Multi-Objective Optimization of an *In Situ* Bioremediation Technology to Treat Perchlorate-Contaminated Groundwater

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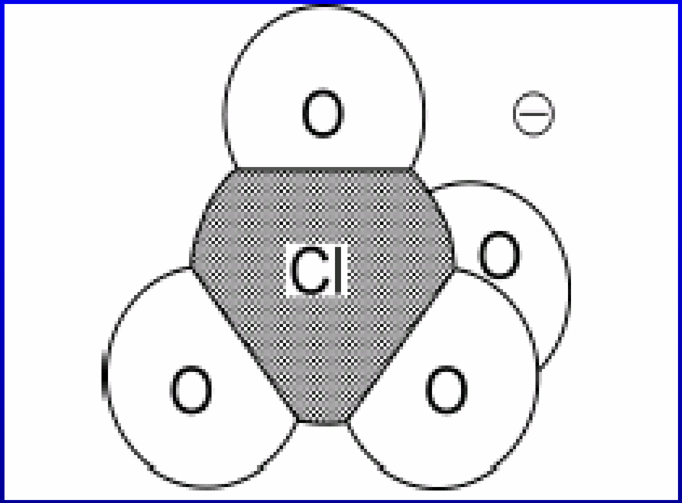
Overview

- The perchlorate problem
- Potential technology solution—*in situ* bioremediation
- Formulate problem for technology optimization
- Optimization approach
  - Technology simulation model
  - Multi-objective genetic algorithm (MOGA)
- Optimization results
- Conclusions

The Perchlorate Problem

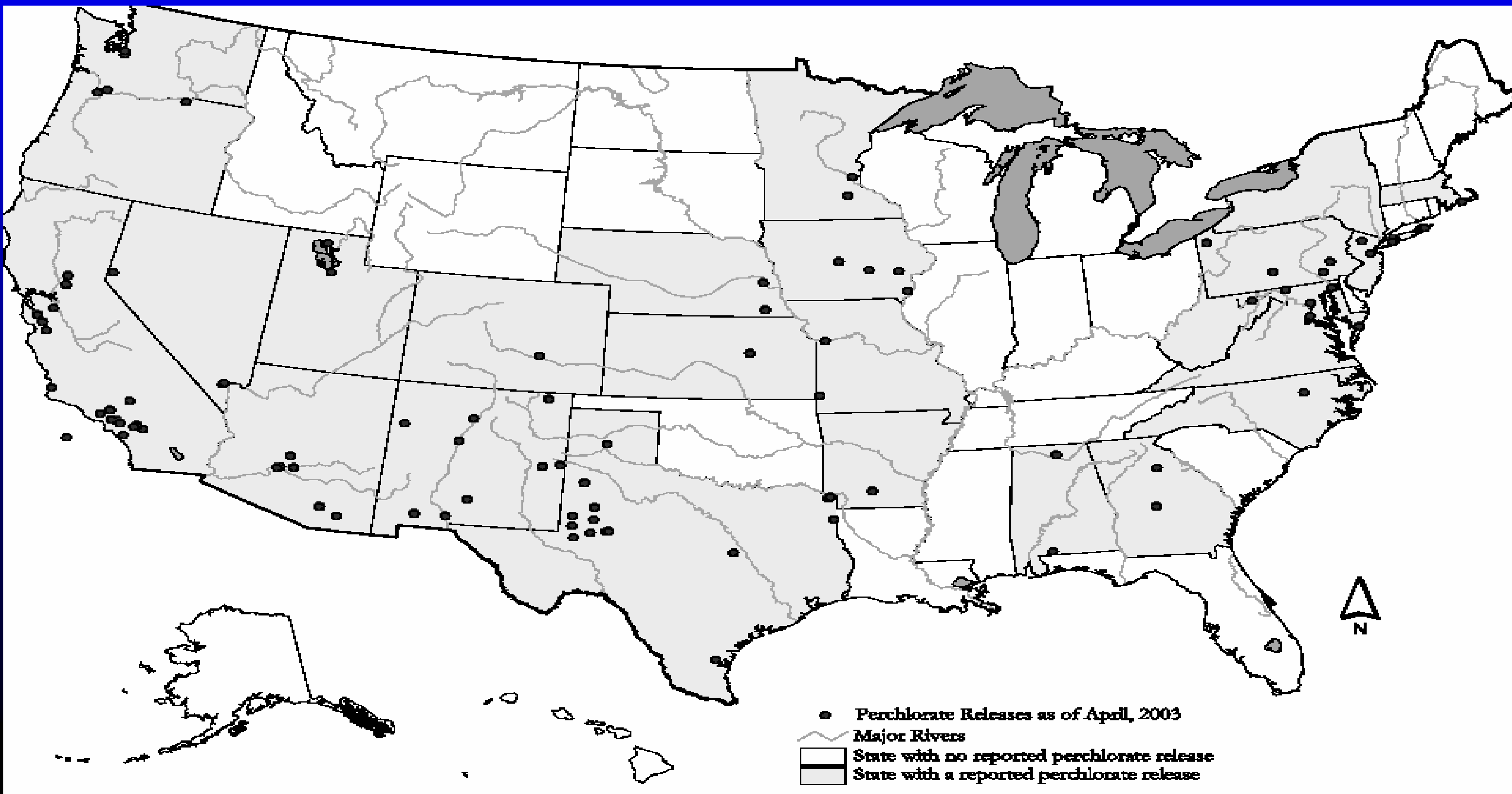
- Used as a constituent in solid rocket boosters and explosives/fireworks
  - Aerospace industry and DoD primary pollution sources
- Chemistry
  - Very mobile in environment
    - Highly soluble (200 g/L)
    - Does not adsorb to soil particles
  - Stable in environment
    - Though energetically favorable, perchlorate reduction is kinetically inhibited



- Health concerns
  - Interferes with uptake of iodine in the thyroid gland
  - CA action level set in March 2004 at 6 μg/L

