Putting the *FLOW* in workflow: Using plume prediction AI to quantify groundwater risk and liability

Nico Higgs B.Sc., M.Sc.
Steven Mamet B.Sc., M.Sc., Ph.D.
Environmental Material Science Inc.

www.ems-inc.ca

ems

Environmental Material Science

Who is EMS?

COMPANY FOUNDING

Early Adopters
FCL, Suncor, Transgas

RELEASE OF SOFTWARE-ENABLED HARDWARE

PlumeFutures

2000 — 2019 — 2022 — 2023 — 2024

R&D

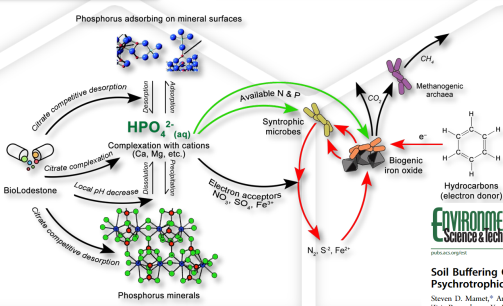
$10M of Sponsored Research by Siciliano Group into In Situ Remediation Technologies

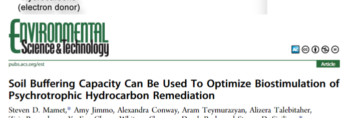
FUNDING

$1.6M Raised from Family Offices, Angels, and Syndicates

EXPANSION & SCALING

US, EU, and Australian Sales

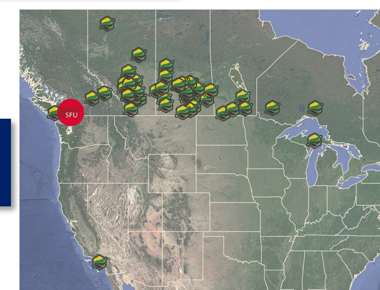



Environmental Science & Technology

Article

Soil Buffering Capacity Can Be Used To Optimize Biostimulation of Psychrotrophic Hydrocarbon Remediation

Steven D. Mamet,* Amy Jimmo, Alexandra Conway, Aram Teymurazyan, Alizera Talebitaher, Zisis Papandreou, Yu-Fen Chang, Whitney Shannon, Derek Peak, and Steven D. Siciliano*



What if we created the world's largest water/soil contaminant database?

HARDWARE
Soil Sensors, Vector Network Analysis, Ionophoric Sensors, Near Infrared

DATA & ANALYTICS
Robust database with 61 million data records powering our analytics

GEO AI
Unlock game-changing insights by expanding to 1.14 billion data records by 2027

Predictive modeling of NSZD
Deep learning (neural networks)

Automated anomaly detection
Unsupervised learning

Site-specific biostim optimization & management actions
Random forests / CNNs

Adaptive management
Stochastic modelling & data assimilation

Apply insights from monitored to unmonitored sites
Transfer learning

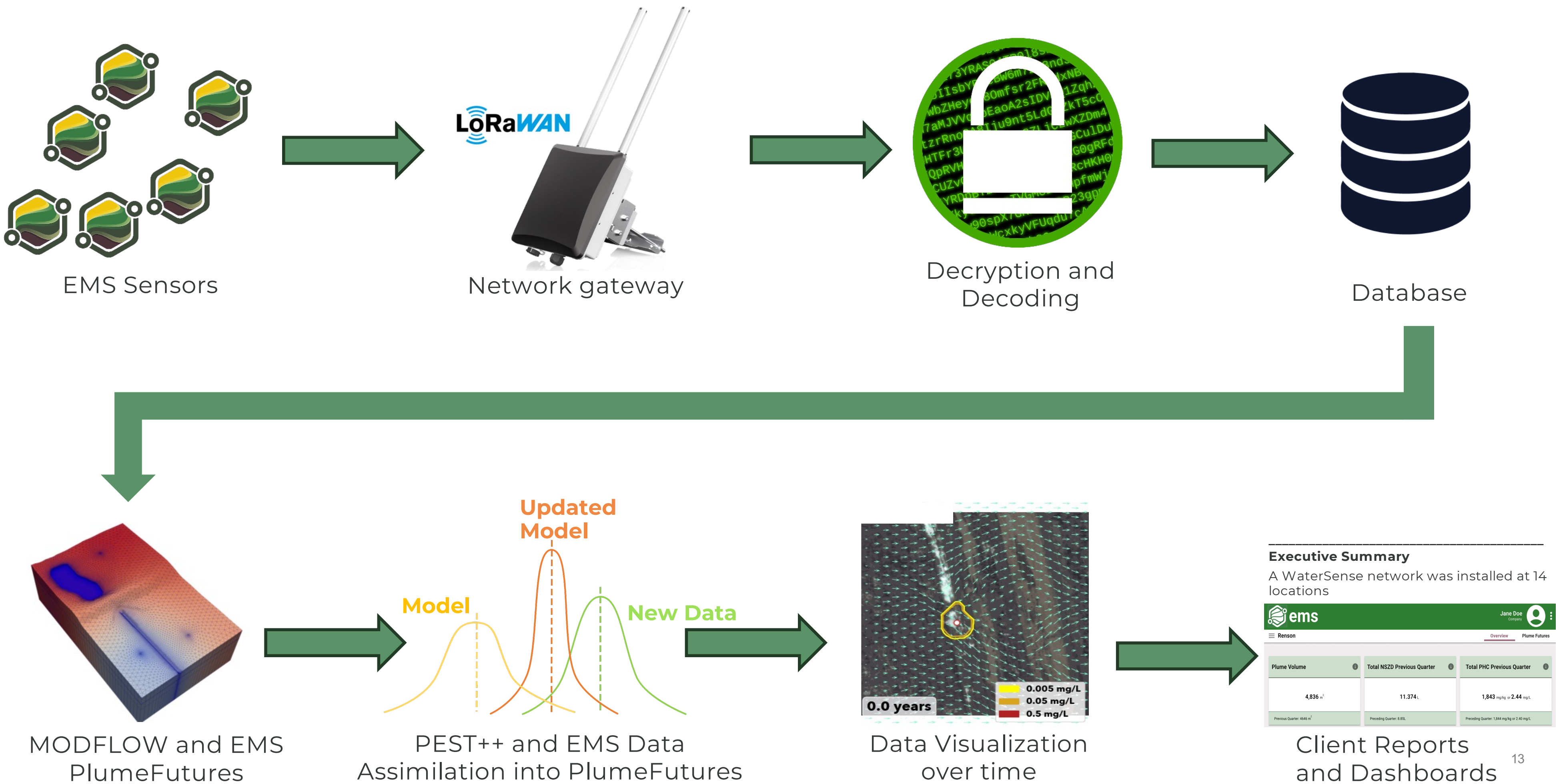
Site portfolio prioritization
Reinforcement learning

