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The More the Merrier: Towards Improved Remedial Outcomes Using Ensemble Methods

Prashanth Khambhammettu, Philippe Renard, Jeremy White, John Doherty, Marc Killingstad, and Michael Kladias

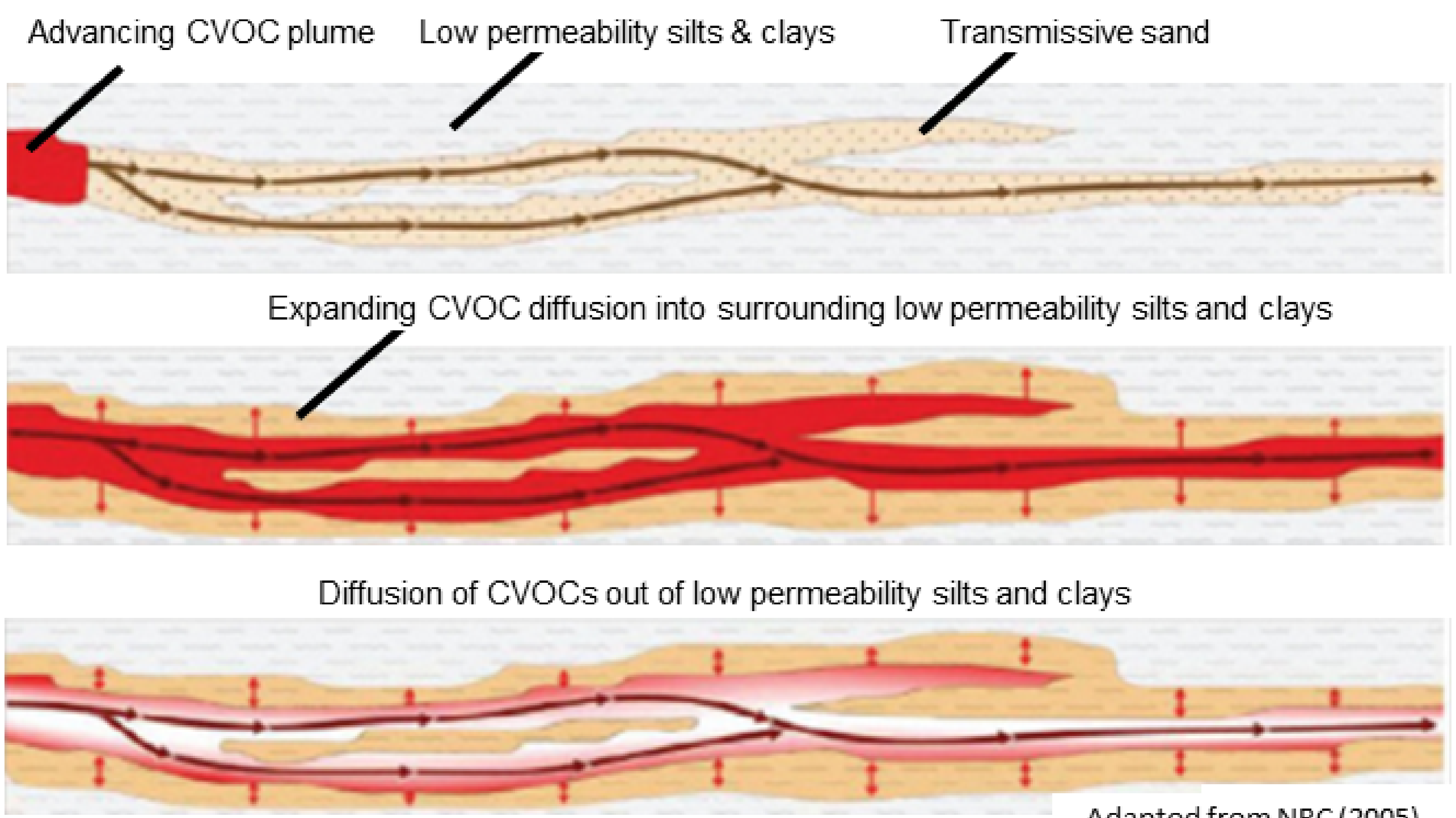
June 6, 2024

Aquifers are complex and heterogeneous

- Groundwater contamination remains above cleanup levels at hundreds of thousands of sites (NRC, 2013)
- Soil and groundwater cleanup at over 300’000 sites in the United States may exceed $200 billion by 2033 (EPA, 2004)
- Emerging contaminants (PFAS) will significantly increase these costs

Can we make a difference ?

Solute transport in heteorogenous settings

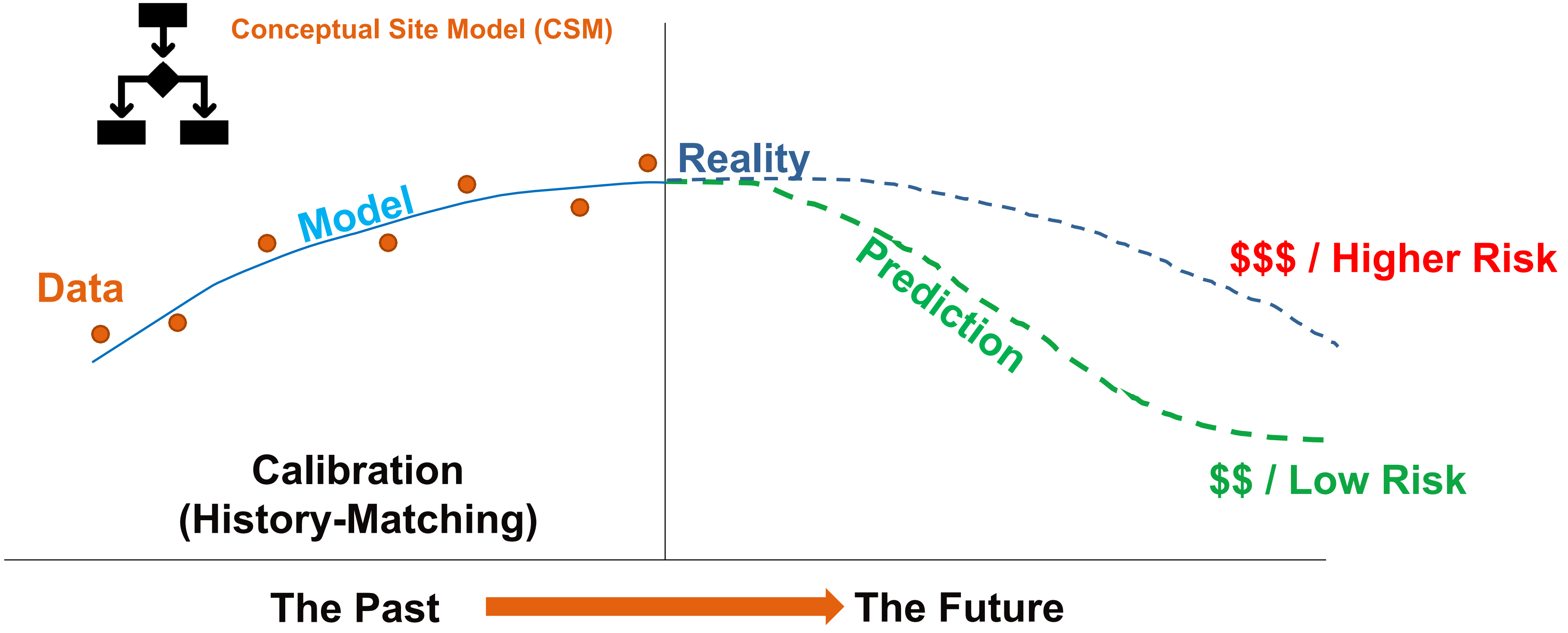


Adapted from NRC (2005)

Remediation requires a clear understanding of the high/low permeabilities

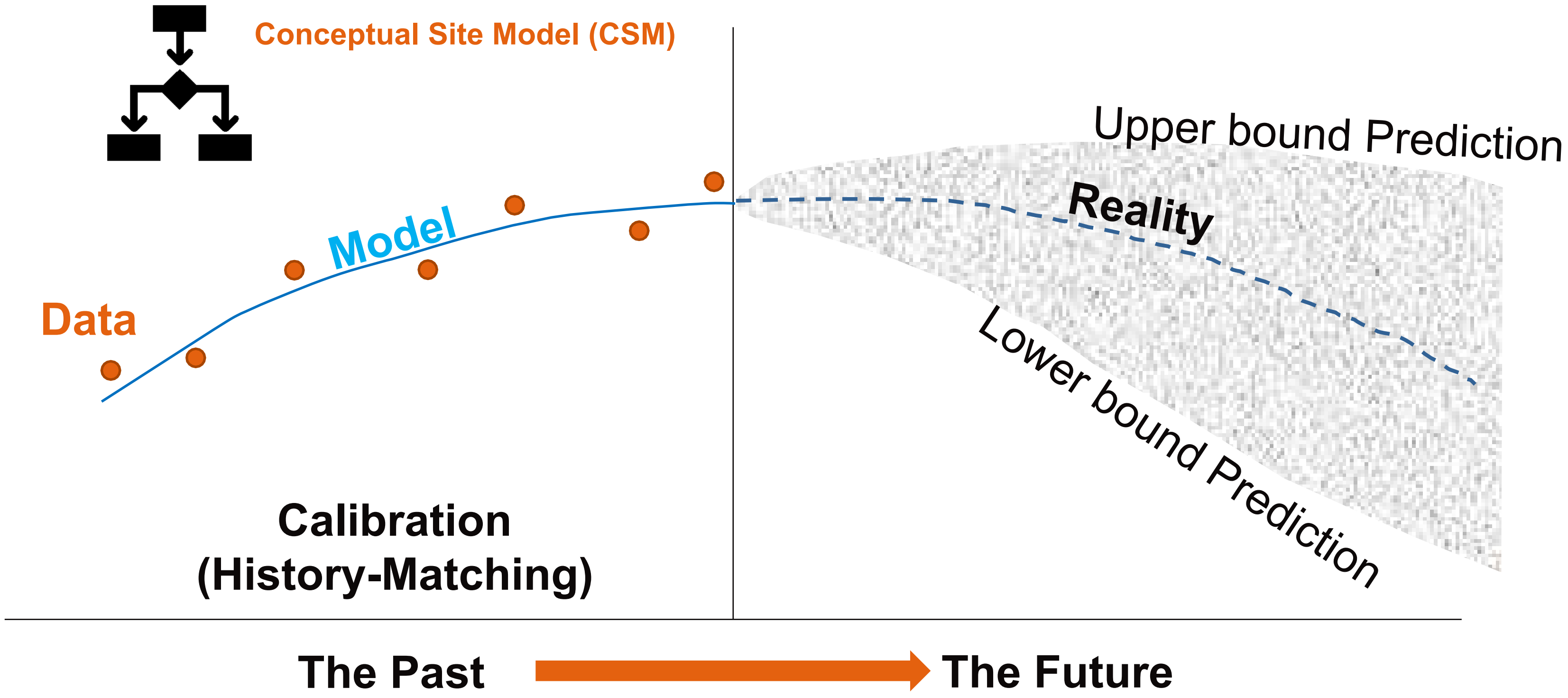
Traditional Modeling Process

A need for a computer model to answer a water resource-related question



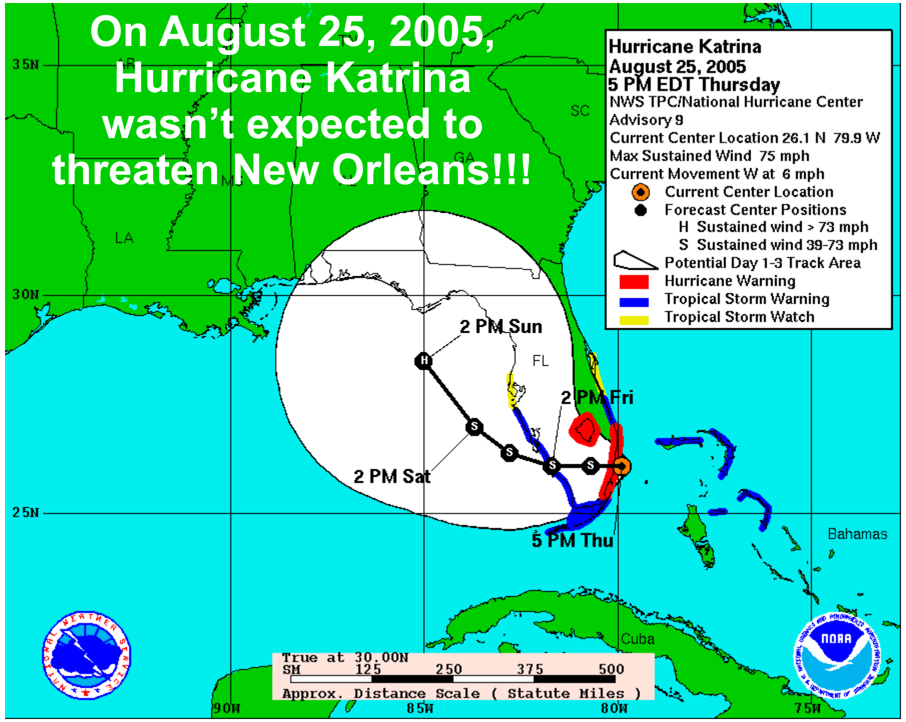
We need to reduce surprises for clients and stakeholders