The Perchlorate Problem

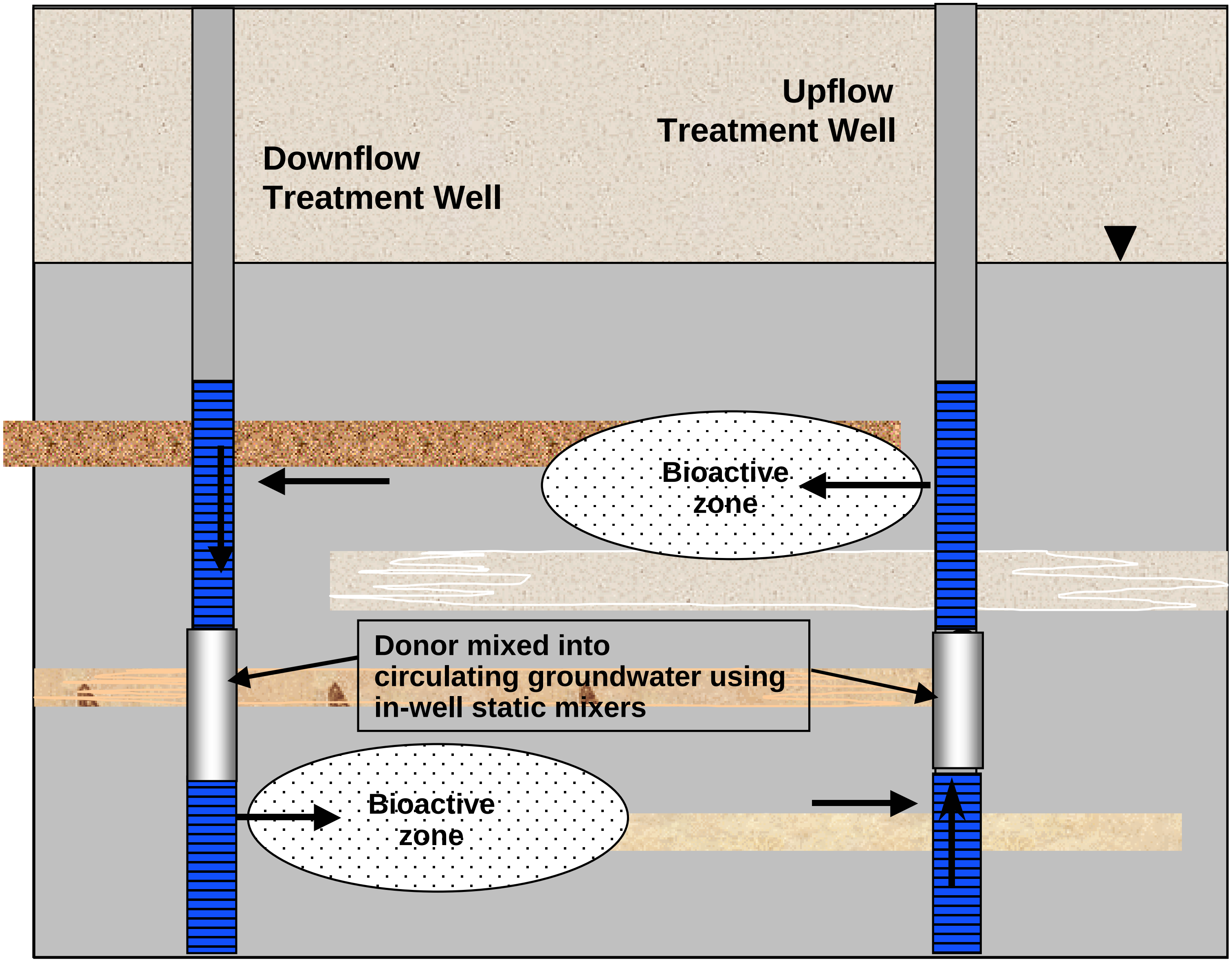
- Groundwater contamination confirmed in 20+ states
- Problem is particularly severe in Southwest

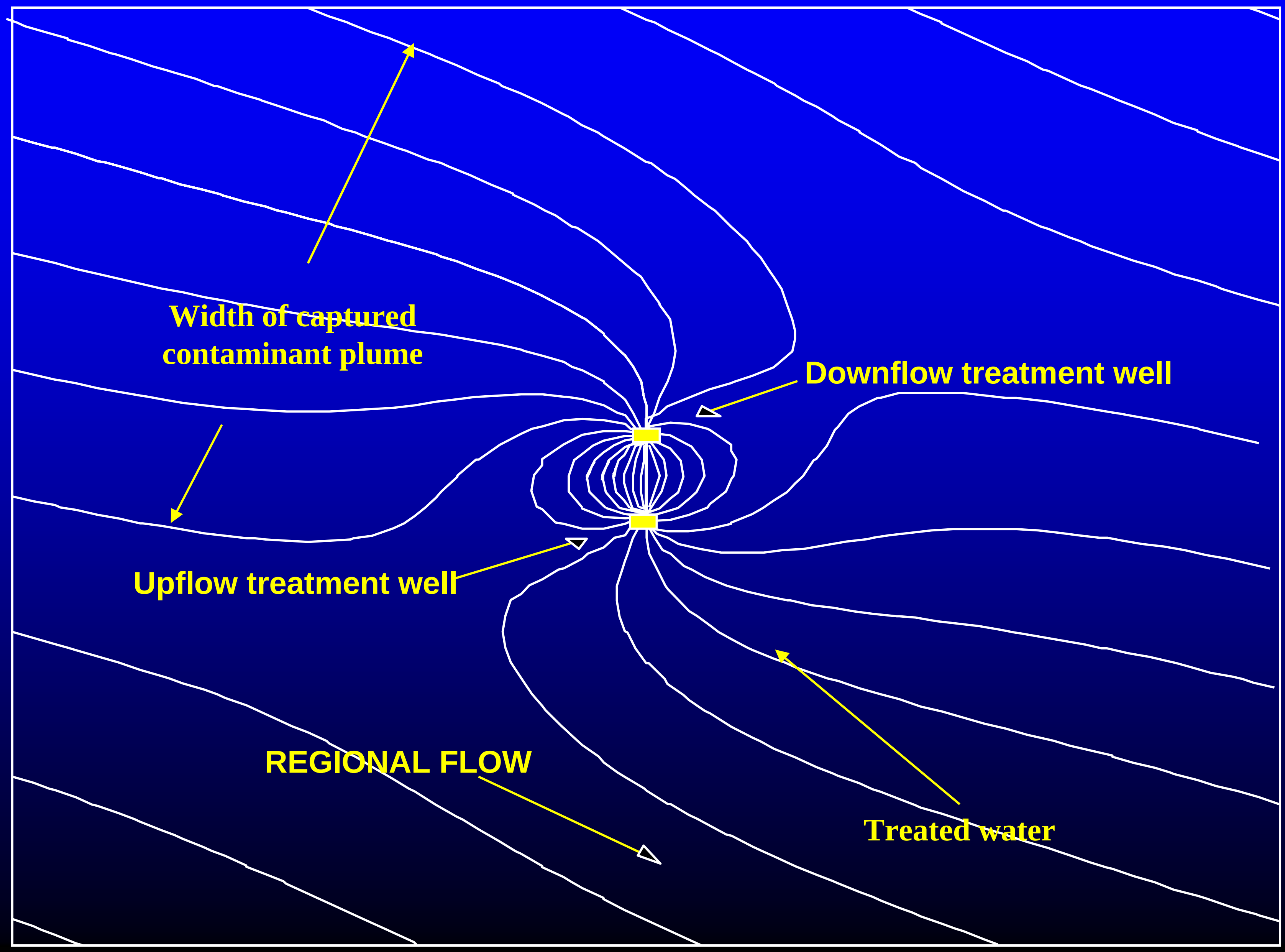


Potential Technology Solution (*In Situ* Bioremediation)

- Perchlorate used as an electron acceptor in the presence of an electron donor
  - *e.g.* acetate, lactate, citrate, ethanol, H_2 gas
- Perchlorate reducing microbes appear to be ubiquitous
  - Capable of reducing perchlorate to low concentrations
- If competing electron acceptors (O_2, NO_3^-) present, microbes will reduce these before using ClO_4^- as an acceptor
- For *in situ* process to work, need to get donor and perchlorate to indigenous bacteria