Real-time decision support
GEO AI

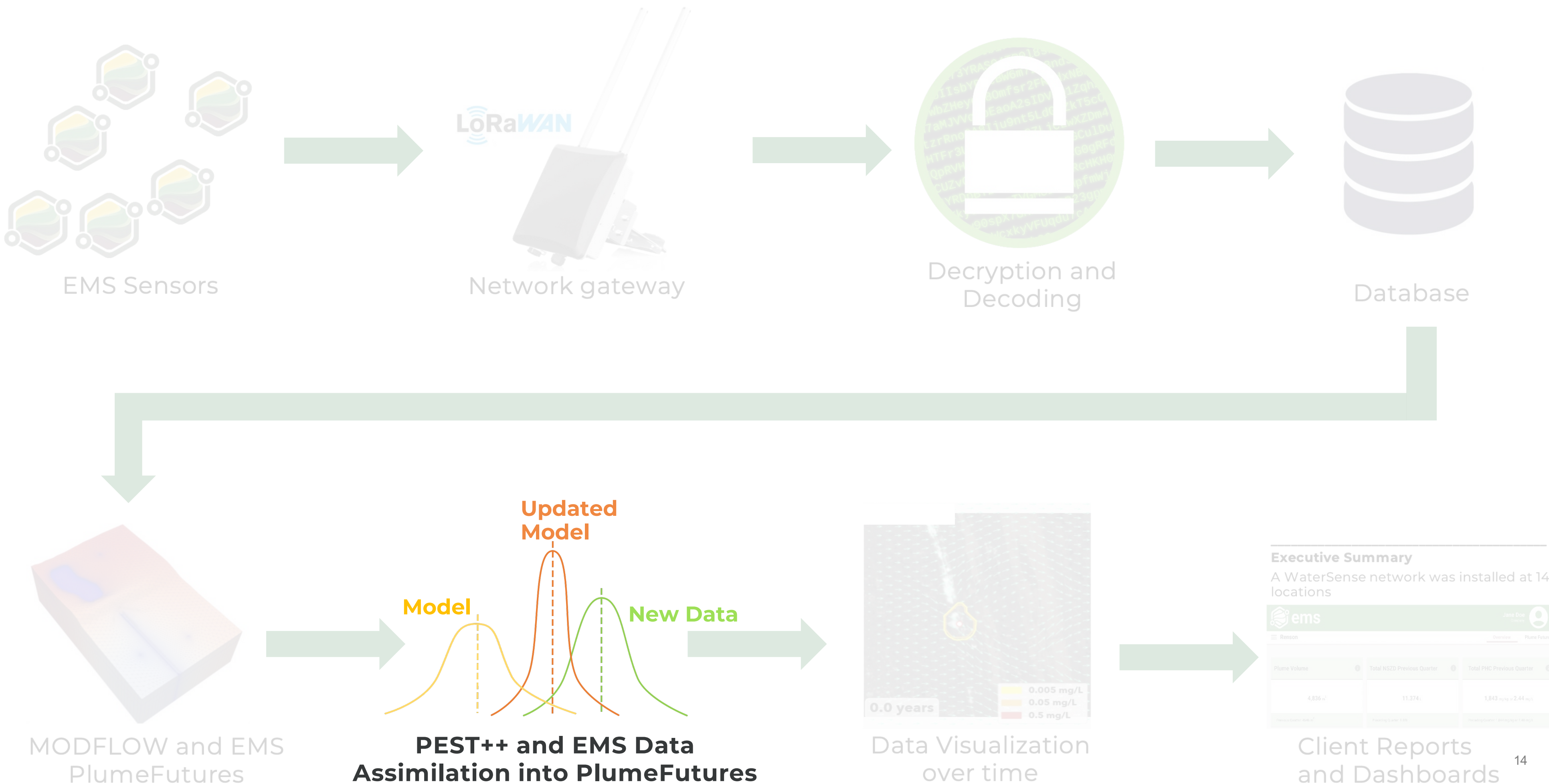
WaterSense Operation

- Gas permeable membrane keeps the sensor **water-proof**, while allowing gases to diffuse to the **NDIR** sensor.
- Measures **CO_2, CH_4**, & **PHC vapours** – calculate dissolved concentrations. Measures **temperature** & **pressure** directly.
- Line or battery powered. **Multi-year battery life**. Solar panel add-on for recharging batteries.
- **Flexible sample times** from minutes to days. Typically, every **30 – 60 minutes**.
- **Automated data communication and storage.** Reduced site trips. Viewable trends on-line.

Data Flow


EMS Sensors
LoRaWAN
Network gateway
Decryption and Decoding
Database
MODFLOW and EMS PlumeFutures
Updated Model
Model
New Data
PEST++ and EMS Data Assimilation into PlumeFutures
0.0 years
0.005 mg/L
0.05 mg/L
0.5 mg/L
Data Visualization over time
Executive Summary
A WaterSense network was installed at 14 locations
ems
Plume Volume
Total NSZD Previous Quarter
Total PHC Previous Quarter
Client Reports and Dashboards

Data Flow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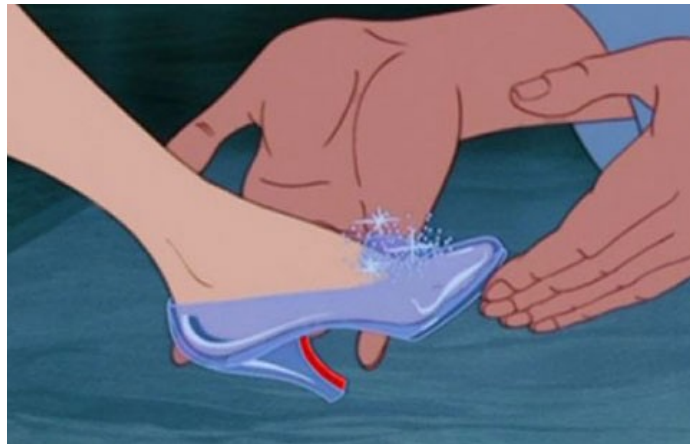
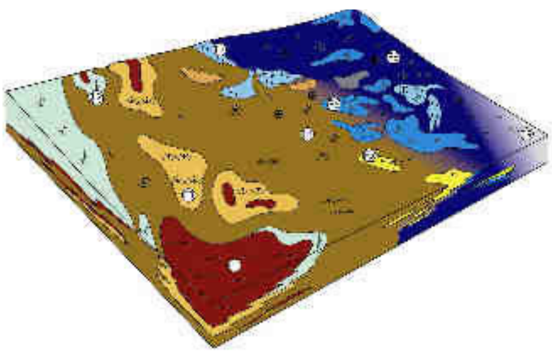
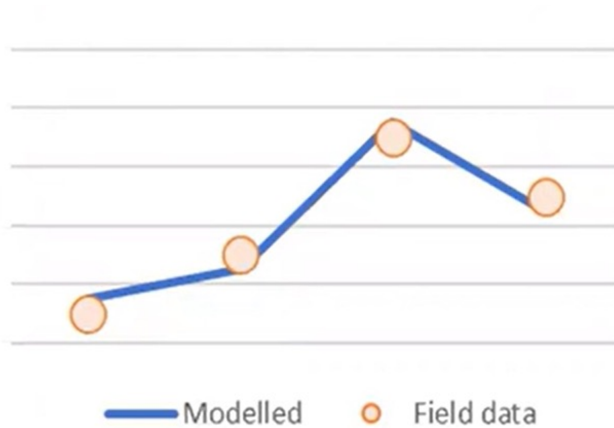
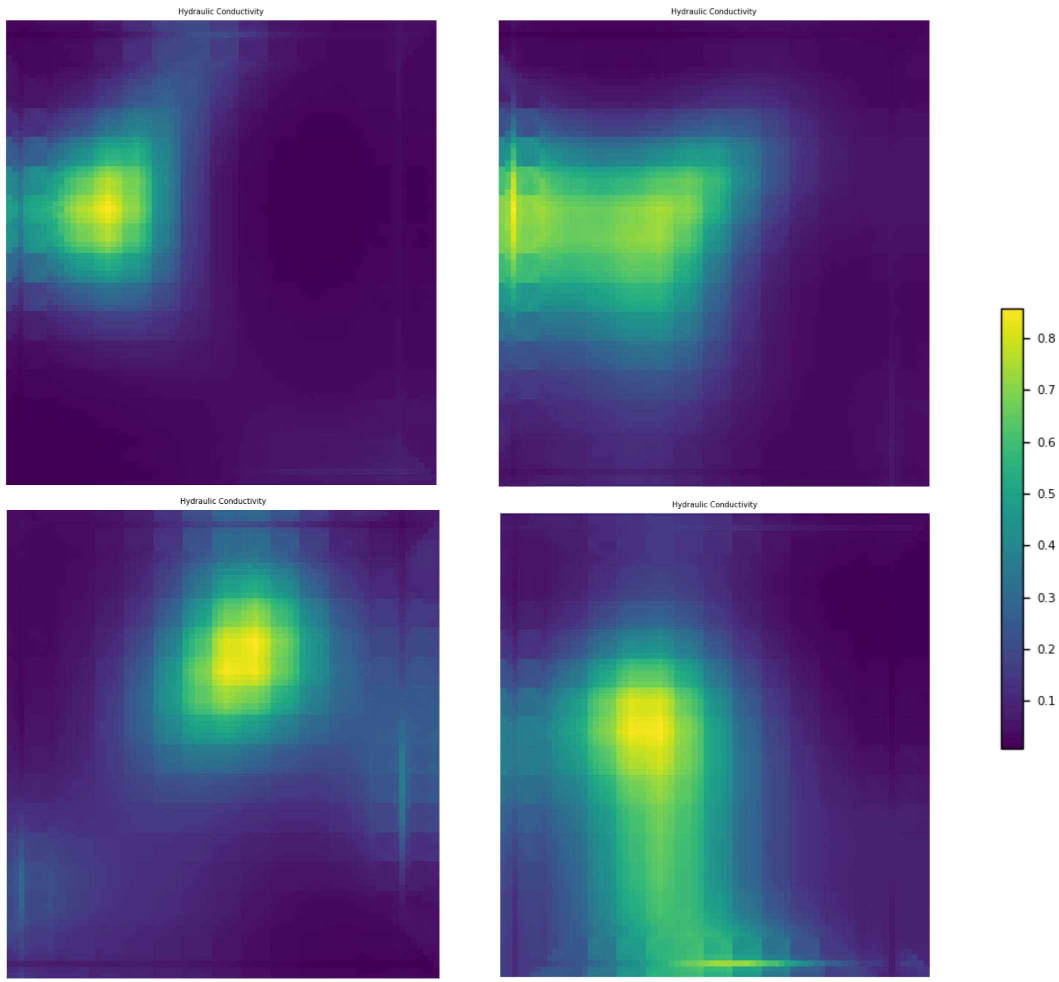
Cinderella Syndrome







