ISCO Design Analysis

February 23, 2008

Introduction

- Goal is to evaluate remedial design strategy using a 3-D groundwater model
- Design parameters:
  - Number of injection wells
  - Injection rate
  - Duration of injection
  - Frequency of injection

Introduction

- Developed custom tools for remedial design analysis, including:
  - Programs to automate model construction, simulation, and output processing
  - Program to calculate oxidant contact time at each model grid cell in source area
  - Program to calculate mass flux of oxidant and contaminant out of source zone over time

Outline

- Sample model construction
- Contact time evaluation
- Mass flux analysis
- Modeling options for reactions and source properties

Sample Model Construction

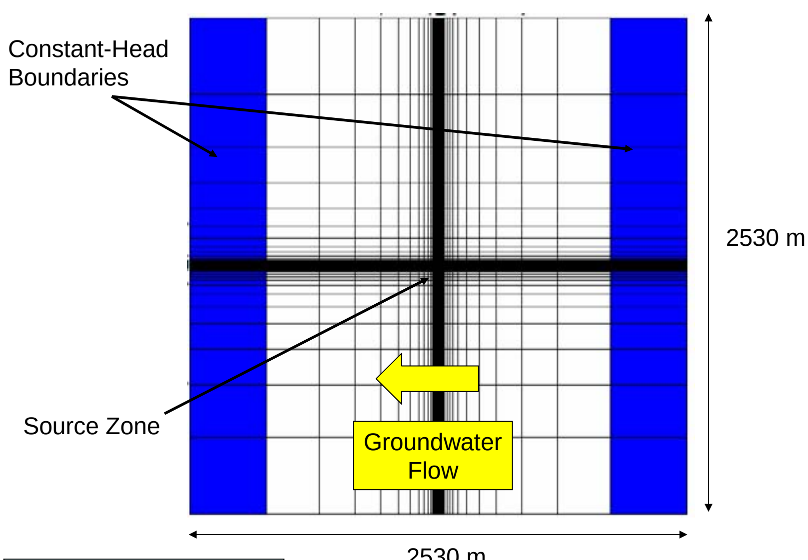
Flow Model Input

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

Transport Model Input

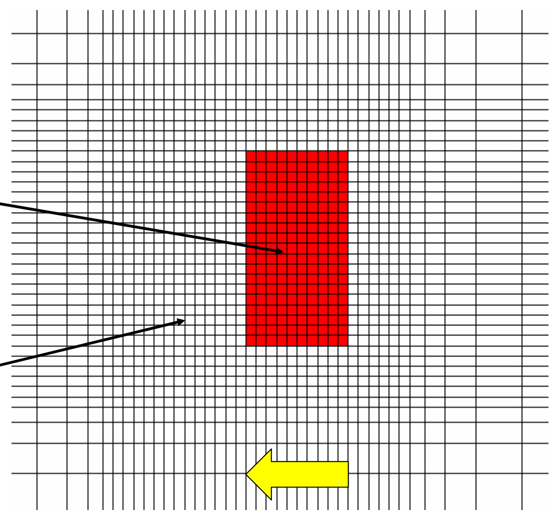
- Injected reactant only
  - Did not simulate contaminant in source zone
- Longitudinal dispersivity = 2 m
- No sorption
- Oxidant half-life = 25 days
- Injected concentration = 1 (normalized)