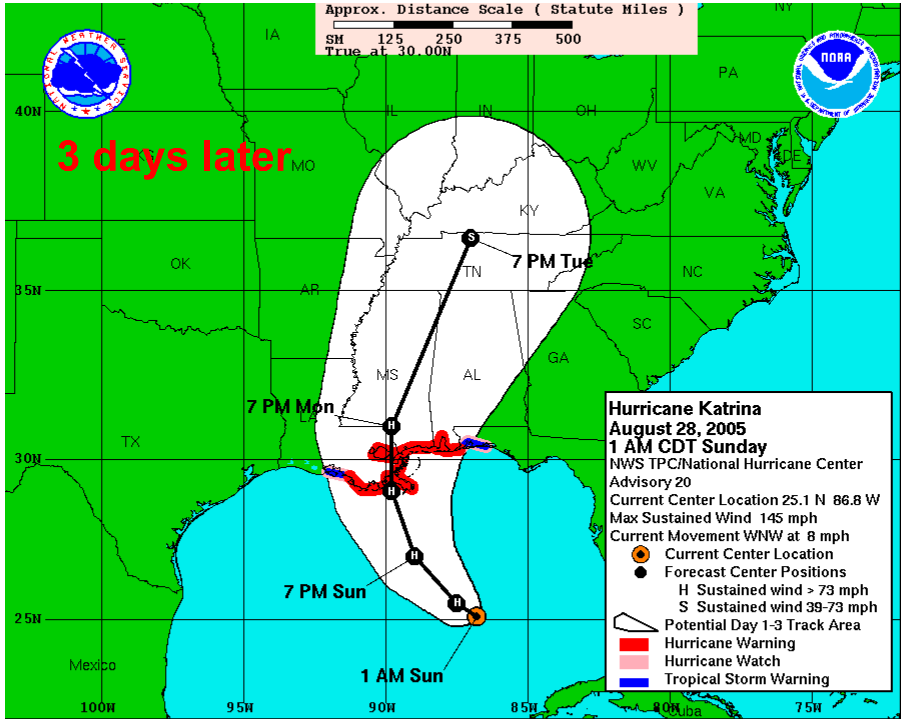
Ensembles can lead to better outcomes



Anticipating and planning for surprises can lead to better outcomes

Why Ensembles? Does anyone else use them?

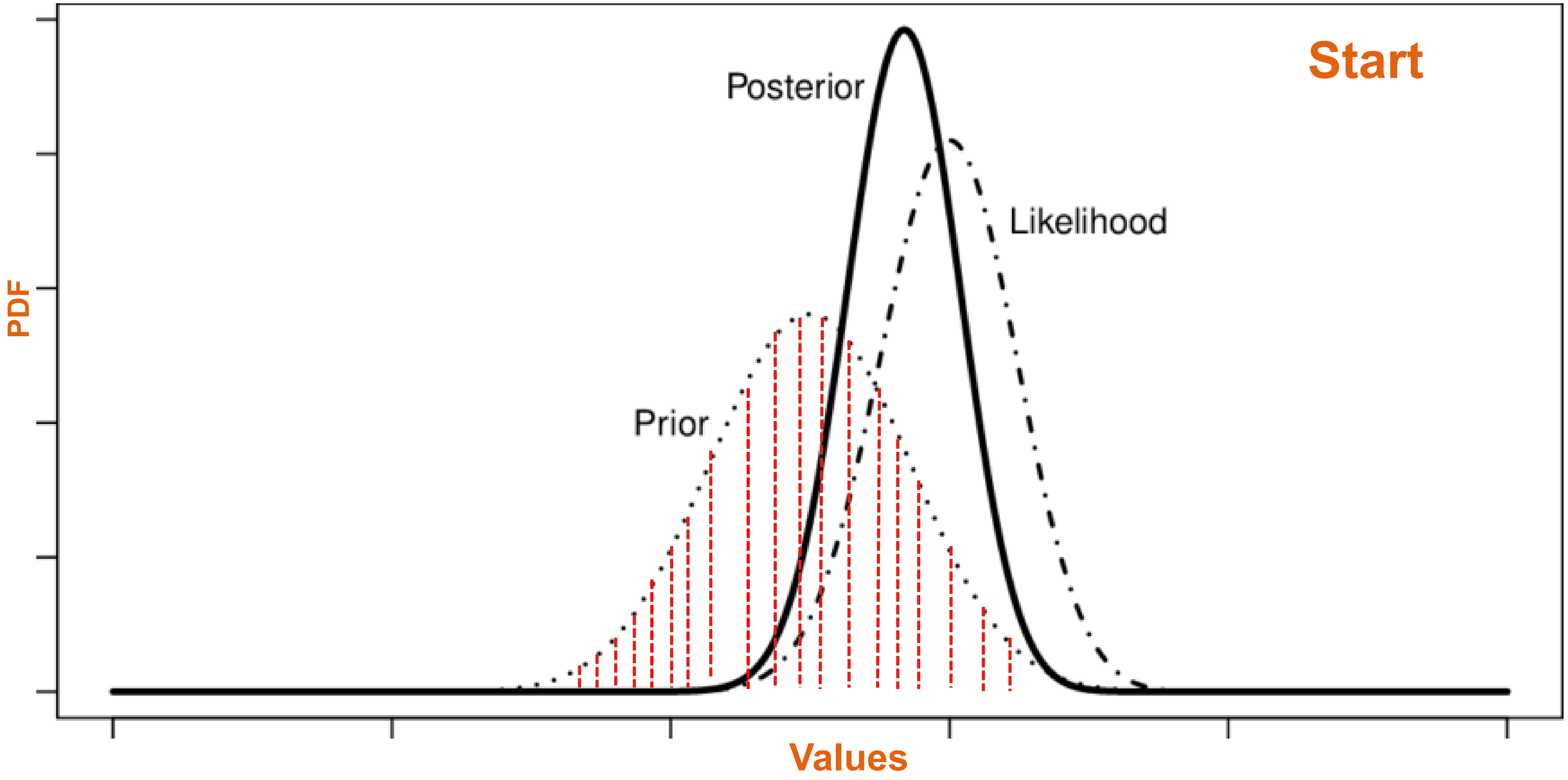




- Prediction uncertainty estimation is not a one-and-done deal
- Repeat analyses as newer datasets become available and/or when the underlying CSM changes

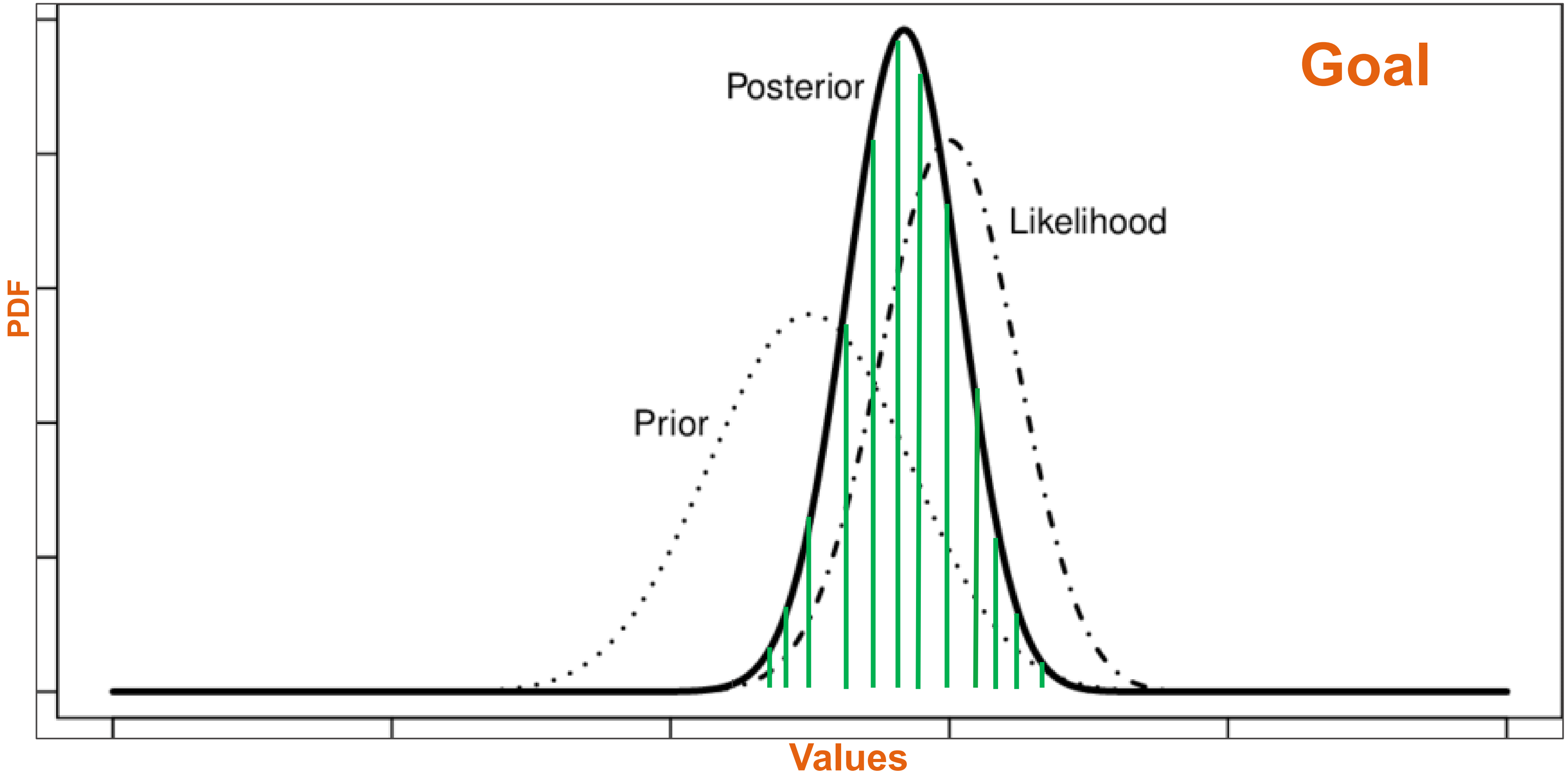
Iterative Ensemble Smoother (IES)

