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Title: Model-driven decision support for monitoring network design based on analysis of data and model uncertainties: methods and applications

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Katzman, Danny

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Web

# Model-driven decision support for monitoring network design based on analysis of data and model uncertainties: methods and applications

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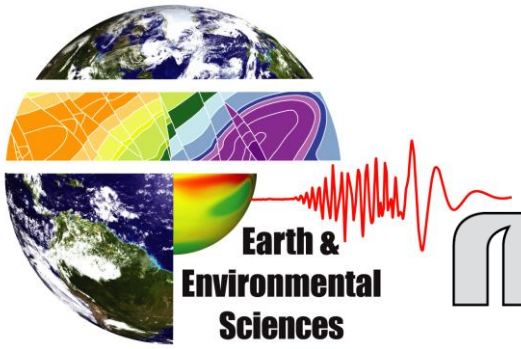
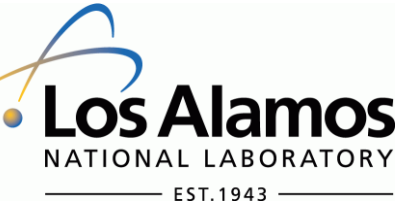
AGU Fall Meeting 2012
H32F. Uncertainty Quantification and Parameter Estimation: Impacts on Risk and Decision Making
December 5, 2012
San Francisco, CA

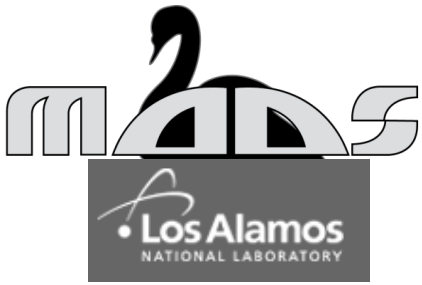



# Outline

- ✧ Model-driven (model-based) decision support
- ✧ Probabilistic vs Non-Probabilistic Decision Methods
- ✧ Information Gap (info-gap) Decision Theory
- ✧ Information Gap (info-gap) Applications:
  - Monitoring Network Design
  - Contaminant Remediation through Source Control
- ✧ Decision Support for Chromium contamination site @ LANL

- ✧ MADS: Model Analyses & Decision Support
  Open source C/C++ computational framework
  Publications, examples & tutorials @
  http://mads.lanl.gov




- ✧ ASCEM: Advanced Subsurface Computing for Environmental Management; Multi-national lab code development project http://ascemdoe.org (U.S. DOE)

ASCEM

BERKELEY LAB

Los Alamos NATIONAL LABORATORY EST. 1943

Pacific Northwest NATIONAL LABORATORY

OAK RIDGE National Laboratory

SRNL SAVANNAH RIVER NATIONAL LABORATORY

# Model-driven (model-based) decision support

- provides decision makers (DM) with model analysis of decision scenarios taking into account site data and knowledge including existing uncertainties (uncertainties in conceptualization, model parameters, and model predictions)
- Model analysis: evaluation, ranking and optimization of alternative decision scenarios
- Decision metric(s): e.g. contaminant concentration at a monitoring well (environmental risk at a point of compliance)
- Decision goal(s): e.g. no exceedance of MCL at a compliance point and/or increase chance of detecting exceedance of MCL at a monitoring well
- Decision scenarios: combinations of predefined activities to achieve the decision goal(s)

# Model-driven decision support (cont.)

- **Activities**:
  - data acquisition campaigns
  - field/lab experiments
  - monitoring
  - remediation
- **Activities** are analyzed in terms of their impact on decision making process (**decision uncertainties**)
- **Decision uncertainties**: uncertainties associated with selection of optimal **decision scenarios**, or performance of specific **decision scenarios**
- **The Game:** Decision maker (DM) vs Nature

**Important:**

- **activities** are selected only to reduce **decision uncertainties**
- **activities** are not selected to reduce model or parameter uncertainties per se (**unconstrained problem**).

# Non-Probabilistic Decision Methods

- Lack of knowledge or information precludes decision analyses requiring unbiased probabilistic distributions or frequency of occurrence (e.g. Bayesian approaches)
- Severe uncertainties (black swans, dragon kings) can have important impact in the decision analyses
- Non-probabilistic decision methods can be applied to effectively incorporate lack of knowledge and severe uncertainties in decision making process
  - Minimax (Maximin) Theory (Wald, 1951)
  - Information Gap Decision Theory (Ben-Haim, 2006)
  - There is a controversy how different are these two theories
- Non-Probabilistic and Probabilistic methods can be coupled (e.g. unknown probability distribution parameters can be a subject of non-probabilistic analysis, e.g. info-gap)

# Information Gap Decision Theory

- Nominal ("best") model prediction intended for decision making (based on nominal / "best estimates" model parameter set)
- Decision metric(s) / performance goal(s)
- Decision scenarios: vector of alternative decisions *d* to compare
- Info-Gap Uncertainty Model (info-gap uncertainty metric = $\alpha$)
  - energy bound (functional uncertainties: objective function, forcing functions, etc.)
  - envelope bound (domain uncertainties: model parameters, calibration targets, etc.)
  - nested sets of uncertain model entities ranked by the largest information gap $\alpha$ that can be included in the set
  - uncertain model entities: parameters, calibrations, functions, etc. with info-gap uncertainties
  - e.g. $U(\alpha,T) = \{ T: abs(T-T') < \alpha \}$ where T' is a nominal values for uncertain model entities
- Model predictions $C(d)$ constrained by $U(\alpha,T)$

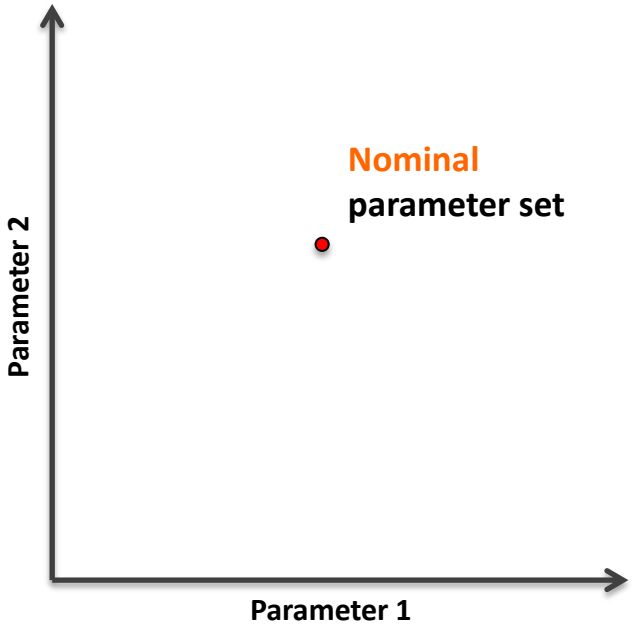
Ben-Haim (2006). *Info-gap decision theory: decisions under severe uncertainty*. Academic Press.

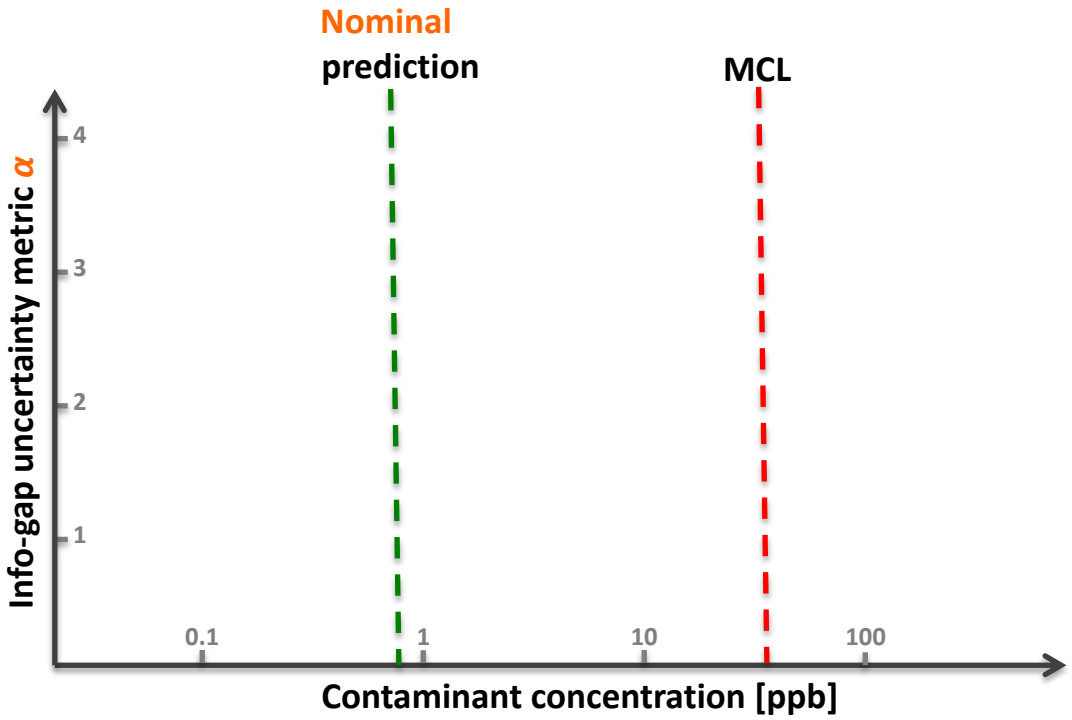
# Information Gap Decision Theory

- **Decision uncertainty** is bounded by **robustness** and **opportuness** functions
- **Robustness** function (immunity to failure of alternate decisions $d$)
  - defines the maximum horizon of uncertainty
  - $R(d) = \max\{ \alpha$: performance goal is satisfied $\}$
    e.g. $R(d) = \max\{ \alpha : ( \max C(d) ) < MCL \}$
- **Opportuness** function (immunity to windfall of alternate decisions $d$)
  - defines the minimum horizon of uncertainty
  - $O(d) = \min\{ \alpha$: performance goal is satisfied $\}$
    e.g. $O(d) = \min\{ \alpha : ( \min C(d) ) < MCL \}$
- Analyses based on Decision Robustness and/or Decision Opportuness:
  - Model selection
  - Remedy selection
  - Performance assessment
  - …

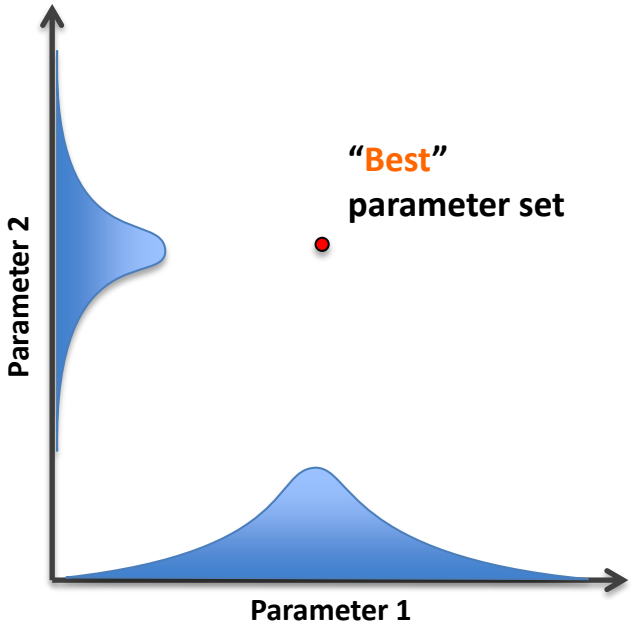
Ben-Haim (2006). *Info-gap decision theory: decisions under severe uncertainty*. Academic Press.

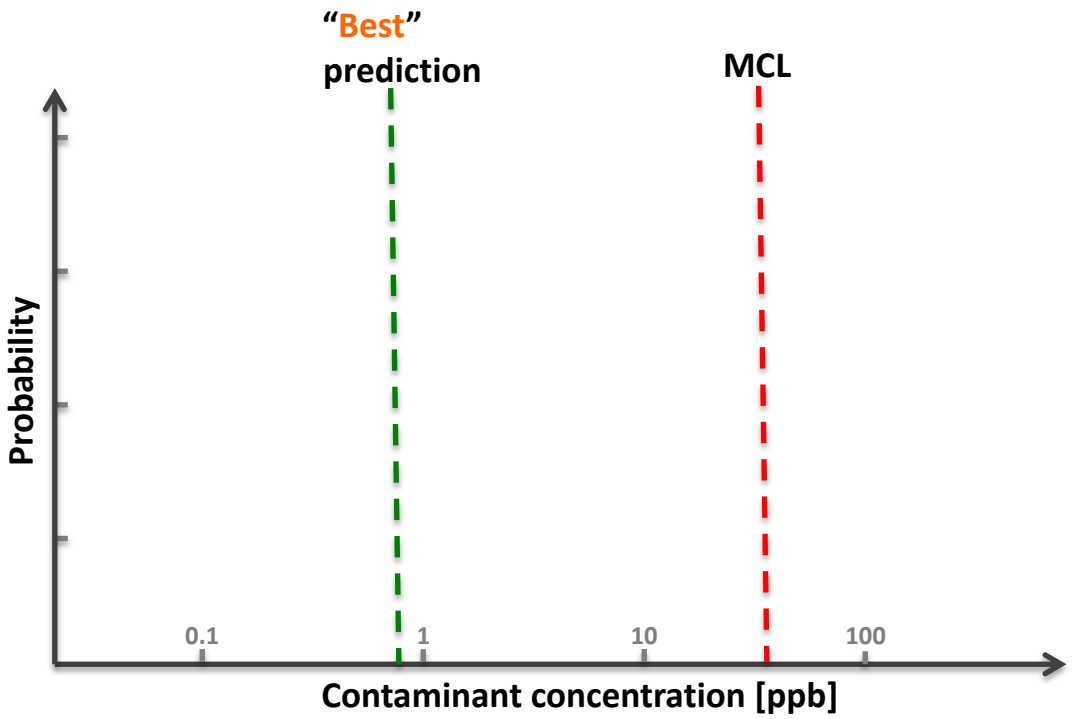
# Info-Gap Analysis: Model parameters



# Bayesian Analysis: Model parameters



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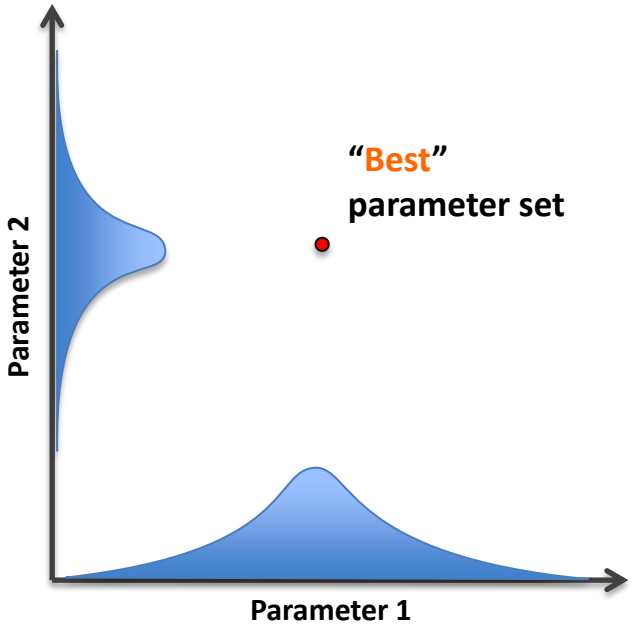


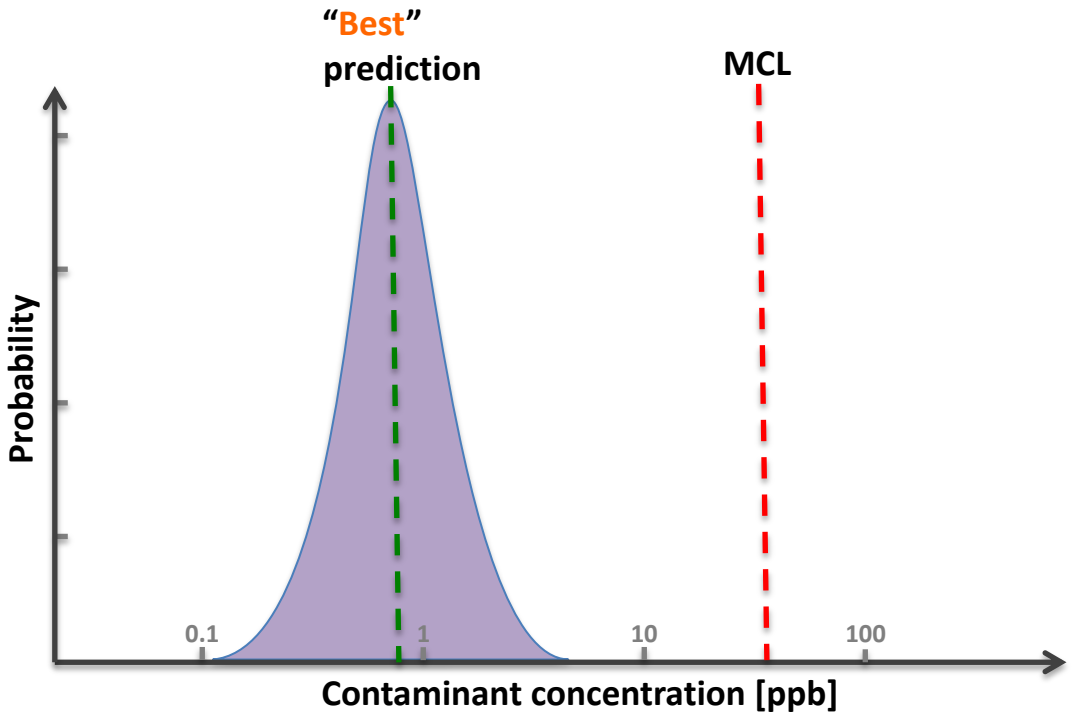

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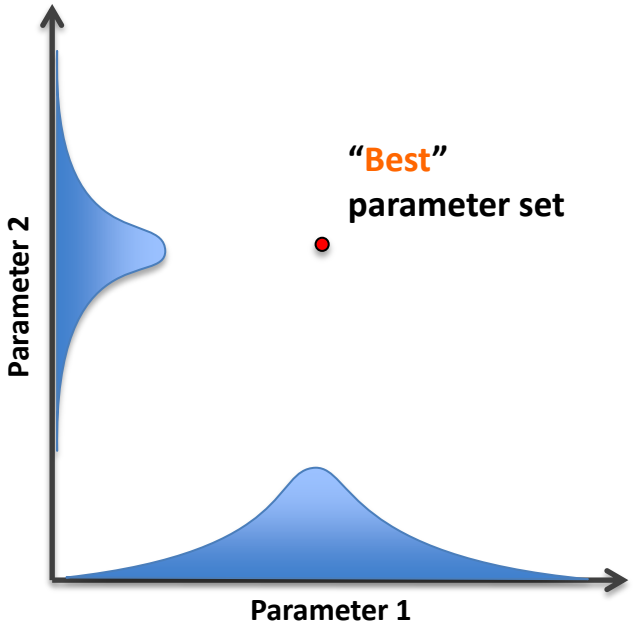
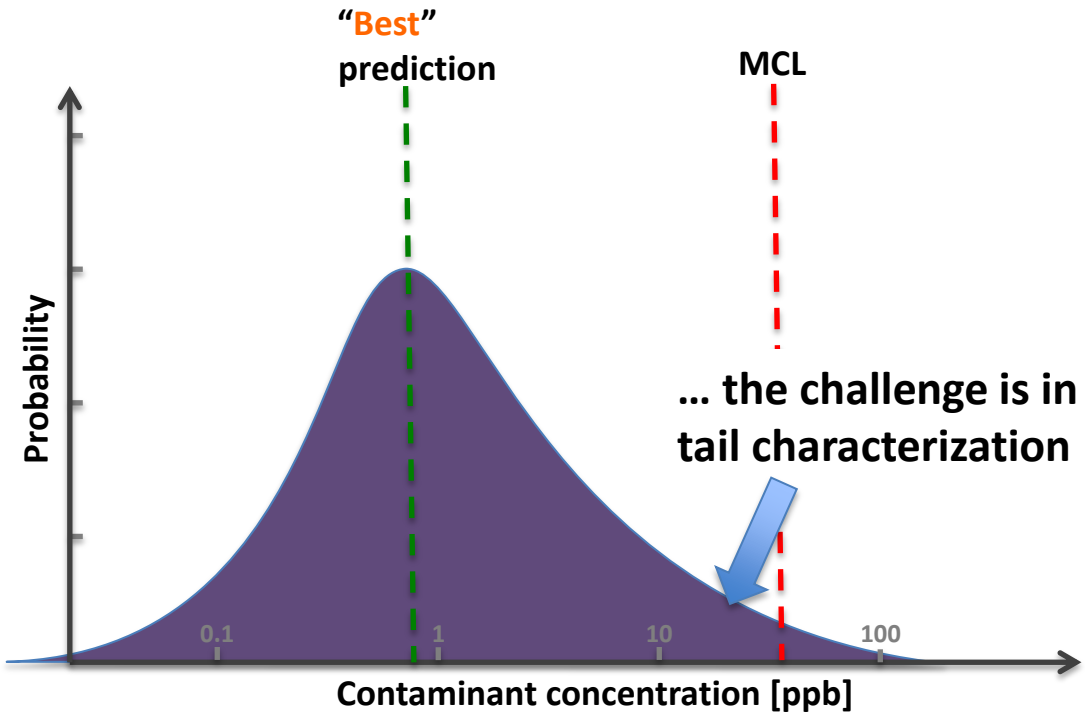
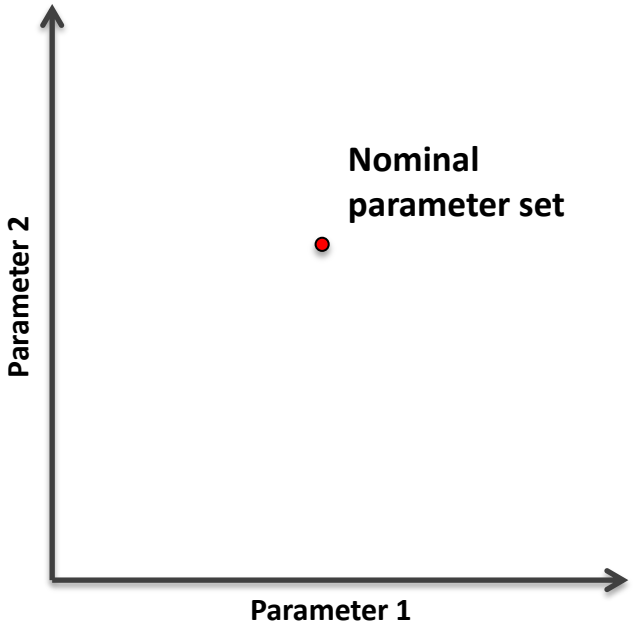
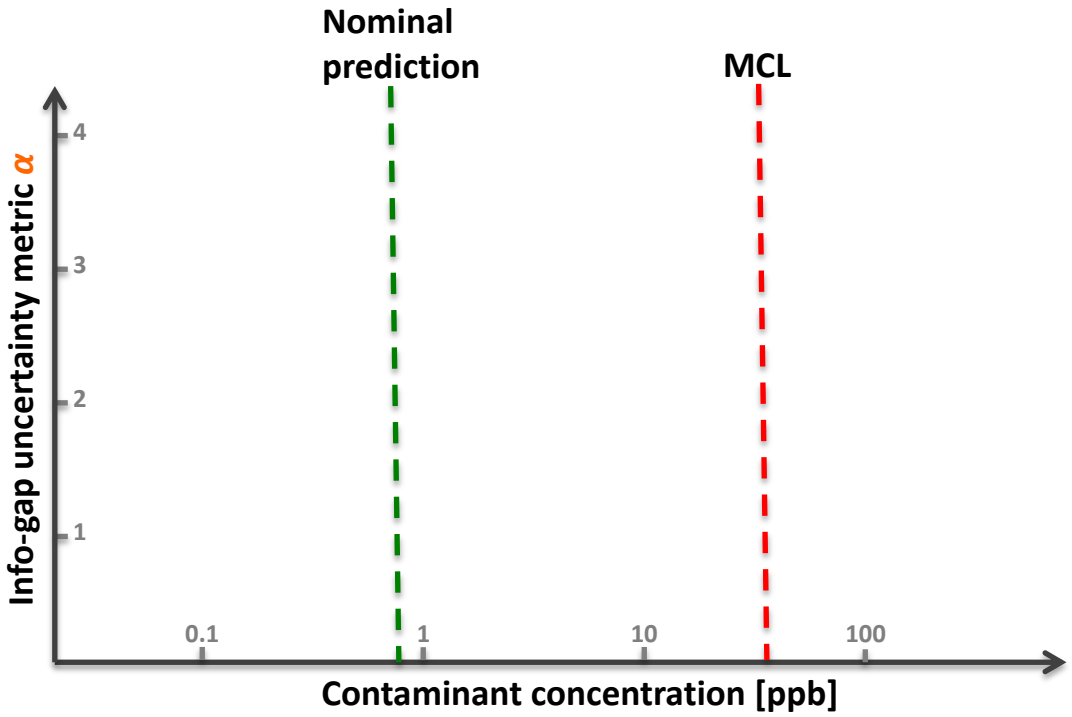


# Info-Gap Analysis: Model parameters (envelope bounds)



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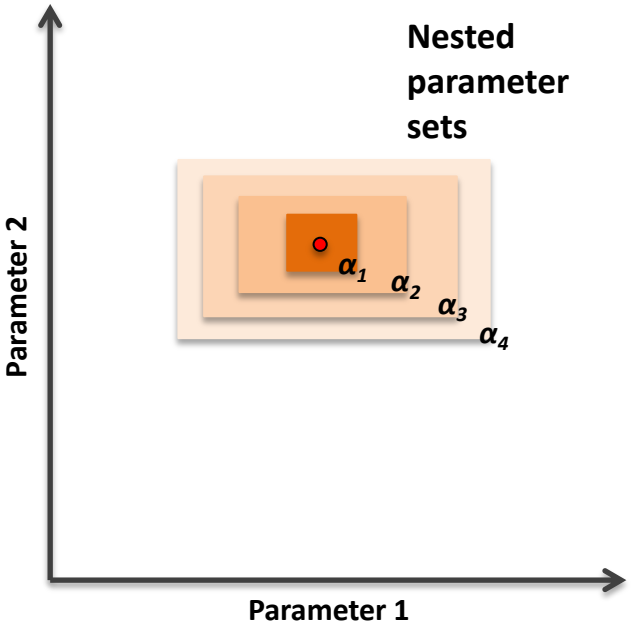


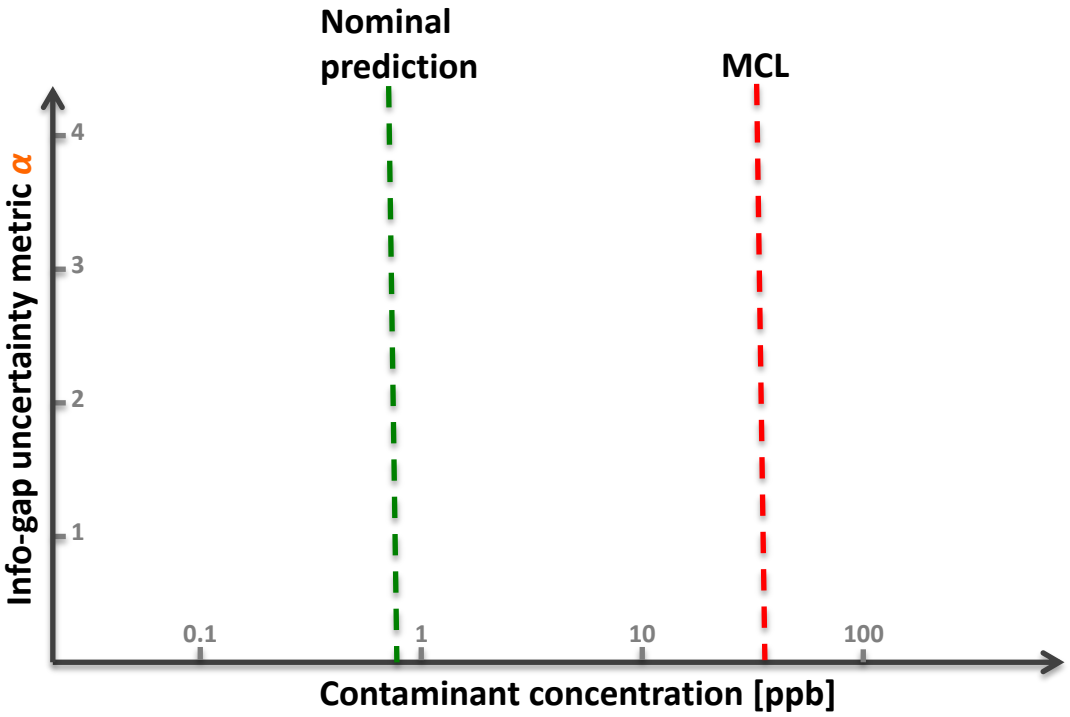


**info-gap uncertainty metric = $\alpha$**

$\alpha_1 < \alpha_2 < \alpha_3 < \alpha_4$

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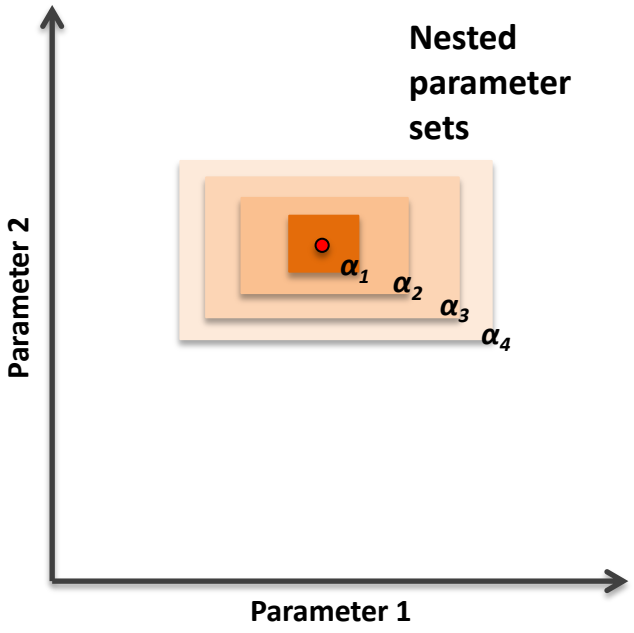


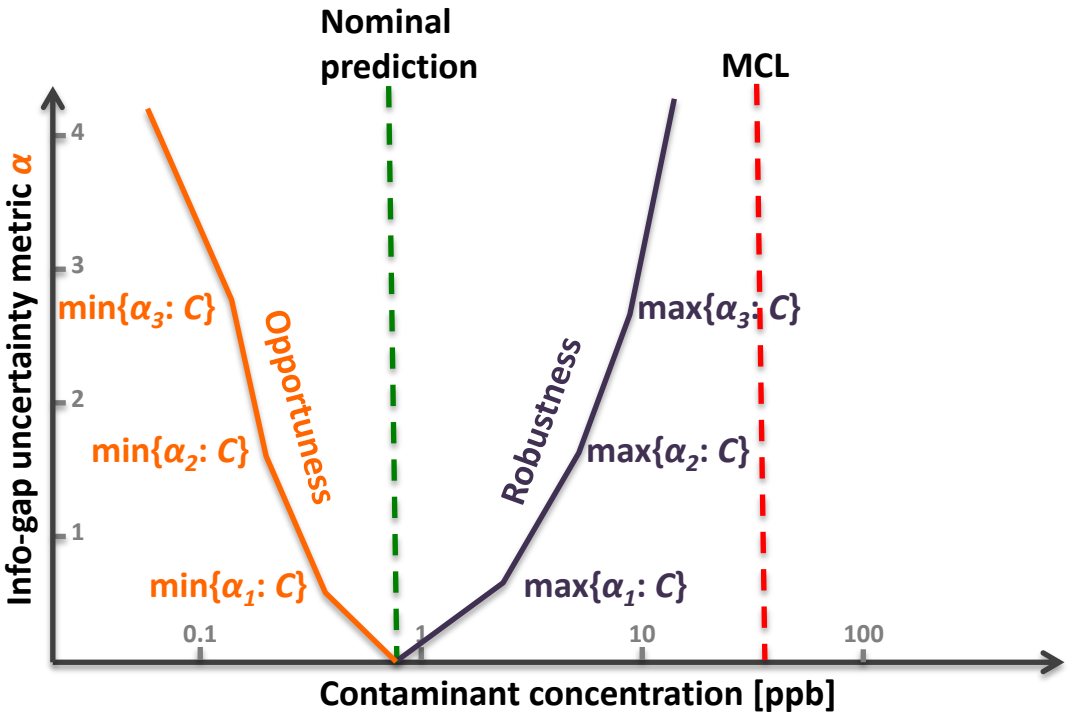


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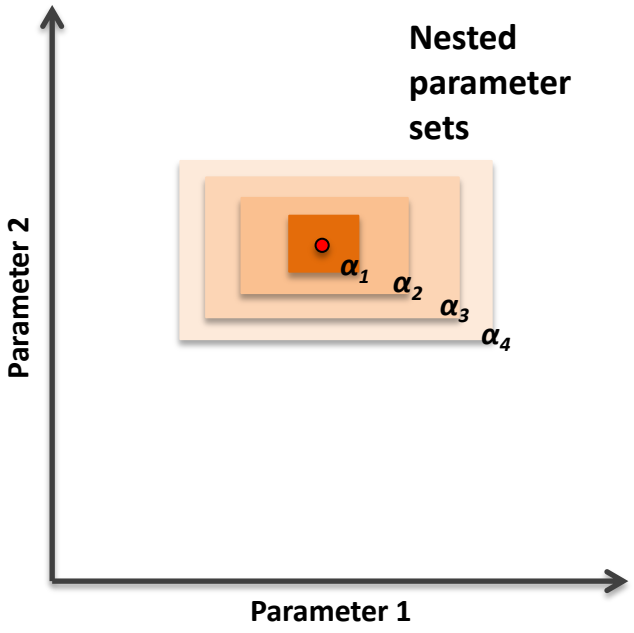