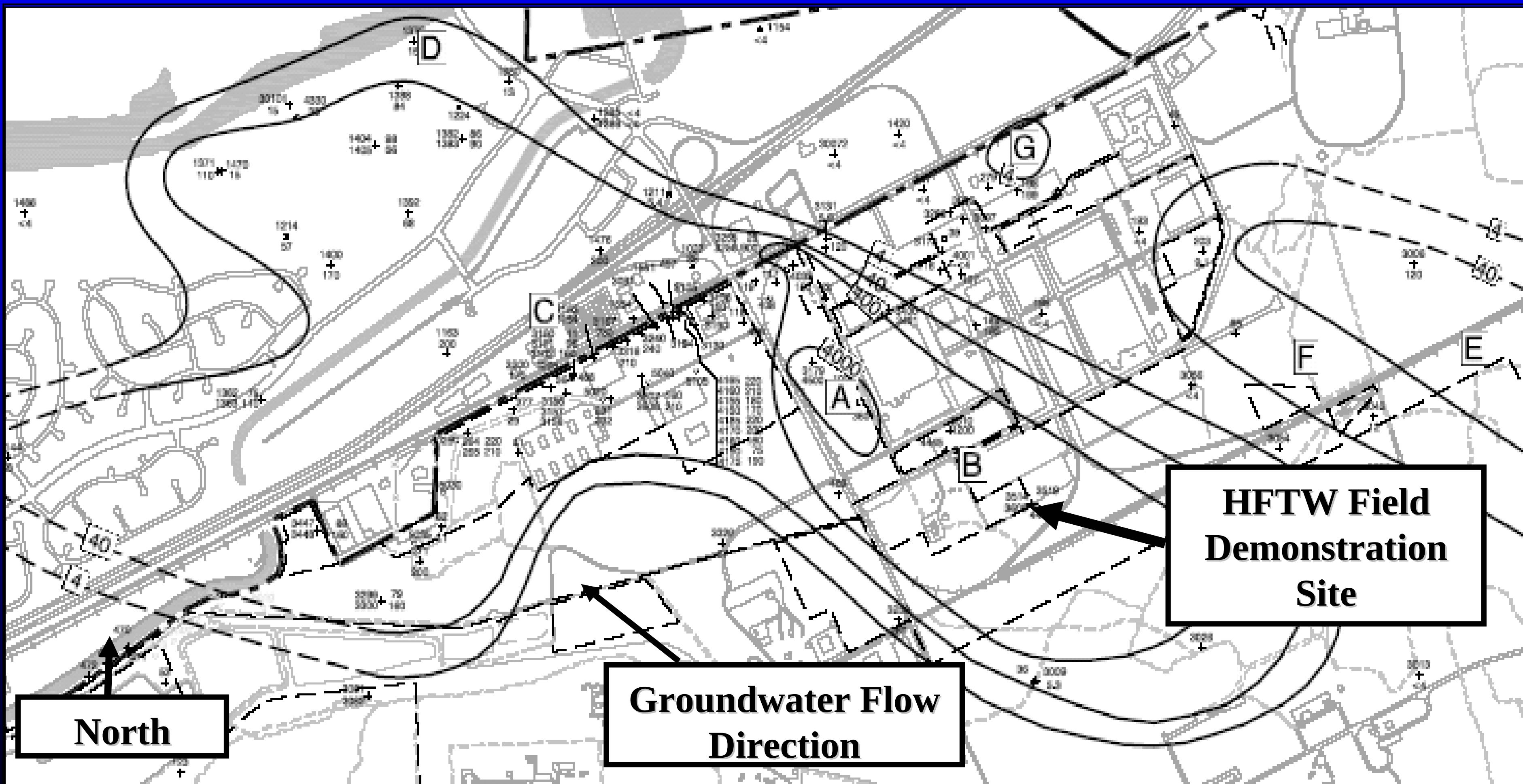
Potential Technology Solution
Horizontal Flow Treatment Wells (HFTWs)

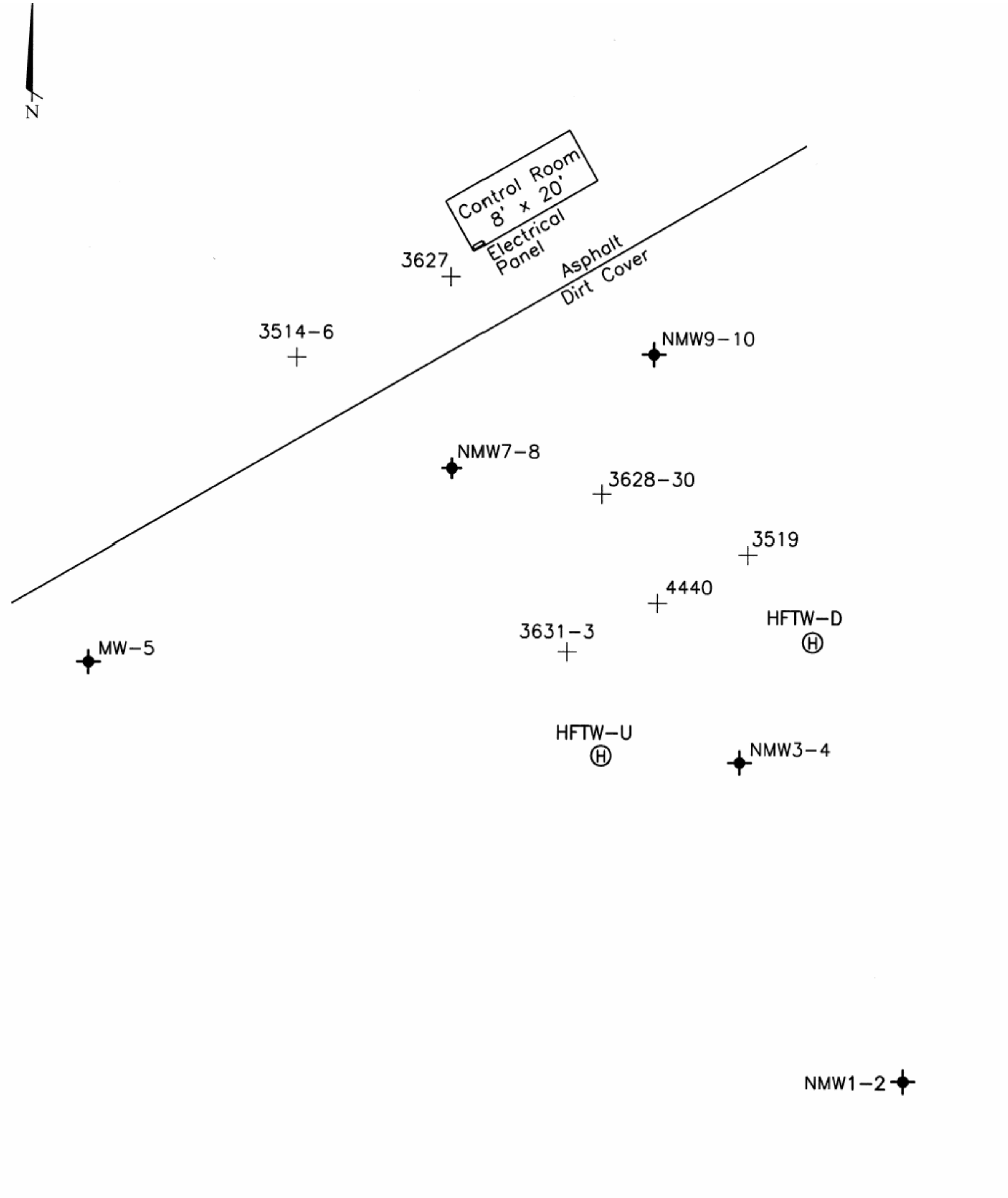




Width of captured
contaminant plume
Downflow treatment well
Upflow treatment well
REGIONAL FLOW
Treated water