Non-Uniqueness



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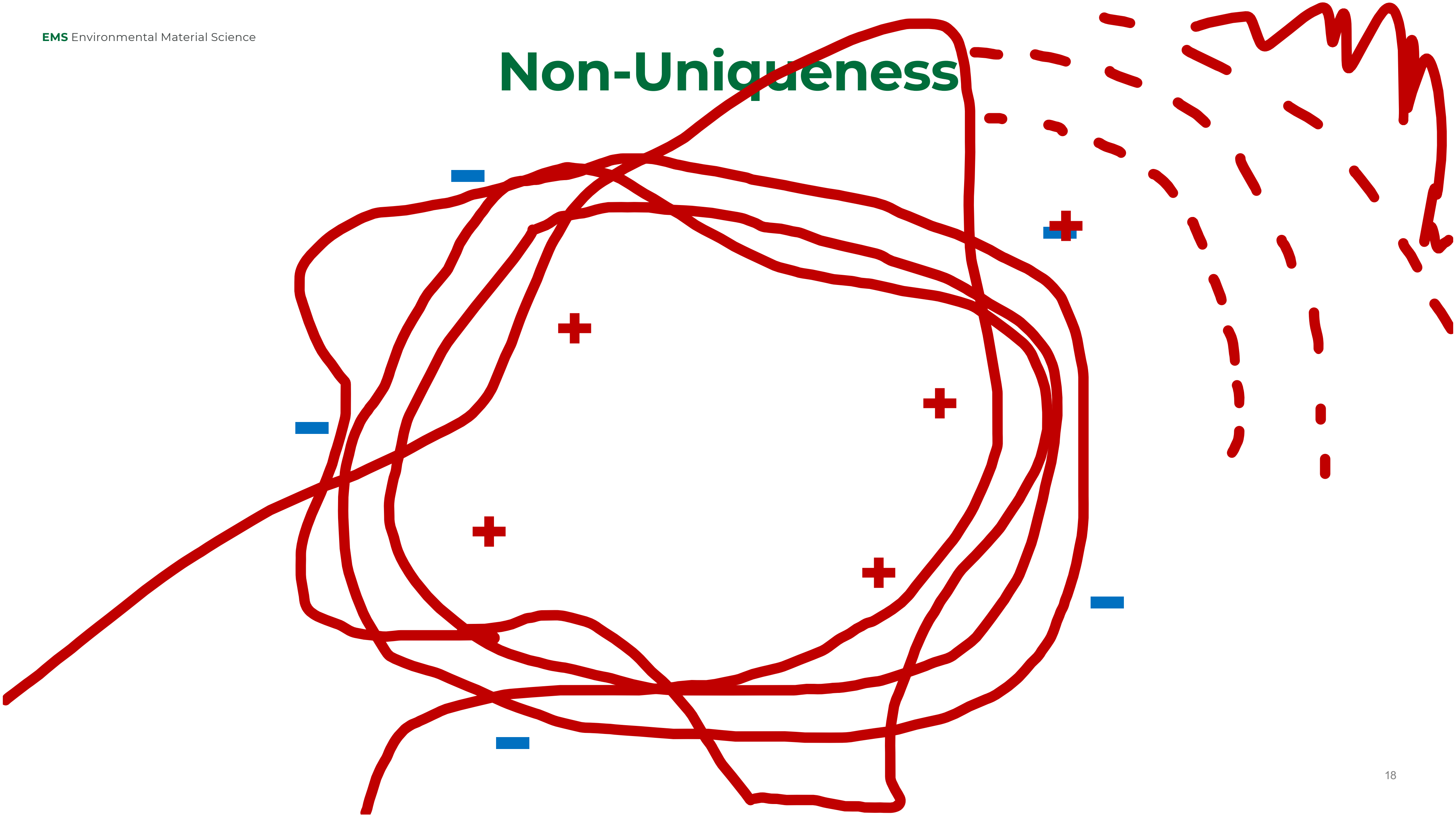

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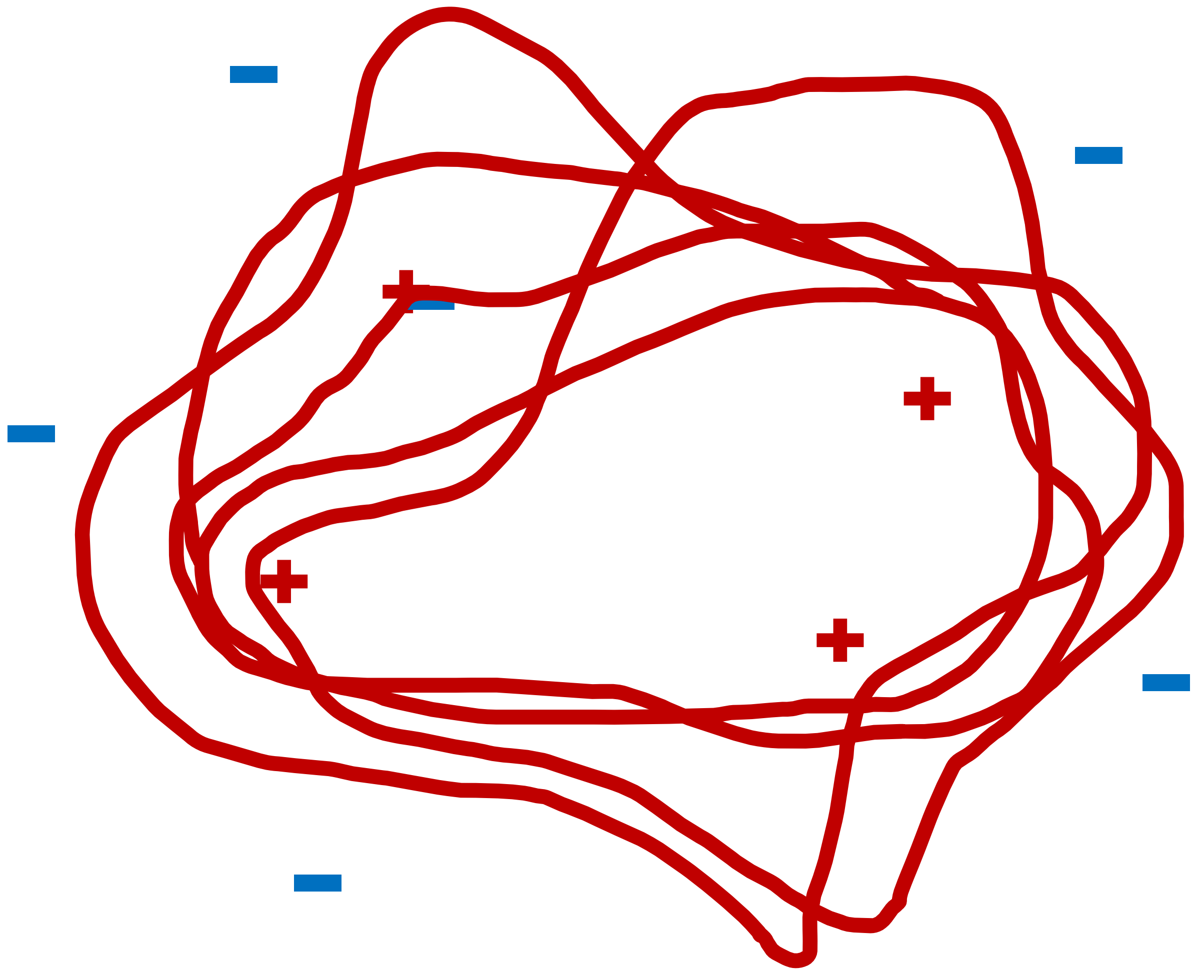
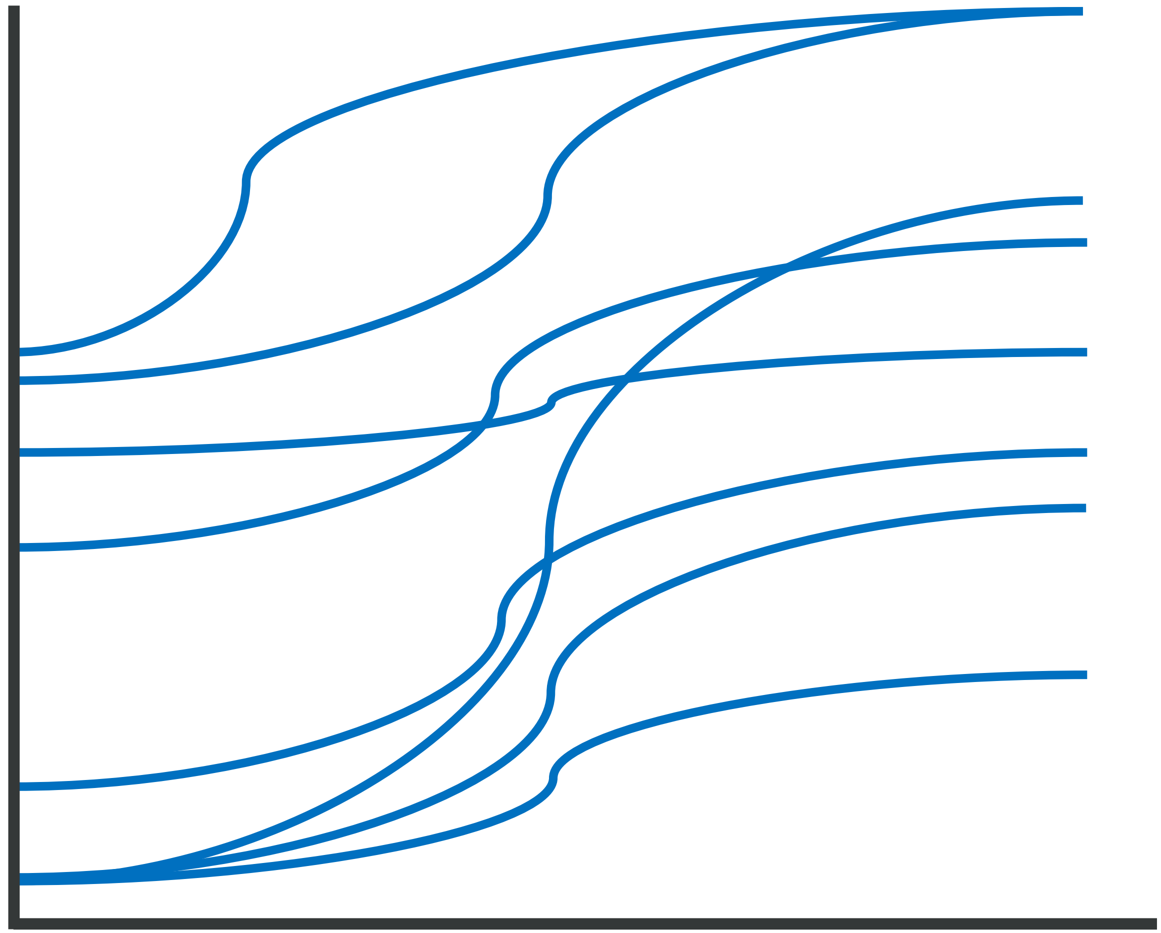


