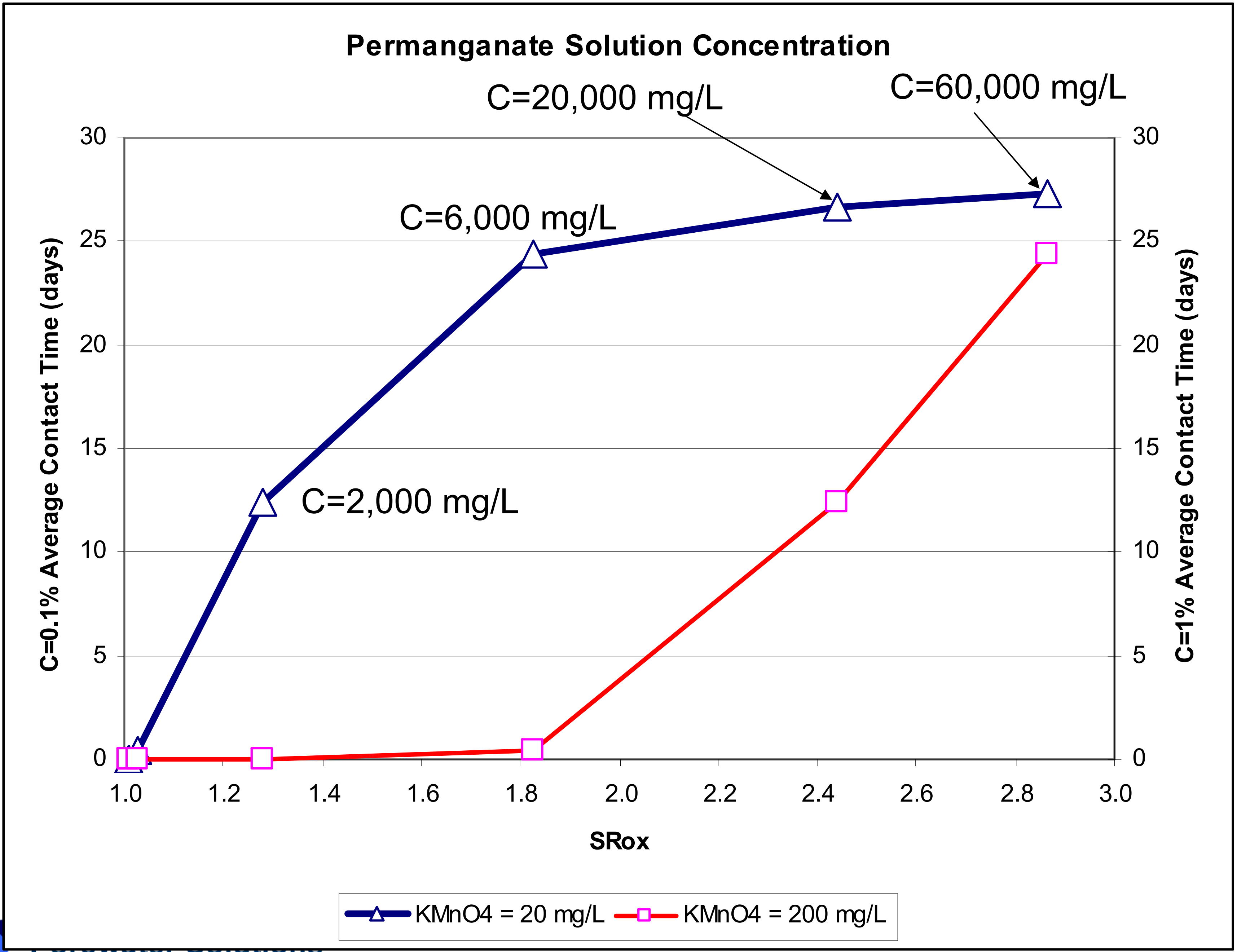
    no-action mass depletion

SRox >= 1

Srox = ISCO dissolution enhancement factor

Transmissivity vs. NAPL Depletion



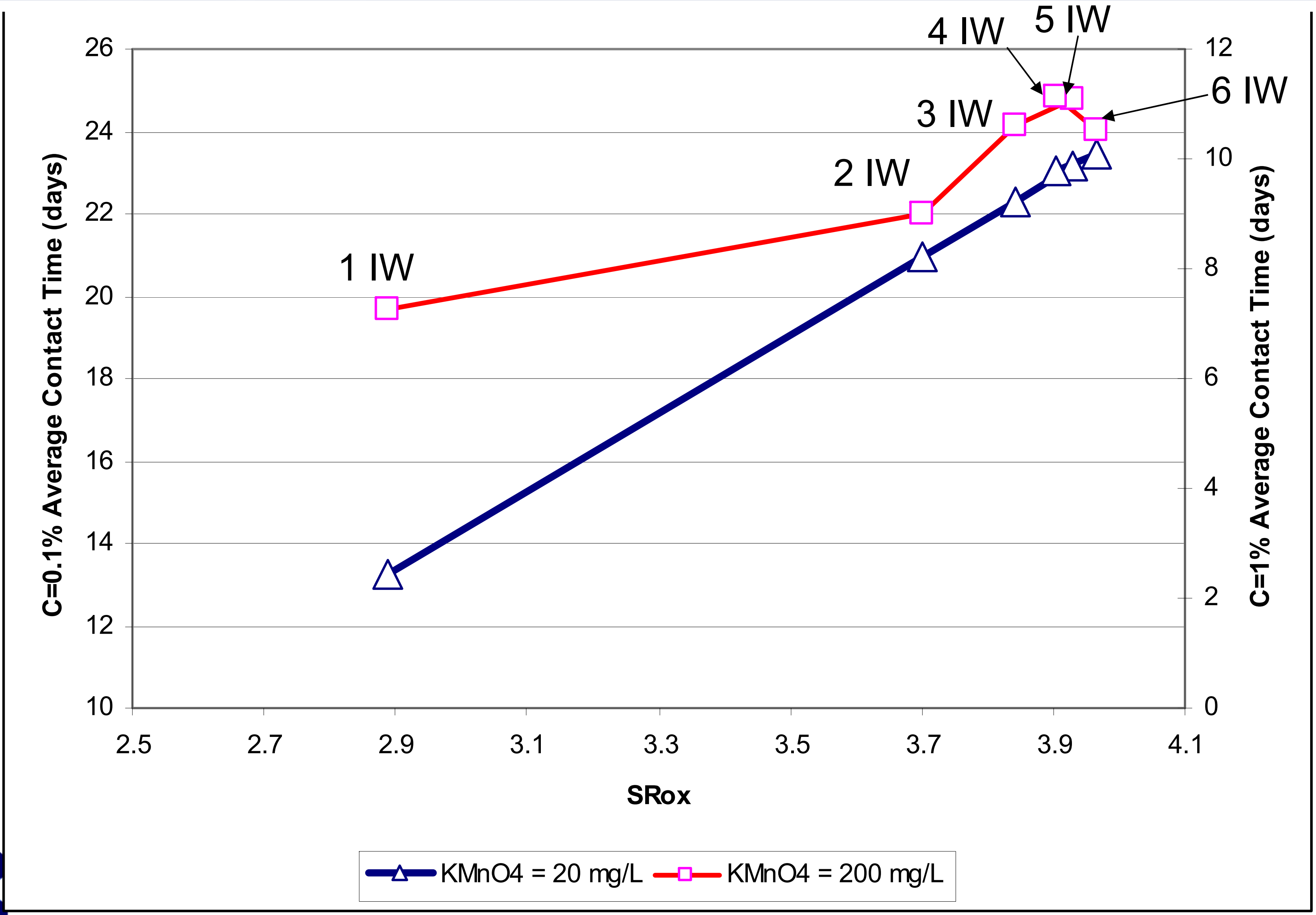

Permanganate Solution Concentration
C=20,000 mg/L
C=60,000 mg/L
C=6,000 mg/L
C=2,000 mg/L
C=0.1% Average Contact Time (days)
C=1% Average Contact Time (days)
0
5
10
15
20
25
30
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
SRox
KMnO4 = 20 mg/L
KMnO4 = 200 mg/L