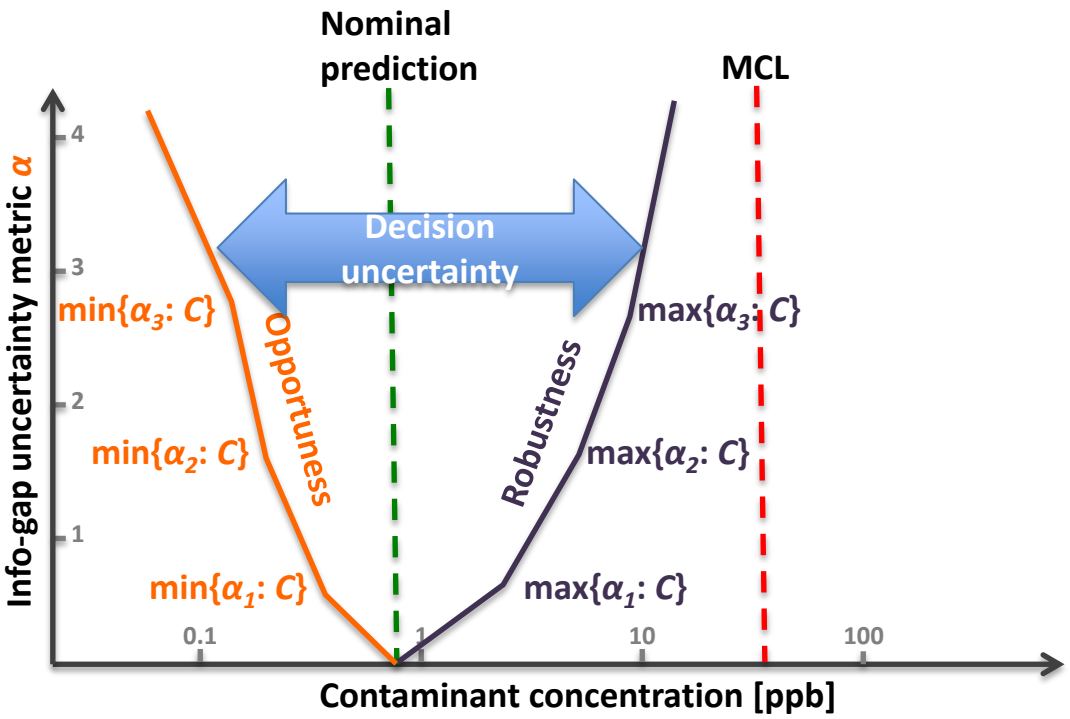


**info-gap uncertainty metric = $\alpha$**

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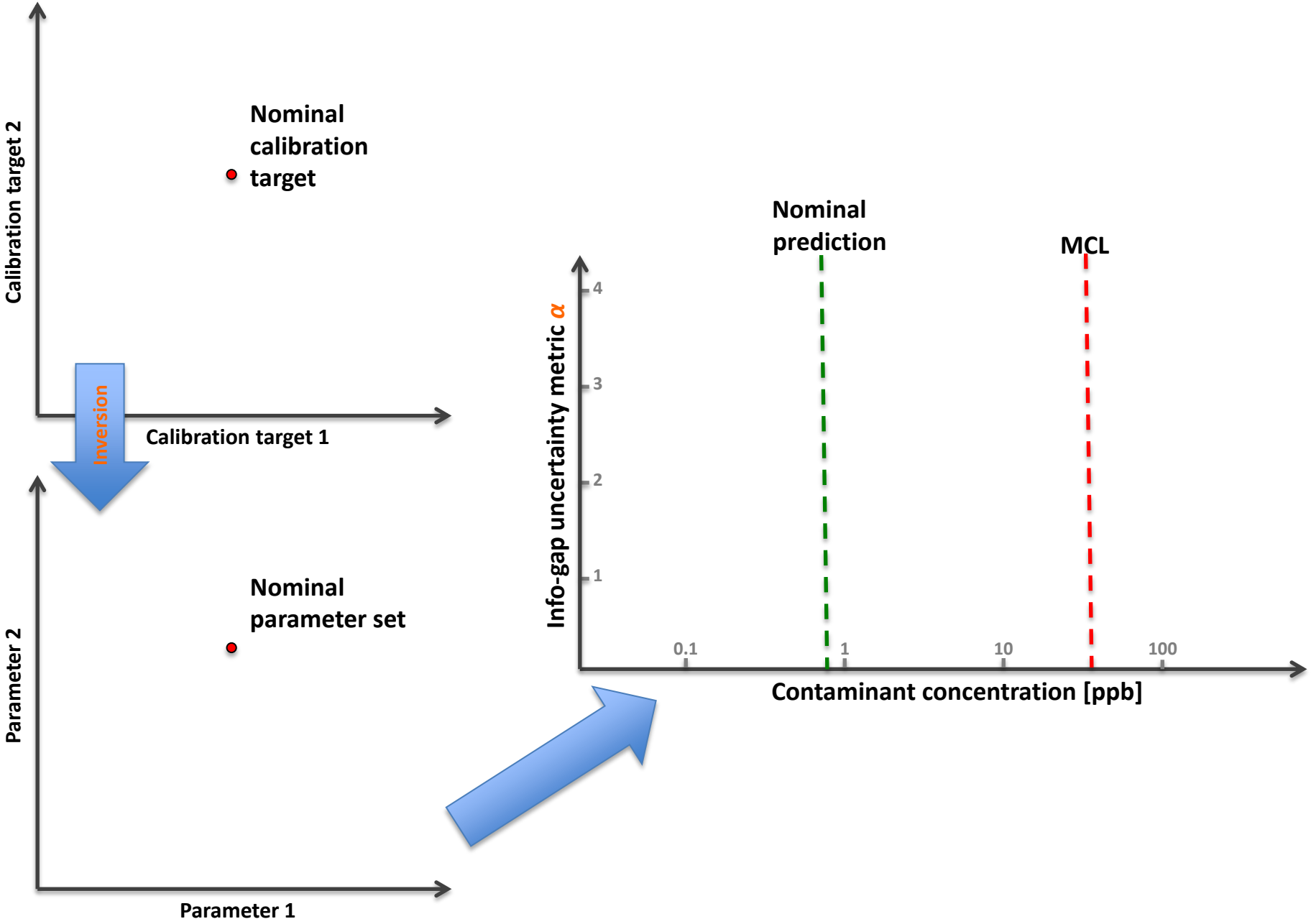
# Info-Gap Analysis: Calibration Targets (envelope bounds)



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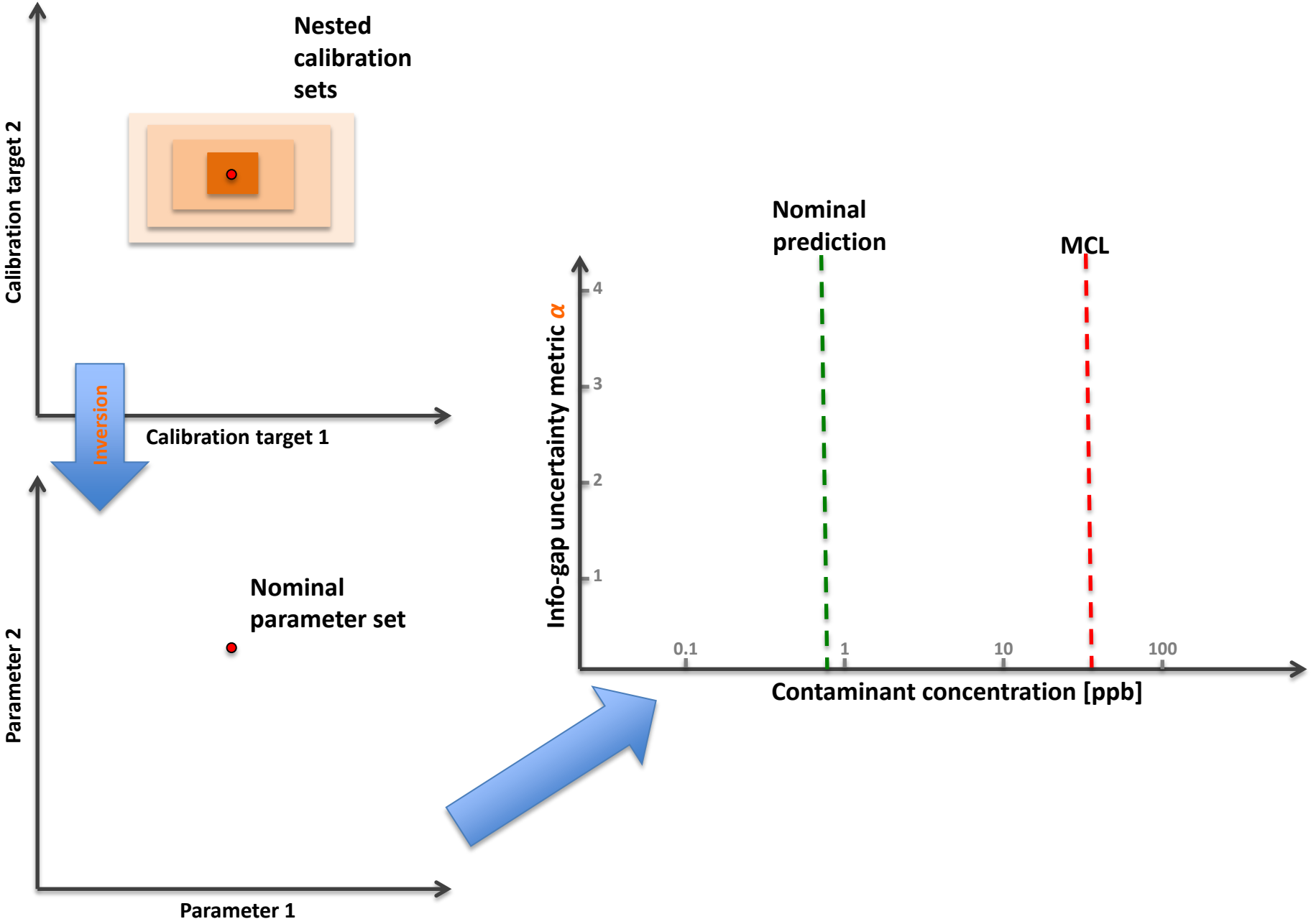

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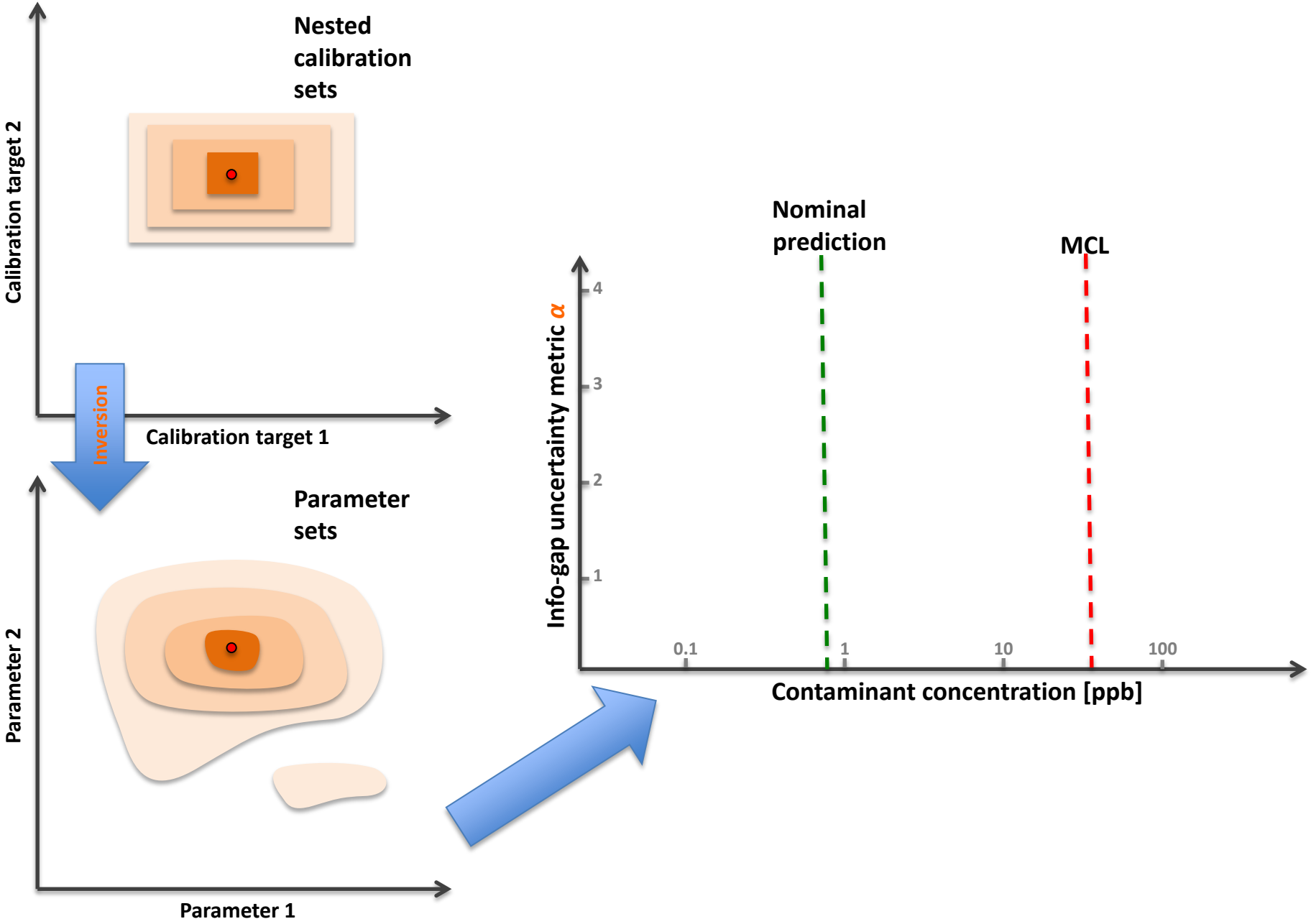

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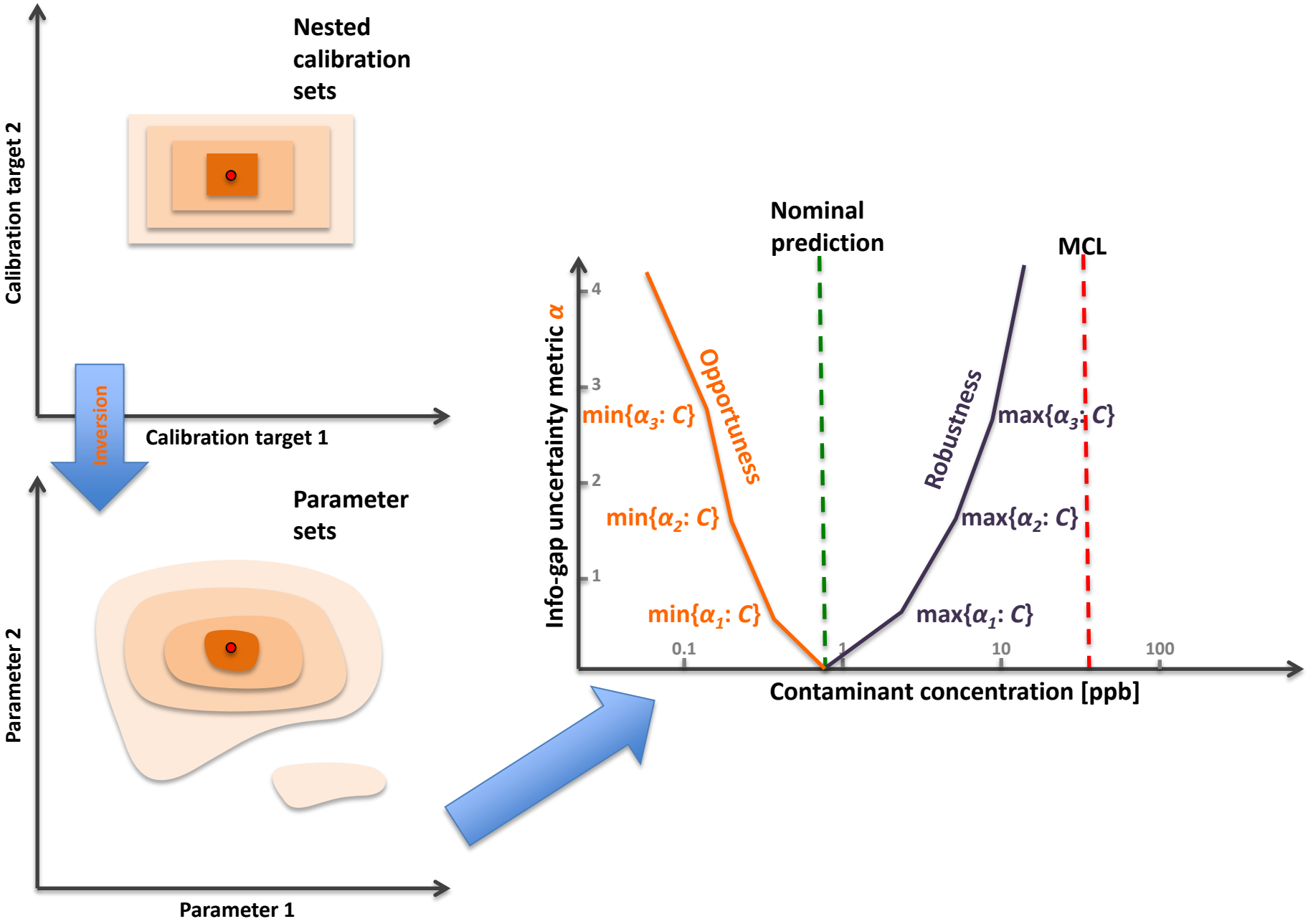
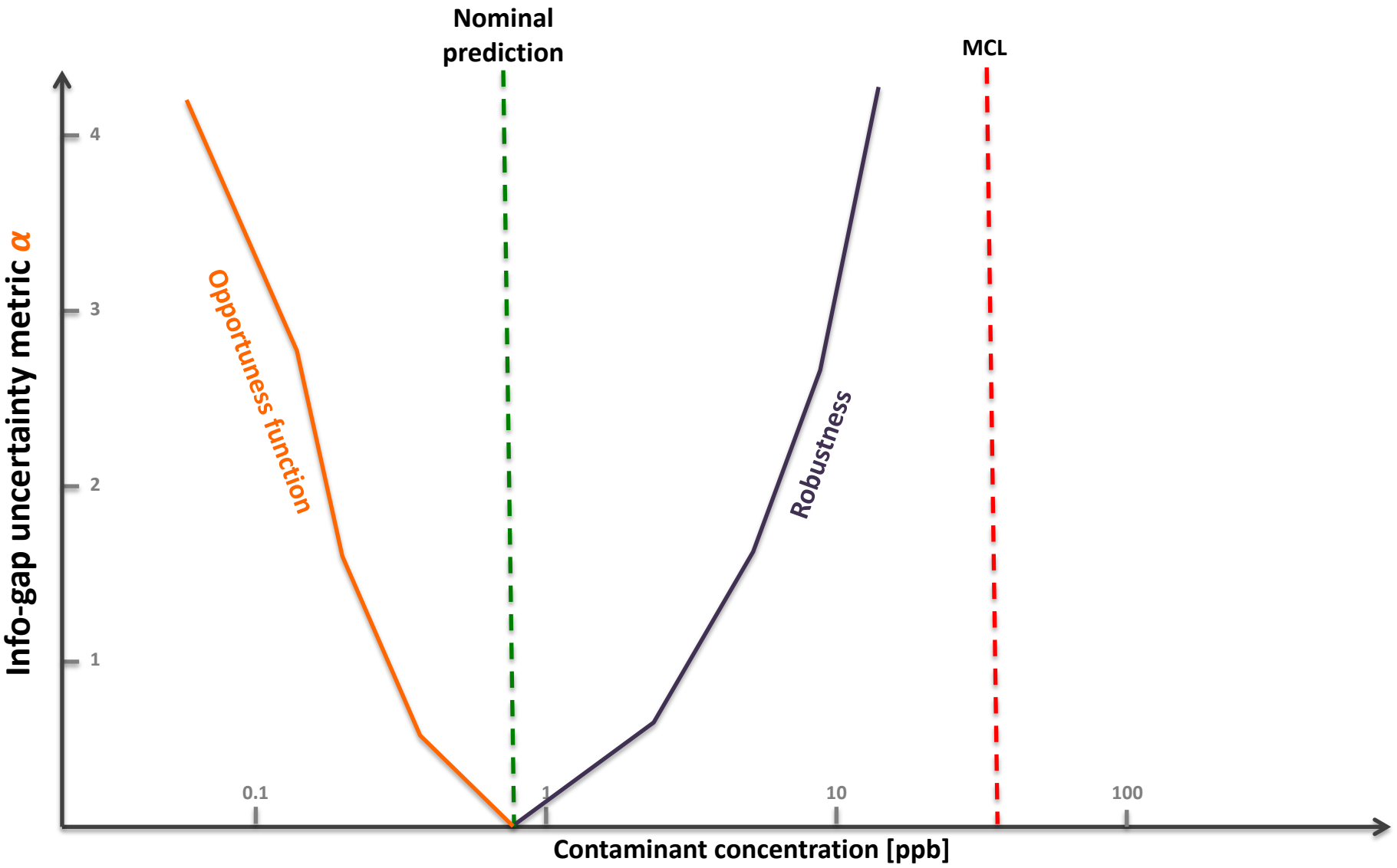


# Info-Gap Analysis: Decision selection based on robustness



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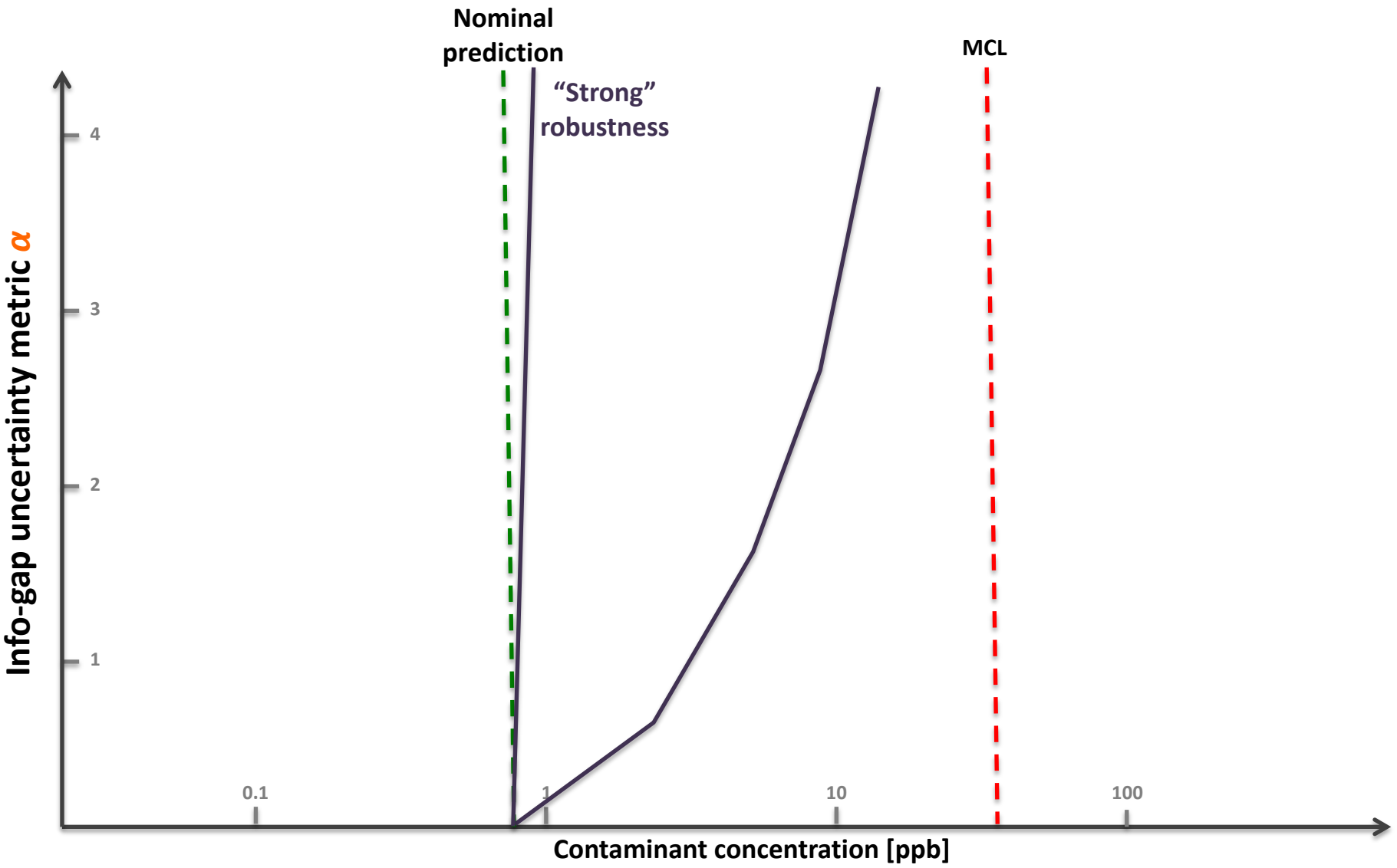

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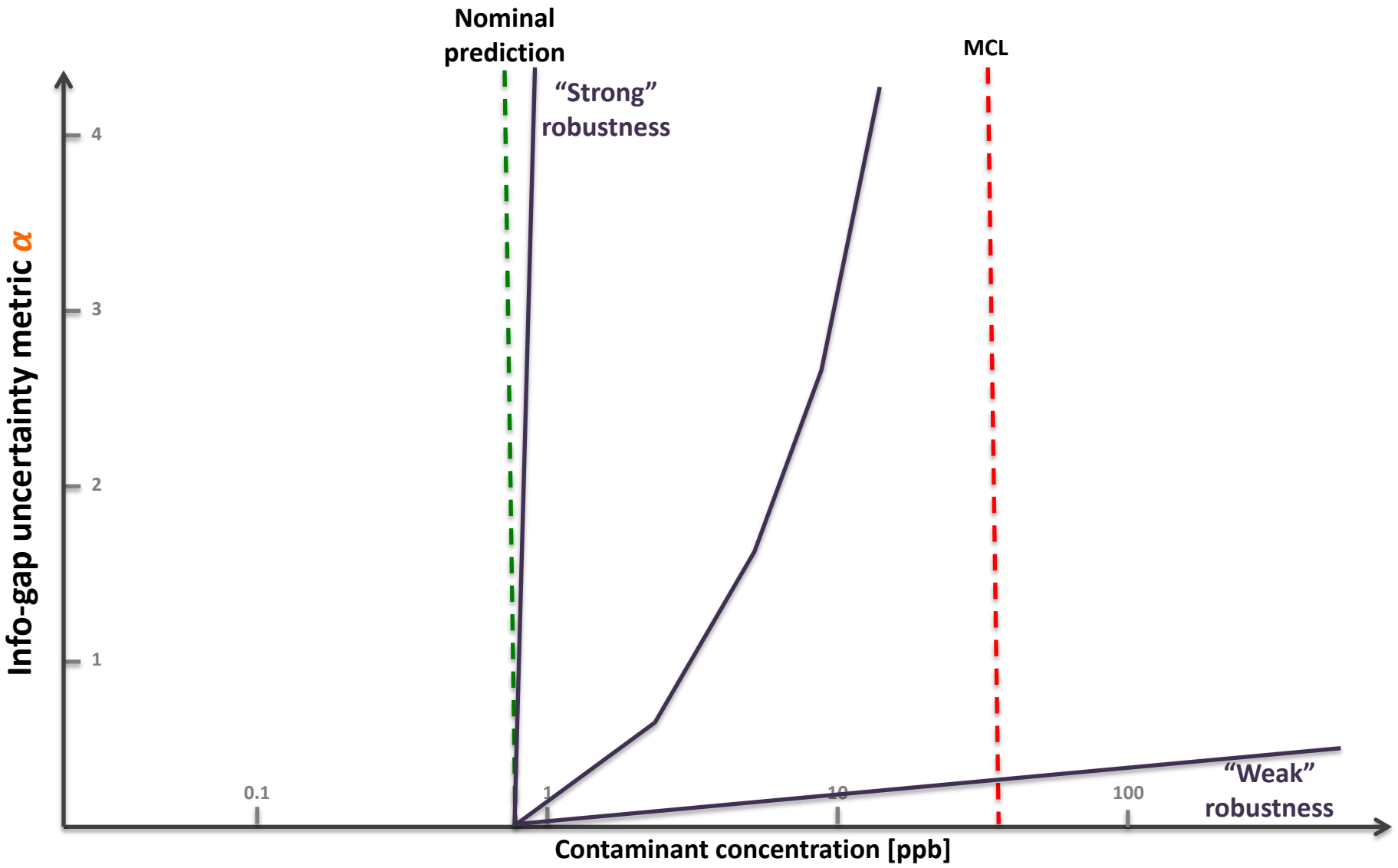

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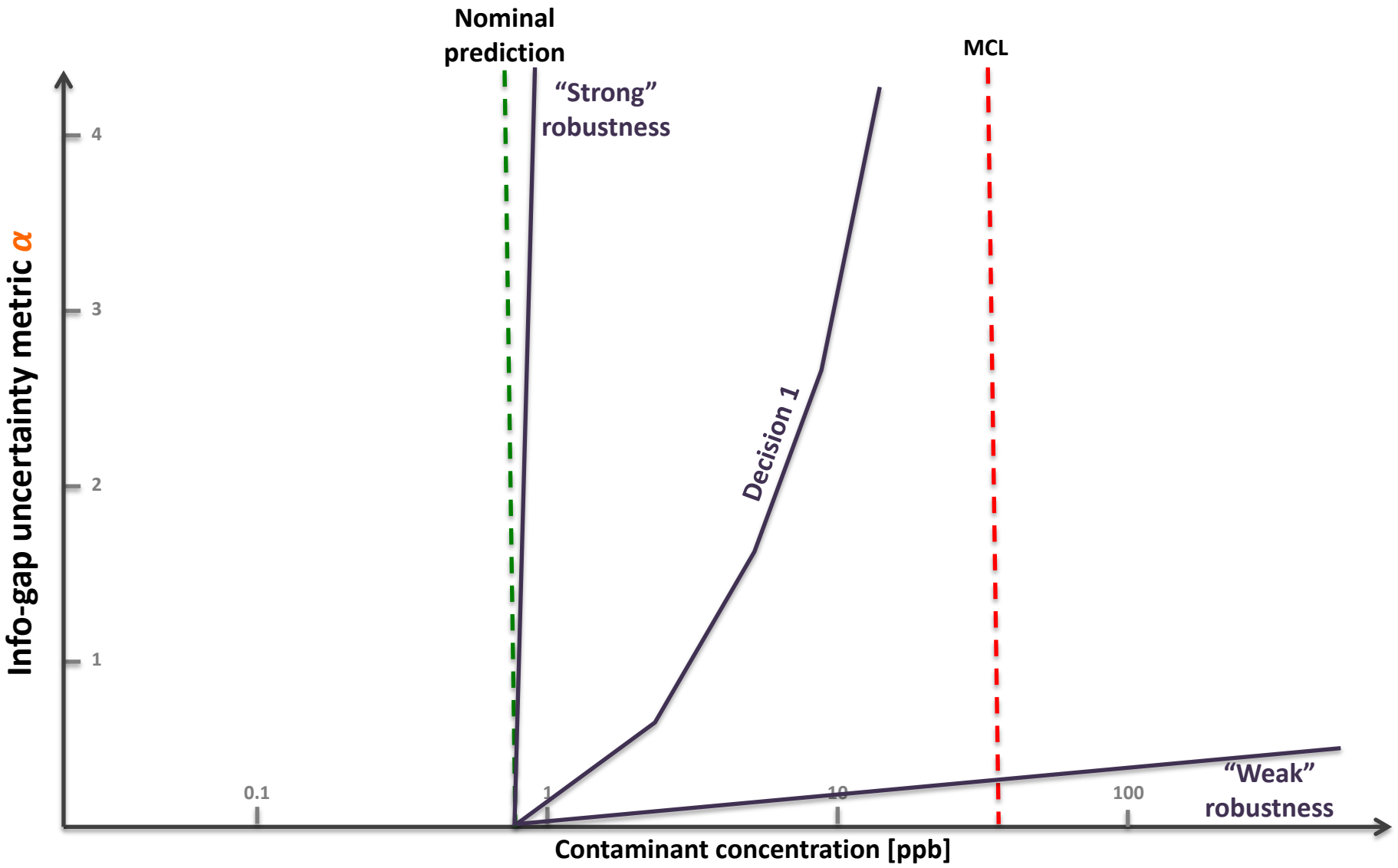

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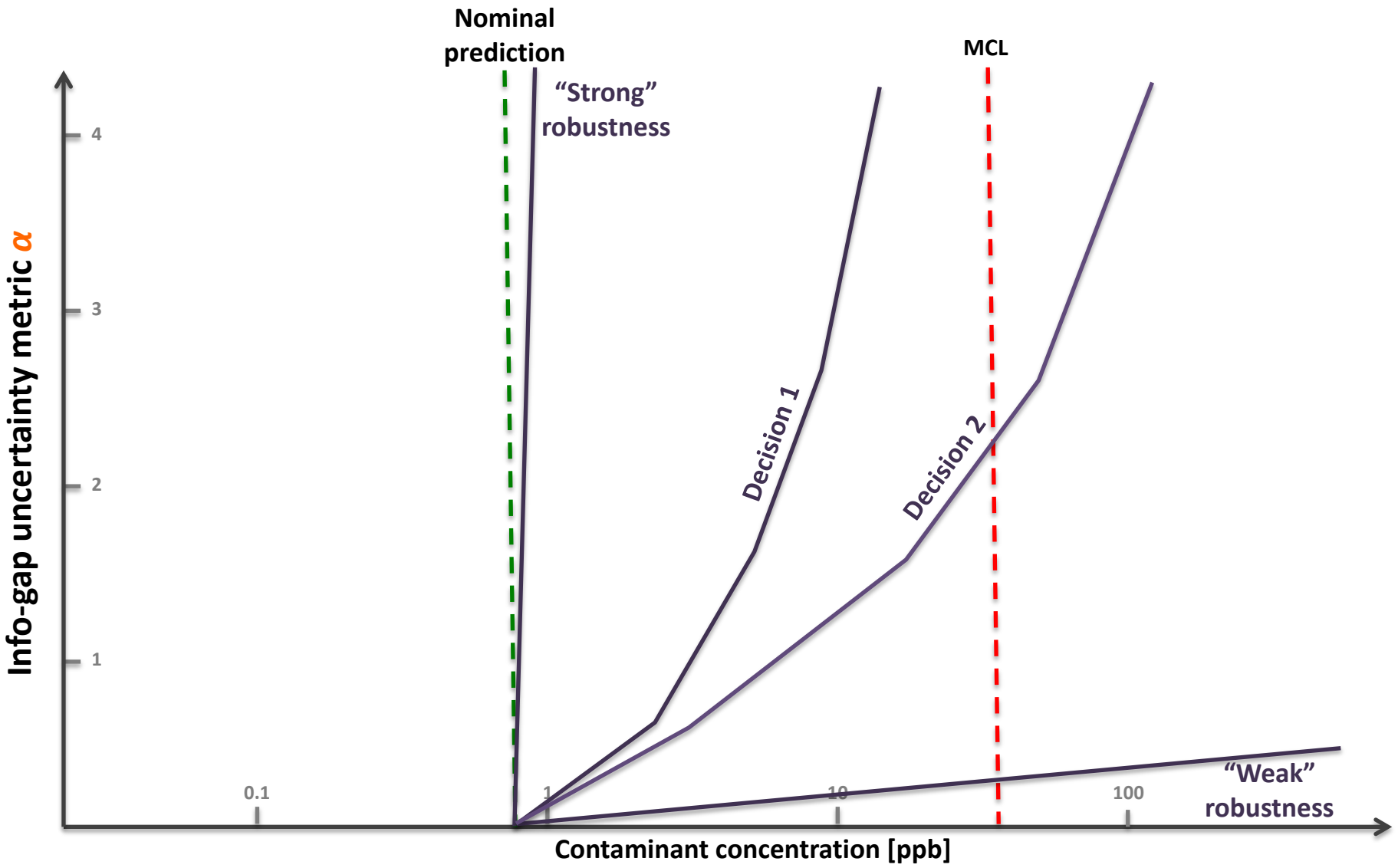