Machine Learning

$$y = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$



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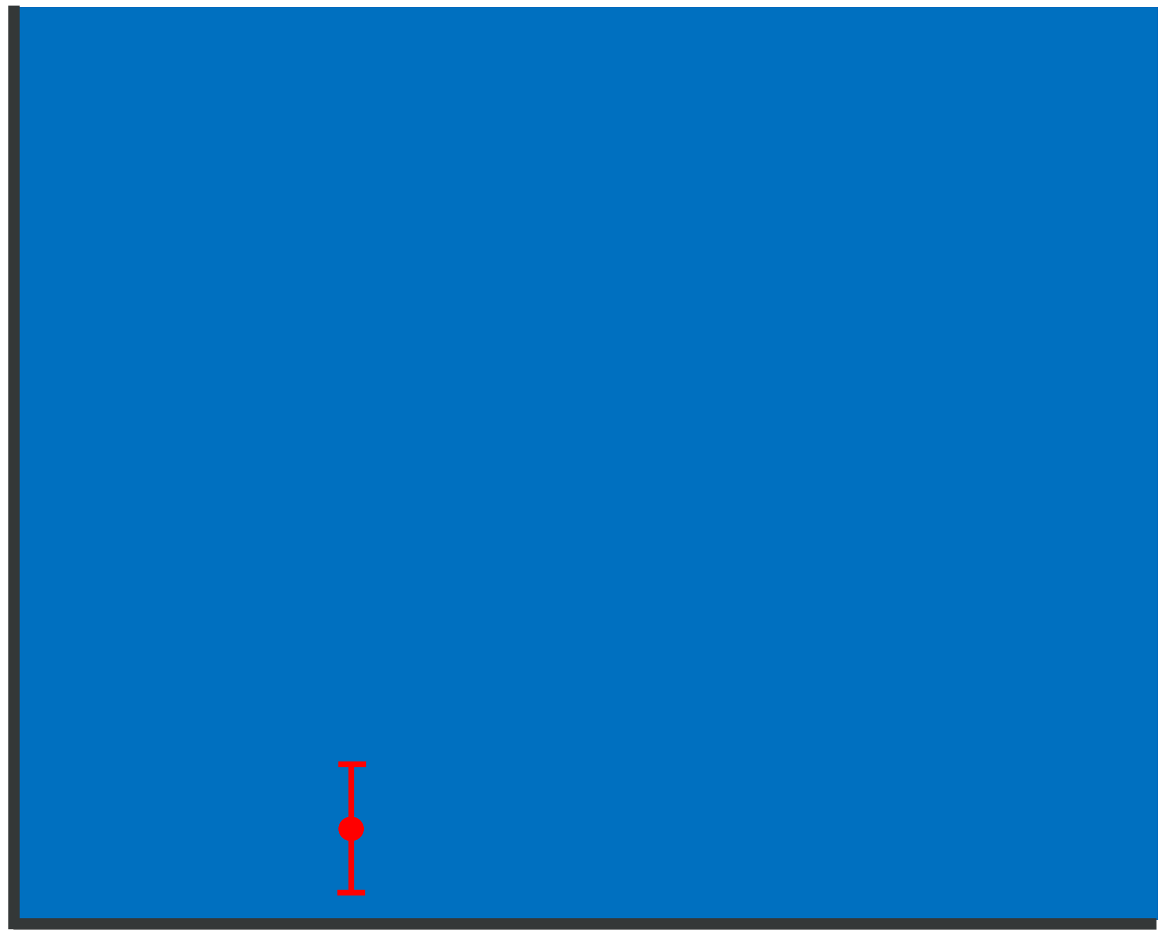

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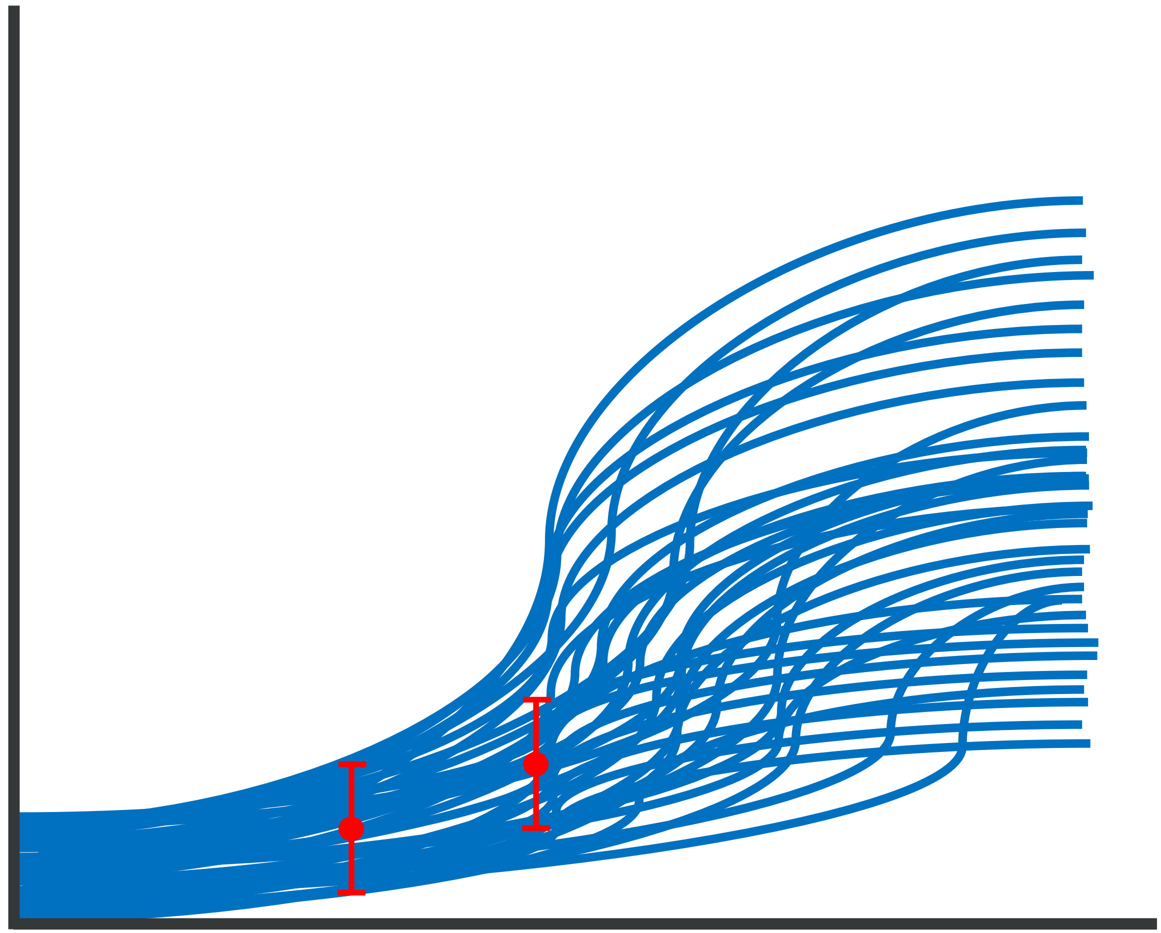

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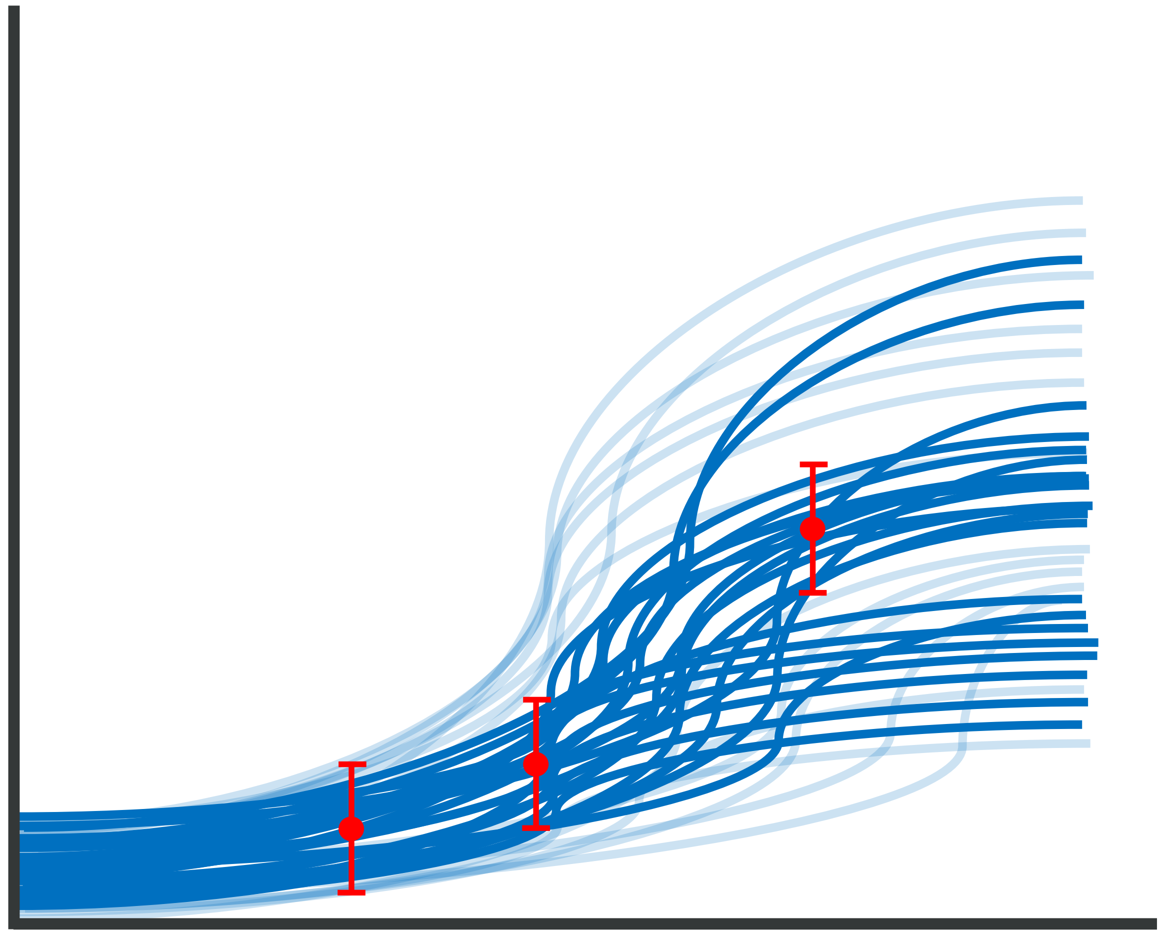

