

Data and Model-Driven Decision Support for Environmental Management of a Chromium Plume at Los Alamos National Laboratory (LANL)

- 13264

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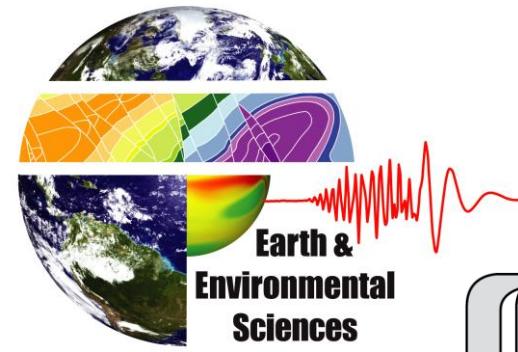
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Outline

- ✧ Model-based Decision Support
- ✧ Deterministic, Probabilistic **vs** Non-Probabilistic Decision Methods
- ✧ Information Gap (**info-gap**) Decision Theory
- ✧ Decision Support for Chromium contamination site @ LANL
 - Site conceptual model
 - Model-based decision analyses
 - Monitoring network design
 - Additional activities related to contaminant remediation

✧ **MADS: Model Analyses & Decision Support**
Open source computational framework
<http://mads.lanl.gov>



✧ **Decision Support in ASCEM (Advanced Subsurface Computing for Environmental Management)** | <http://ascemdoe.org>



Model-based Decision Support

- ✧ provides decision makers with **model analysis of decision scenarios**:
evaluation, ranking and optimization of alternative **decision scenarios**
- ✧ takes into account site data and knowledge including existing uncertainties
(uncertainties in conceptualization, model parameters, and model predictions)
- ✧ Decision metric(s): e.g. contaminant concentration or environmental risk at a point of compliance, etc.
- ✧ Decision goal(s): e.g. no exceedance of MCL's, dose limits, or risk levels at compliance points
- ✧ Decision scenarios: combinations of predefined activities to achieve the decision goal(s)

Model-based 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 vs. Nature

Important:

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

Decision Methods

- ❖ Deterministic methods (“traditional” performance assessment): a single model simulation representing worst-case or expected (“best” estimated) system behavior

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Decision Methods

- ✧ **Deterministic methods (“traditional” performance assessment):** a single model simulation representing **worst-case or expected (“best” estimated) system behavior**
- ✧ **Probabilistic methods (Bayesian techniques, GoldSim):** analyses based on a series of model simulations **capturing expected probabilistic uncertainties (Monte Carlo, Markov Chain Monte Carlo, Null Space Monte Carlo, etc.)**
- ✧ **Non-probabilistic methods:** analyses based on a series of model simulations representing **unknown uncertainties (Minimax/Maximin Theory, Information Gap Decision Theory, etc.)**

Non-Probabilistic Decision Methods

- ✧ Lack of knowledge or information precludes decision analyses requiring probabilistic distributions (e.g. Bayesian approaches)
 - probability distributions cannot be defined (!)
 - uniform distributions frequently applied instead (causing biased decision analyses)
- ✧ Severe uncertainties can have important impact in the decision analyses
 - heavy tails: non-Gaussian distributions will infinite variances
 - black swans: low probability events in distribution tails with significant decision impacts
 - dragon kings: unexpected high probability events in the distribution tails
- ✧ Non-probabilistic decision methods can be applied to effectively incorporate lack of knowledge and severe uncertainties in decision making process
- ✧ 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)

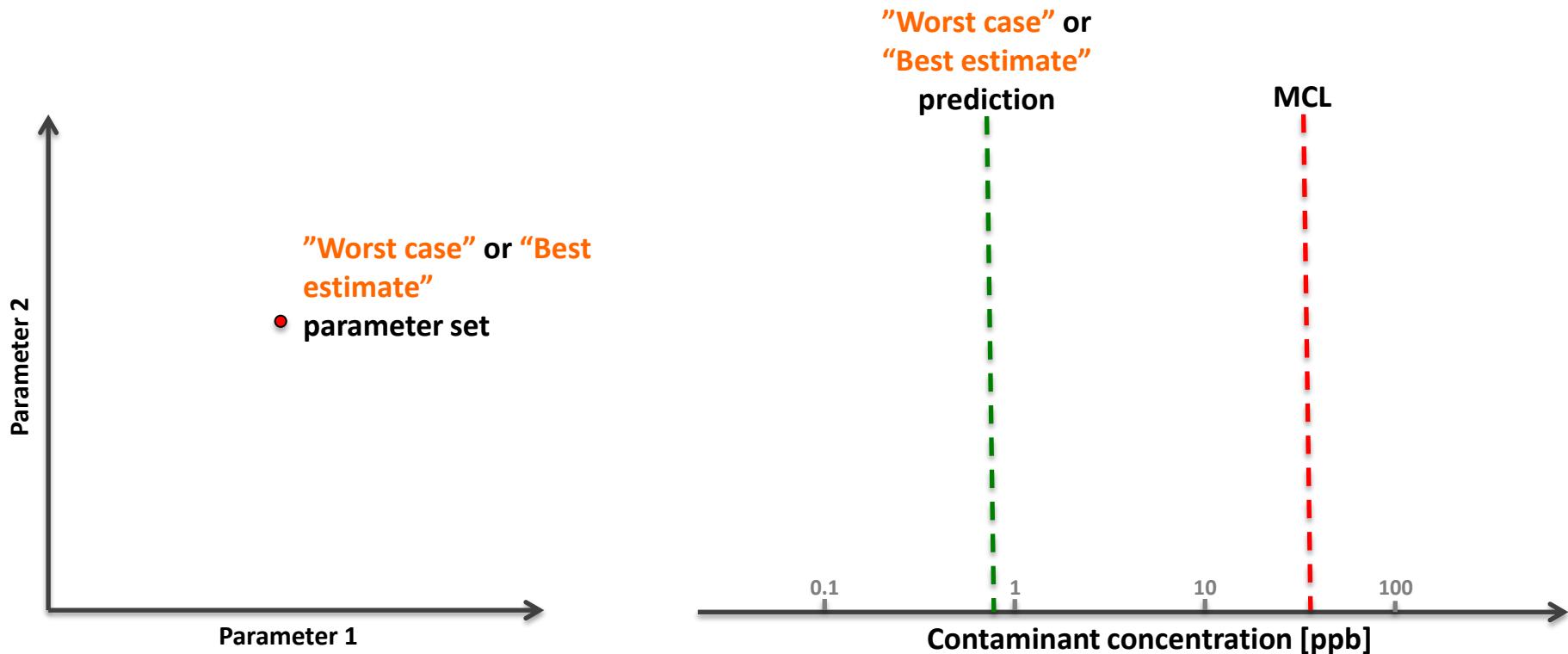
Information Gap Decision Theory

- ✧ Non-probabilistic methodology for comparison of alternative decision scenarios
 - ✧ Decision uncertainty is bounded by robustness and opportuness functions
 - ✧ Robustness function (immunity to failure)
 - ✧ Opportuness function (immunity to windfall)
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- ✧ Information Gap Decision Theory @ <http://mads.lanl.gov>

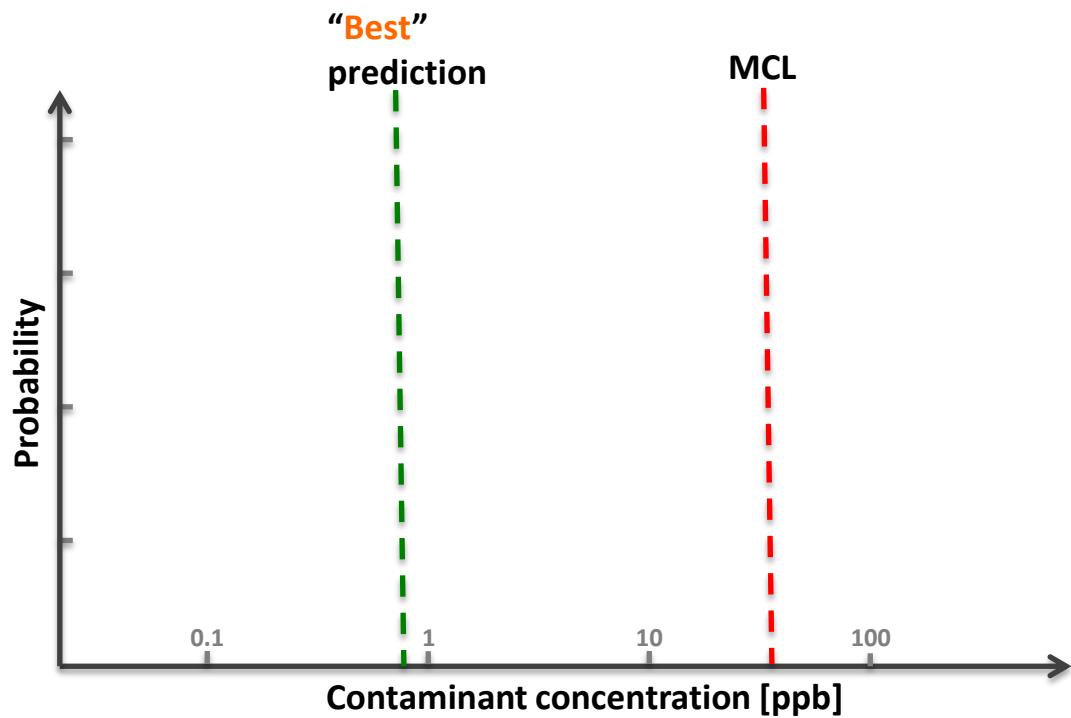
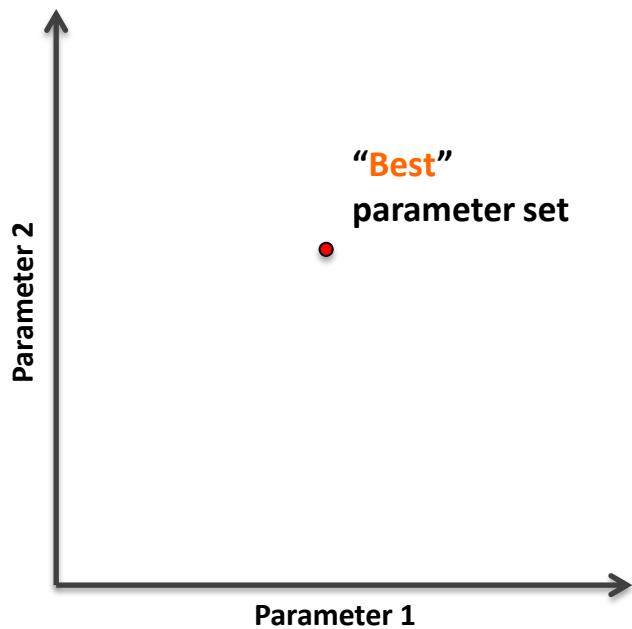
Example analyses:

- Deterministic
- Probabilistic (Bayesian)
- Non-probabilistic (Info-Gap)

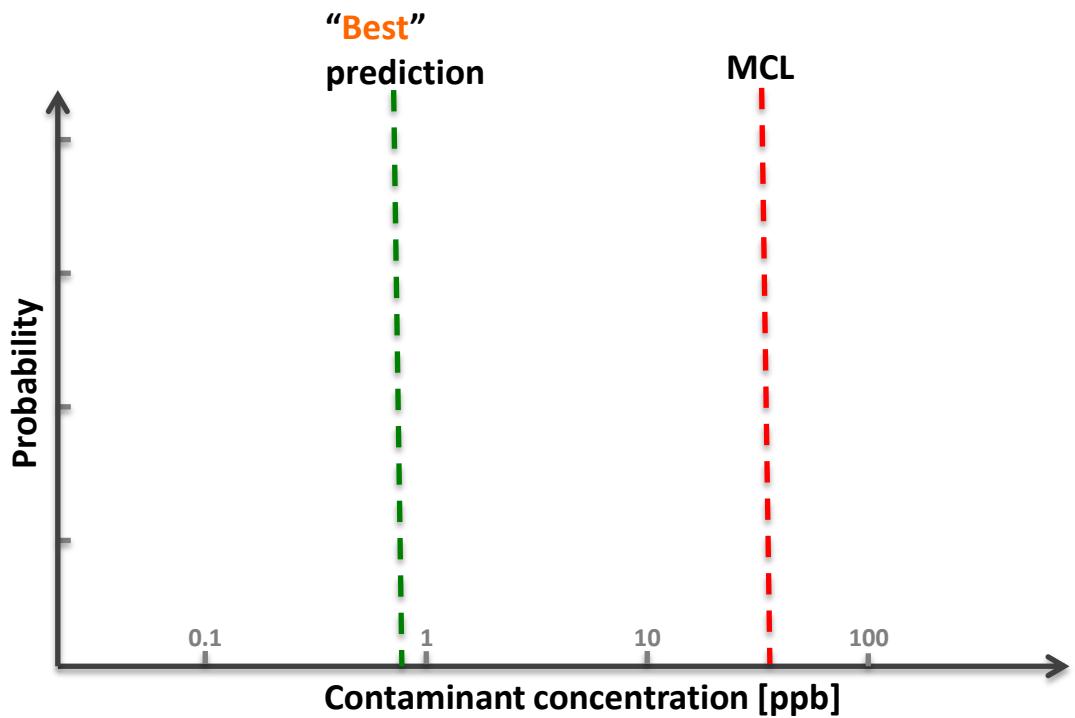
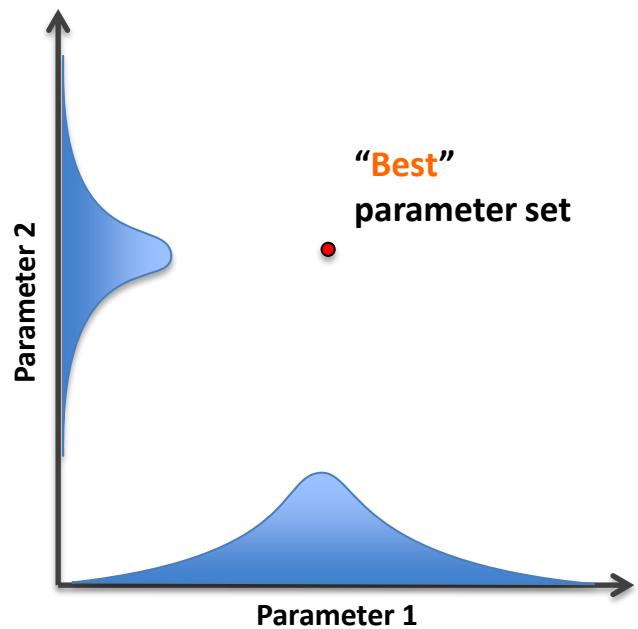
Deterministic analysis



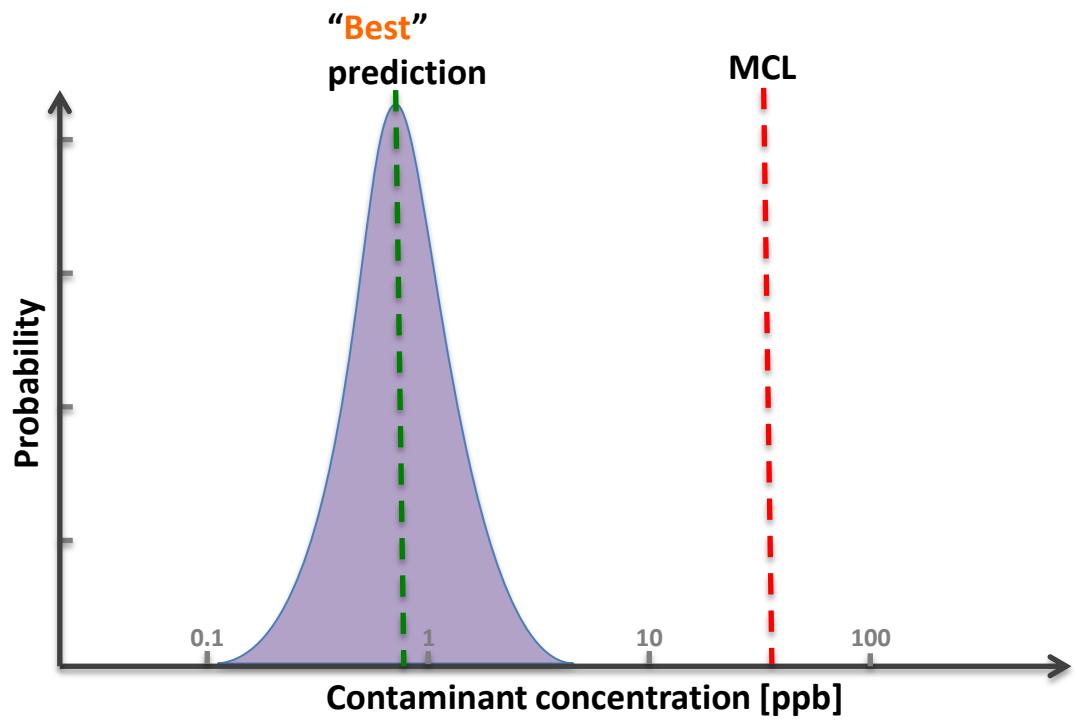
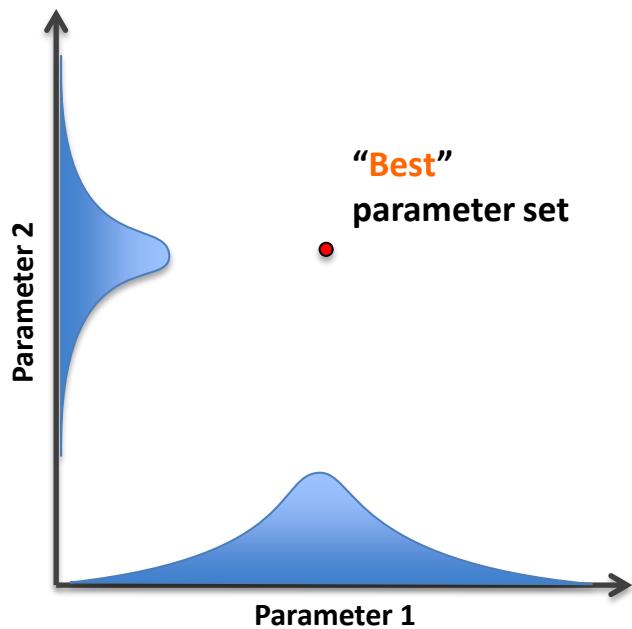
Bayesian (probabilistic) analysis



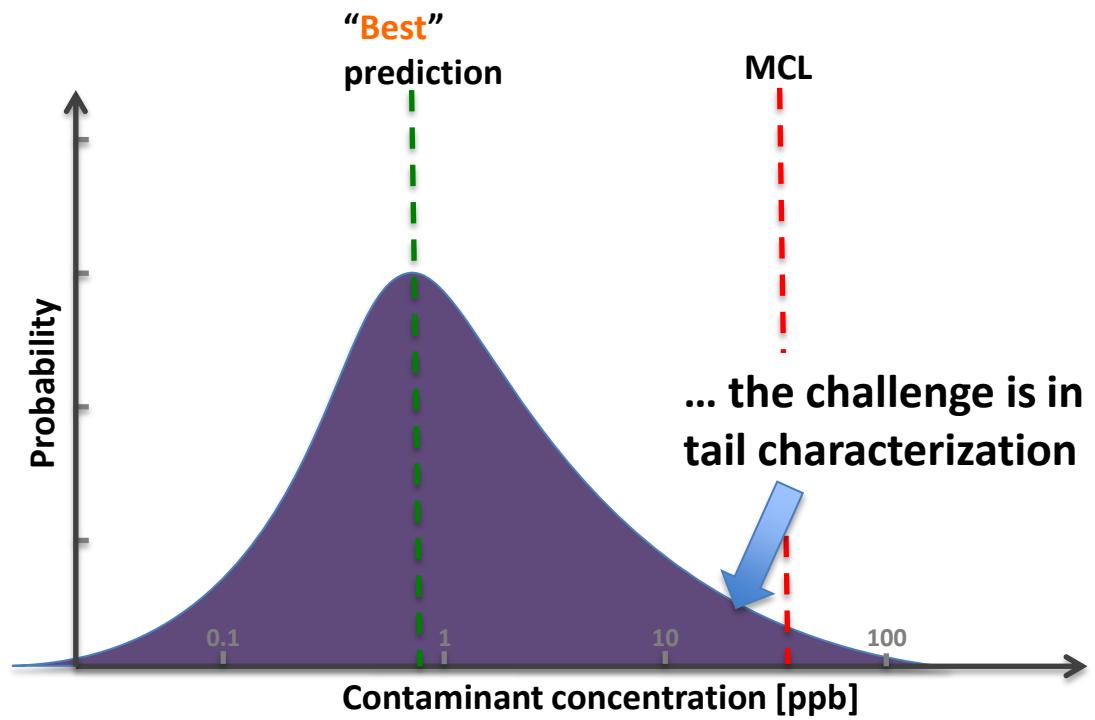
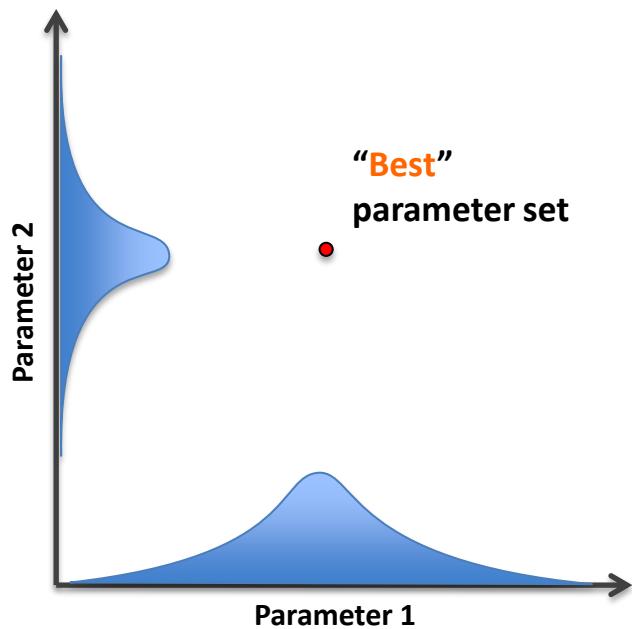
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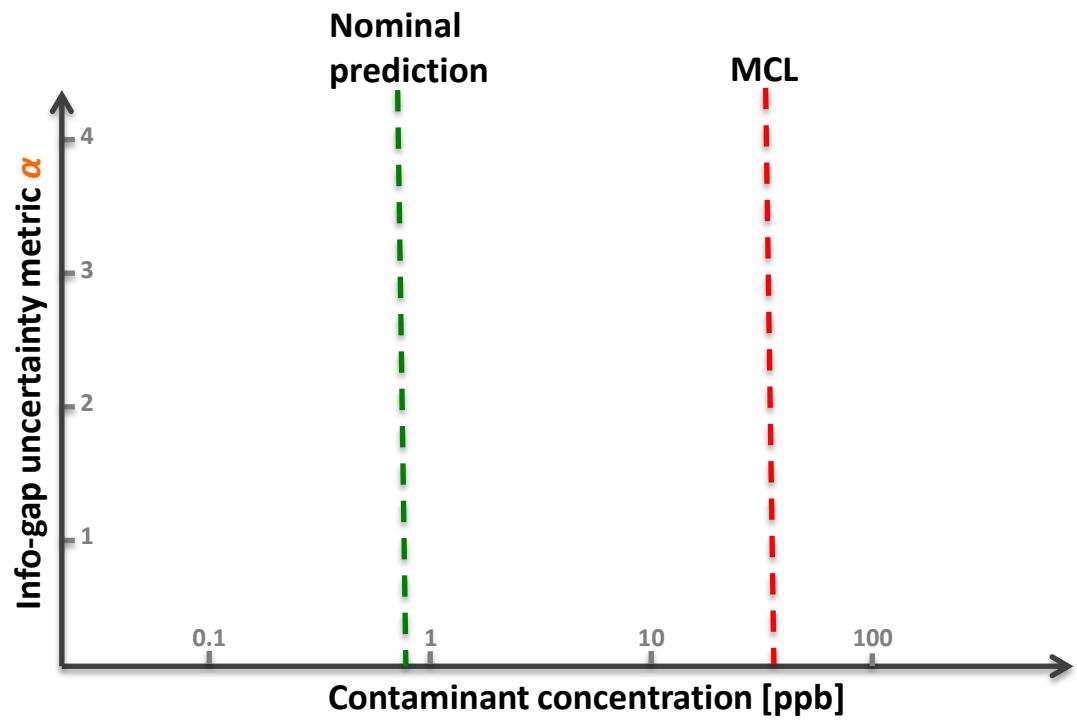
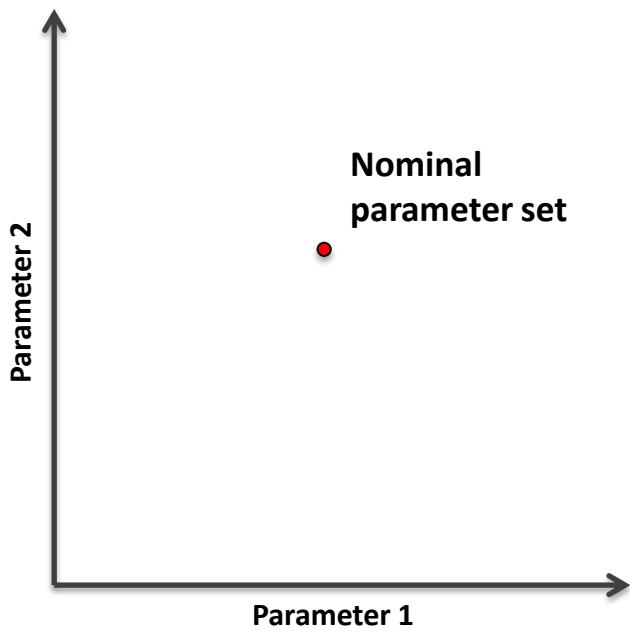
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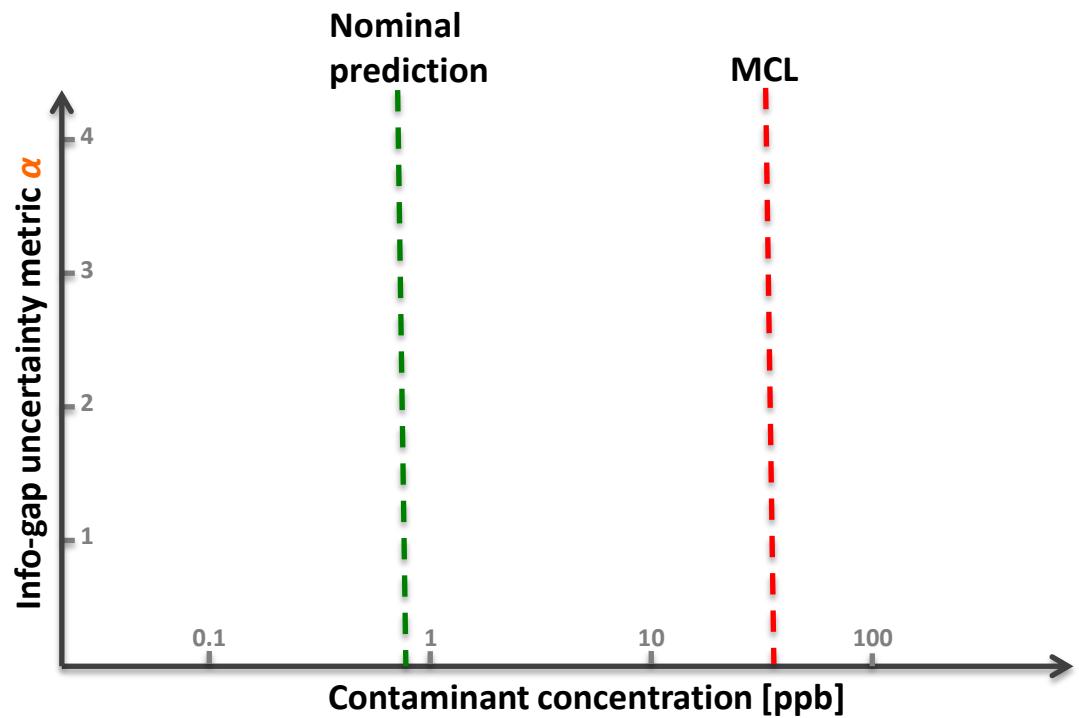
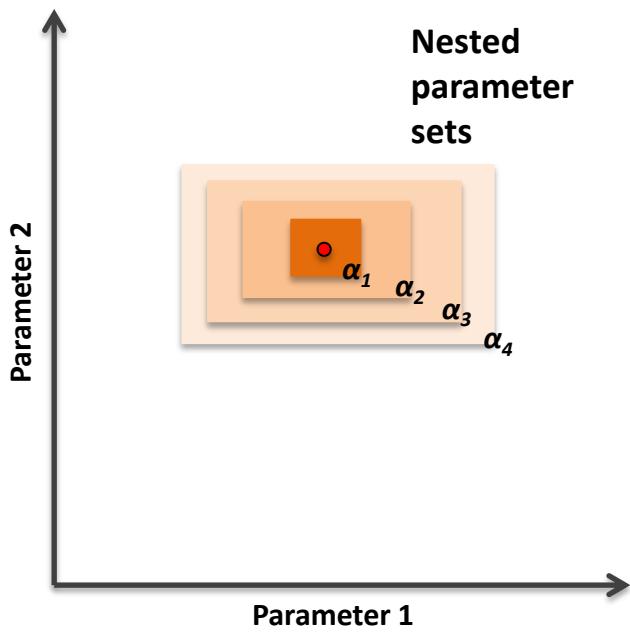
Bayesian (probabilistic) analysis



Info-Gap (non-probabilistic) analysis



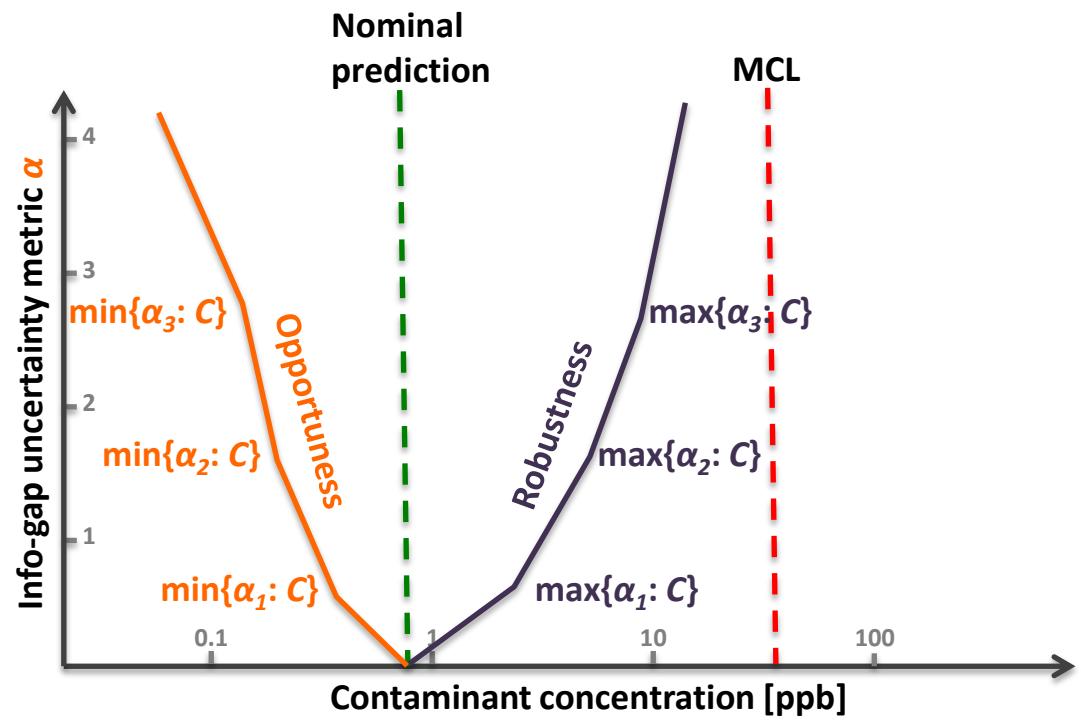
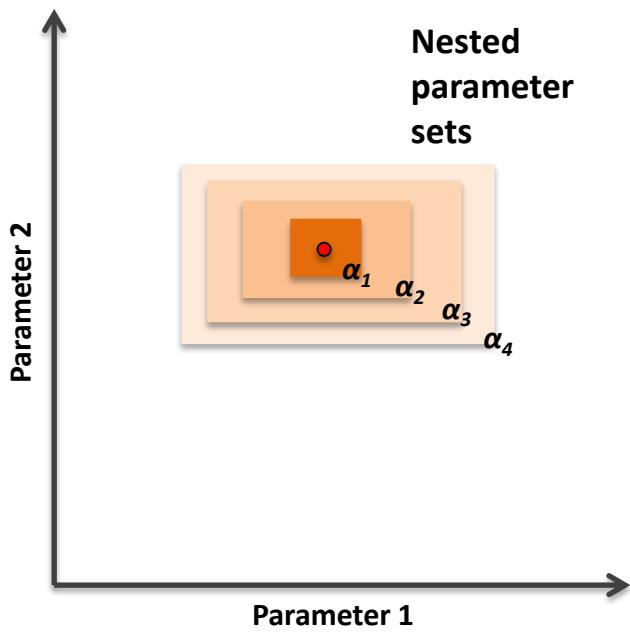
Info-Gap (non-probabilistic) analysis