Potential Technology Solution
Upcoming HFTW Field Evaluation




N
Control Room
8' x 20'
Electrical
Panel
Asphalt
Dirt Cover
3627
3514-6
NMW9-10
NMW7-8
3628-30
3519
4440
HFTW-D
3631-3
MW-5
HFTW-U
NMW3-4
NMW1-2

Optimization Problem Formulation

- Objectives
  - MAXIMIZE mass ClO_4^- destroyed
  - MINIMIZE operating cost
- Decision variables
  - Pump rate (*Q*)
  - Well spacing (*d*)
  - Concentration of injected electron donor (C_{in})
  - Injection pulse duration (*p*)
- Constraints – decision variable bounds

Conceptual Optimization Approach

Select potential solutions

↓

Run cost and technology models to evaluate how well each potential solution meets objectives

↓

Determine “best” solutions

Technology Model (Parr *et al*., 2003)

- Flow-and-transport model
- Biological treatment submodel
- Site model

Technology Model

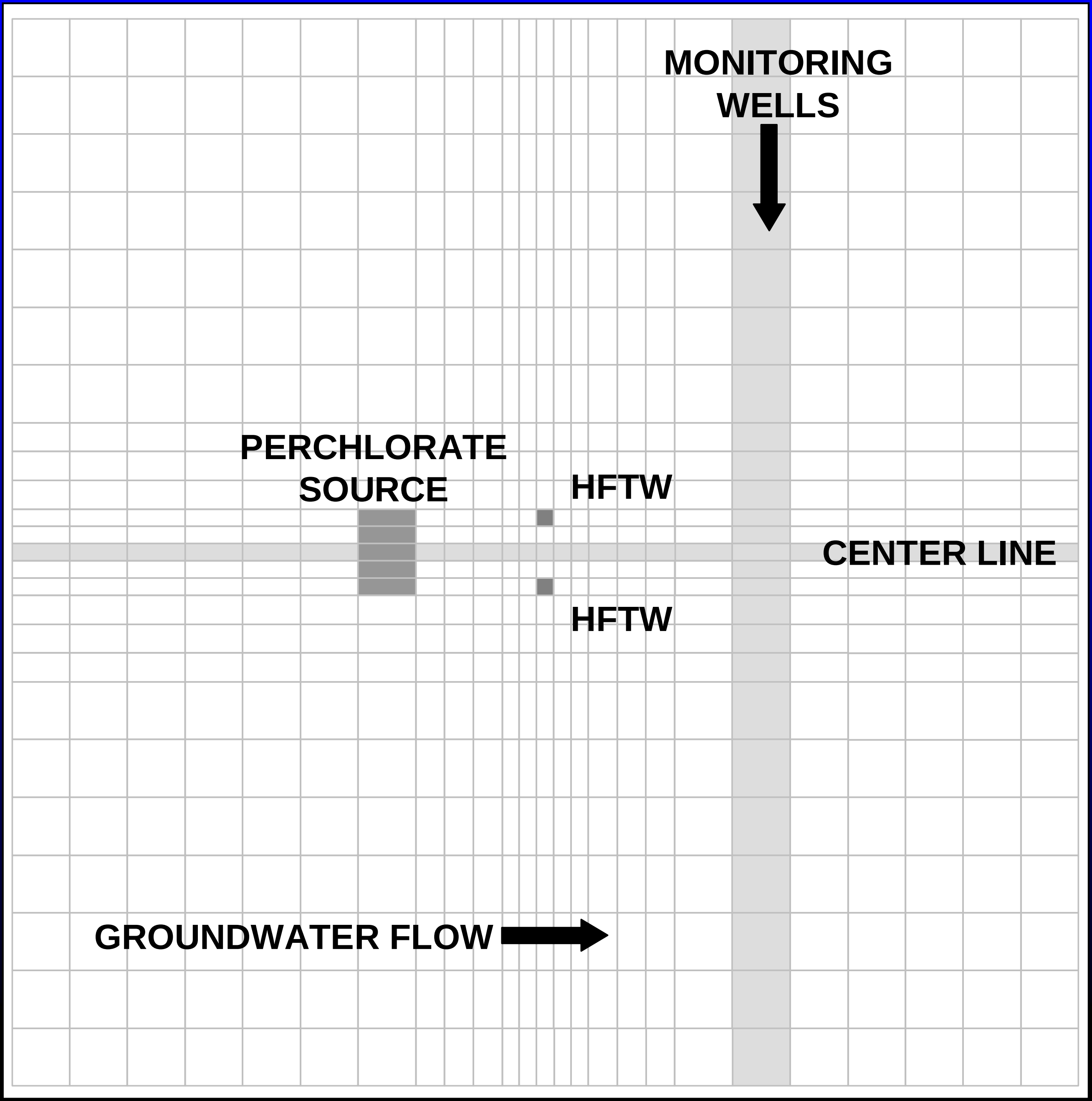
- Flow-and-transport model
  – Steady-state flow equation solved using MODFLOW
  – PDEs for advection, dispersion, and reaction of electron donor, O_2, NO_3^-, & ClO_4^-
    - Equations solved using finite differences
    - Reactions defined in biological submodel
  – Bacteria are assumed immobile

Technology Model

- Biological treatment submodel
  - Consumption rates of dissolved species (electron donor, O_2, NO_3^-, ClO_4^-) due to microbially mediated redox reactions
    - Described by dual-Monod kinetics (degradation rate dependent on both donor and acceptor concentrations)
  - Immobile biomass growth also described by dual-Monod kinetics with first-order die-off
  - Multiple acceptors (O_2, NO_3^-, ClO_4^-) compete for electrons from the donor

Technology Model

Site Model



Cost Model

- For comparison purposes, operating cost modeled as simple function of pumping rate and cost of electron donor