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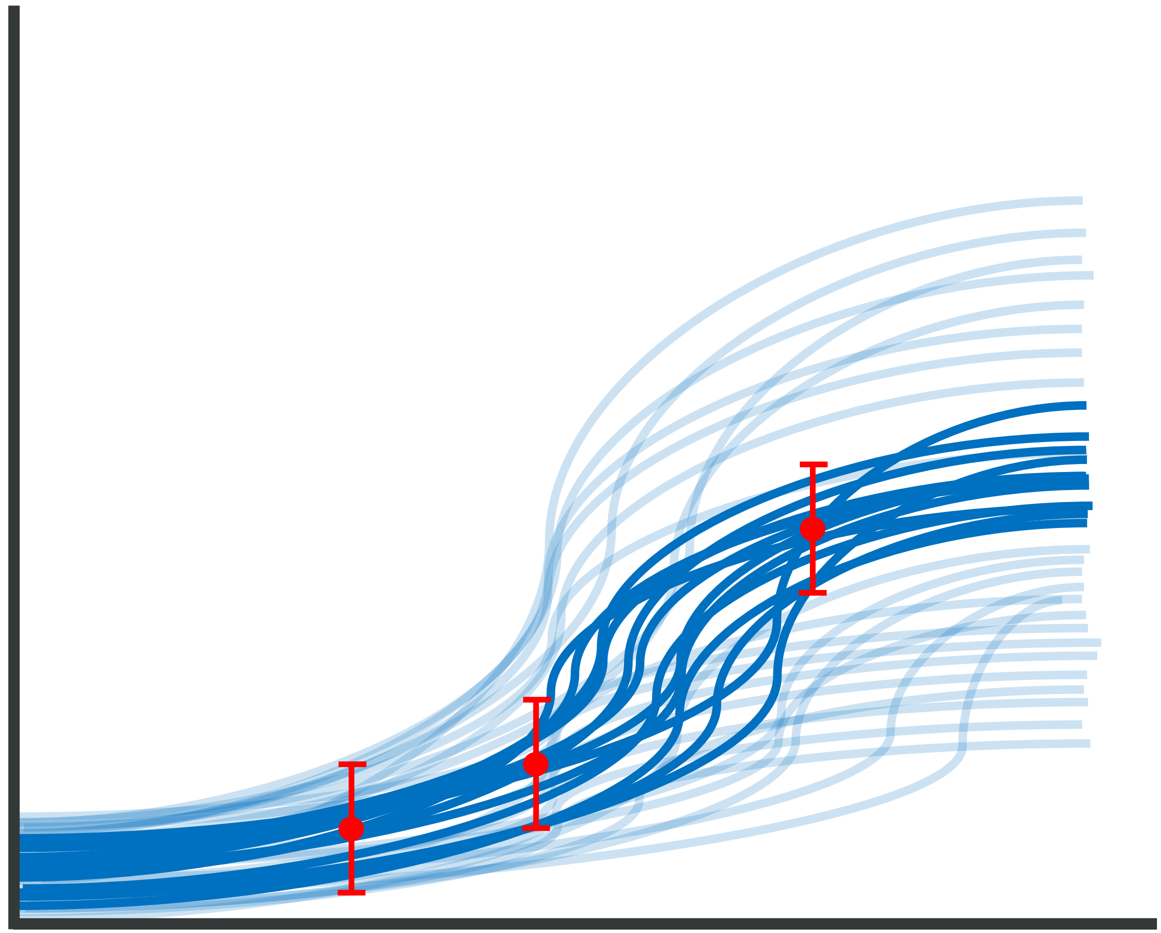

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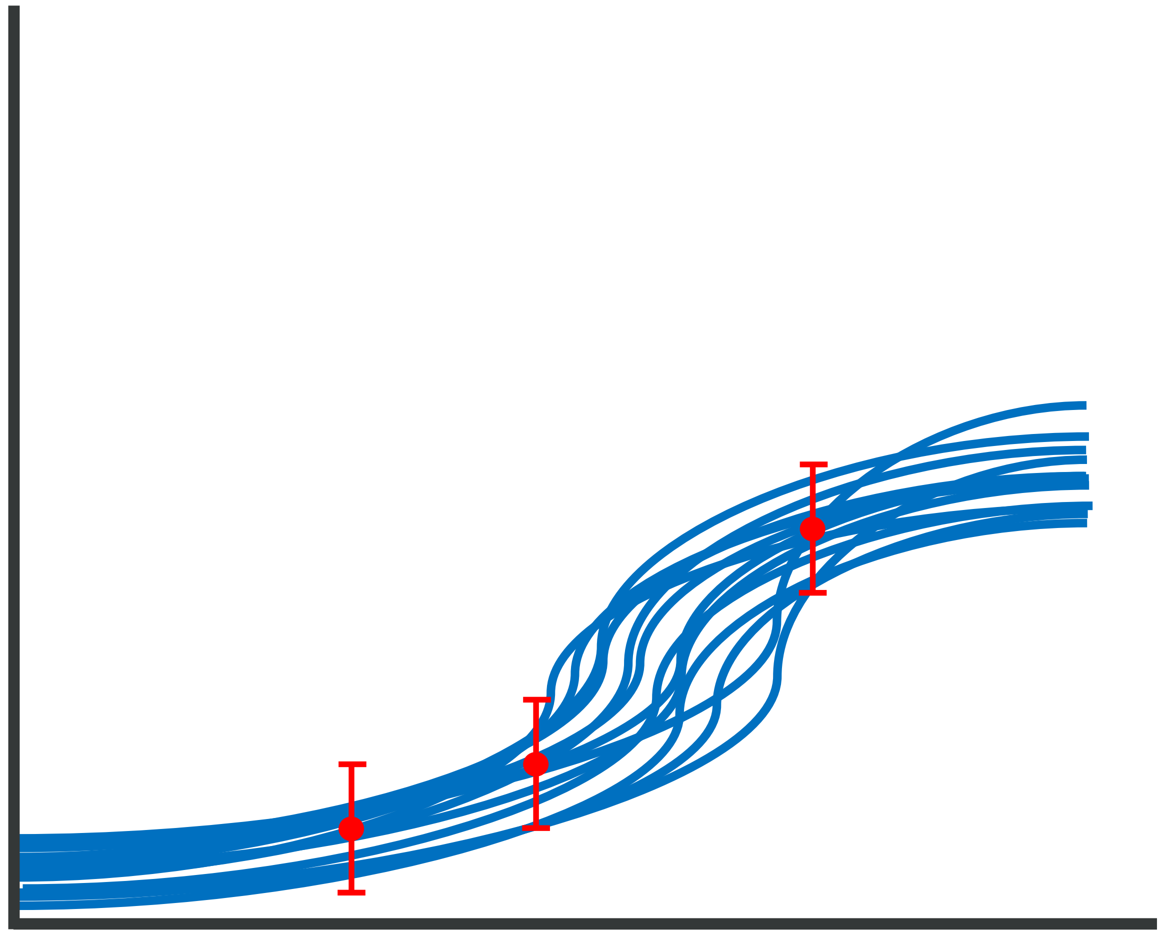