info-gap uncertainty metric (horizon of unknown uncertainty) = α

$$\alpha_1 < \alpha_2 < \alpha_3 < \alpha_4 \dots < \alpha_{\infty}$$

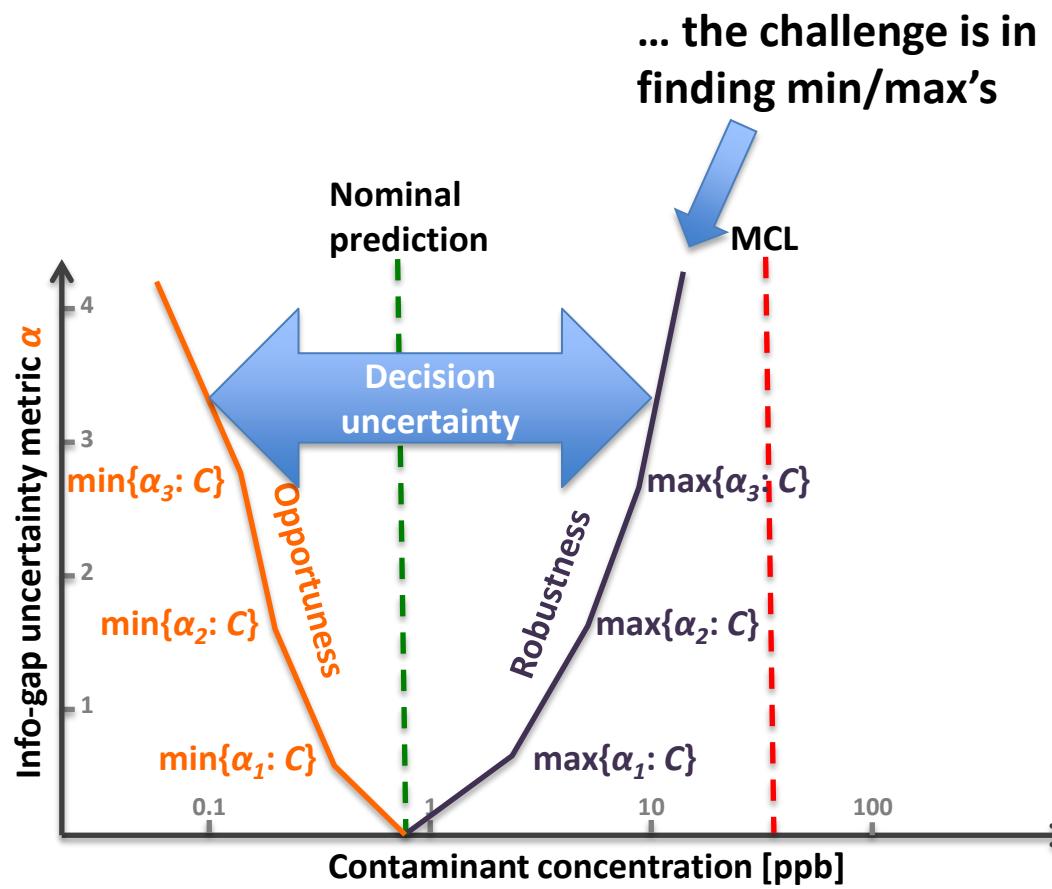
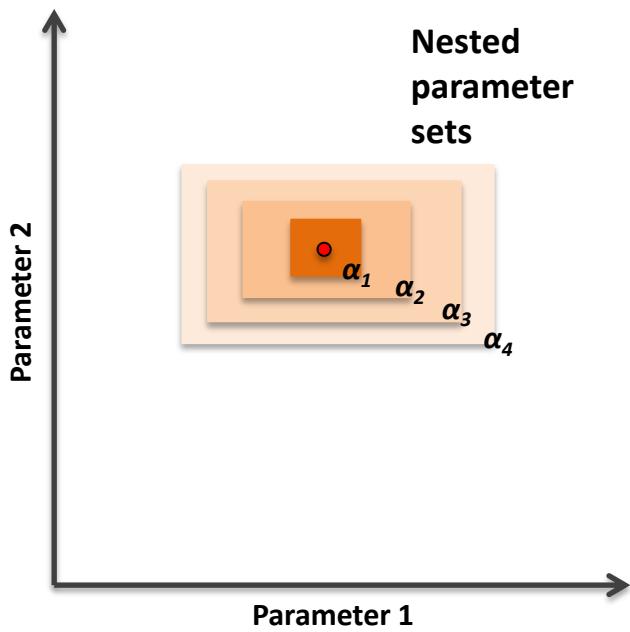
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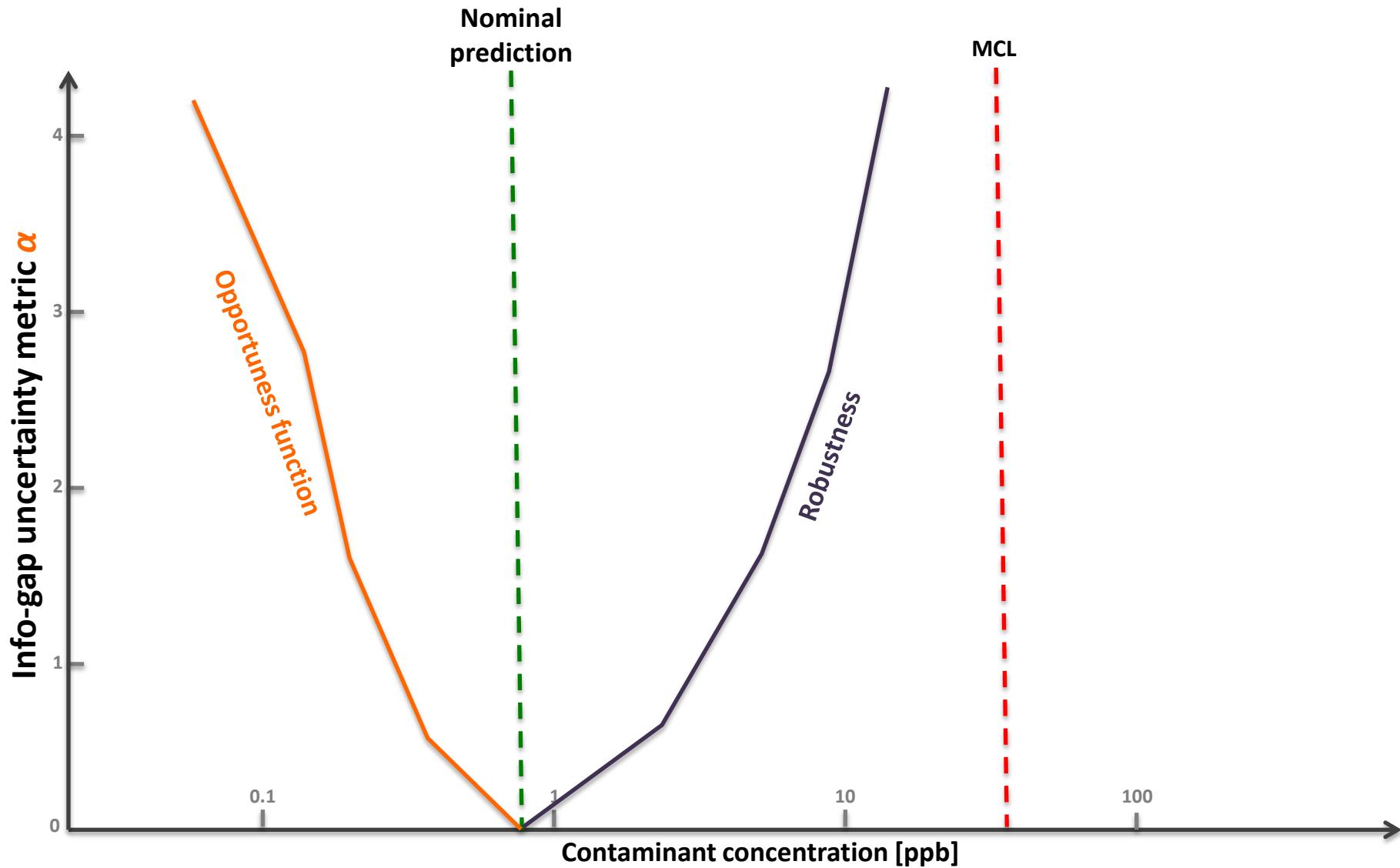
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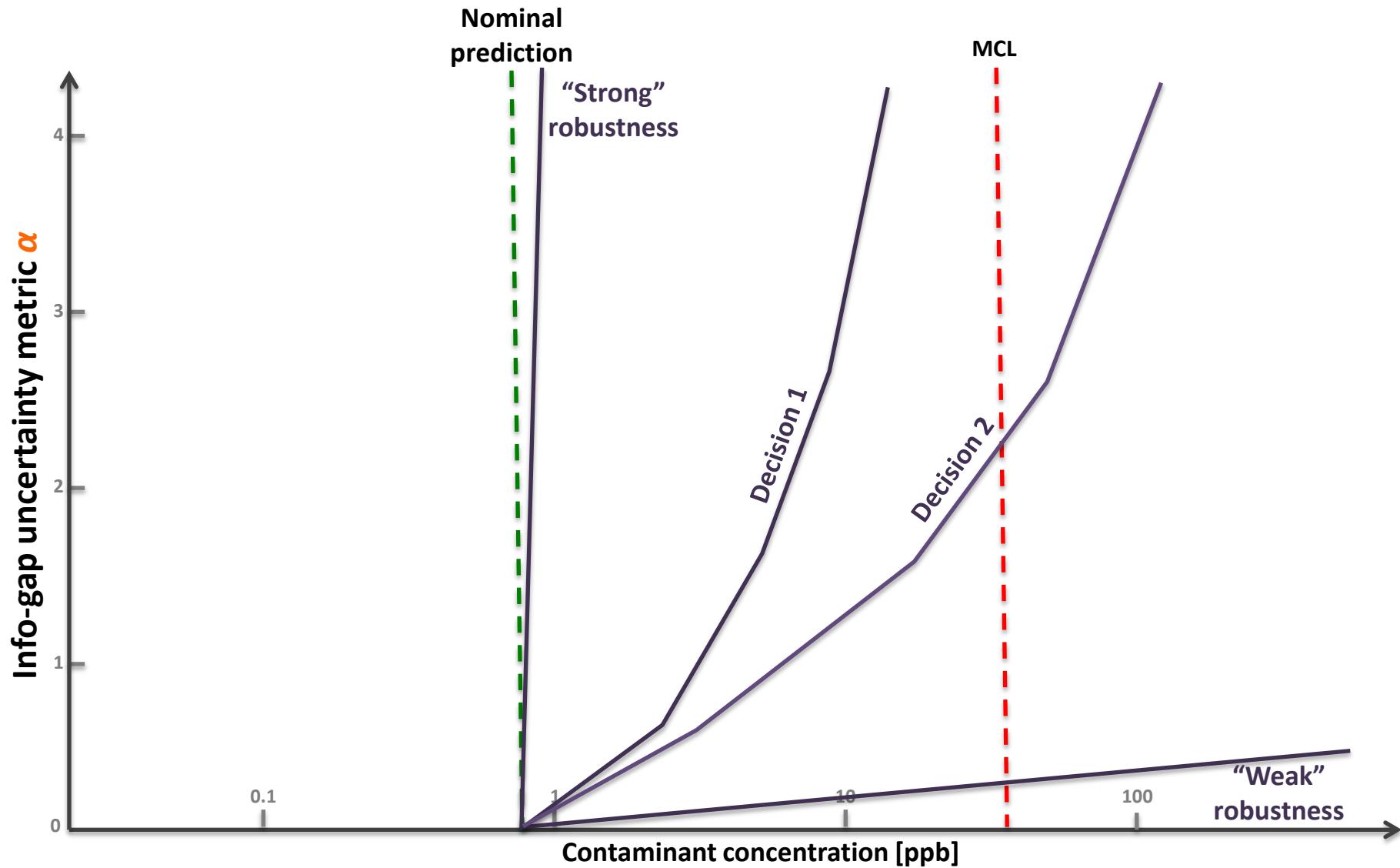
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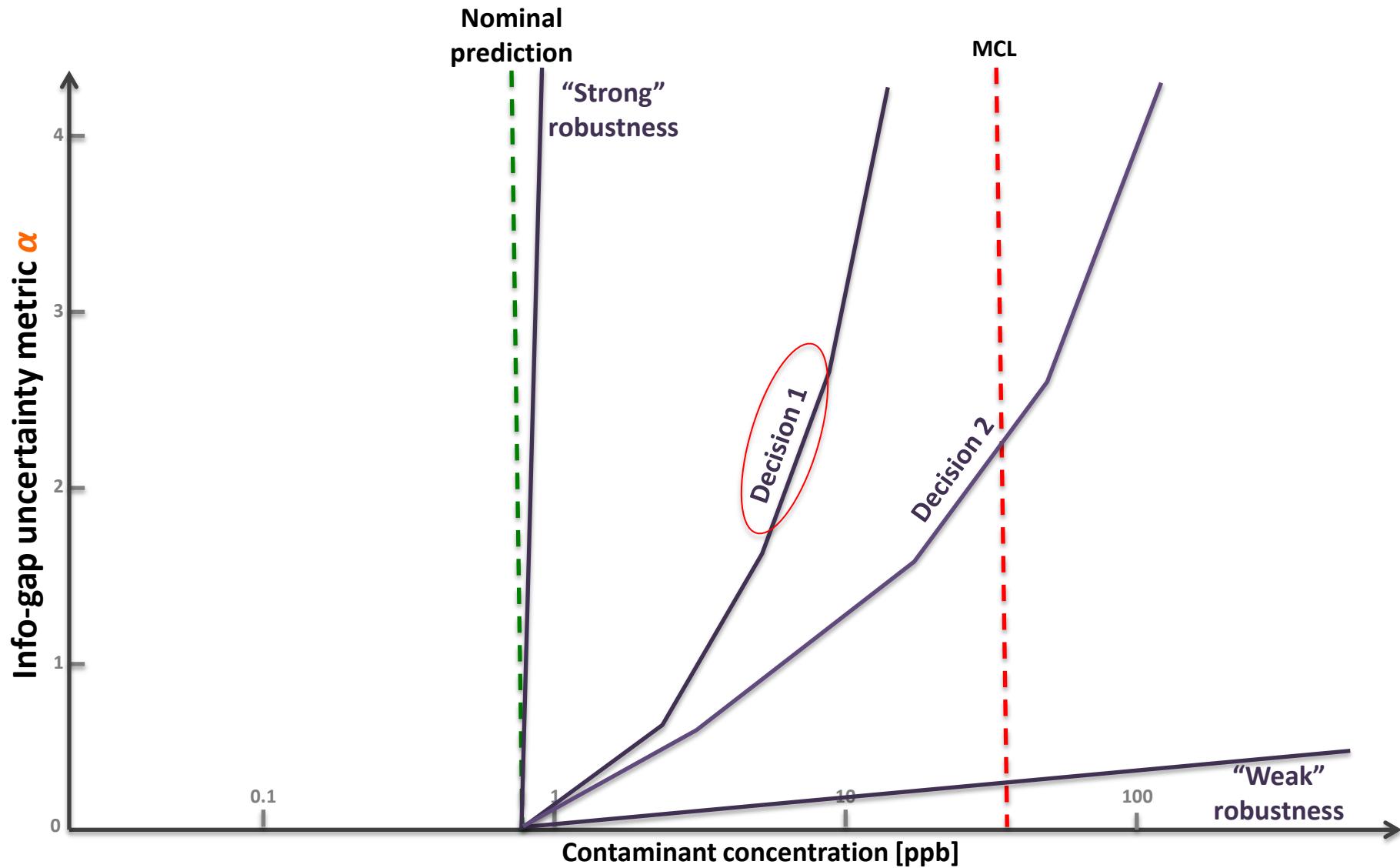
Info-Gap Analysis: Decision selection based on robustness



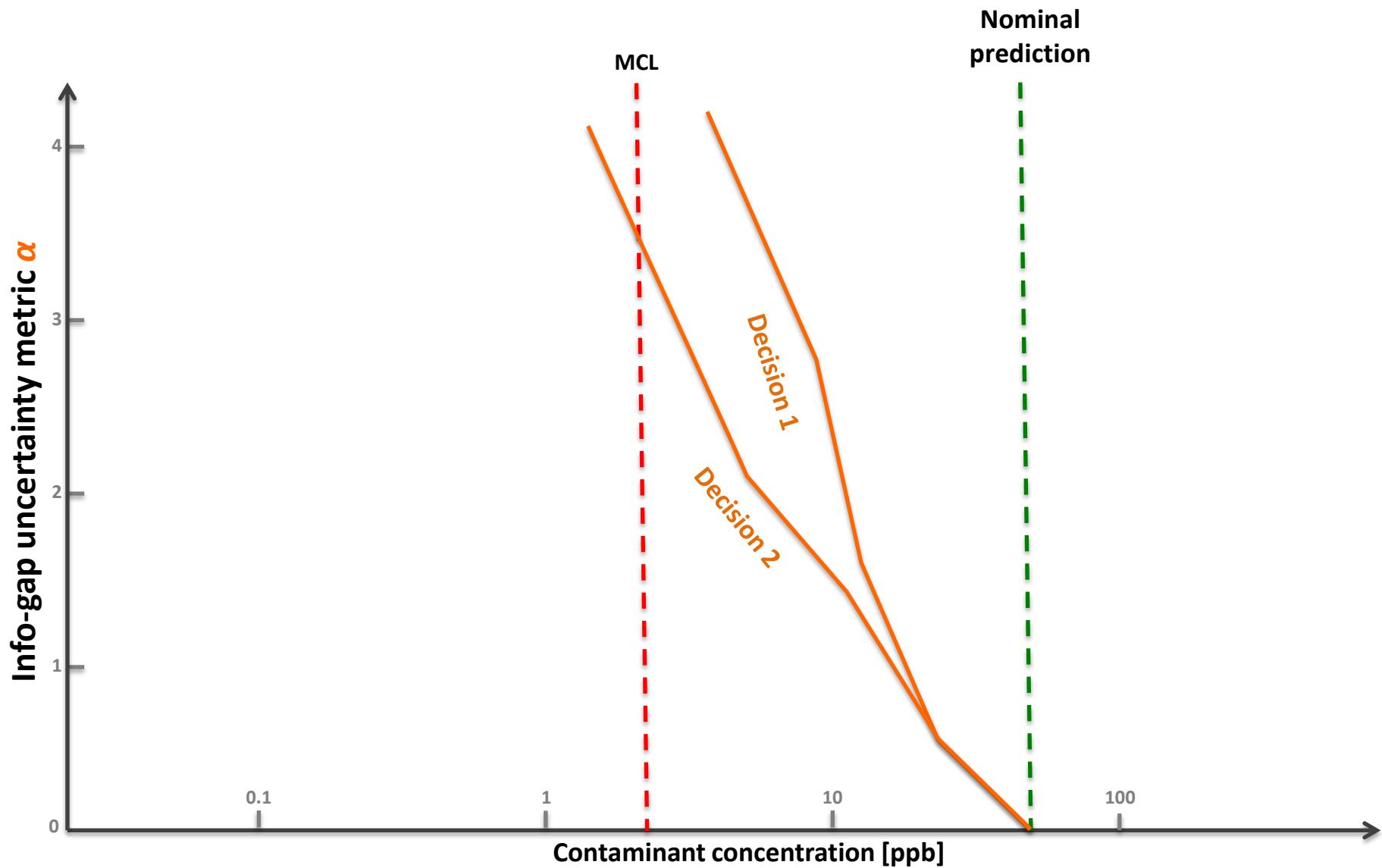
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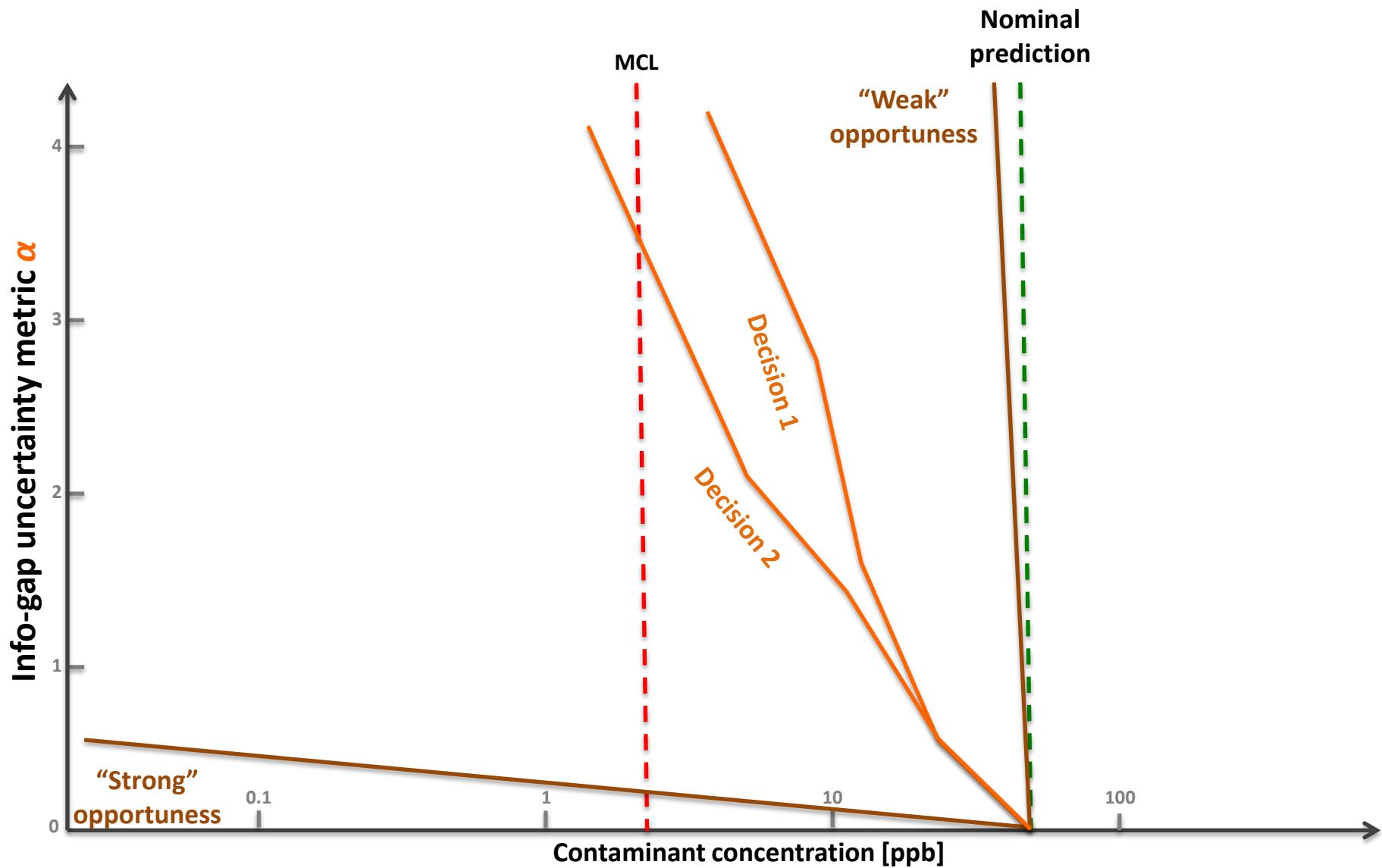
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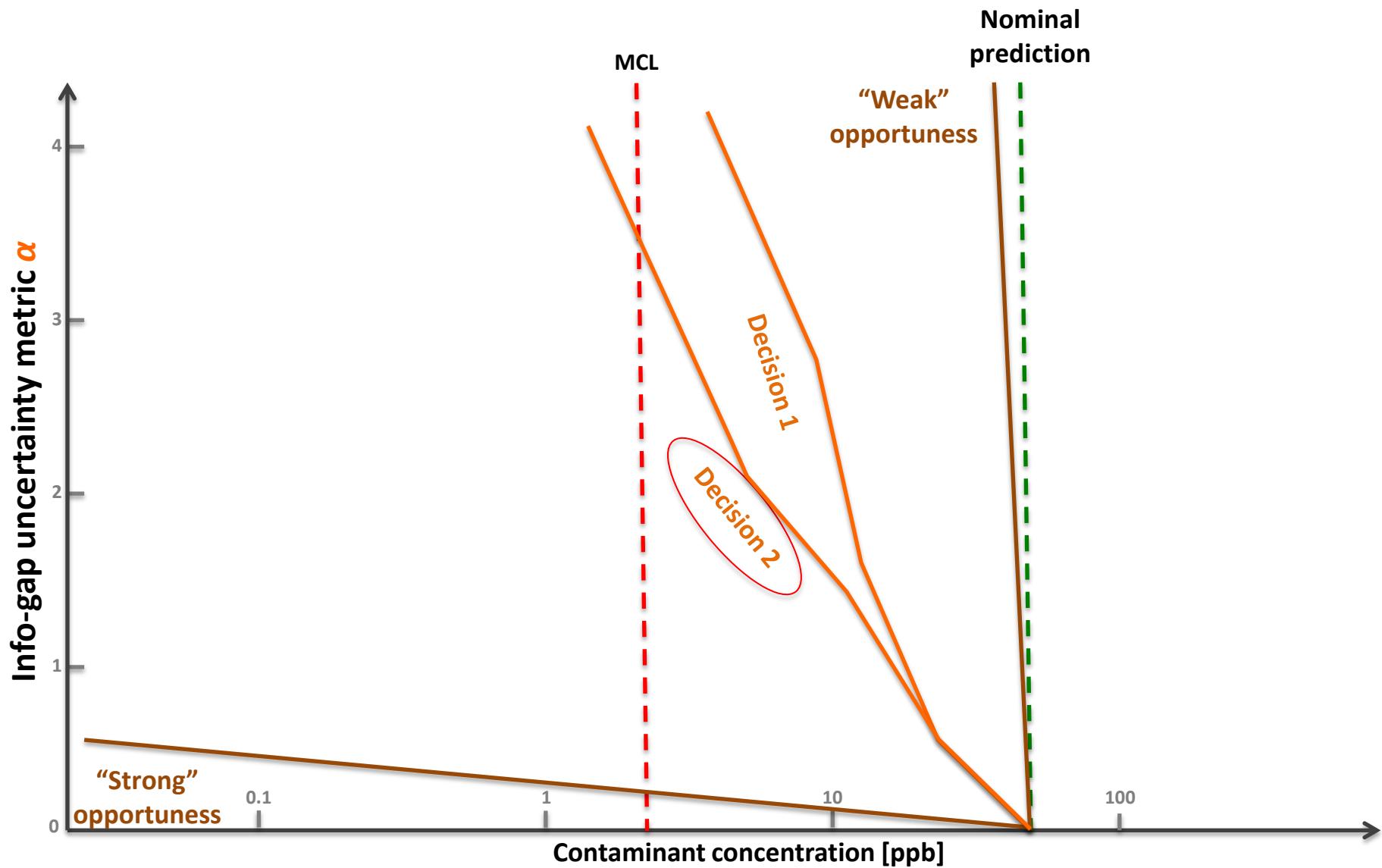
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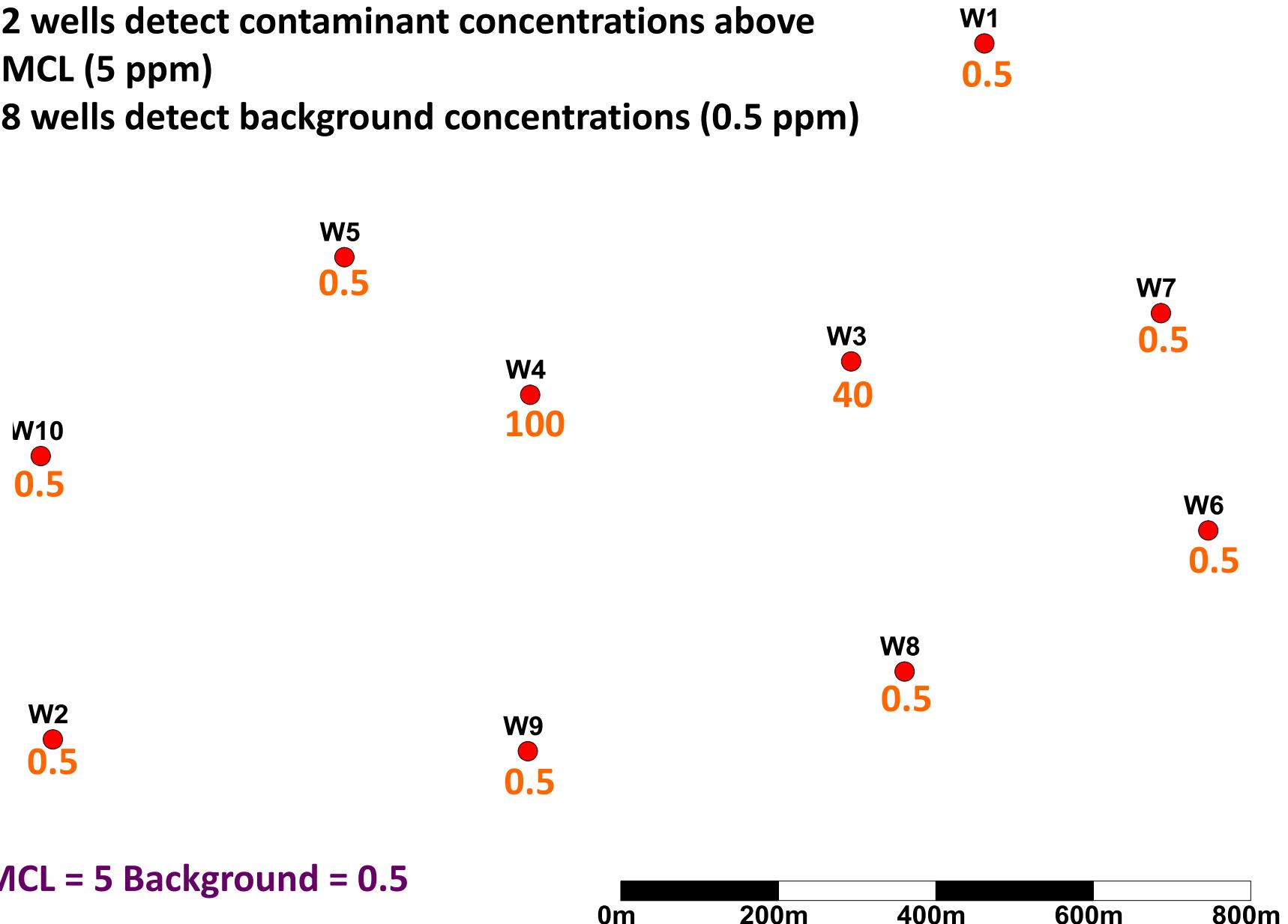


Info-Gap Analysis: Decision selection based on opportuness



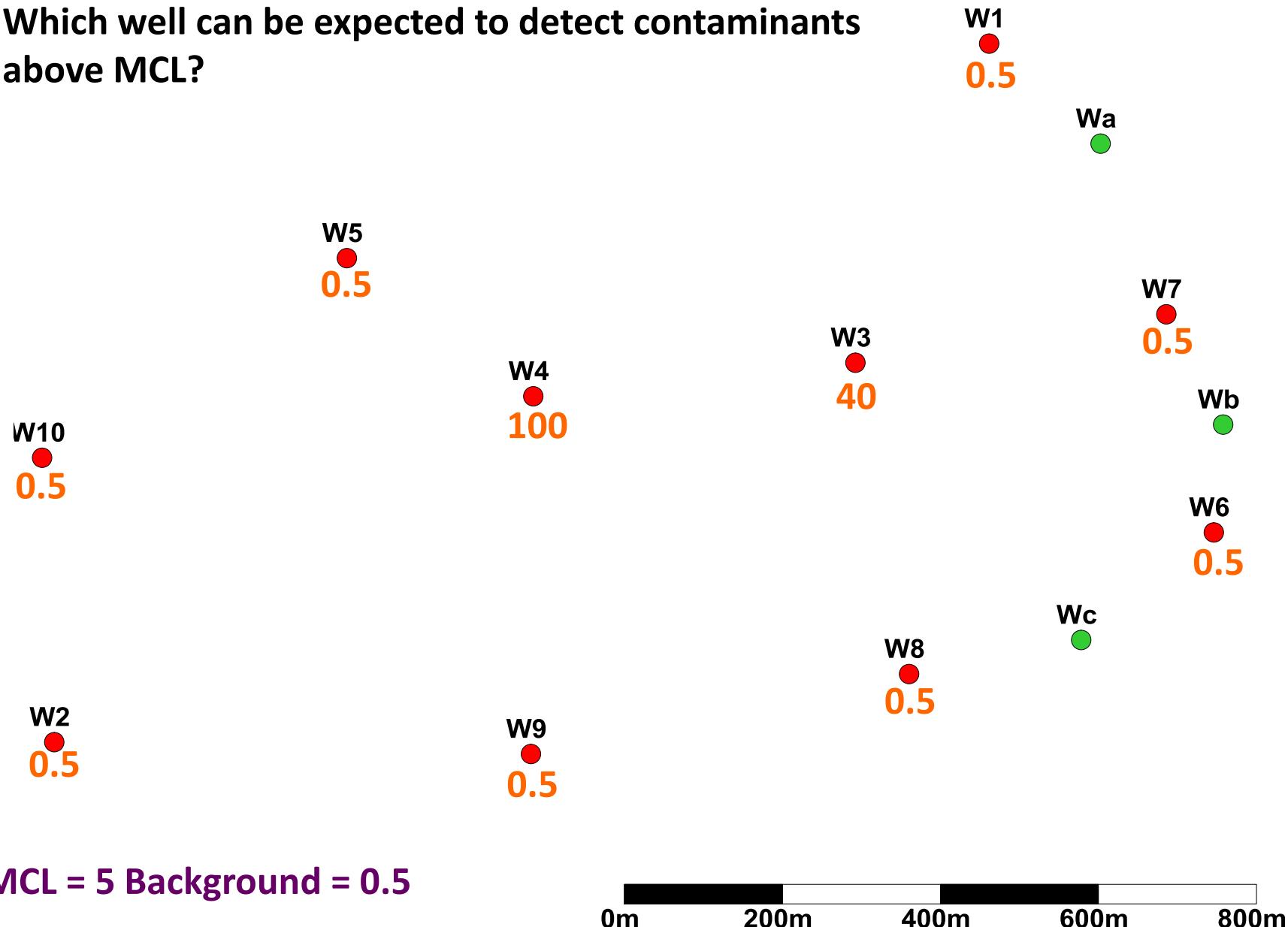
Info-Gap Analysis: Synthetic Network Design

- ✧ 10 monitoring wells in an aquifer
- ✧ 2 wells detect contaminant concentrations above MCL (5 ppm)
- ✧ 8 wells detect background concentrations (0.5 ppm)



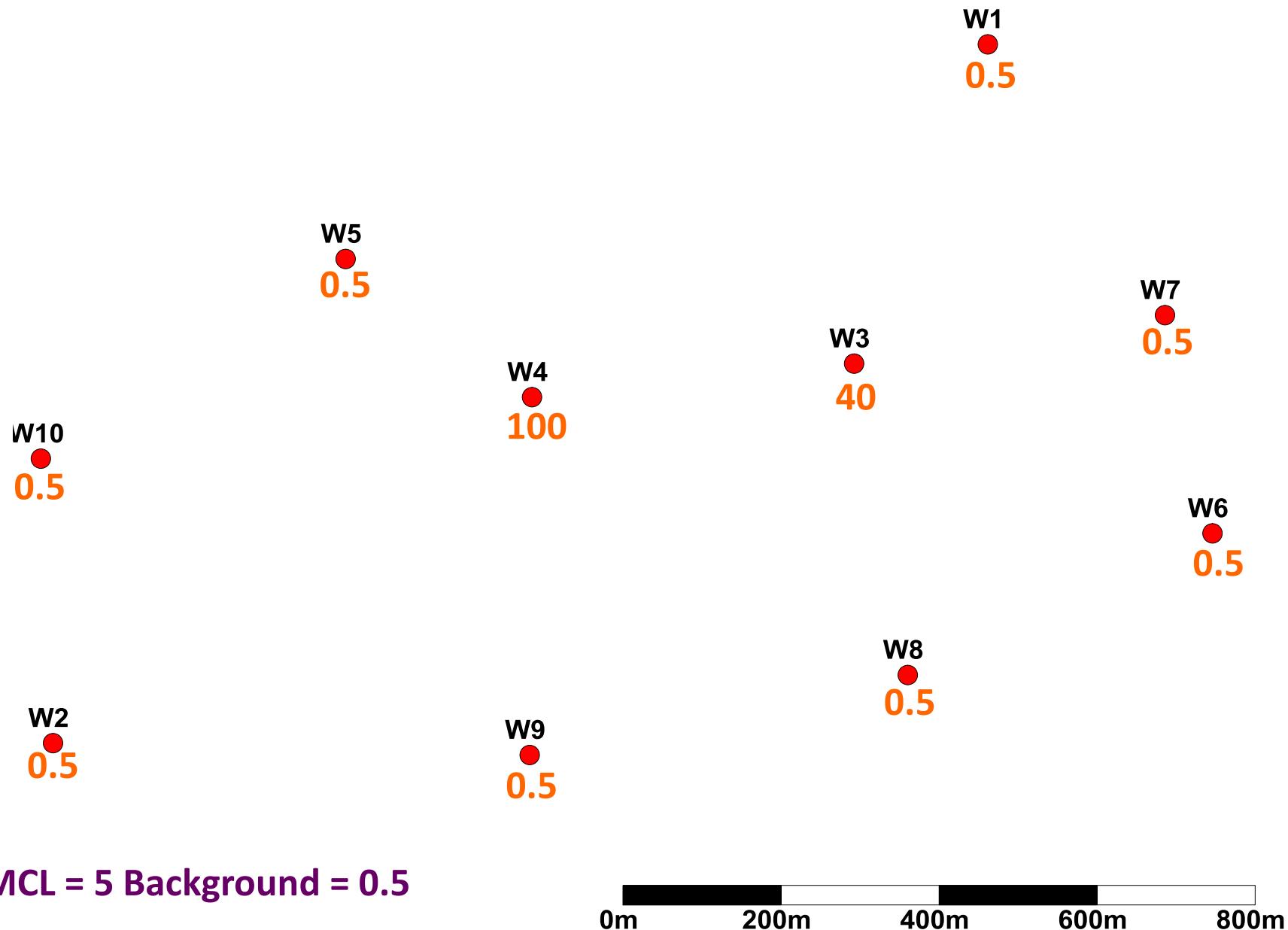
Info-Gap Analysis: Synthetic Network Design

- ✧ 3 new proposed monitoring well locations (green dots)
- ✧ Which well can be expected to detect contaminants above MCL?



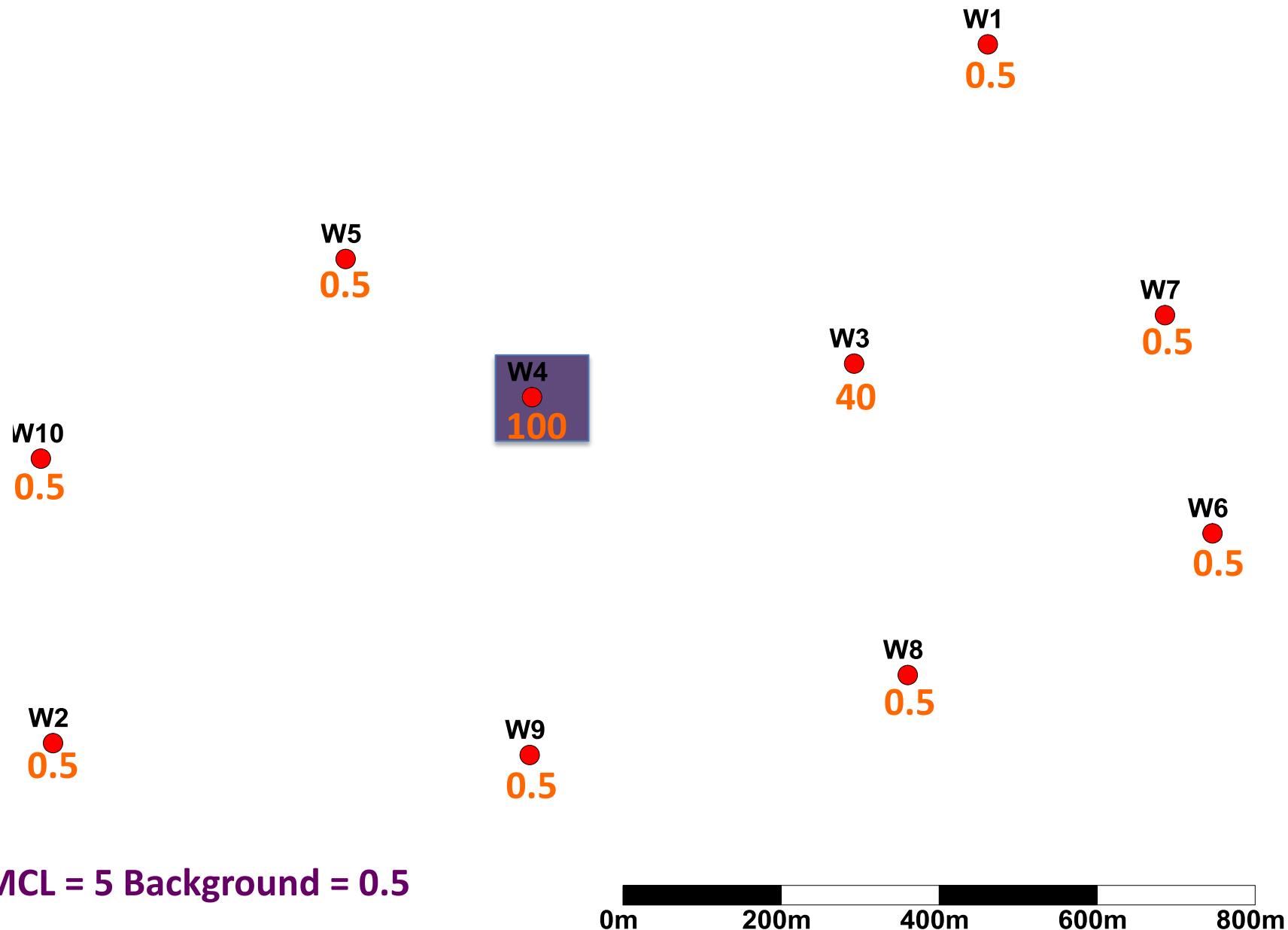
Info-Gap Analysis: Synthetic Network Design

❖ Where is the contaminant source?