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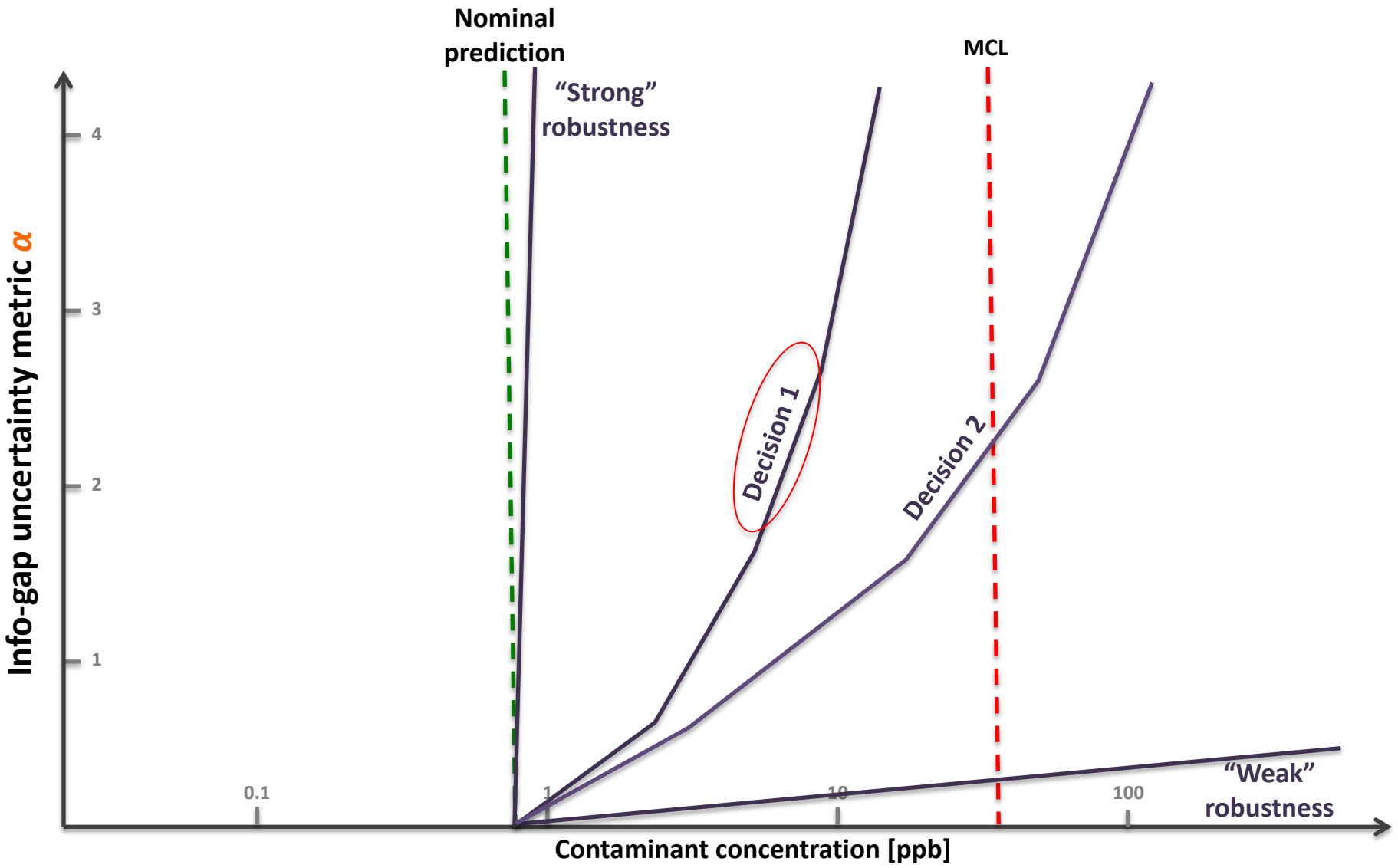

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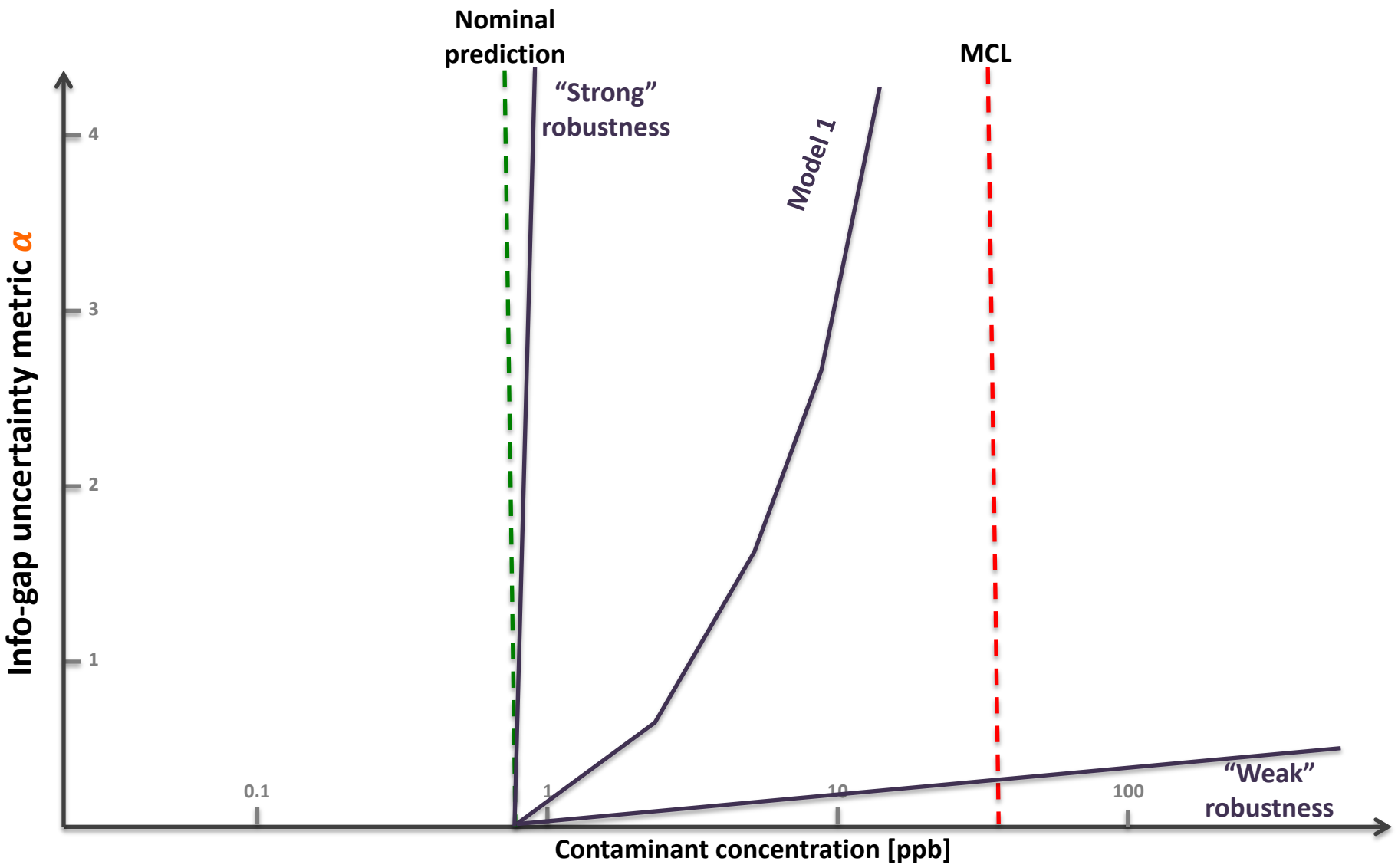

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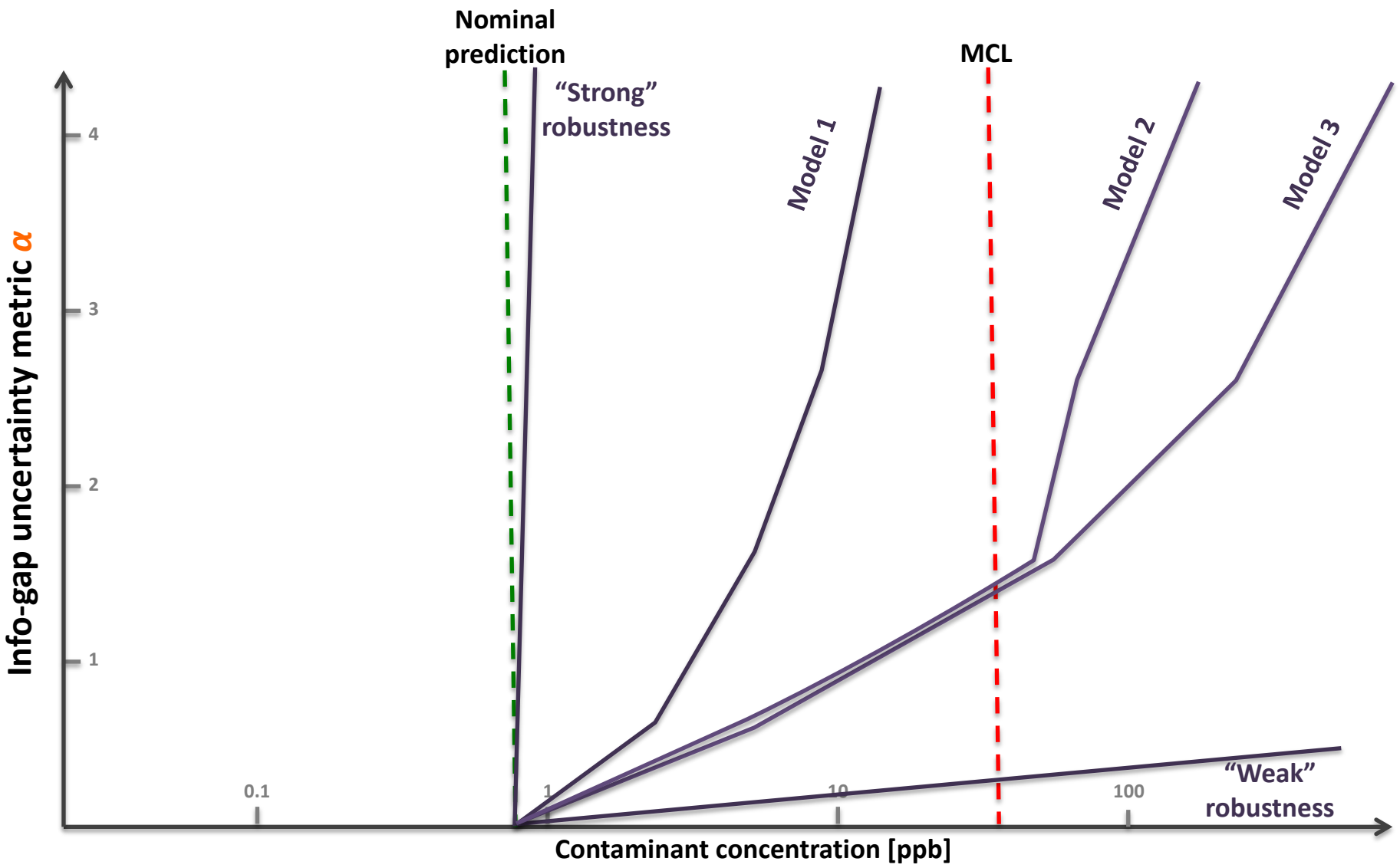

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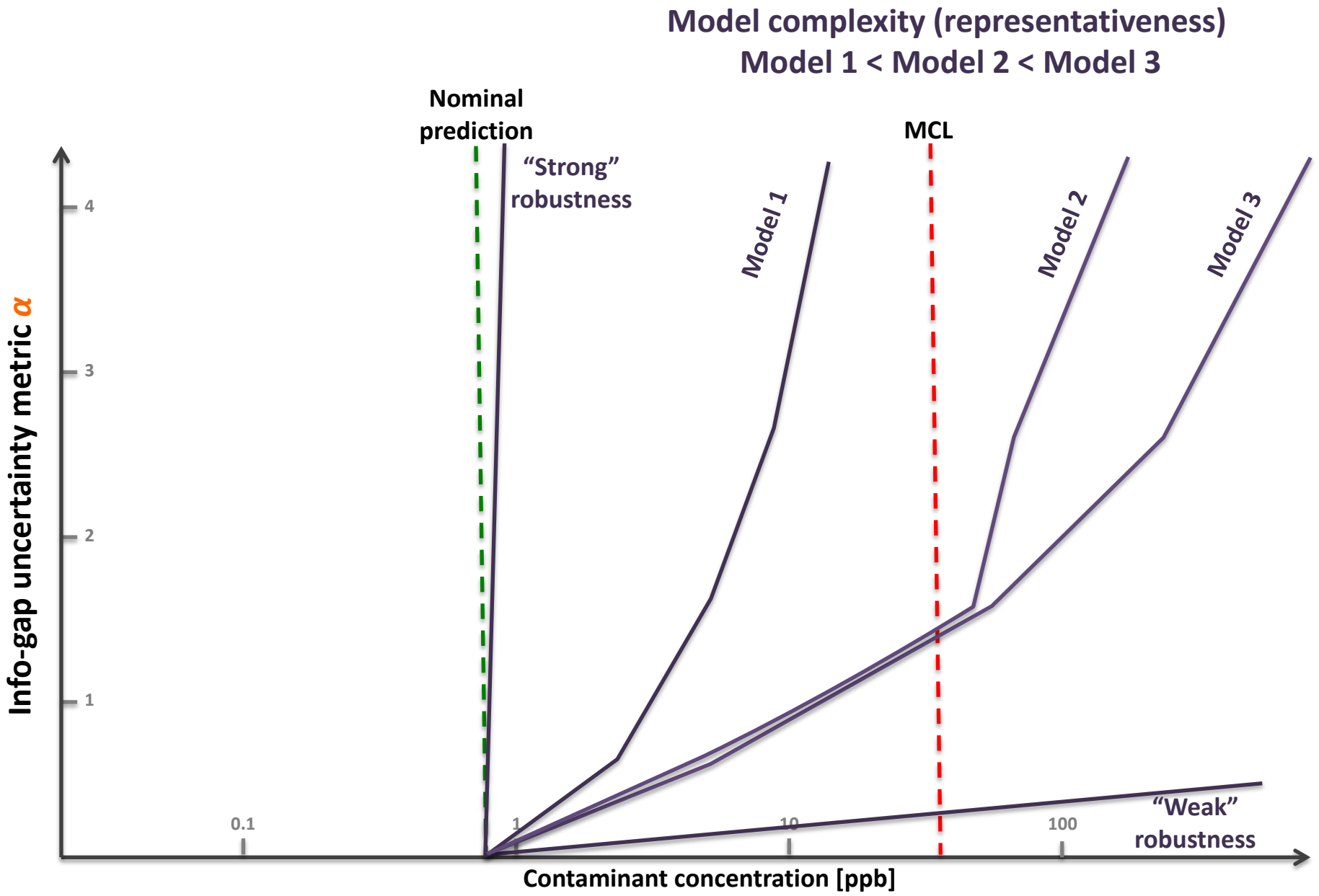

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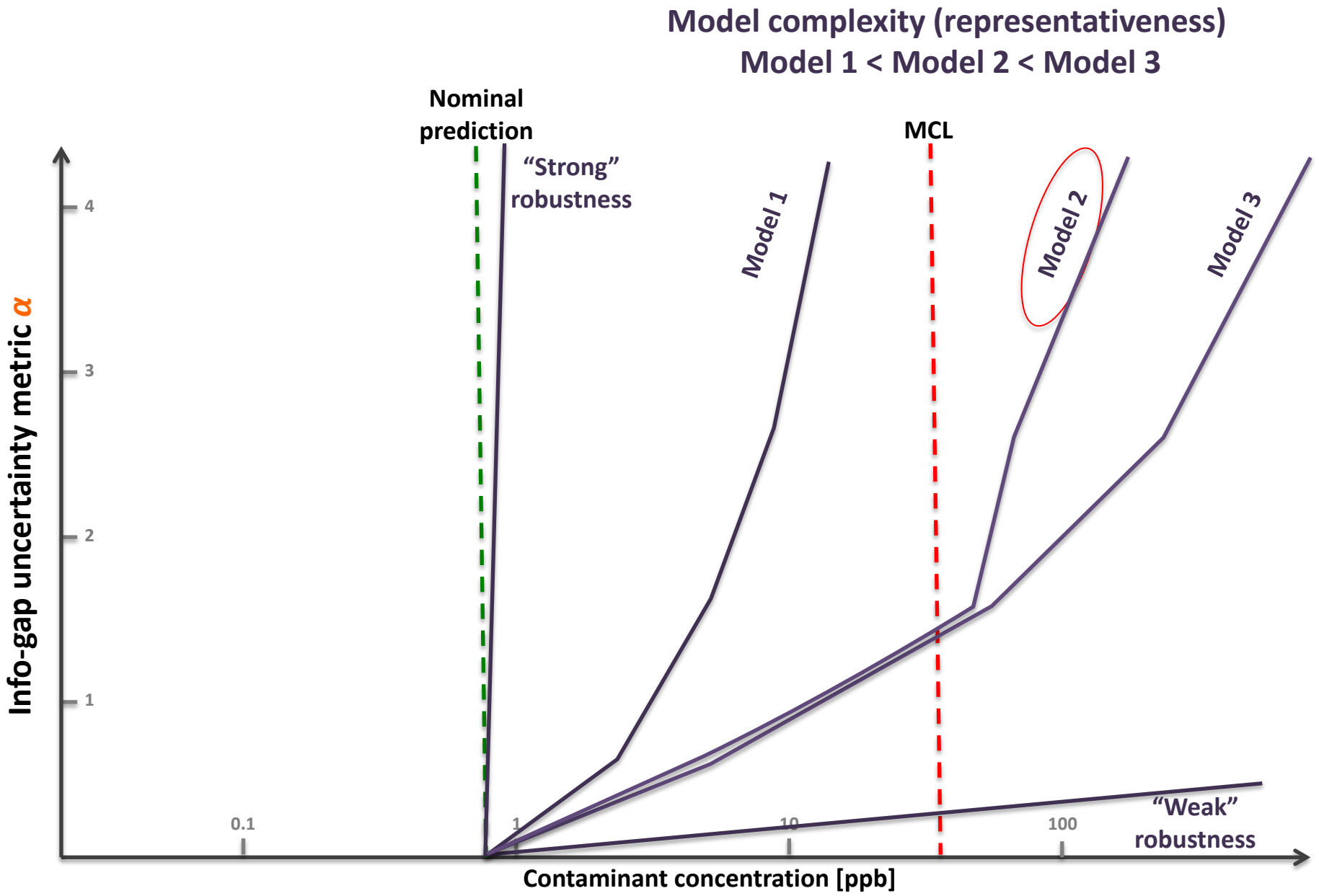
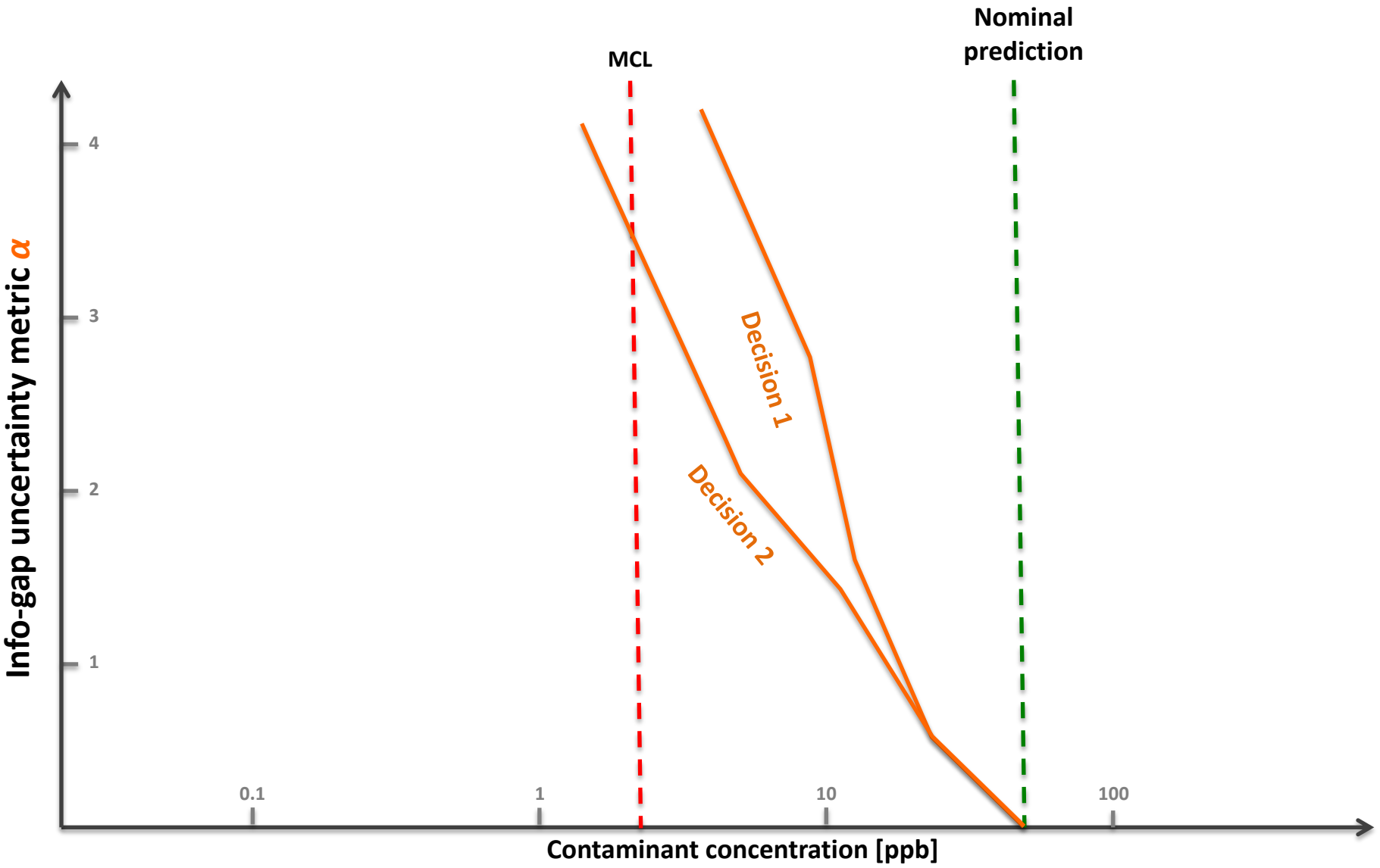


# Info-Gap Analysis: Decision selection based on opportuness



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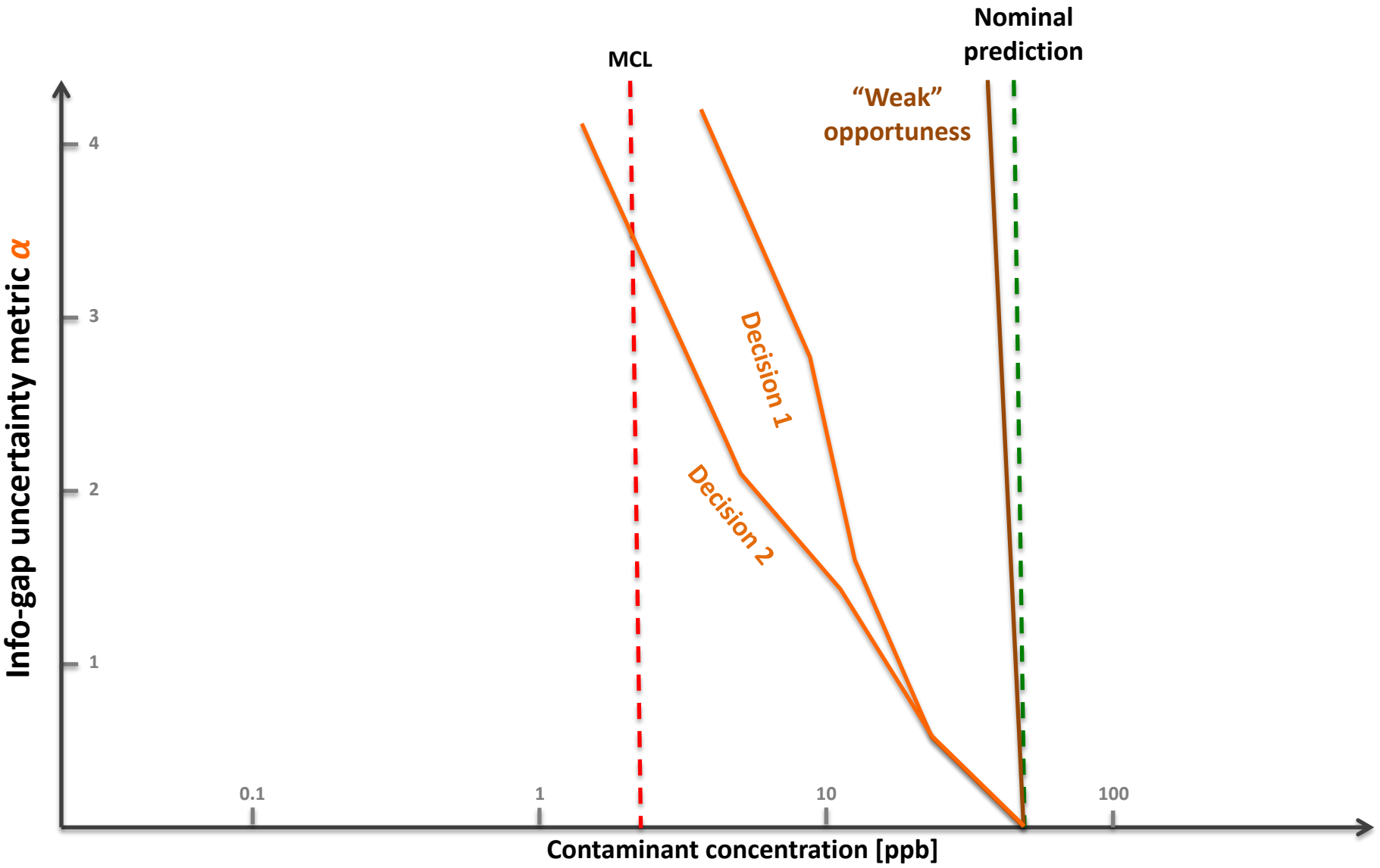

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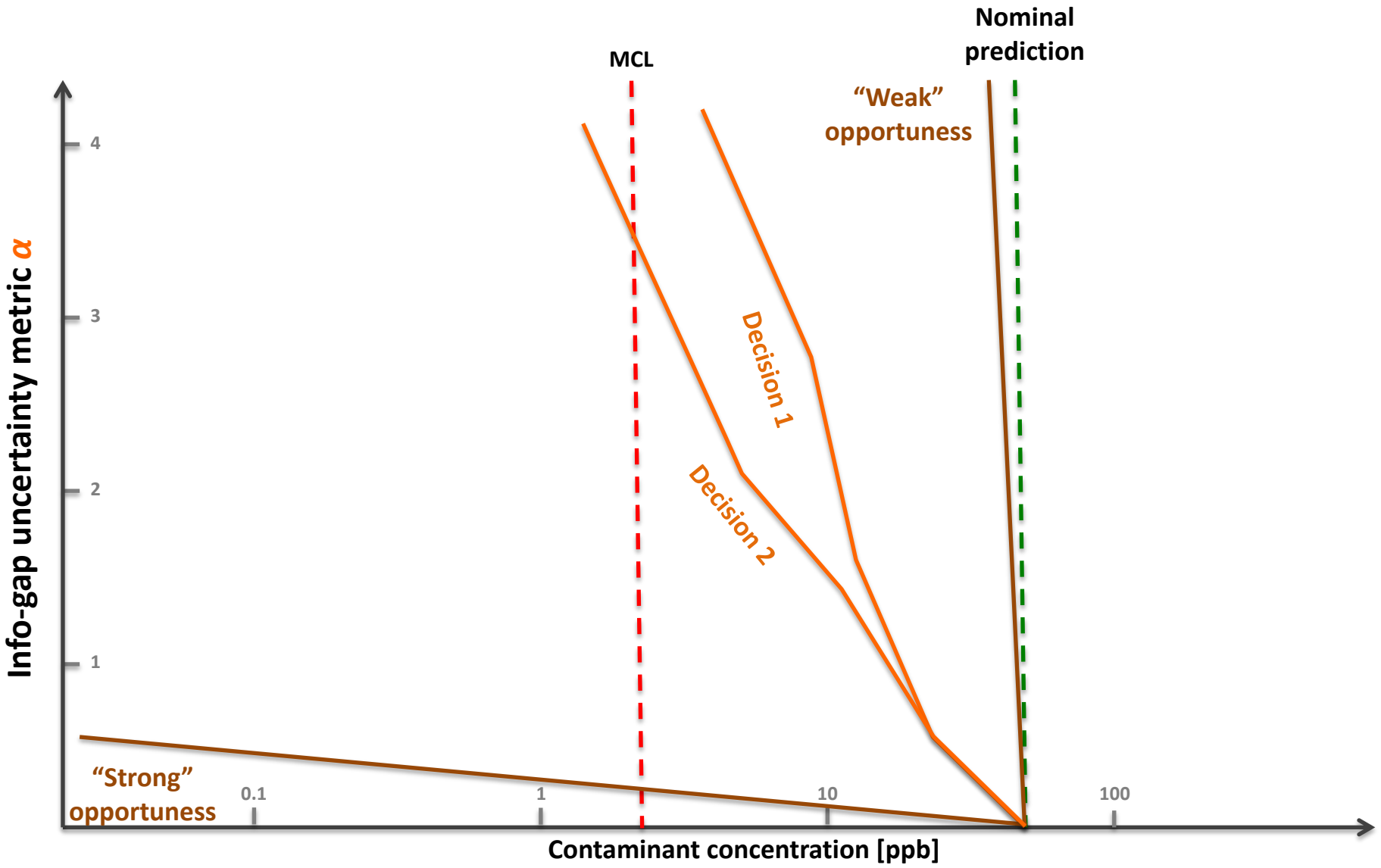

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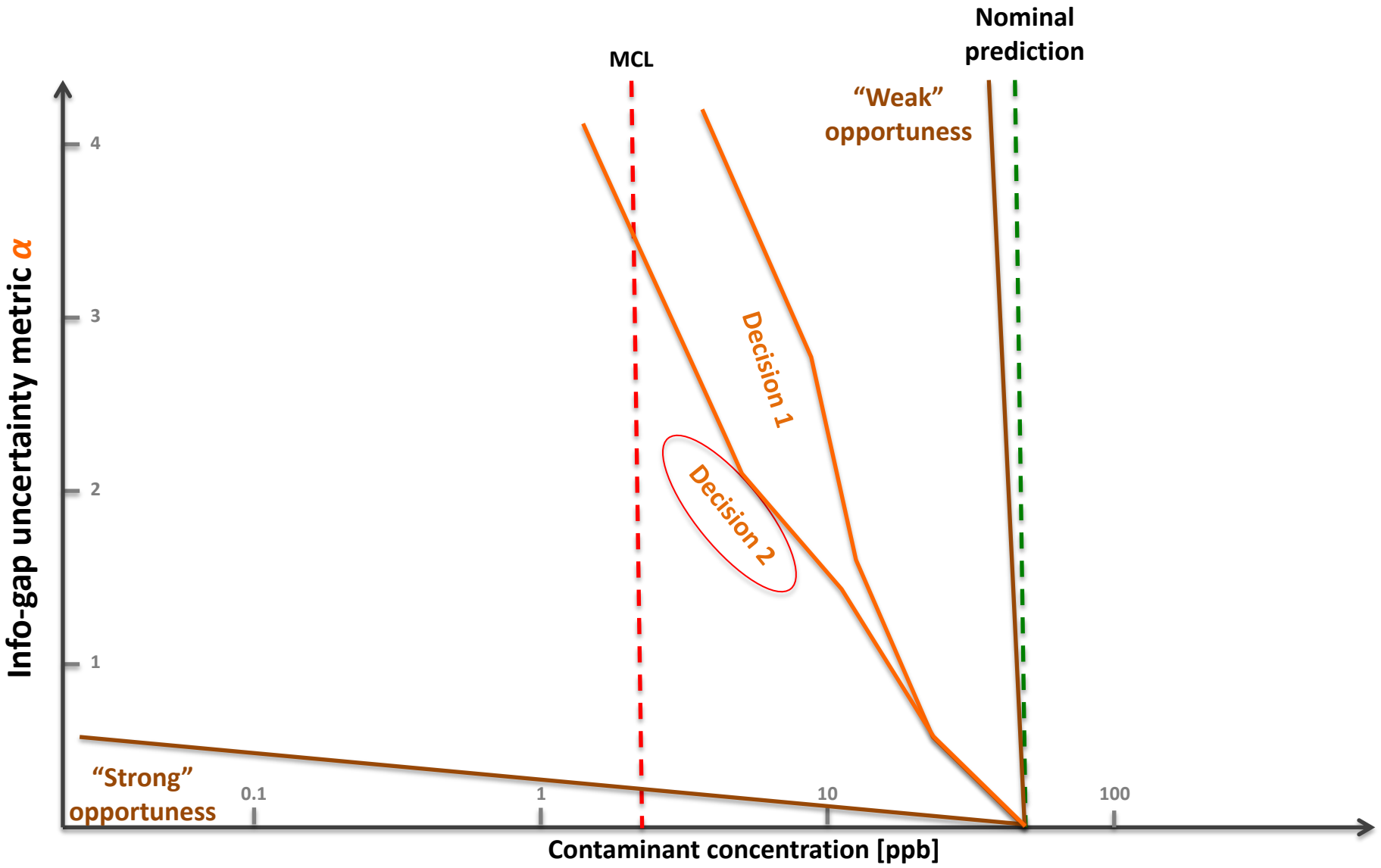
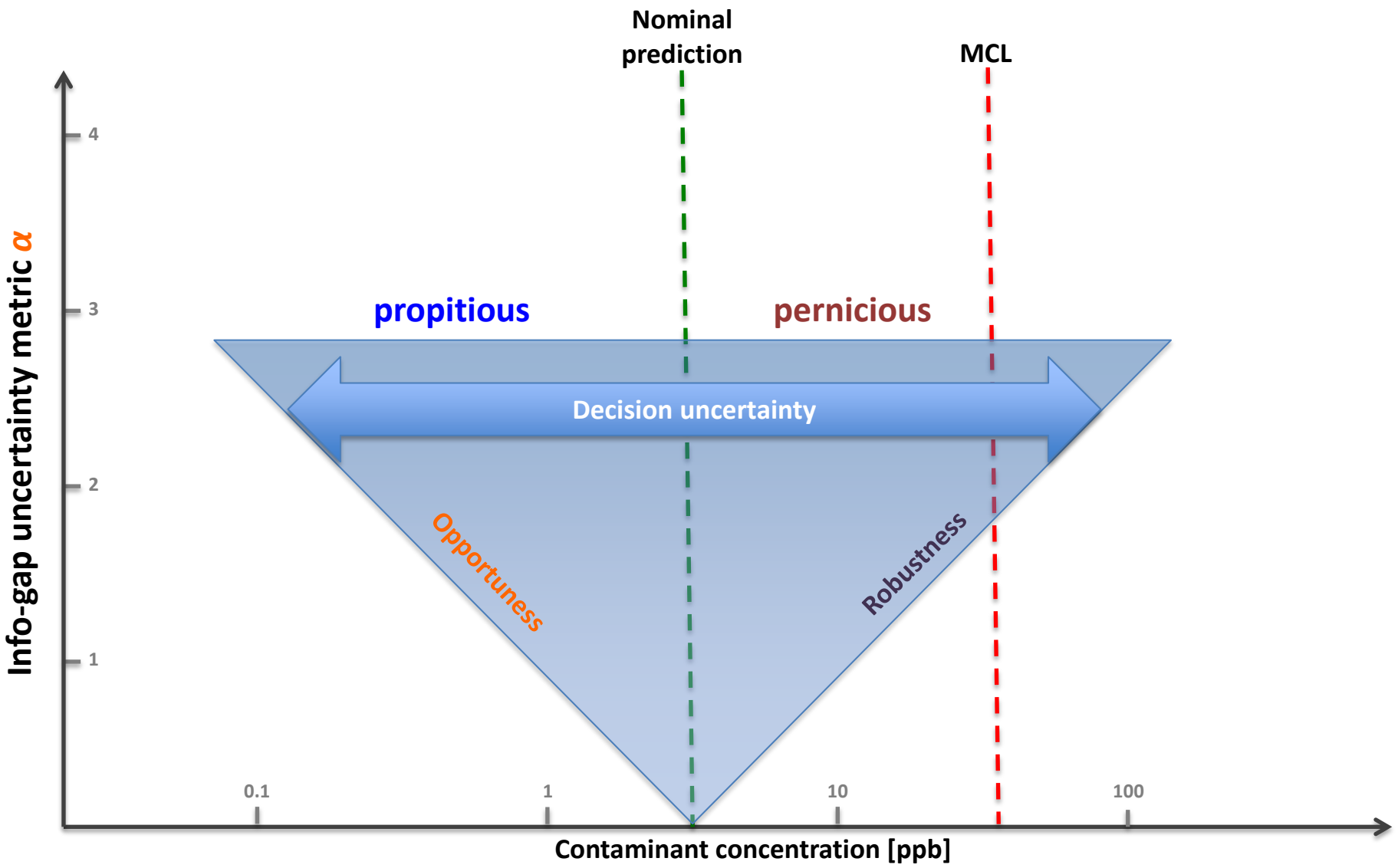