- Iteratively “smooth” a prior ensemble to sample the posterior

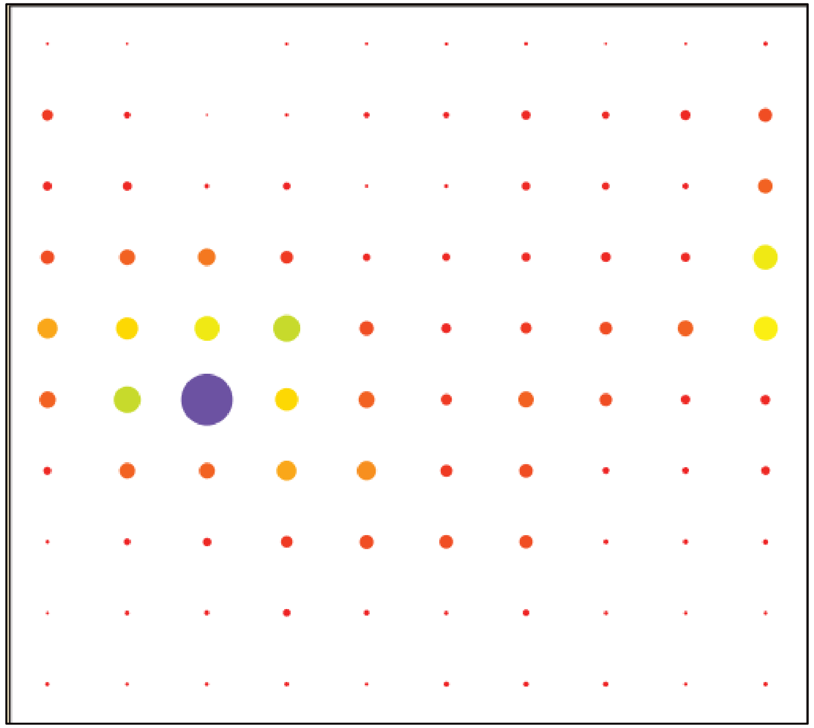


Iterative Ensemble Smoother (IES)

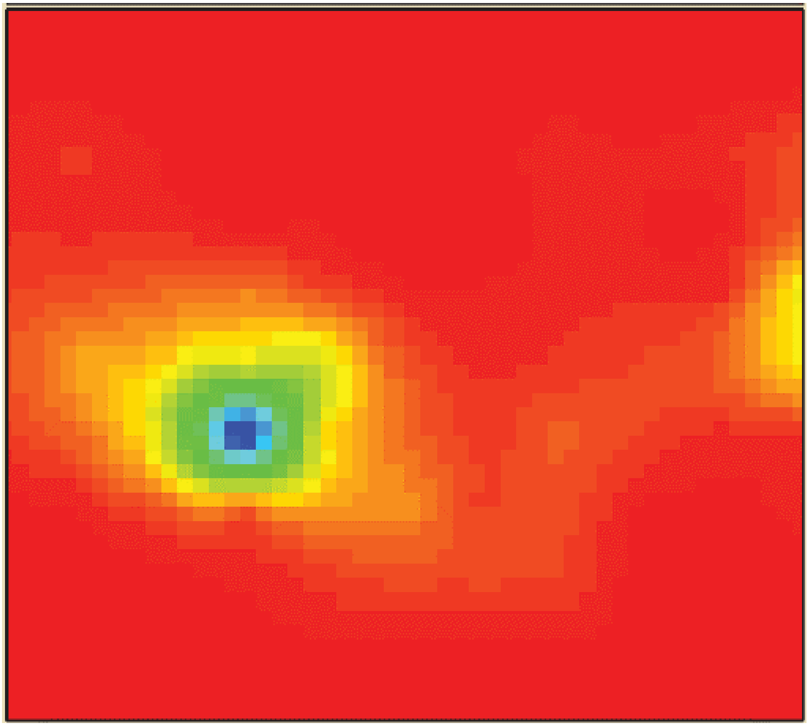
- ❑ Iteratively "smooth" a prior ensemble to sample the posterior



Pilot Points as a tool for representing heteogeneity



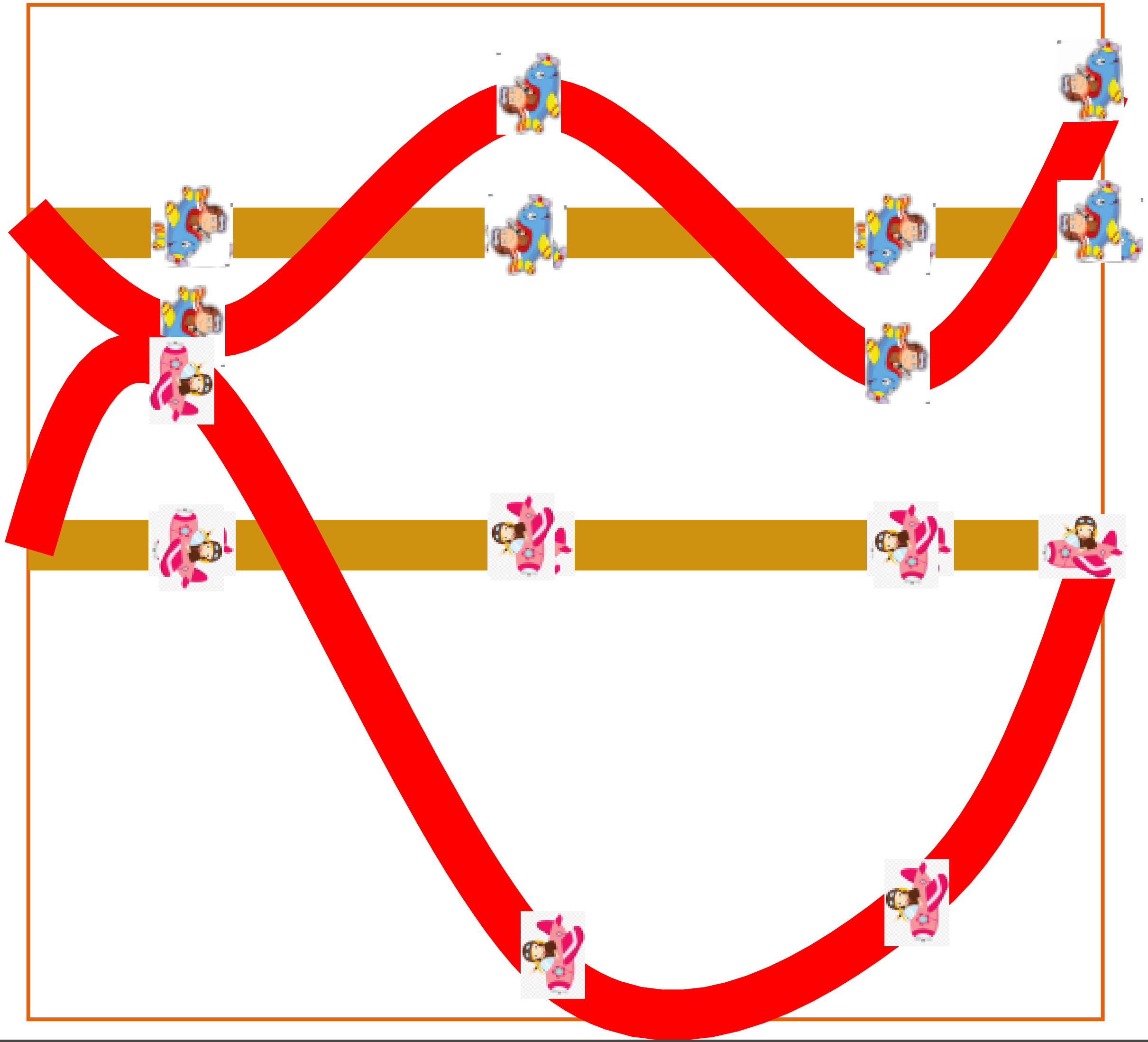
Pilot points colored and sized by associated value



Surface created by interpolating to model grid scale

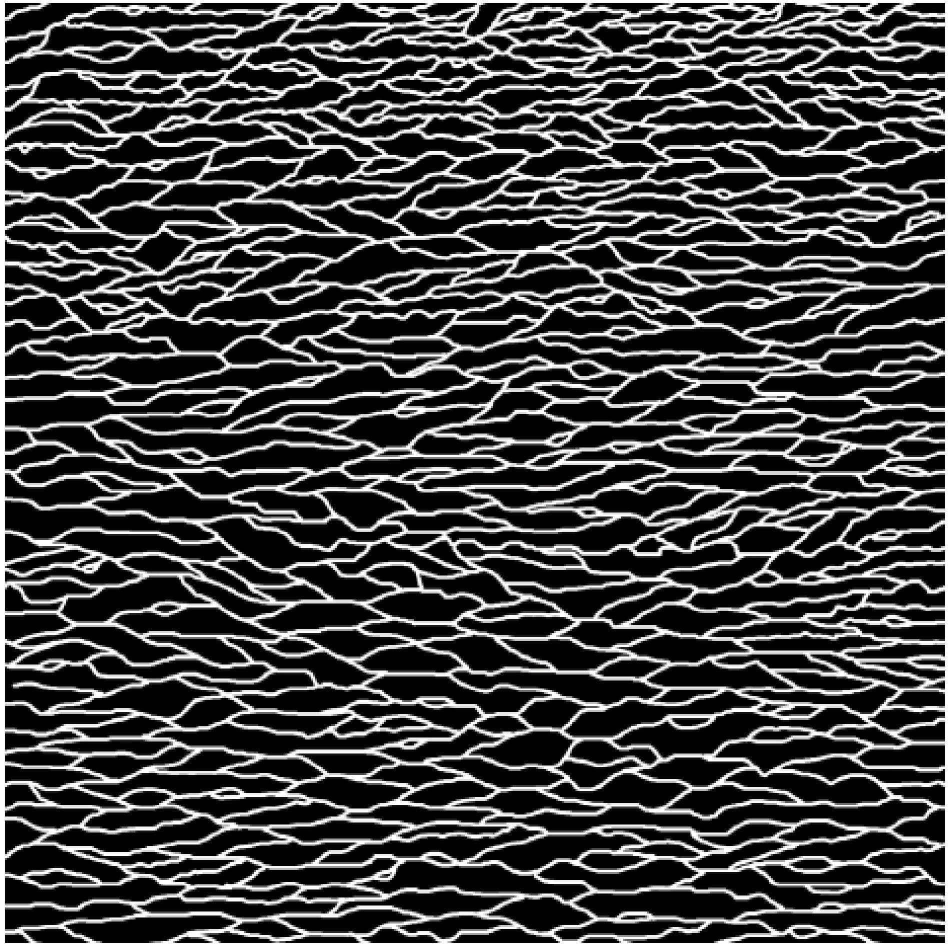
Source: USGS SIR 2010-5168

Traveling Pilot Points (TRIPS)