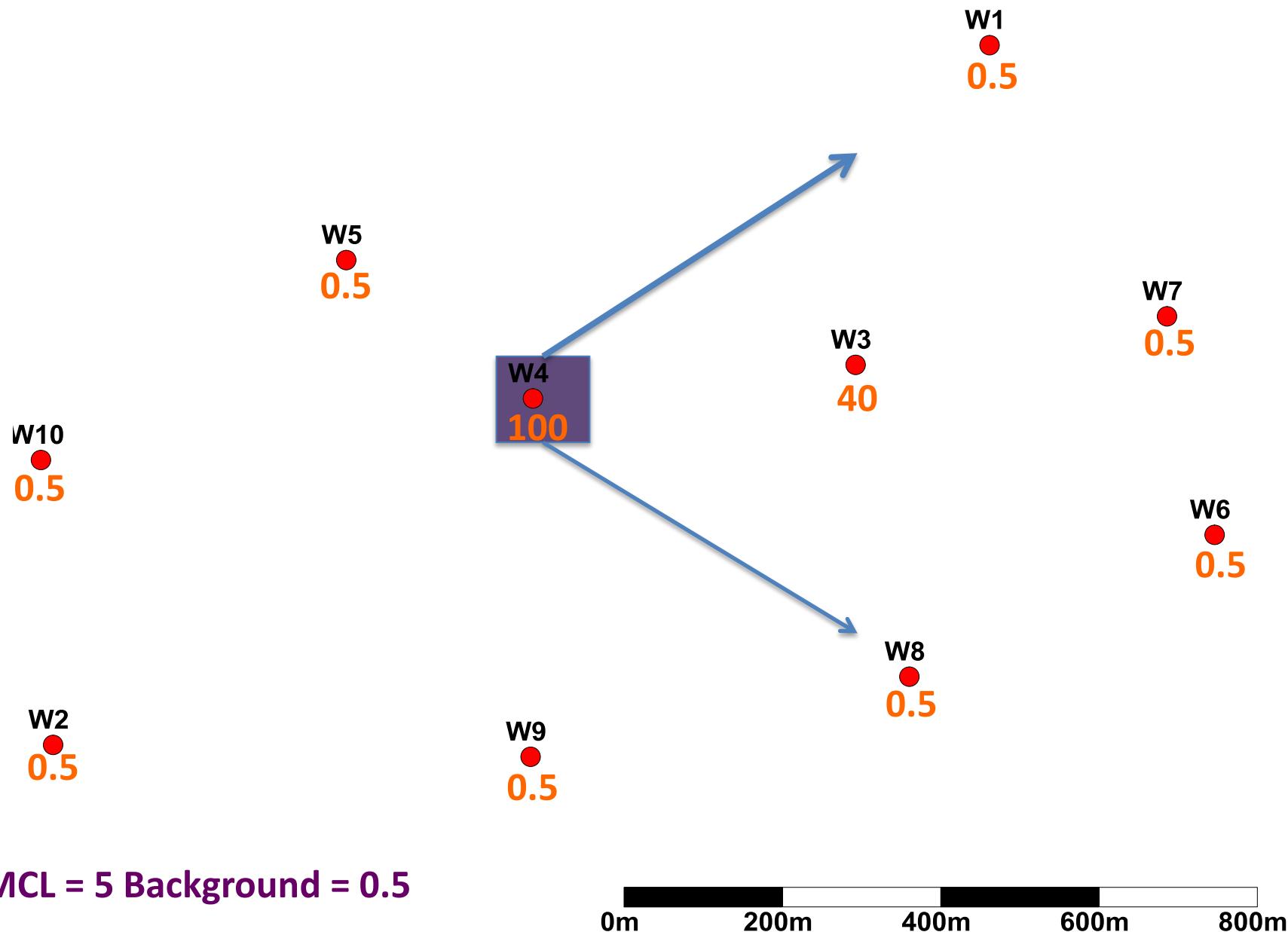
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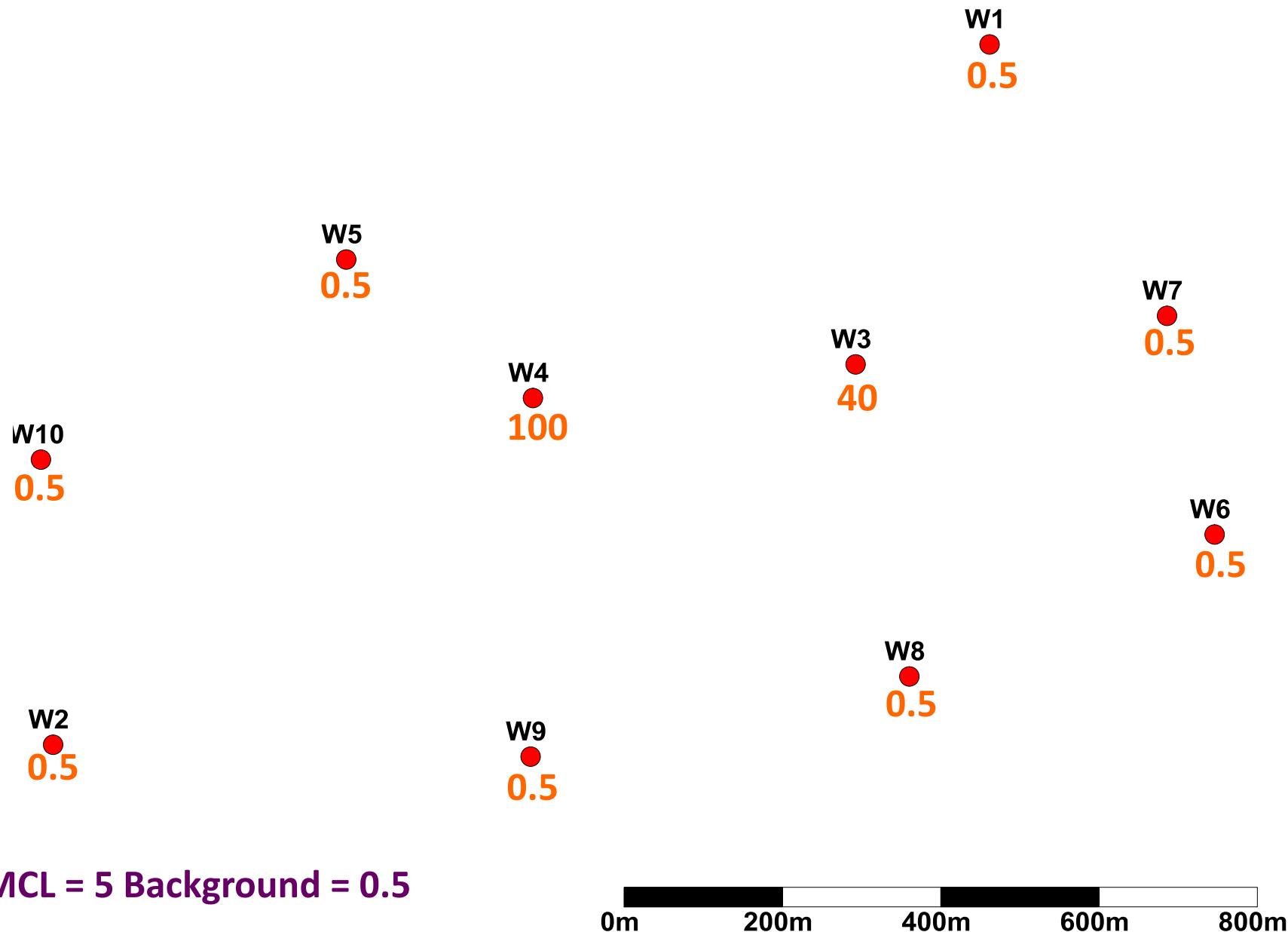
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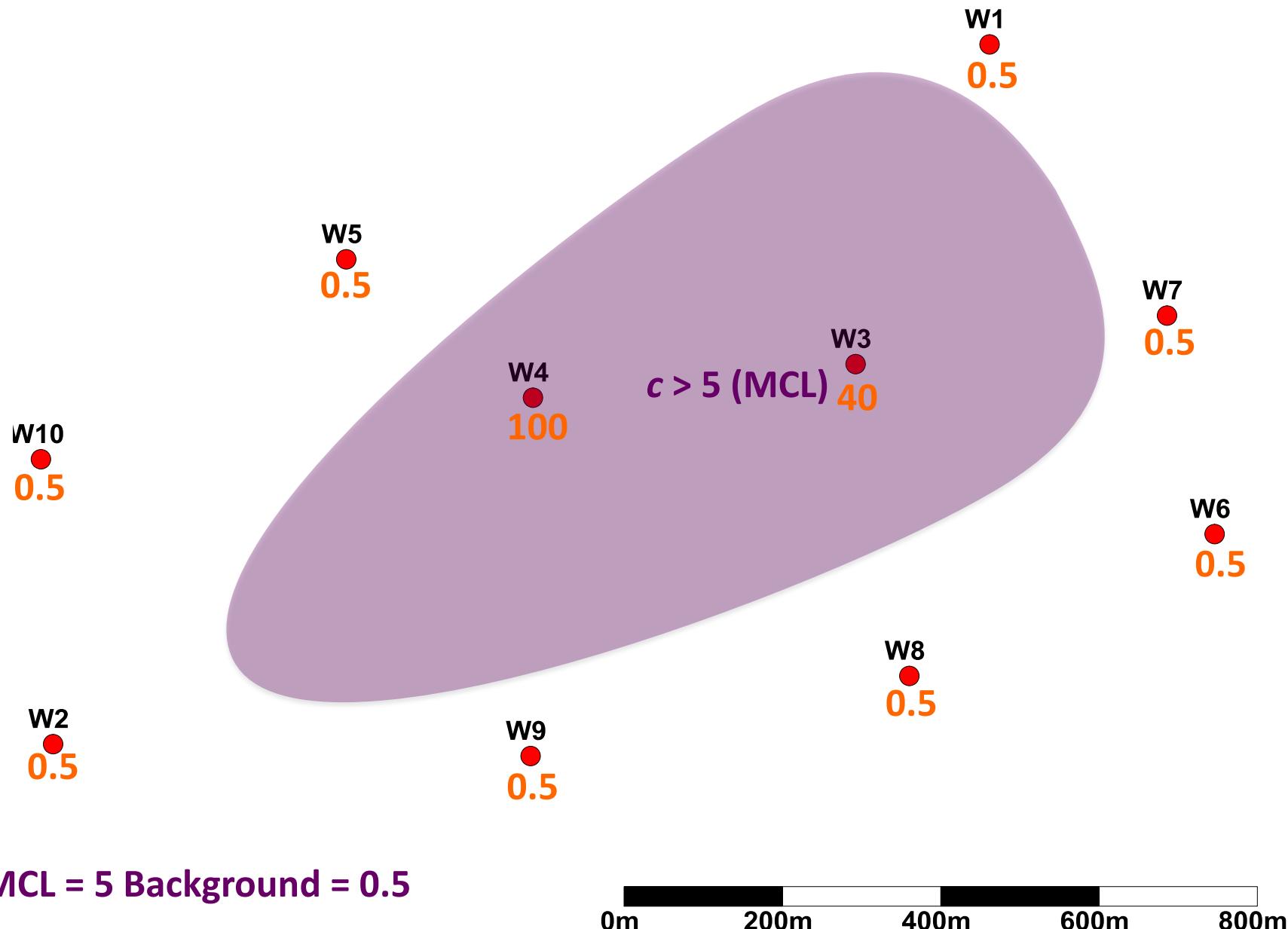
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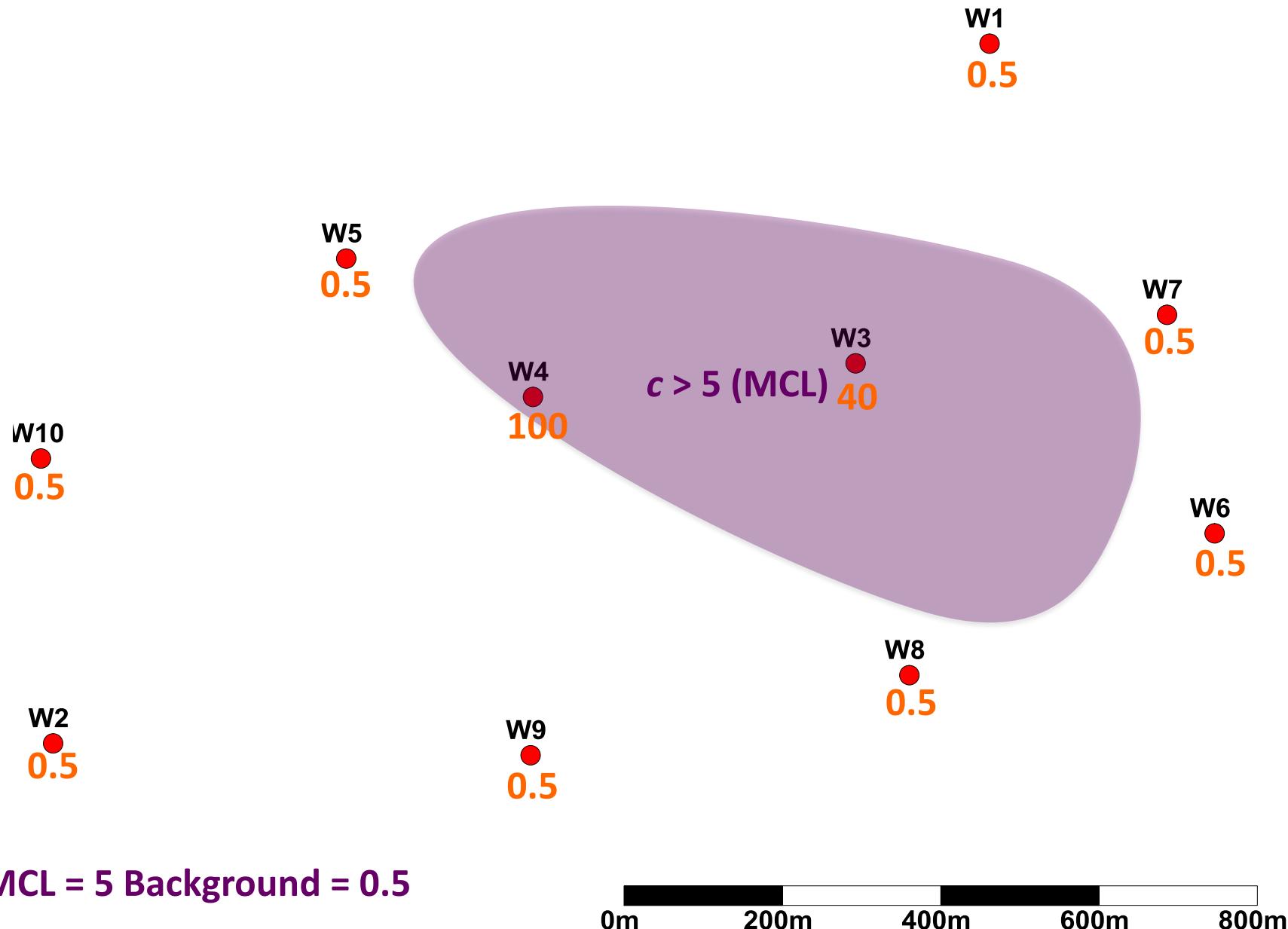
Info-Gap Analysis: Synthetic Network Design

✧ Multiple plausible plume configurations ...



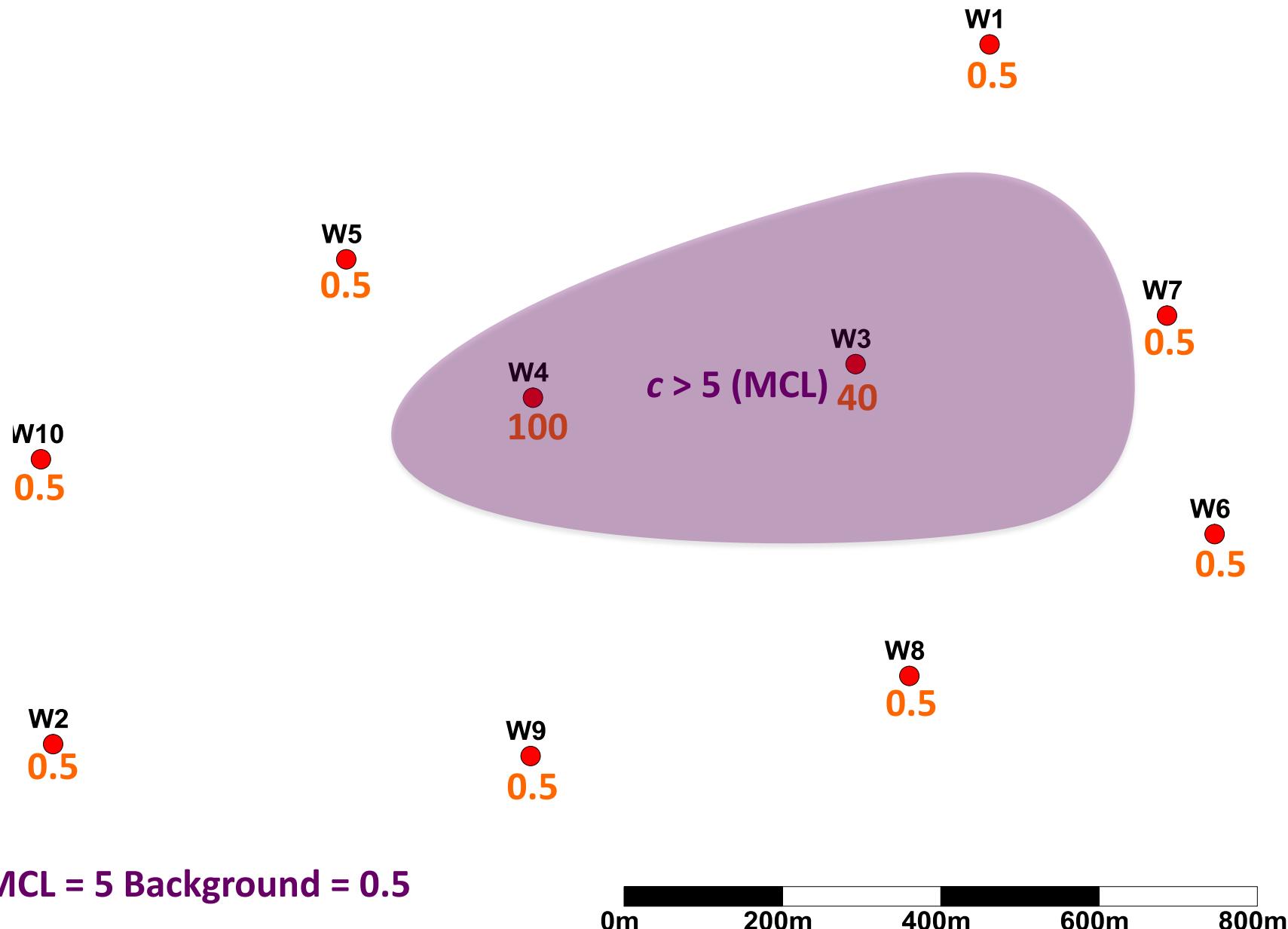
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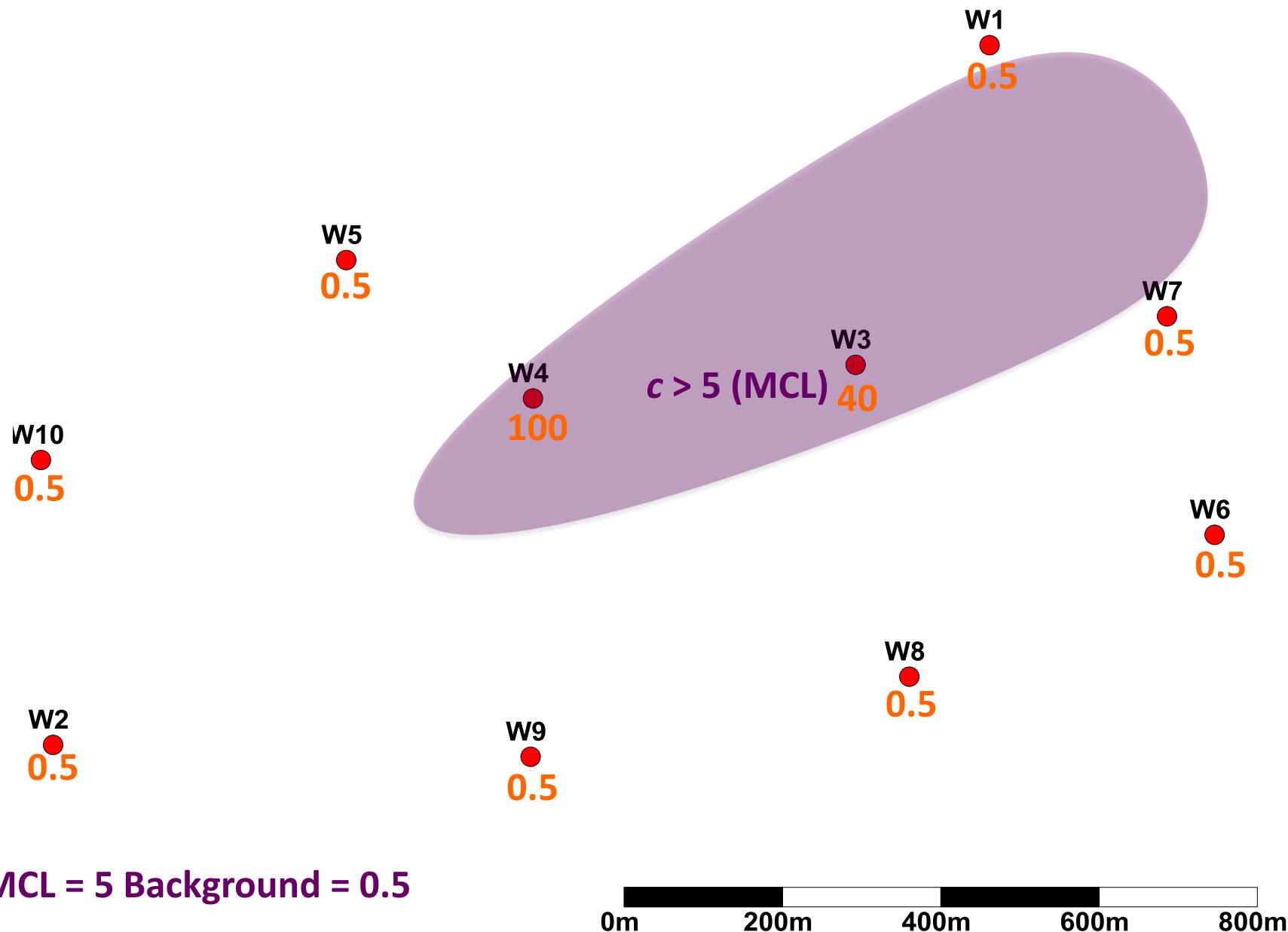
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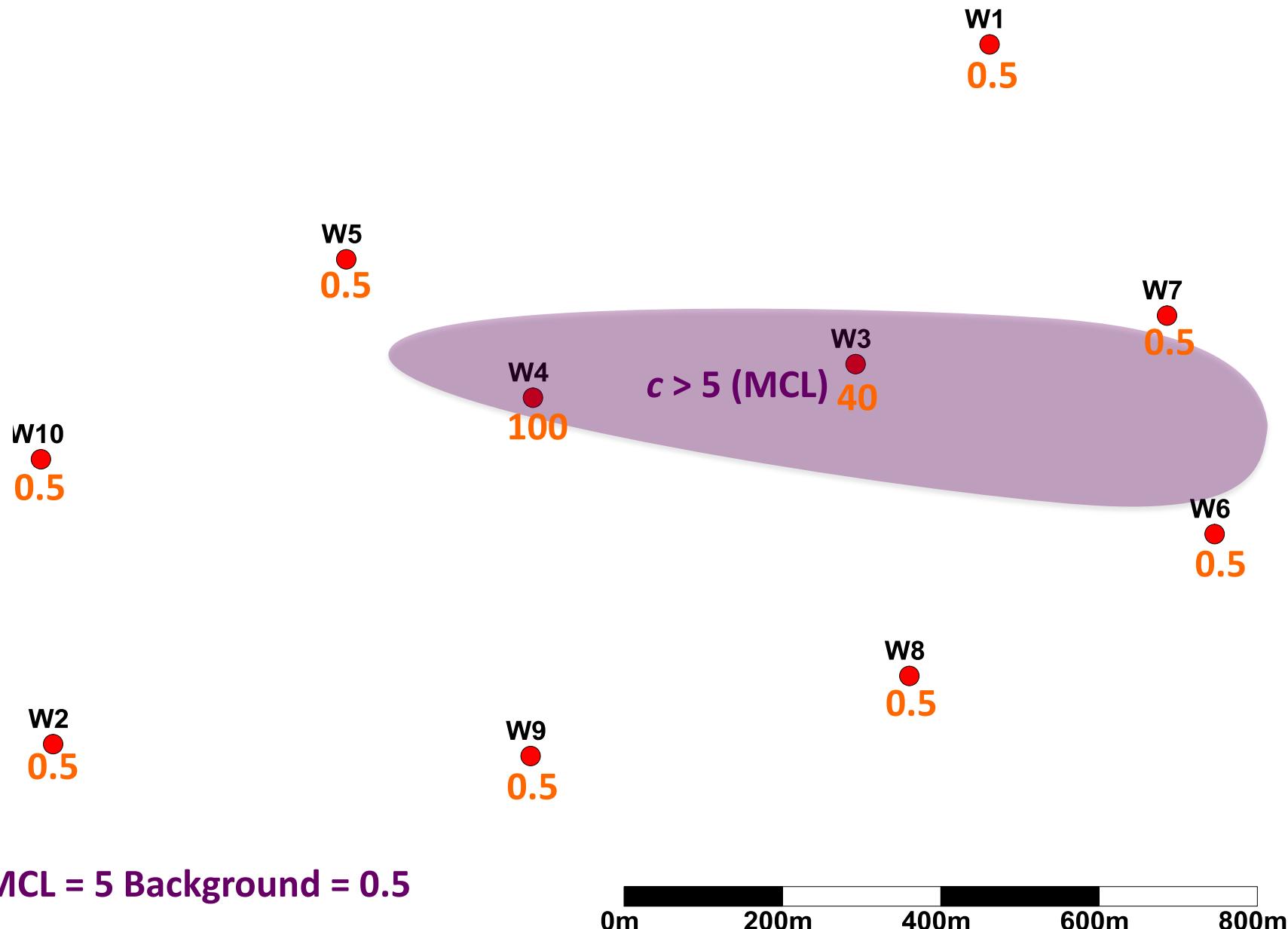
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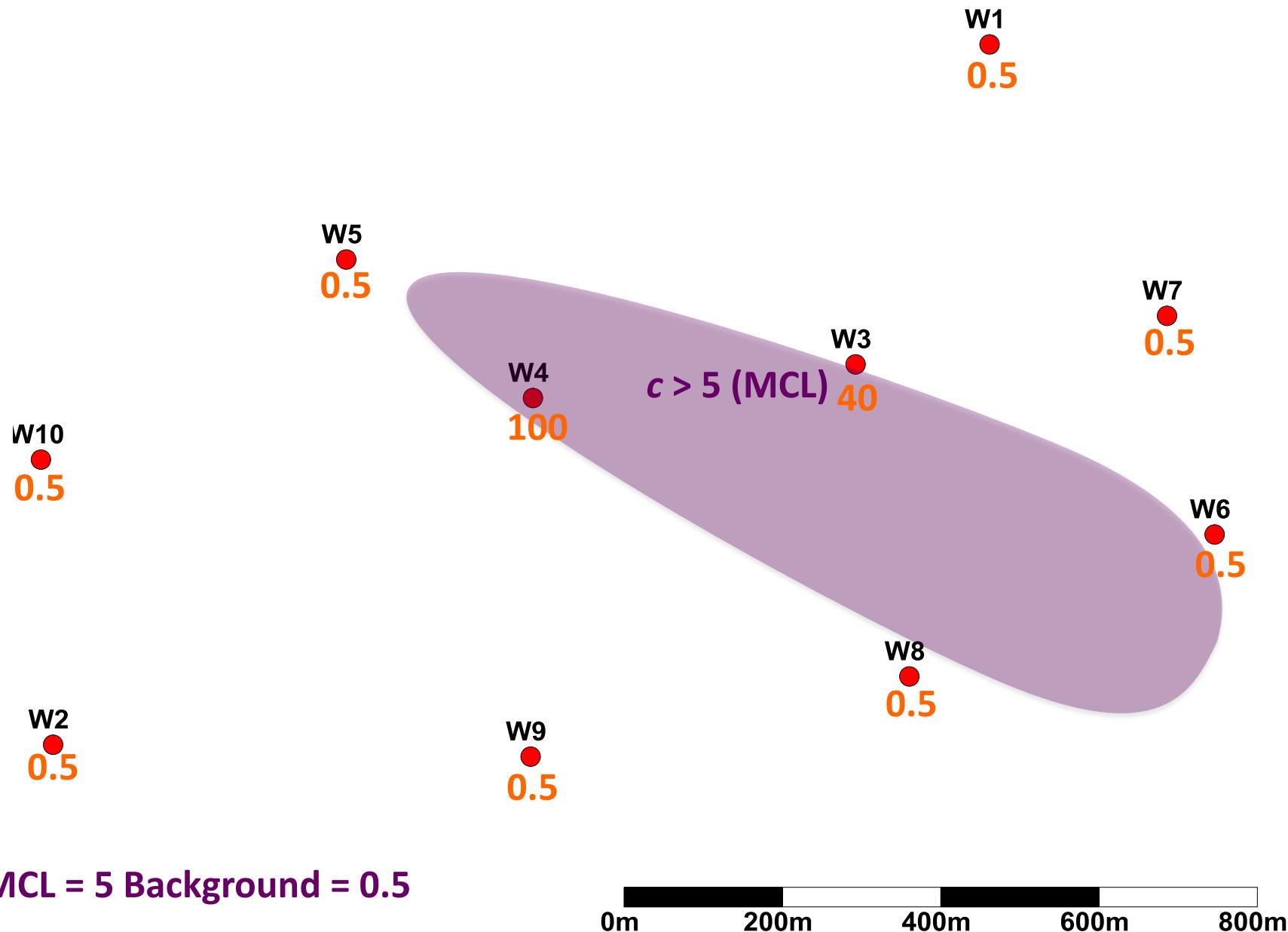
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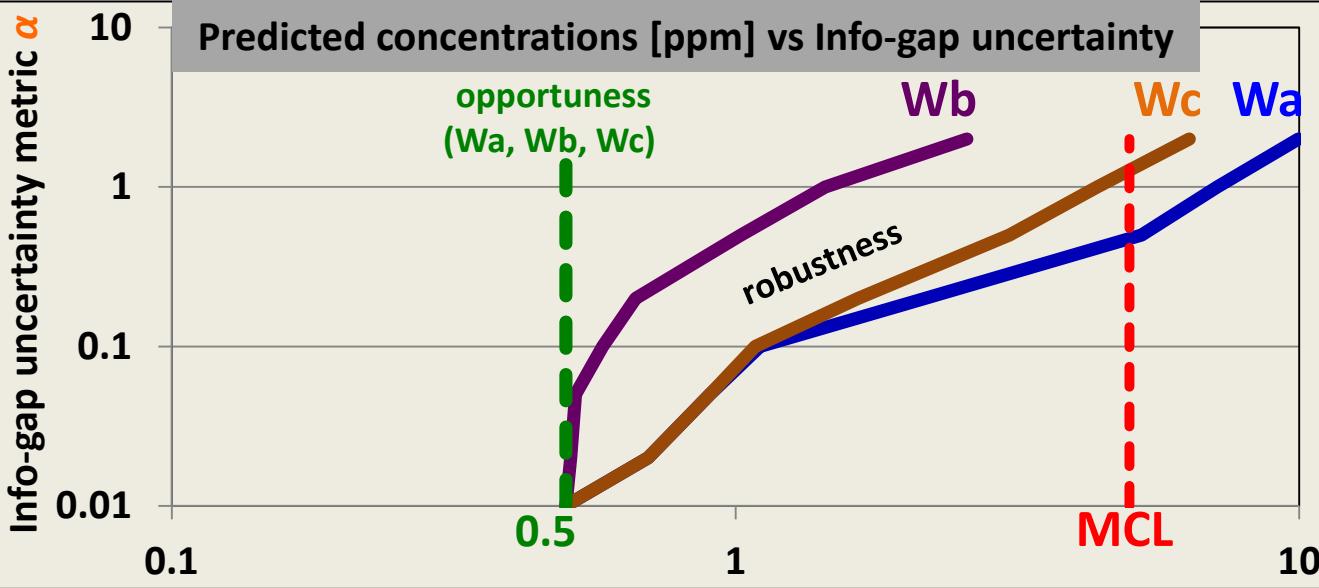


Info-Gap Analysis: Synthetic Network Design

✧ Multiple plausible plume configurations ...



Info-Gap Analysis: Network Design



W10
0.5

W4
100

W3
40

W6
0.5

W2
0.5

W9
0.5

W8
0.5

Wc

Wa

W7
0.5

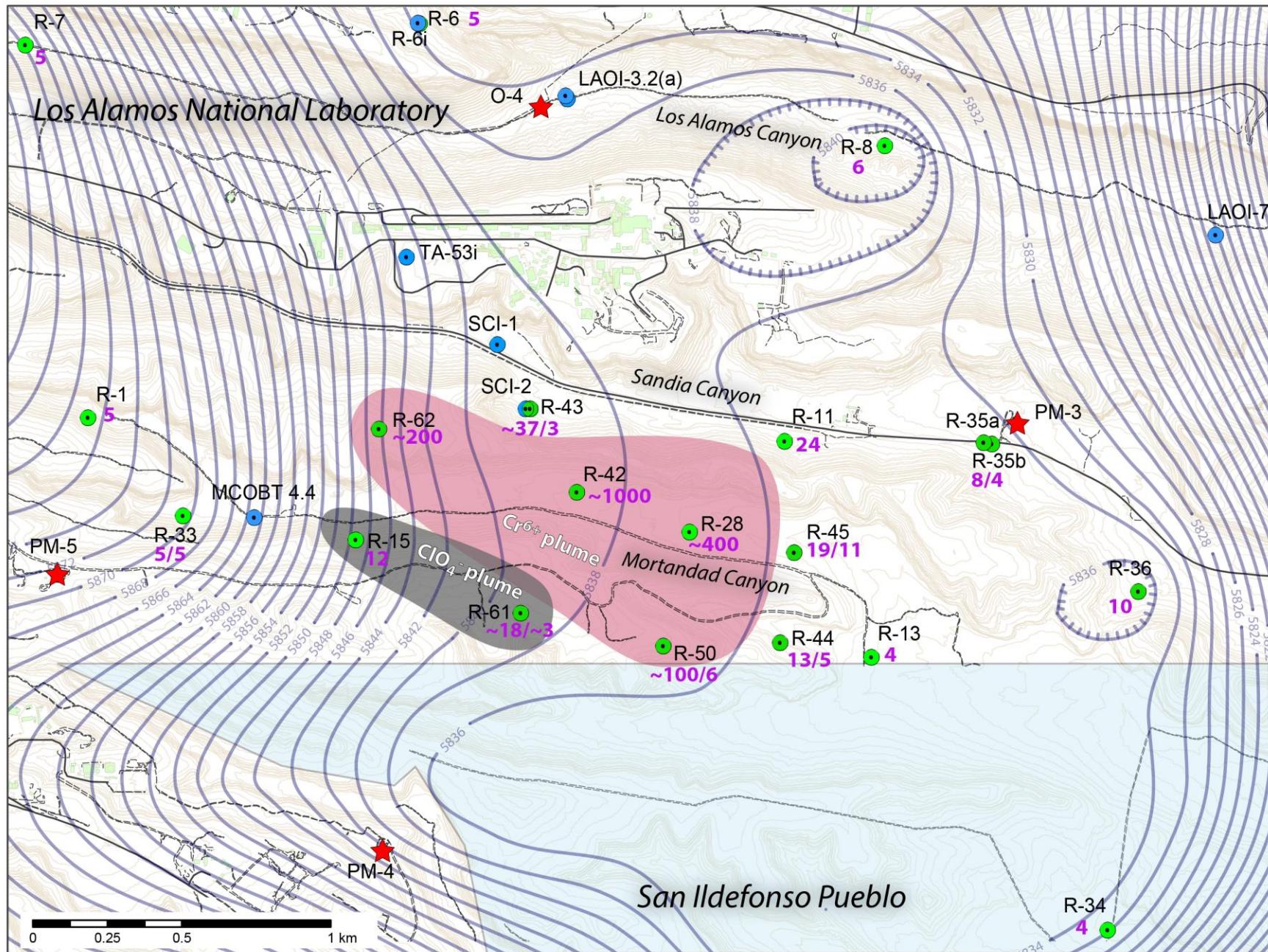
Wb

MCL = 5 Background = 0.5

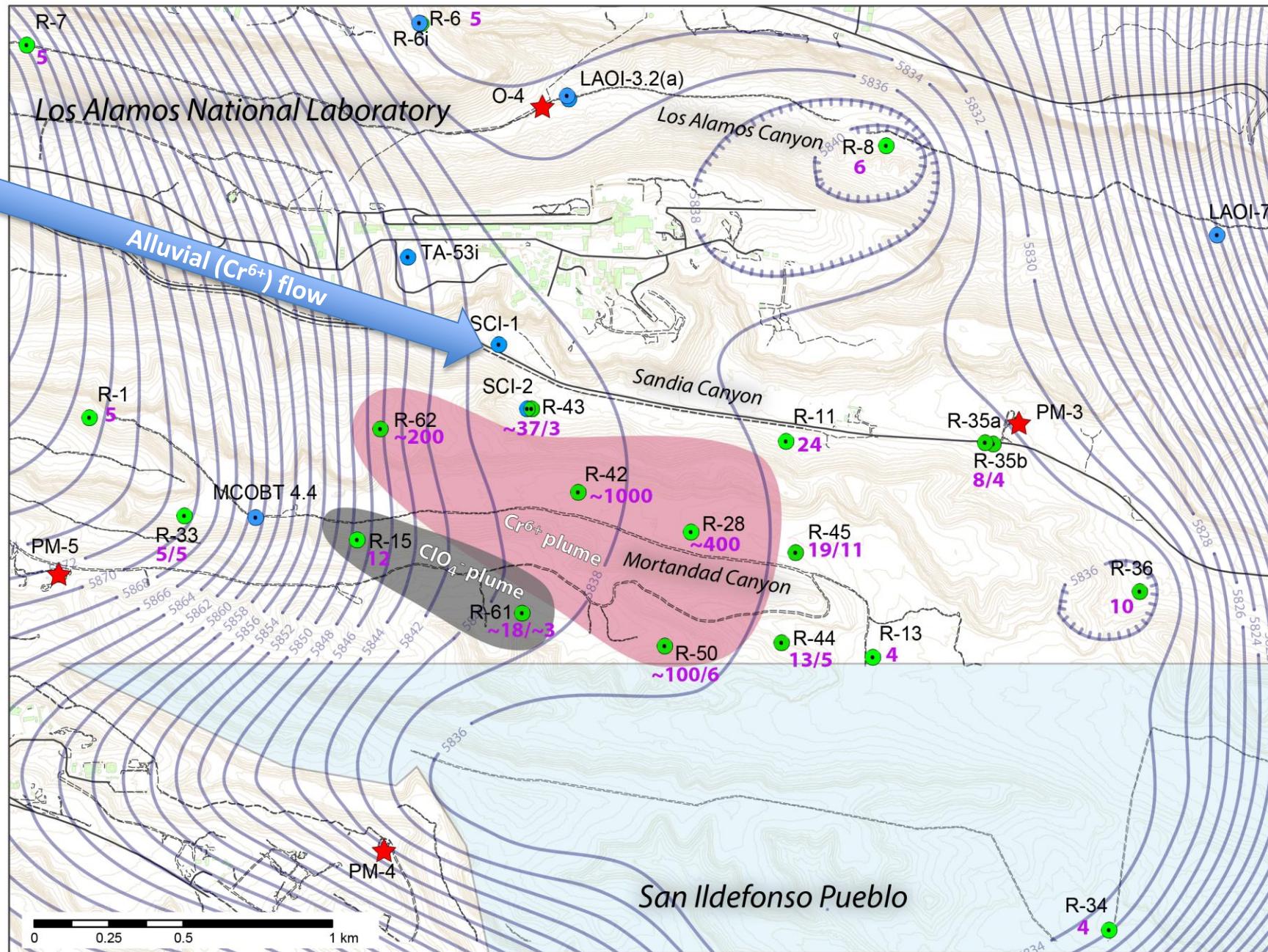
For more information: <http://mads.lanl.gov>

0m 200m 400m 600m 800m

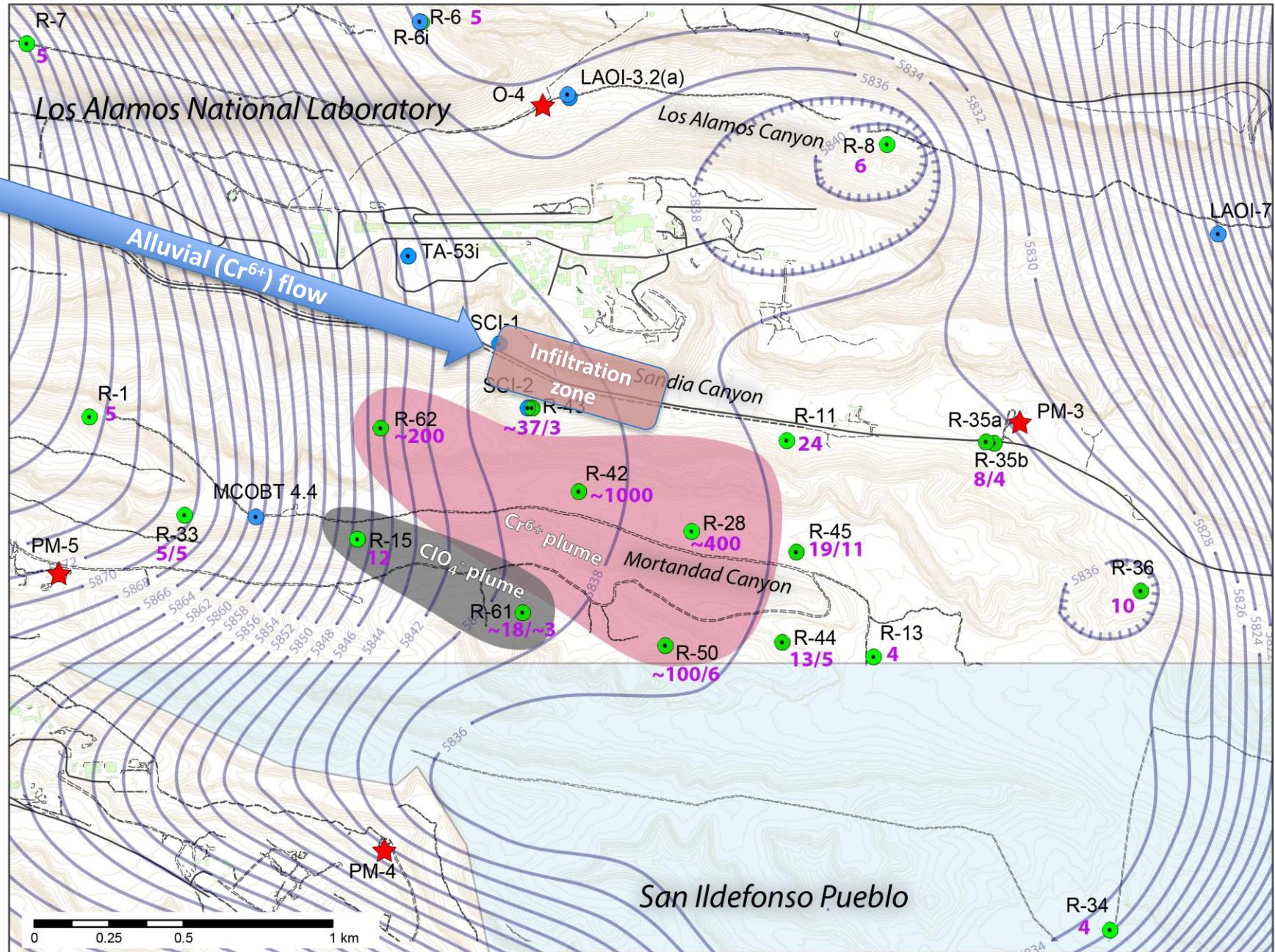
Chromium plume in the regional aquifer at LANL