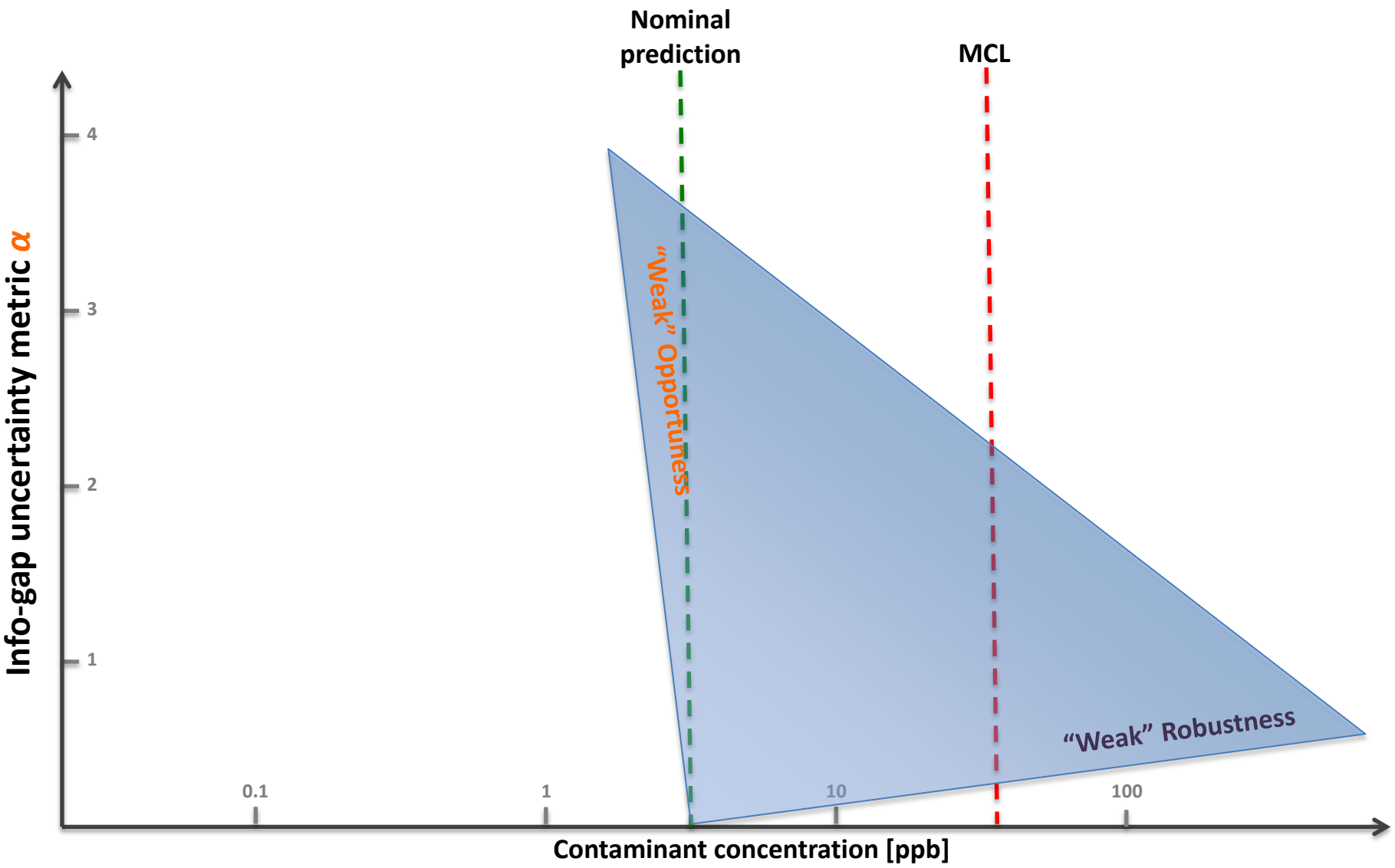
# Info-Gap Analysis: Decision uncertainty

## … duality of decision uncertainty



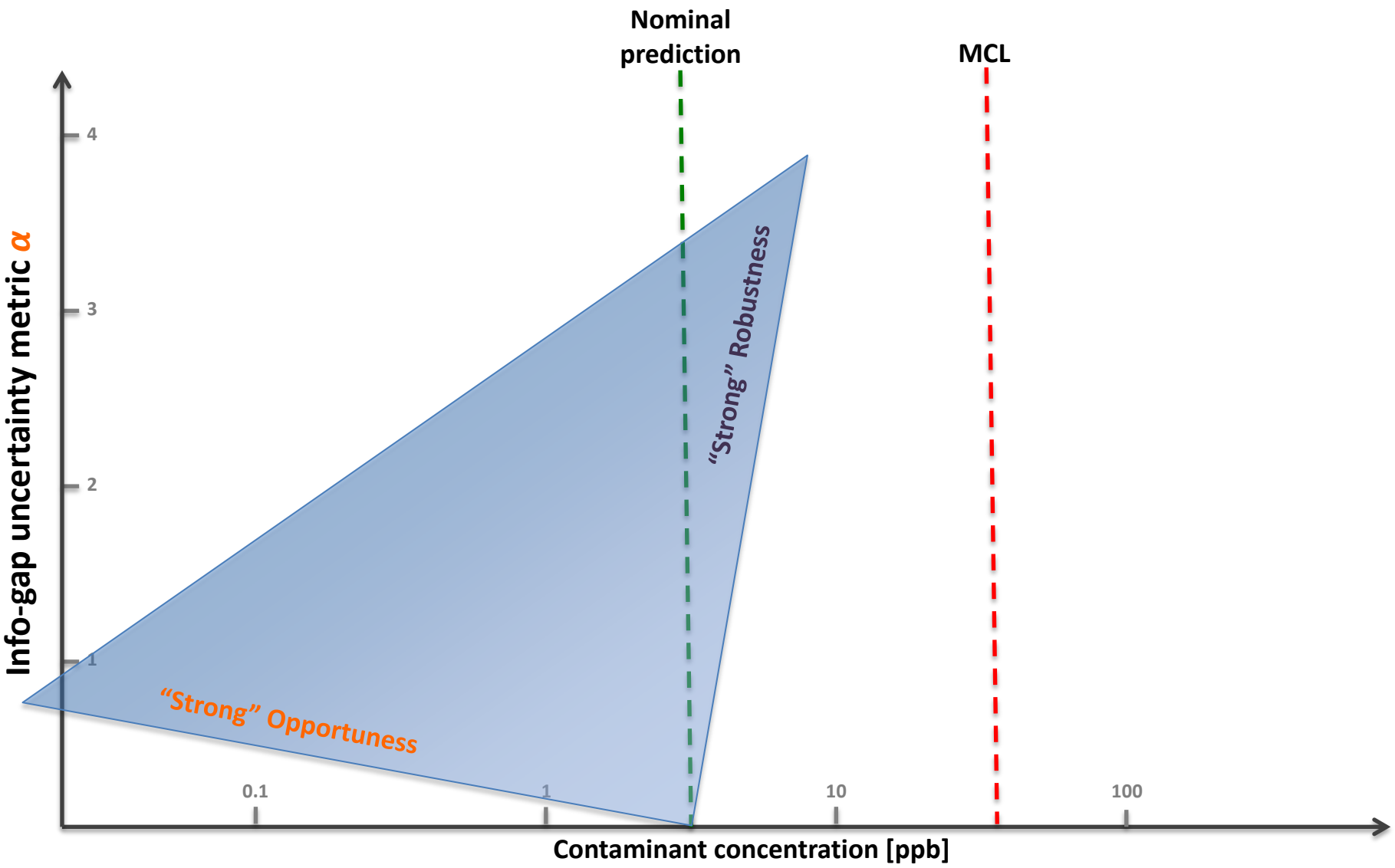
# Info-Gap Analysis: Decision uncertainty

… not preferred decision bounds



# Info-Gap Analysis: Decision uncertainty

## … preferred decision bounds

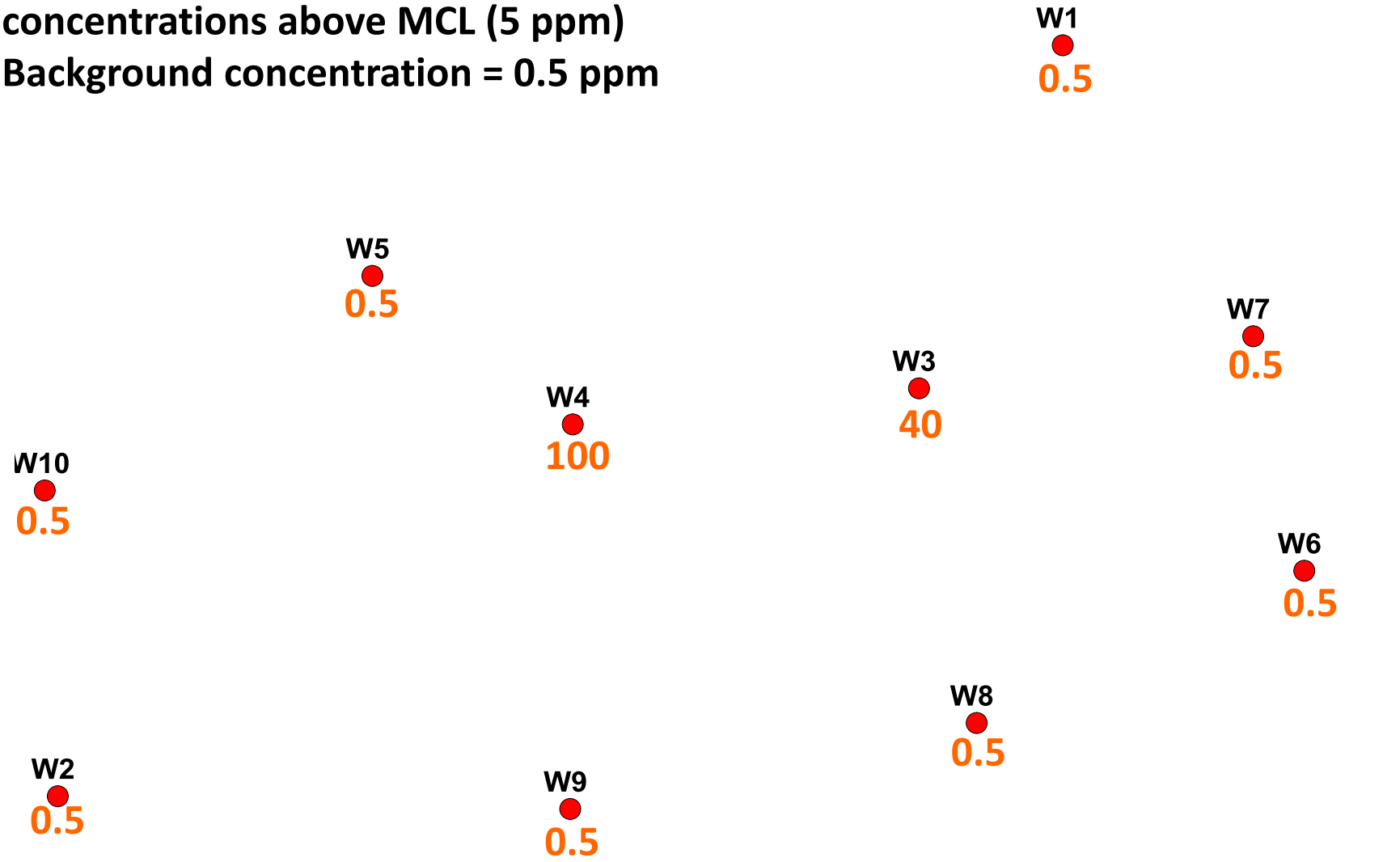


# Info-Gap Application: Case 1

**Optimization of monitoring network**

# Info-Gap Analysis: Network Design

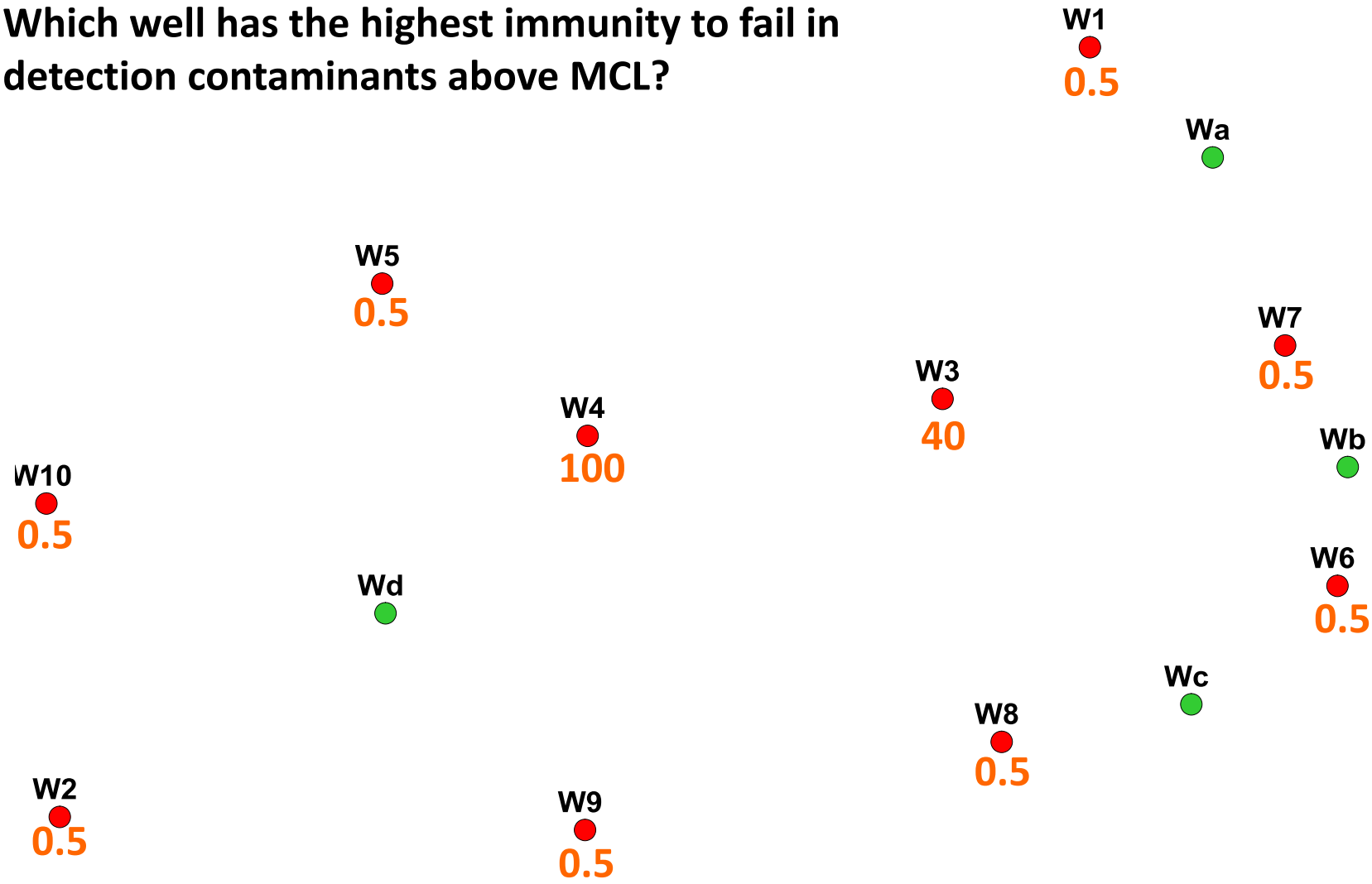
- Two monitoring wells in an aquifer with contaminant concentrations above MCL (5 ppm)
- Background concentration = 0.5 ppm




MCL = 5 Background = 0.5

# Info-Gap Analysis: Network Design

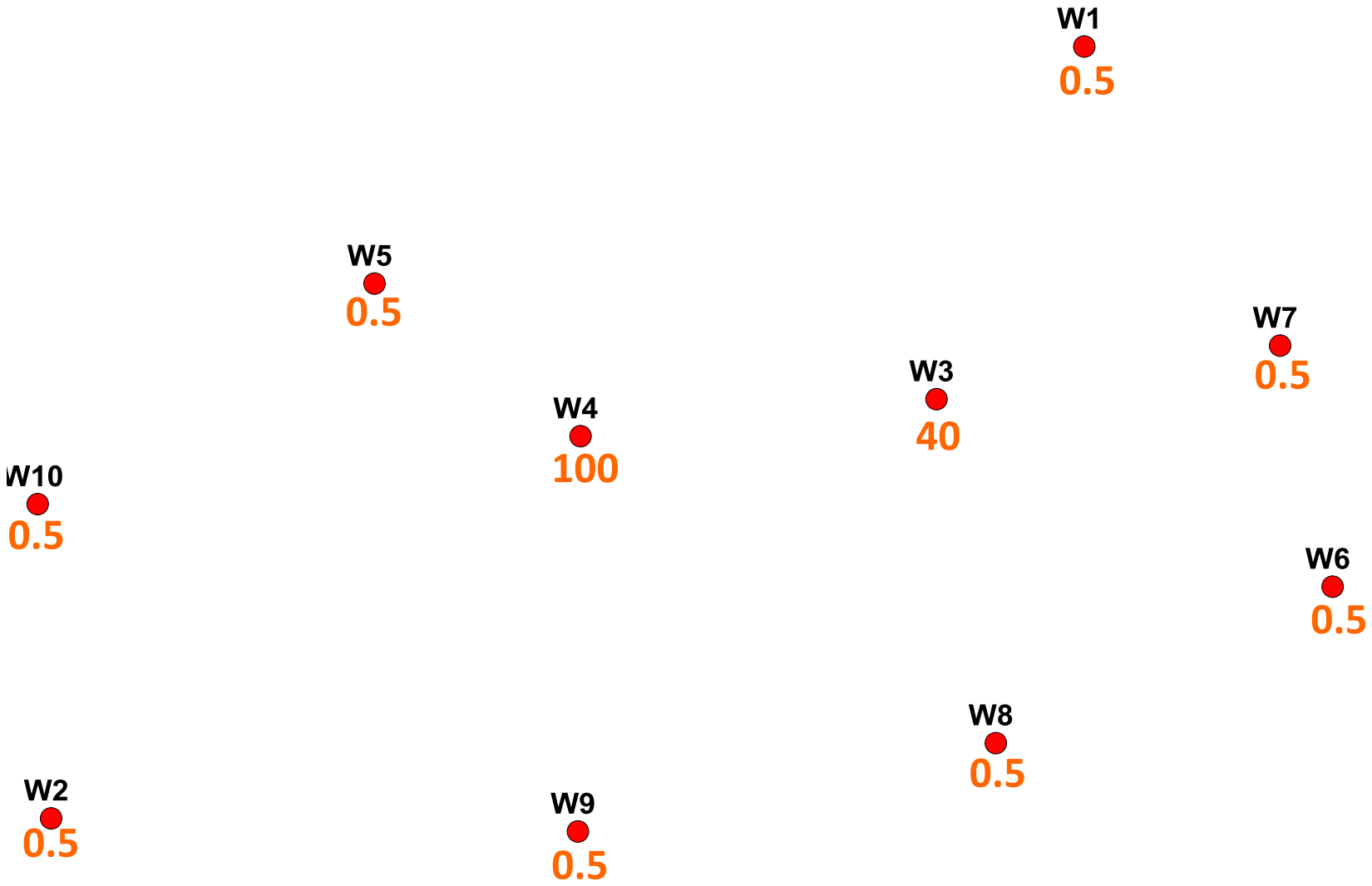
- 4 new proposed monitoring well locations
- Which well has the highest immunity to fail in detection contaminants above MCL?




MCL = 5 Background = 0.5

# Info-Gap Analysis: Network Design

✧ Where is the contaminant source?

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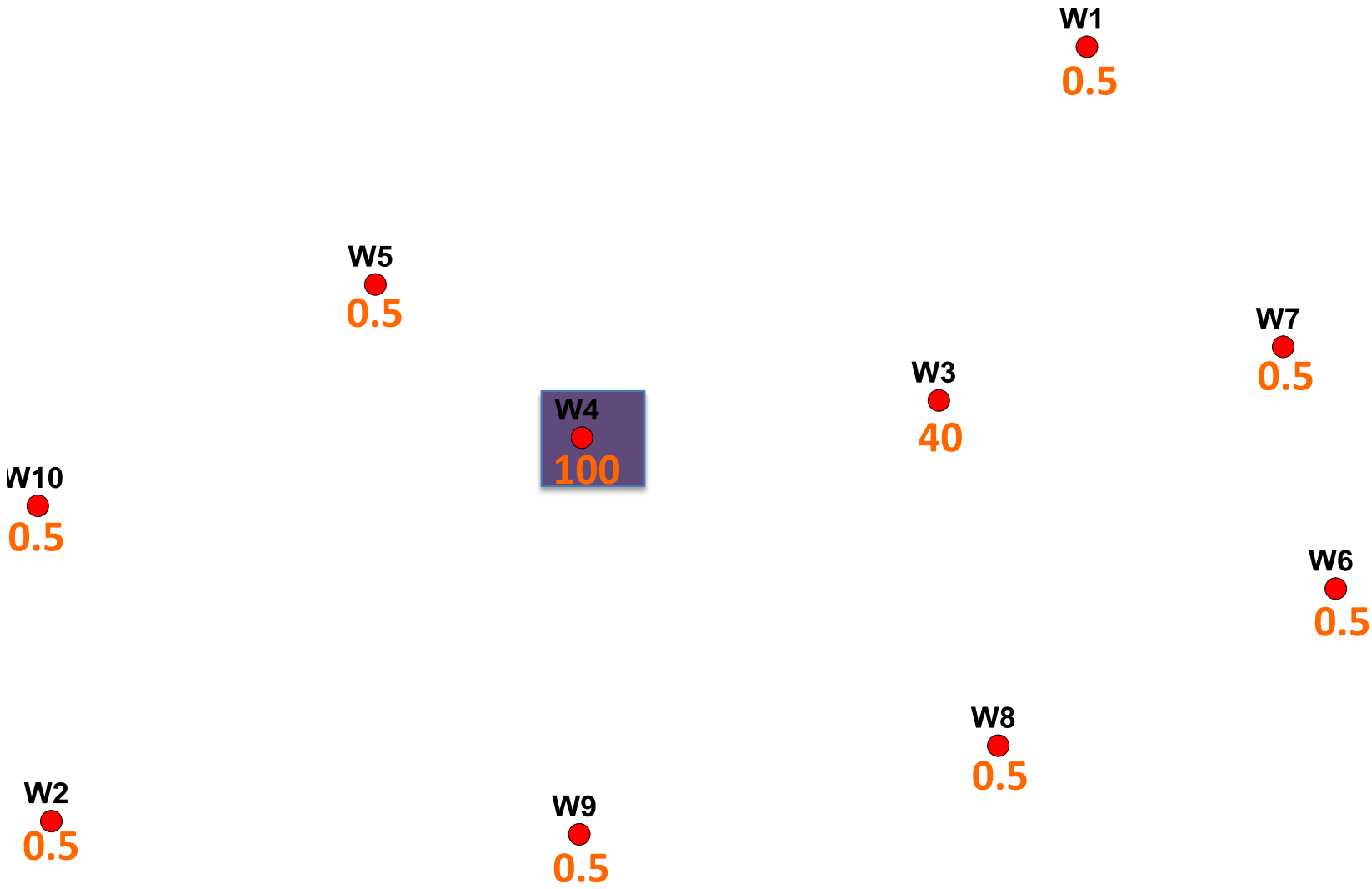
# Info-Gap Analysis: Network Design

- Where is the contaminant source?

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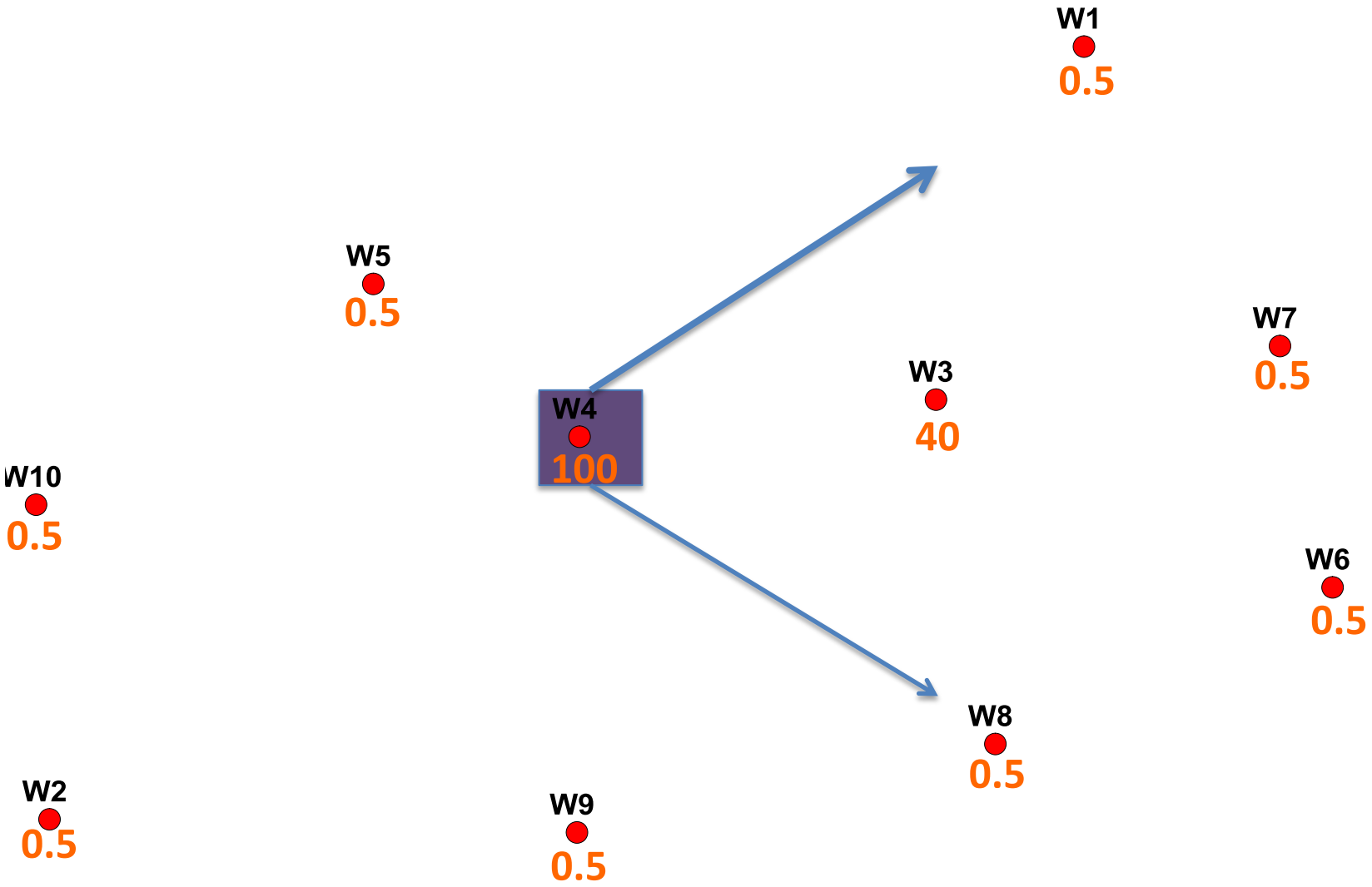
# Info-Gap Analysis: Network Design

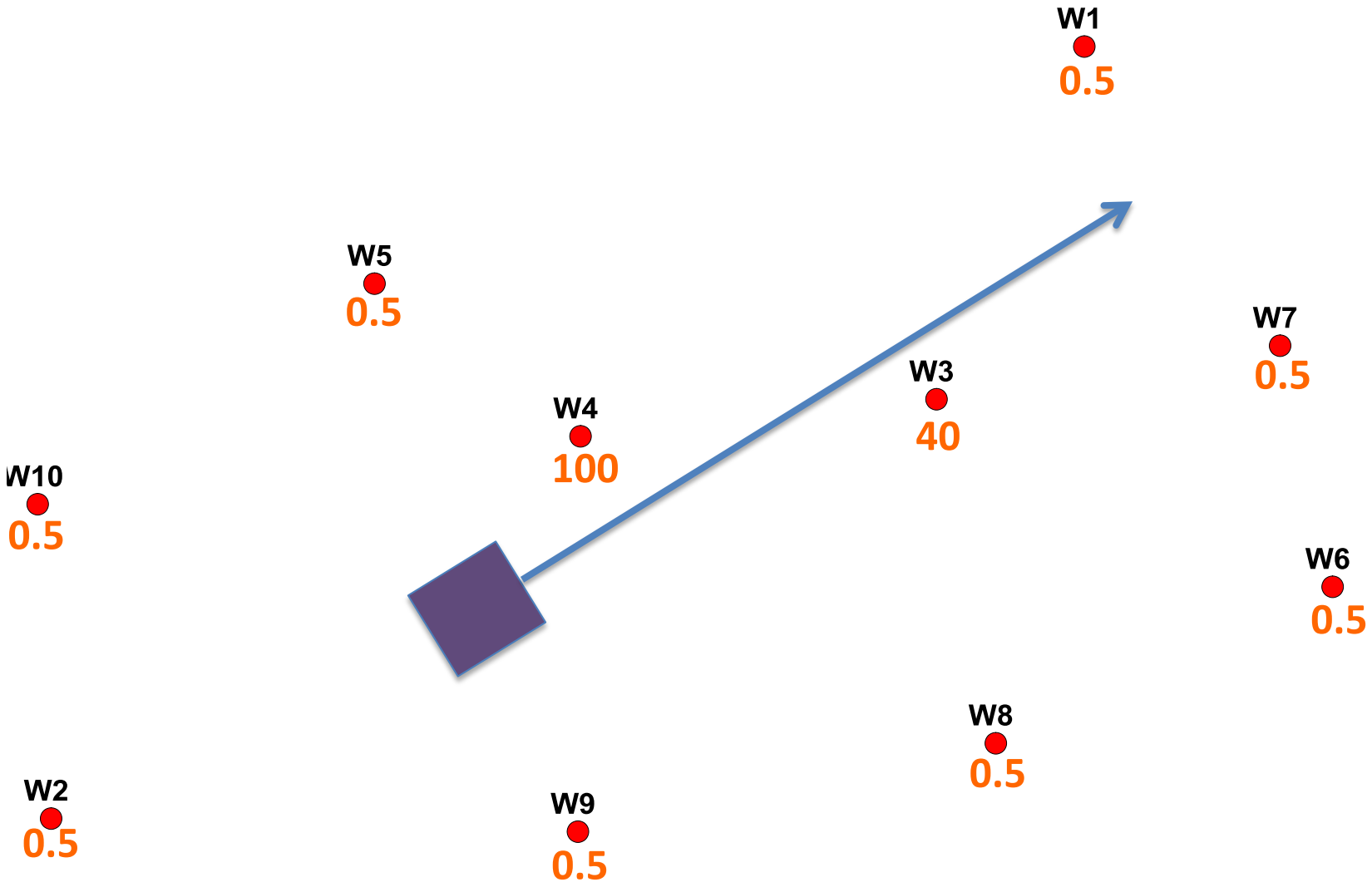
✧ Where is the contaminant source?




MCL = 5 Background = 0.5

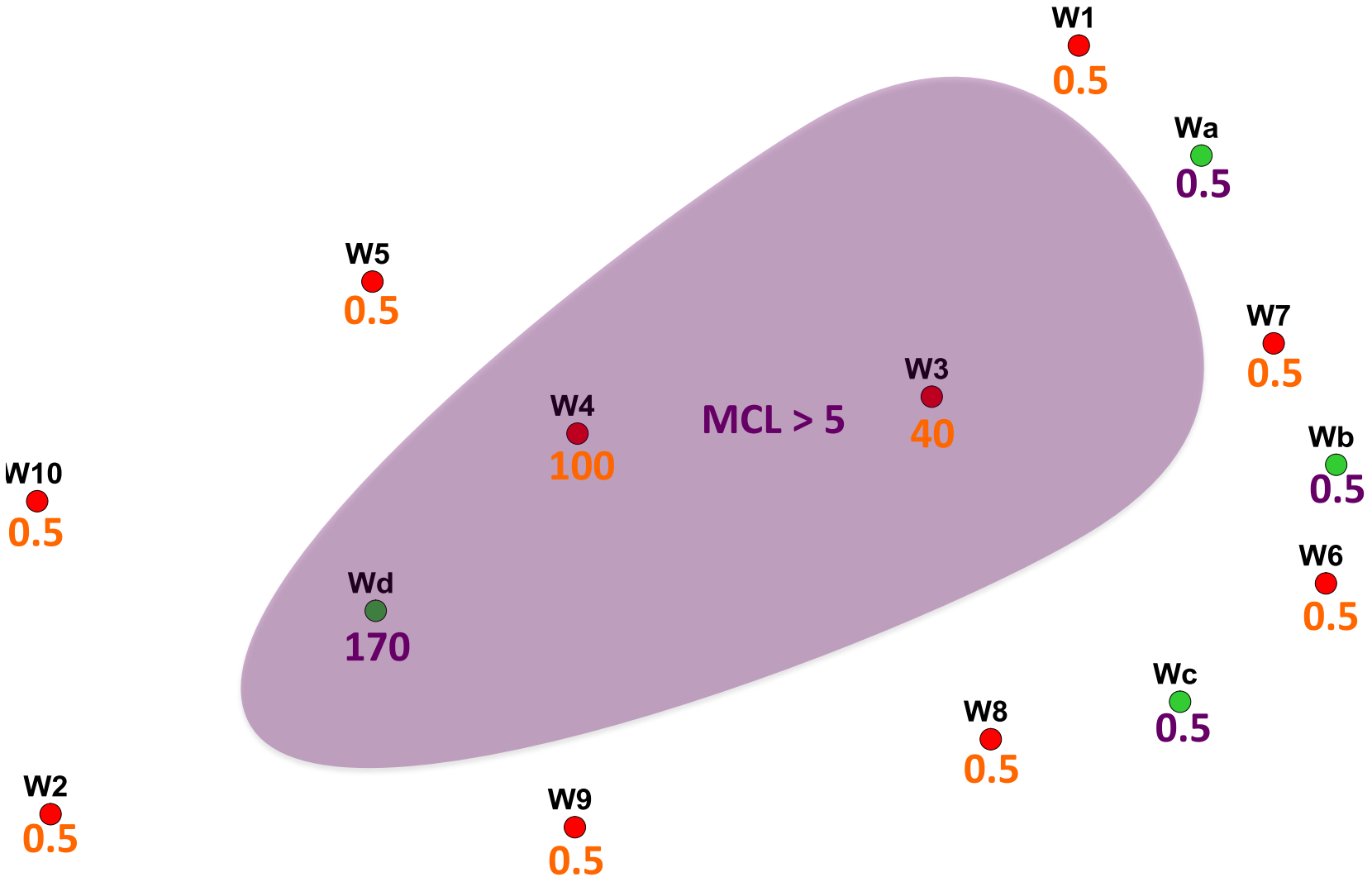
# Info-Gap Analysis: Network Design

- Where is the contaminant source?