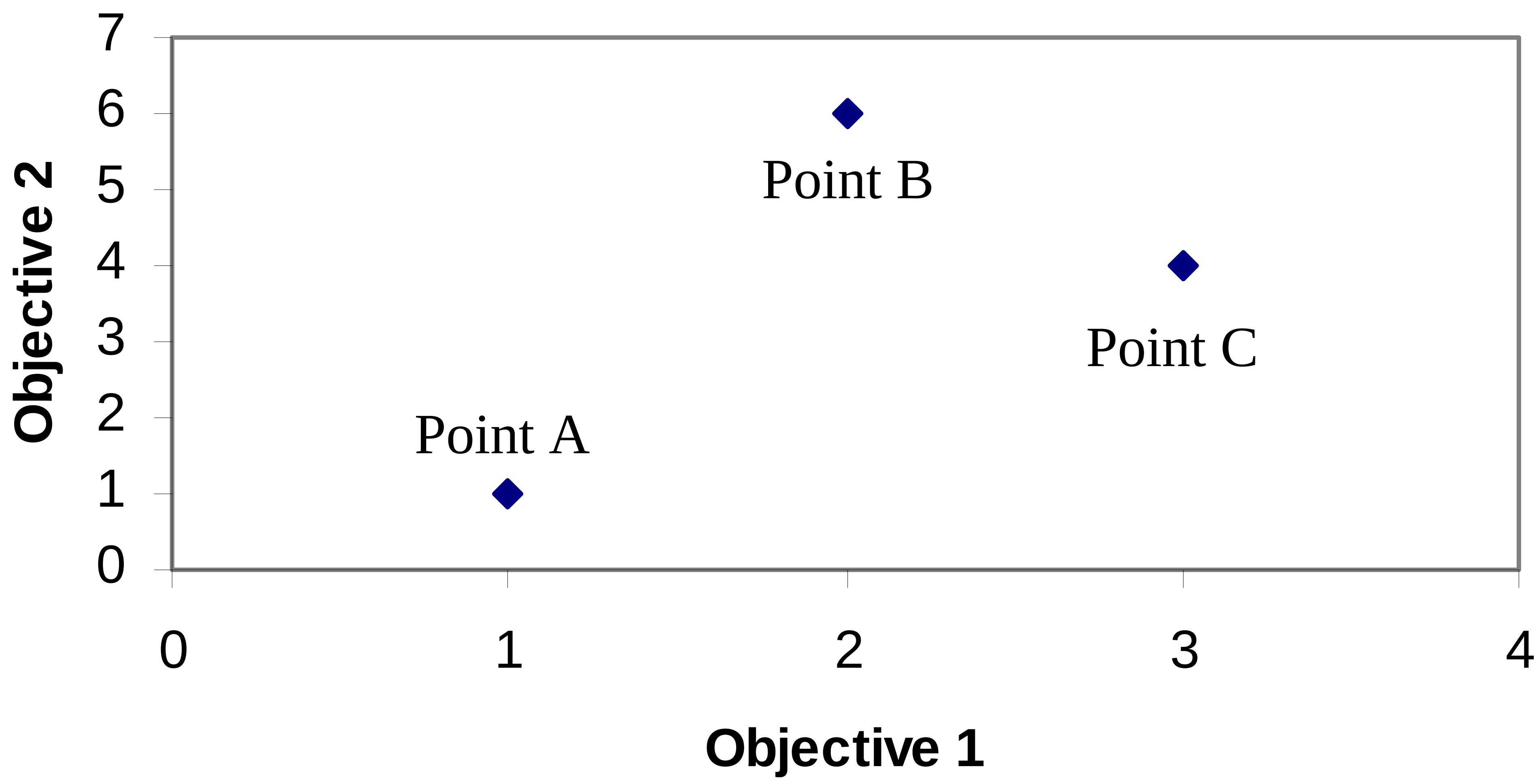
Multi-Objective Genetic Algorithm (MOGA)
Genetic algorithm (GA)

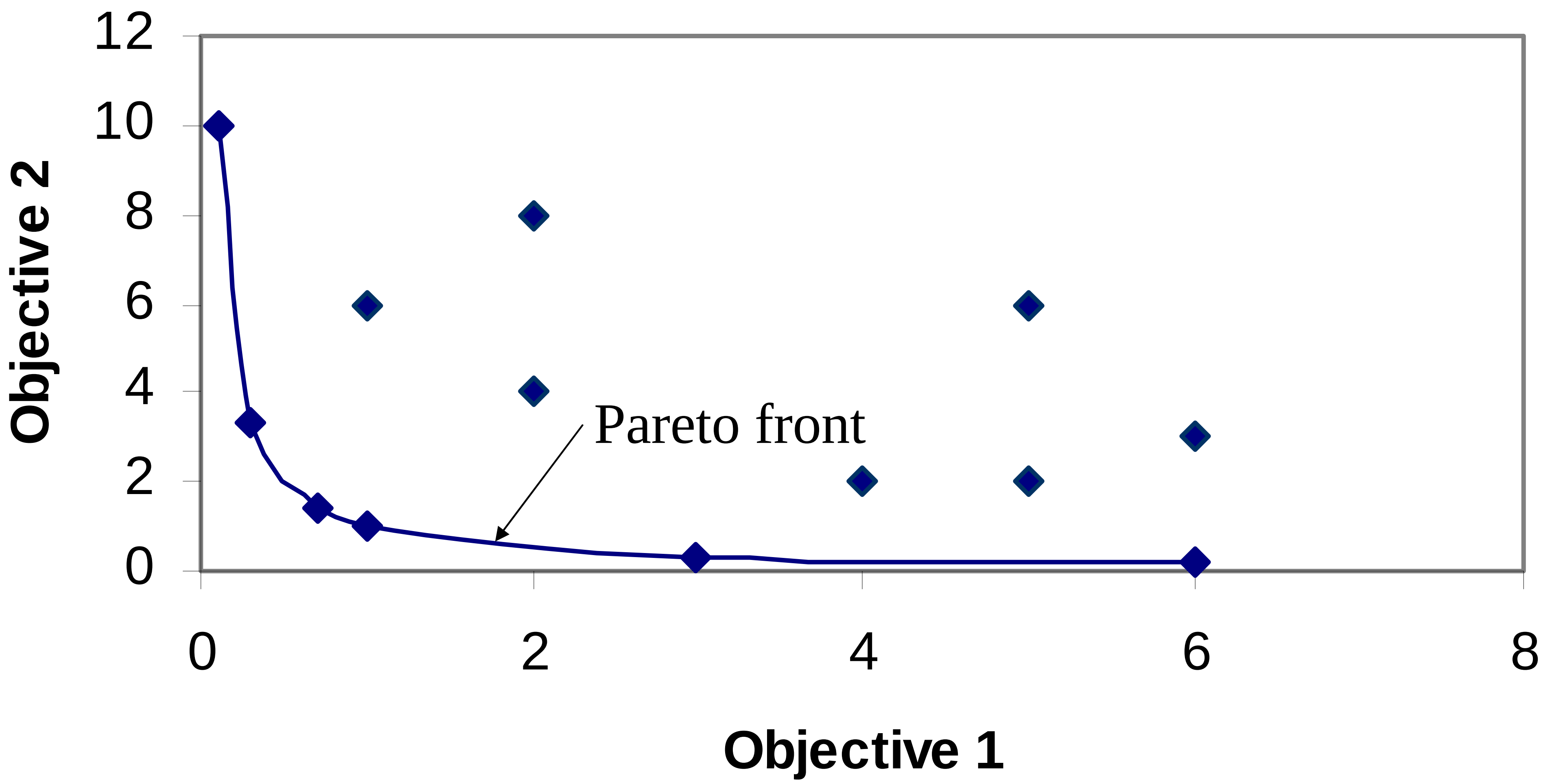
- Chromosome defined as set of decision variables
  - [Q, d, C_{in}, p]
- Initialize population of chromosomes (potential solutions)
- Repeat the following "generation cycle" N times
  - Evaluate chromosomes using the objective function
  - Select "fittest" chromosomes
  - Recombine "fittest" chromosomes to make new generation
    - Mutation
    - Crossover