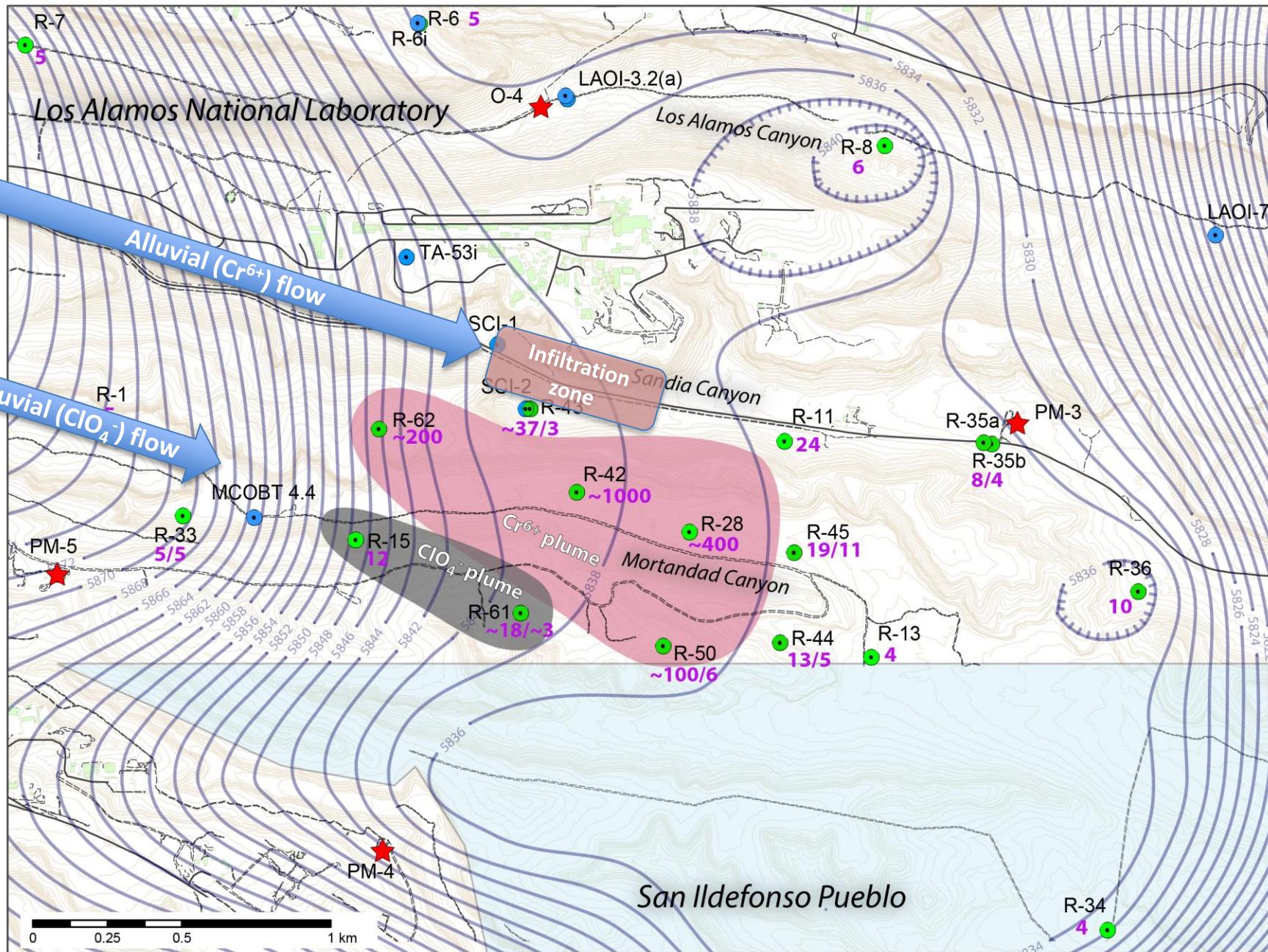
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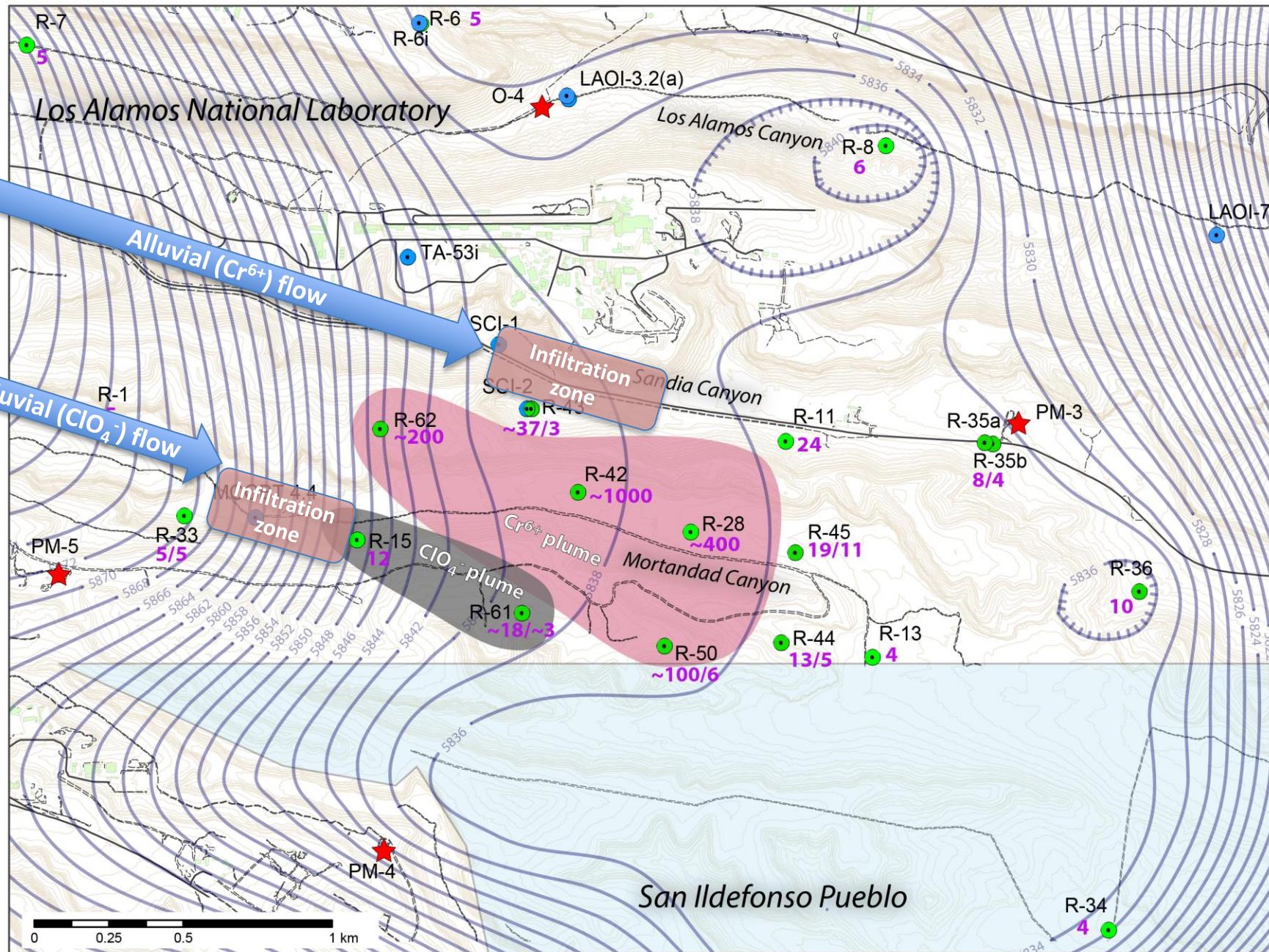
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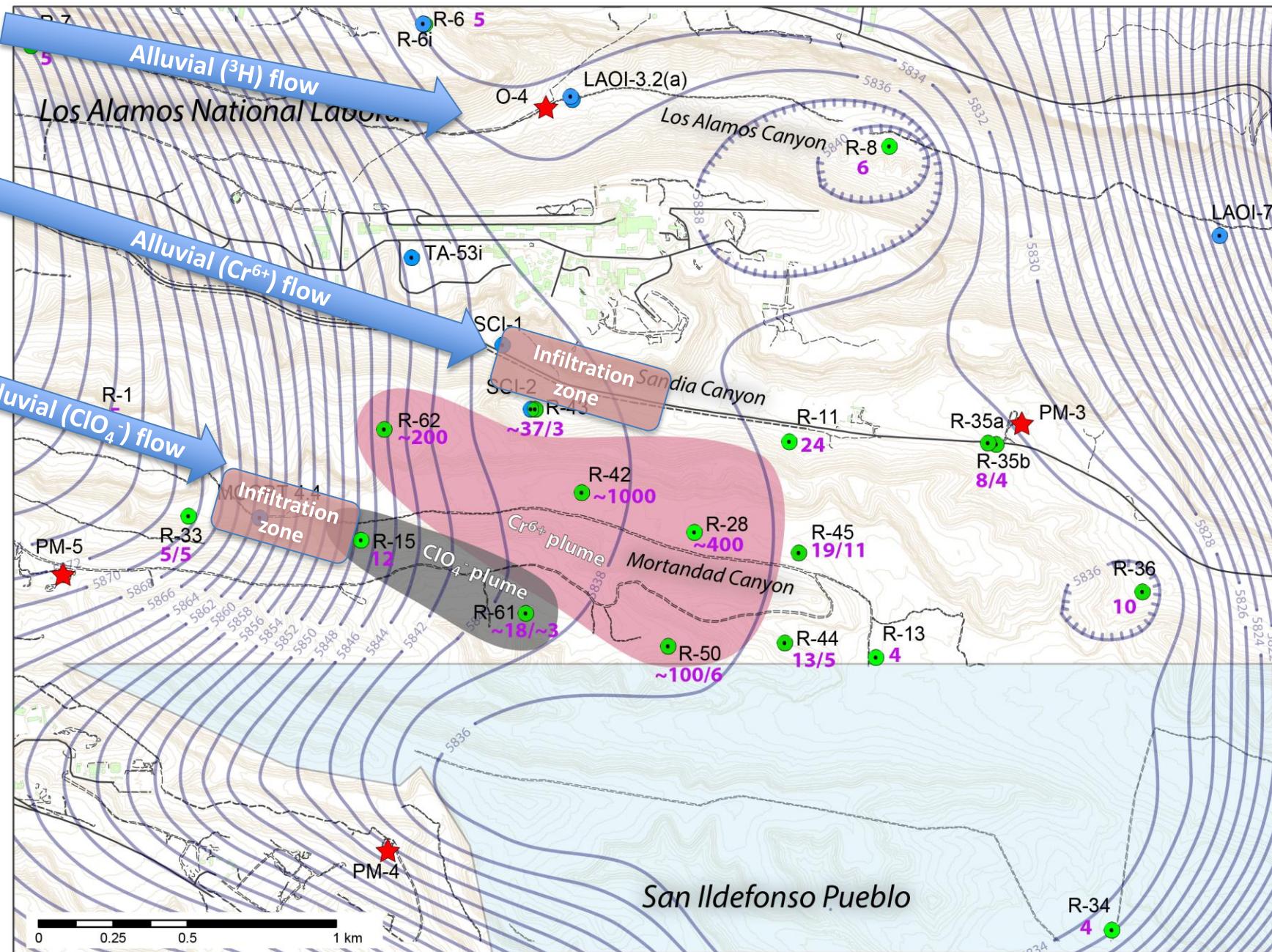
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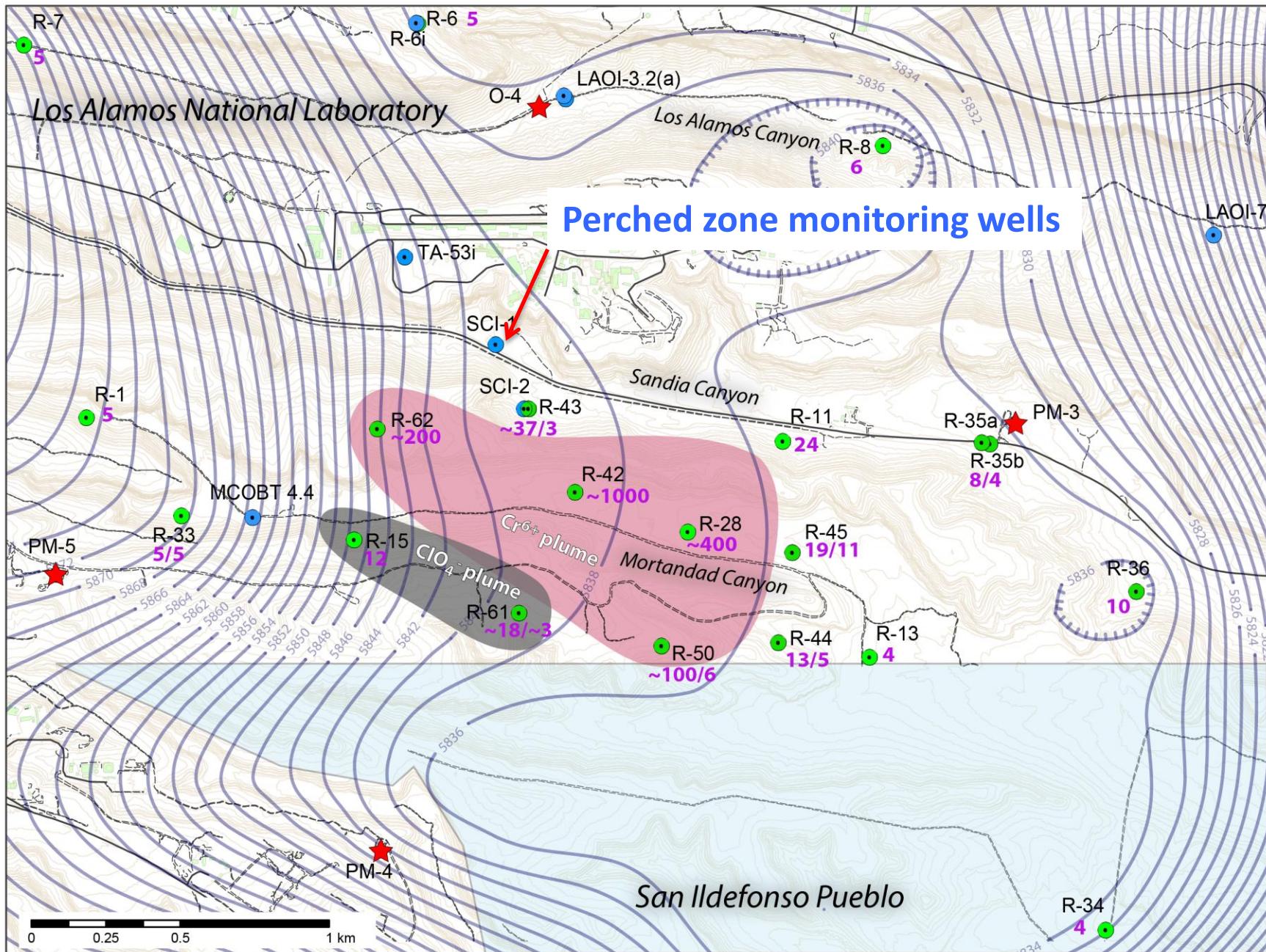
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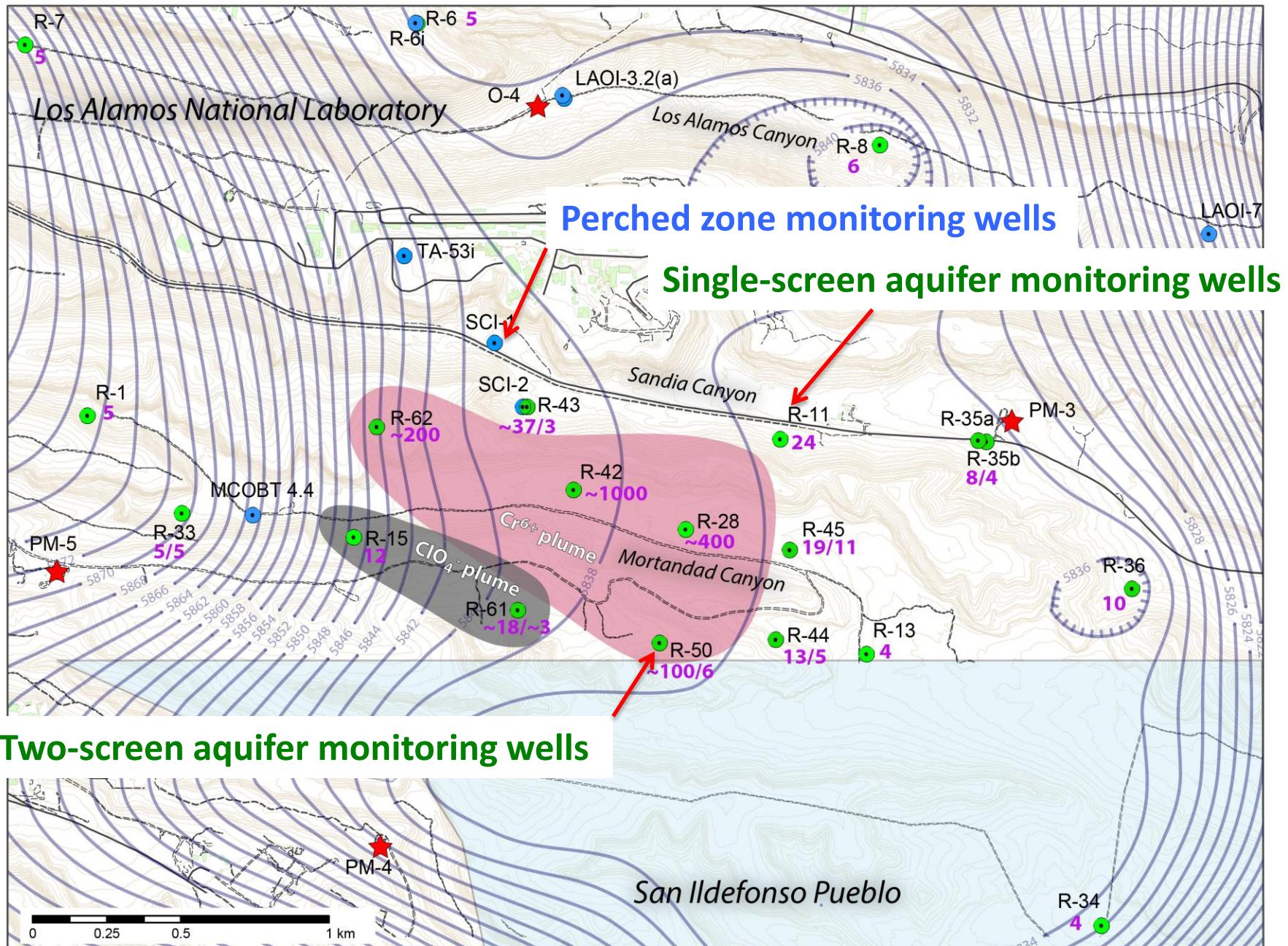
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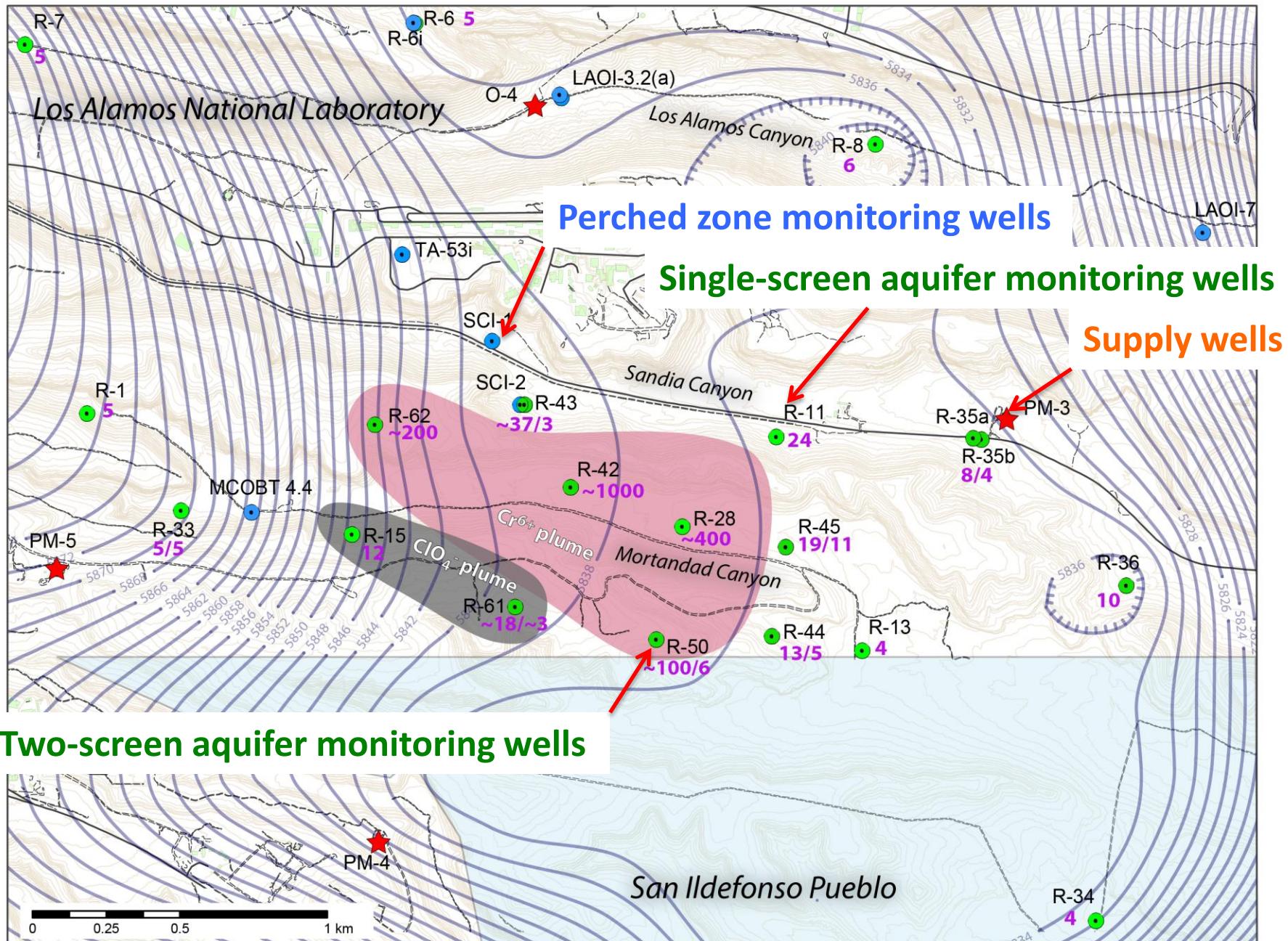
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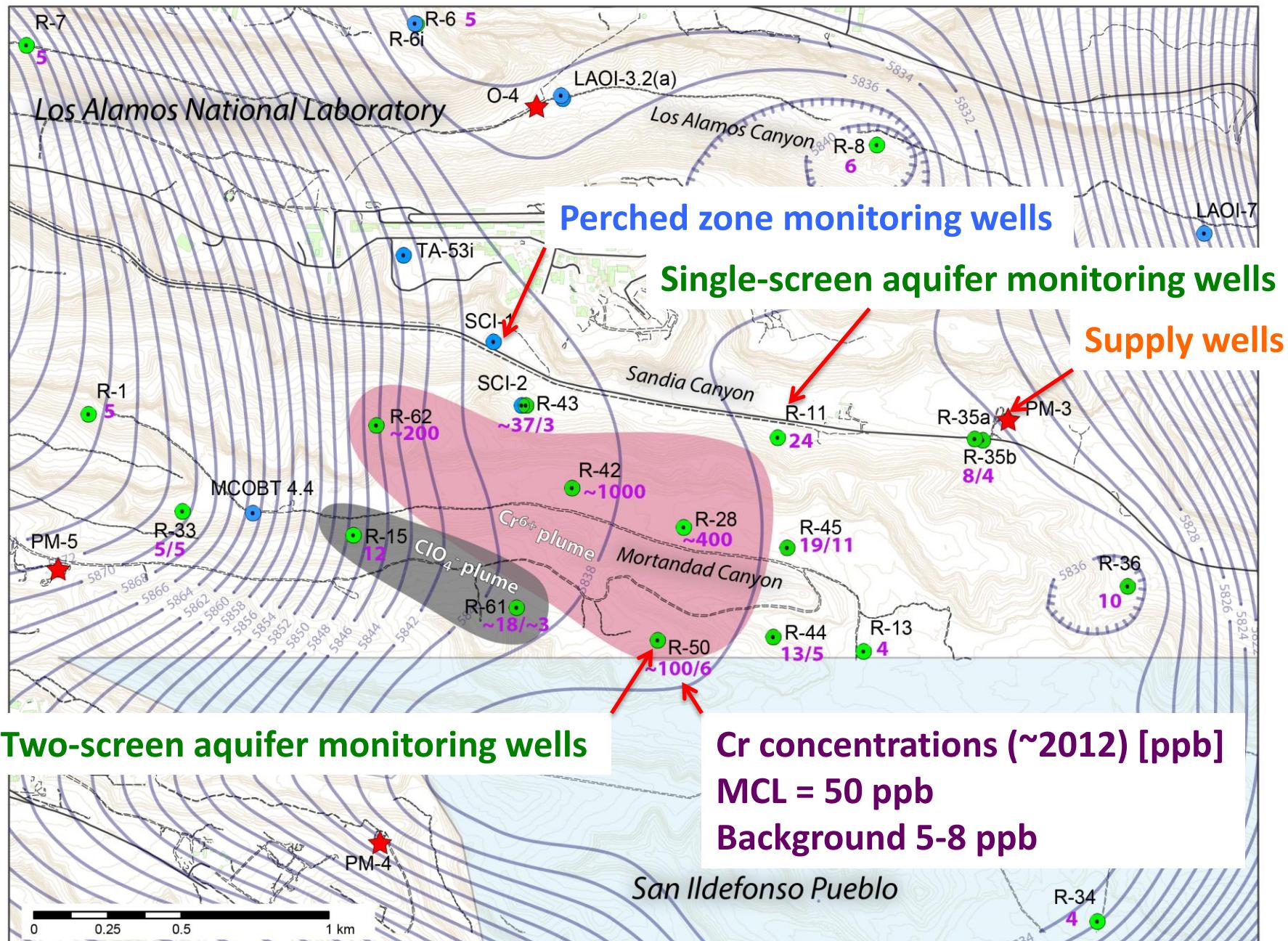
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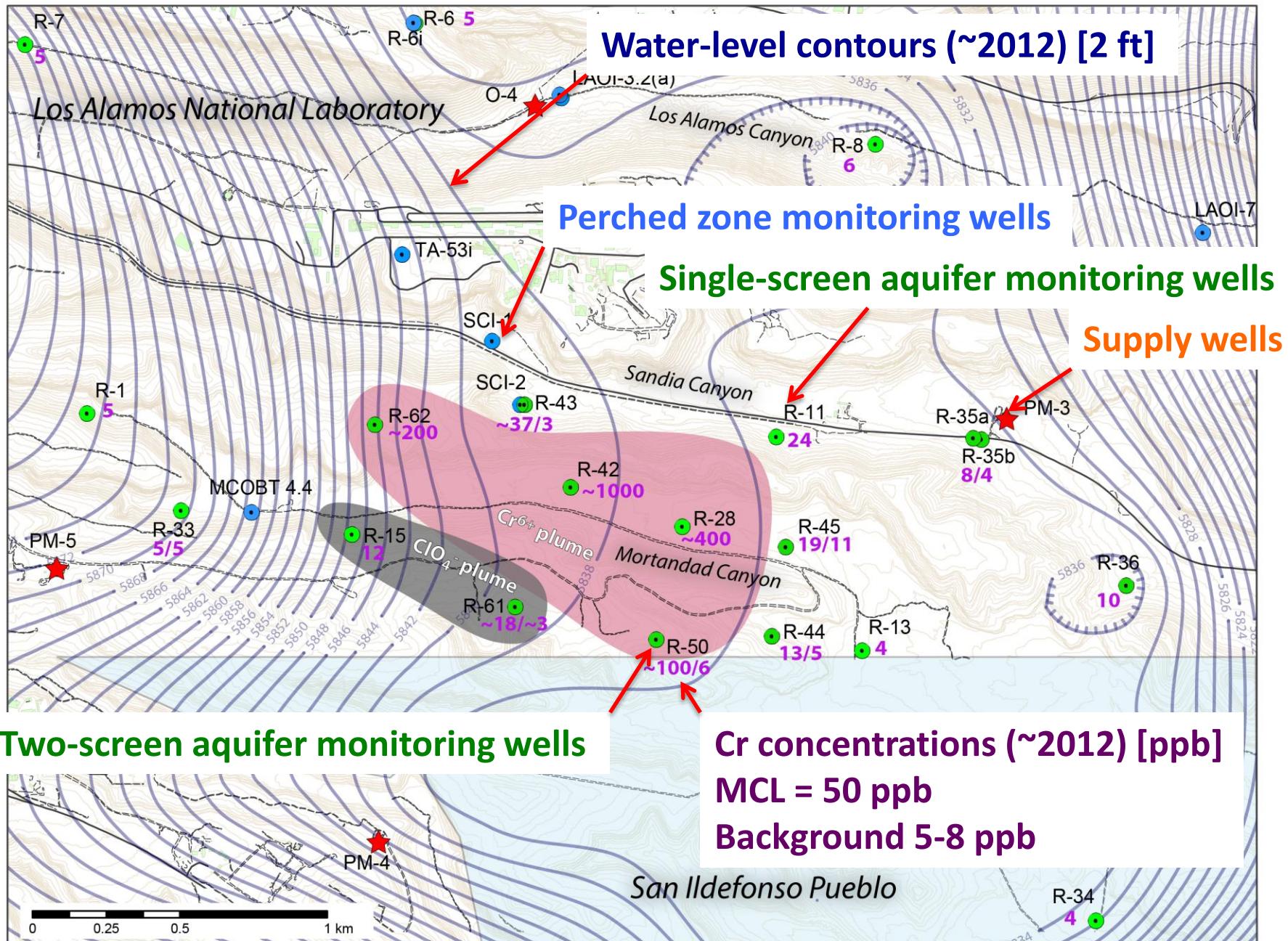
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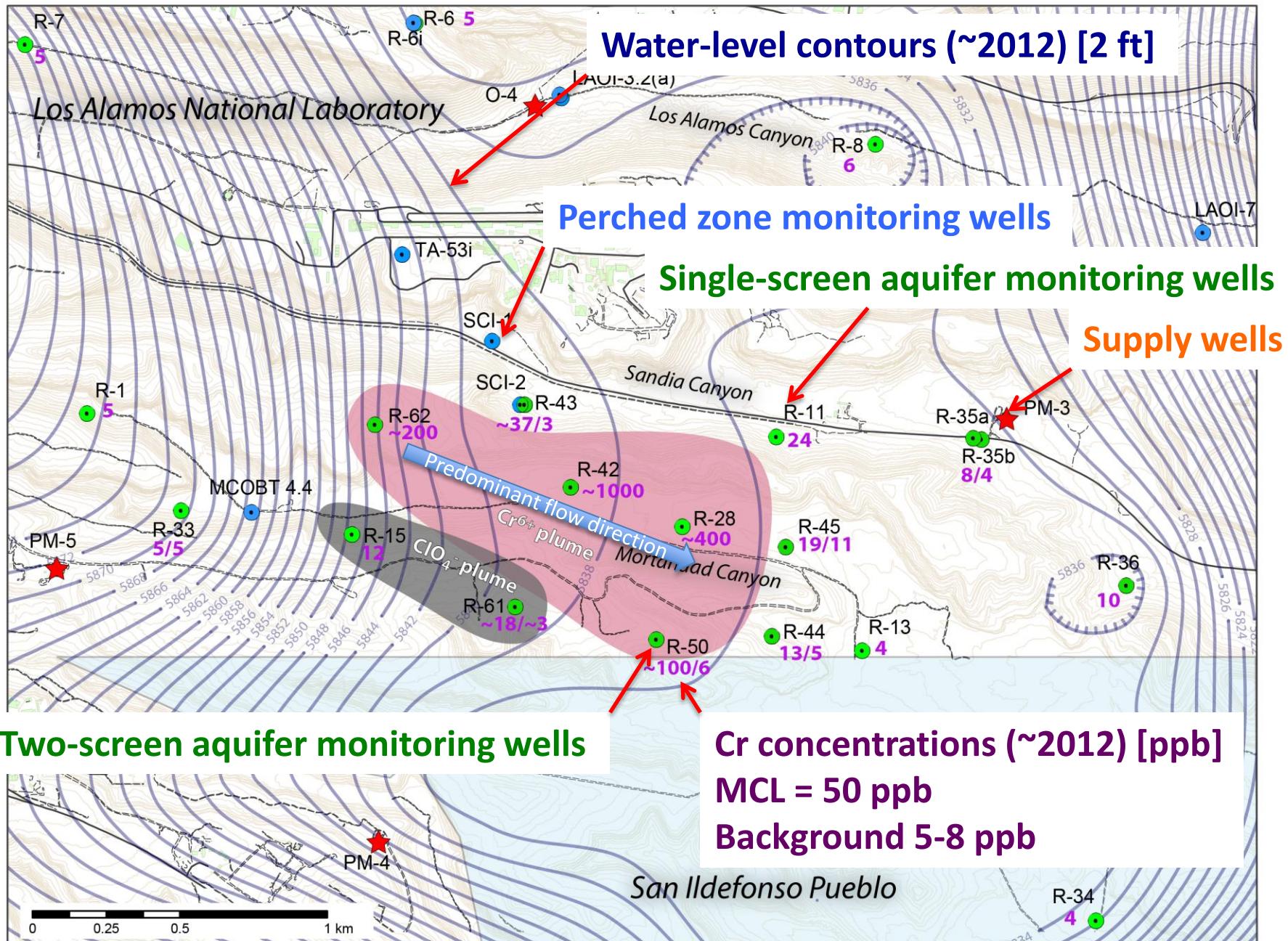
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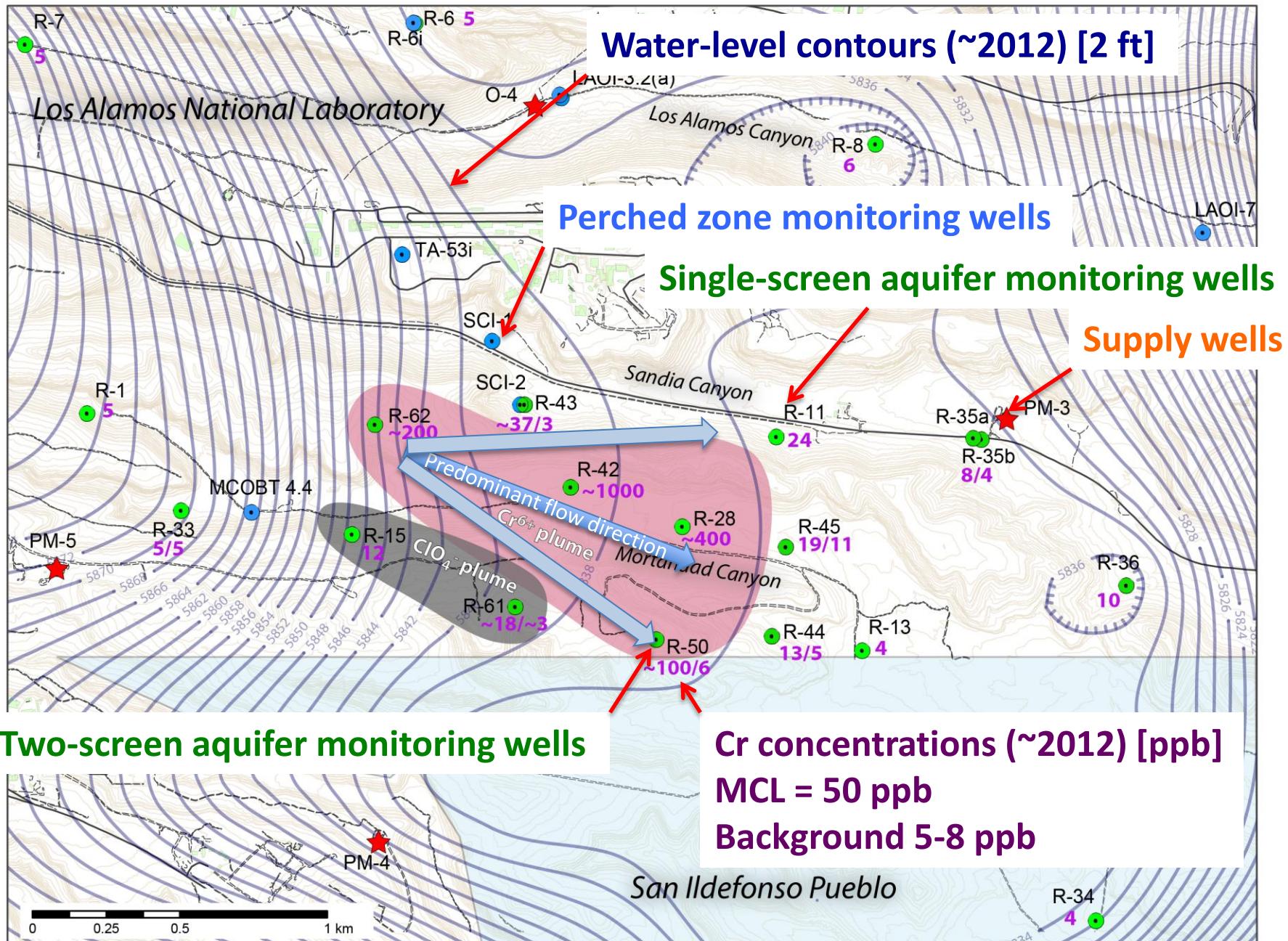
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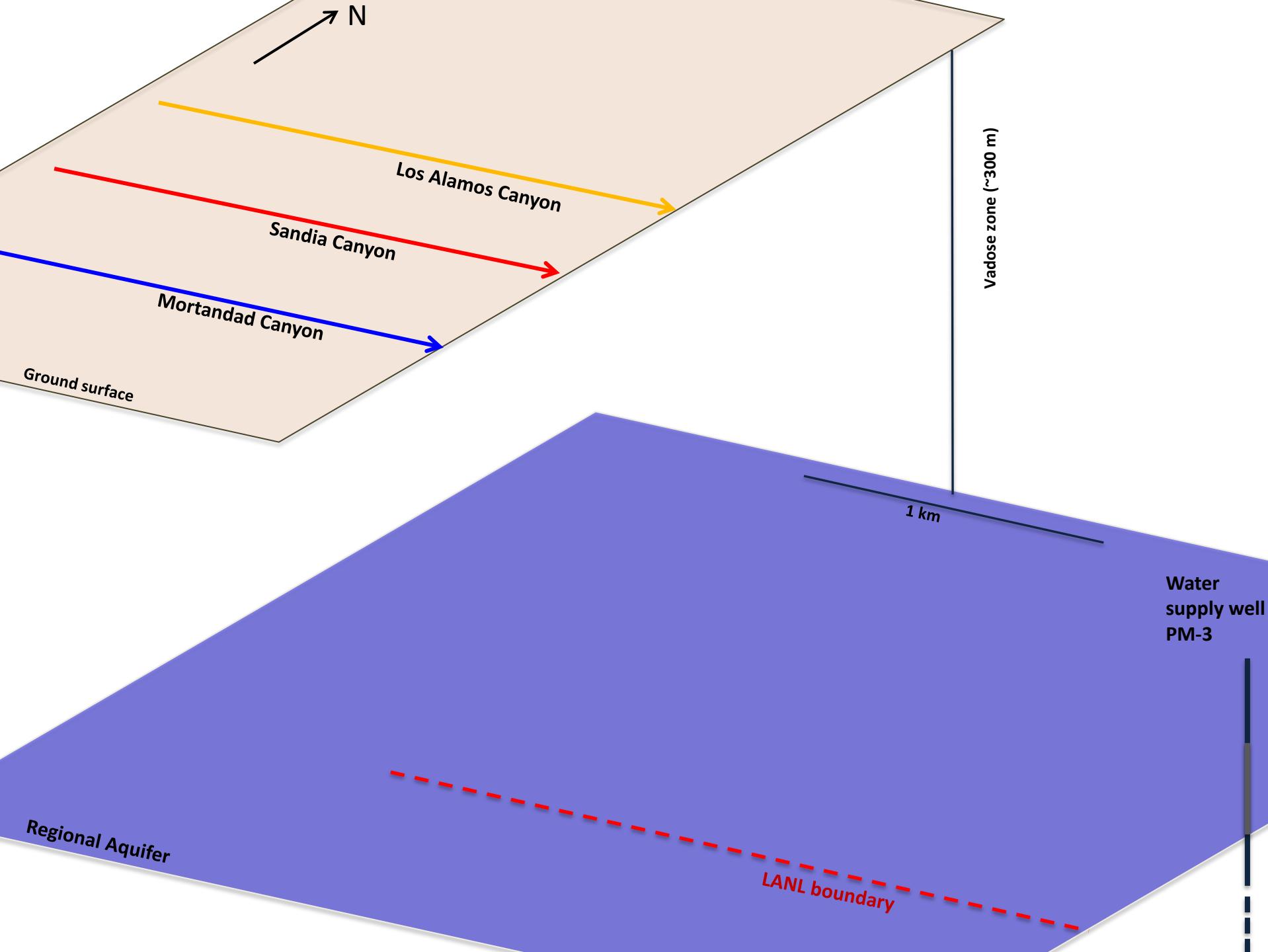