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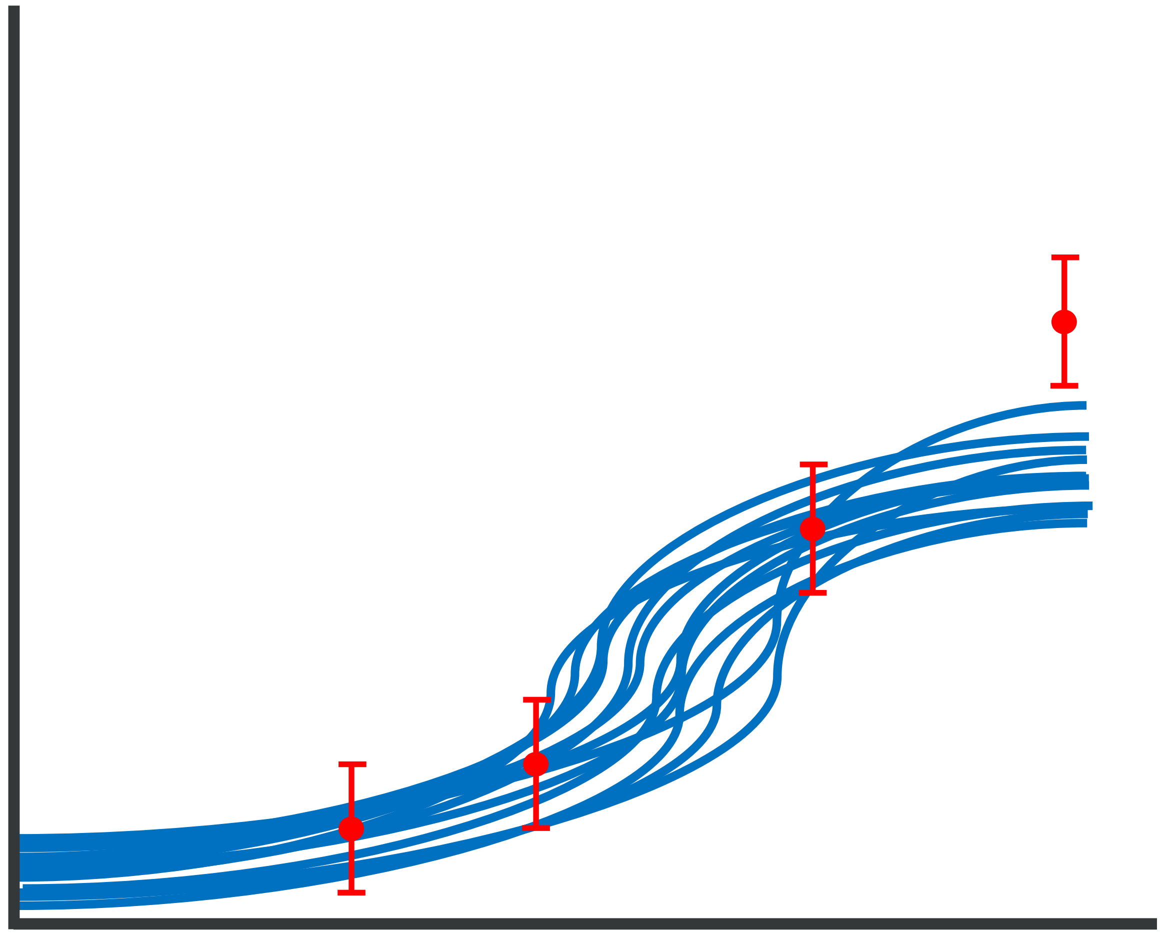

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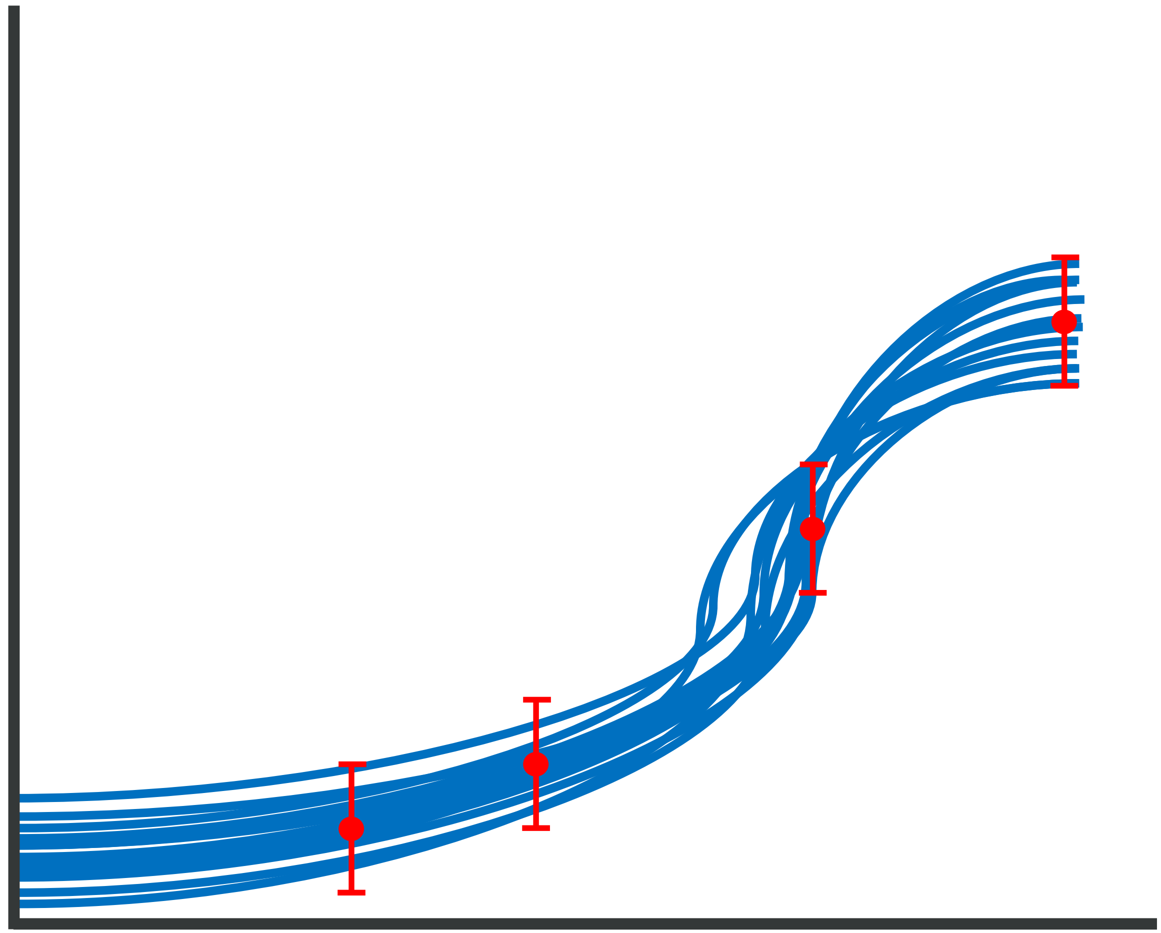
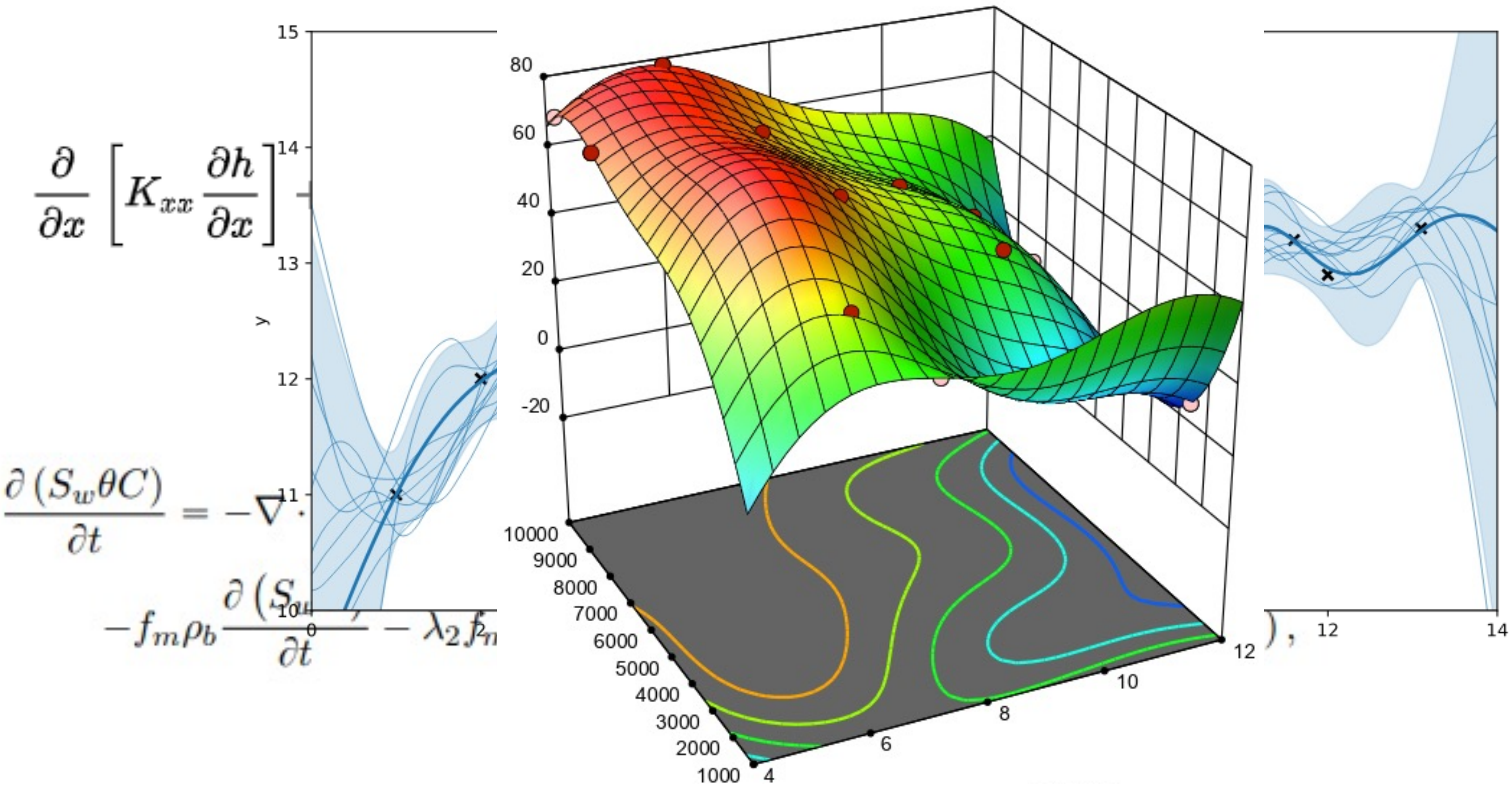
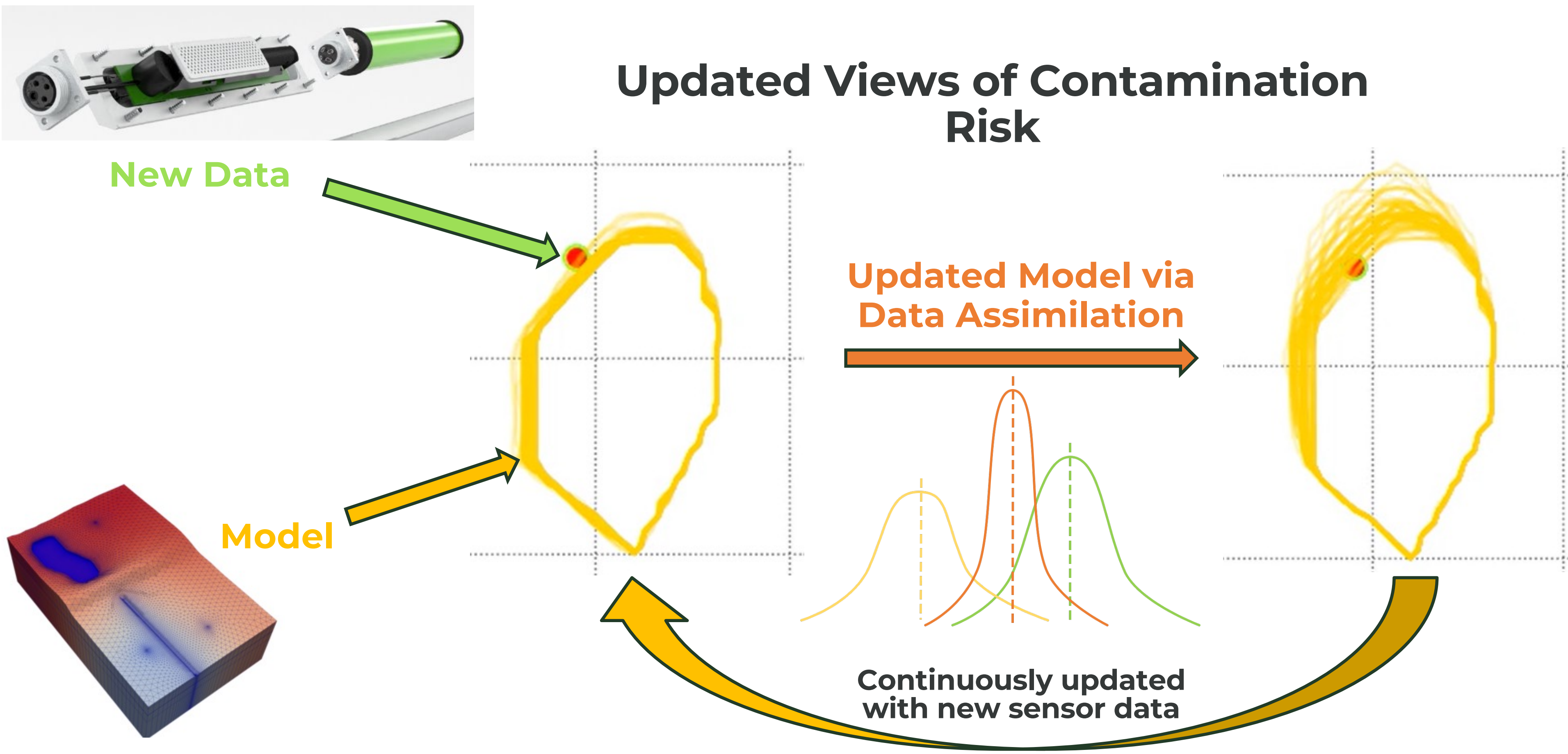