Multi-Objective Genetic Algorithm (MOGA)
Pareto-based approach to multi-objective optimization

- Objective functions are not combined into a single objective function; no "weights" or "penalties"
- Each objective has equal importance
- Distinguish superior/inferior solutions using concept of **domination**

Domination Concept





12
10
8
6
4
2
0
Objective 2
Pareto front
0
2
4
6
8
Objective 1

MOGA

Create population of chromosomes (solutions)

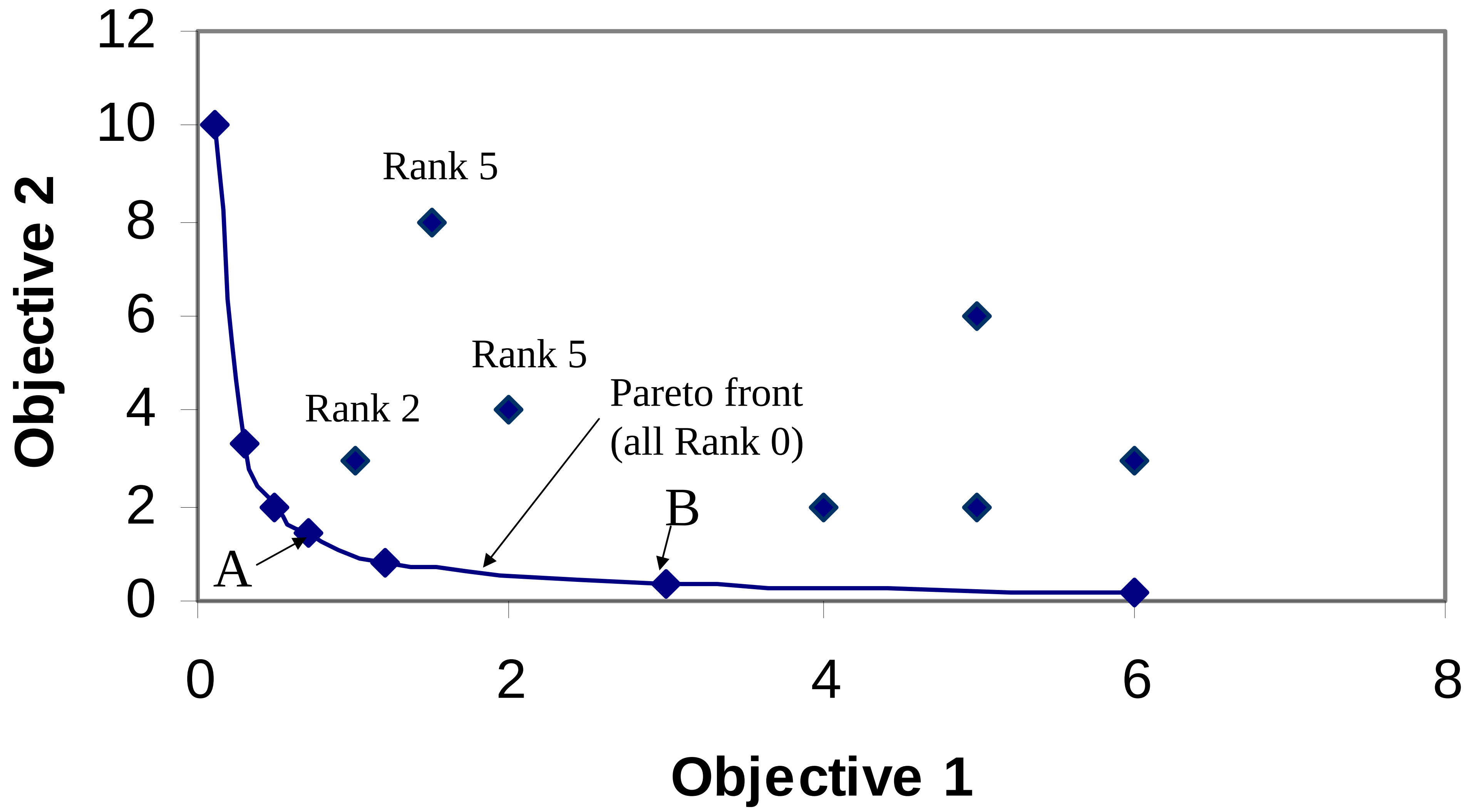
Run technology and cost models (in parallel) to quantify how well each chromosome satisfies the two objectives

Pareto rank all chromosomes

Select "fittest" chromosomes for reproduction (based on Pareto rank and crowding)

Quit after N generations

Crossover and mutation



12
10
8
6
4
2
0
Objective 2
Rank 5
Rank 5
Rank 2
Pareto front
(all Rank 0)
A
B
0
2
4
6
8
Objective 1

MOGA Application

Evaluate two different sites at two operation times

Determine Pareto front

Report maximum downgradient ClO_4^- concentration

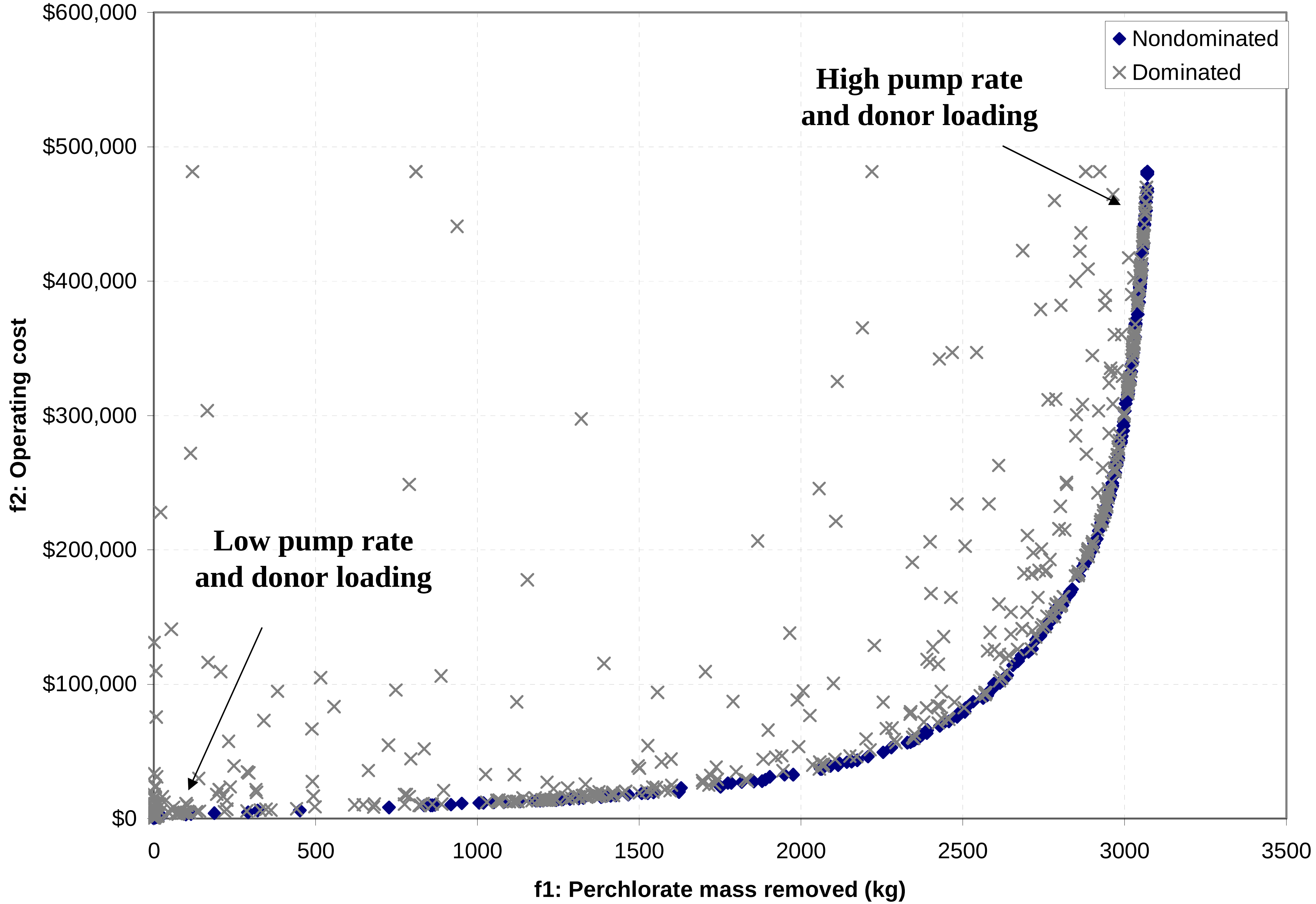
	NV	CA
Hyd conductivity (m/day)	7.60	2.59
Hydraulic gradient	10^{-2}	10^{-3}
Initial [ClO_4^-] (mg/L)	330	160
Initial [O_2] (mg/L)	2.8	0.55
Initial [NO_3^-] (mg/L)	60.0	0.50