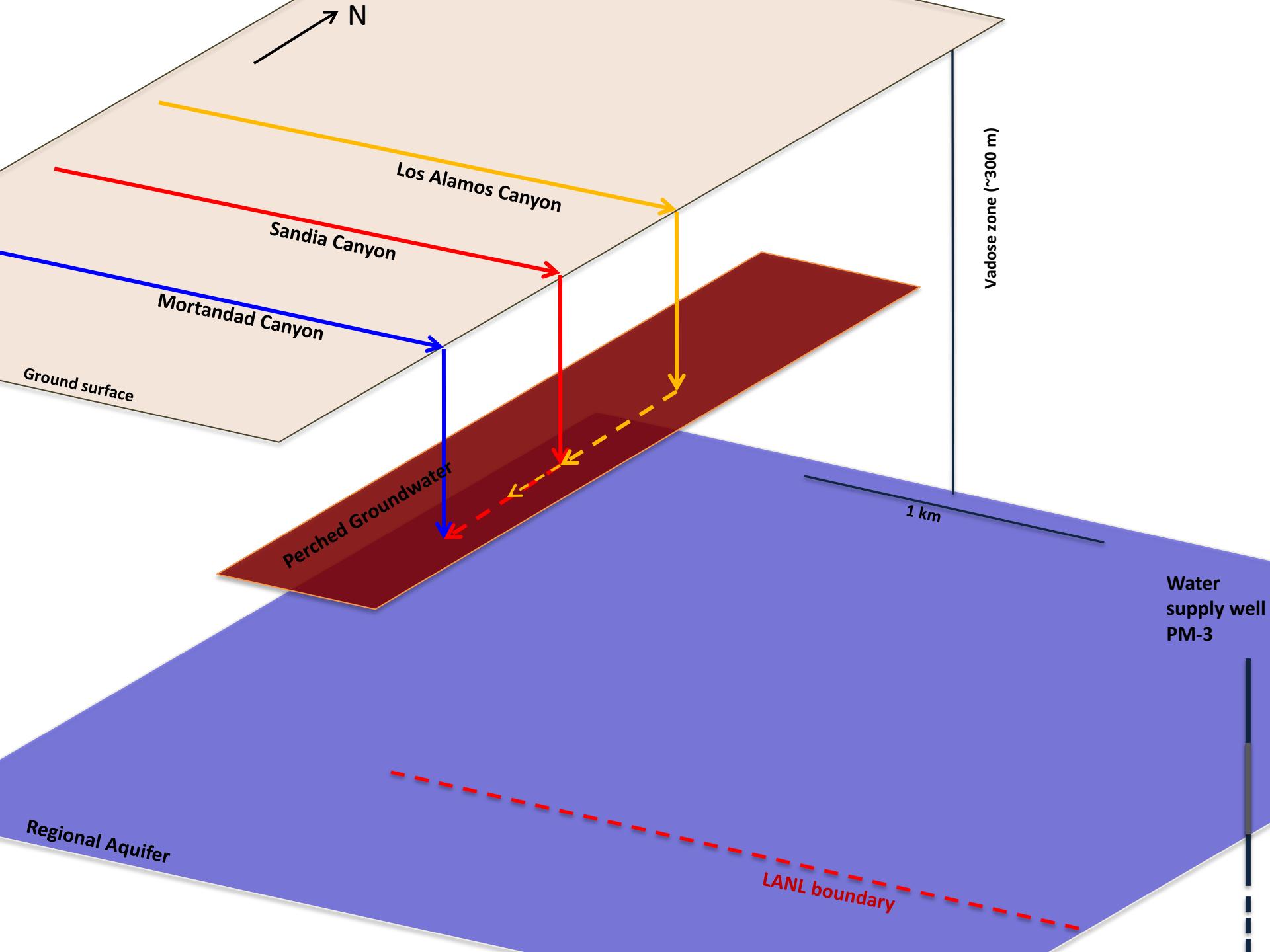
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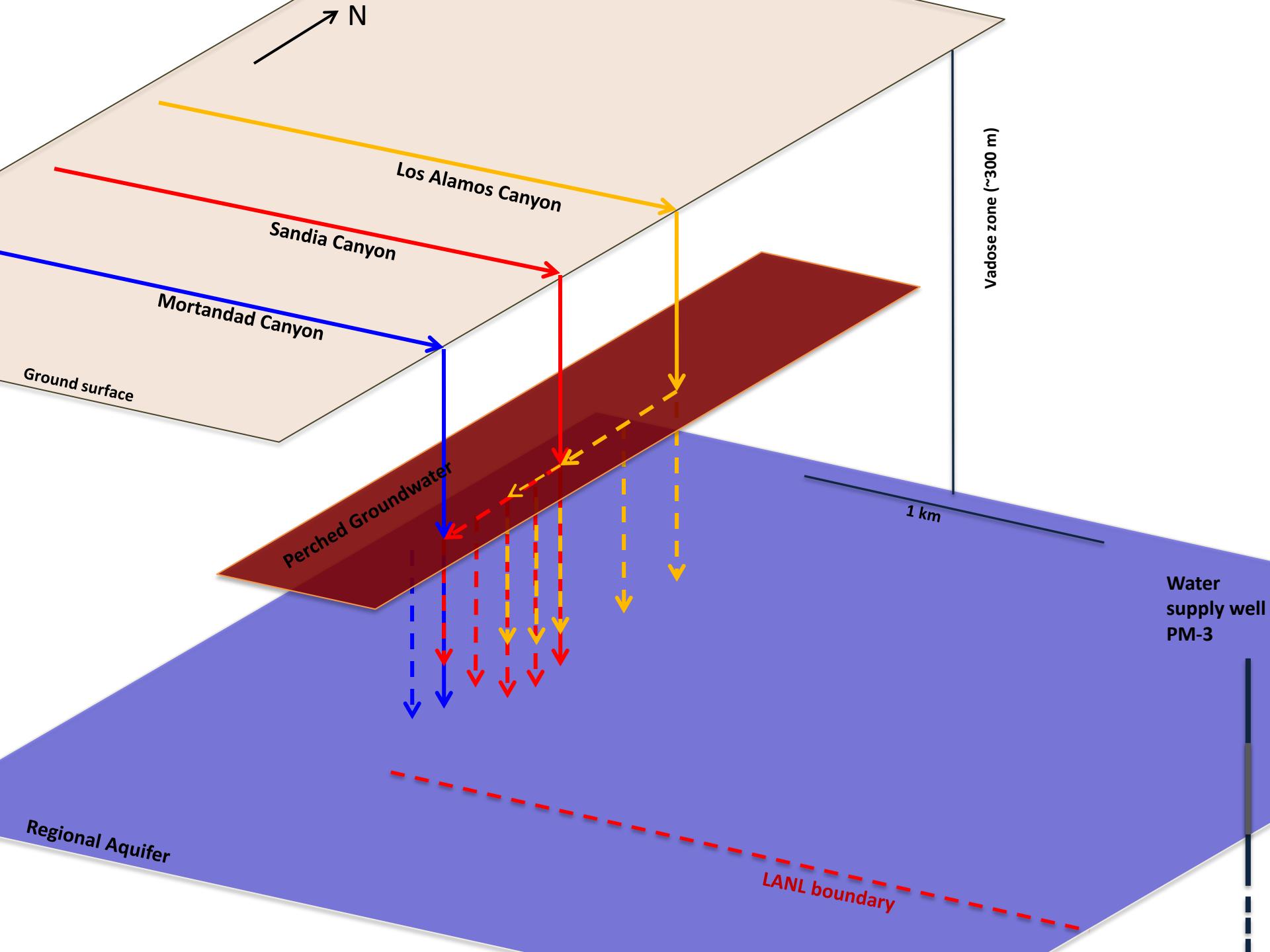


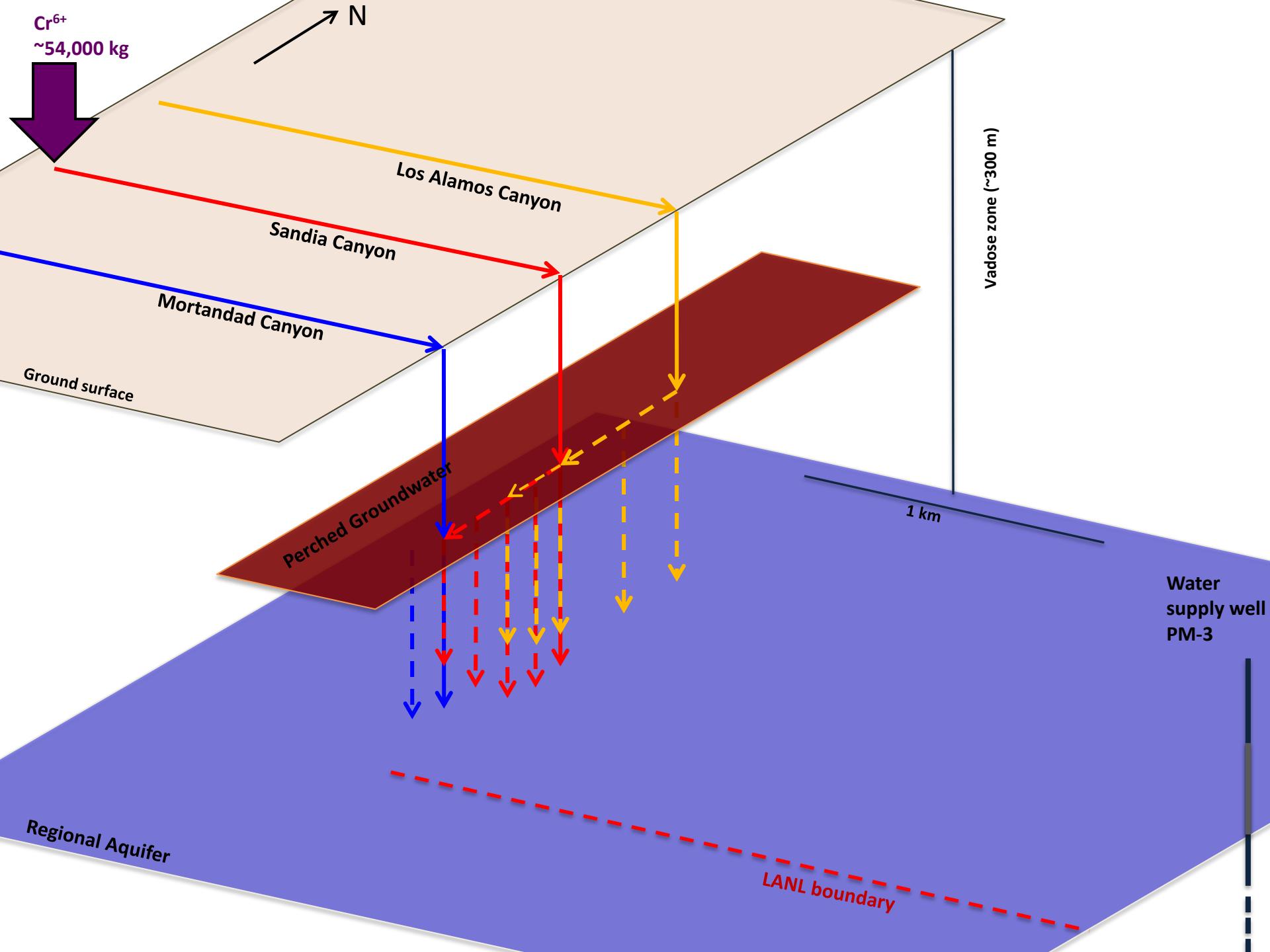
LANL Chromium site

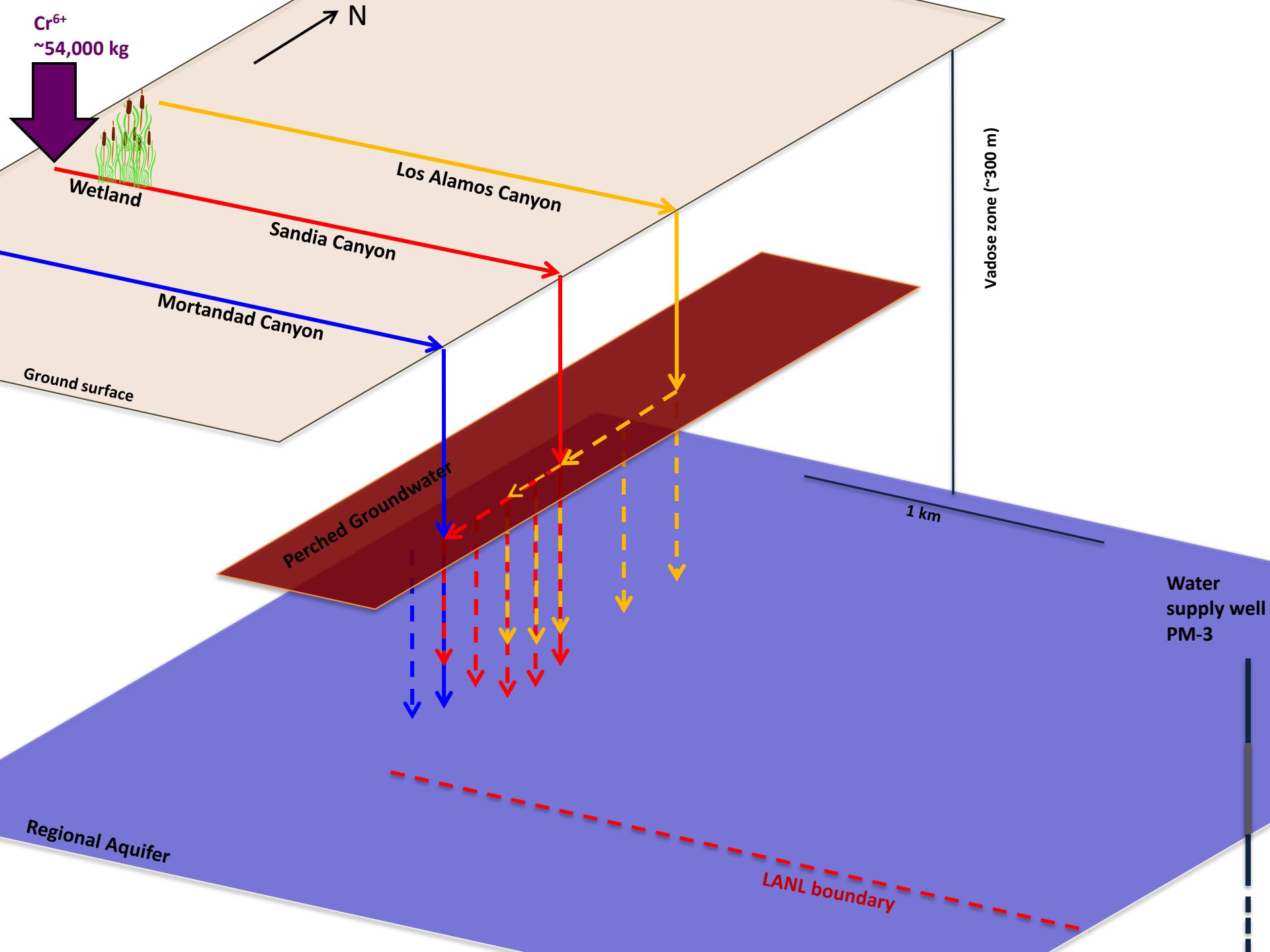
- ✧ ~54,000 kg of Cr⁶⁺ released in Sandia Canyon between 1956 and 1972
- ✧ Cr⁶⁺ detected above MCL (50 ppb; NM standard) in 4 monitoring wells in the regional aquifer beneath LANL
- ✧ Cr⁶⁺ plume size is about 2 km² (region above MCL)
- ✧ Cr⁶⁺ plume is located near LANL site boundary
- ✧ Series of water-supply wells are located nearby
- ✧ Contaminant source location and mass flux at the top of the regional aquifer are unknown due to complex 3D pathways through the vadose zone
- ✧ Limited remedial options due to aquifer depth (~300 m below the ground surface) and complexities in the subsurface flow
- ✧ Current conceptual model for chromium migration in the subsurface is supported by multiple lines of evidence (hydrogeological, geophysical, mineralogic, petrographic, and geochemical studies and model analyses)