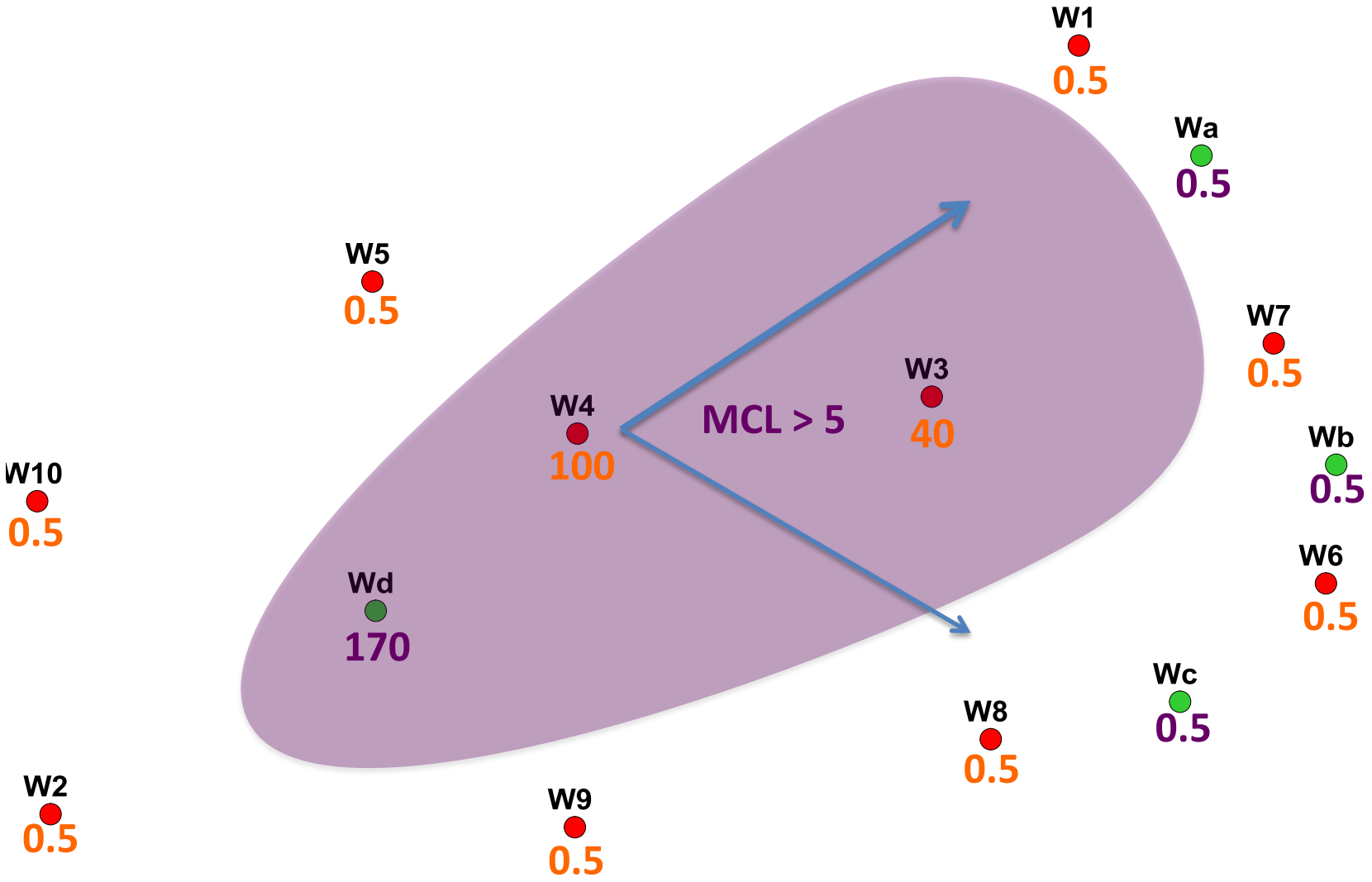

MCL = 5 Background = 0.5

# Info-Gap Analysis: Network Design



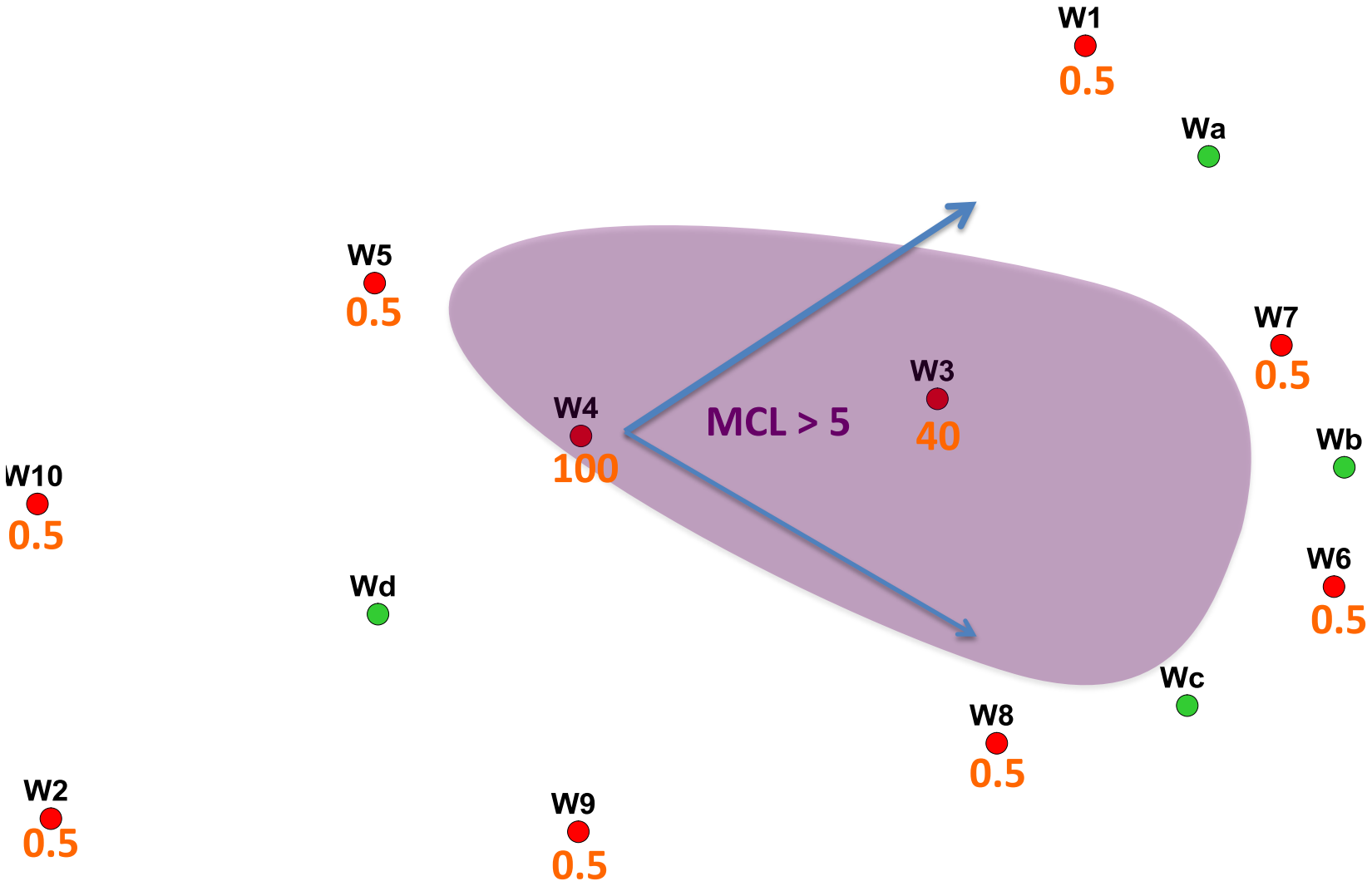

MCL = 5 Background = 0.5

# Info-Gap Analysis: Network Design




MCL = 5 Background = 0.5

# Info-Gap Analysis: Network Design

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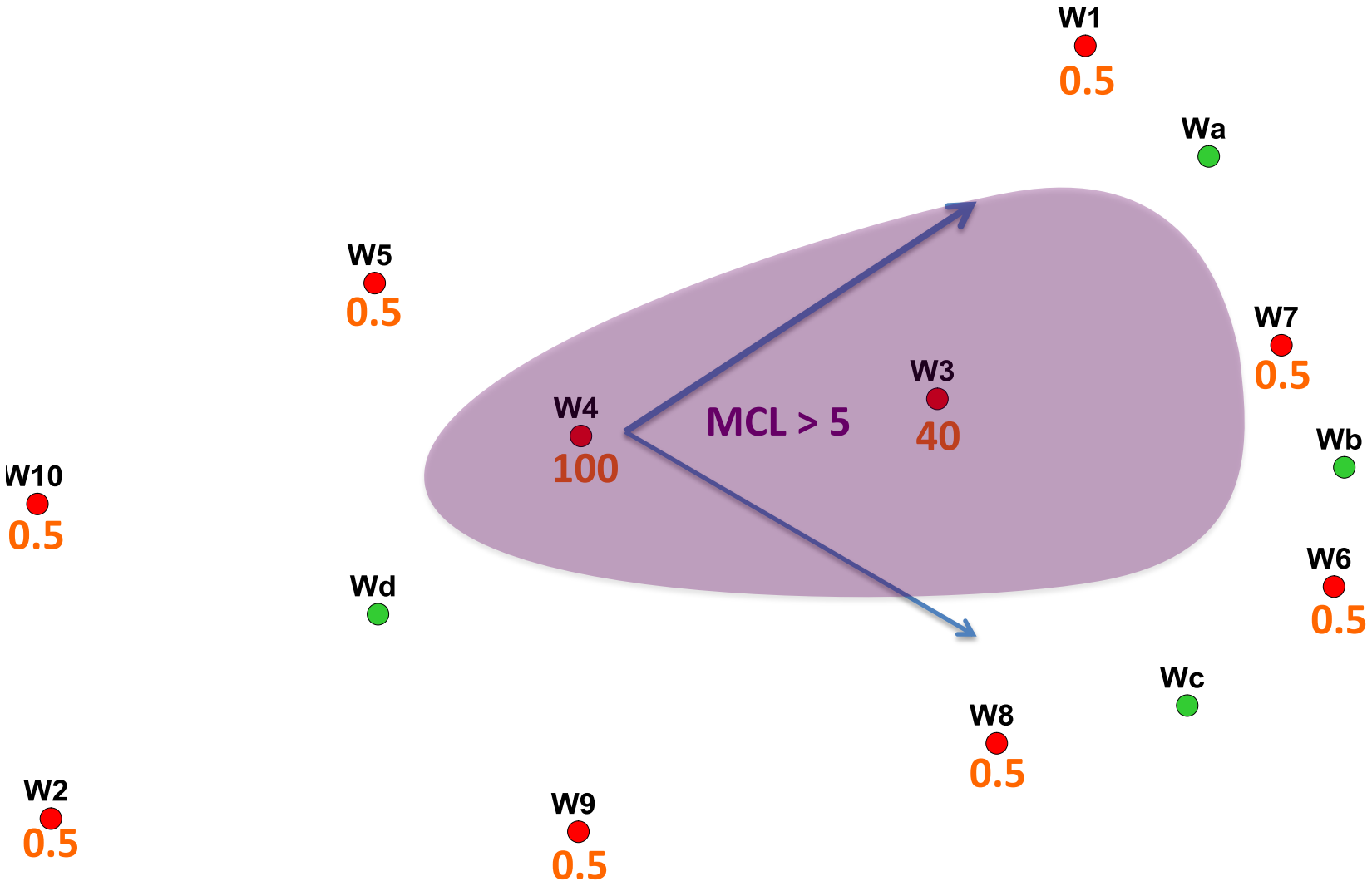
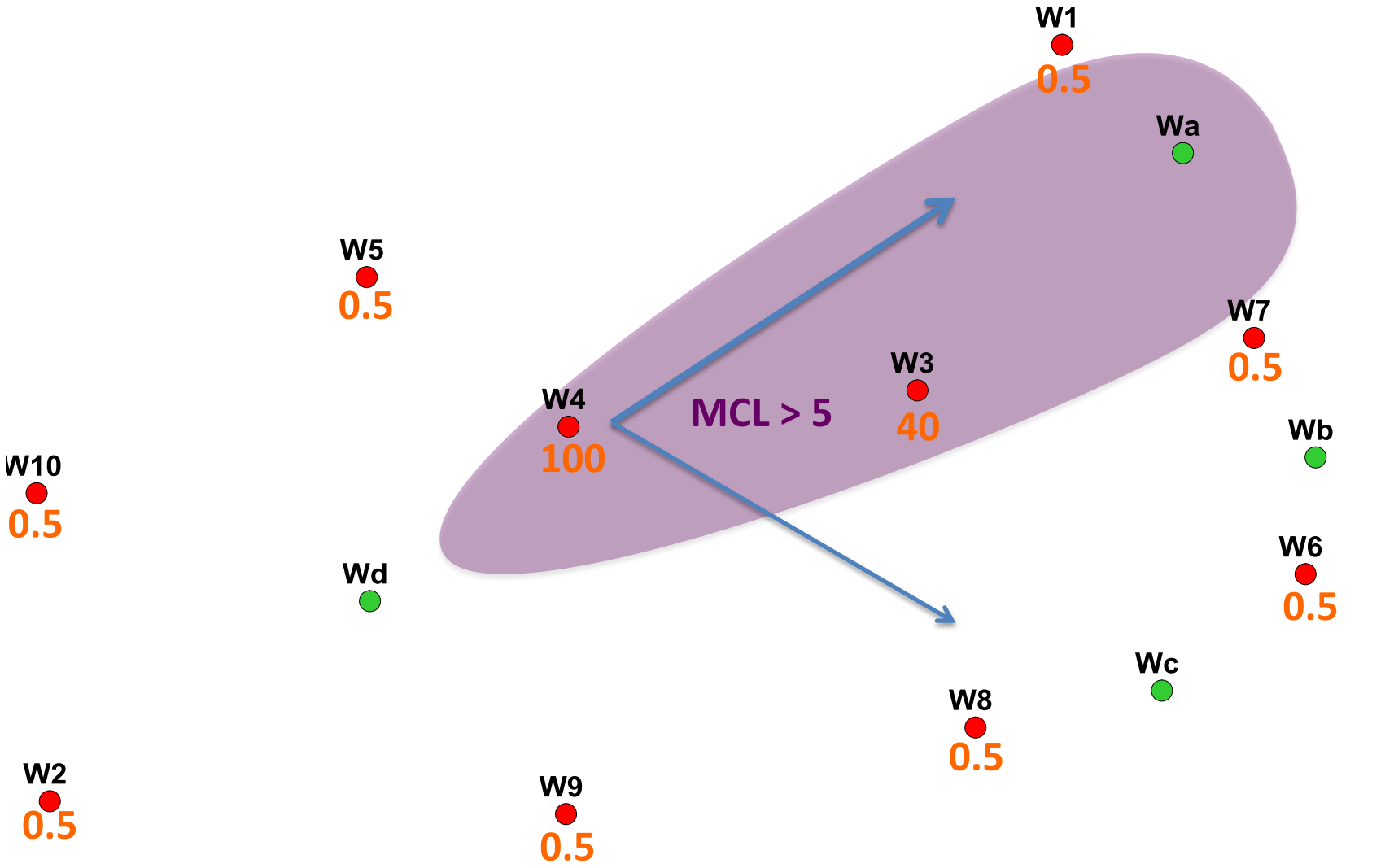
# Info-Gap Analysis: Network Design




MCL = 5 Background = 0.5

# Info-Gap Analysis: Network Design

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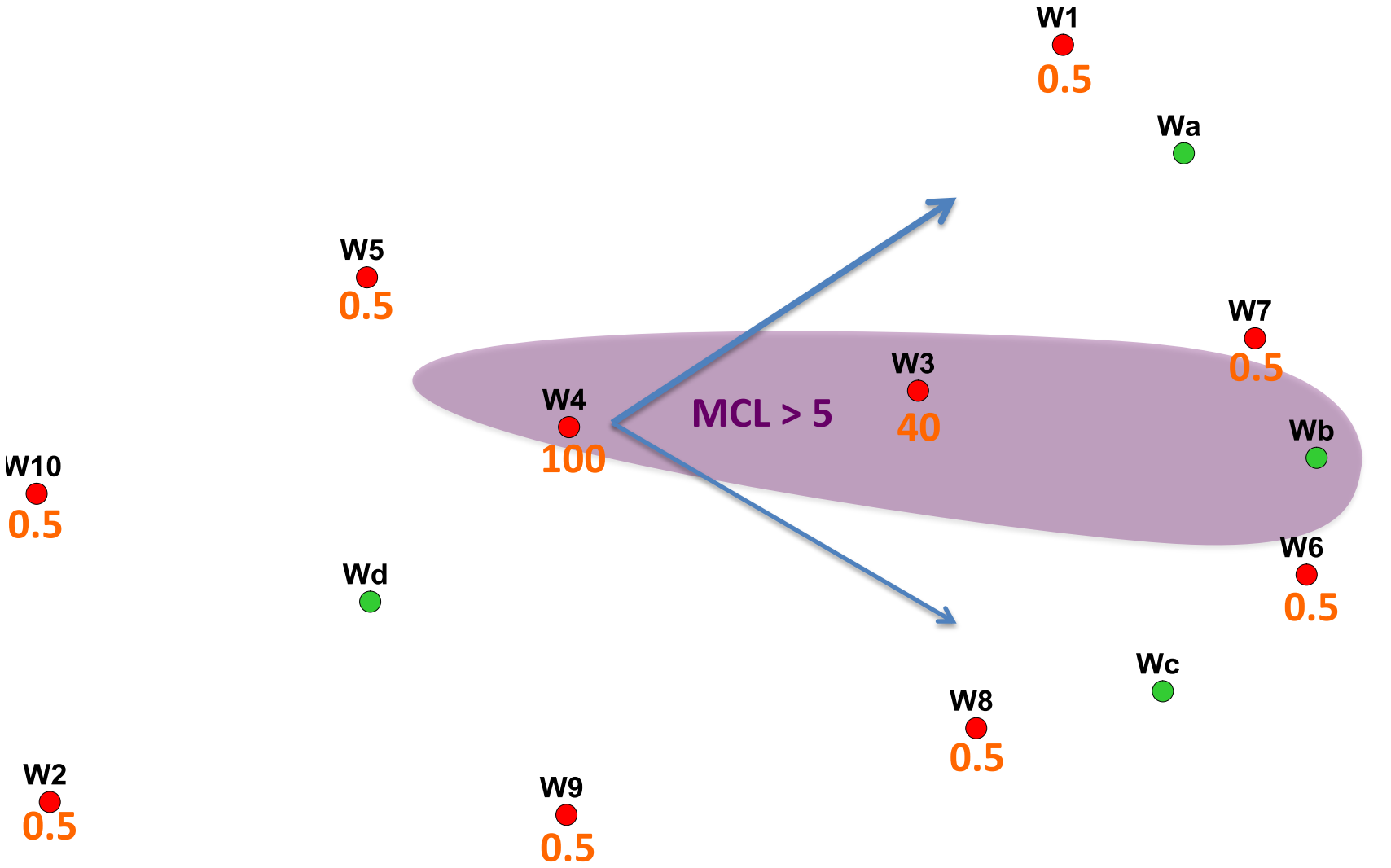
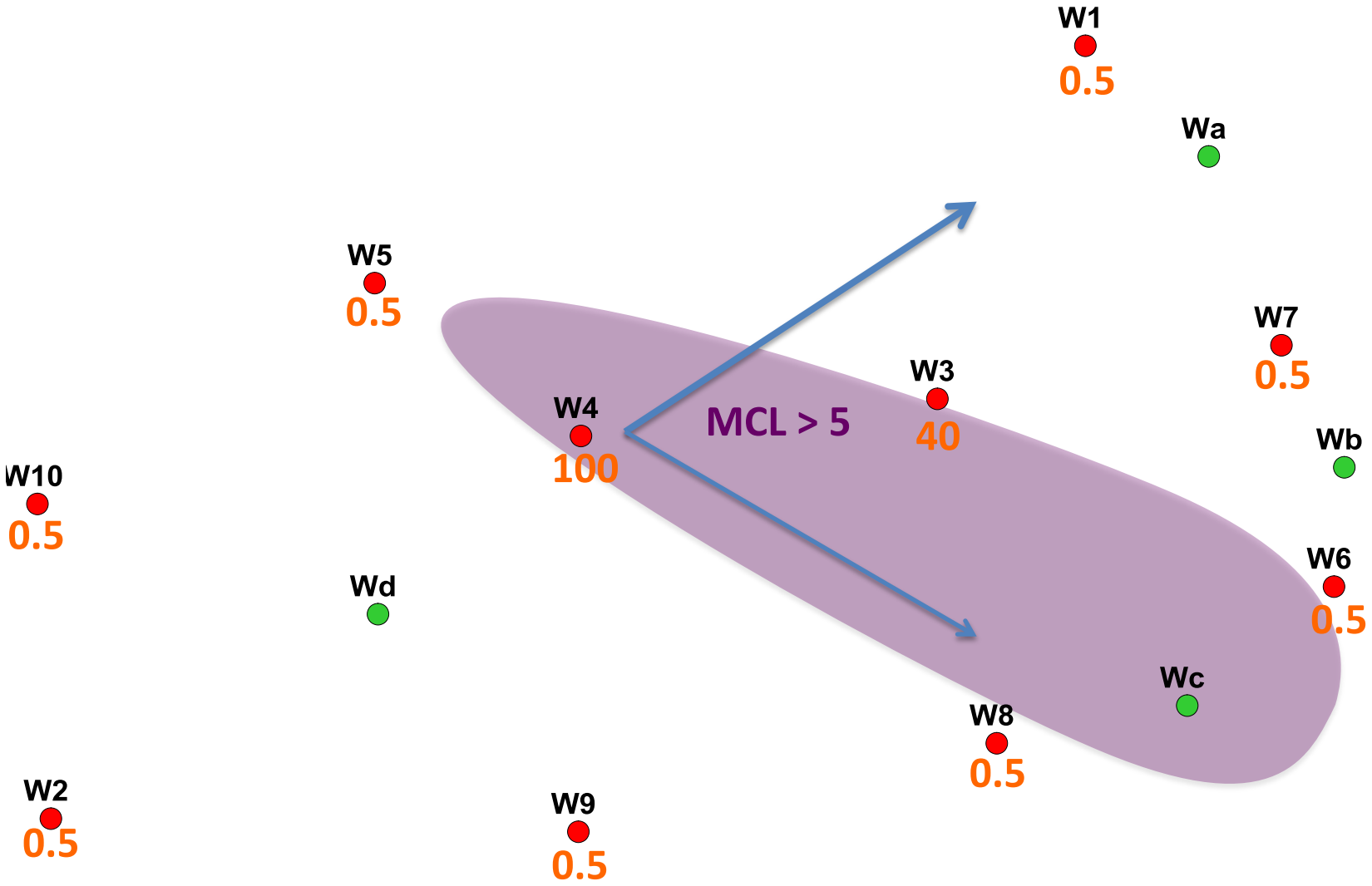



MCL = 5 Background = 0.5

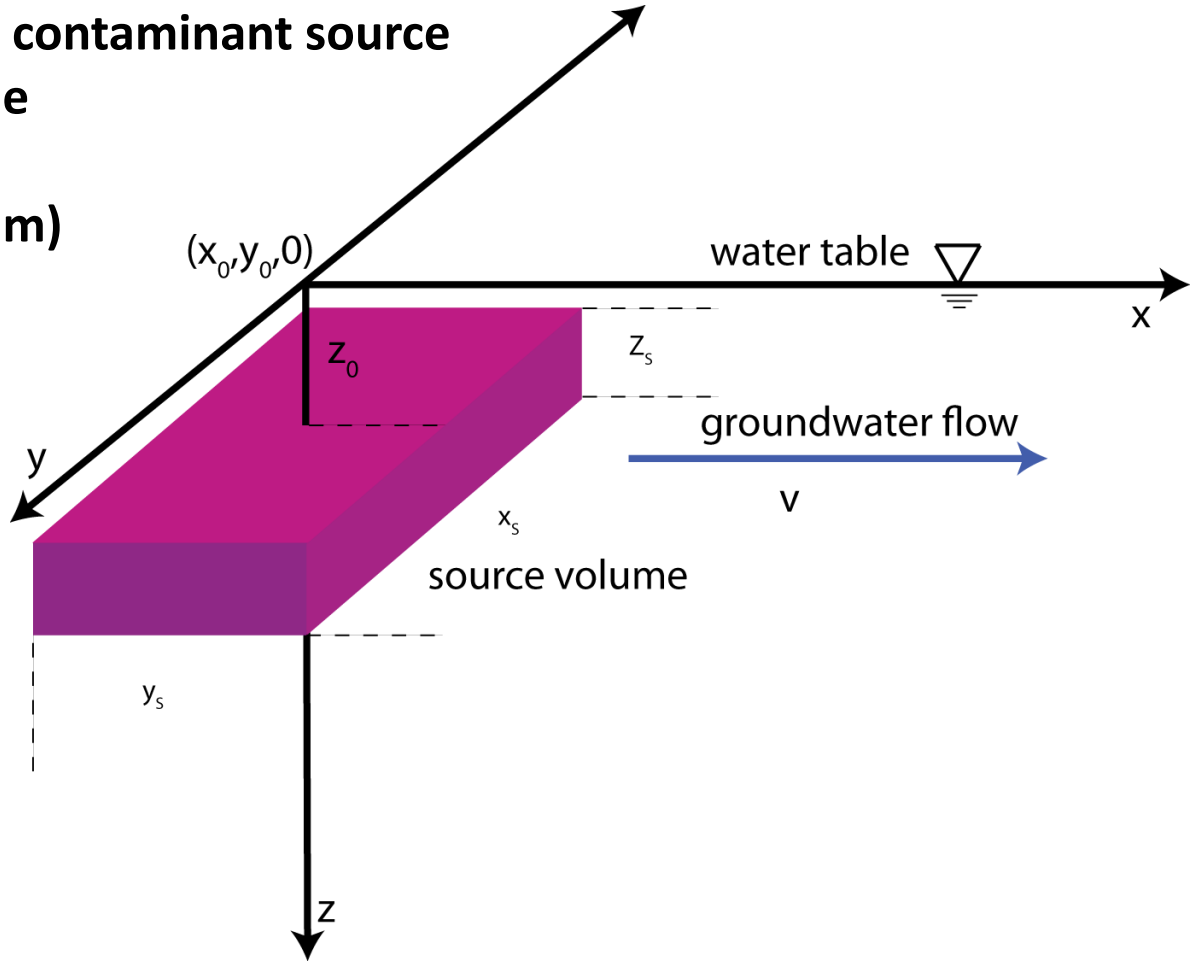
# Info-Gap Analysis: Network Design




MCL = 5 Background = 0.5

# Info-Gap Analysis: Network Design

- Analytical contaminant flow model:
  - 3D steady-state uniform groundwater flow in unbounded aquifer
  - 3D contaminant source at the top of the aquifer
  - 3D contaminant migration (advection, dispersion)
- Deterministic model parameters
  - contaminant flux at the contaminant source
  - contaminant arrival time
  - groundwater velocity
  - source thickness ($z_s$ = 1 m)



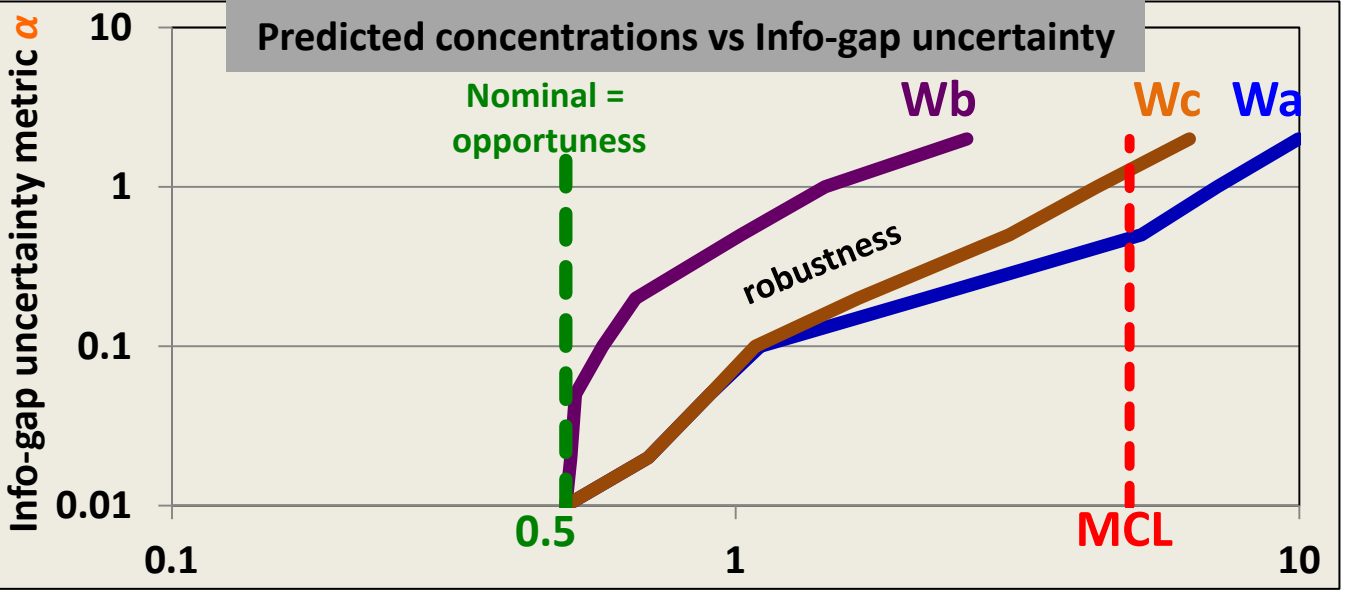
# Info-Gap Analysis: Network Design

- Unknown model parameters (8)
  - source coordinates ($x$, $y$)
  - source size ($x_S$, $y_S$)
  - flow direction
  - aquifer dispersivities (longitudinal, horizontal/vertical transverse)
- Uncertain observations (calibration targets) (10):
  - concentrations at the monitoring wells
- Unknown model parameters estimated using inversion
- Impact of uncertainty in calibration targets on model parameters is estimated using info-gap analyses
- Robustness and opportuness functions associated with predicted contaminant concentrations at the proposed new well locations are applied for decision analyses
- Decision question: which of the new proposed well location has the highest immunity of failure/windfall to detect concentrations above MCL ($c$ > 5 ppm)
  i.e. which well provides the most robust/opportune decision to improve the monitoring network

# Info-Gap Analysis: Network Design

- Calibration targets are highly uncertain (PDF's cannot be defined) due to:
  - measurement errors
  - uncertain background concentrations
  - uncertain local hydrogeological and geochemical conditions

# Info-Gap Analysis: Network Design

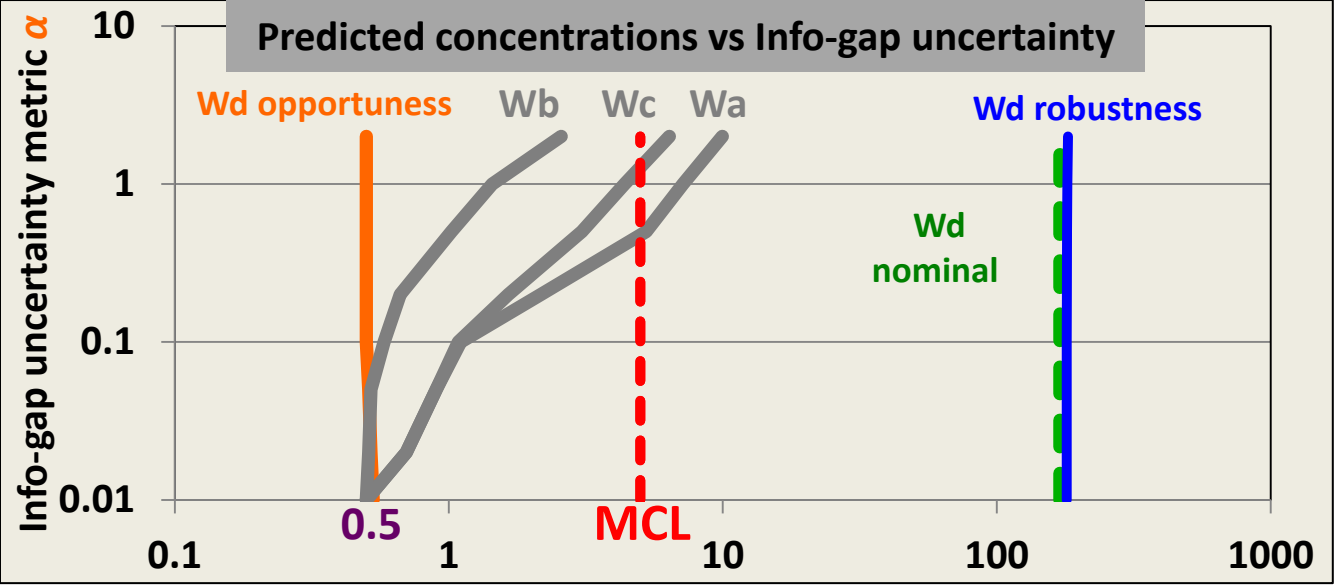


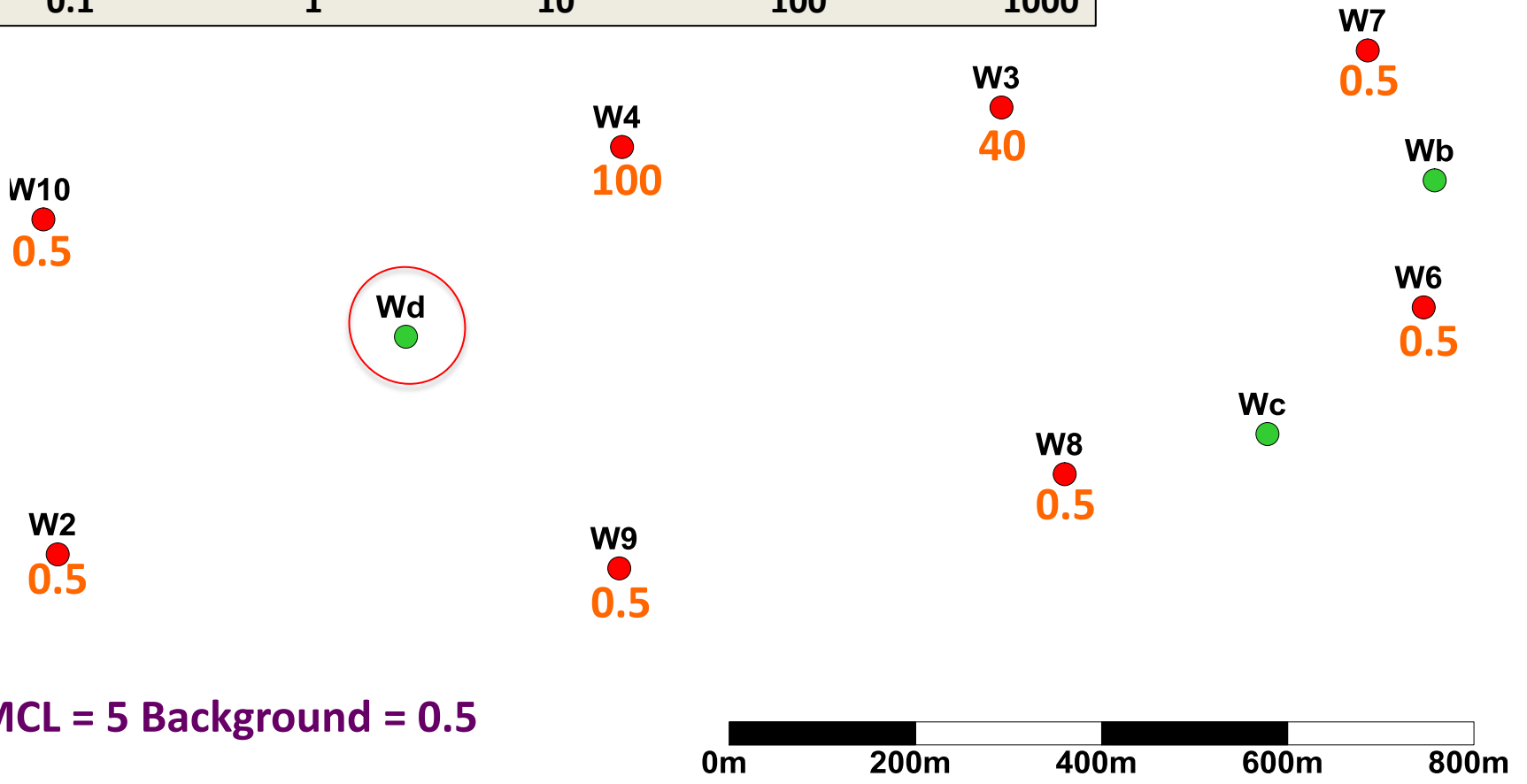




MCL = 5 Background = 0.5

# Info-Gap Analysis: Network Design




MCL = 5 Background = 0.5

# Info-Gap Application: Case 2

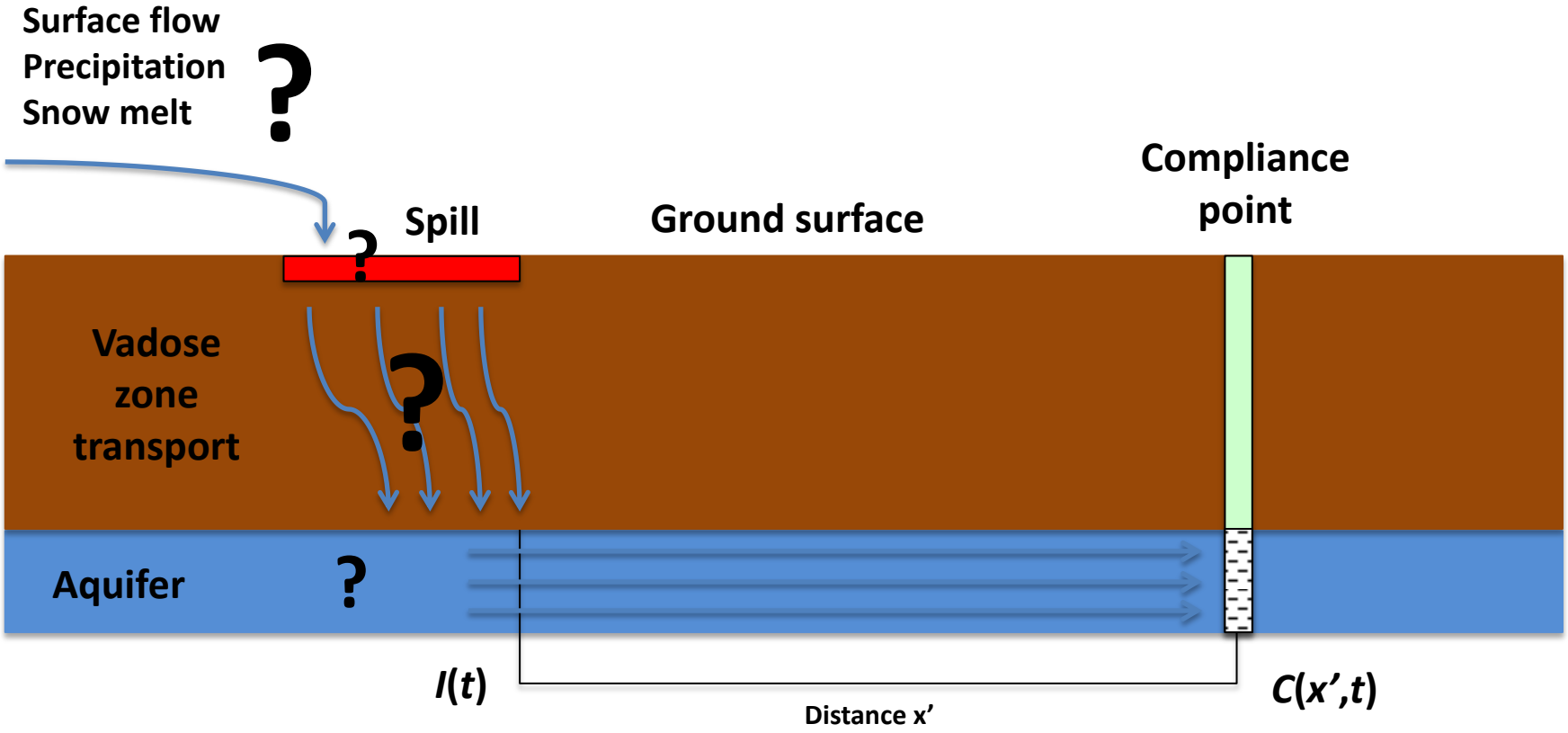
**Remediation of contamination in a aquifer through contaminant source control**

Harp & Vesselinov (2011). *Contaminant remediation decision analysis using information gap theory*. SERRA.