Model Domain

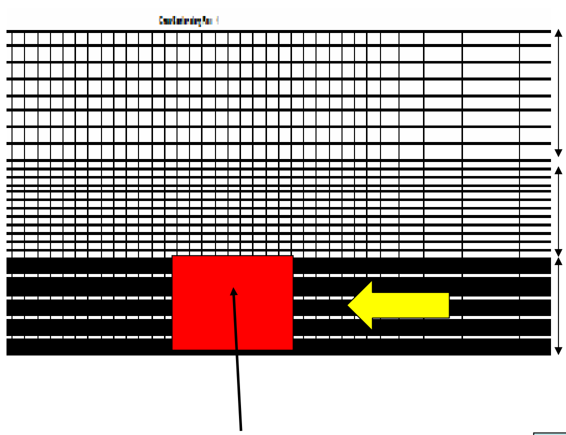


62 rows and 62 columns

Close-up of source zone



Domain Cross-Section



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

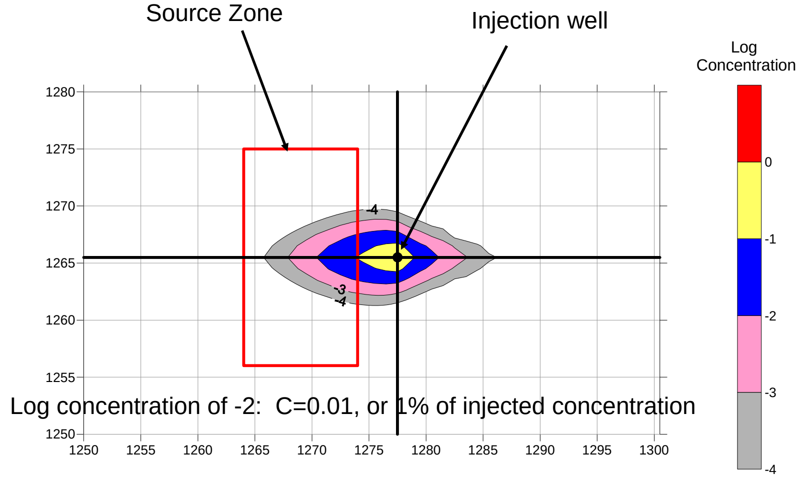
- Contact Time = total time during simulation that permanganate exceeds the target concentration in a model grid cell
- Contouring contact time provides a measure of efficiency in oxidant distribution in the source area over entire simulation
- Evaluating the % of source area with a minimum contact time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

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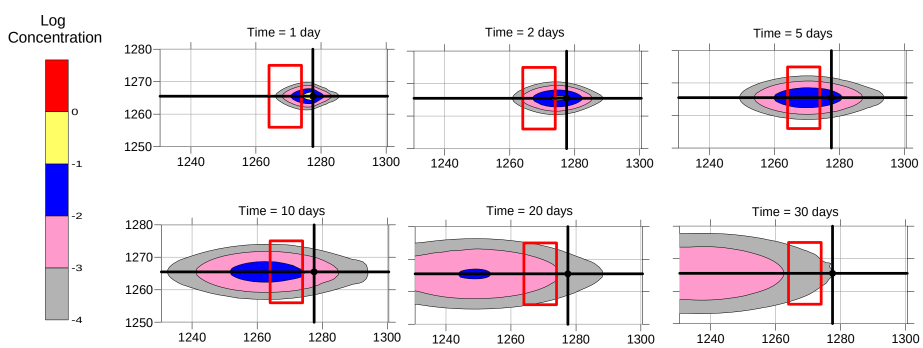
PERM conc. over time