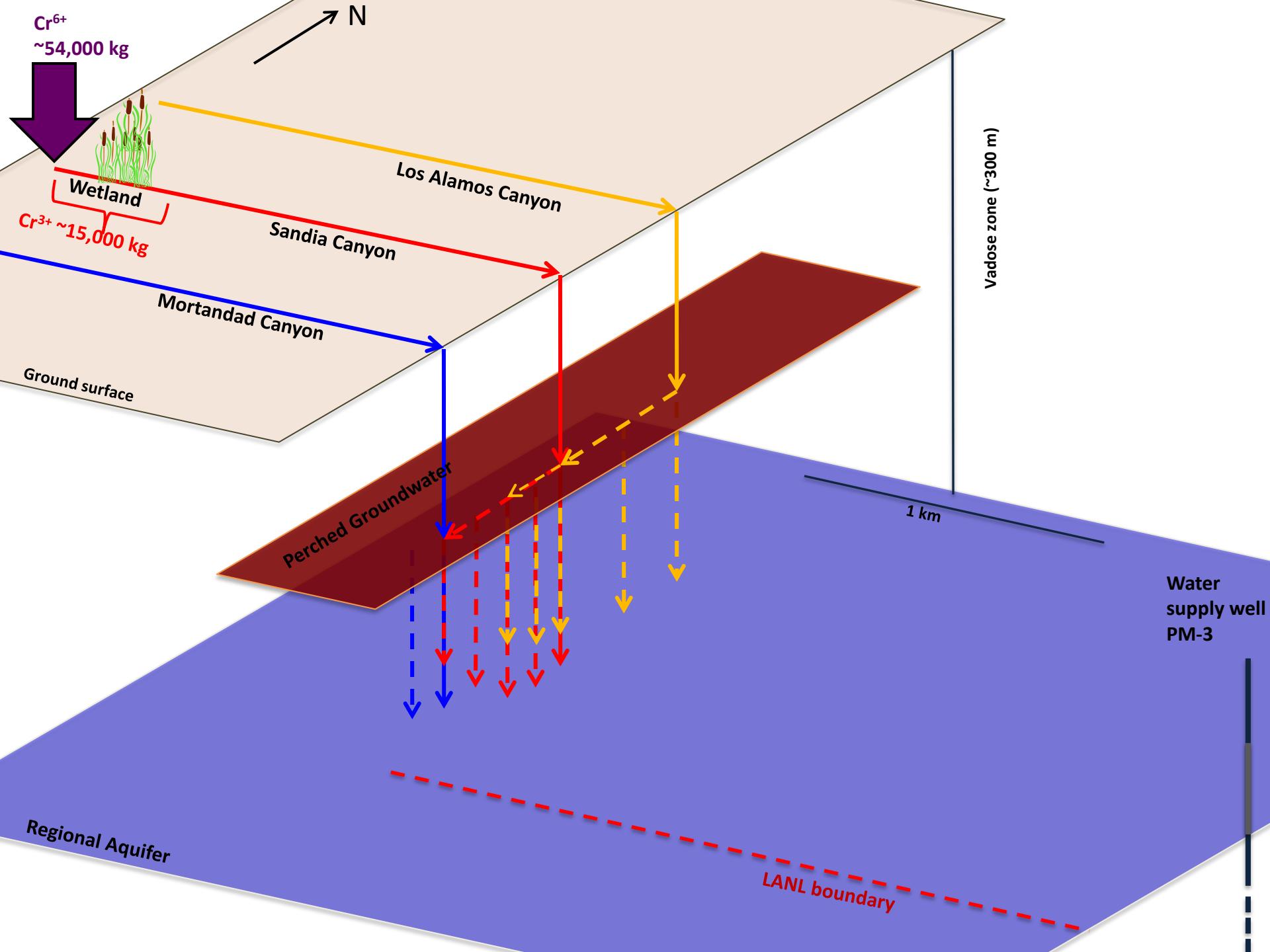


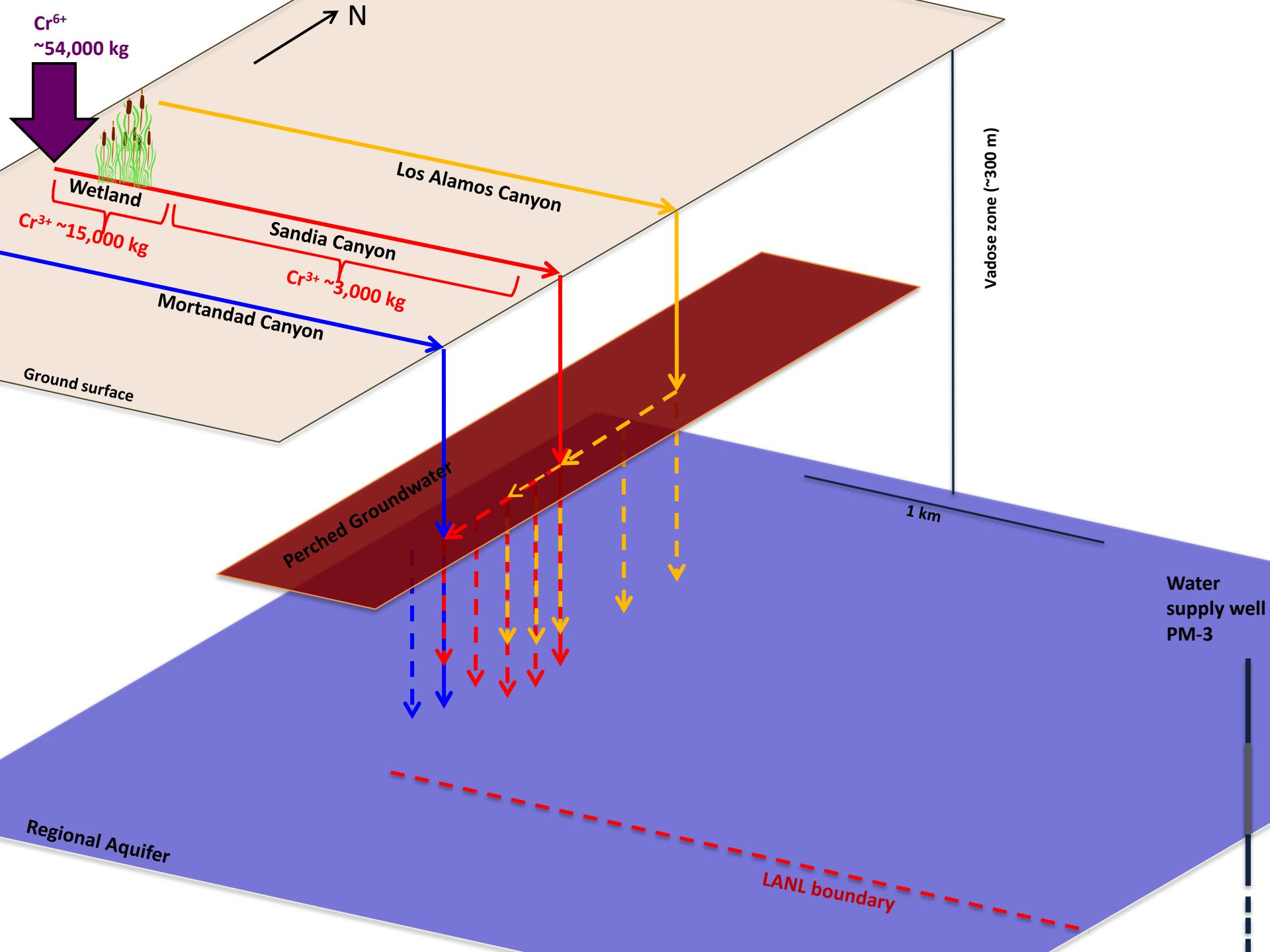


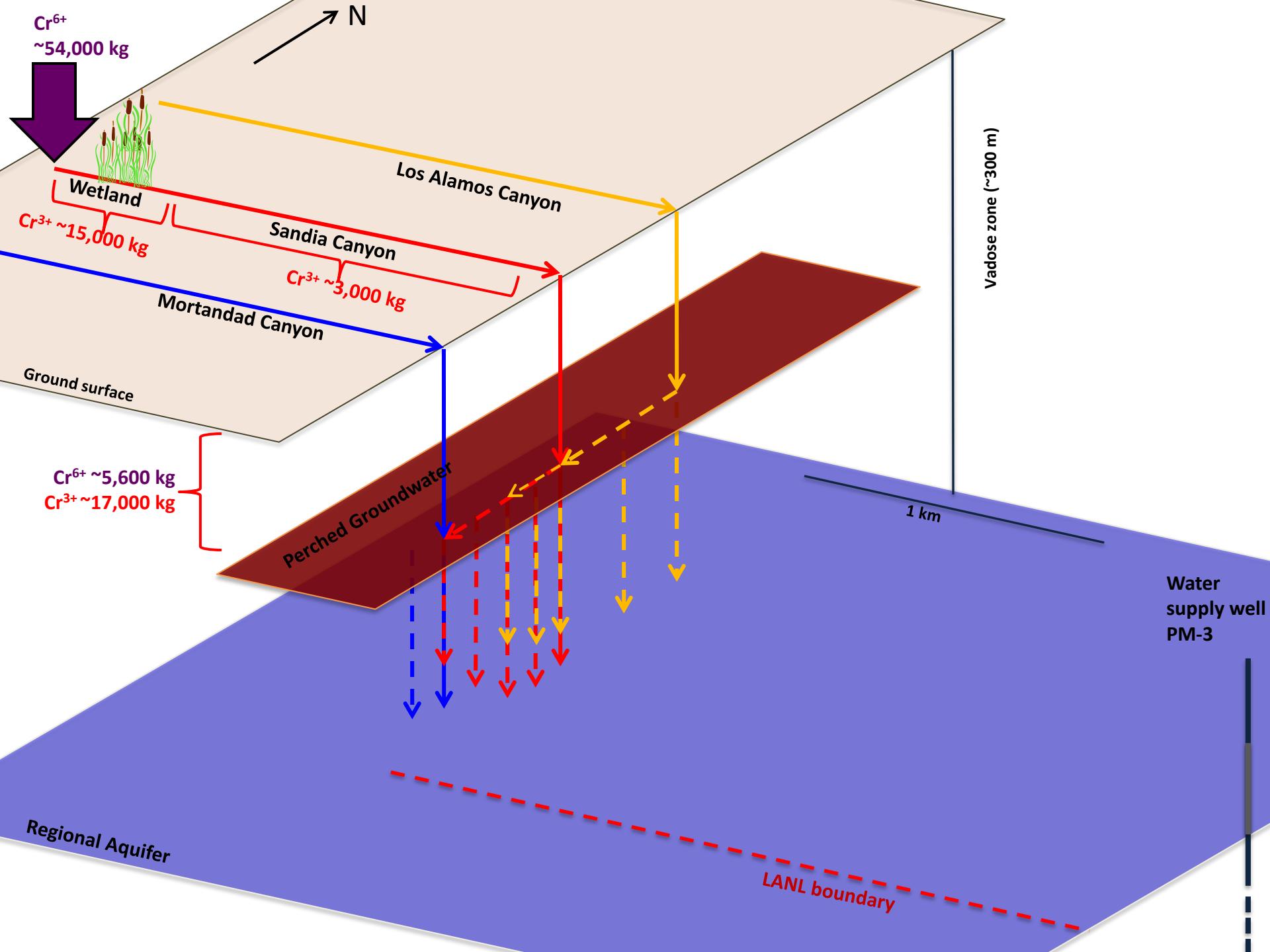


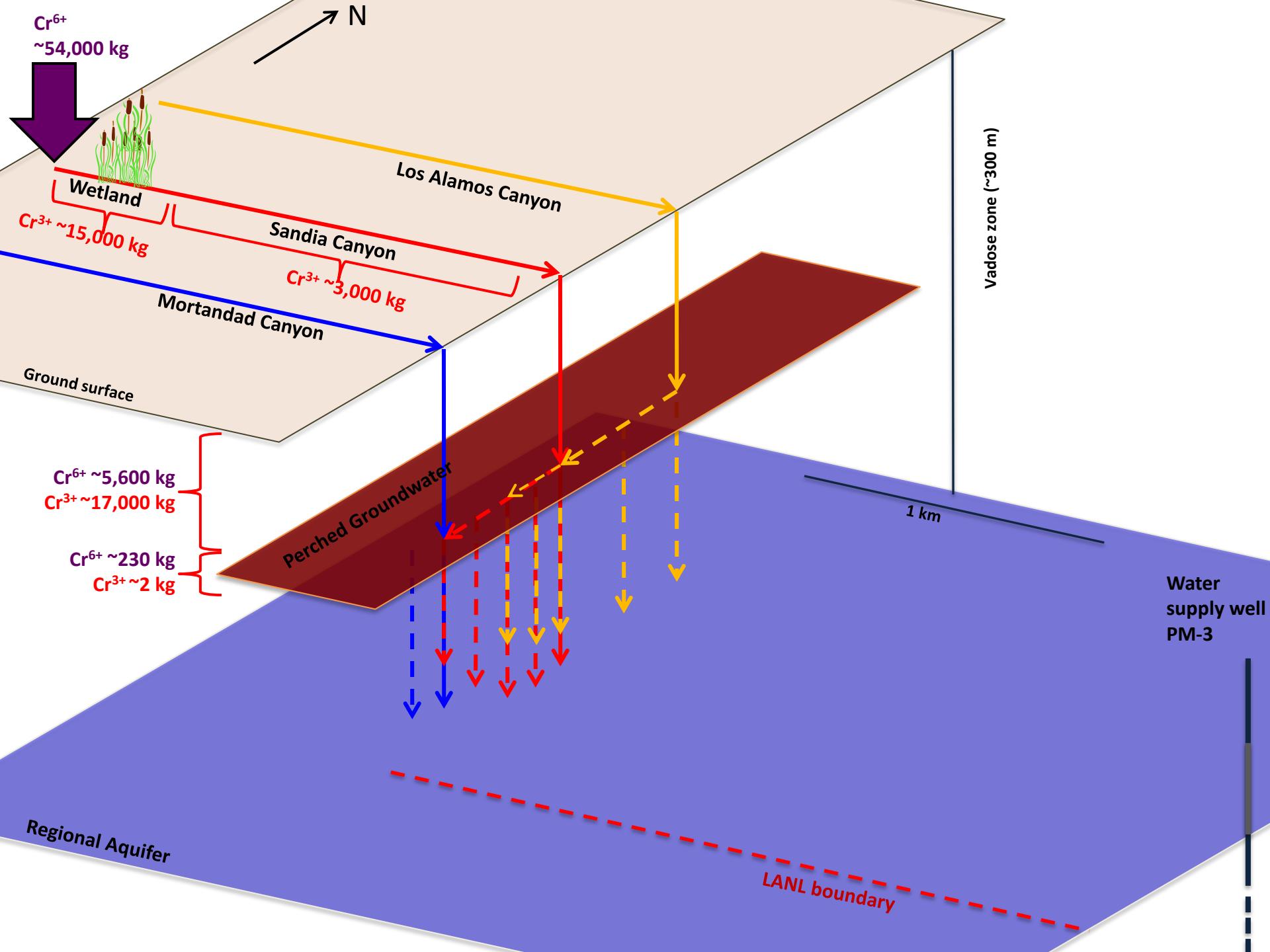


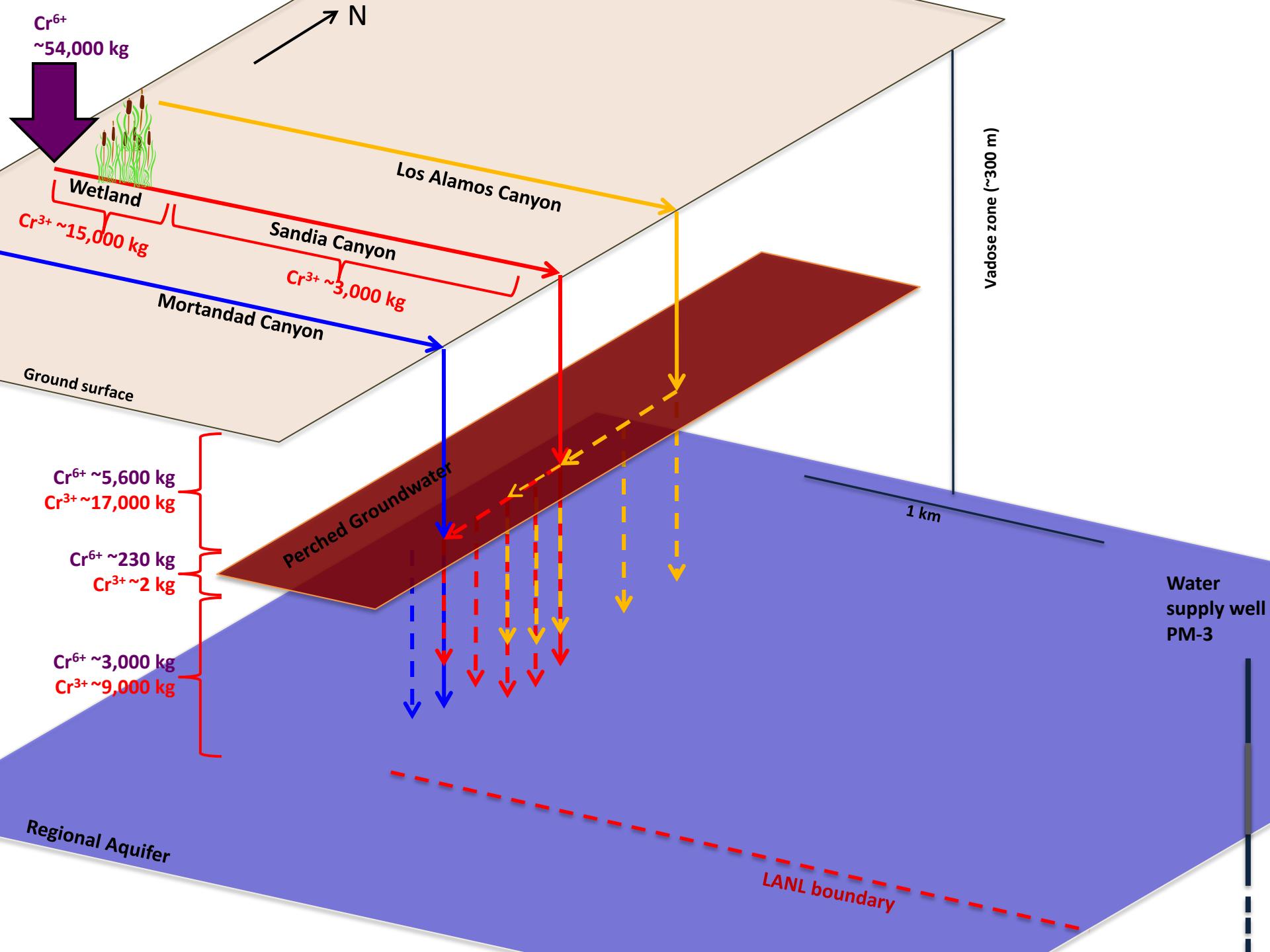


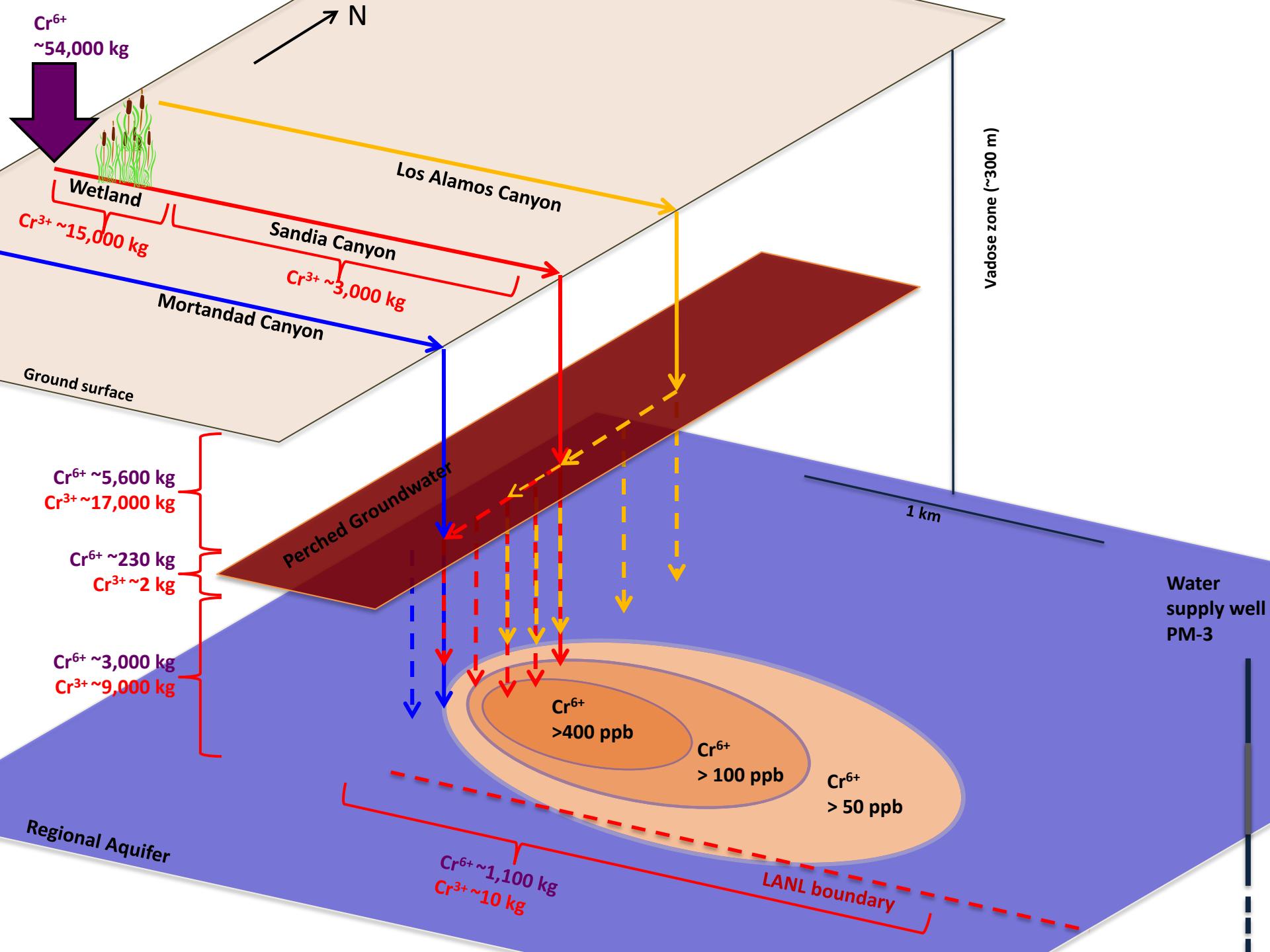


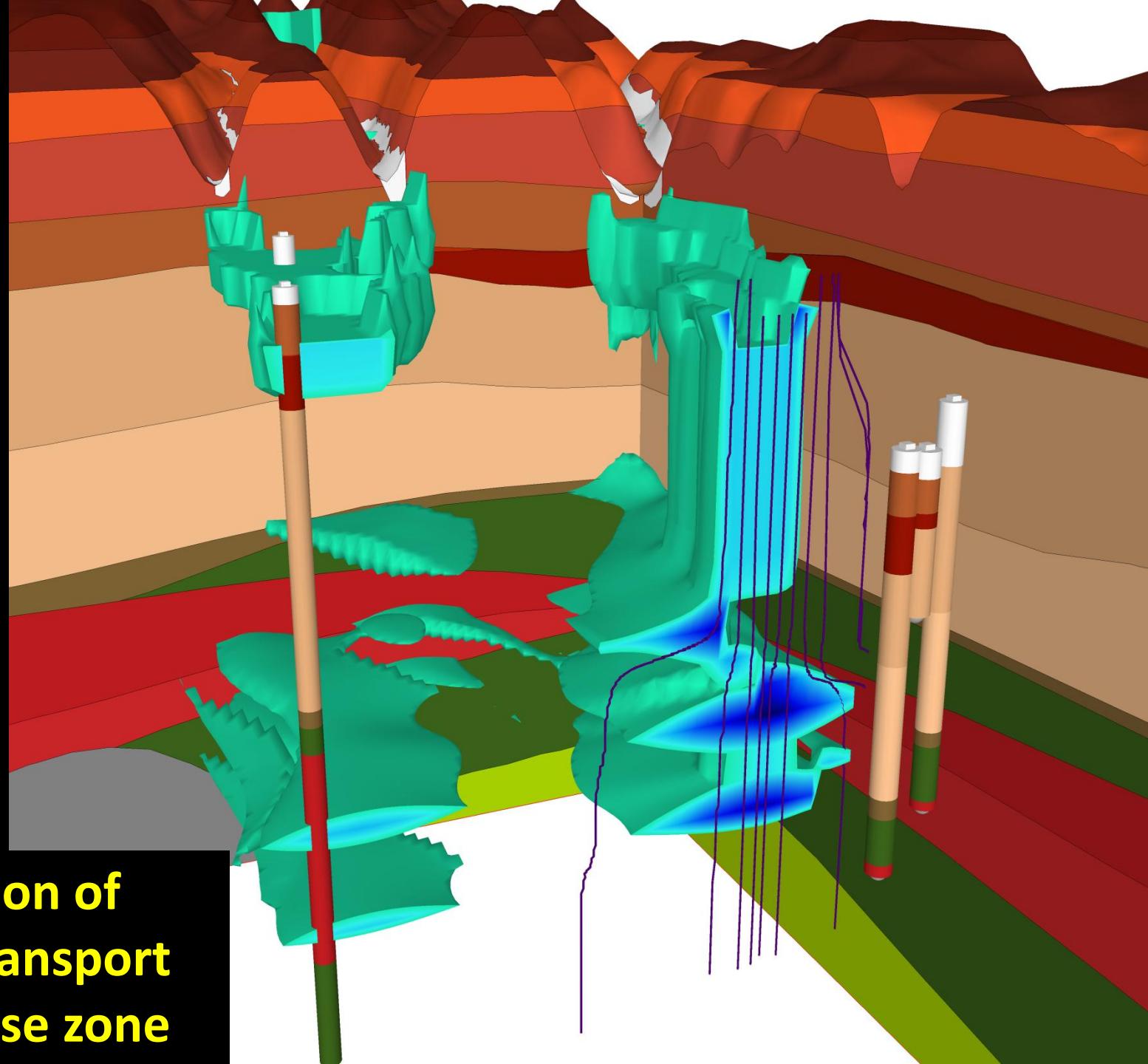








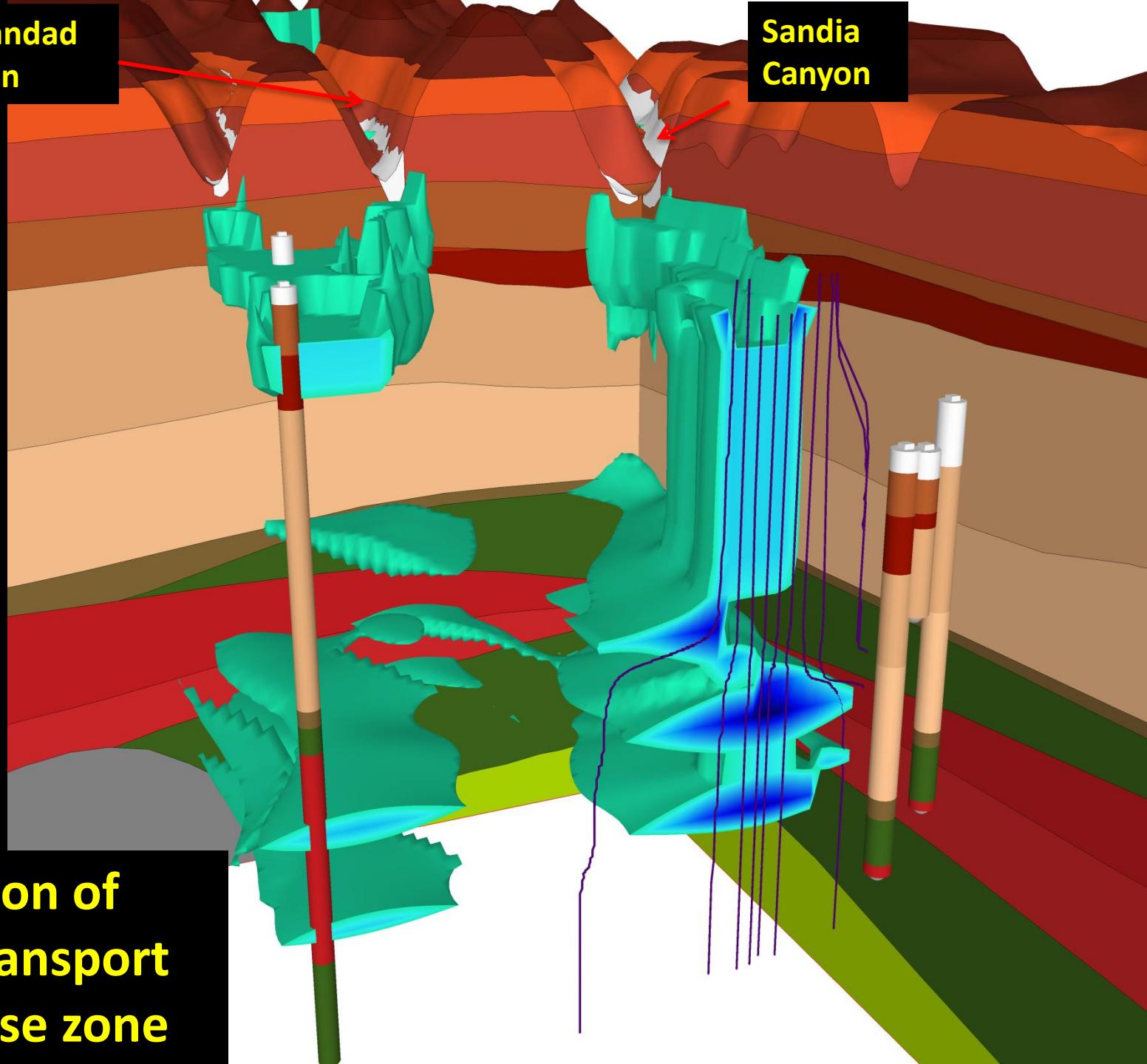




**3D simulation of
flow and transport
in the vadose zone**

Mortandad
Canyon

Sandia
Canyon



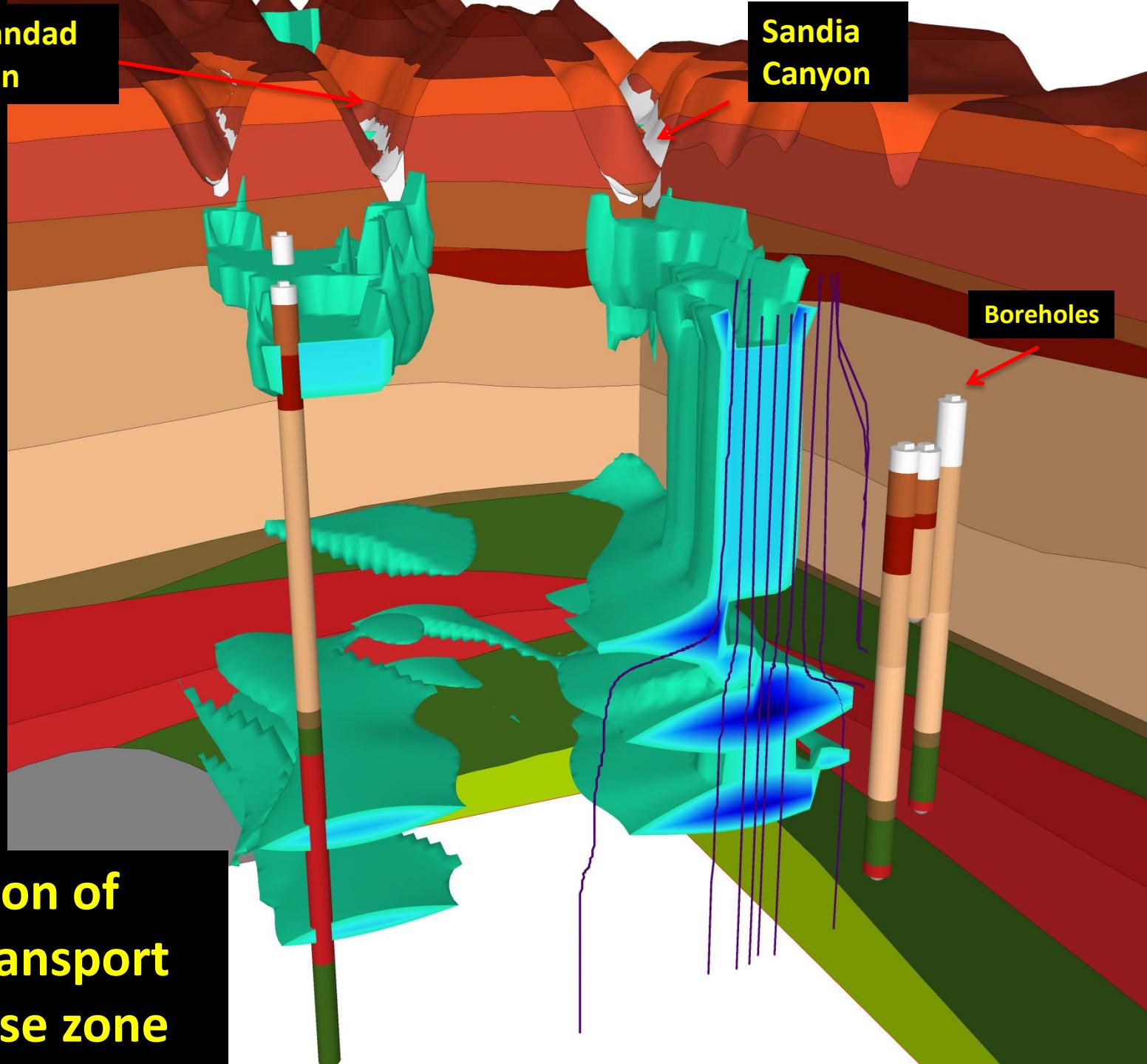
**3D simulation of
flow and transport
in the vadose zone**

Mortandad
Canyon

Sandia
Canyon

Boreholes

3D simulation of
flow and transport
in the vadose zone



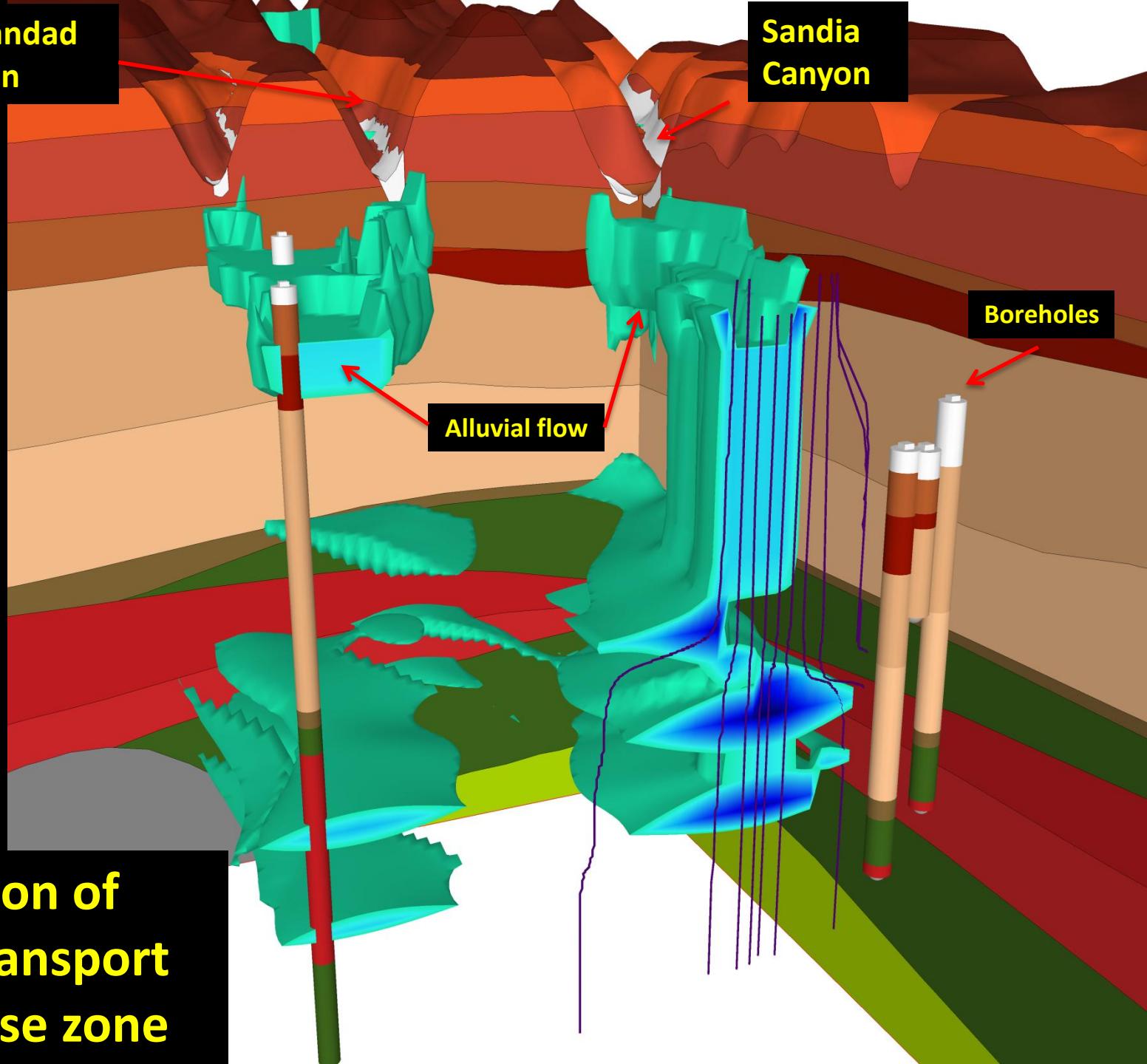
Mortandad
Canyon

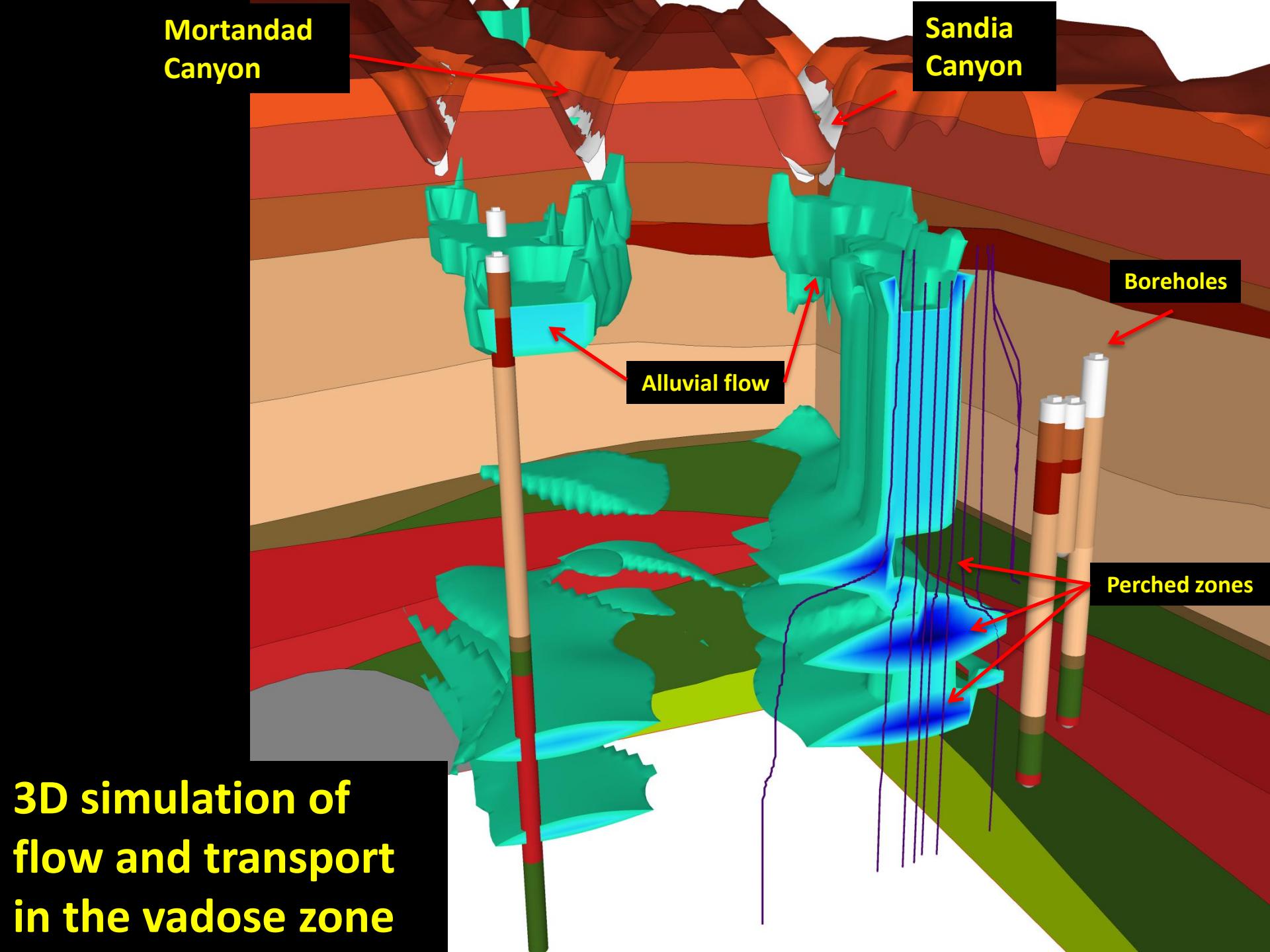
Sandia
Canyon

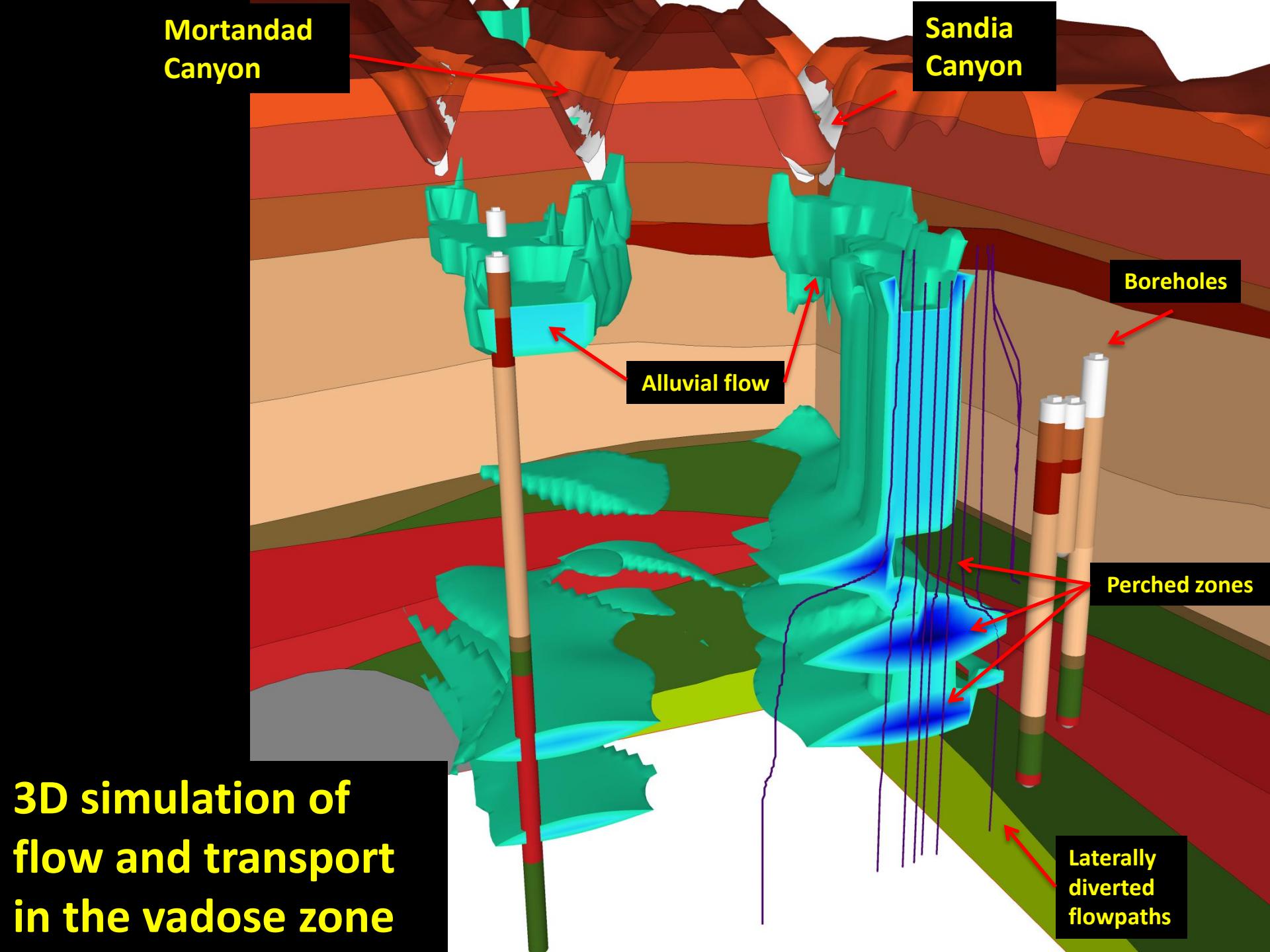
Boreholes

Alluvial flow

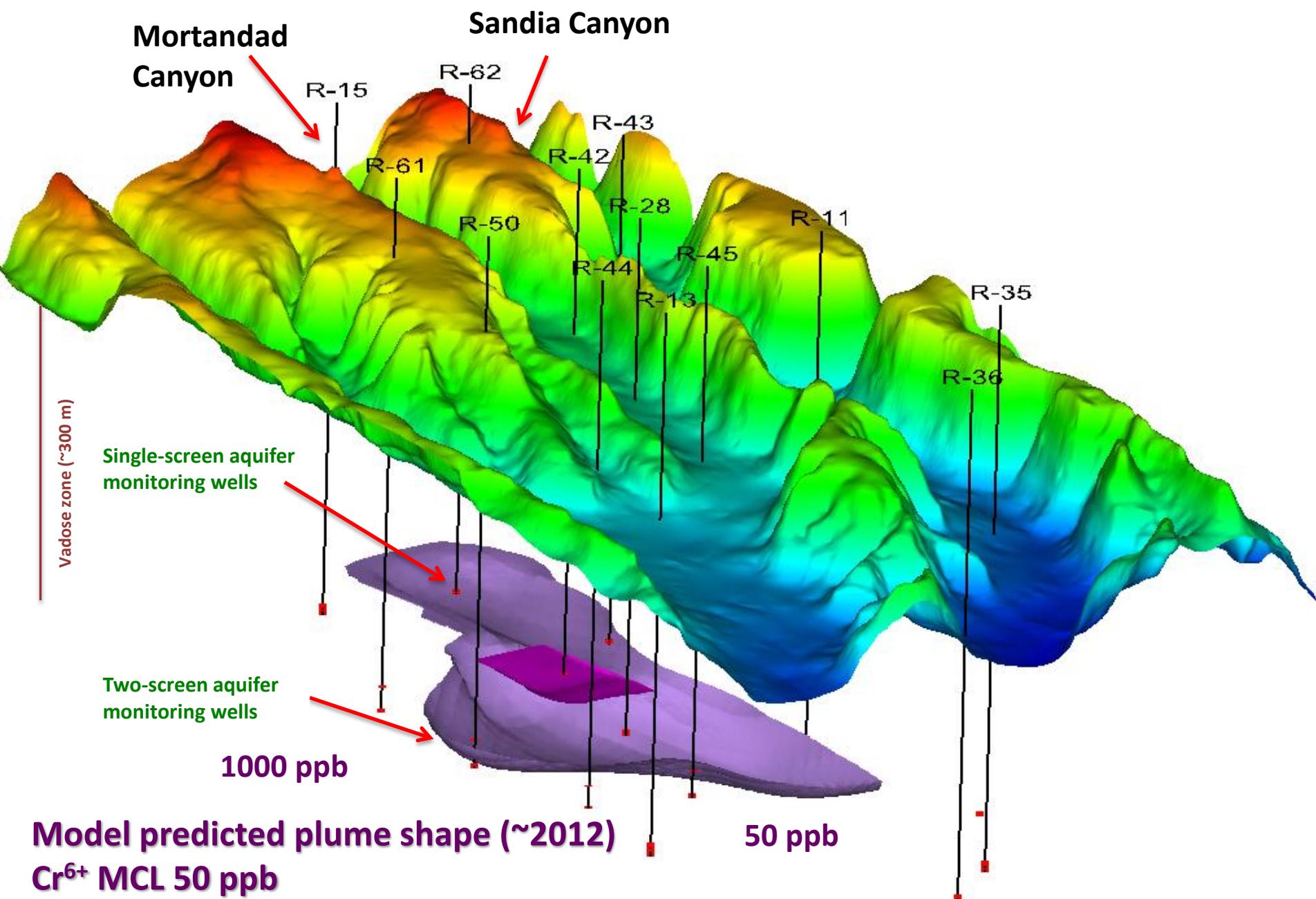
3D simulation of
flow and transport
in the vadose zone



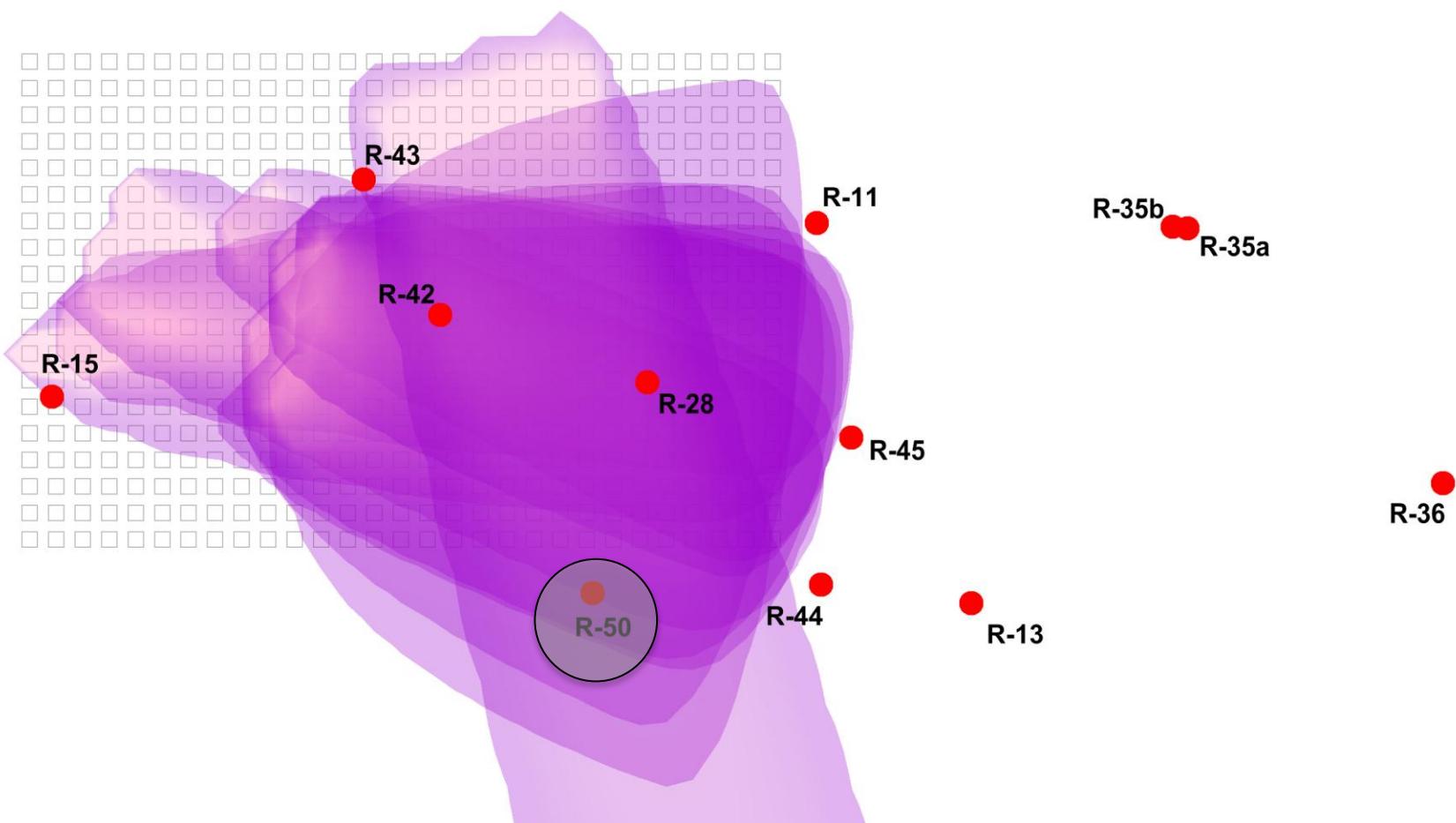




LANL chromium site

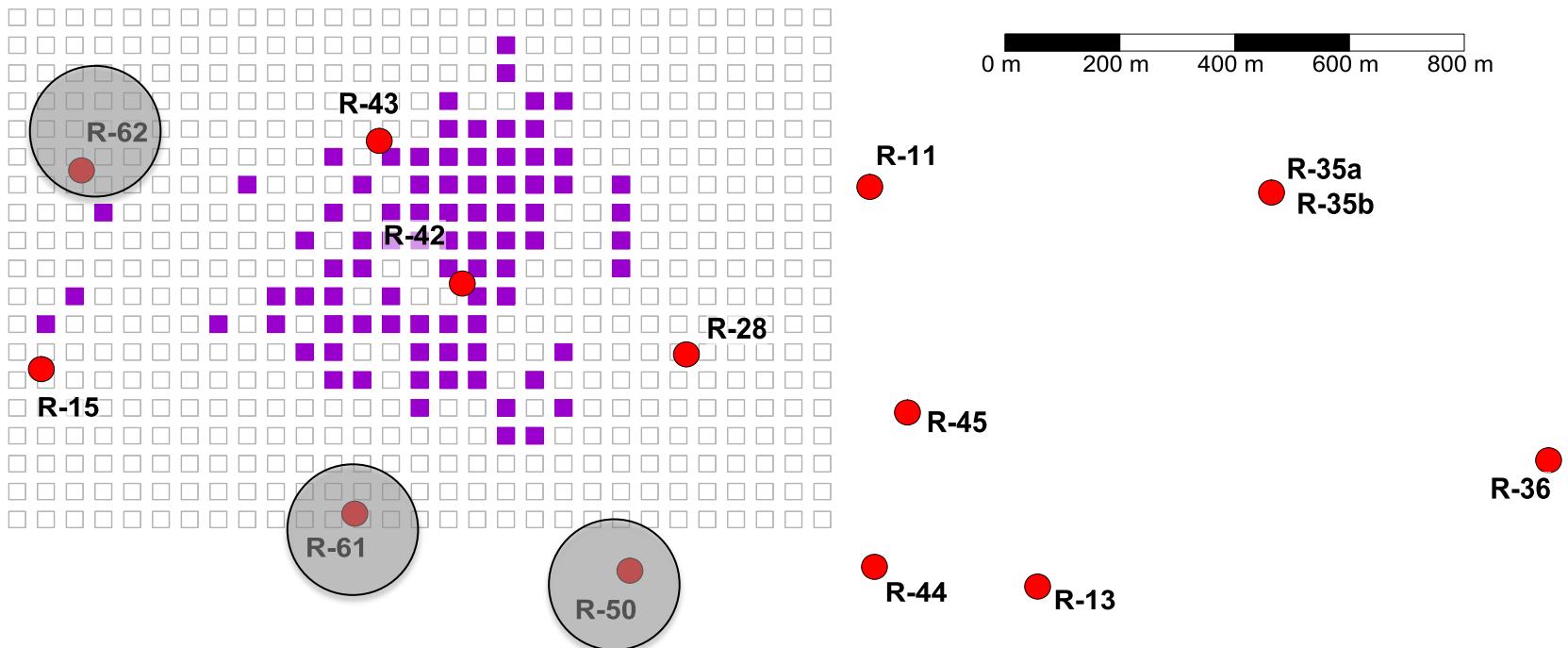


2009 model analyses for source identification / network design



- Due to uncertainties, a series of alternative models (plumes) are plausible
- Model predictions are constrained by all the available regional-aquifer data (hydrogeological and geochemical)
- 11 out 83 plausible plumes shown

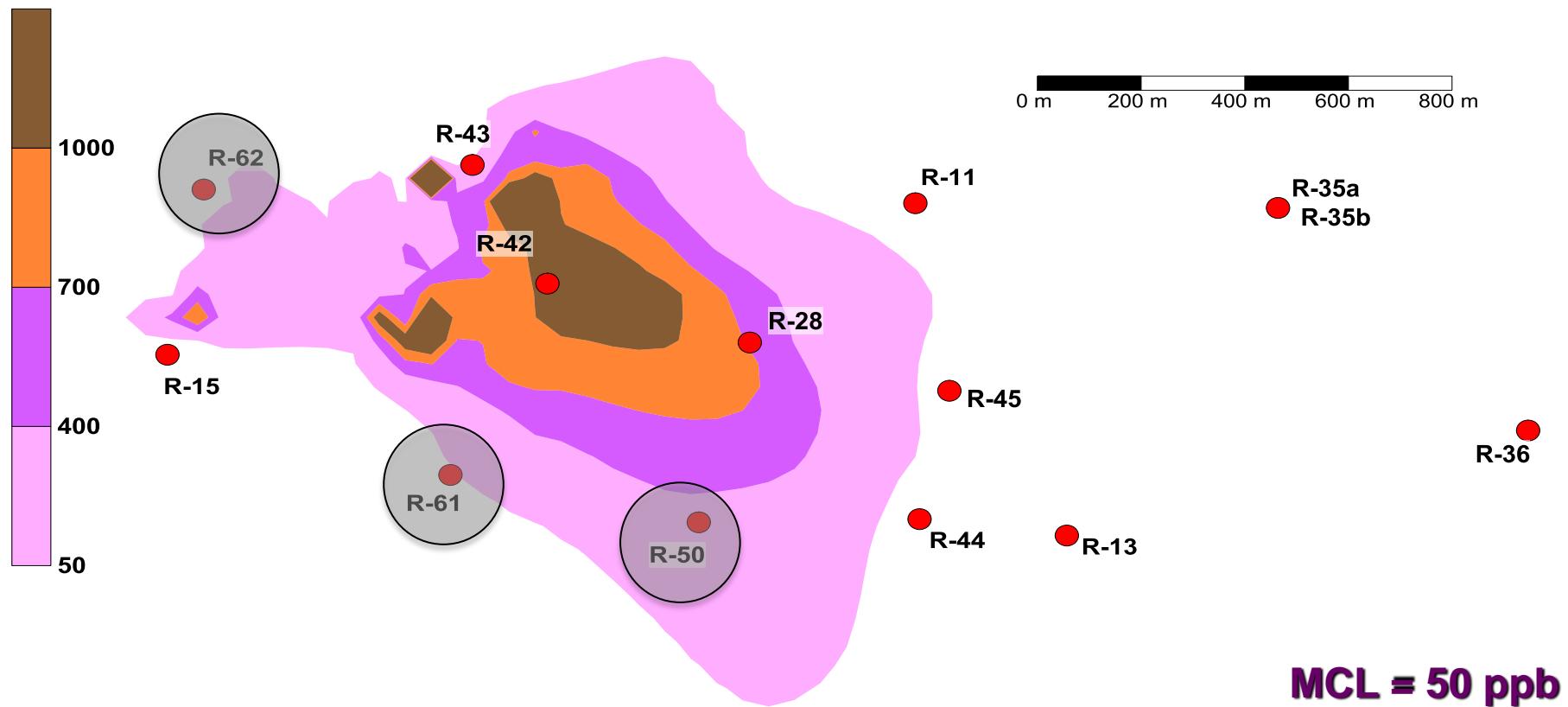
2009 model analyses for source identification / network design



Plausible contaminant-arrival locations (83 out of 551)
Wells R-62, R-61 and R-50 were not drilled yet

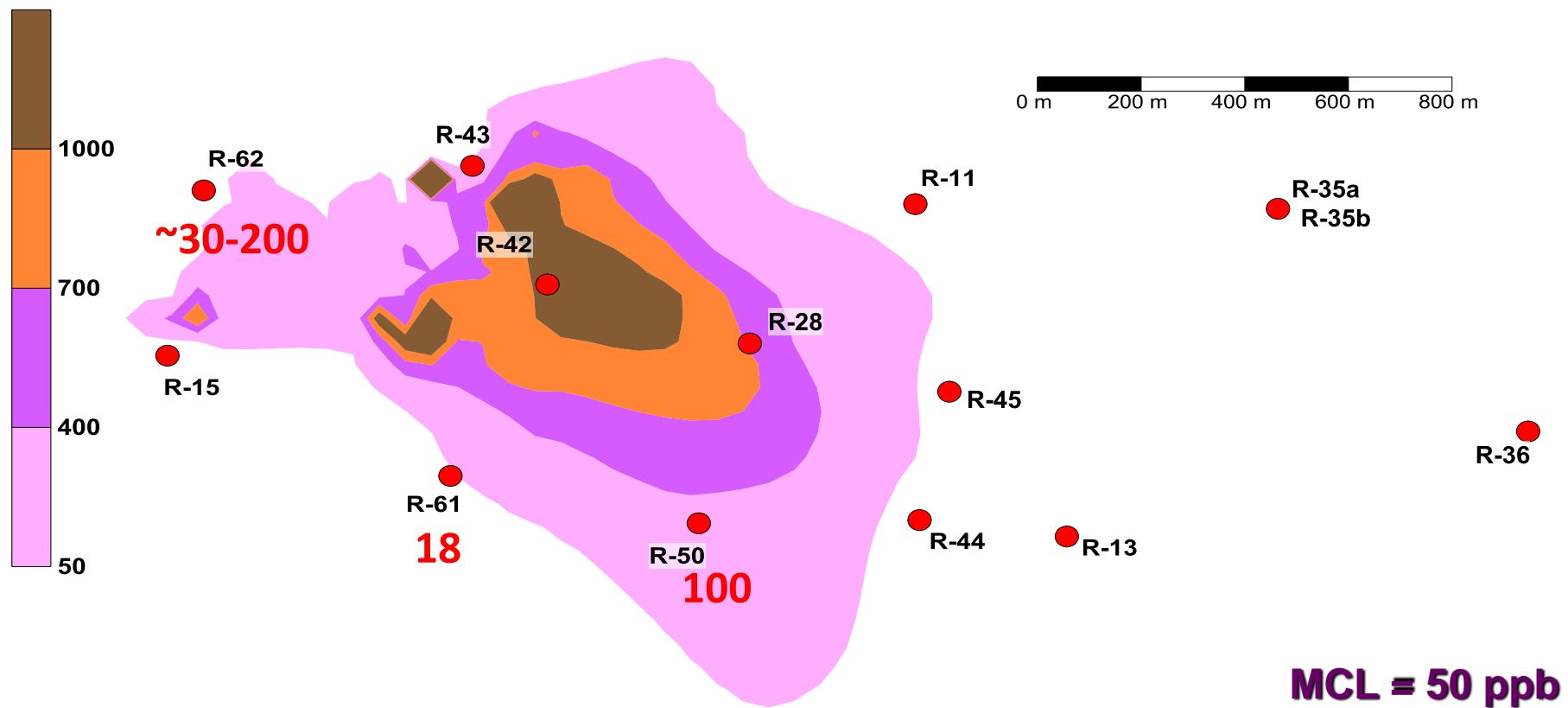
2009 model estimate of the plausible Cr⁶⁺ [ppb] along the regional aquifer water table