# Info-Gap Analysis: Remediation of contaminant source

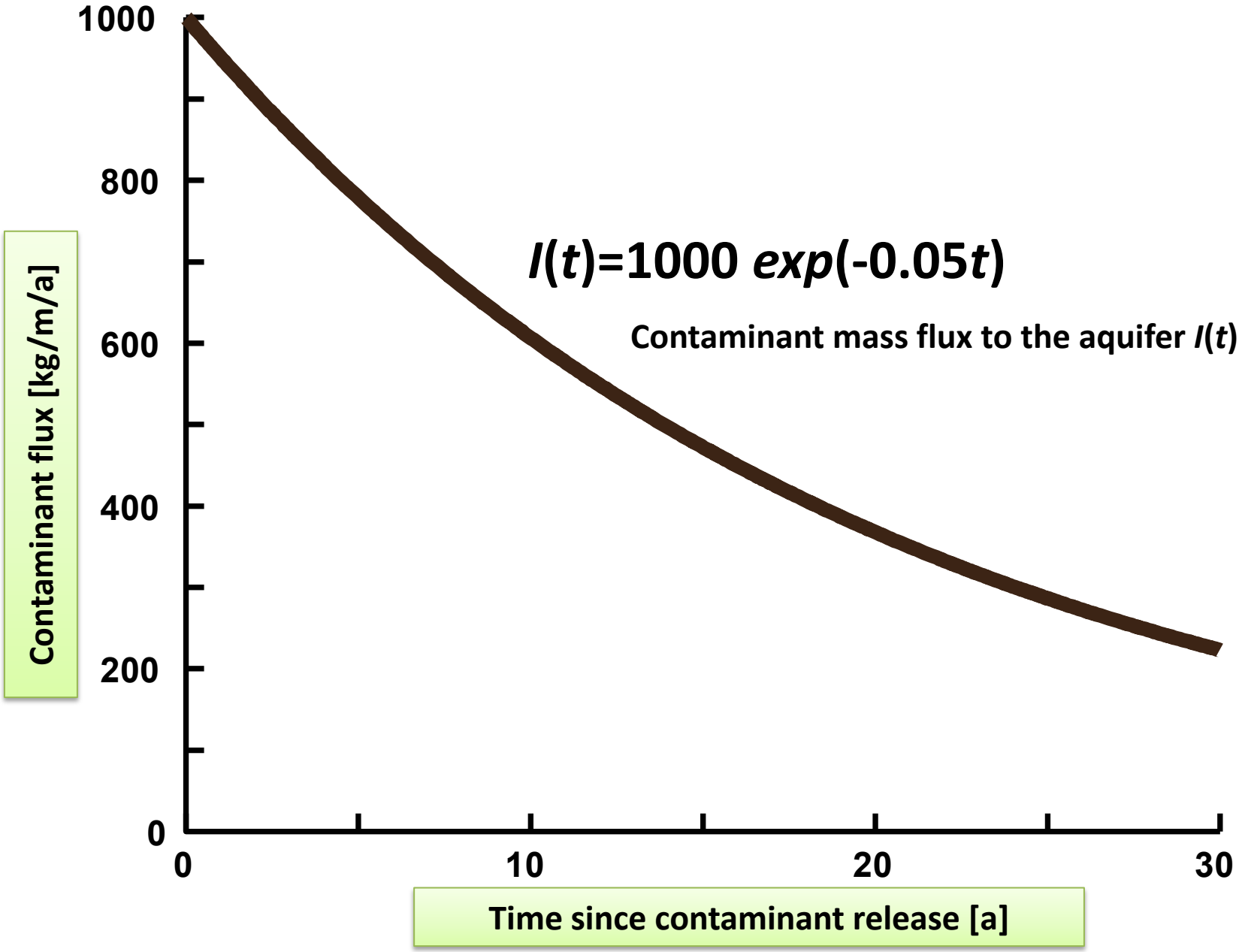
**Simple contaminant remediation problem:**

- ✧ how much contaminant mass needs to be removed to satisfy compliance requirement $C(x',t) < \text{MCL}$
- ✧ lack of probabilistic (frequency of occurrence) information about the contaminant mass flux to aquifer $I(t)$

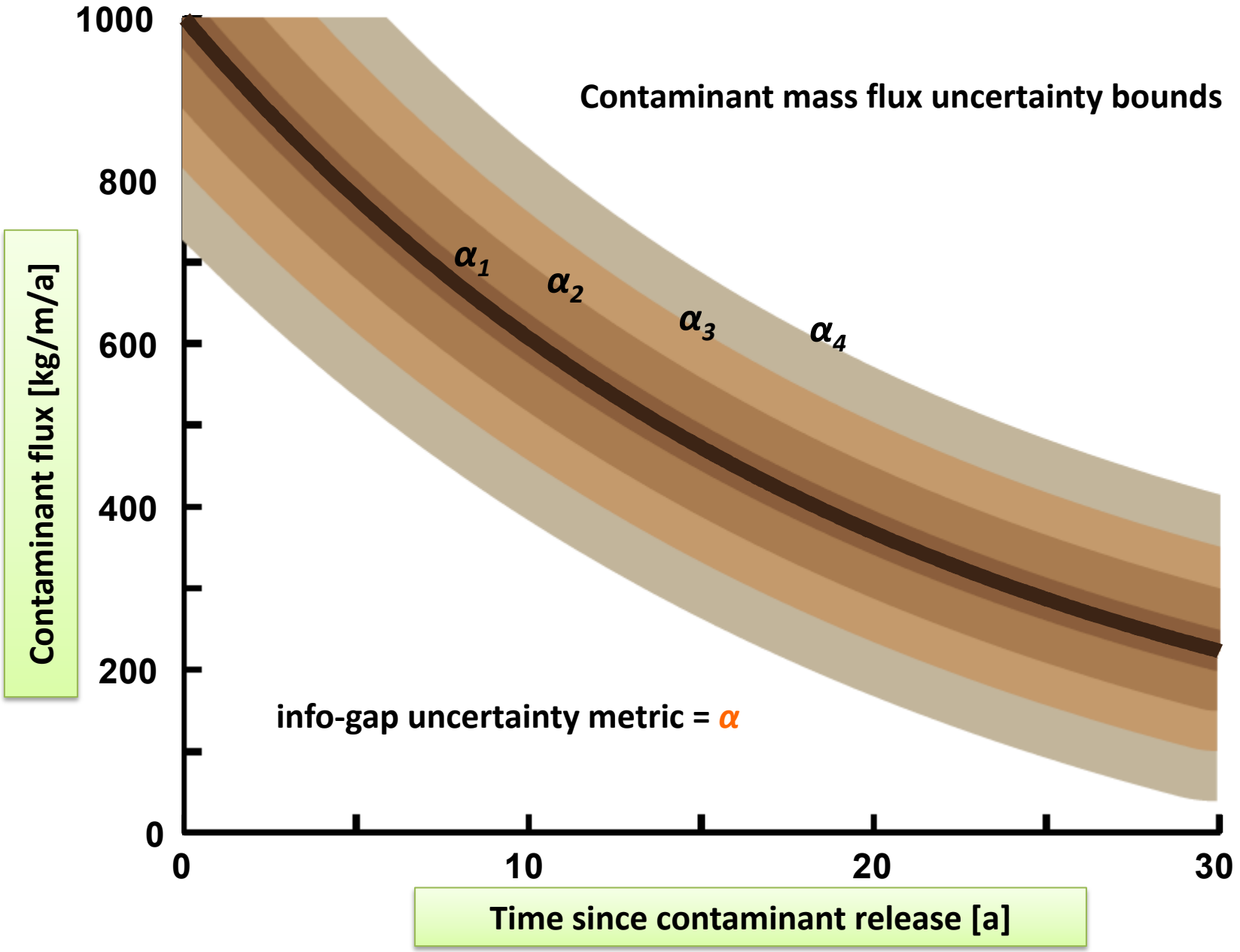



Harp & Vesselinov (2011). *Contaminant remediation decision analysis using information gap theory*. SERRA.

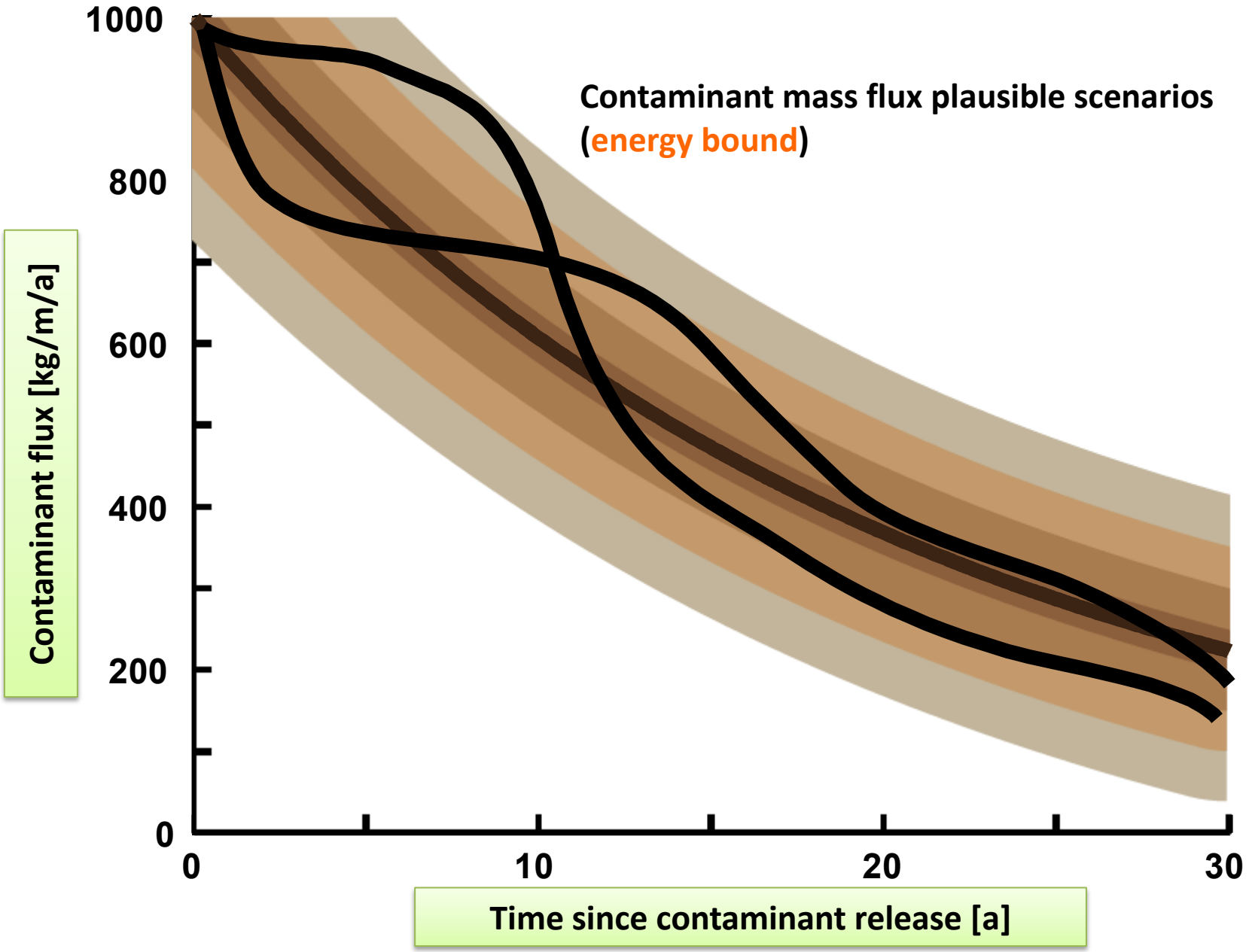
# Info-Gap Analysis: Remediation of contaminant source



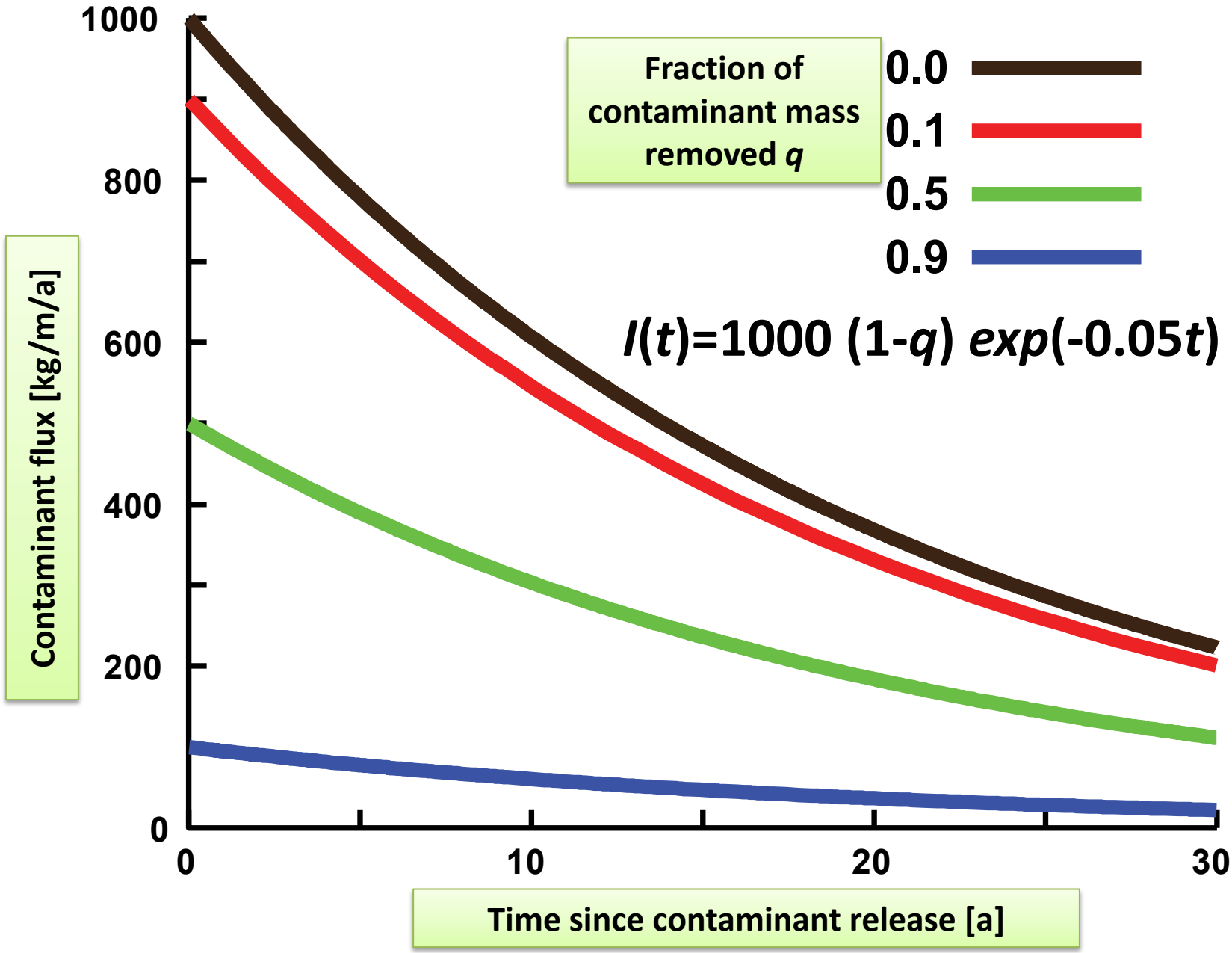
# Info-Gap Analysis: Remediation of contaminant source



# Info-Gap Analysis: Remediation of contaminant source

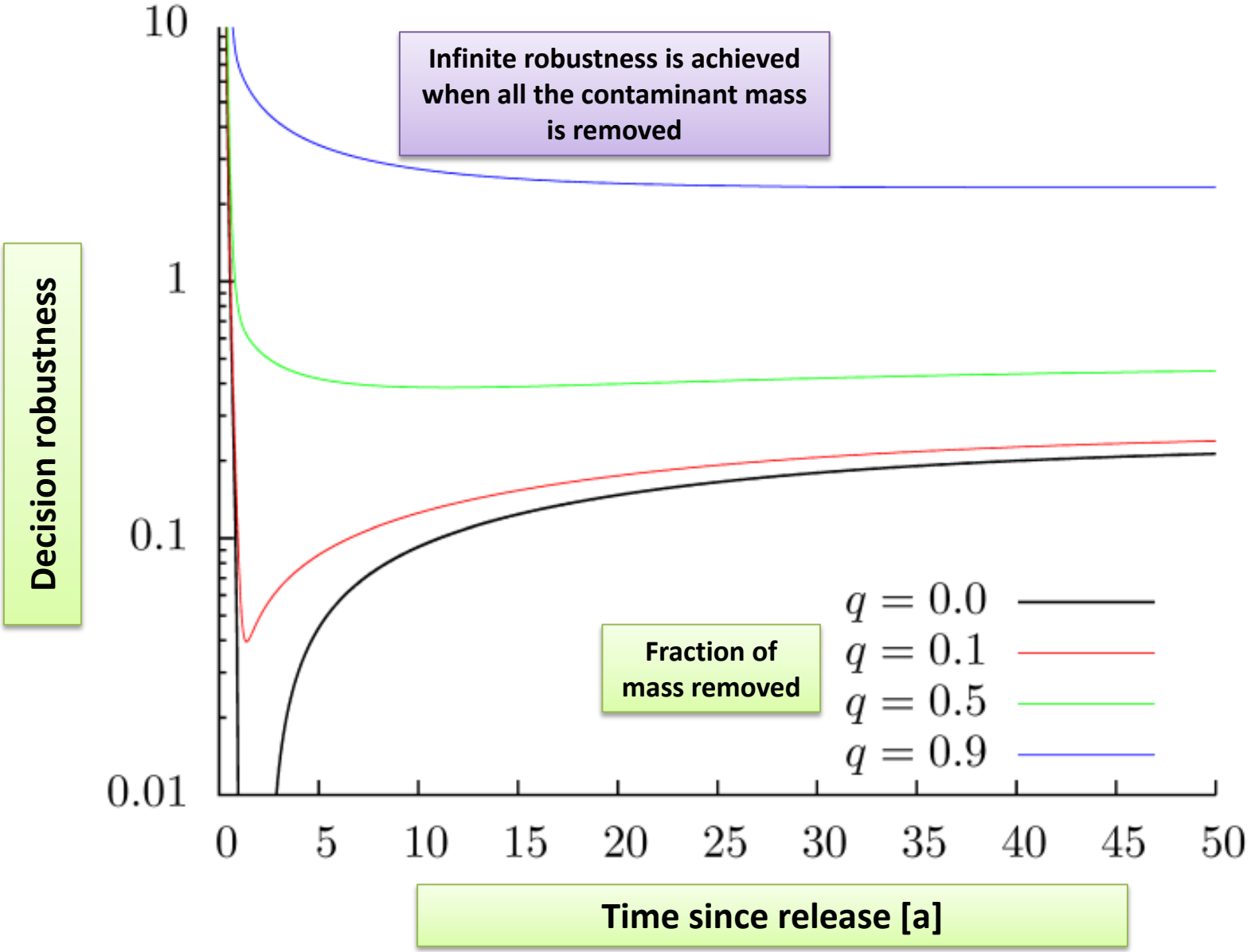


# Info-Gap Analysis: Remediation of contaminant source

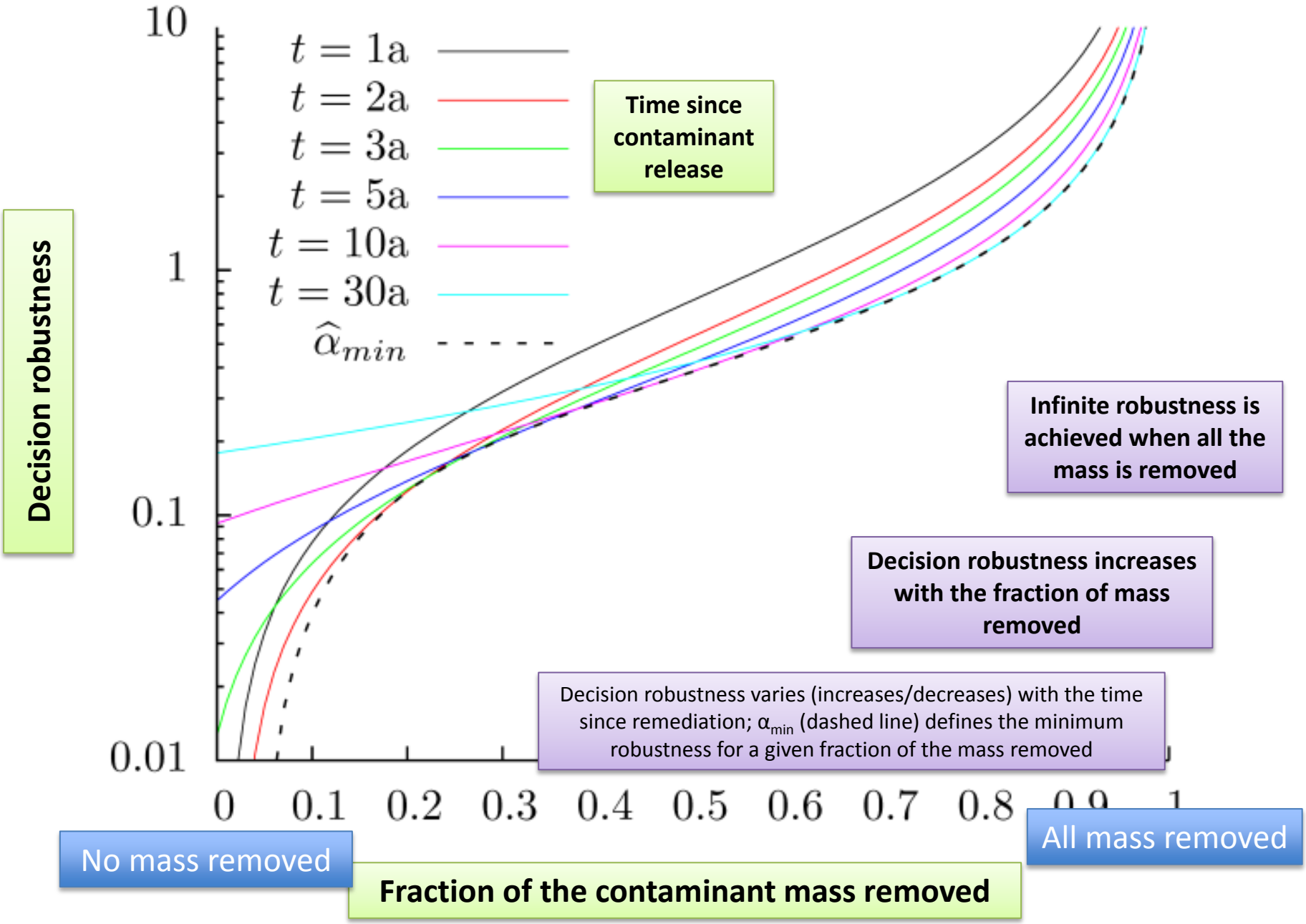


# Info-Gap Analysis: Remediation of contaminant source

**Decision robustness defines how much contaminant mass should be removed and still be immune to failure considering lack of information about the contaminant mass flux**



# Info-Gap Analysis: Remediation of contaminant source

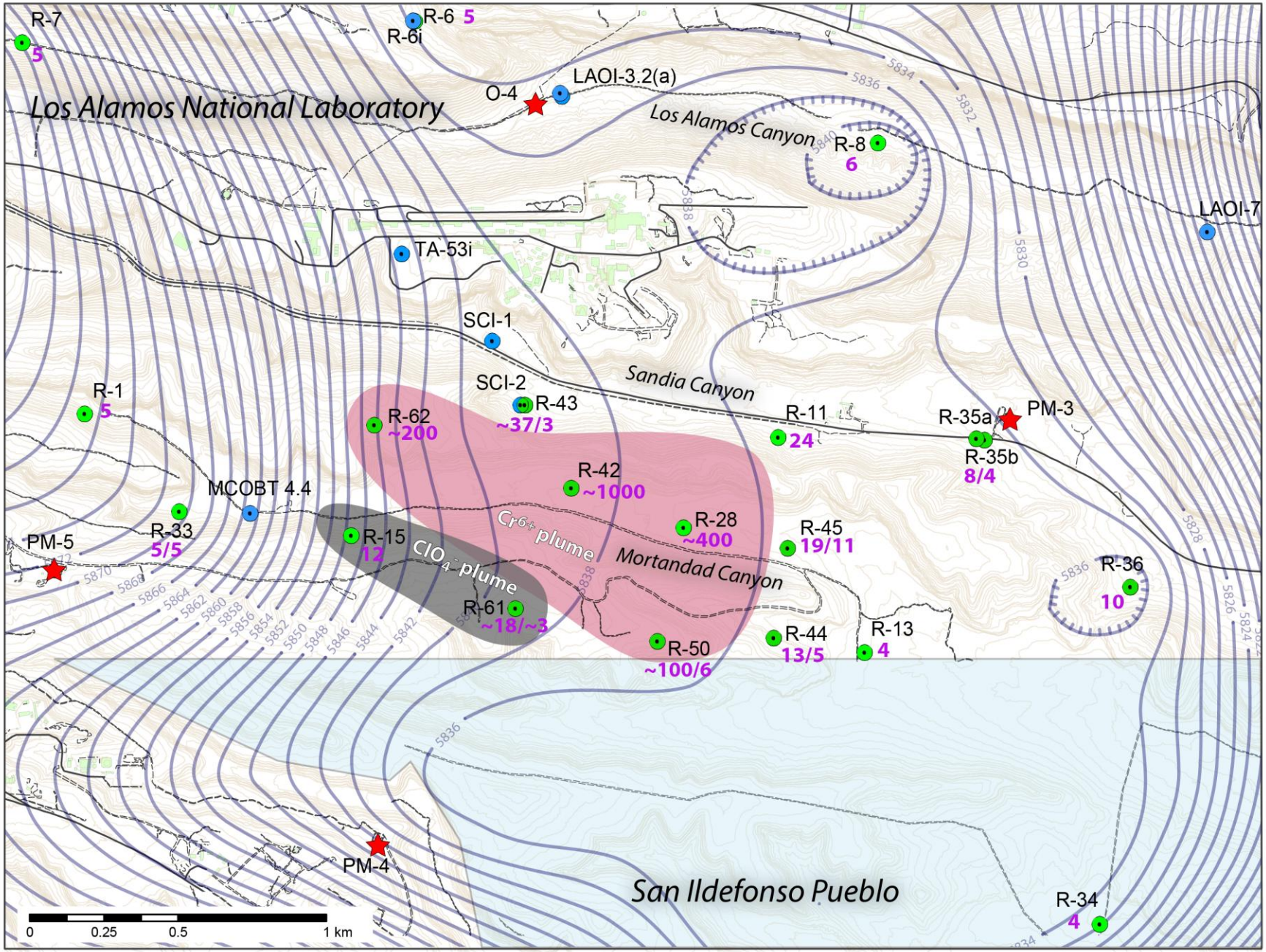


# Chromium plume in the regional aquifer at LANL

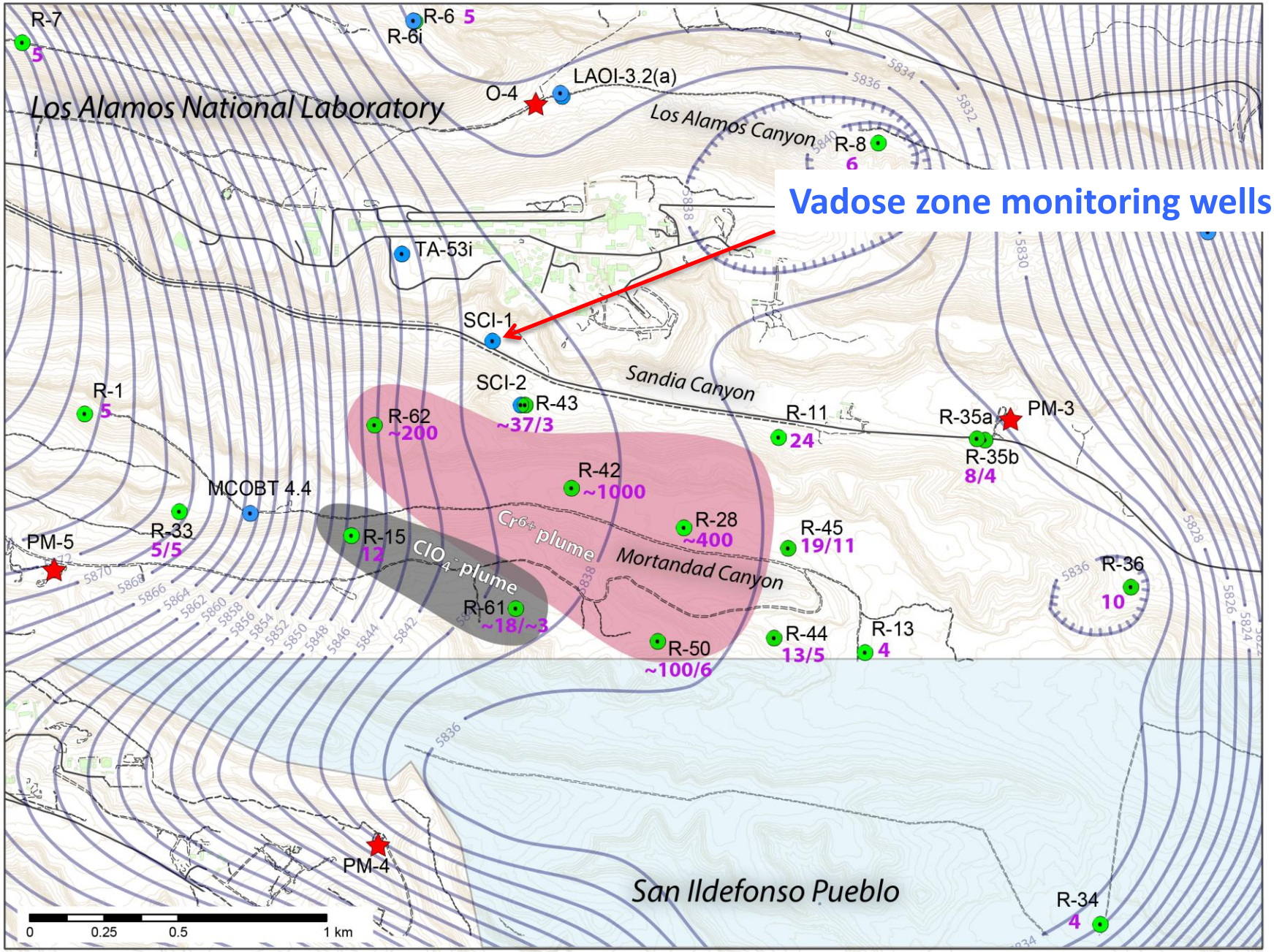
**GOALS**:

- ✧ **provide model-based decision support related to chromium transport in the vadose zone and regional aquifer at LANL**
- ✧ **apply advanced computationally efficient methods for:**
  - ○ **parameter estimation (PE)**
  - ○ **model calibration**
  - ○ **model-based uncertainty quantification (UQ)**
  - ○ **risk analysis (RA), and**
  - ○ **decision support (DS)**
- ✧ **utilize high-performance computing due to high computational demands for model simulations and model analyses**