Infer the extents of the channels and their properties simultaneously

Training Image to Covariance



	y11	y12	y13	y14	y15	y21	y22	y23	y24	y25	y31	y32	y33	y34	y35	$log_{10}(K_c)$	$log_{10}(K_m)$
y11	253.8	231.1	203.5	186.3	173.8	107.7	102.4	92.3	90.9	85.0	52.2	34.5	28.6	36.7	31.1	0.0	0.0
y12	231.1	244.5	219.6	206.4	193.9	104.8	98.3	89.3	90.4	85.5	45.6	32.2	24.5	31.8	25.0	0.0	0.0
y13	203.5	219.6	247.7	237.2	222.4	98.1	97.4	96.1	96.7	91.8	44.0	34.7	32.4	38.6	34.2	0.0	0.0
y14	186.3	206.4	237.2	273.1	262.2	89.3	92.0	95.0	100.5	94.8	37.1	32.0	35.2	39.9	38.4	0.0	0.0
y15	173.8	193.9	222.4	262.2	295.2	82.6	85.7	96.8	99.6	95.1	25.9	23.4	26.1	26.3	27.4	0.0	0.0
y21	107.7	104.8	98.1	89.3	82.6	231.6	217.7	204.9	187.1	176.5	103.2	94.5	85.2	80.7	68.7	0.0	0.0
y22	102.4	98.3	97.4	92.0	85.7	217.7	240.3	225.6	207.3	198.4	102.0	95.3	84.7	82.0	69.6	0.0	0.0
y23	92.3	89.3	96.1	95.0	96.8	204.9	225.6	262.0	243.8	227.9	95.9	91.6	90.7	97.0	87.4	0.0	0.0
y24	90.9	90.4	96.7	100.5	99.6	187.1	207.3	243.8	270.0	252.5	87.5	84.6	87.8	103.6	95.6	0.0	0.0
y25	85.0	85.5	91.8	94.8	95.1	176.5	198.4	227.9	252.5	273.4	86.5	83.2	81.2	94.9	89.7	0.0	0.0
y31	52.2	45.6	44.0	37.1	25.9	103.2	102.0	95.9	87.5	86.5	168.2	142.0	129.0	115.5	110.6	0.0	0.0
y32	34.5	32.2	34.7	32.0	23.4	94.5	95.3	91.6	84.6	83.2	142.0	167.6	155.6	146.1	137.8	0.0	0.0
y33	28.6	24.5	32.4	35.2	26.1	85.2	84.7	90.7	87.8	81.2	129.0	155.6	186.8	185.1	172.2	0.0	0.0
y34	36.7	31.8	38.6	39.9	26.3	80.7	82.0	97.0	103.6	94.9	115.5	146.1	185.1	235.3	222.5	0.0	0.0
y35	31.1	25.0	34.2	38.4	27.4	68.7	69.6	87.4	95.6	89.7	110.6	137.8	172.2	222.5	253.4	0.0	0.0
$log_{10}(K_c)$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	0
$log_{10}(K_m)$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.01

TABLE A.2: Covariance Matrix for prior parameters

Contents lists available at ScienceDirect

Advances in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

The Traveling Pilot Point method. A novel approach to parameterize the inverse problem for categorical fields

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ARTICLE INFO

Keywords:
Inverse problem
Categorical inversion
Traveling pilot points
Multiple-point statistics
Null Space Monte Carlo
Linear sub-space methods

ABSTRACT

Categorical parameter distributions are common-place in hydrogeological systems consisting of geologic facies/categories with distinct properties, e.g., high-permeability channels embedded in a low-permeability matrix. Parameter estimation is difficult in such systems because the discontinuities in the parameter space hinder the inverse problem. Previous research in this area has been focused on the use of stochastic methods. In this paper, we present a novel approach based on Traveling Pilot points (TRIPS) combined with subspace parameter estimation methods to generate realistic categorical parameter distributions that honor calibration constraints (e.g., - measured water levels). In traditional implementations, aquifer properties (e.g., hydraulic conductivity) are estimated at fixed pilot point locations. In the TRIPS implementation, both the properties associated with the pilot points and their locations are estimated. Tikhonov regularization constraints are incorporated in the parameter estimation process to produce realistic parameter depictions. For a synthetic aquifer system, we solved the categorical inverse problem by combining the TRIPS methodology with two subspace methods: Null Space Monte Carlo (NSMC) and Posterior Covariance (PC). A posterior ensemble developed with the rejection sampling (RS) method is compared against the TRIPS ensembles. The comparisons indicated similarities between the various ensembles and to the reference parameter distribution. Between the two subspace methods, the NSMC method produced an ensemble with more variability than the PC method. These preliminary results suggest that the TRIPS methodology has promise and could be tested on more complicated problems.

Groundwater

Towards Improved Remedial Outcomes in Categorical Aquifers with an Iterative Ensemble Smoother

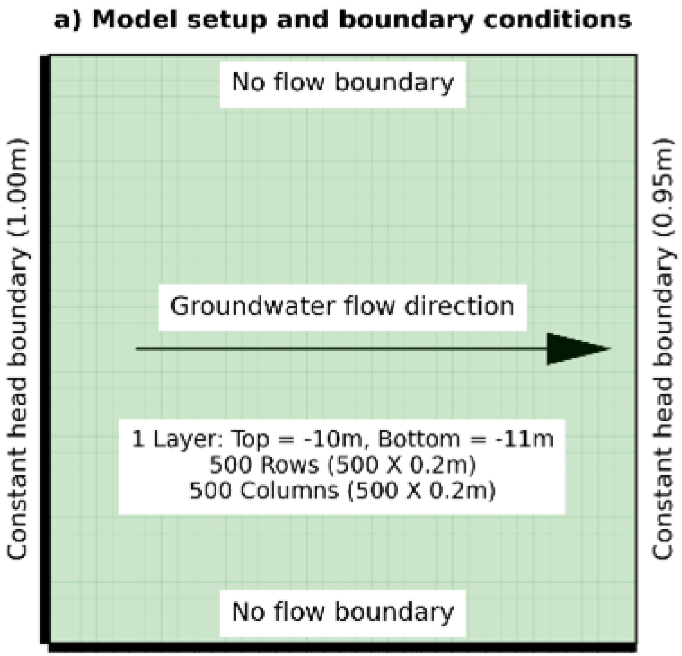
by Prashanth Khambhammettu[1], Philippe Renard[2], John Doherty[3], Jeremy White[4], Marc Killingstad[5], and Michael Kladias[5]

Abstract

Categorical parameter distributions consisting of geologic facies with distinct properties, for example, high-permeability channels embedded in a low-permeability matrix, are common at contaminated sites. At these sites, low-permeability facies store solute mass, acting as secondary sources to higher-permeability facies, sustaining concentrations for decades while increasing risk and cleanup costs. Parameter estimation is difficult in such systems because the discontinuities in the parameter space hinder the inverse problem. This paper presents a novel approach based on Traveling Pilot Points (TRIPS) and an iterative ensemble smoother (IES) to solve the categorical inverse problem. Groundwater flow and solute transport in a hypothetical aquifer with a categorical parameter distribution are simulated using MODFLOW 6. Heads and concentrations are recorded at multiple monitoring locations. IES is used to generate posterior ensembles assuming a TRIPS prior and an approximate multi-Gaussian prior. The ensembles are used to predict solute concentrations and mass into the future. The evaluation also includes an assessment of how the number of measurements and the choice of the geological prior determine the characteristics of the posterior ensemble and the resulting predictions. The results indicate that IES was able to efficiently sample the posterior distribution and showed that even with an approximate geological prior, a high degree of parameterization and history matching could lead to parameter ensembles that can be useful for making certain types of predictions (heads, concentrations). However, the approximate geological prior was insufficient for predicting mass. The analysis demonstrates how decision-makers can quantify uncertainty and make informed decisions with an ensemble-based approach.

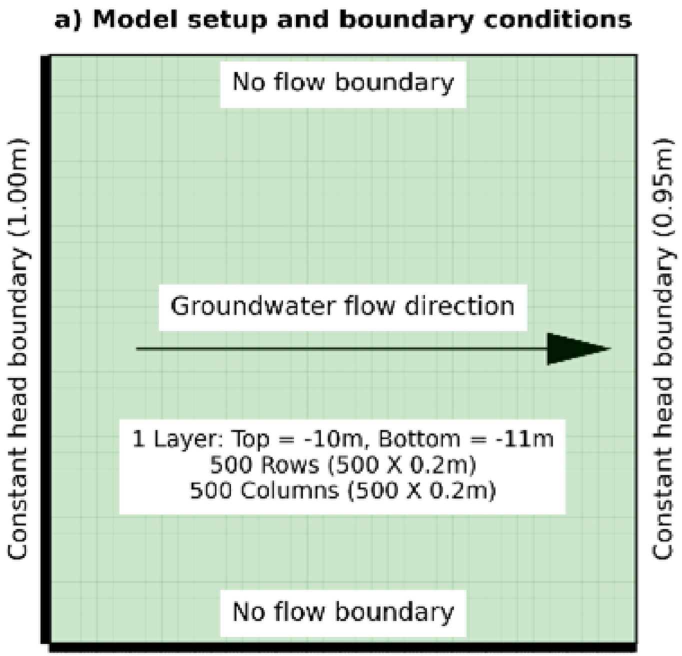
A Flow and Transport Example

- Infer categorical facies from groundwater heads and solute concentrations
- Quantify remedial uncertainty after 30 years



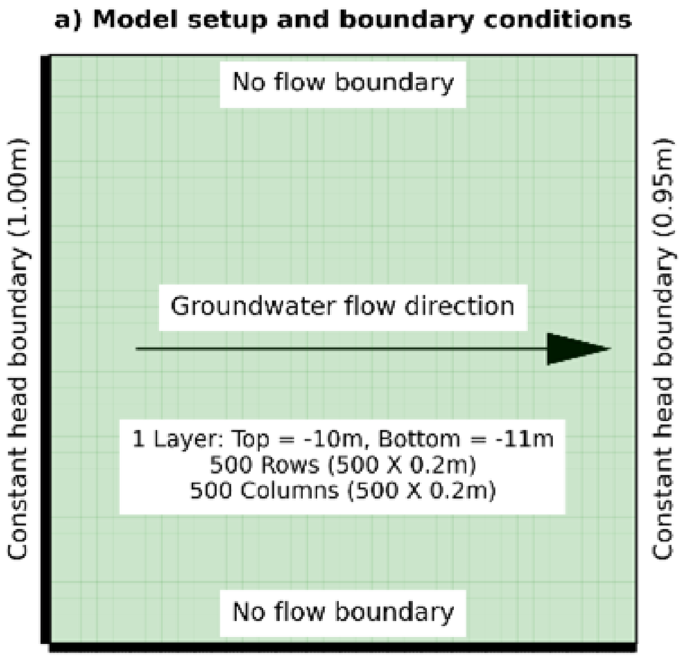
Gradient = 10^{-4}

Steady-state groundwater flow



Constant Concentration Source (10^4 µg/l)

Active for the first two years (Column 2)