Optimization Runs

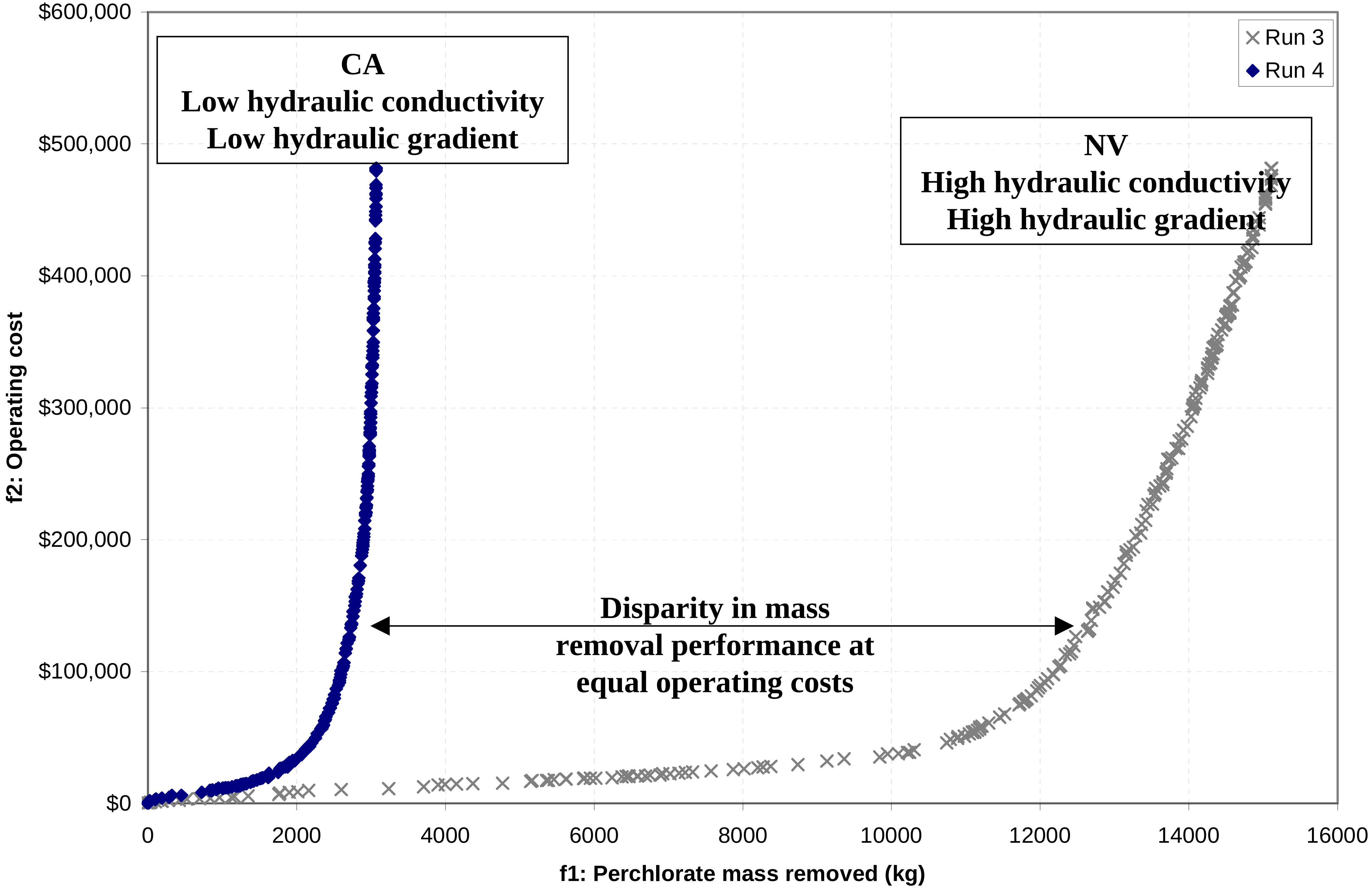
Run 1	Run 2	Run 3	Run 4
300 days	300 days	600 days	600 days
NV	CA	NV	CA