- ❖ 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



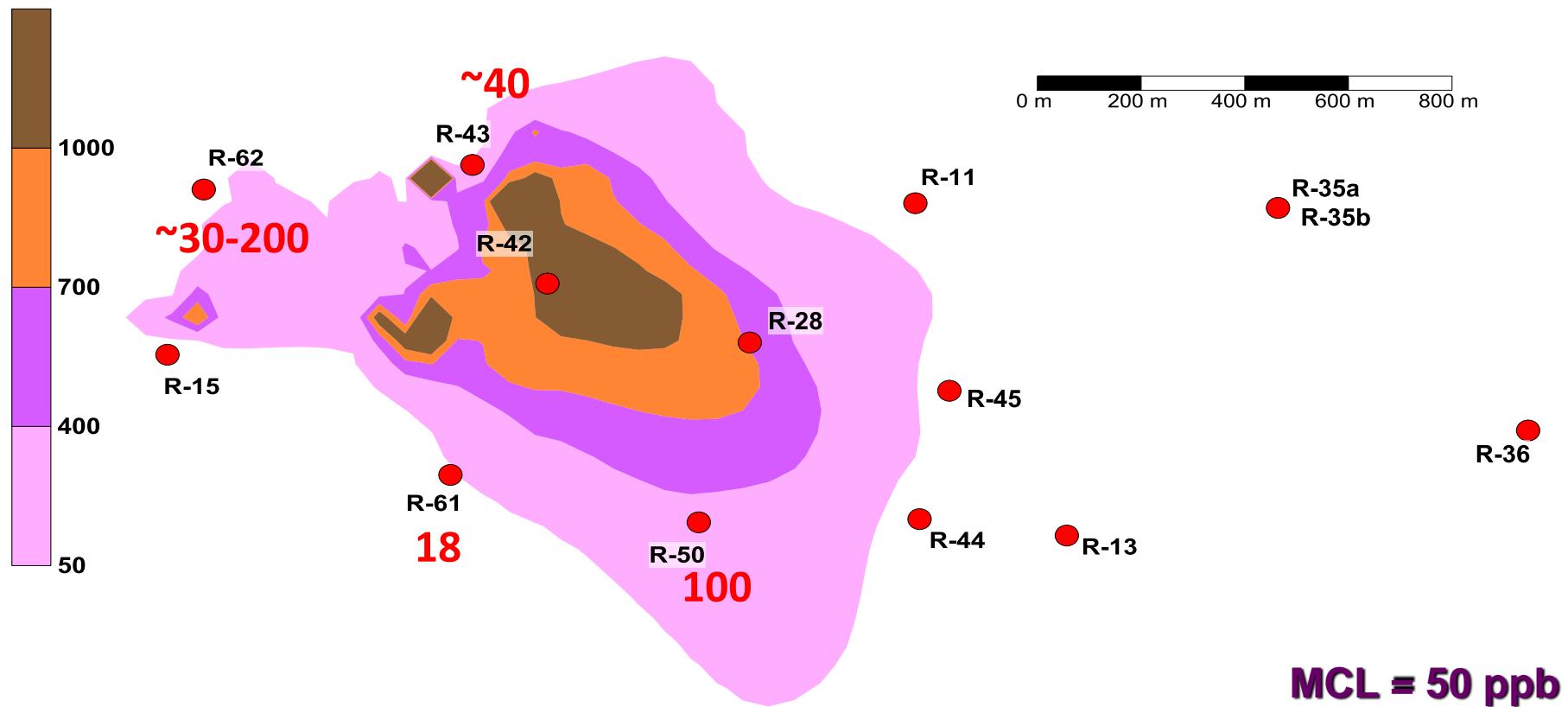
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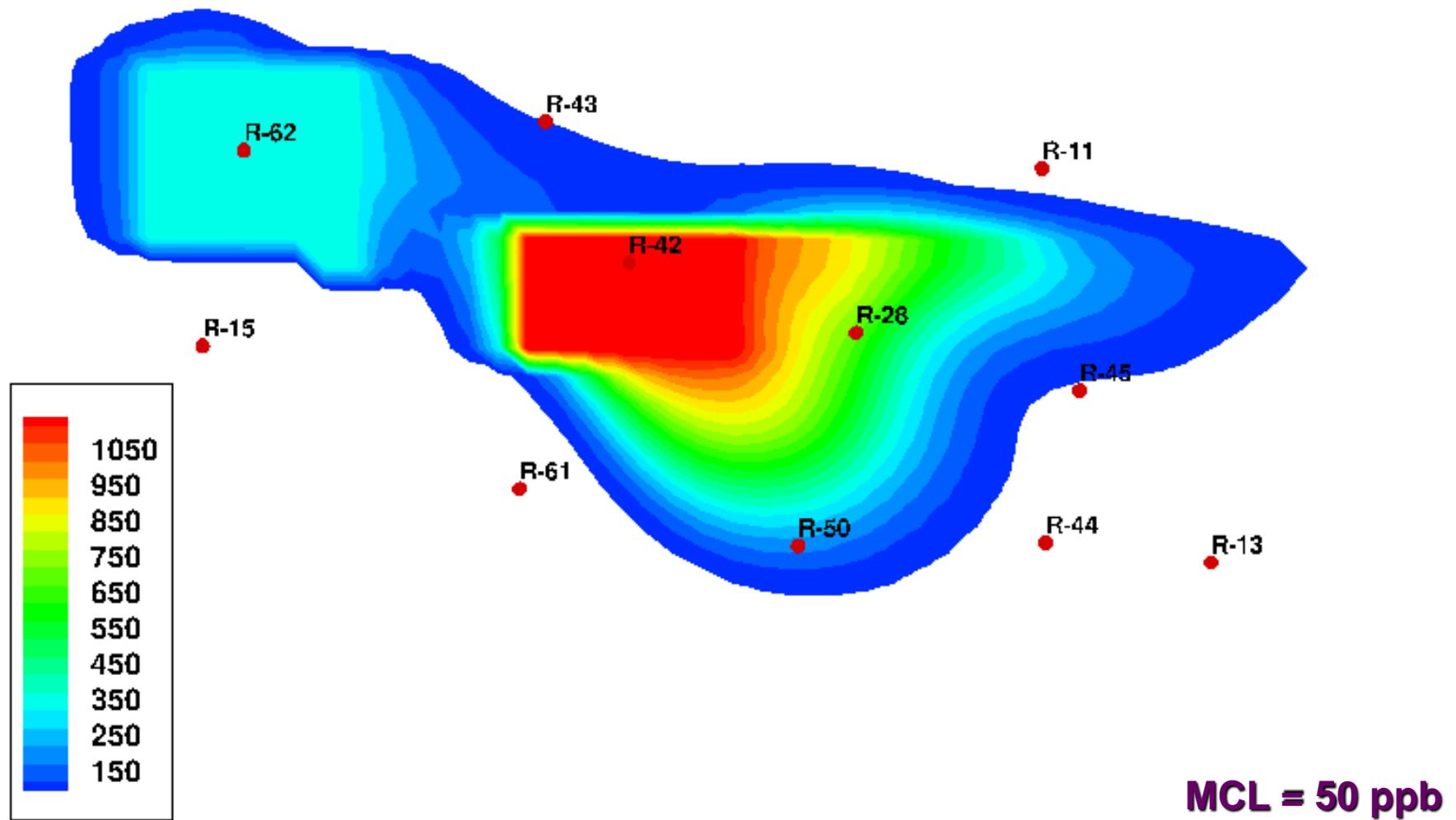


2009 model estimate of the plausible Cr⁶⁺ [ppb] along the regional aquifer water table

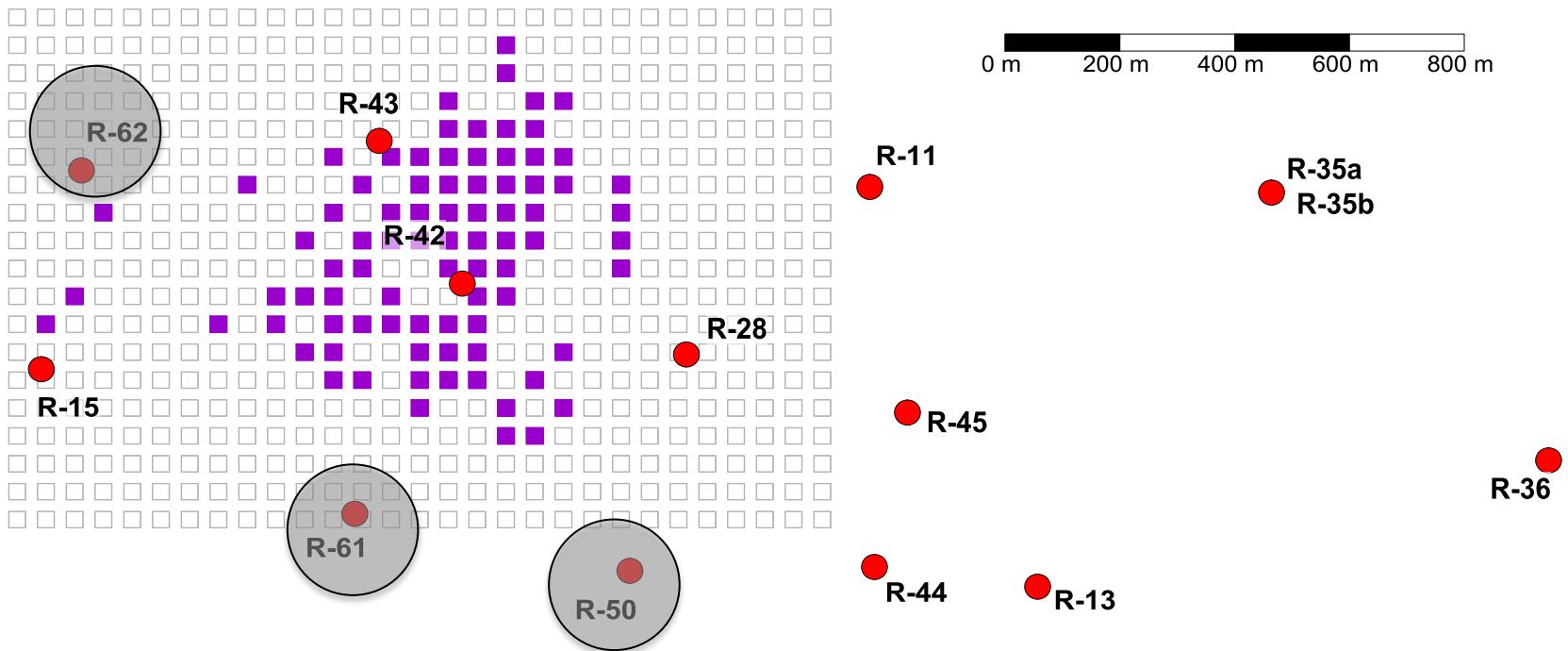
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2012 model estimate of the plausible Cr⁶⁺ [ppb] along the regional aquifer water table

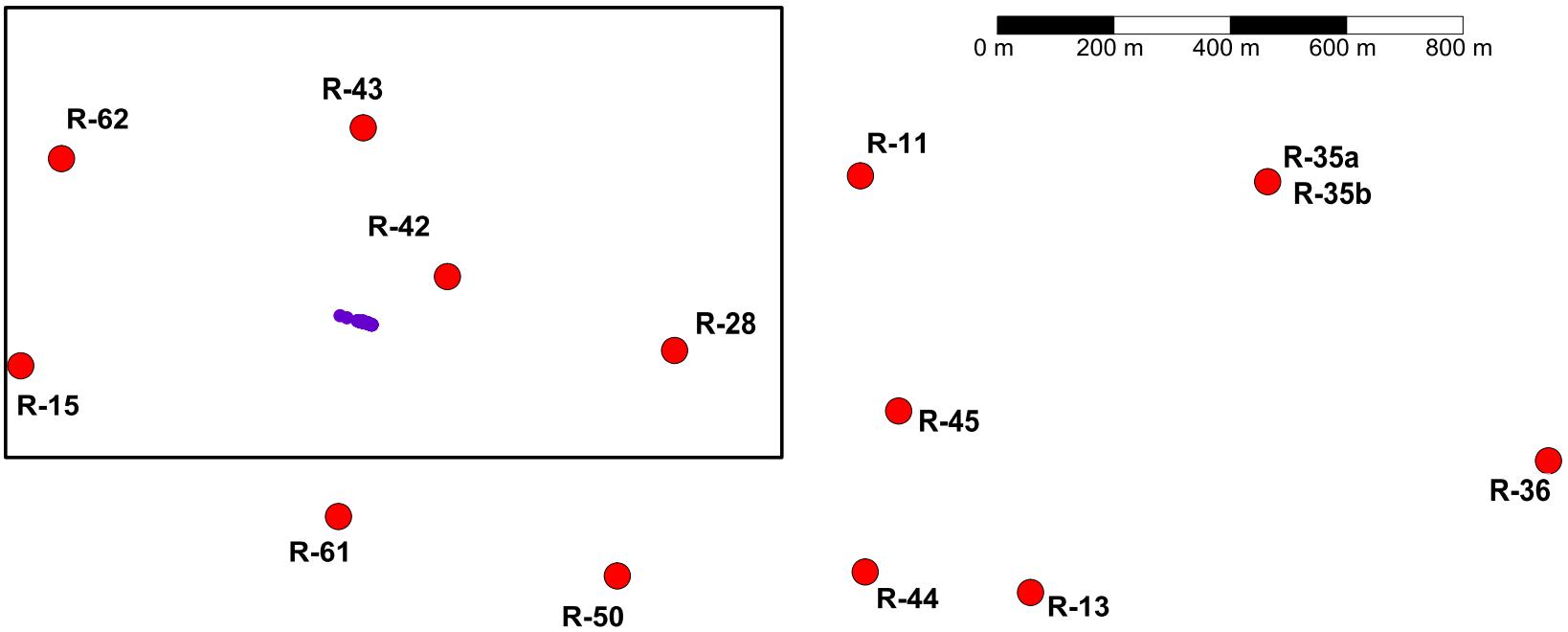


2009 model analyses for source identification / network design



Plausible contaminant-arrival locations (83 out of 551)

2012 model analyses for source identification / network design

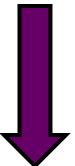


- Series of plausible contaminant-arrival locations in a well-constrained region
- All the obtained solutions (492) are almost equivalent
- Additional analyses are performed considering multiple contaminant arrival locations

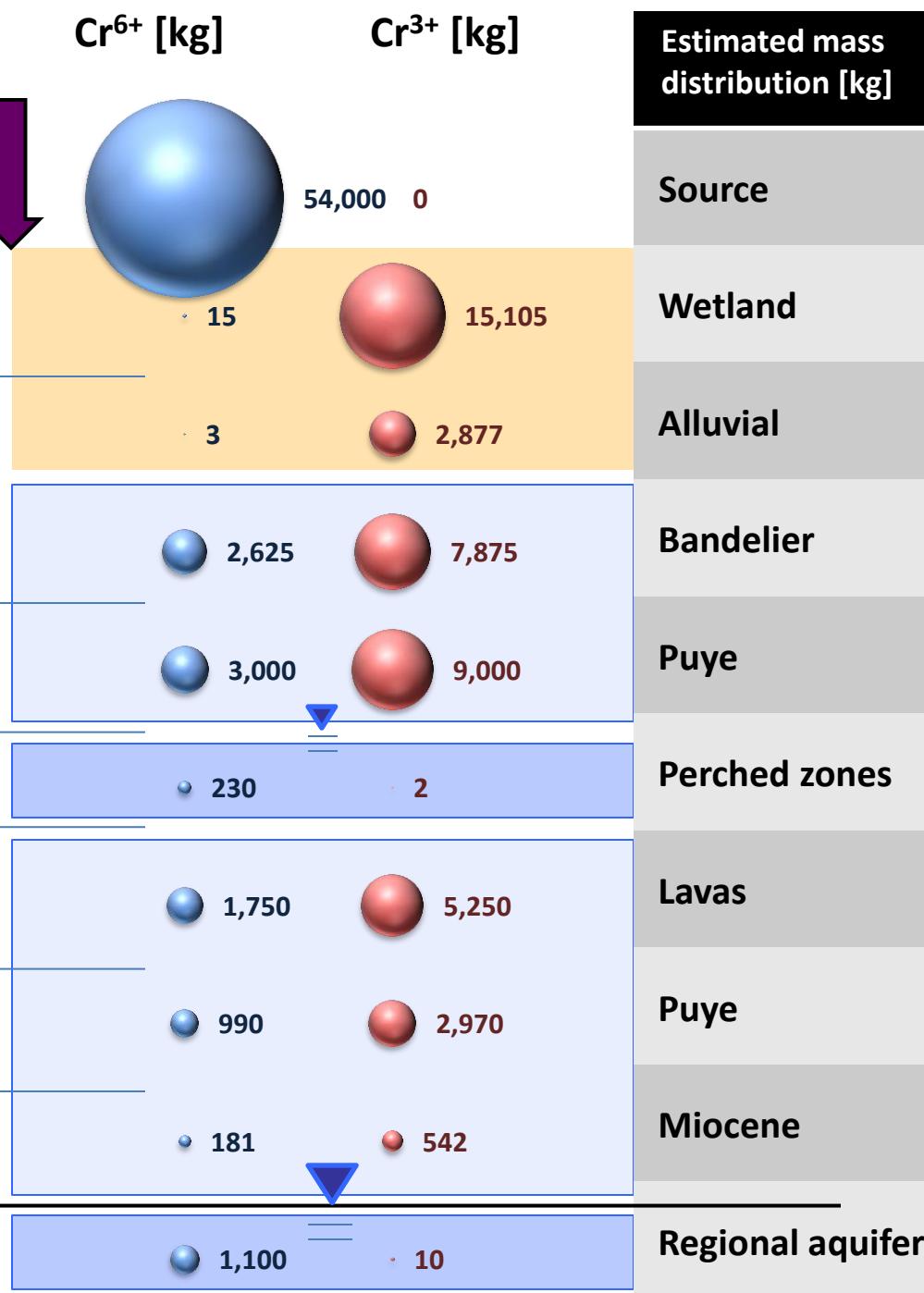
Cr^{6+} [kg]

Cr^{3+} [kg]

Estimated mass distribution [kg]



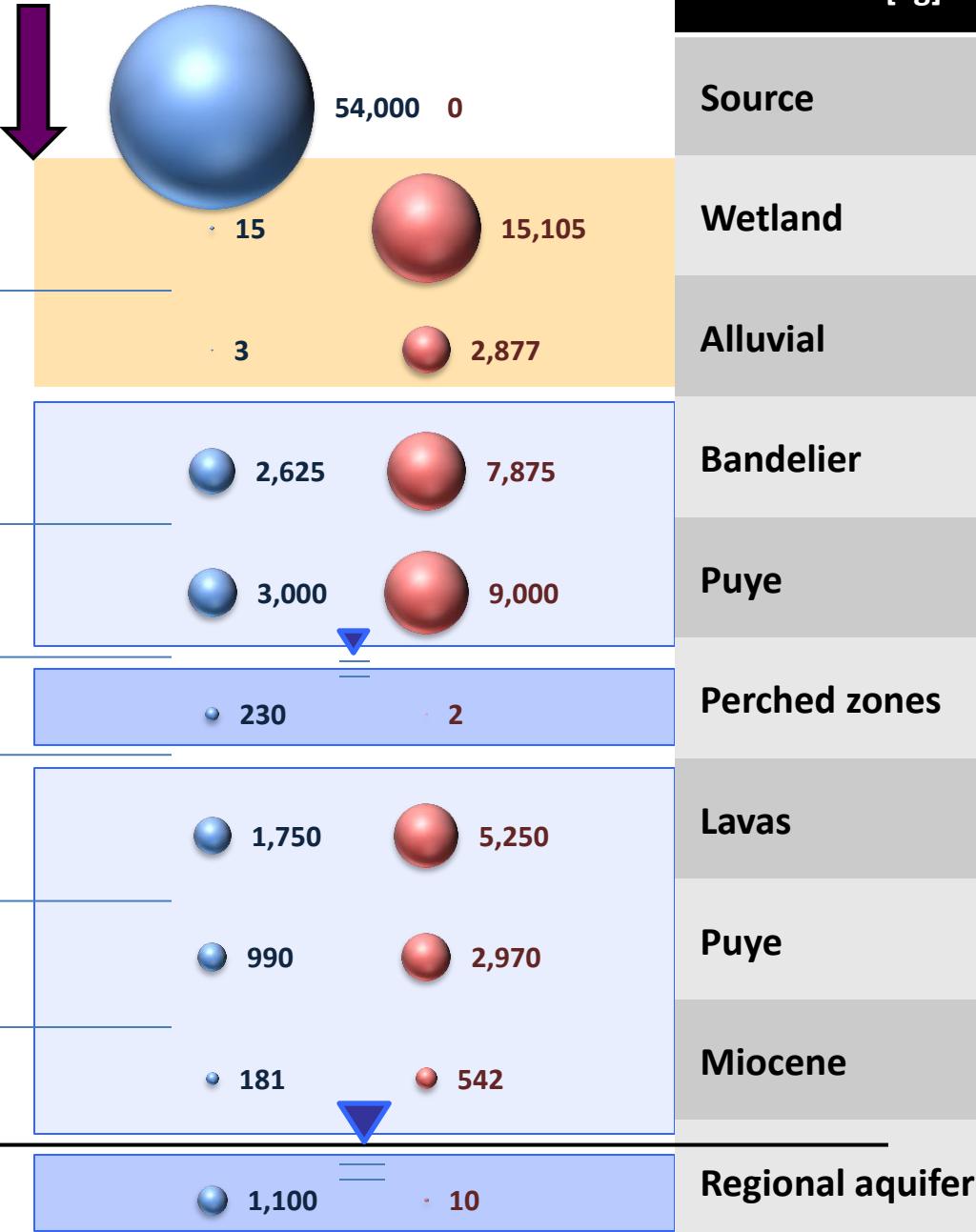
Cr^{6+} mass distribution



Cr^{6+} [kg]

Cr^{3+} [kg]

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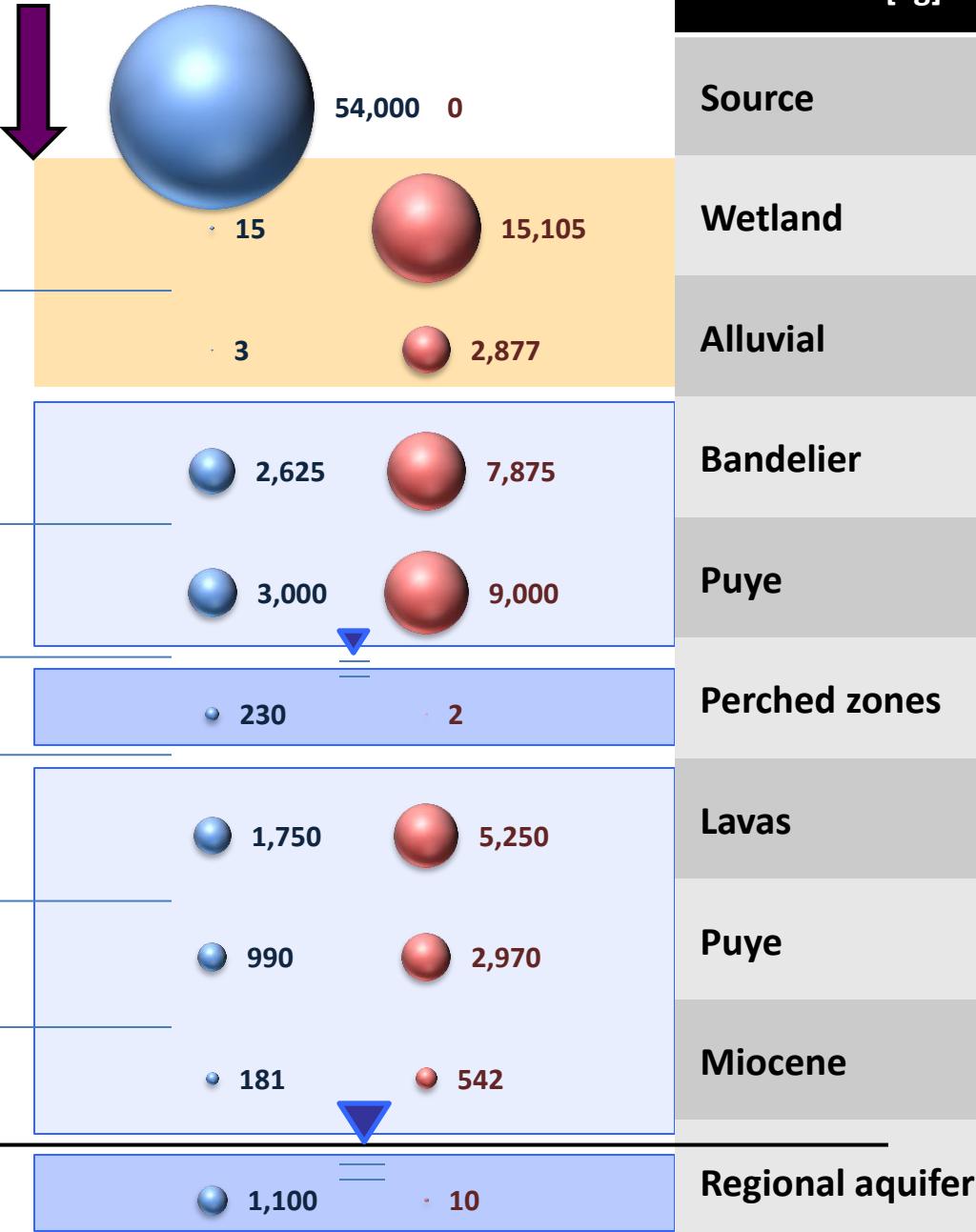
Cr^{6+} mass distribution

There are uncertainties associated with these estimates. For example, source mass may vary between 31,000 and 72,000 kg, and mass in the aquifer may vary between 300 and 3,300 kg.

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Estimated mass distribution [kg]



Cr^{6+} mass distribution

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Series of additional activities are identified to reduce decision uncertainties related to contaminant mass distribution (source)

Cr⁶⁺ [kg]

Cr³⁺ [kg]

Estimated mass distribution [kg]



54,000

15



15,105

3



2,877



2,625



7,875



3,000



9,000



230



2



1,750



5,250



990



2,970



181



542



1,100



10

Regional aquifer

Planned activities

Grade Control Structure

- immediate effect
- stabilize wetland to control Cr, PCBs, and other

Reduced effluent volume (infiltration)

- mid-term effect
- reduce flux of secondary Cr source

Geochemical lab-scale analyses (cores)

- key support for optimizing CME – MNA
- attenuation potential
- reduction potential

Pumping/tracer tests at existing wells

- immediate affect
- source removal
- capture zone analysis
- characterize field-scale hydrogeologic and geochemical properties
- characterize secondary Cr source

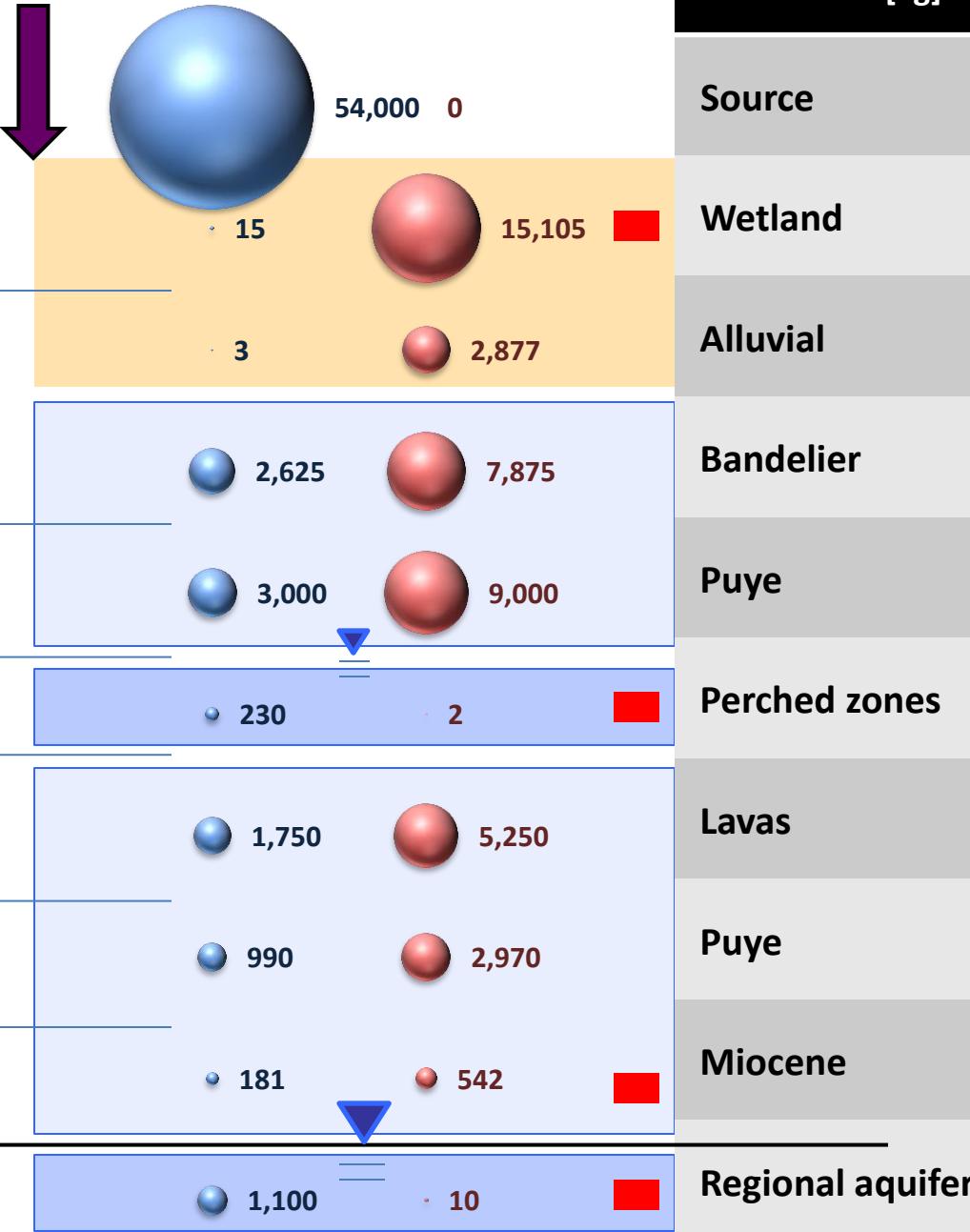
Groundwater flow & transport modeling

- key for interpretation of the collected data
- key support for optimizing CME - MNA

Cr⁶⁺ [kg]

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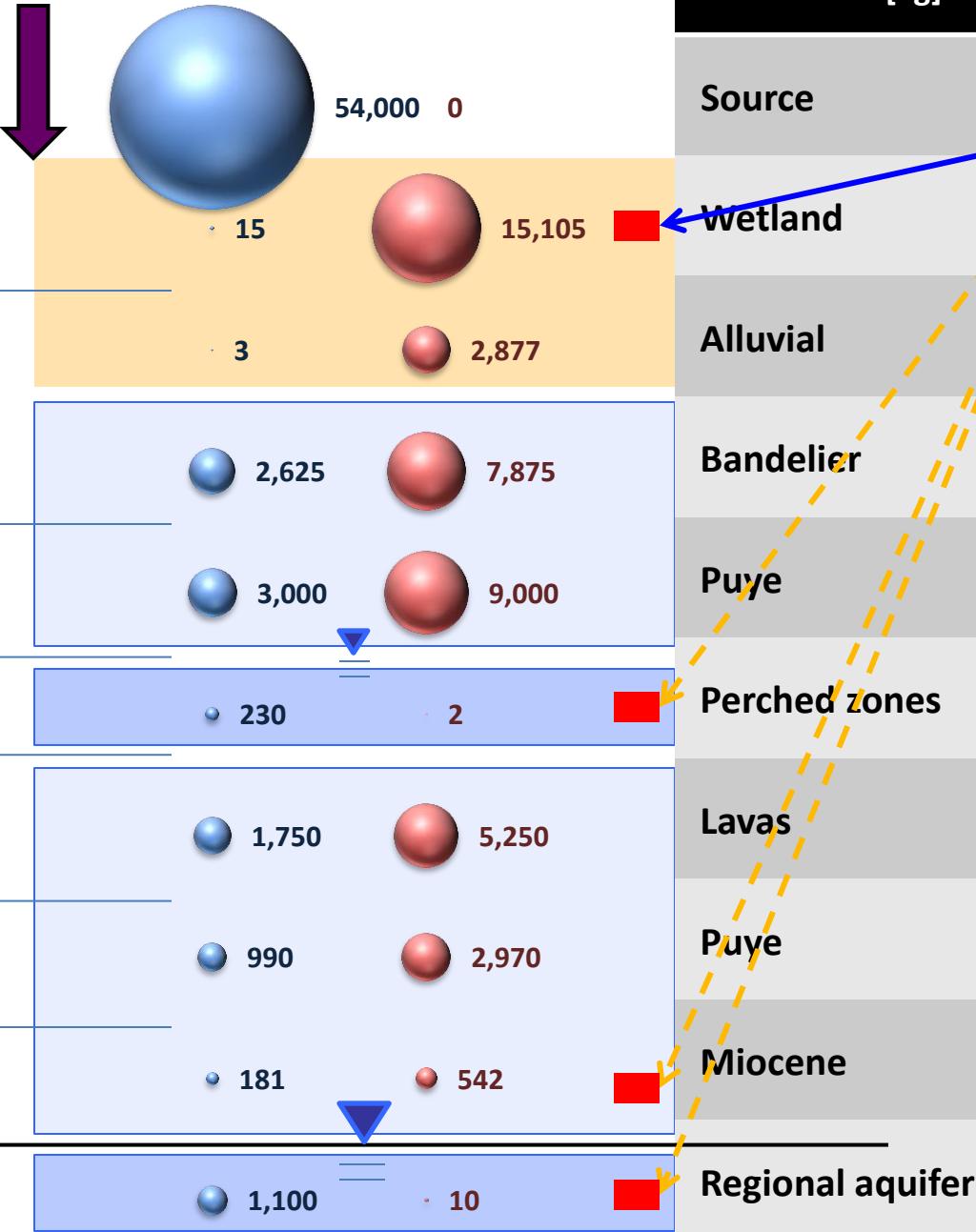
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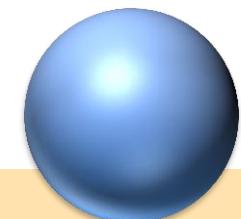
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Estimated mass distribution [kg]