Findings

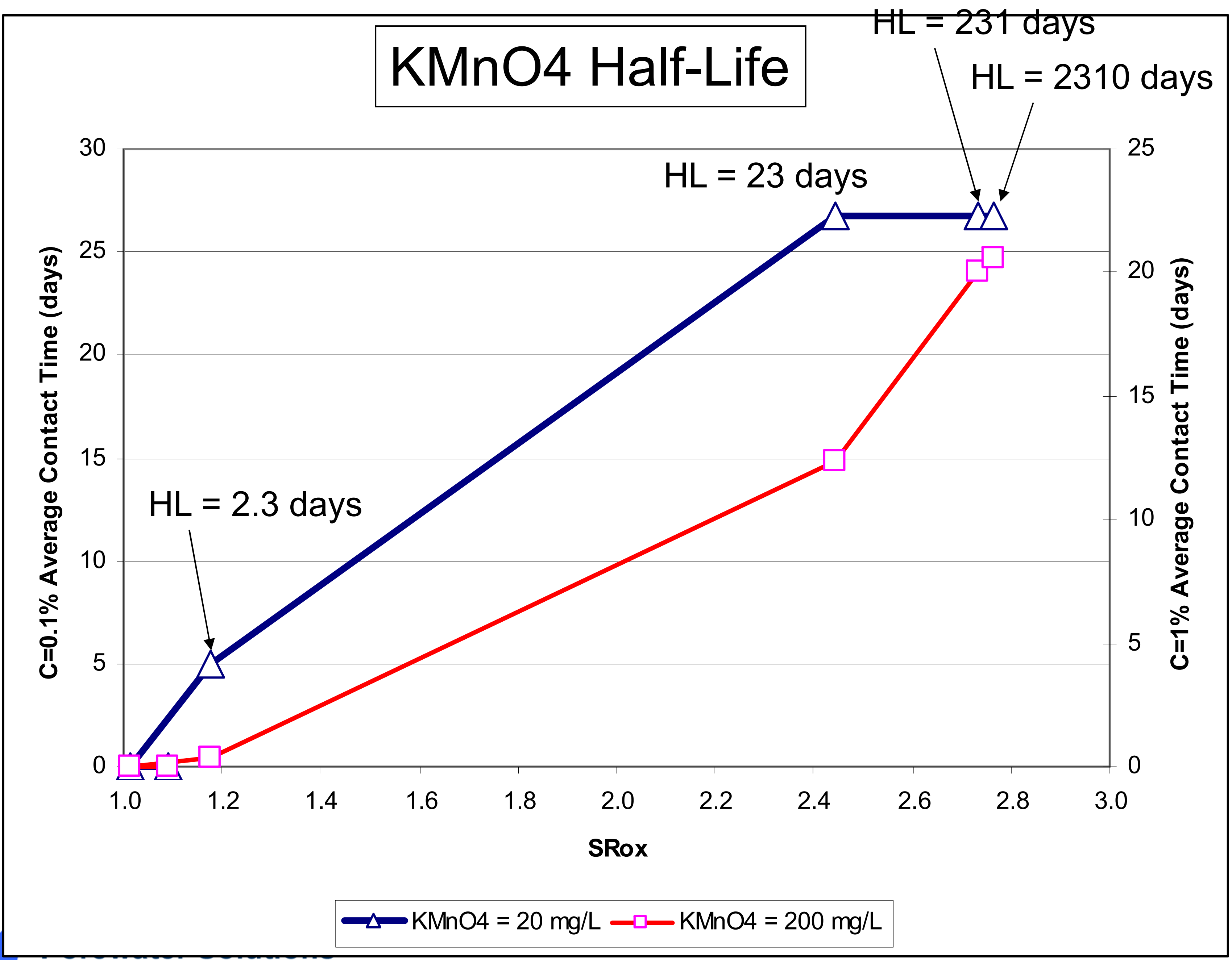
- Results match Petri et al. (2008)
  1. high velocity systems less impacted by ISCO because of higher natural dissolution rate; and
  2. Increasing permanganate concentration increased rate of DNAPL depletion.

- Indicates modeling of NAPL dissolution represents trends observed in lab experiments conducted by Petri et al.