Results

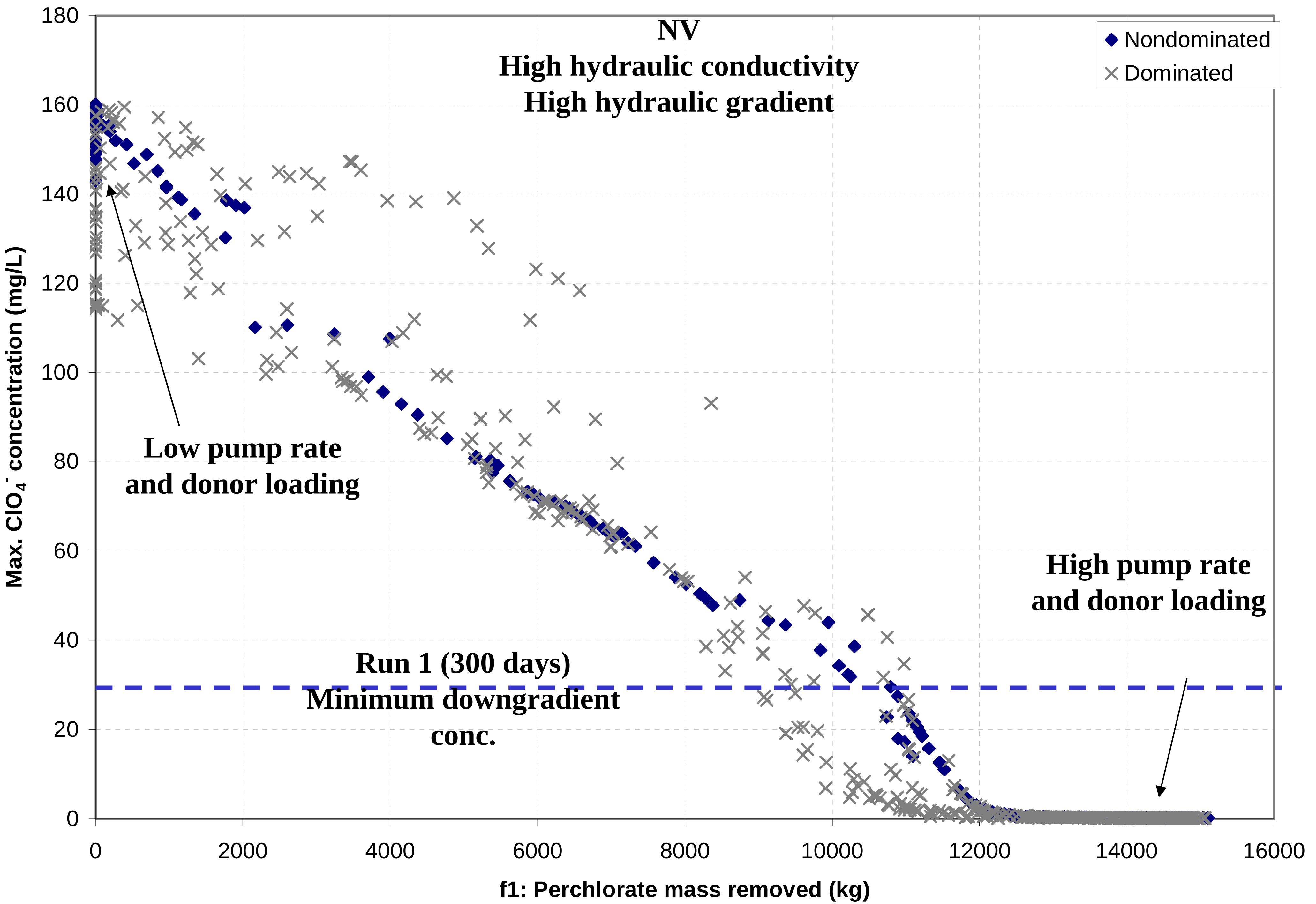
Pareto Front – Run 4
Low Conductivity Site, 600 day Operation



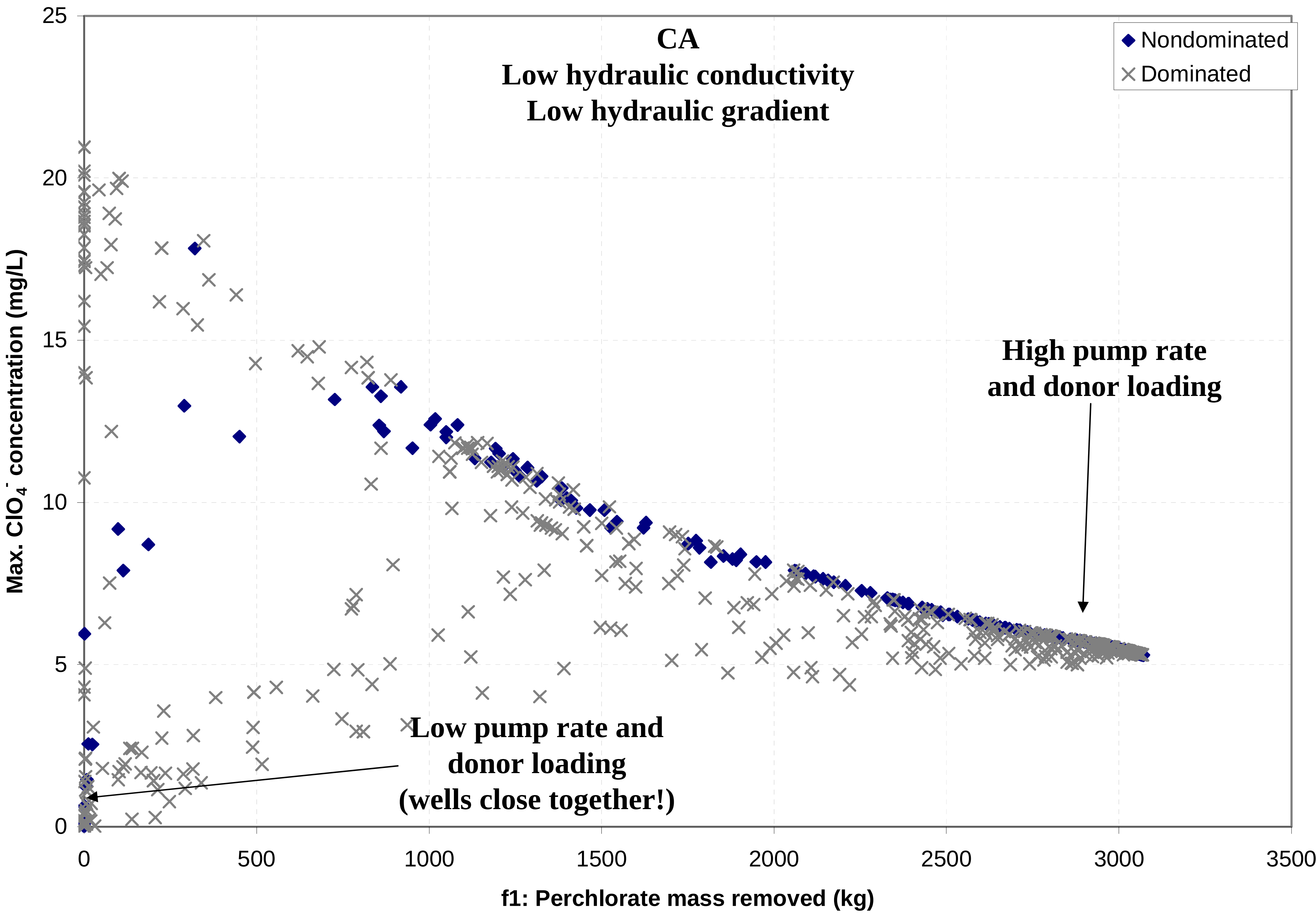
Pareto Fronts – NV and CA Sites



Downgradient Concentration vs Mass Removed (Run 3)



Downgradient Concentration vs Mass Removed (Run 4)



Conclusions

- MOGA, applied in conjunction with a technology model, provides useful insights into impact of environmental and design parameters on technology performance and operating cost
  - Incremental operating cost per unit mass removed increases as overall mass removal increases
  - Downgradient concentrations decrease with increased time of technology operation
  - Increased mass removal (and operating cost) does not necessarily correlate with decreased downgradient concentrations

Conclusions

- Pareto front provides decision maker with tool to easily visualize performance and cost tradeoffs