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

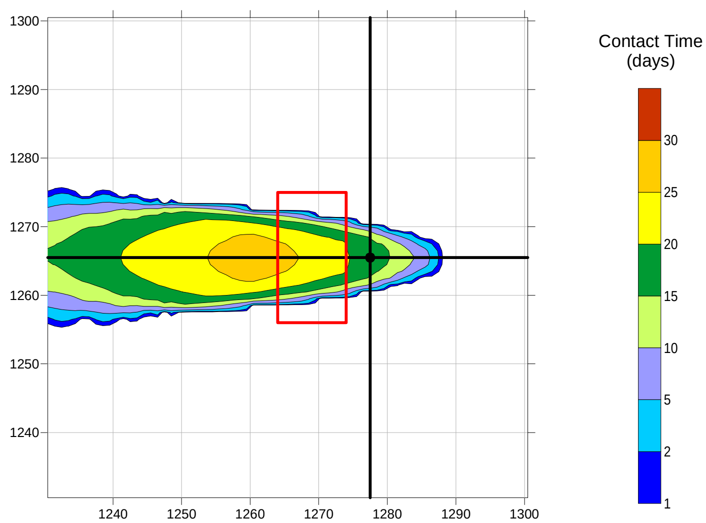
Contact Time Calculation

- 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

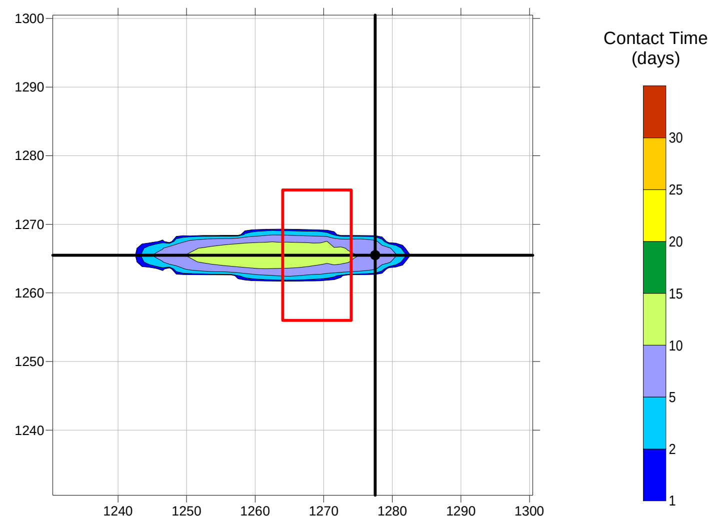
Contact Time Calculation

- 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

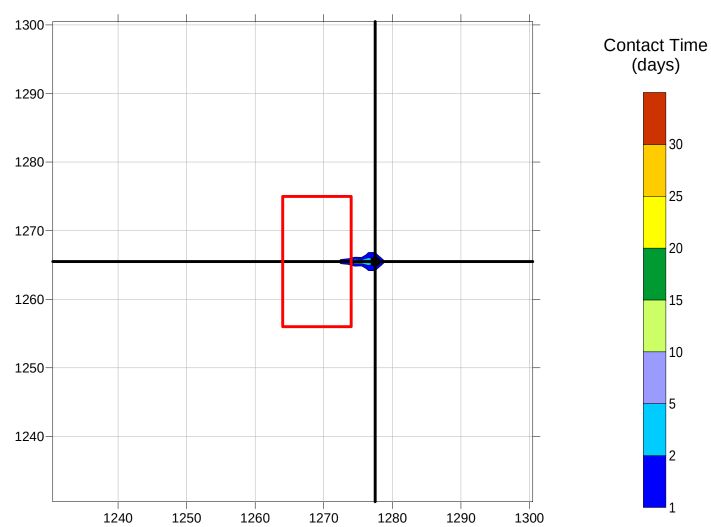
Contact Time: Reactant C > 0.1%



Contact Time: Reactant C > 1%