Vary No. of Injection Wells (IW)



KMnO4 Half-Life



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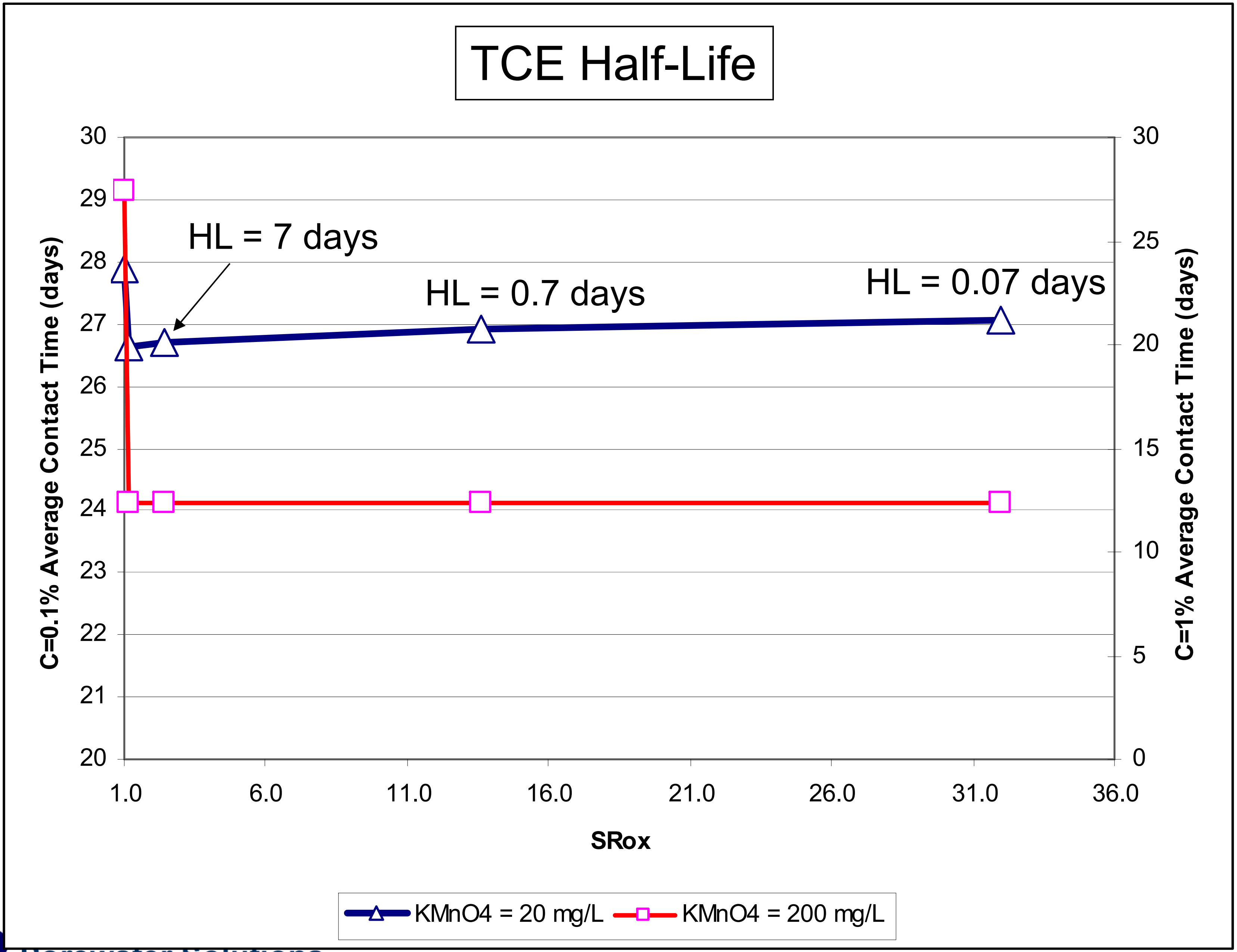
TCE Half-Life
HL = 7 days
HL = 0.7 days
HL = 0.07 days
C=0.1% Average Contact Time (days)
30
29
28
27
26
25
24
23
22
21
20
C=1% Average Contact Time (days)
30
25
20
15
10
5
0
1.0
6.0
11.0
16.0
21.0
26.0
31.0
36.0
SRox
KMnO4 = 20 mg/L
KMnO4 = 200 mg/L

Conclusions

- Parameters that result in higher contact time also result in higher DNAPL depletion rate for site conditions
- Contact time is reasonable surrogate for evaluating relative influence of design parameters on DNAPL flushing rate