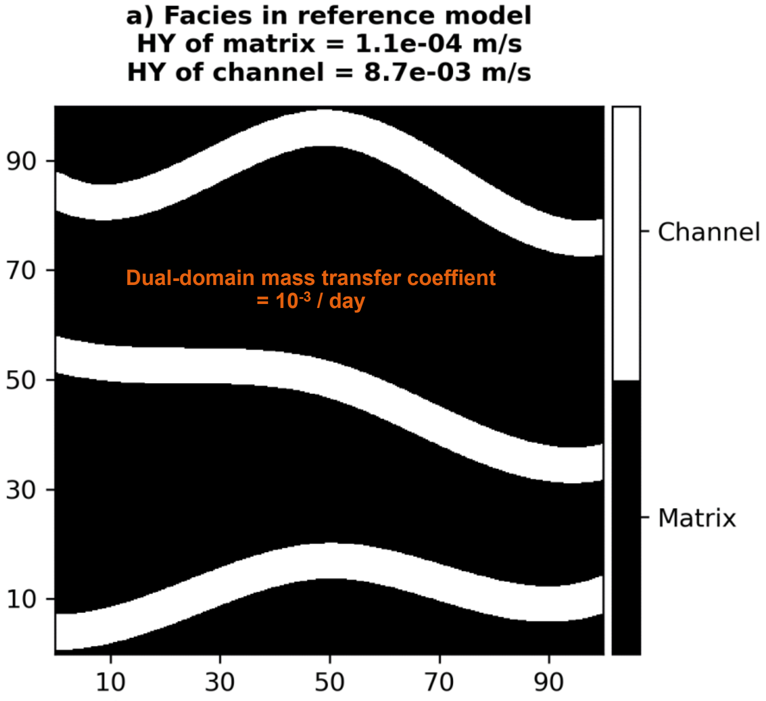


Source removed after two years

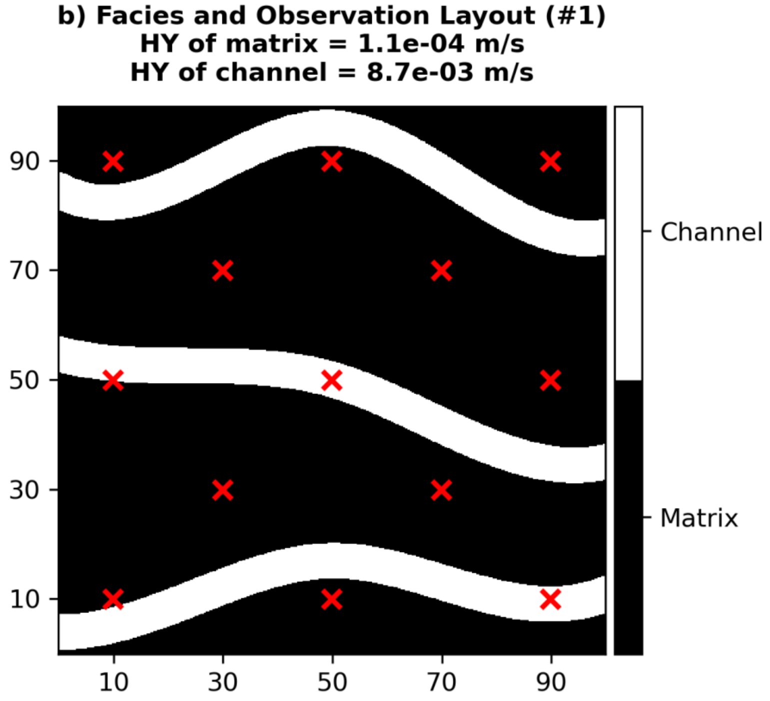
Solute transport evaluated for another 28 years

Transport Process and Monitoring Locations

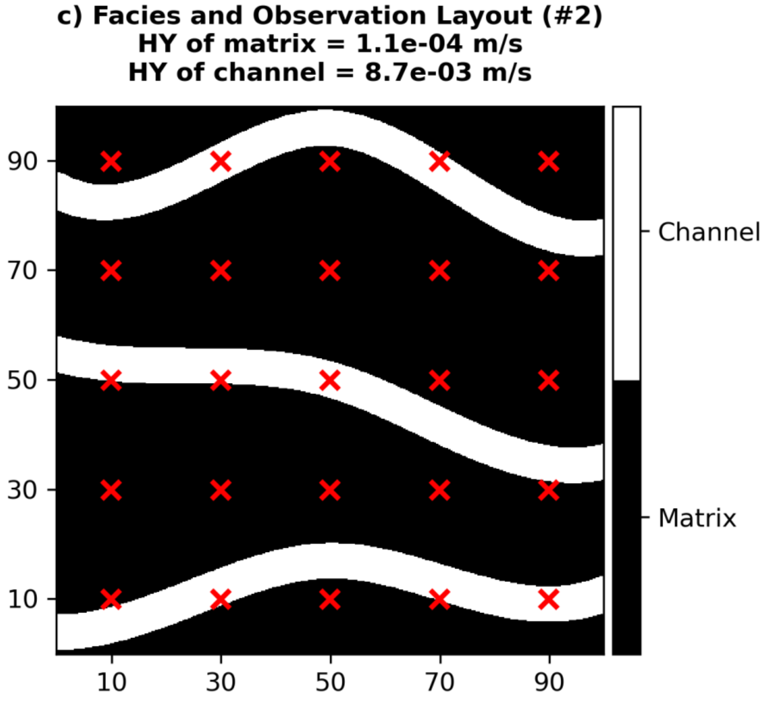
- Dual-domain(mobile/immobile) approach for simulating solute transport
- Dispersion/sorption/decay not simulated



Facies	Total Porosity	Mobile porosity	Immobile porosity
Channel	35%	10%	25%
Matrix	43%	1%	42%



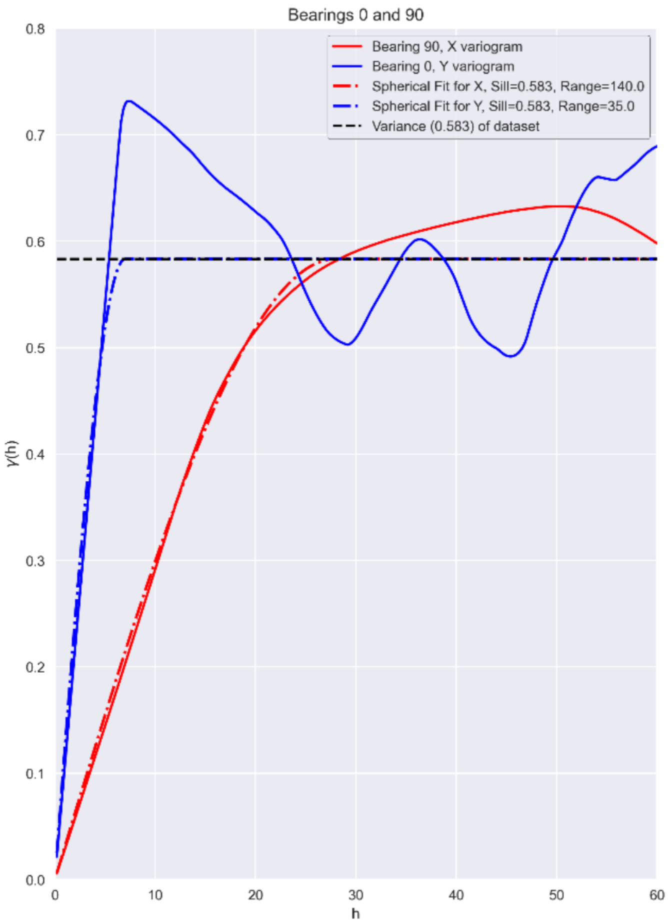
13 Monitoring Locations
Monitor quarterly for four years
13 heads, 208(13*16) concentrations

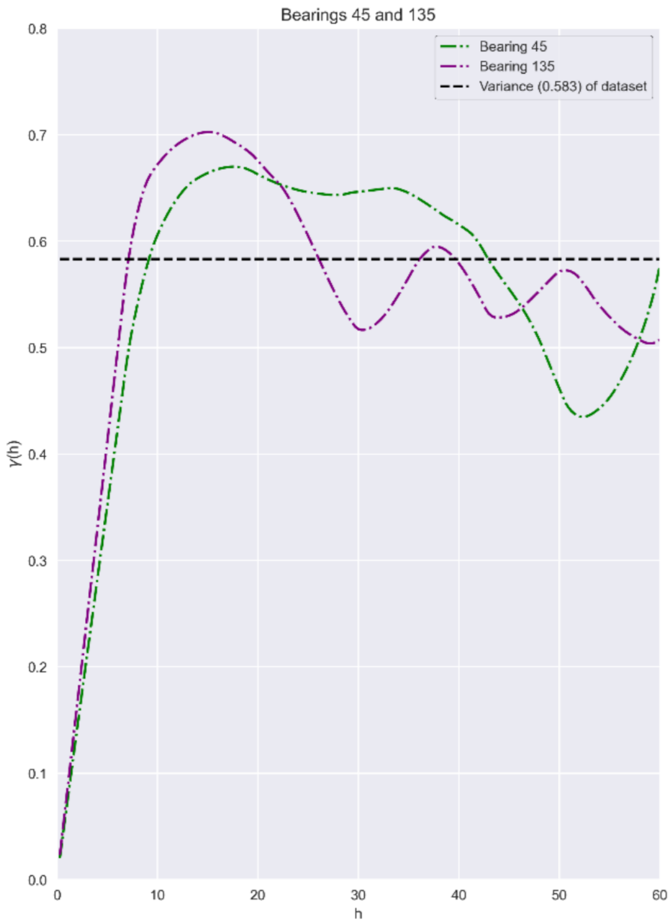


25 Monitoring Locations
Monitor quarterly for four years
25 heads, 400(25*16) concentrations

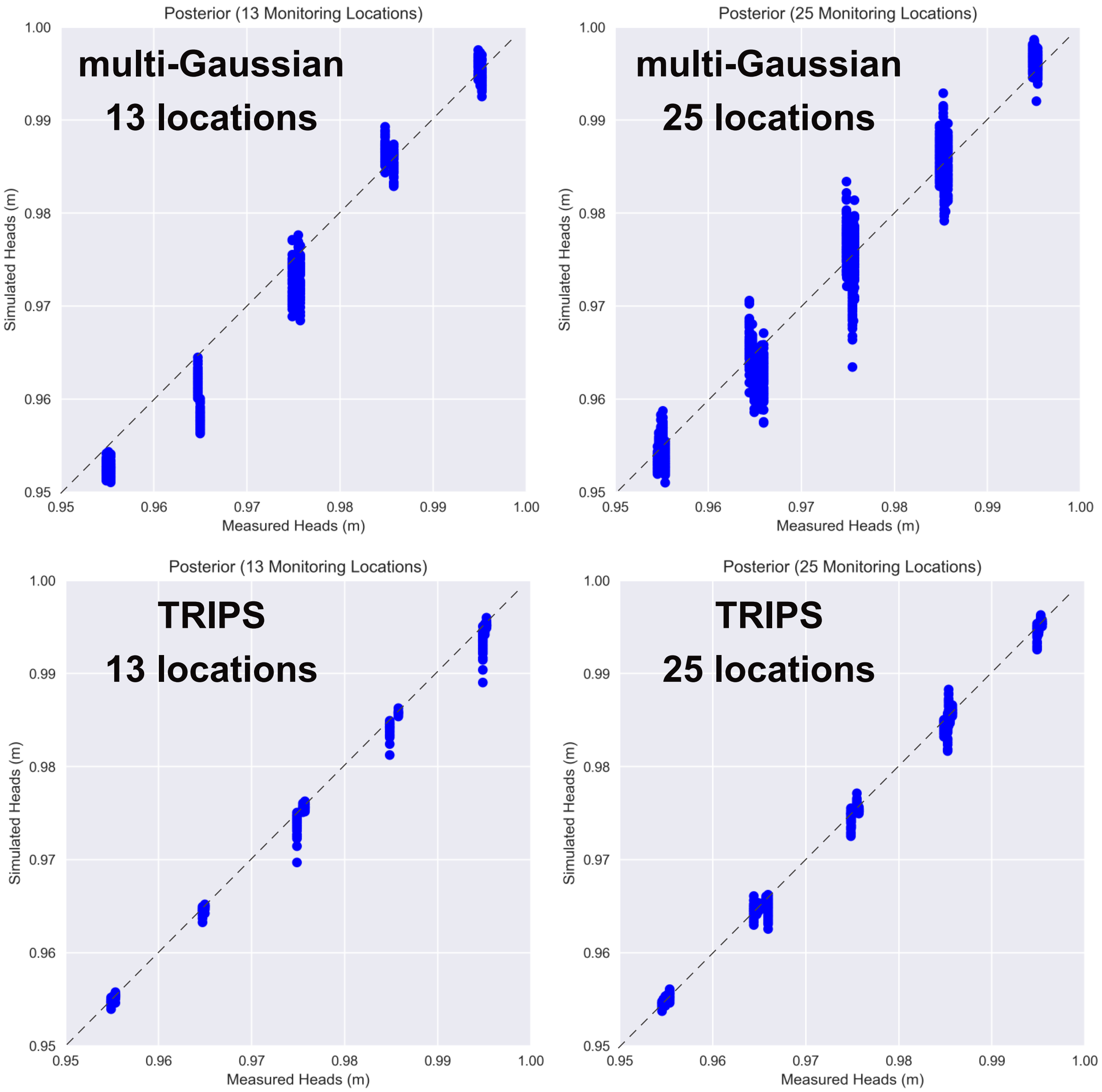
Heterogeneity Simulation Approaches

- Discrete(TRIPS-based) approach (15 TRIP locations, 2 hydraulic conductivity values)
- Continuous(multi-Gaussian) prior (simulate HY in every grid cell)
  - 250’000 parameters