Contact Time: Reactant C > 10%



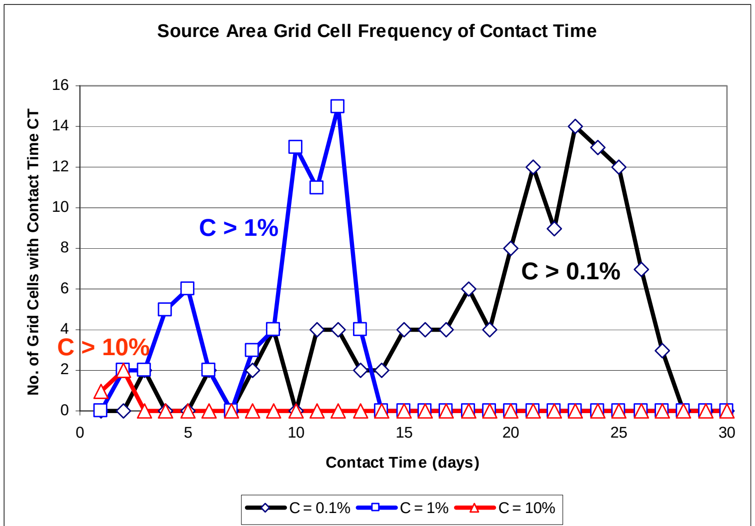
Findings

- 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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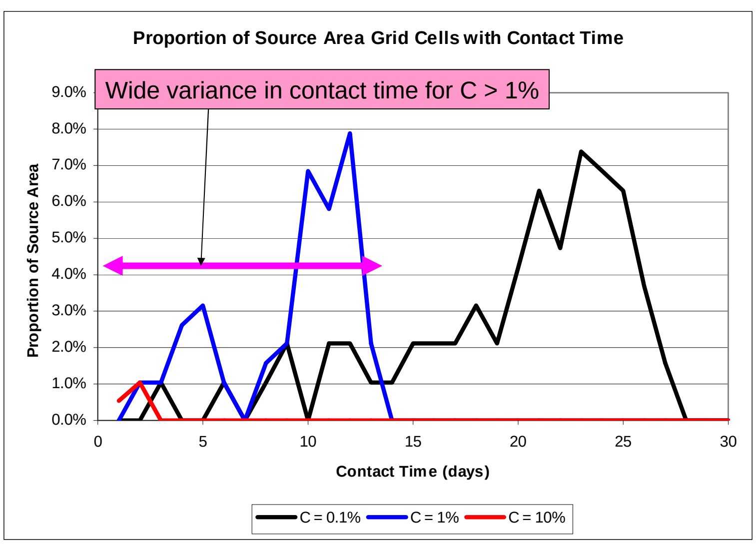
Contact Time Distribution in Source Zone



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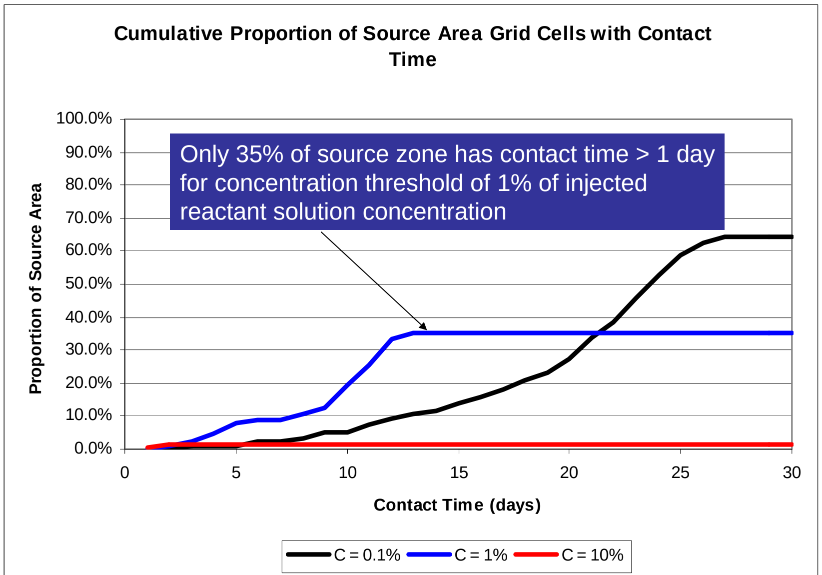
Cumulative Distribution