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Bandelier

Puye

Perched zones

Lavas

Puye

Miocene

Regional aquifer

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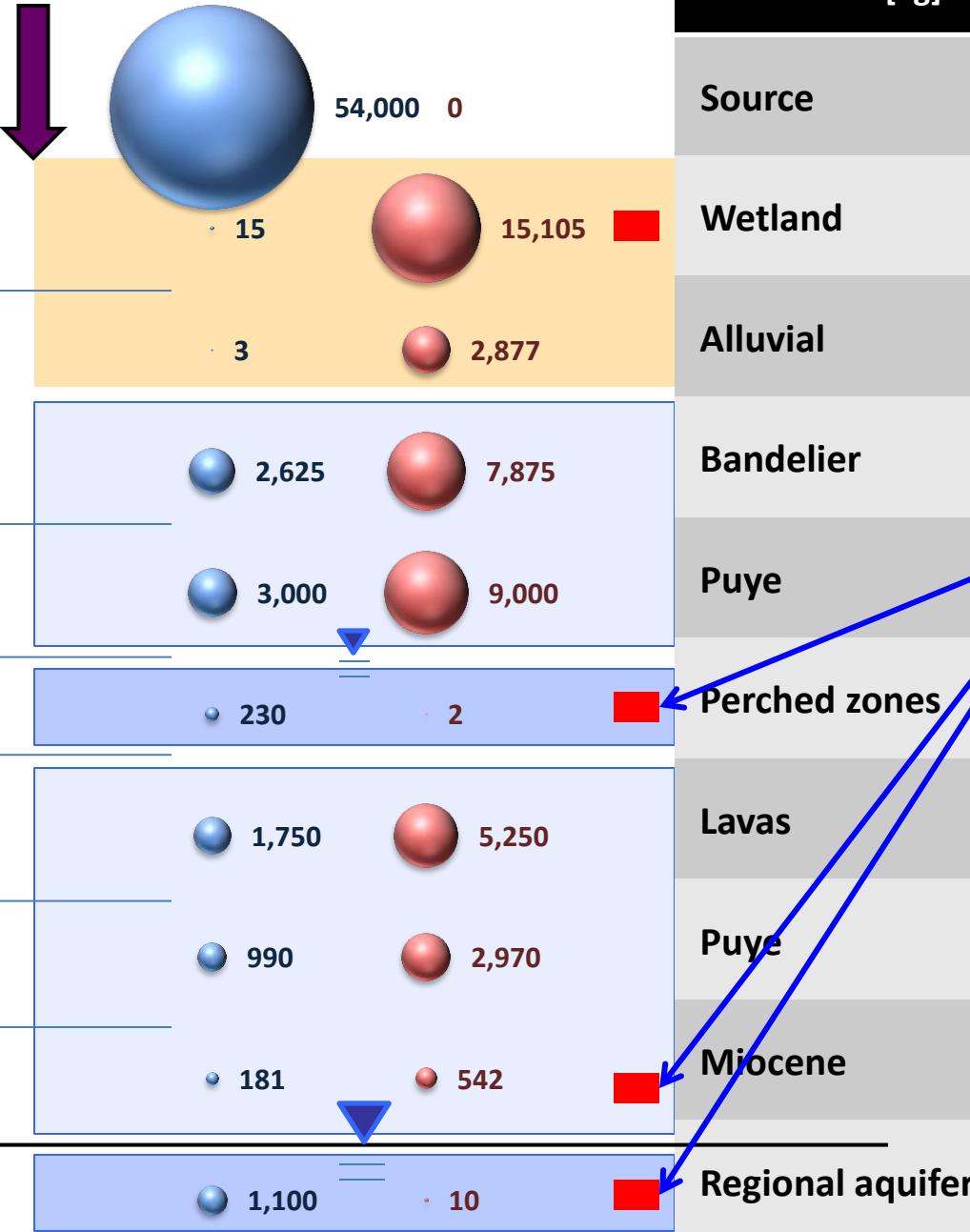
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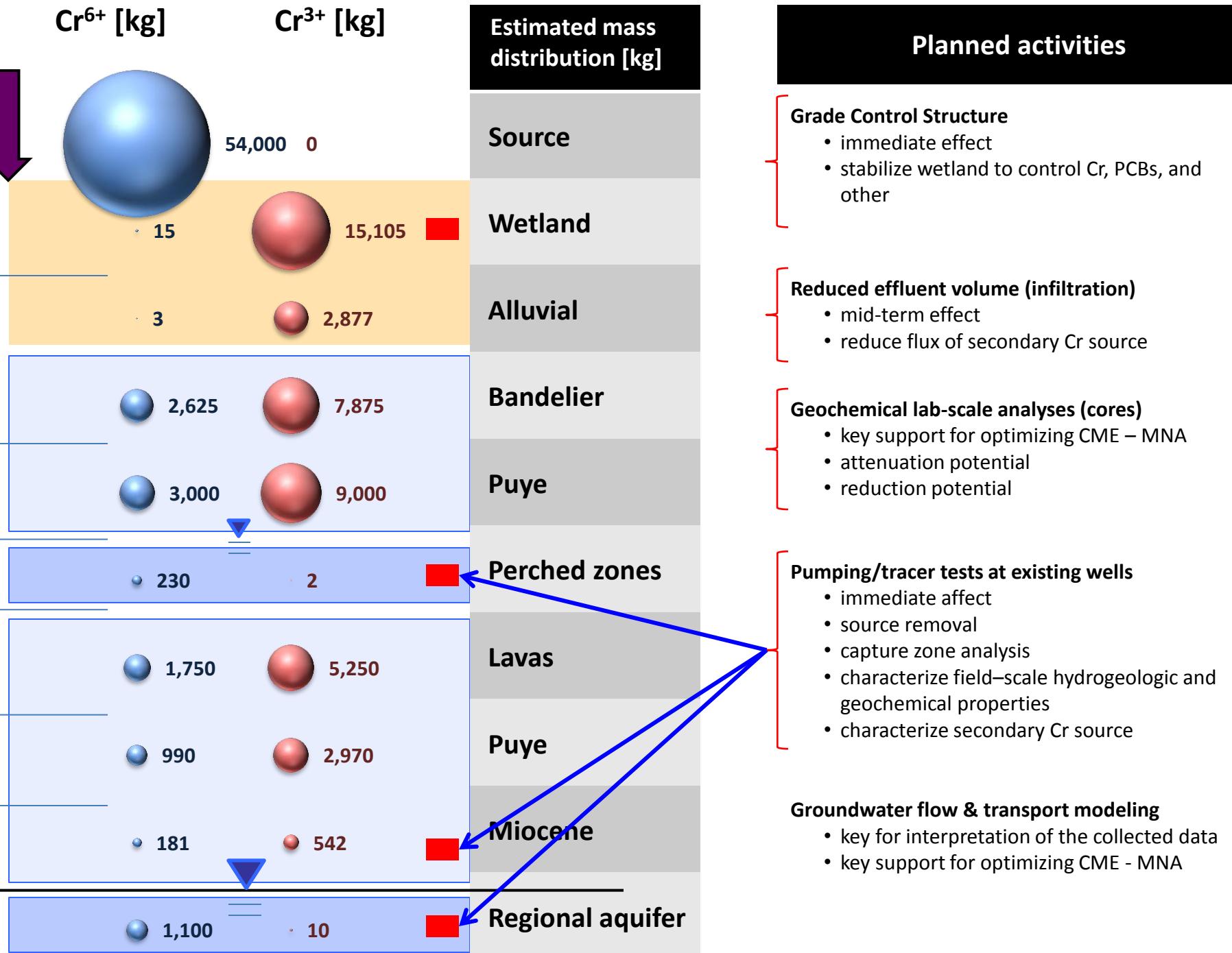
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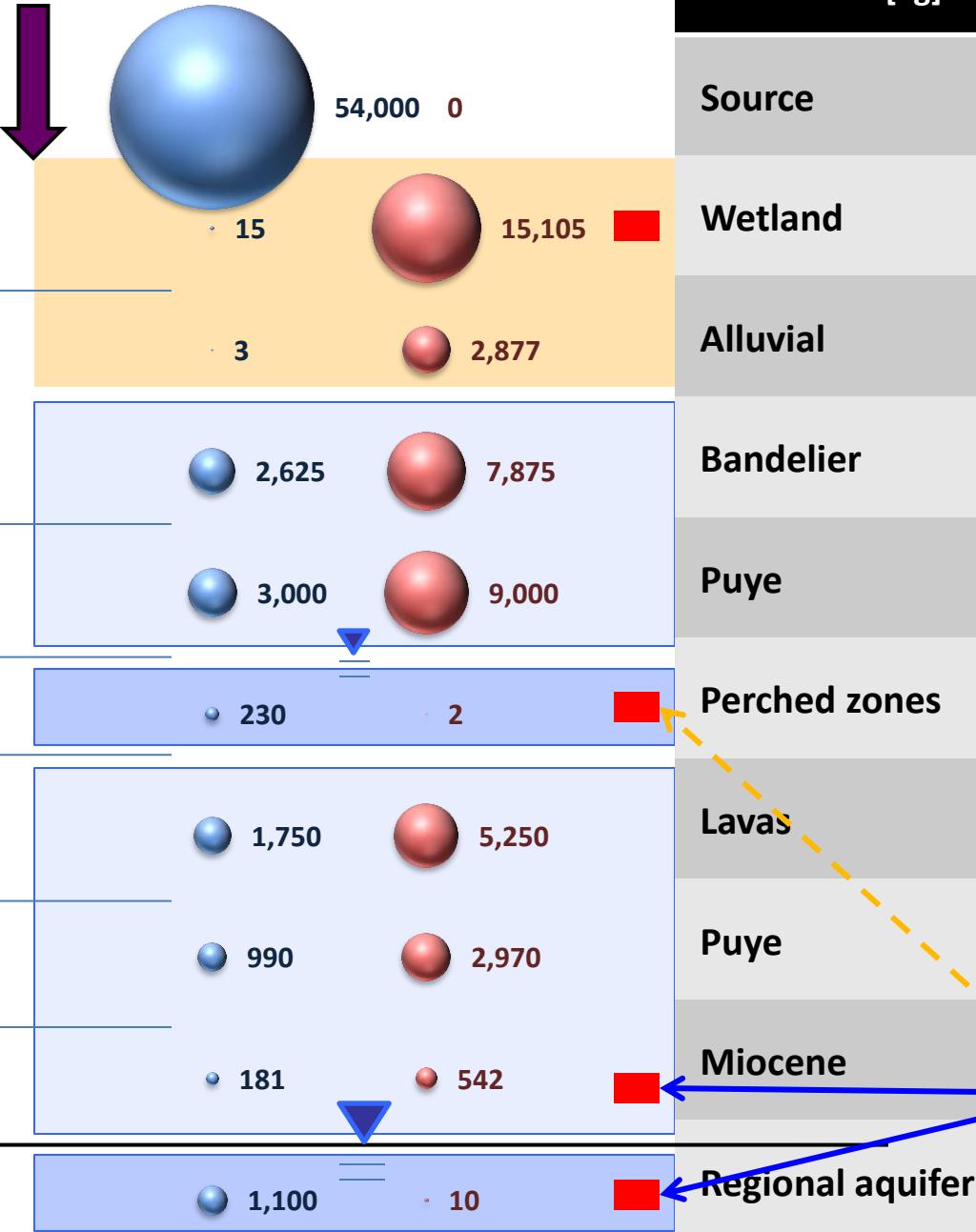
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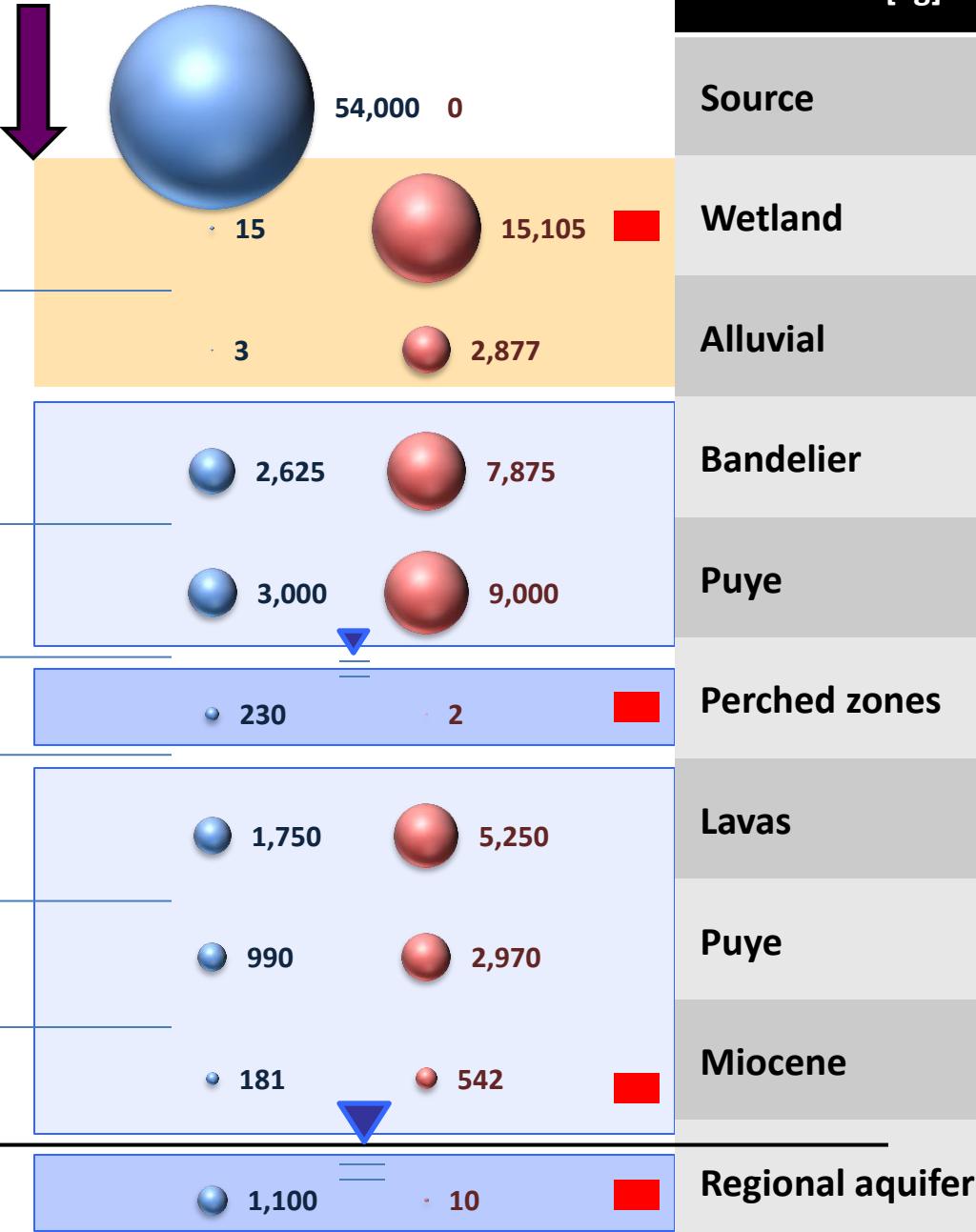
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Model Analysis and Decision Support



- ✧ an open-source high-performance computational framework for **Model Analyses** and **Decision Support (MADS)**
- ✧ advanced **adaptive** computational techniques:
 - **sensitivity analysis** (local / global);
 - **uncertainty quantification** (local / global);
 - **optimization / calibration / parameter estimation** (local / global);
 - **model ranking & selection**
 - **decision support** (probabilistic / non-probabilistic)
- ✧ novel robust 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 3D contaminant transport solvers
- ✧ external coupling with any process simulator (e.g. ModFlow, FEHM, Amanzi, PFLOTRAN, STOMP/eSTOMP, TOUGH, TOUGHREACT, ...)
- ✧ source code, examples, performance comparisons, and tutorials @ <http://mads.lanl.gov>
- ✧ **MADS** tools will be implemented in the **ASCEM** project



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- ❖ advanced **adaptive** computational techniques:
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Summary:

- ✧ Both **Non-Probabilistic** and **Probabilistic** uncertainties often exist in decision problems
- ✧ In the case of **probabilistic** methods, definition of prior probability distributions for model parameters 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 for waste and environmental management
 - Harp & Vesselinov (2011). *Contaminant remediation decision analysis using information gap theory.*
 - Vesselinov & Harp (2013). *Model-driven decision support for monitoring network design using information gap theory.*
- ✧ MADS provides a computationally efficient framework for decision analyses using **non-probabilistic** and **probabilistic** methods (<http://mads.lanl.gov>)

Summary:

- ✧ Current conceptual model for chromium migration in the subsurface is supported by **multiple lines of evidence** (hydrogeological, geophysical, mineralogic, petrographic, and geochemical studies and model analyses)
- ✧ **Data- and model-based (systems-based) decision analyses** are successfully implemented to progress characterization and performance assessment at the site (monitoring network design, additional characterization activities)
- ✧ Plume characterization is a **challenging** and **nonunique** problem because multiple models are consistent with the site data and conceptual knowledge
- ✧ Decision analyses are facilitated by implementation of **robust** techniques and **high-performance computing**
- ✧ Activities are currently planned to constrain uncertainties impacting decision analyses:
 - aquifer heterogeneity: spatial distribution of low-permeable zones that can act as secondary contaminant sources
 - contaminant mass distribution
 - spatial and temporal distribution of contaminant mass flux to the aquifer
 - implementation of remedial activities

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mads
Monty Desseinou
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Chromium plume in the regional aquifer at LANL

Challenges:

- ✧ define site conceptual model and existing uncertainties:
 - complex hydrostratigraphy, geochemistry, flow and transport regimes
 - data characterized with different support volumes and uncertain due to various factors
 - multiple contaminant pathways
 - hydrogeological, geophysical, mineralogic, petrographic, and geochemical studies applied
 - current conceptual model is supported by multiple lines of evidence
- ✧ perform computationally efficient analyses:
 - parameter estimation (PE)
 - model calibration
 - uncertainty quantification (UQ)
 - decision support (DS)
- ✧ high computational demands for model simulations and analyses (requiring utilization of LANL high-performance computing capabilities)
- ✧ uncertainties associated with application of the remedial options

Work related to LANL Chromium site

✧ Model-driven decision support

- evaluation and optimization of additional characterization activities (e.g. field pumping and tracer tests)
- evaluation and optimization of monitoring network design (well locations)
- evaluation and optimization of remedial activities (ongoing)

✧ Characterization activities:

- exploration, analysis & evaluation of **alternative conceptual models**
- estimation of nature/extent/fate of contaminant plumes (Cr^{6+} , ClO_4^-)
- source identification (estimating location/flux of contaminant mass arriving at the top of regional aquifer)
- estimation of vadose zone & aquifer heterogeneity (hydrogeology and geochemistry)

Estimates of chromium mass distribution in the subsurface including existing uncertainties

Estimates of chromium mass distribution	Cr ⁶⁺ [kg]			Cr ³⁺ [kg]			Cr ⁶⁺ + Cr ³⁺ [kg]			Cr ³⁺ /Cr ⁶⁺ ratio [%]
	mean	min	max	mean	min	max	mean	min	max	
Source	54,000	31,000	72,000	0	0	0	54,000	31,000	72,000	0
Canyon alluvial sediments	18	6	27	17,982	5,694	26,973	18,000	5,700	27,000	99.9
---- Wetland	15	5	23	15,105	4,783	22,657	15,120	4,788	22,680	99.9
---- Downstream sediment	3	1	4	2,877	911	4,316	2,880	912	4,320	99.9
Bandelier	2,625	250	12,750	7,875	750	38,250	10,500	1,000	51,000	75
Puye	3,000	600	15,000	9,000	1,800	45,000	12,000	2,400	60,000	75
Perched zones	230	100	500	0	0	0	230	100	500	0
Lavas	1,750	225	2,250	5,250	675	6,750	7,000	900	9,000	75
Puye	990	250	2,000	2,970	750	6,000	3,960	1,000	8,000	75
Miocene	181	25	1,000	542	75	3,000	722	100	4,000	75
Aquifer	1,100	270	3,300	0	0	0	1,100	270	3,300	0
Total	9,894	1,726	36,827	43,619	9,744	125,973	53,512	11,470	162,800	

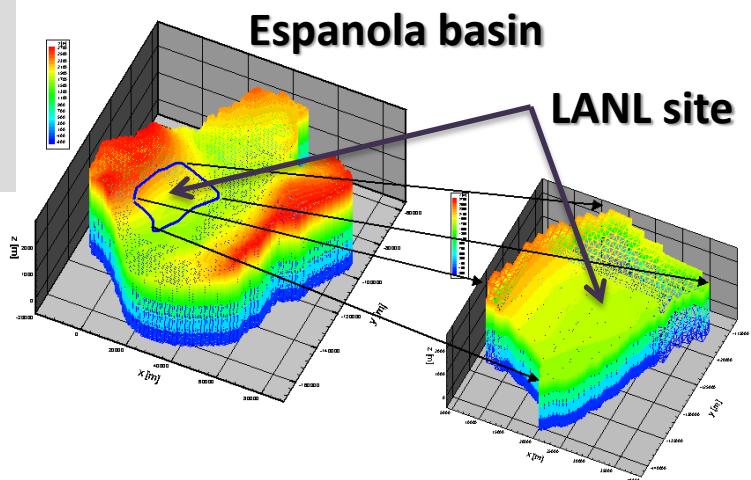
Information Gap Decision Theory

- ✧ Nominal (“best”) model prediction intended for decision making (based on nominal / “best estimates” model parameter set)
- ✧ Decision metric(s)
- ✧ Decision goal(s)
- ✧ Decision scenarios: a series of alternative decisions to compare
- ✧ Info-Gap Uncertainty Model
- ✧ Model predictions for each decision scenario constrained by Info-Gap Uncertainty Model

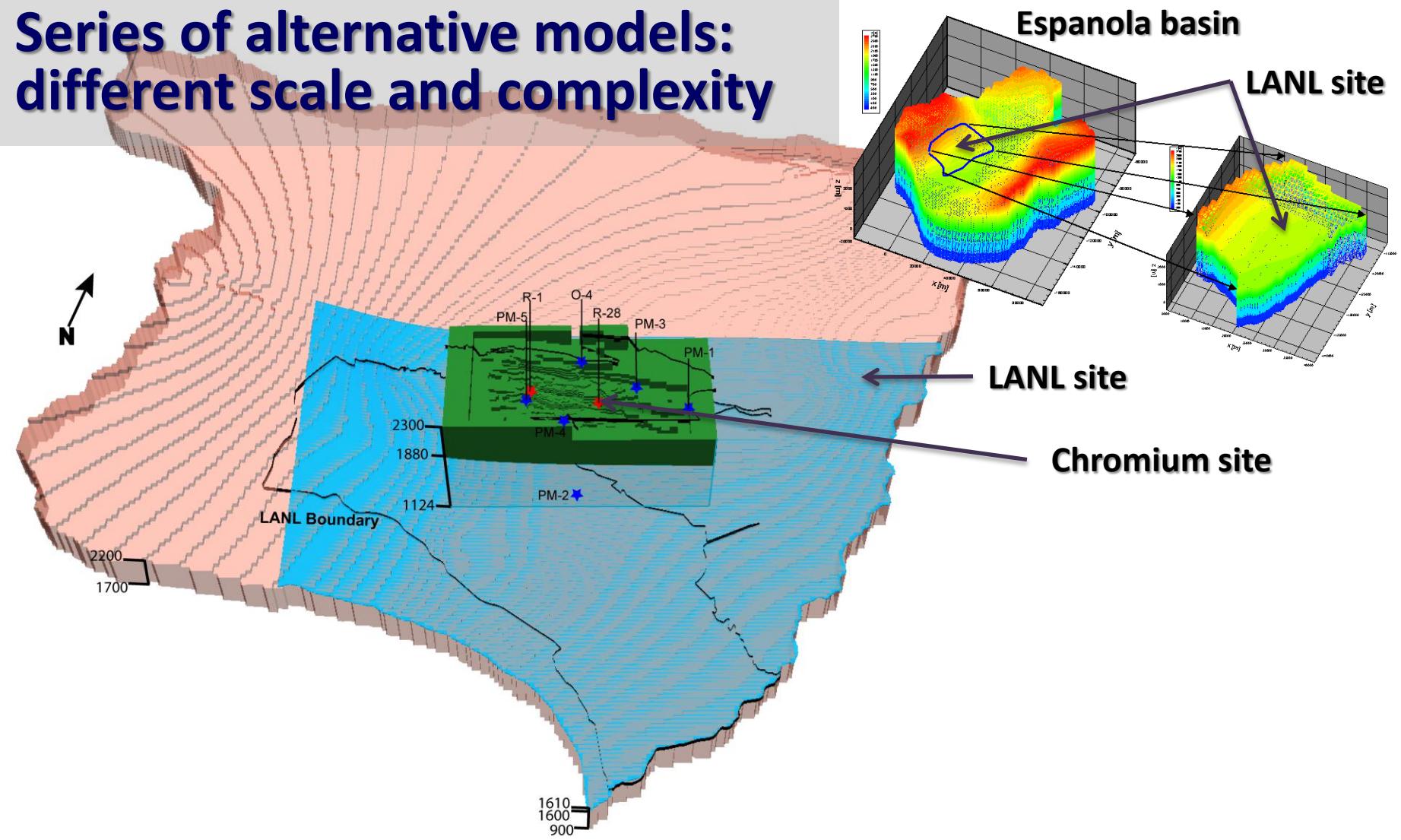
Info-Gap Analysis: Synthetic Network Design

- ✧ Unknown model parameters (8) characterizing plume size:
 - source locations (coordinates x, y)
 - source lateral size (x_s, y_s)
 - flow direction
 - aquifer dispersivities (longitudinal, horizontal/vertical transverse)
- ✧ Uncertain concentration observations (calibration targets) (10) due to:
 - measurement errors
 - uncertain background concentrations
 - uncertain local hydrogeological and geochemical conditions
- ✧ Analytical model of the 3D contaminant flow
- ✧ Unknown model parameters estimated using inversion
- ✧ Decision question: which of the new proposed well location has the highest immunity of failure to detect concentrations above MCL ($c > 5$ ppm)
i.e. which well provides the most robust decision to improve the monitoring network

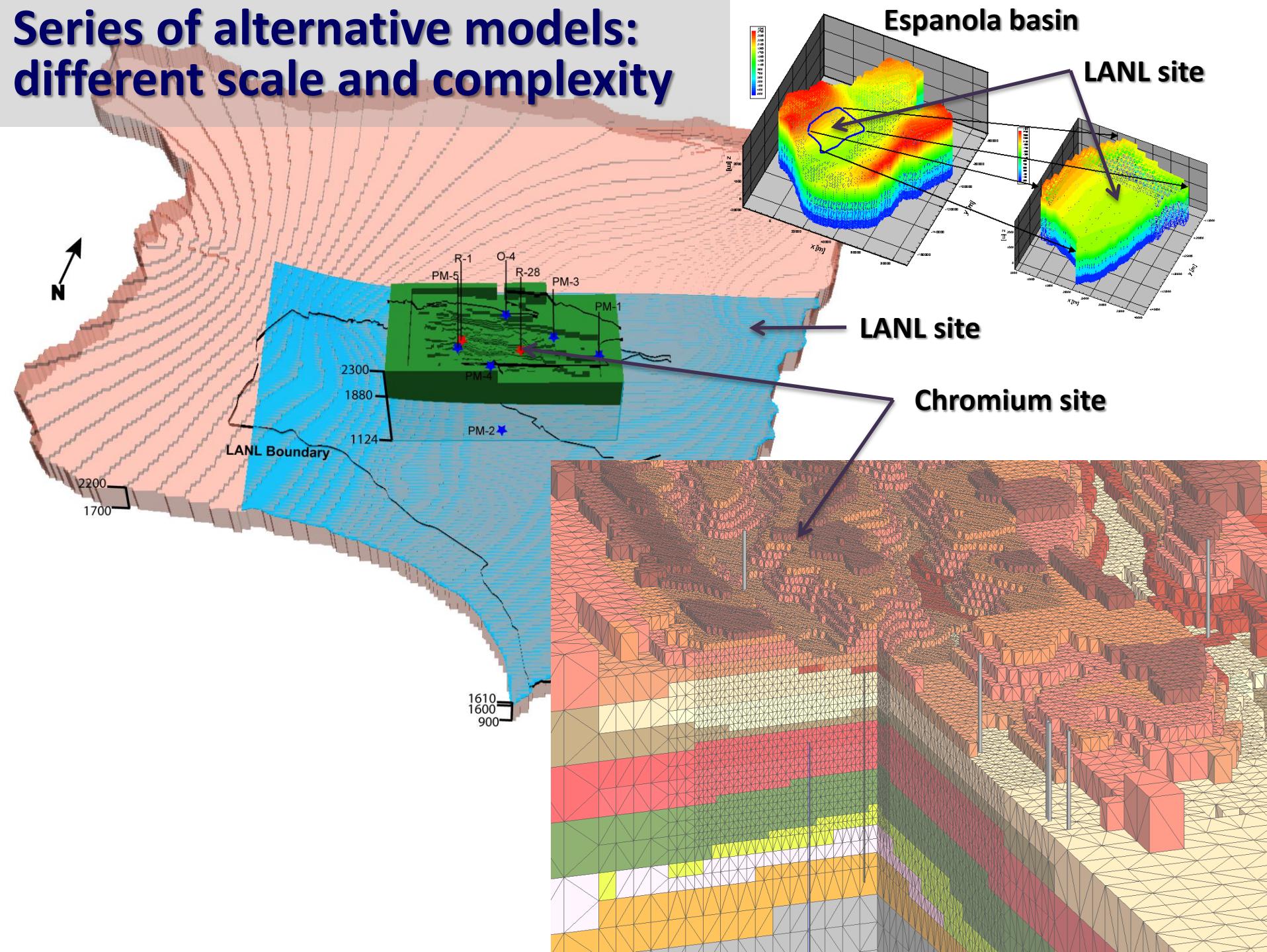
Series of alternative models: different scale and complexity



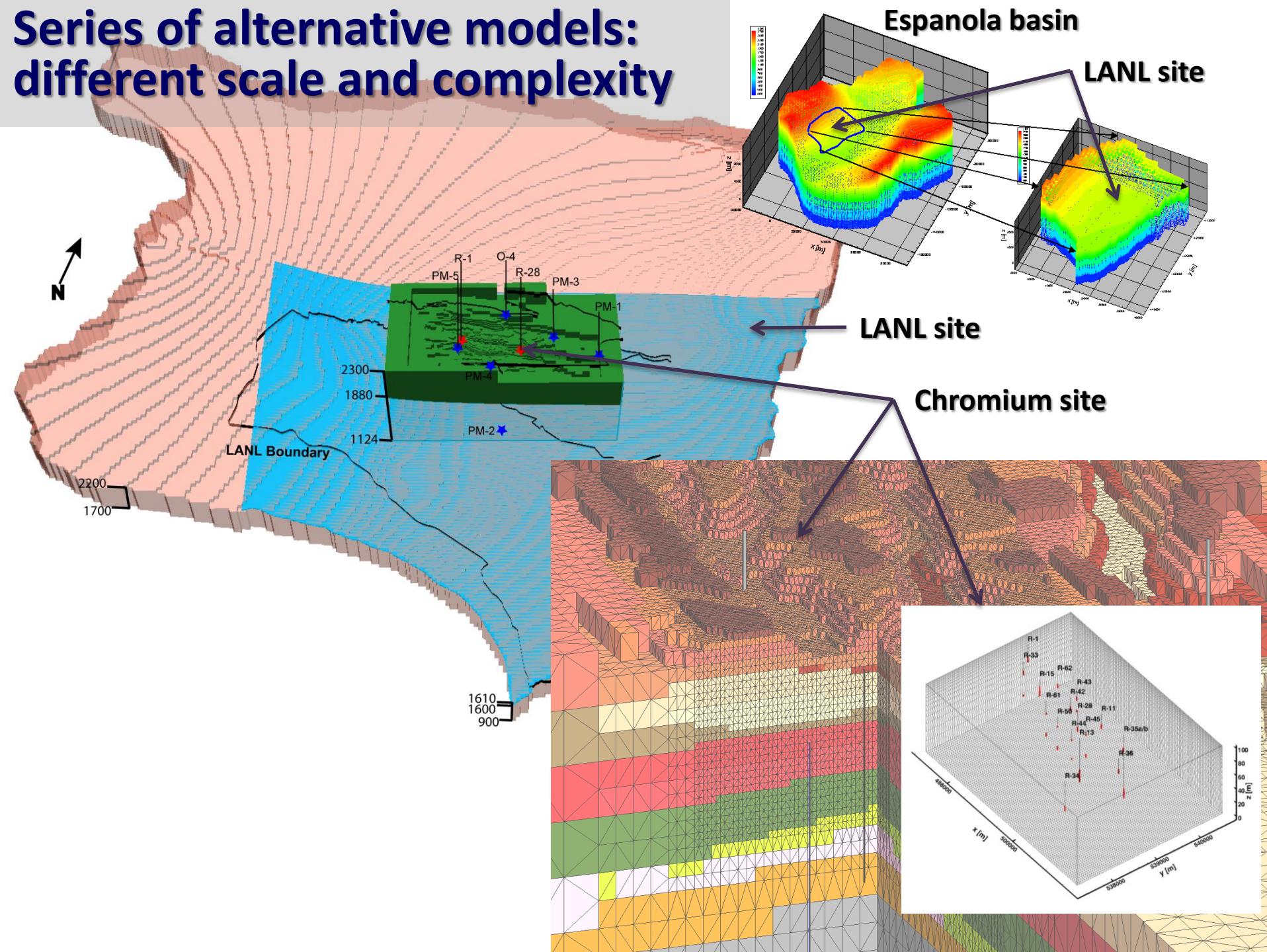
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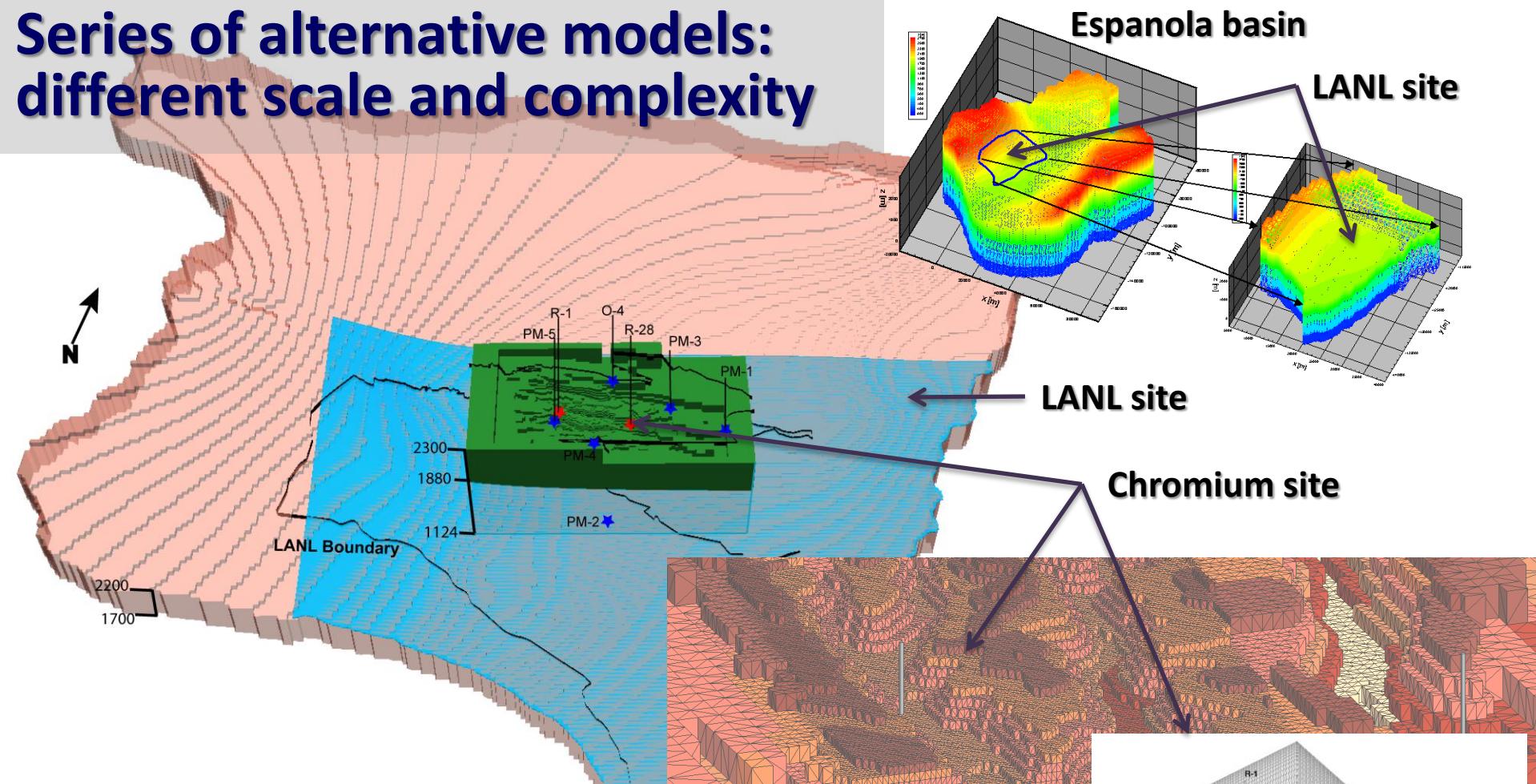
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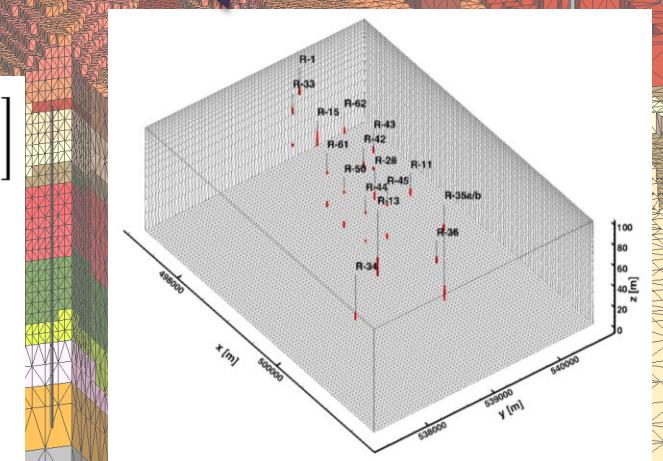
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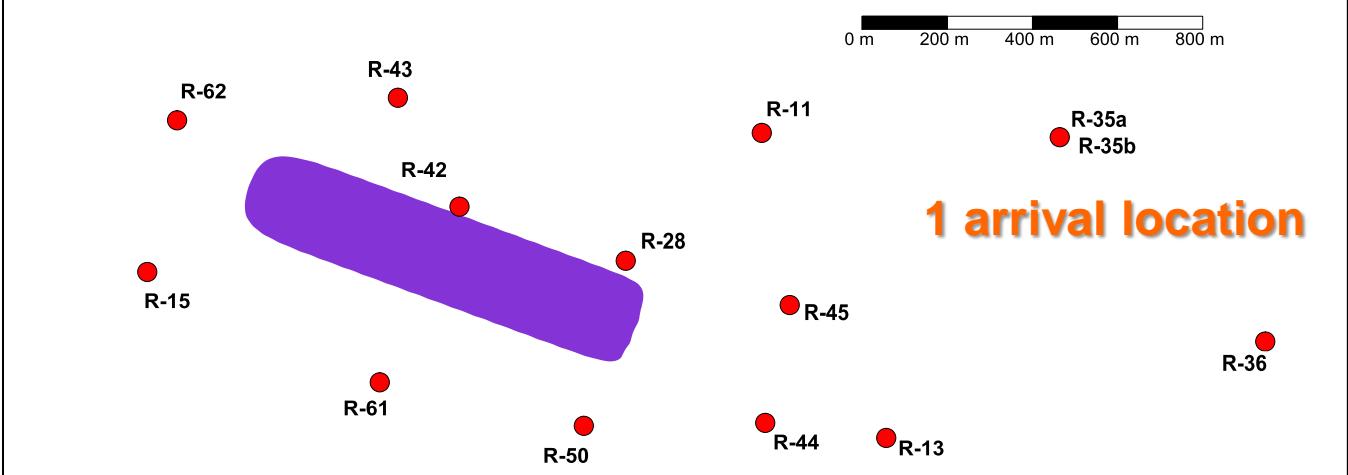
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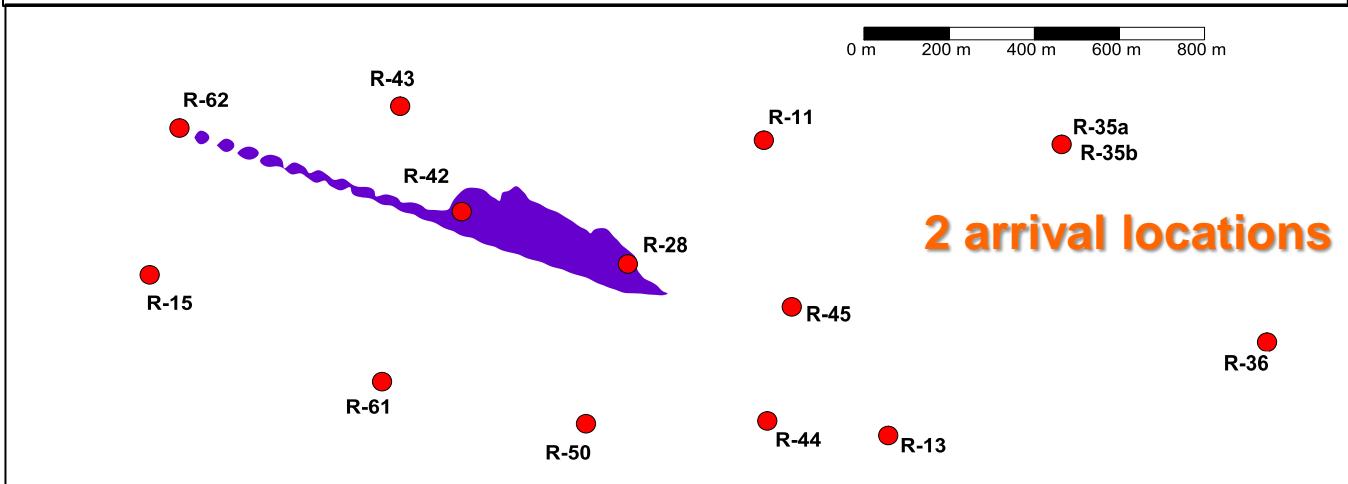
$$c(x, y, z, t) = \frac{1}{8\pi\theta x_S y_S z_S} \int_0^t I(t-\tau) \exp(-\lambda\tau) \left[\text{erfc}\left(\frac{x - \frac{1}{2}x_S - v\tau}{2\sqrt{\alpha_L v\tau}}\right) - \text{erfc}\left(\frac{x + \frac{1}{2}x_S - v\tau}{2\sqrt{\alpha_L v\tau}}\right) \right. \\ \times \left[\text{erfc}\left(\frac{y - \frac{1}{2}y_S - v\tau}{2\sqrt{\alpha_{TH} v\tau}}\right) - \text{erfc}\left(\frac{y + \frac{1}{2}y_S - v\tau}{2\sqrt{\alpha_{TH} v\tau}}\right) \right] \\ \times \left[\text{erfc}\left(\frac{z - (z_0 + z_S)}{2\sqrt{\alpha_{TV} v\tau}}\right) - \text{erfc}\left(\frac{z - z_0}{2\sqrt{\alpha_{TV} v\tau}}\right) + \text{erfc}\left(\frac{z + (z_0 + z_S)}{2\sqrt{\alpha_{TV} v\tau}}\right) \right. \\ \left. - \text{erfc}\left(\frac{z + z_0}{2\sqrt{\alpha_{TV} v\tau}}\right) \right] d\tau \alpha_L$$



2012 model analyses

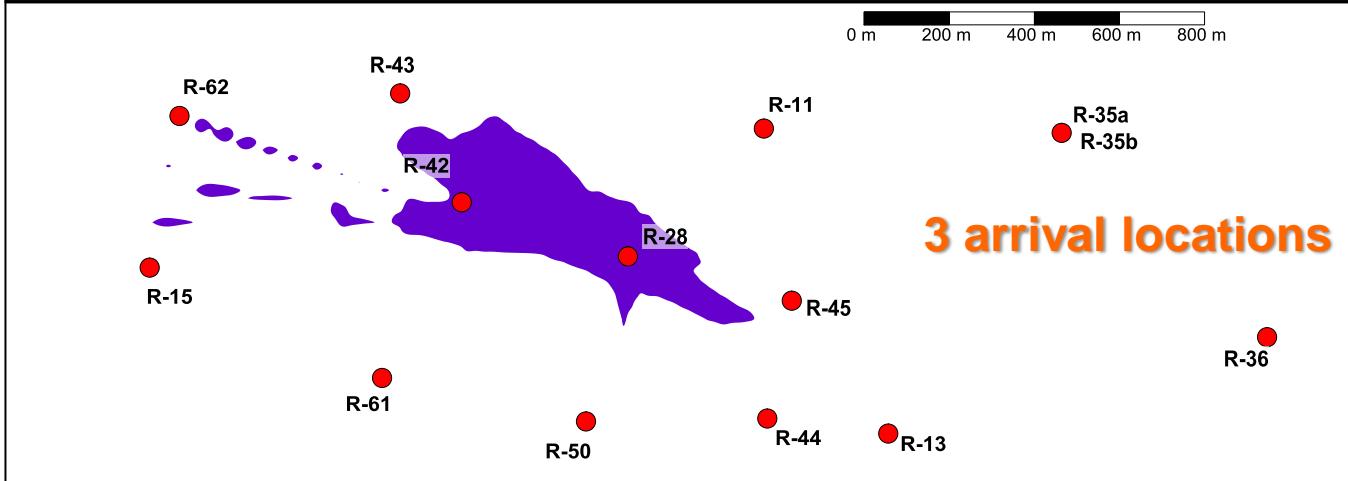


1 arrival location



2 arrival locations

Regions along the top the regional aquifer where the calculated Cr⁶⁺ concentrations exceed 1500 ppb based on averaging of all the acceptable model solutions



3 arrival locations

Cr⁶⁺ [kg]

Cr³⁺ [kg]

Estimated mass distribution [kg]

Planned activities



54,000

15

3

2,625

3,000

230

1,750

990

181

1,100

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15,105

2,877

7,875

9,000

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Source

wetland

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Perched zones

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- reduce flux of secondary Cr source

Geochemical lab-scale analyses (cores)

- key support for optimizing CME – MNA
- attenuation potential
- reduction potential

Pumping/tracer tests at existing wells

- immediate affect
- source removal
- capture zone analysis
- characterize field-scale hydrogeologic and geochemical properties
- characterize secondary Cr source

Groundwater flow & transport modeling

- key for interpretation of the collected data
- key support for optimizing CME - MNA