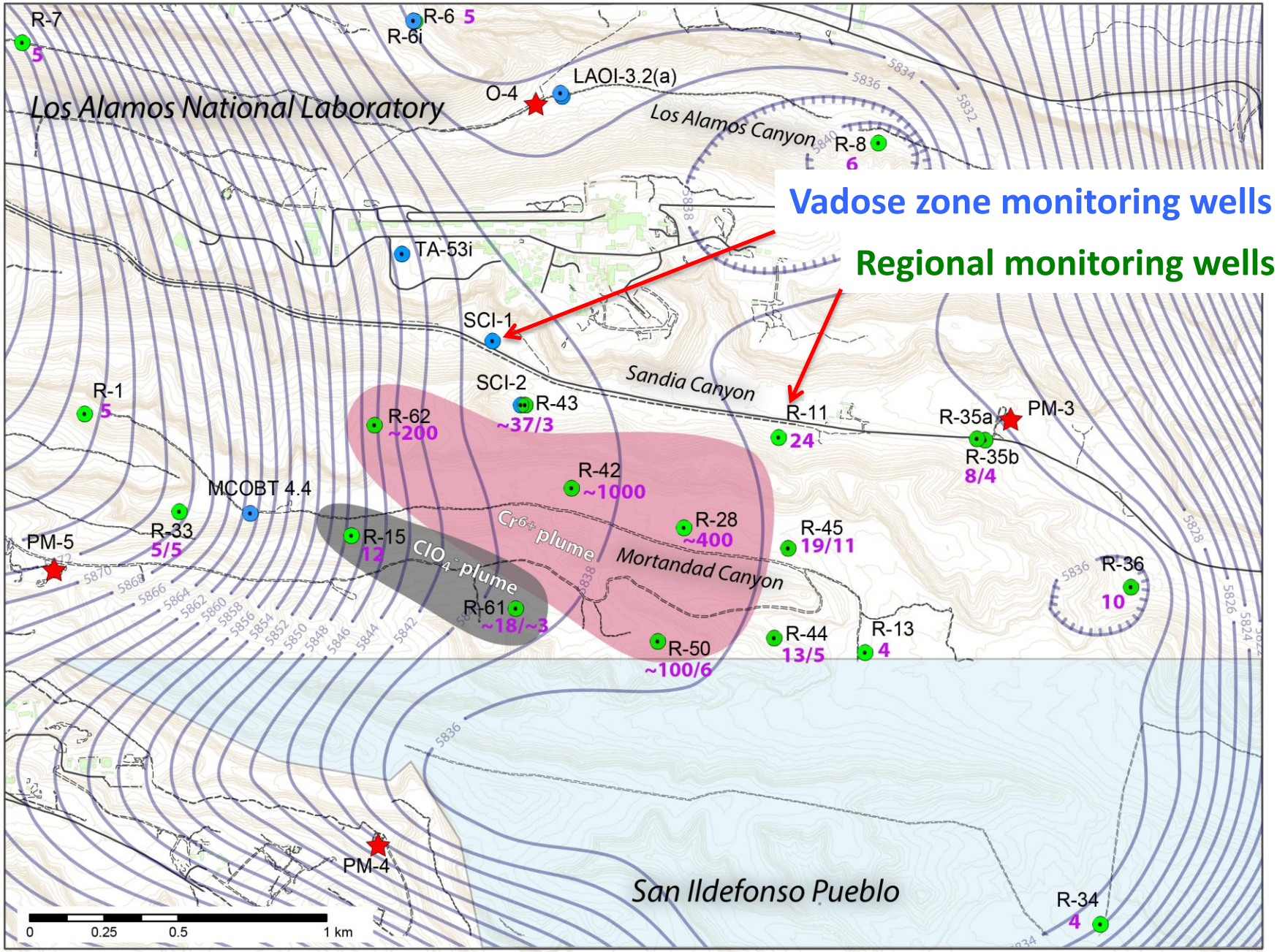
# Chromium plume in the regional aquifer at LANL



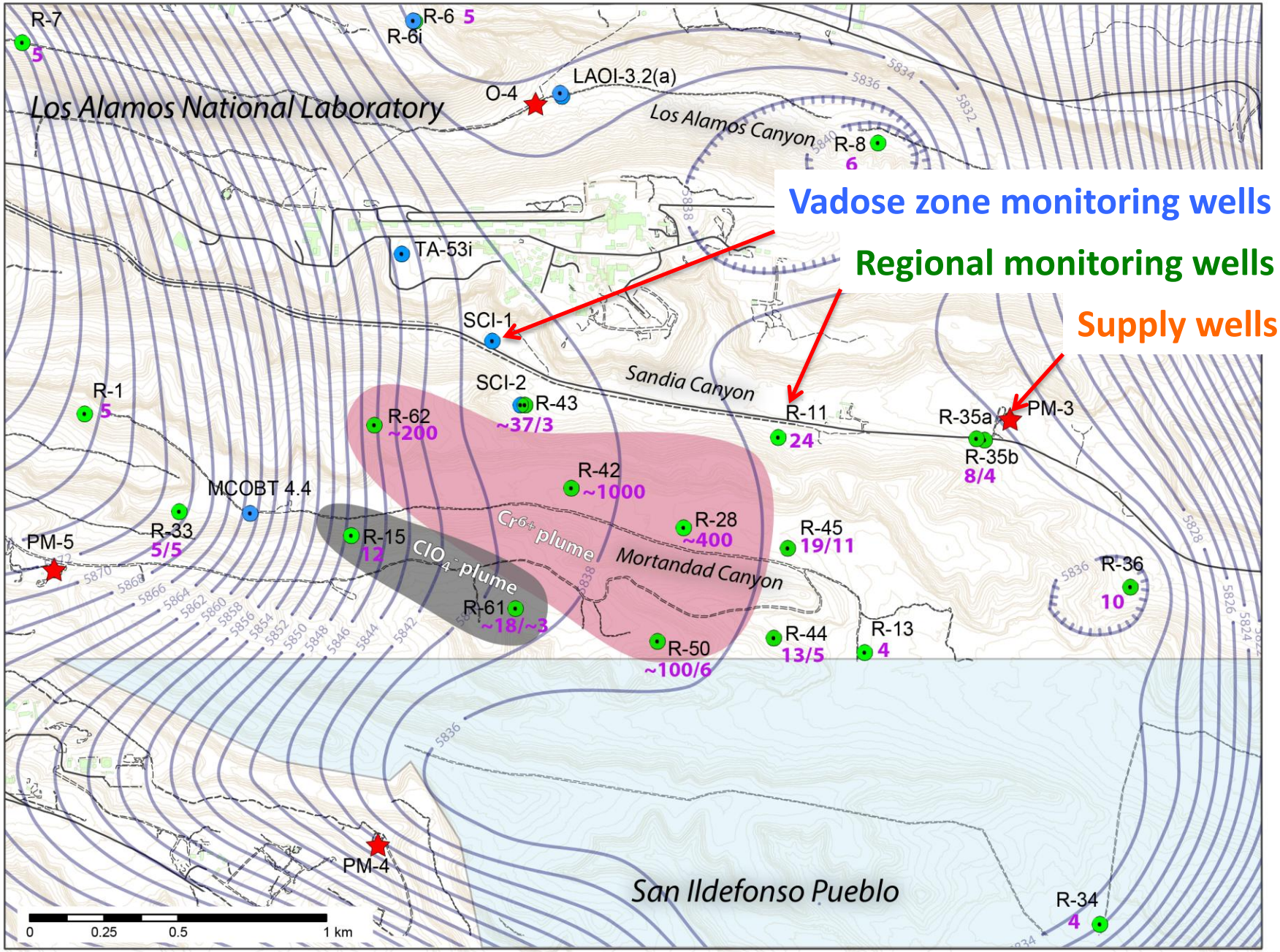
# Chromium plume in the regional aquifer at LANL



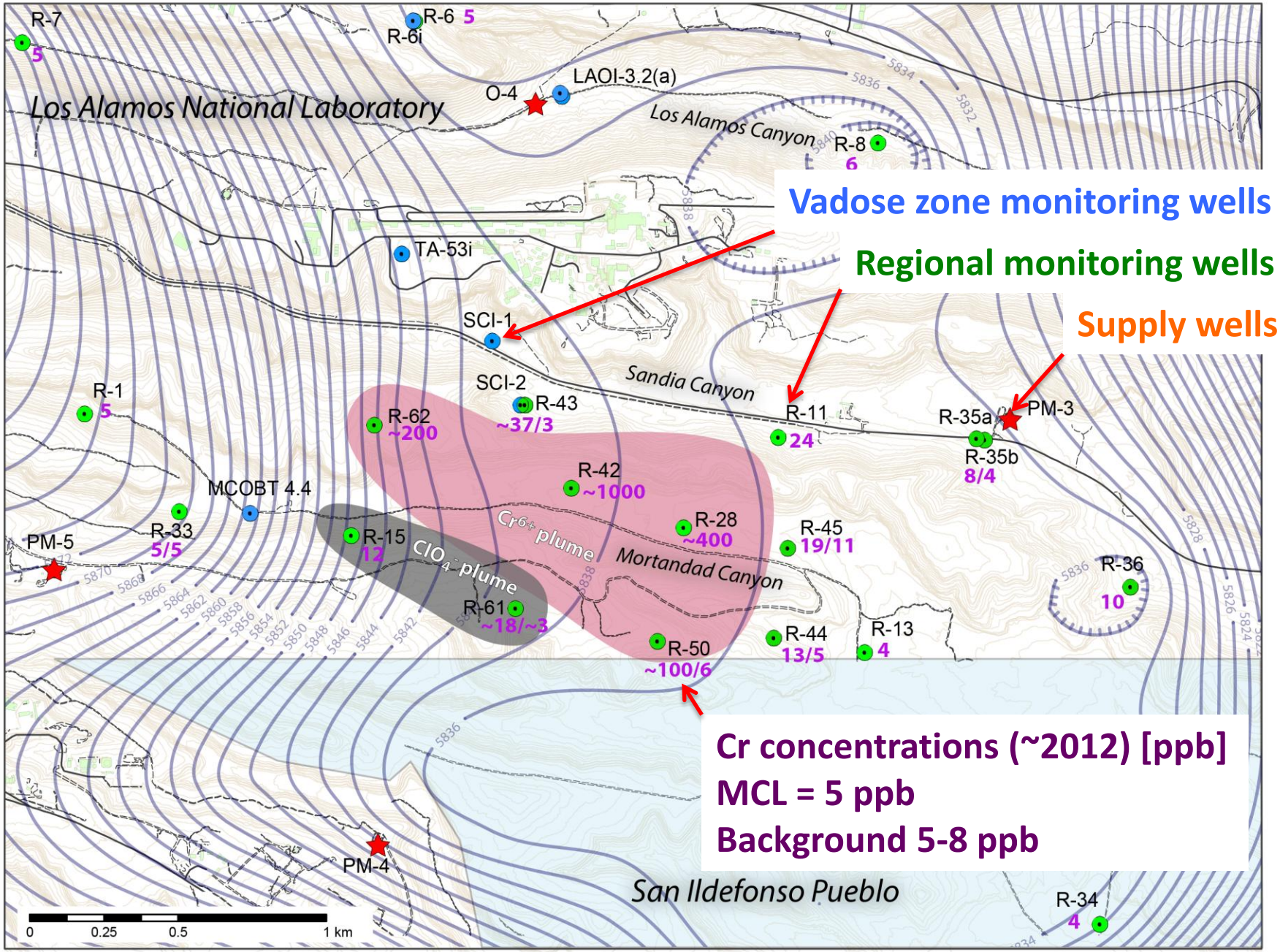
# Chromium plume in the regional aquifer at LANL

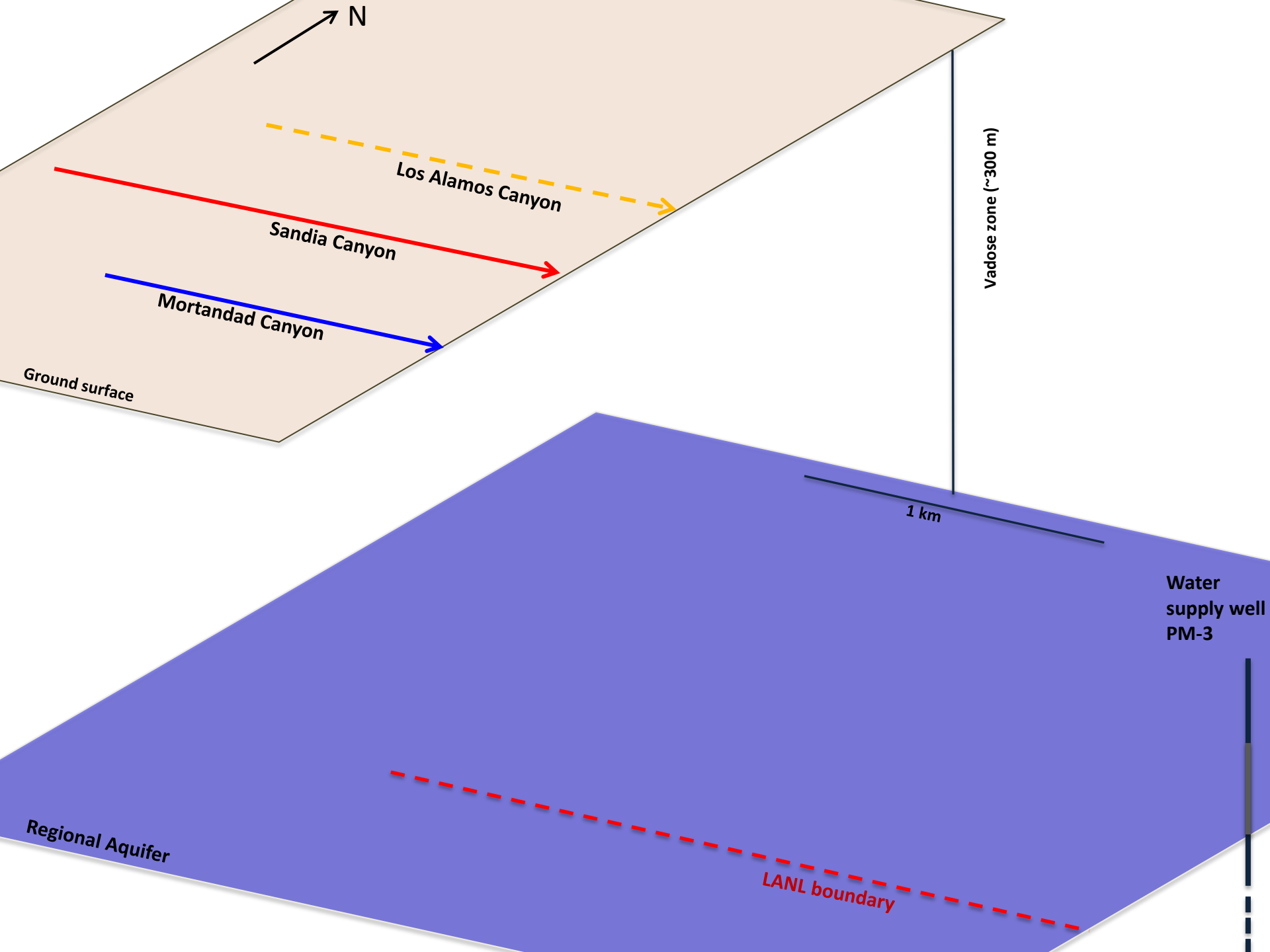


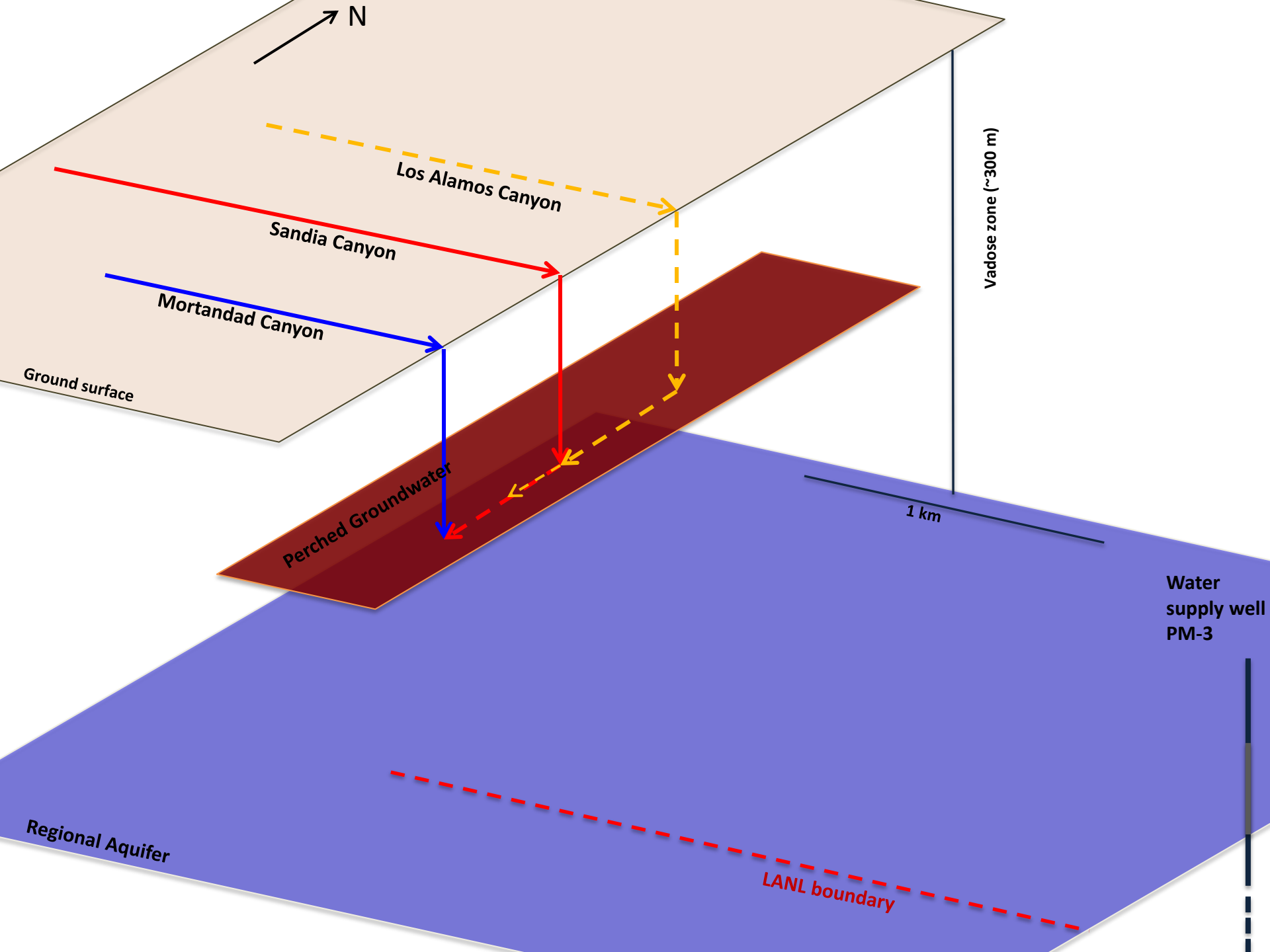
# Chromium plume in the regional aquifer at LANL

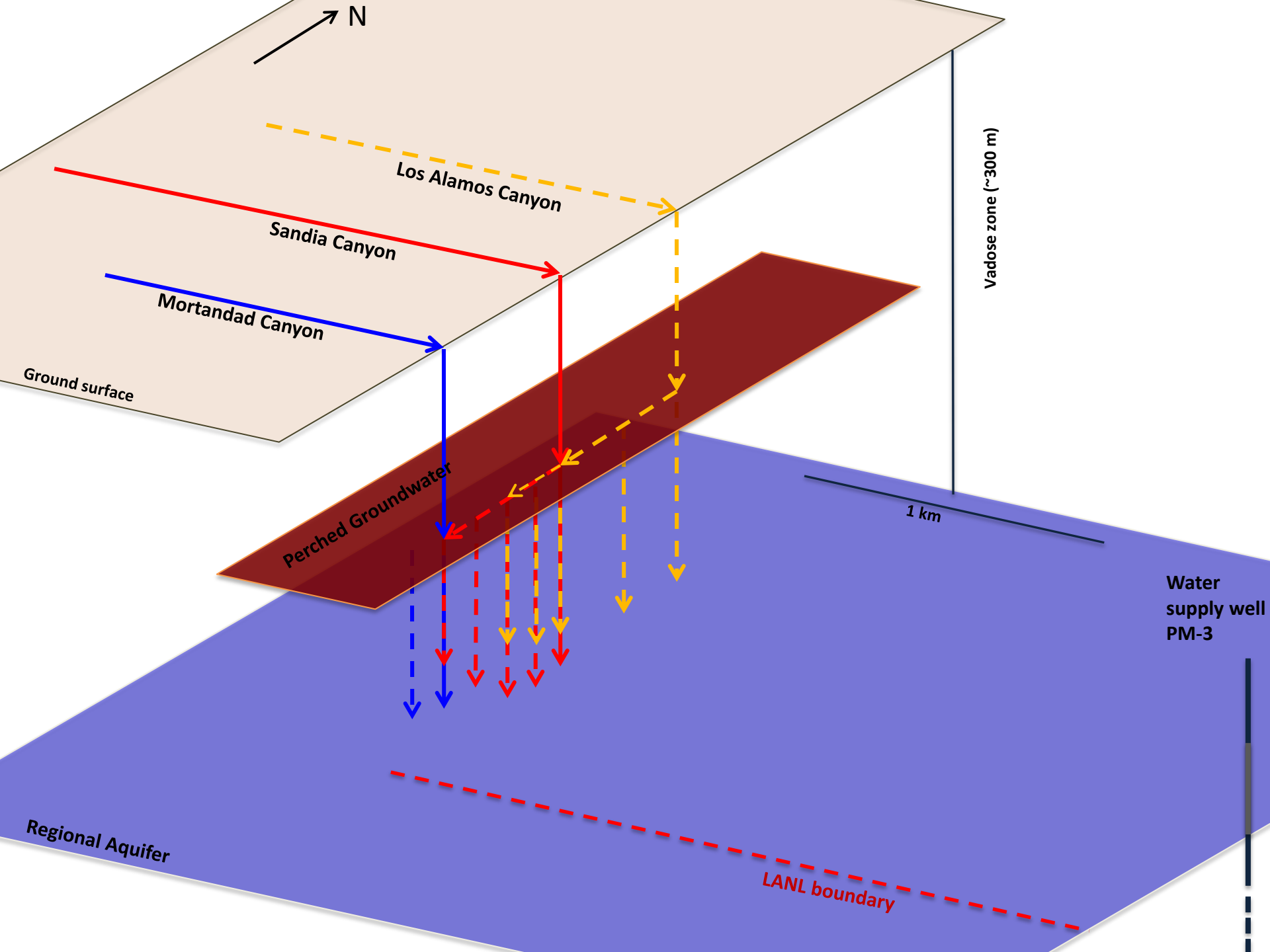


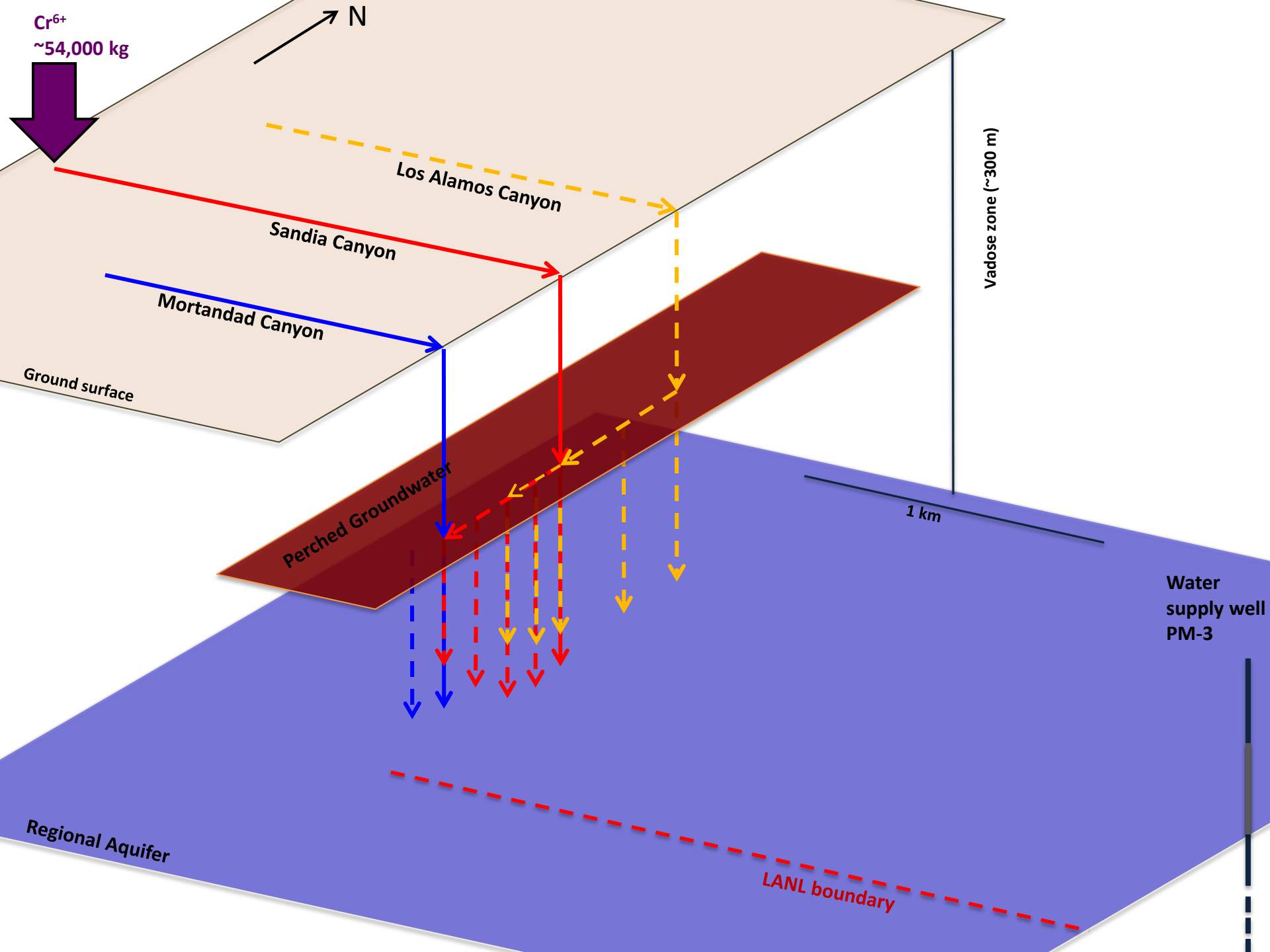
# Chromium plume in the regional aquifer at LANL

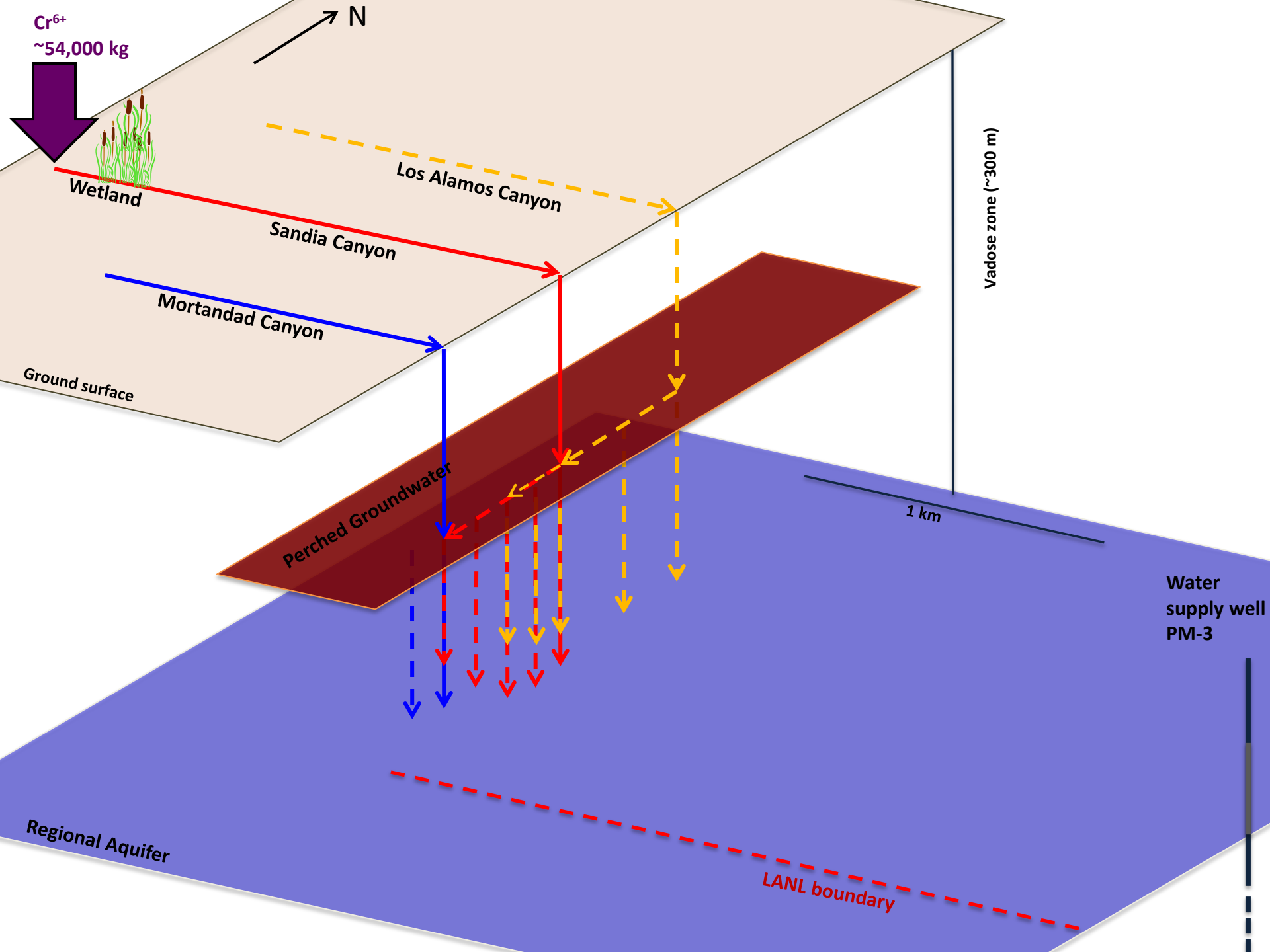


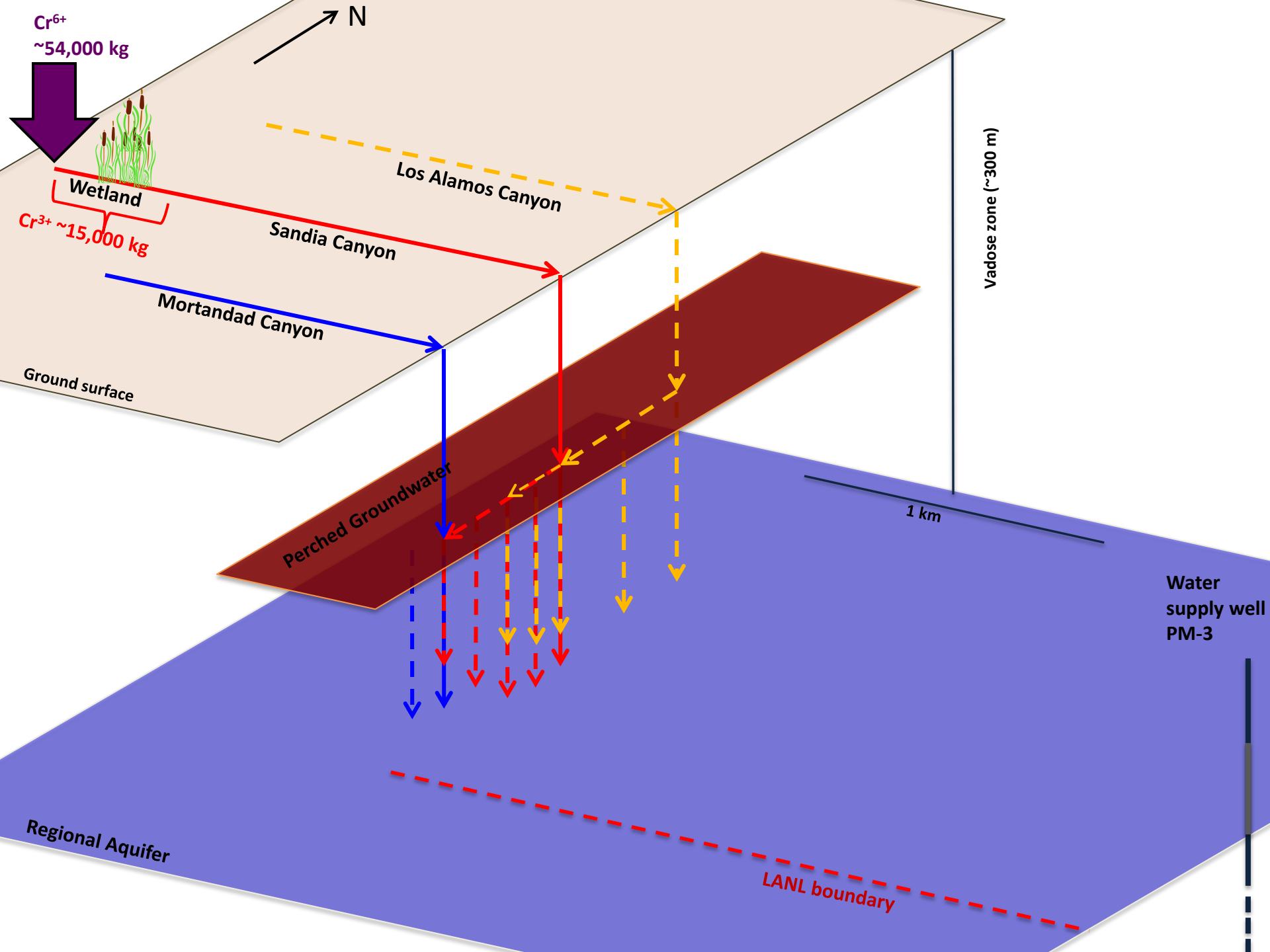

N
Los Alamos Canyon
Sandia Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary

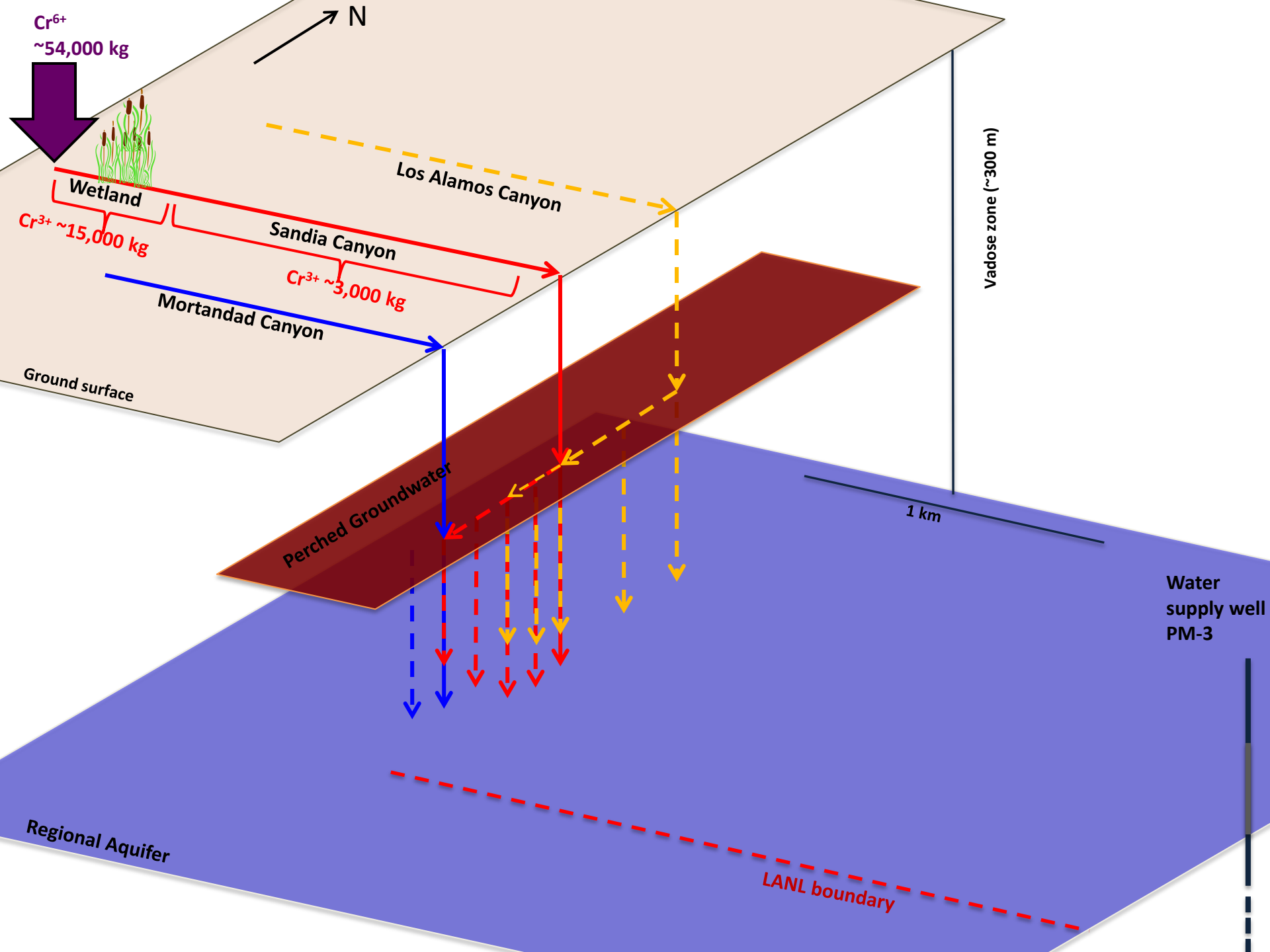

N
Los Alamos Canyon
Sandia Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
Perched Groundwater
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary