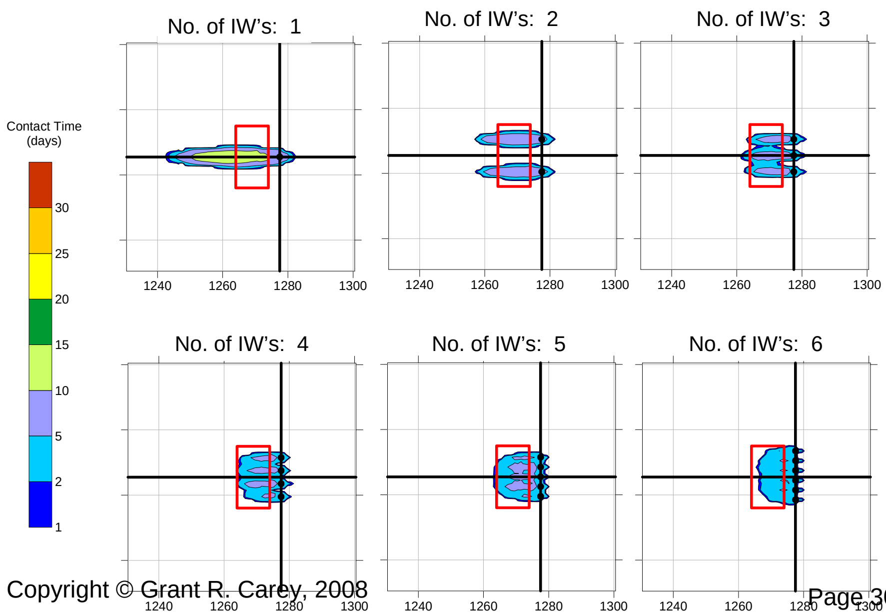
Contact Time Evaluation

Multiple Injection Well Scenarios

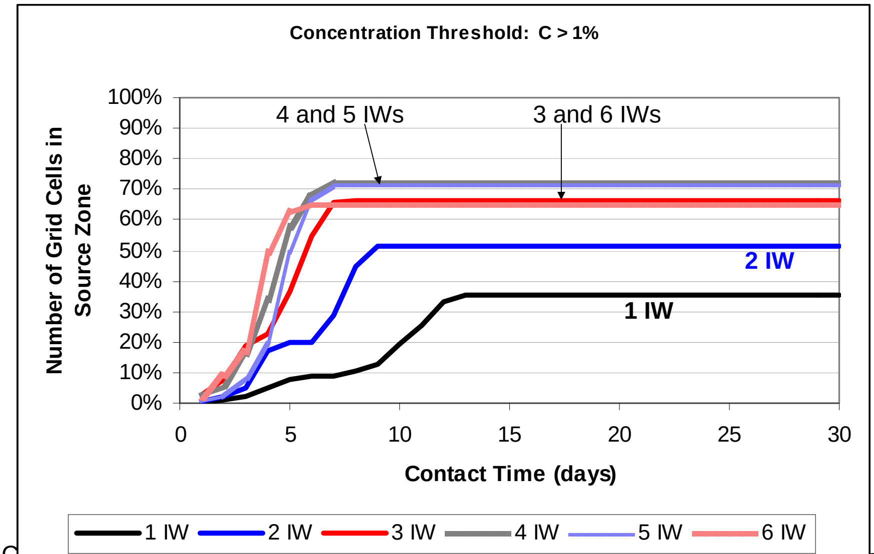
Multiple Well Scenarios

- 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



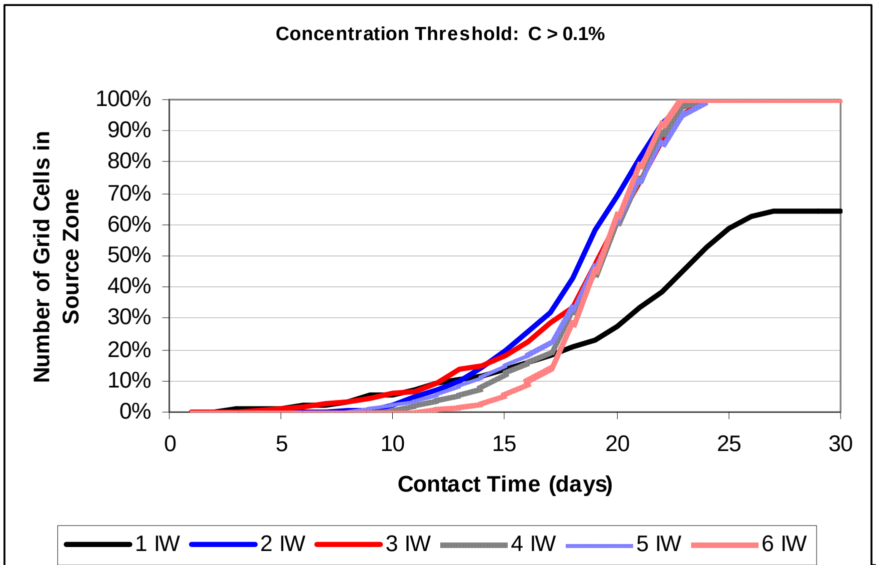
Cumulative Frequency: Reactant C > 1%



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%



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

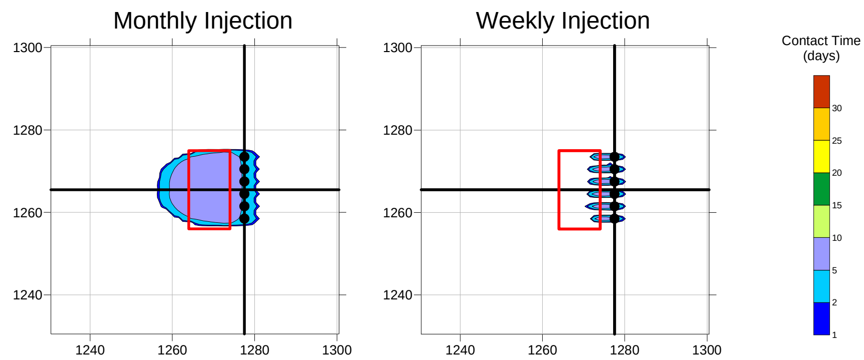
Goal

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

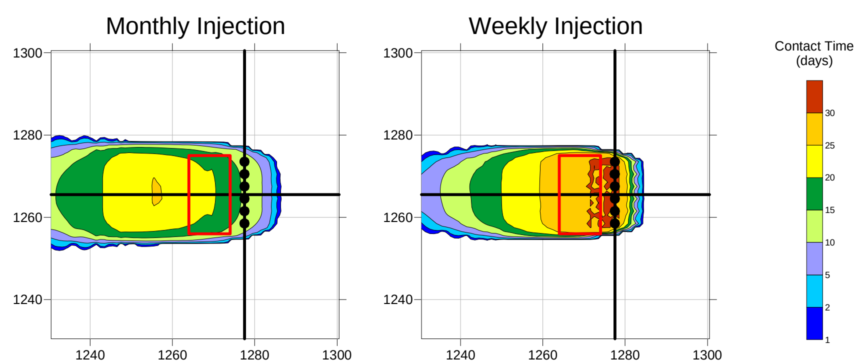
Injection Scenarios

- 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%