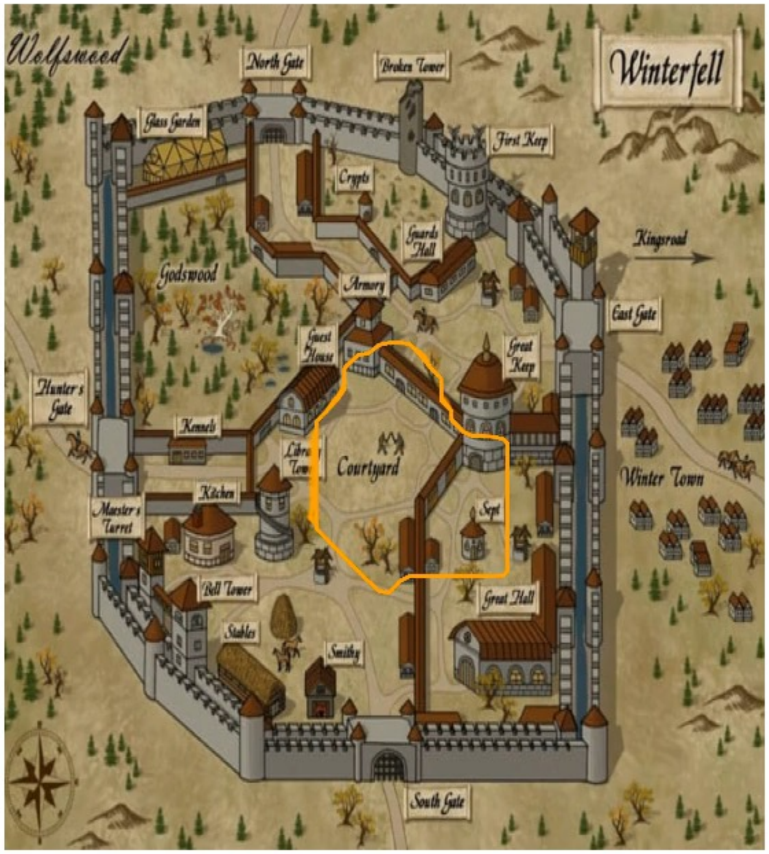
Data Assimilation



What is the value of PlumeFutures and continuous data?



Data Assimilation



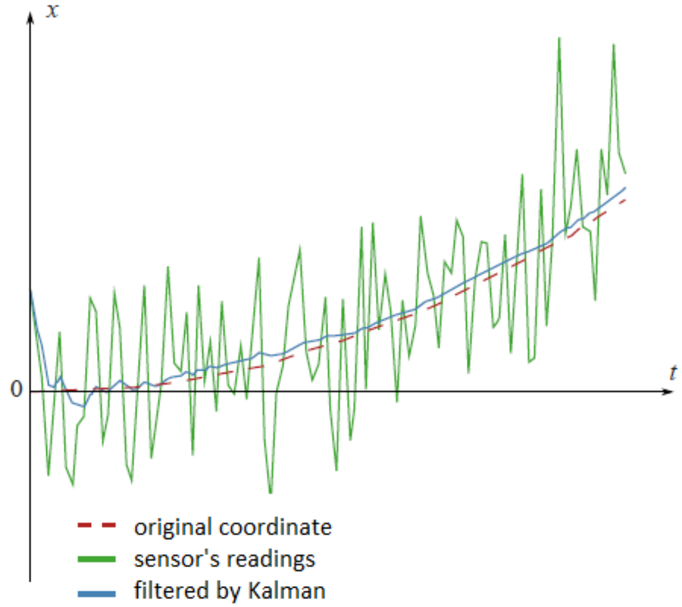
Kalman Filter

The optimal* way to combine noisy estimates to produce a better and less noisy estimate

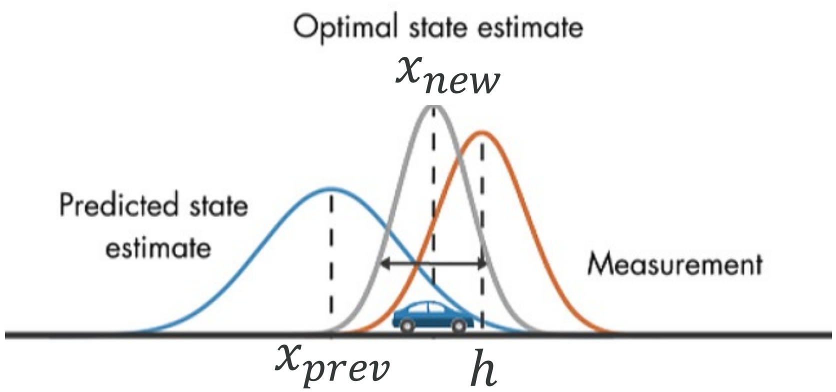
Seemingly endless list of applications:

- Target tracking (e.g. missiles, kamikaze drones)
- Unmanned vehicles and robots (e.g. self-driving cars, drones, submarines etc.)
- Numerical Weather Prediction
- GPS devices (e.g. google maps)
- Signal Processing
- Econometrics
- Apollo program
- NASA Space Shuttle
- Navy submarines