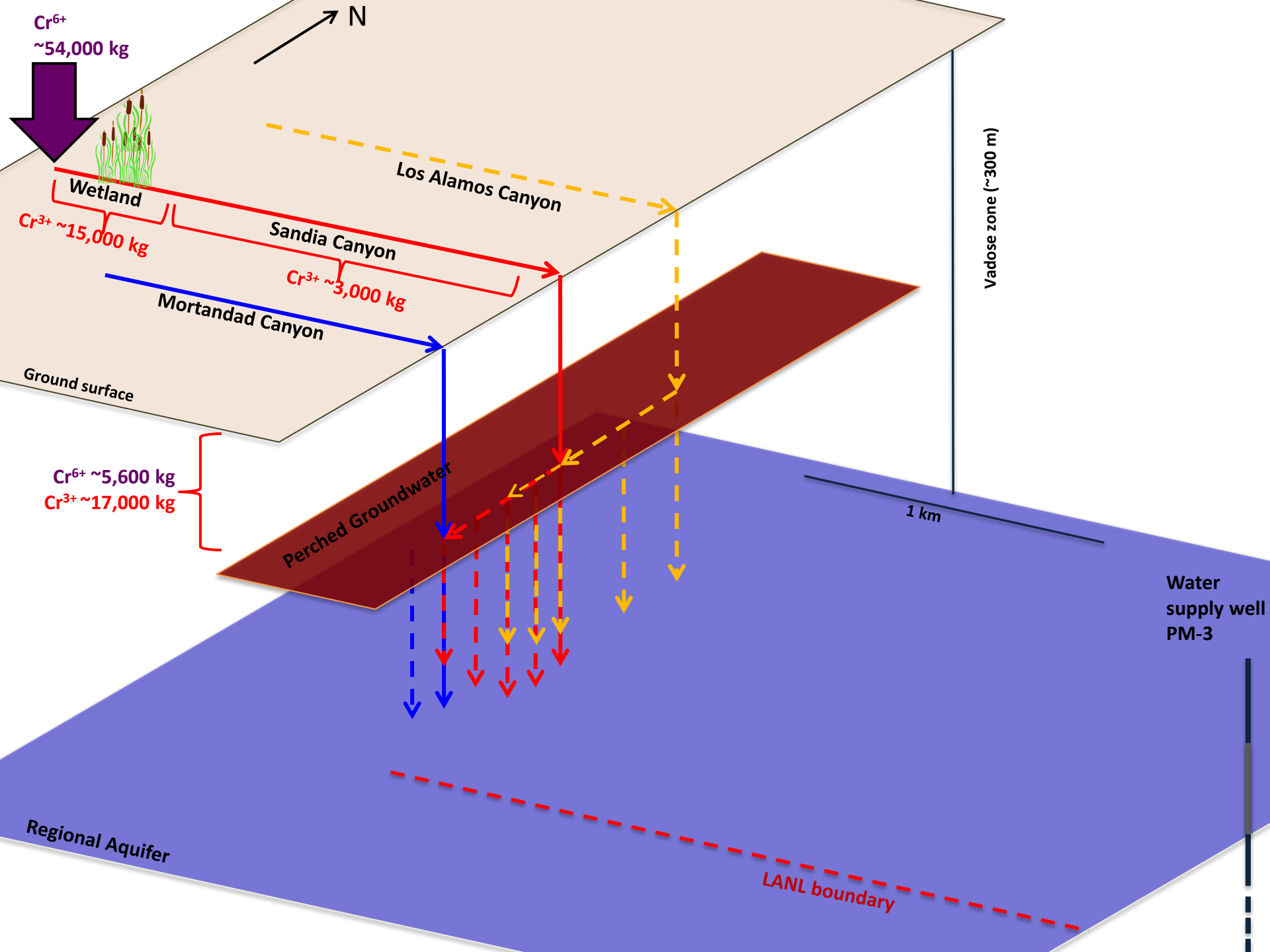

N
Los Alamos Canyon
Sandia Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
Perched Groundwater
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary

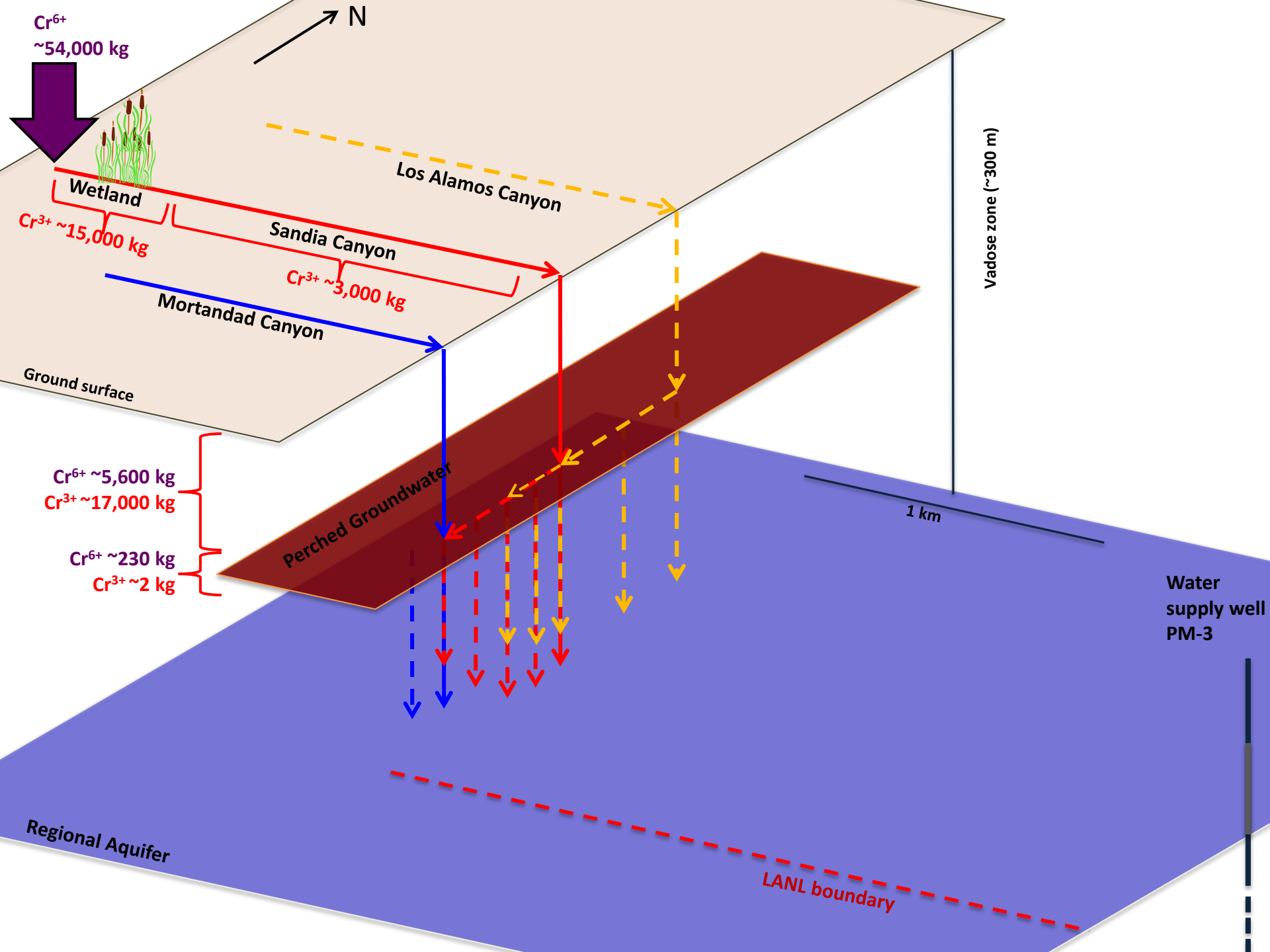

$Cr^{6+}$
~54,000 kg
N
Los Alamos Canyon
Sandia Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
Perched Groundwater
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary

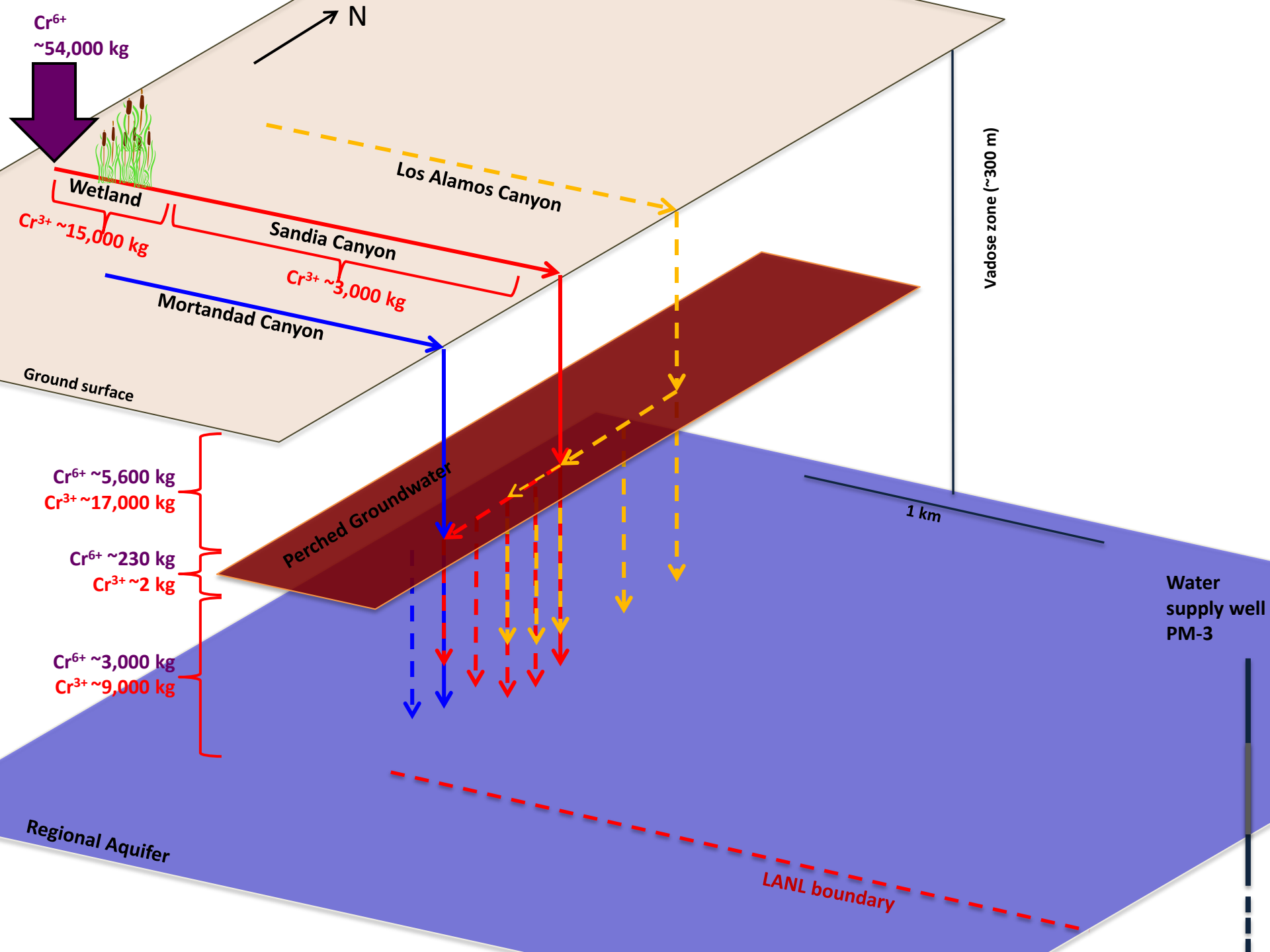

$Cr^{6+}$
~54,000 kg
N
Wetland
Sandia Canyon
Los Alamos Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
Perched Groundwater
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary

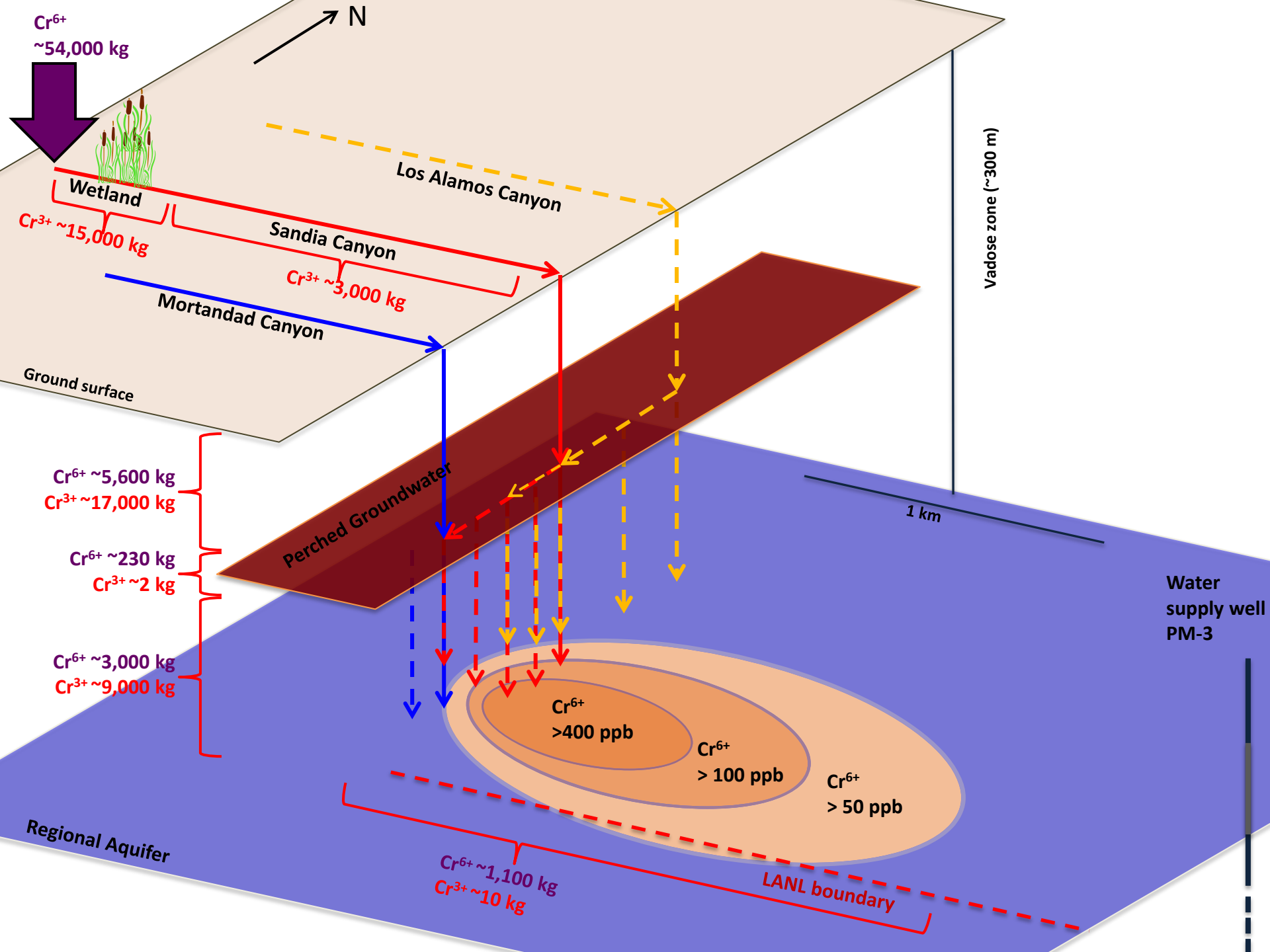

$Cr^{6+}$
~54,000 kg
N
Wetland
$Cr^{3+}$ ~15,000 kg
Sandia Canyon
Los Alamos Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
Perched Groundwater
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary


$Cr^{6+}$
~54,000 kg
N
Wetland
$Cr^{3+}$ ~15,000 kg
Sandia Canyon
$Cr^{3+}$ ~3,000 kg
Mortandad Canyon
Los Alamos Canyon
Ground surface
Vadose zone (~300 m)
Perched Groundwater
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary


Cr6+
~54,000 kg
N
Wetland
Cr3+ ~15,000 kg
Sandia Canyon
Cr3+ ~3,000 kg
Los Alamos Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
Cr6+ ~5,600 kg
Cr3+ ~17,000 kg
Perched Groundwater
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary

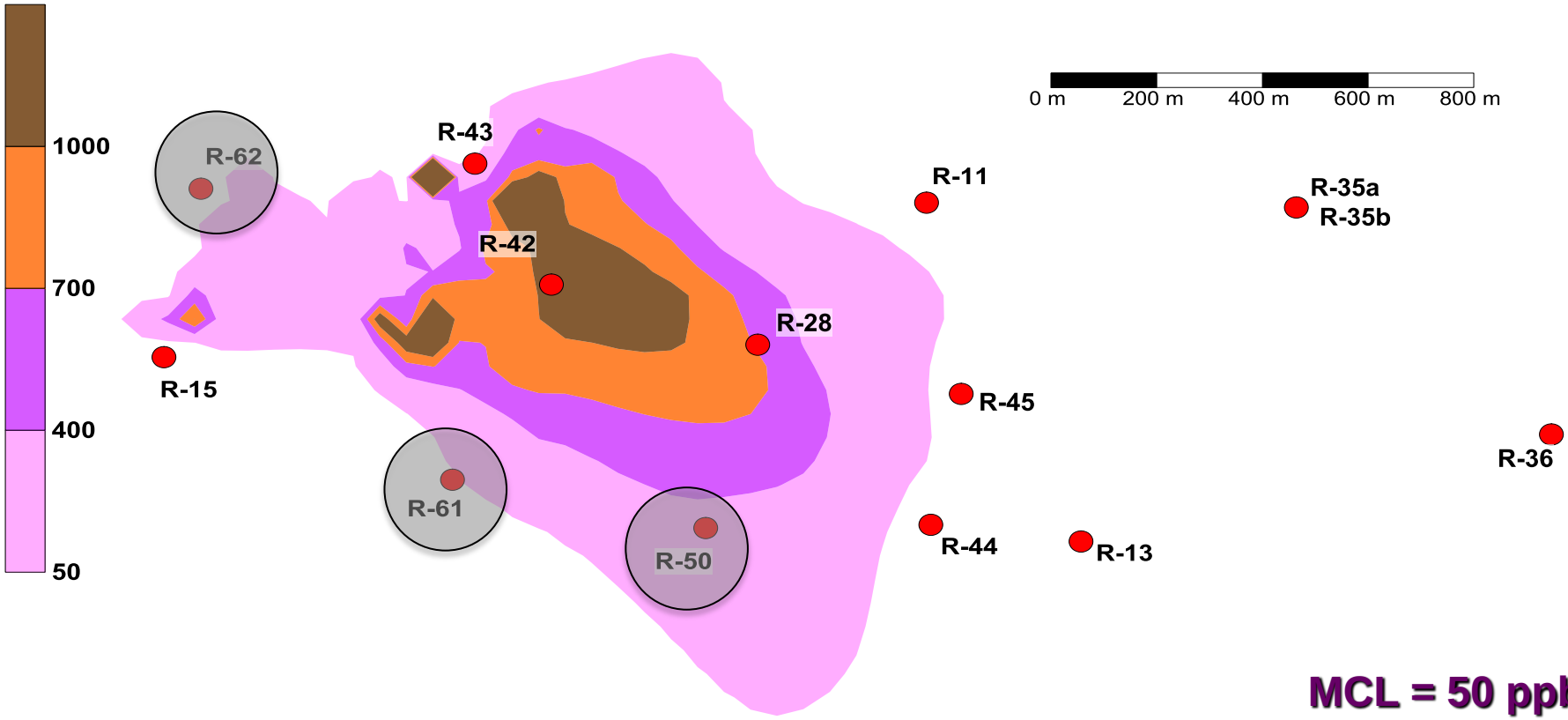

Cr6+
~54,000 kg
N
Wetland
Cr3+ ~15,000 kg
Sandia Canyon
Cr3+ ~3,000 kg
Los Alamos Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
Cr6+ ~5,600 kg
Cr3+ ~17,000 kg
Perched Groundwater
Cr6+ ~230 kg
Cr3+ ~2 kg
1 km
Water
supply well
PM-3
Regional Aquifer
LANL boundary


$Cr^{6+}$
~54,000 kg
N
Wetland
$Cr^{3+}$ ~15,000 kg
Sandia Canyon
$Cr^{3+}$ ~3,000 kg
Mortandad Canyon
Los Alamos Canyon
Ground surface
Vadose zone (~300 m)
$Cr^{6+}$ ~5,600 kg
$Cr^{3+}$ ~17,000 kg
Perched Groundwater
1 km
$Cr^{6+}$ ~230 kg
$Cr^{3+}$ ~2 kg
Water supply well PM-3
$Cr^{6+}$ ~3,000 kg
$Cr^{3+}$ ~9,000 kg
Regional Aquifer
LANL boundary


Cr6+
~54,000 kg
N
Wetland
Cr3+ ~15,000 kg
Sandia Canyon
Cr3+ ~3,000 kg
Los Alamos Canyon
Mortandad Canyon
Ground surface
Vadose zone (~300 m)
Perched Groundwater
1 km
Cr6+ ~5,600 kg
Cr3+ ~17,000 kg
Cr6+ ~230 kg
Cr3+ ~2 kg
Cr6+ ~3,000 kg
Cr3+ ~9,000 kg
Water
supply well
PM-3
Cr6+
>400 ppb
Cr6+
> 100 ppb
Cr6+
> 50 ppb
Regional Aquifer
Cr6+ ~1,100 kg
Cr3+ ~10 kg
LANL boundary

# 2009 model estimate of the plausible contaminant concentrations [ppb] along the regional aquifer water table

- Wells R-62, R-61 and R-50 were not drilled yet
- Locations of wells R-62, R-61 and R-50 were optimized based on model analyses
- Observed concentrations at R-62, R-61 and R-50 confirmed model predictions
- R-43 concentration were at background when the analyses were performed
- Since 2010, R-43 concentrations are increasing and approaching the model predicted concentration




MCL = 50 ppb

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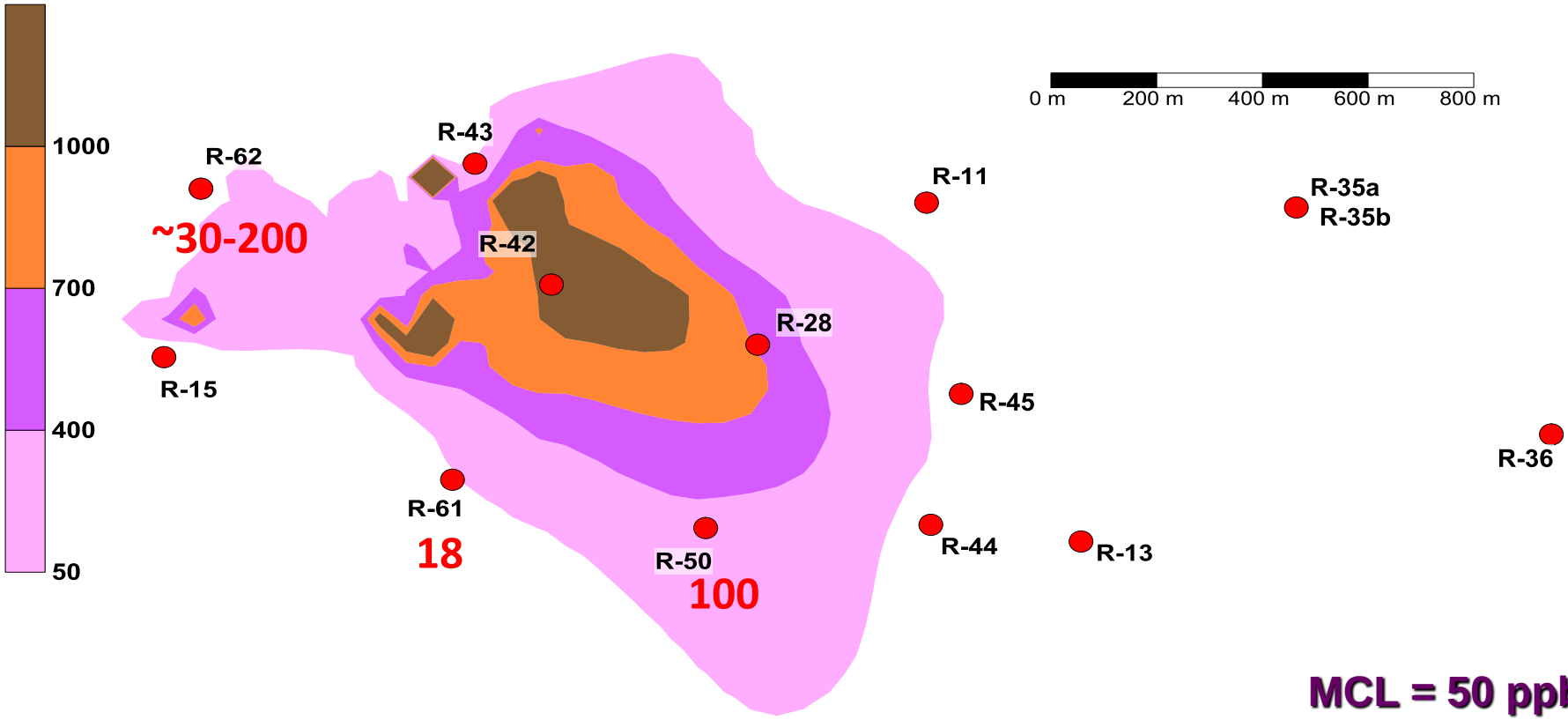

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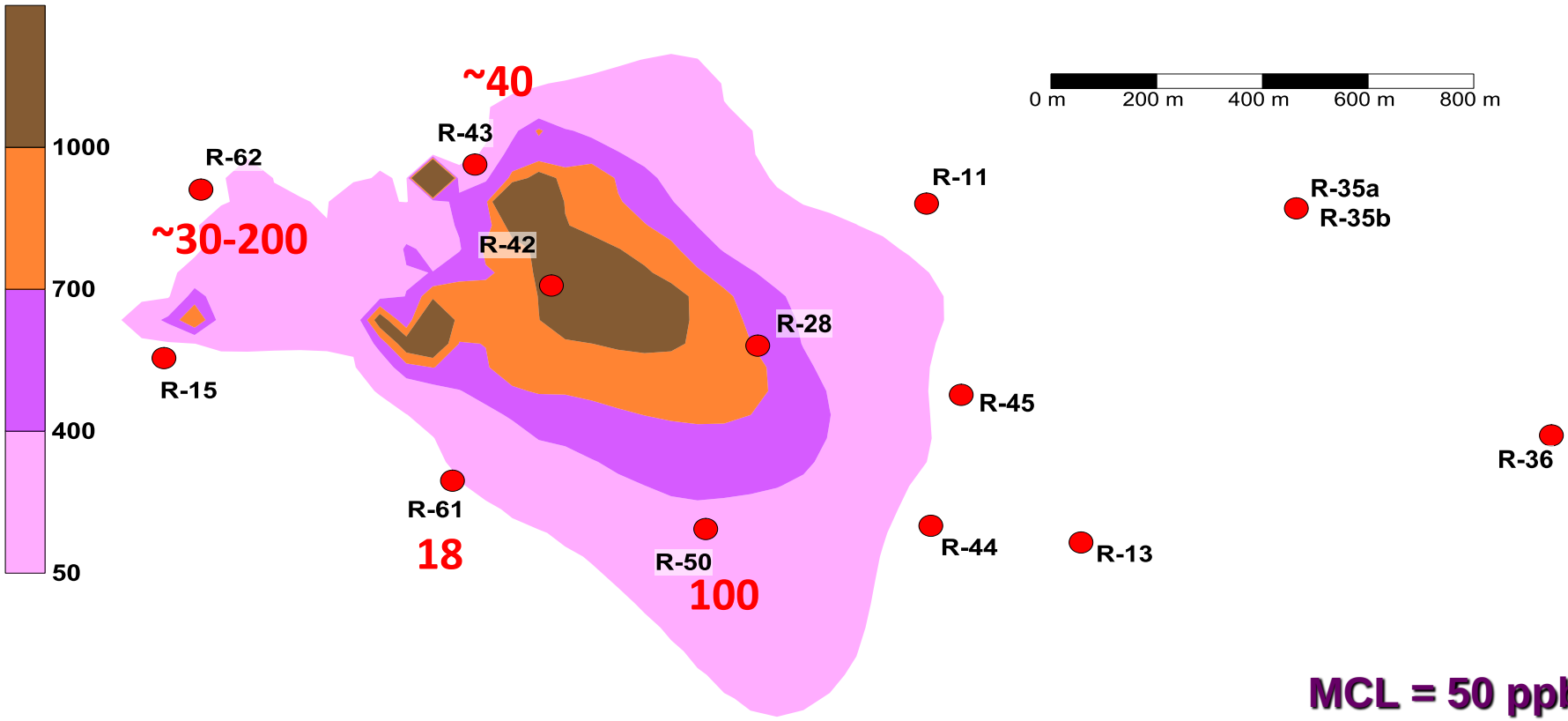
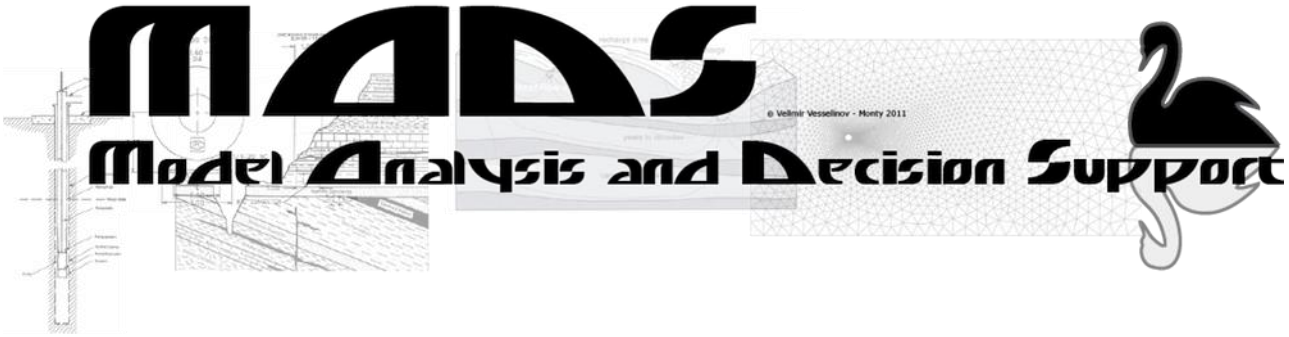



MCL = 50 ppb




**MADS is applied to perform all the presented info-gap decision analyses …**

# MADS
## Model Analysis and Decision Support


Los Alamos NATIONAL LABORATORY

SEREN DIP ITY

- an open-source high-performance computational framework for analyses and decision support based on complex process models
- advanced adaptive computational techniques:
  - sensitivity analysis (local / global);
  - uncertainty quantification (local / global);
  - optimization / calibration / parameter estimation (local / global);
  - model ranking & selection
  - decision support (GLUE, info-gap)
- novel algorithms
  - Agent-Based Adaptive Global Uncertainty and Sensitivity (ABAGUS)
    Harp & Vesselinov (2012) An agent-based approach to global uncertainty and sensitivity analysis. *Computers & Geosciences*.
  - Adaptive hybrid (local/global) optimization strategy (Squads)
    Vesselinov & Harp (2012) Adaptive hybrid optimization strategy for calibration and parameter estimation of physical process models. *Computers & Geosciences*.
- internal coupling with analytical contaminant transport solvers and test problems
- external coupling with existing process simulators (ModFlow, TOUGH, FEHM, eSTOMP, Amanzi, …)
- Source code, examples, performance comparisons, and tutorials @ http://mads.lanl.gov

# ASCEM Advanced Subsurface Computing for Environmental Management

**Regulatory**
Public Interface
Reviews
Decision Making

**Programmatic**
Project Management
Oversight
Decision Making

**Scientific**
Model Setup and Execution
Model Analyses
Decision Support

- an open-source interactive decision support system (Akuna/Agni) coupled a process simulator (Amanzi)
- high-performance computing (HPC)
- data- and model-driven decision support to provide standardized, consistent, site-specific and scientifically defensible decision analyses across DOE-EM complex
- **Challenge:**
  - develop tools to make better use of complex information and capabilities to explore problems in greater detail
  - address the most challenging performance assessment and waste-disposal problems
- **Impact:**
  - provide technical underpinnings for current U.S. DOE-EM risk and performance assessments
  - inform strategic data collection for model improvement and decision support
  - support scientifically defensible and standardized assessments and remedy selections

http://ascemdoe.org

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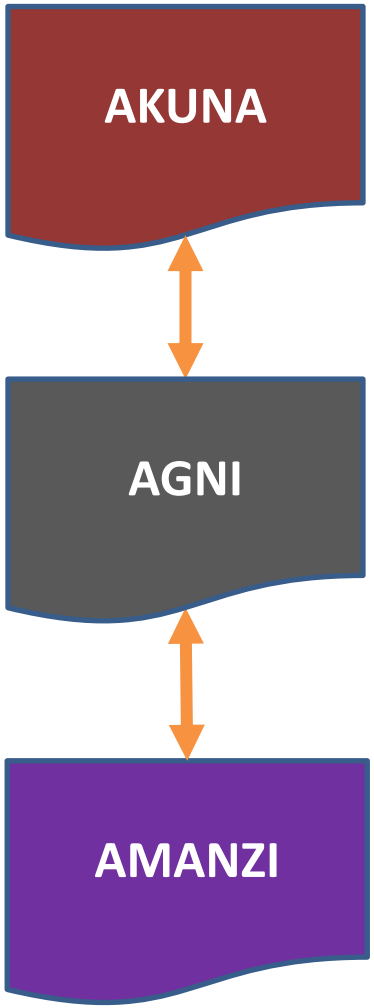
# ASCEM Modules




**Akuna ("no worries"): Graphic User Interface**
(**Karen Schuchardt**, *PNNL*)

- Open Source Eclipse/Java based
- Incorporates data management, visualization, and model development tools

**Agni ("fire"): Simulation controller and Toolset driver**
(**George Pau**, *LBNL*, **Velimir Vesselinov**, *LANL*)

- Open Source C++ object oriented
- Provides coupling between **Akuna** and **Amanzi**
- Performs various model-based analyses (SA, UQ, PE, DS, … )

**Amanzi ("water"): HPC Flow and Transport Simulator**
(**David Moulton**, *LANL*)

- Open Source C++ object oriented
- Saturated / unsaturated groundwater flow, …
- Structured / unstructured / adaptive gridding
- …

# ASCEM Model-Analysis Toolsets in Agni

- **Sensitivity Analysis (SA)** (*Stefan Finsterle*, *Elizabeth Keating*)
- **Parameter Estimation (PE)** (*Stefan Finsterle*, *LBNL*)
- **Uncertainty Quantification (UQ)** (*Elizabeth Keating*, *LANL*)
- **Risk Assessment (RA)** (*Wilson McGinn*, *ORNL*)
- **Decision Support (DS)** (*Velimir Vesselinov*, *LANL*)

# Conclusions and recommendations:

- Both Non-Probabilistic and Probabilistic uncertainties often exist in a decision problem
- Non-Probabilistic and Probabilistic methods should be applied to their appropriate uncertainties in the decision analyses
- In the case of probabilistic methods, definition of prior probability distributions for model parameters or calibration targets with unknown/uncertain distribution can produce biased predictions and decision analyses
- In the case of non-probabilistic methods, lack of knowledge and severe uncertainties can be captured
- Non-probabilistic methodologies have been successfully applied for a series of synthetic and real-world problems, though less often in hydrology
  - Remediation of unknown contaminant source
    Harp & Vesselinov (2011). *Contaminant remediation decision analysis using information gap theory*. SERRA
- MADS provides a computationally efficient framework for decision analyses using non-probabilistic and probabilistic methods ( http://mads.lanl.gov )
- ASCEM tools are currently actively developed and will become available for testing and benchmarking in 2013 ( http://ascemdoe.org )


SERENDIPITY
MADS
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