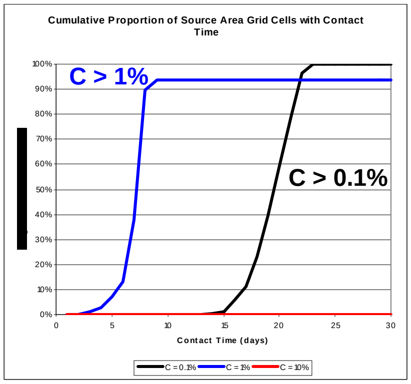


Contact Time for C > 0.1%

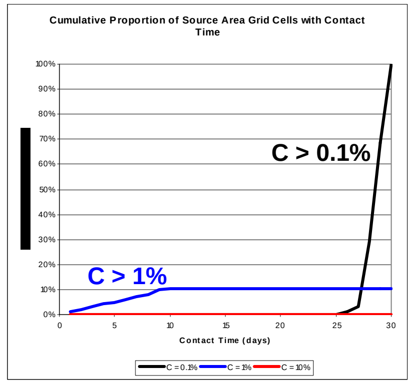


Contact Time Distribution

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

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Flux Analysis

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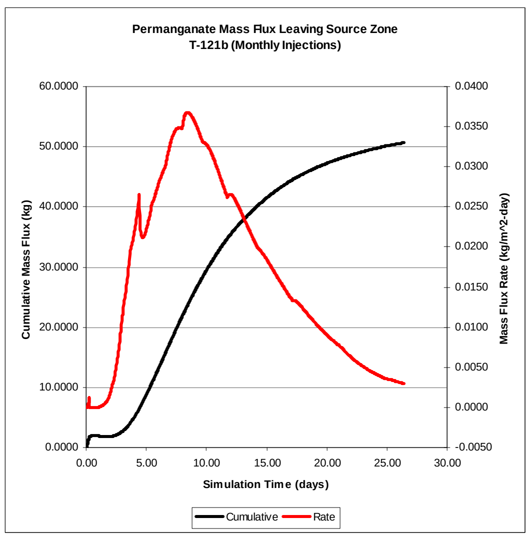
Flux Analysis

- 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

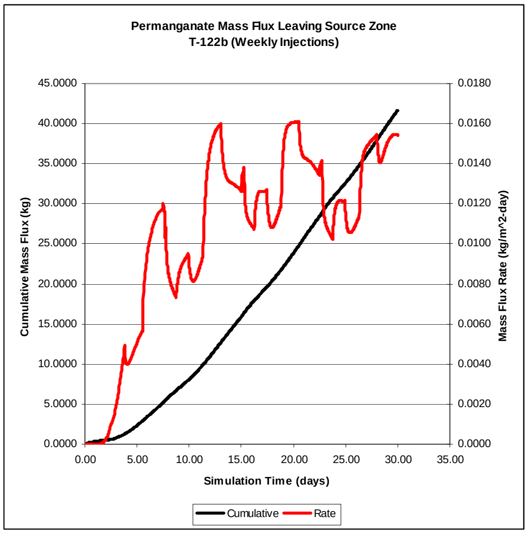


Advective flux

Flux Analysis – Weekly Injection

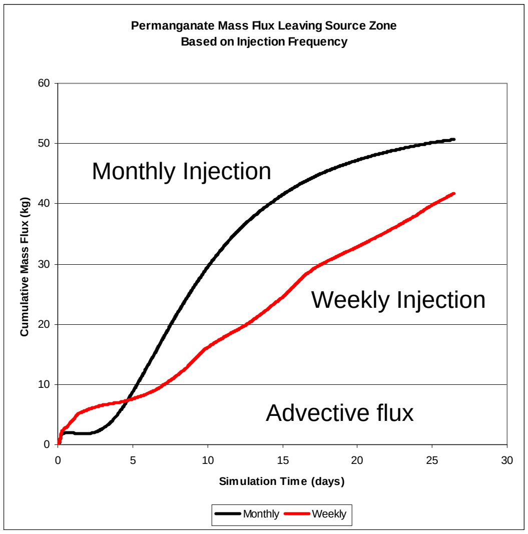
Total Mass Injected = 80 kg

50% leaving Source area



Advective flux

Permanganate Mass Leaving Source Area



Modeling Options

Modeling Options

- Add native organic demand (NOD)
  - Oxidant reaction depends on NOD
    - Model phased changes to injection strategy to account for degradation of NOD over time
- Add contaminant with rates that depend on OXD concentration
- Multicomponent DNAPL source with equilibrium or rate-limited dissolution

Summary

- Custom modeling tools can be used to:
  - Provide competitive advantage when submitting proposals
  - Compare remedial efficiency for different options
  - Justify design to regulators and public