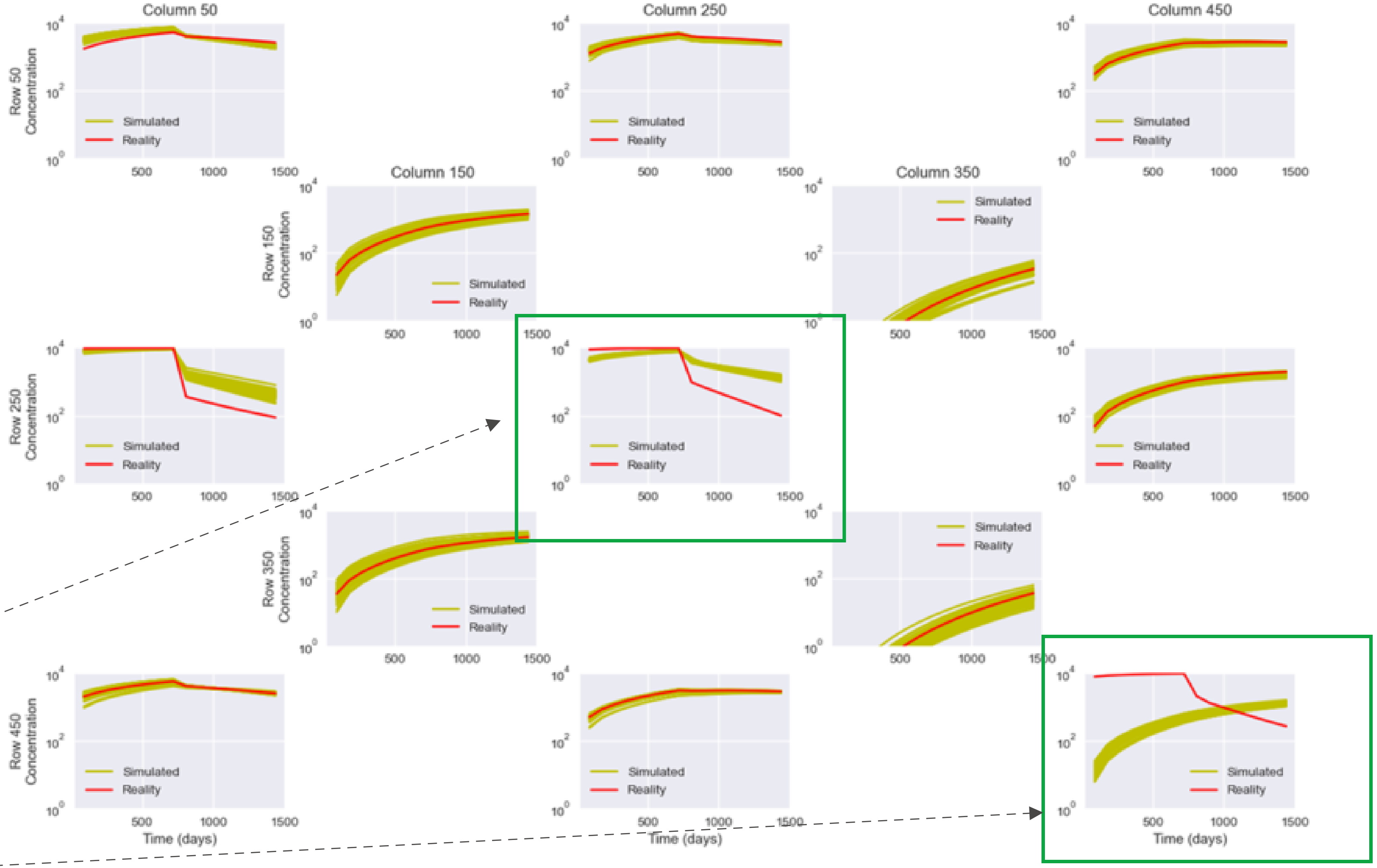


Simulated Vs. Observed Heads

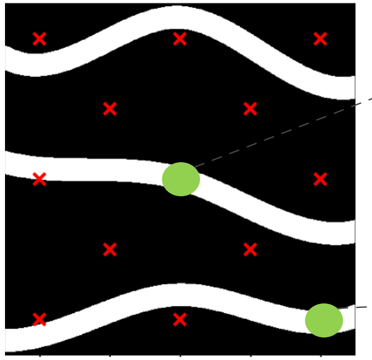


Simulated vs. Observed Concentrations

multi-Gaussian Continuous Posterior 13 monitoring

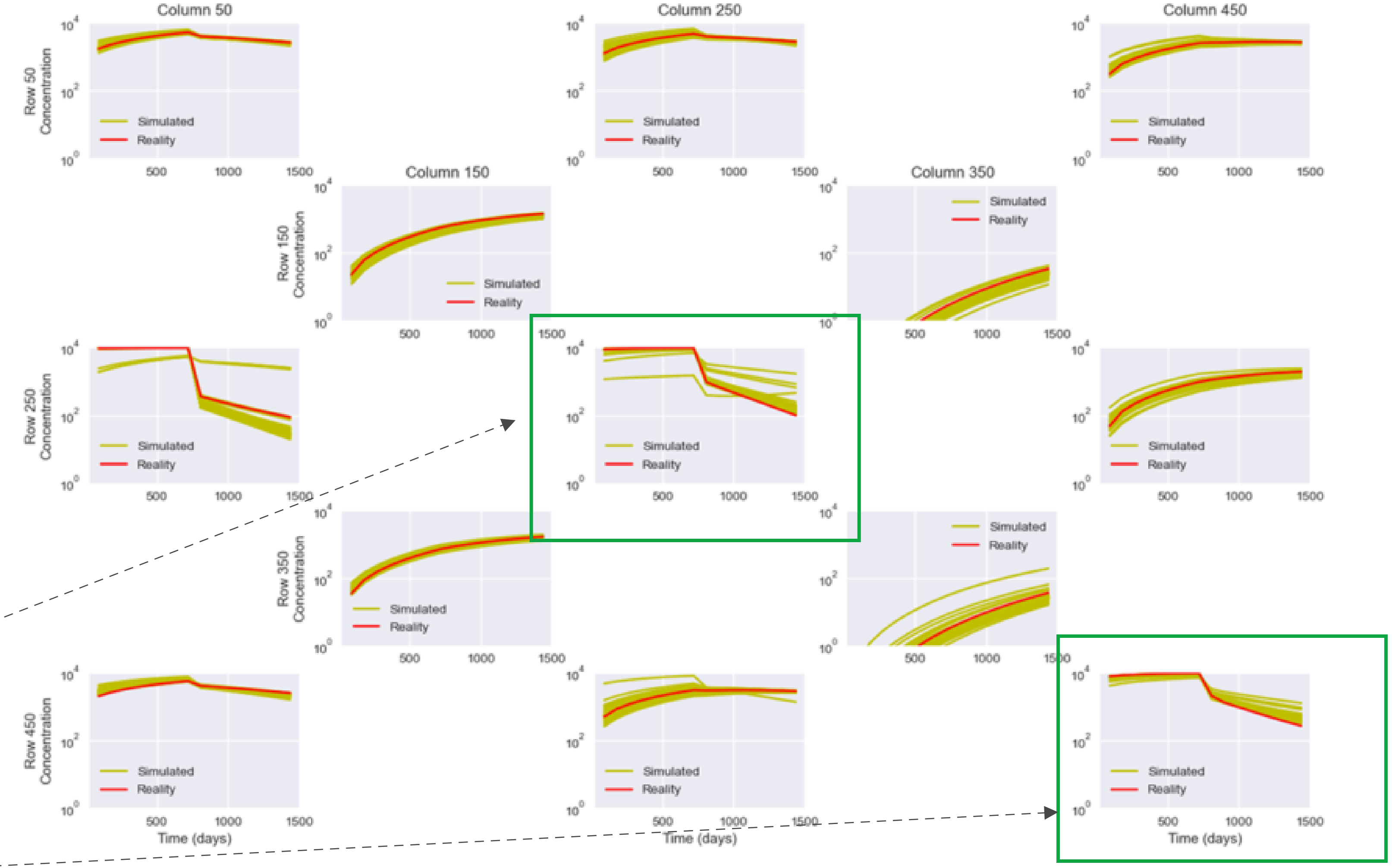


location of observations

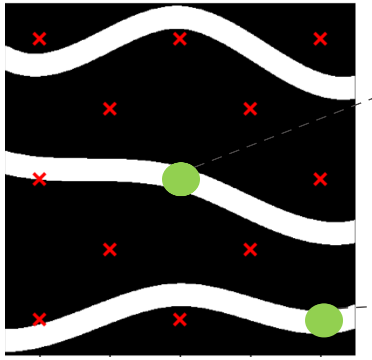


Simulated vs. Observed Concentrations

**TRIPS
Discrete
Posterior
13 monitoring**

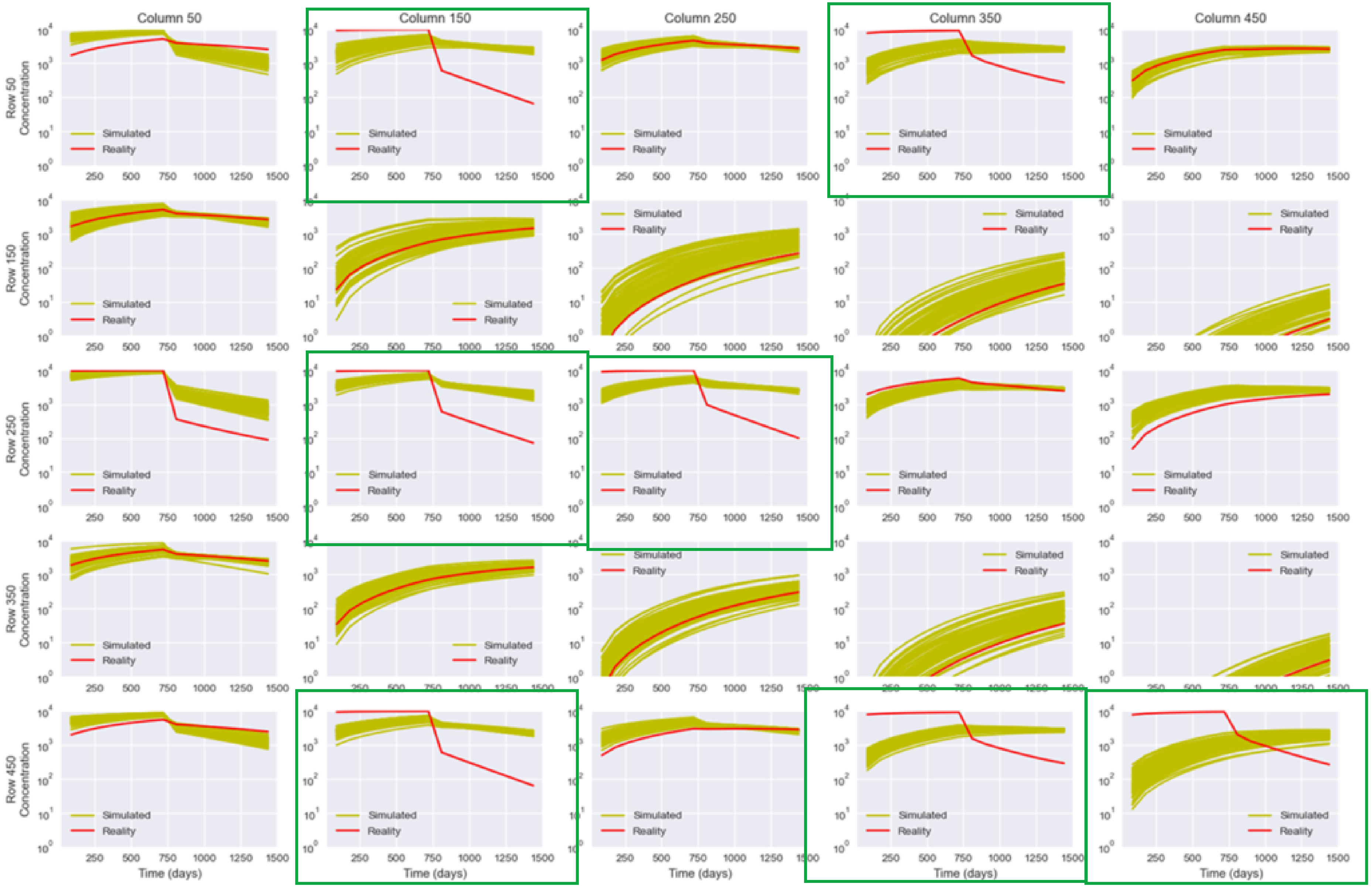


location of observations

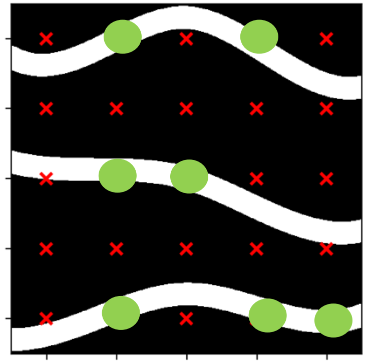


Simulated vs. Observed Concentrations

multi-Gaussian Continuous Posterior 25 monitoring

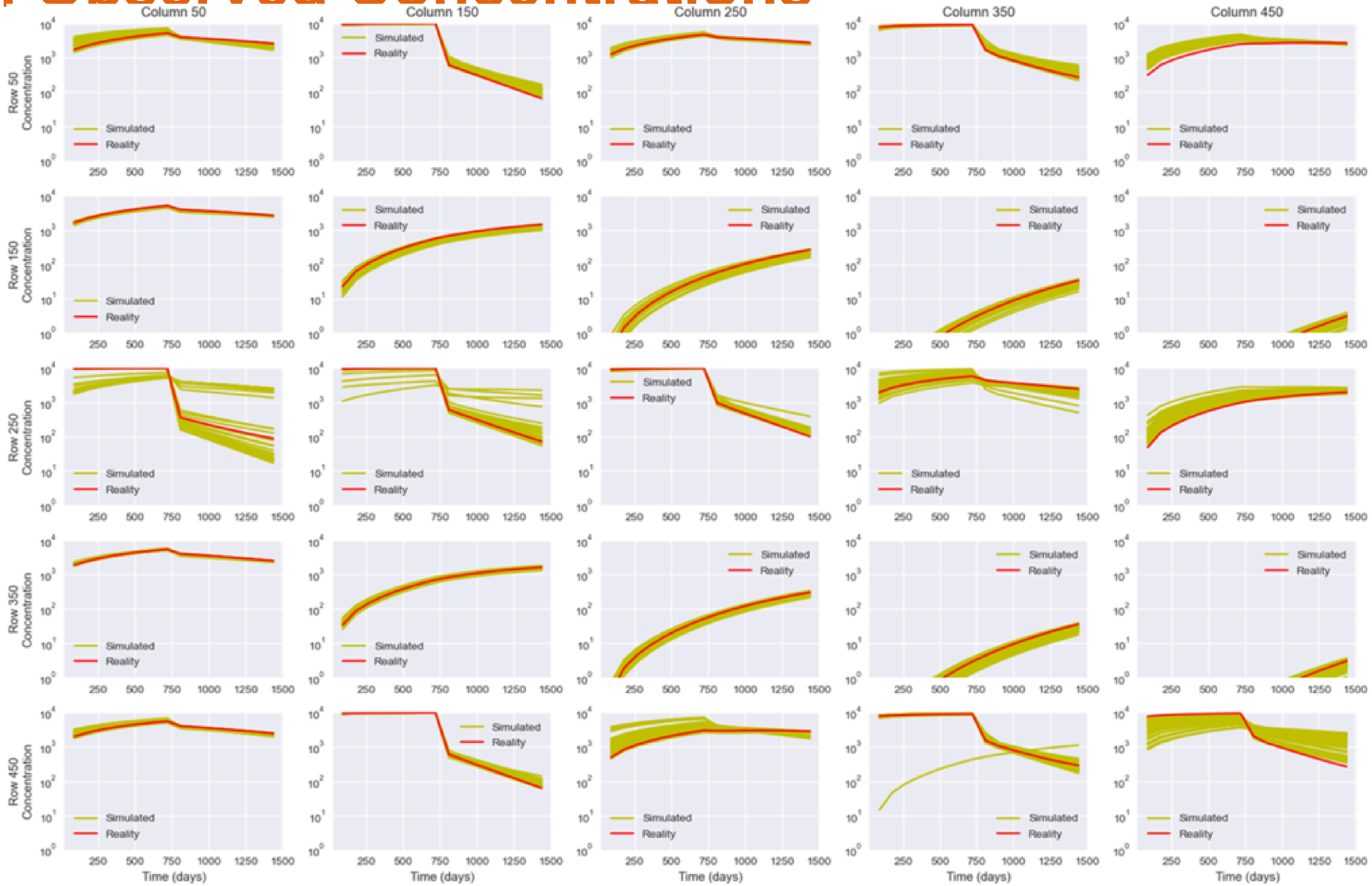


location of observations

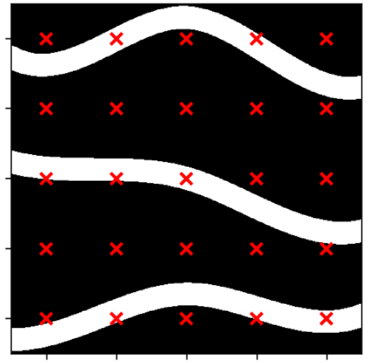


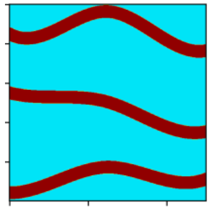
Simulated vs. Observed Concentrations

TRIPS
Discrete
Posterior
25 monitoring

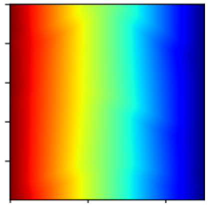


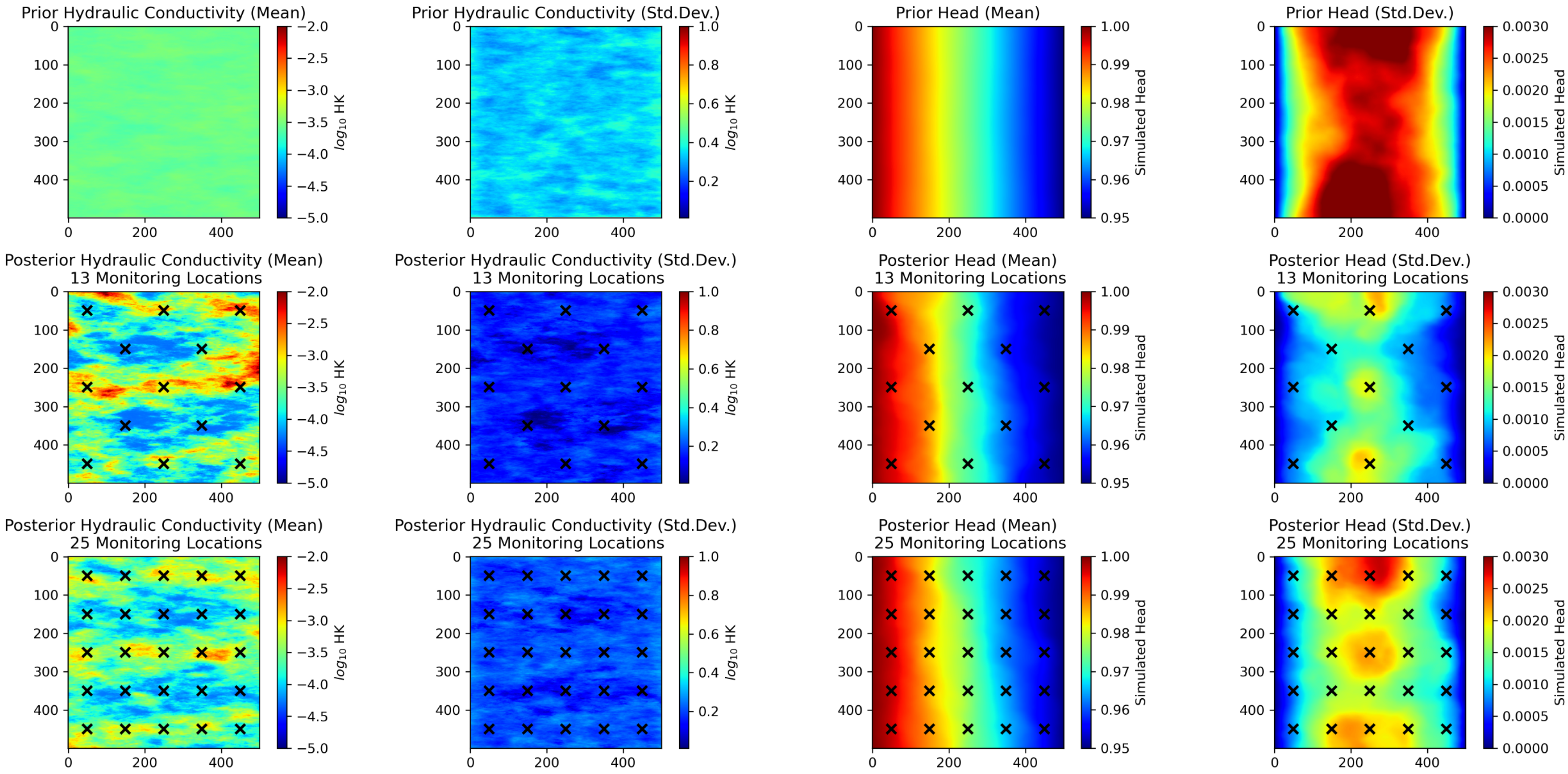
location of observations

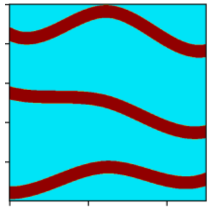




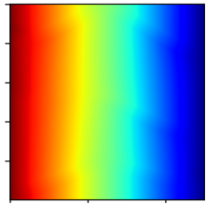
Multi-Gaussian Ensemble

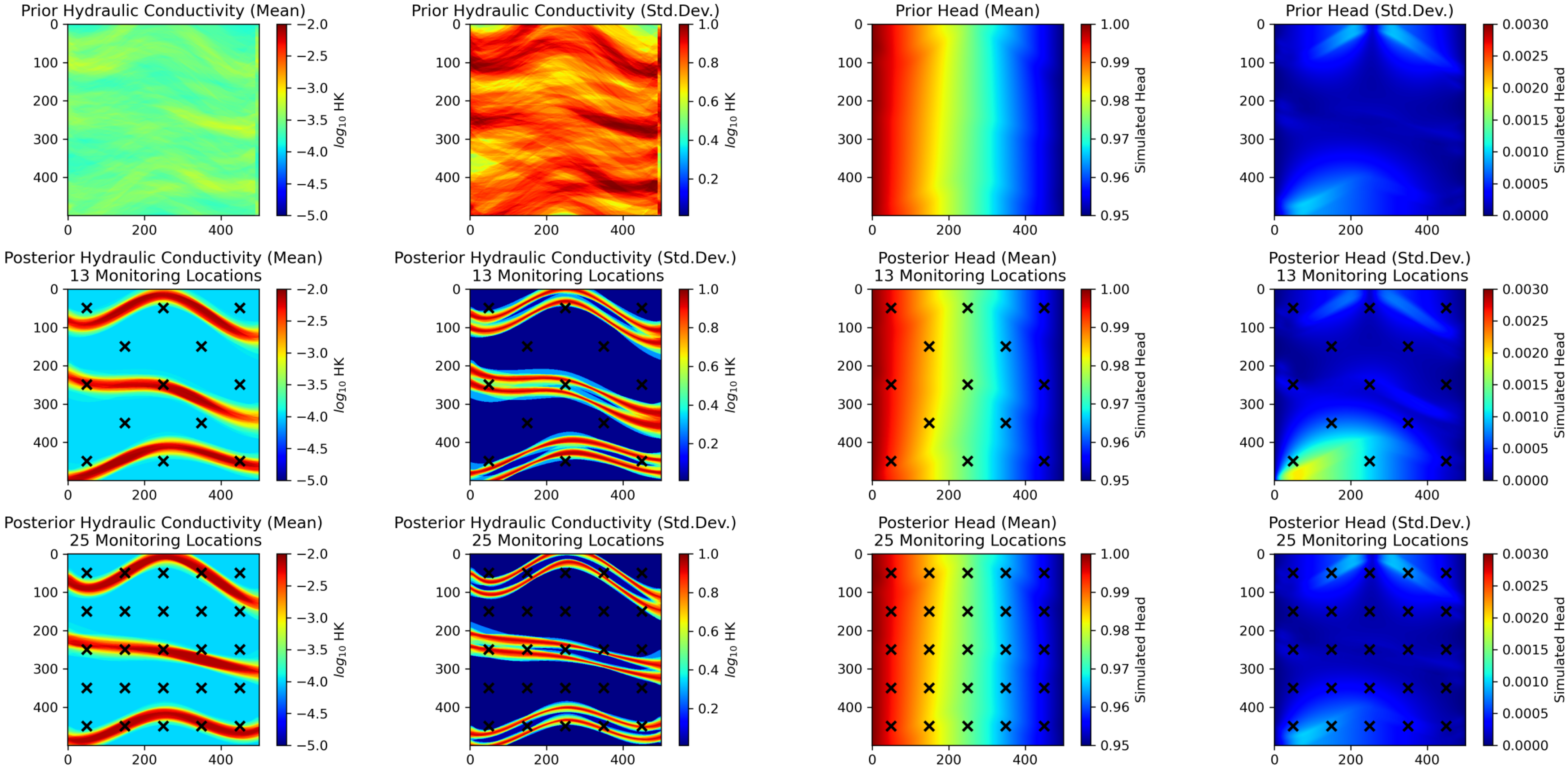




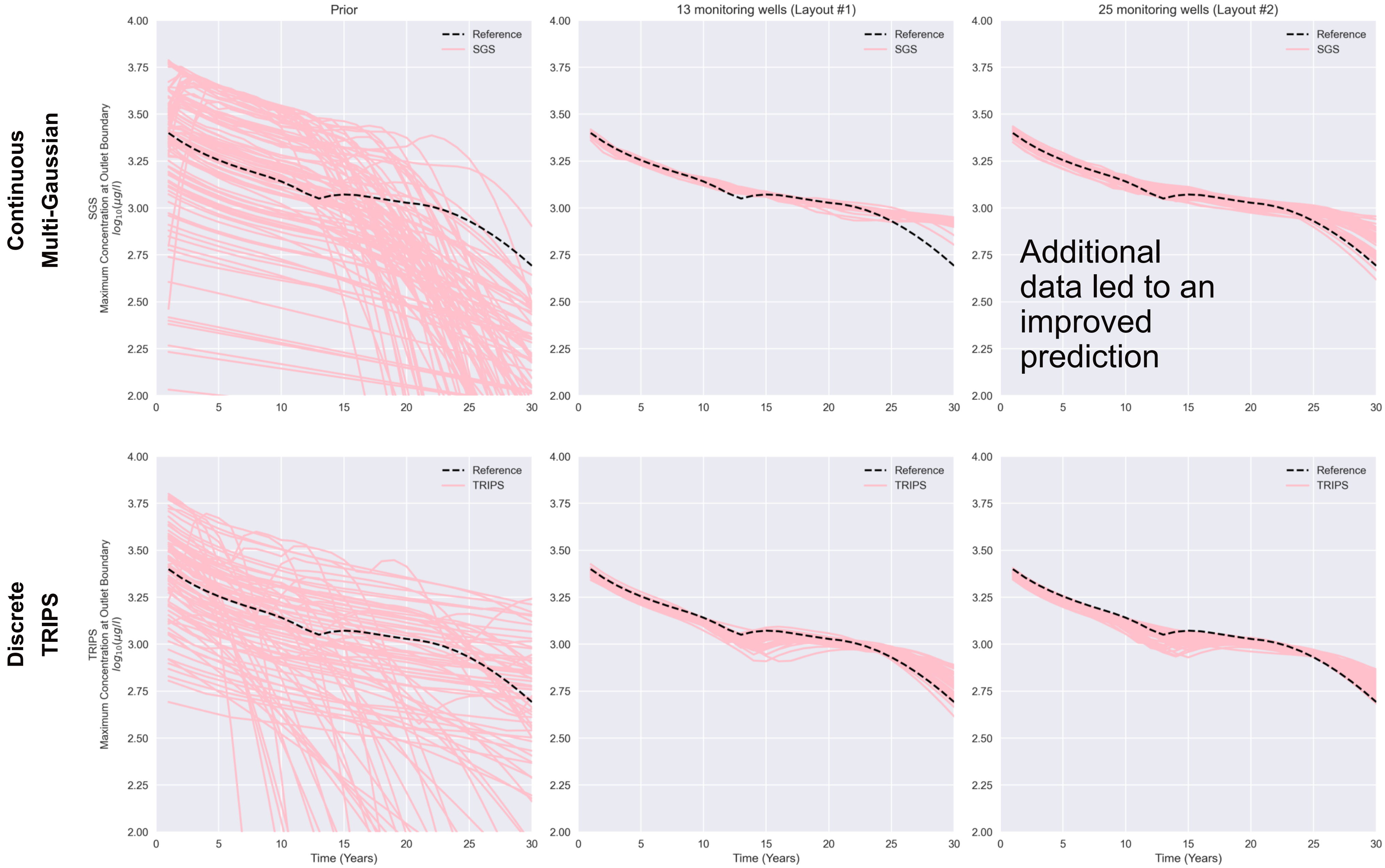


TRIPS Ensemble

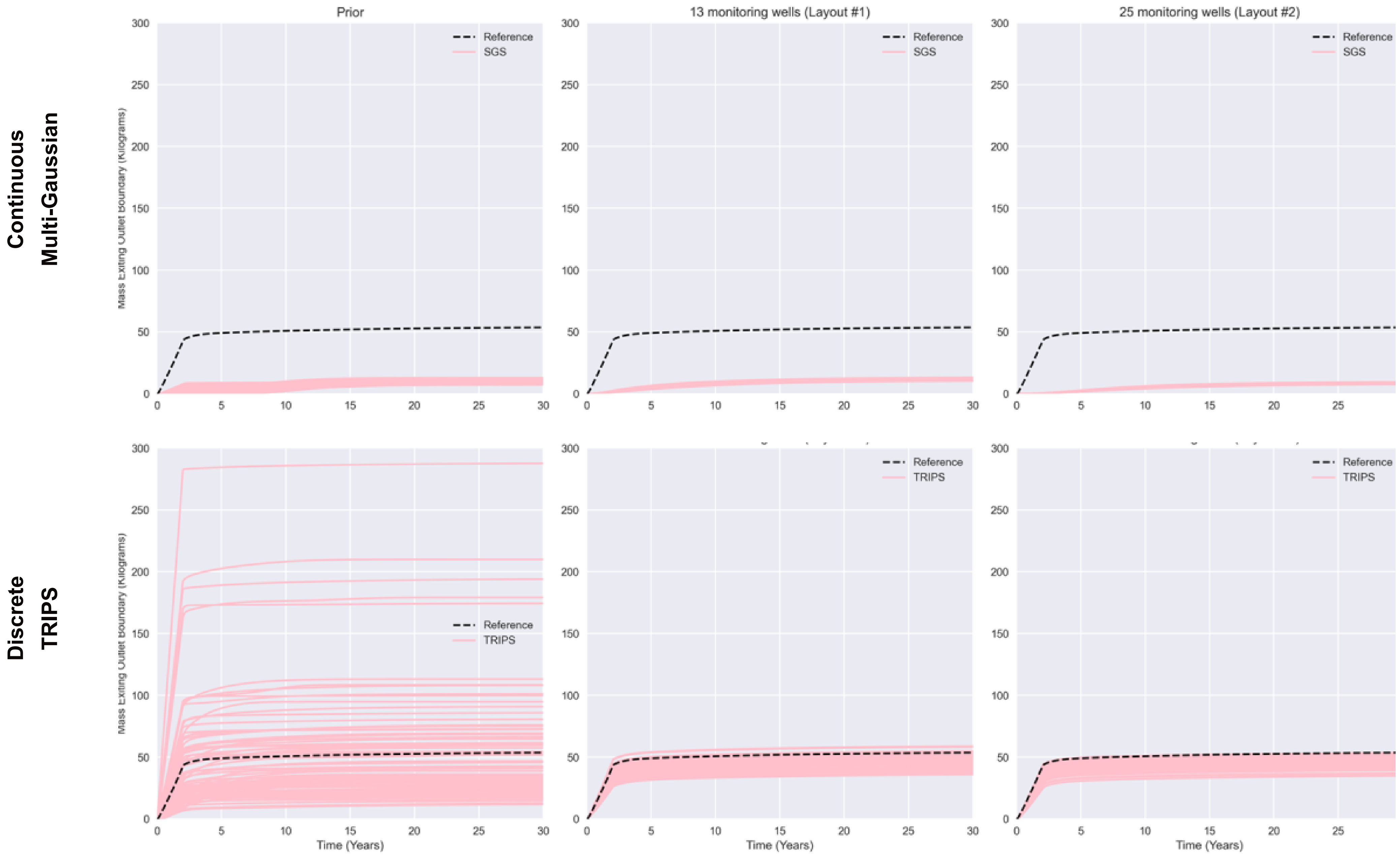




Prediction #1
Uncertainty in Maximum Predicted Concentrations at Outlet Boundary (µg/l)



<u>Prediction #2</u>
Uncertainty in Mass leaving the Outlet Boundary (Kilograms)



Final remarks

- Letting pilot points travel to define geometry of facies in combination with iterative ensemble smoothers) can be used to infer categorical facies
- High-degree of parameterization and history matching can compensate for a bad geological prior for certain predictions
- However, for complex predictions, uncertainty analysis cannot undo the harm of choosing an inappropriate geological prior.
- Be prepared to revise your CSM and predict periodically. That is the norm with a lot of predictive models outside our industry!

Thank you for joining us!

Questions? please reach out to:

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