Rudolf E. Kálmán



Kalman Filter



$$x_{new} = x_{prev} + Kr$$

$$r = \underbrace{h}_{\text{measurement}} - \underbrace{Zx}_{\text{model}}$$

$$K = \frac{\sigma_z^2}{\sigma_z^2 + \sigma_h^2}$$

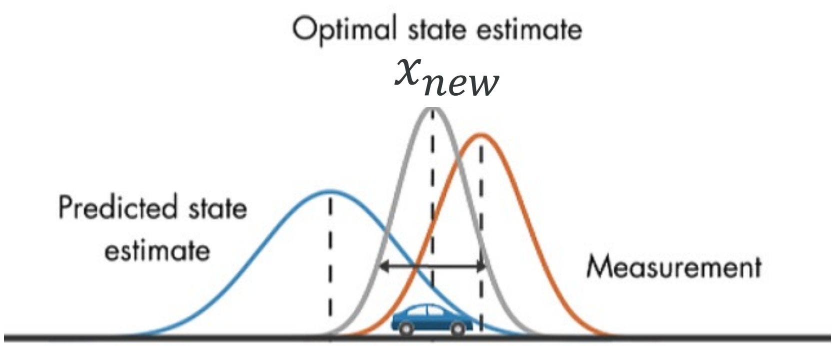
"Kalman gain"

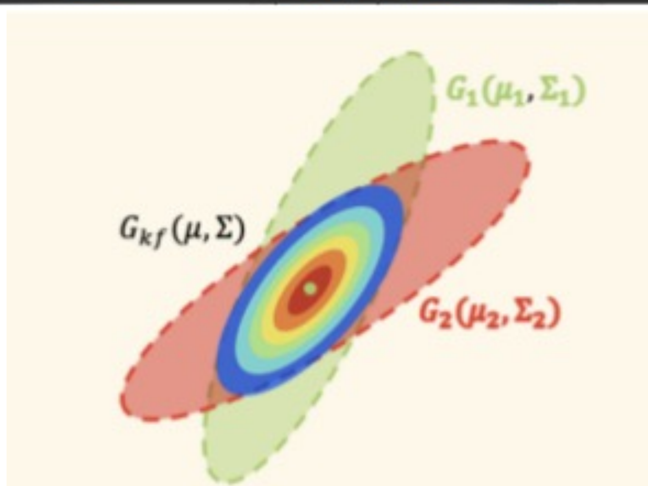
Size of update determined by the relative difference between the model uncertainty (σ_z^2) and the measurement uncertainty (σ_h^2).

If the model uncertainty is lower $(\sigma_z^2 < \sigma_h^2)$ then we have a smaller update.

If the model uncertainty is higher $(\sigma_z^2 > \sigma_h^2)$ then we have a larger update.

Kalman Filter





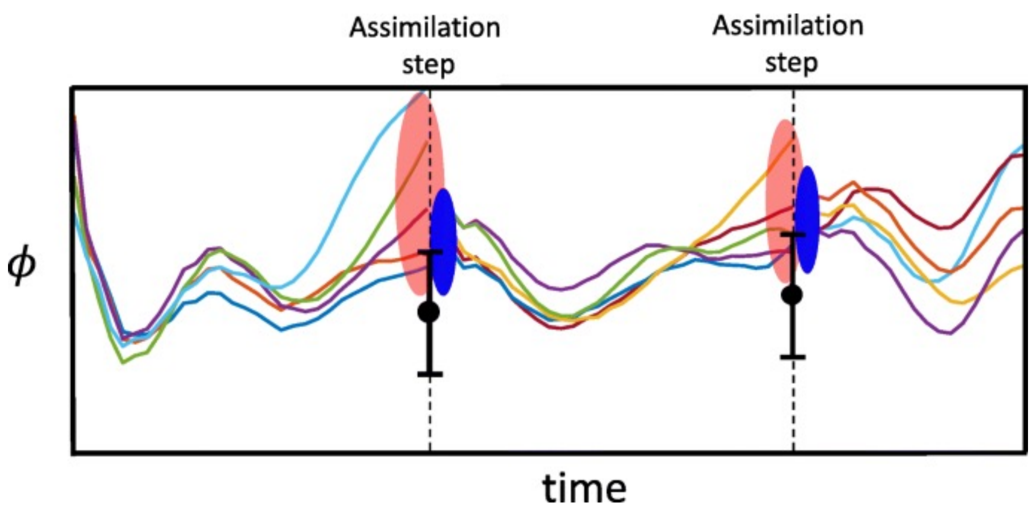
$$x_{new} = x_{prev} + Kr \qquad r = h - Zx$$

$$K = C(x)Z^T[ZC(x)Z^T + C(\varepsilon)]^{-1}$$

“Kalman gain”

$$K = \frac{\sigma_Z^2}{\sigma_Z^2 + \sigma_h^2} \qquad K = \frac{C(x)Z^T}{[ZC(x)Z^T + C(\varepsilon)]}$$

Ensemble Kalman Filter



$$x_{new} = x_{prev} + Kr \qquad r = h - Z(x)$$

$$K = C(x)Z^T[ZC(x)Z^T + C(\varepsilon)]^{-1}$$

Approximated with the statistics of the ensembles

Ensemble Kalman Filter

$$x_{new} = x_{prev} + Kr$$

$$r = h - Z(x)$$

$$r = h - o$$

$$K = C(x)Z^T[ZC(x)Z^T + C(\varepsilon)]^{-1}$$

$$C(x)Z^T \approx \frac{1}{N-1}(x - \bar{x})(o - \bar{o})^T$$

$$ZC(x)Z^T \approx \frac{1}{N-1}(o - \bar{o})(o - \bar{o})^T$$

$$x_{new} = x_{prev} + C(x,o)[C(o) + C(\varepsilon)]^{-1}r$$

Iterative Ensemble Smoother

$$x_1 = x_{prev} + \Delta x_1$$
$$x_2 = x_1 + \Delta x_2$$
$$\dots$$
$$x_{new} = x_i + \Delta x_i$$

$$r = h - Z(x)$$
$$r = h - o$$

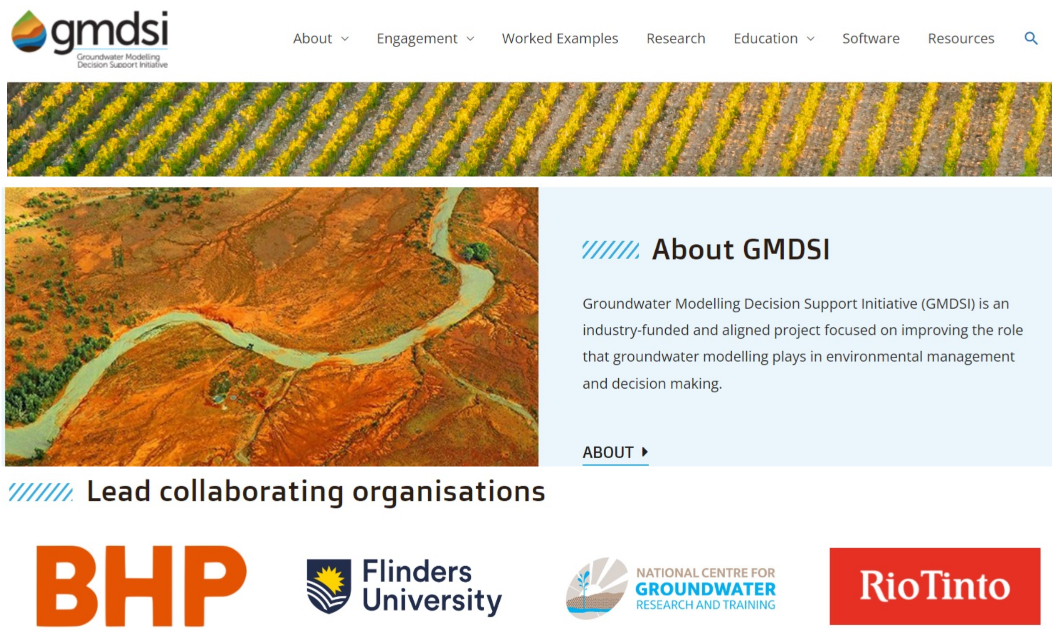
$$\Delta x_i = -((J_e^T C(\varepsilon)^{-1} J_e) + (1+\lambda)C(x)^{-1})^{-1}(C(\varepsilon)^{-1}(x_i - x_{i-1}) + J_e^T r)$$

$$J_e = C(\varepsilon)^{\frac{1}{2}} \frac{\Delta_{sim}}{\Delta_{par}} C(\varepsilon)^{-\frac{1}{2}}$$

$$\Delta_{par} \approx \frac{1}{N-1}(x - \bar{x})(o - \bar{o})^T$$

$$\Delta_{sim} \approx \frac{1}{N-1}(o - \bar{o})(o - \bar{o})^T$$

Data Assimilation Resources



FloPy

a Python package to create, run, and post-process MODFLOW-based models

pyEMU

PEST++

Software Suite for Parameter Estimation, Uncertainty Quantification, Management Optimization, and Sensitivity Analysis

PlumeFutures

Machine learning AI has enabled:

- Model prep time reduced from **weeks to 1-3 hours**.
- Model updating fully **automated**.
- Model predictions targeted at **what clients care about** (**risk and liability**), not what ~~nerds~~ modelers care about (parameters).
- **Revolutionizing scale**: from manual modeling of select sites to analyzing **thousands of locations**, processing **millions of data points**.

White, 2017. Forecast First: An Argument for Groundwater Modeling in Reverse. Groundwater 55(5): 660-664.

Case Study: Deliberate Delineation

Contours of the groundwater Benzene threshold from 200 models that equally fit the available data.

Identified potential plume instability.

AI informed borehole locations to delineate risk.

ems

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Material Science

Nico Higgs
nicohiggs@ems-inc.ca

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stevemamet@ems-inc.ca

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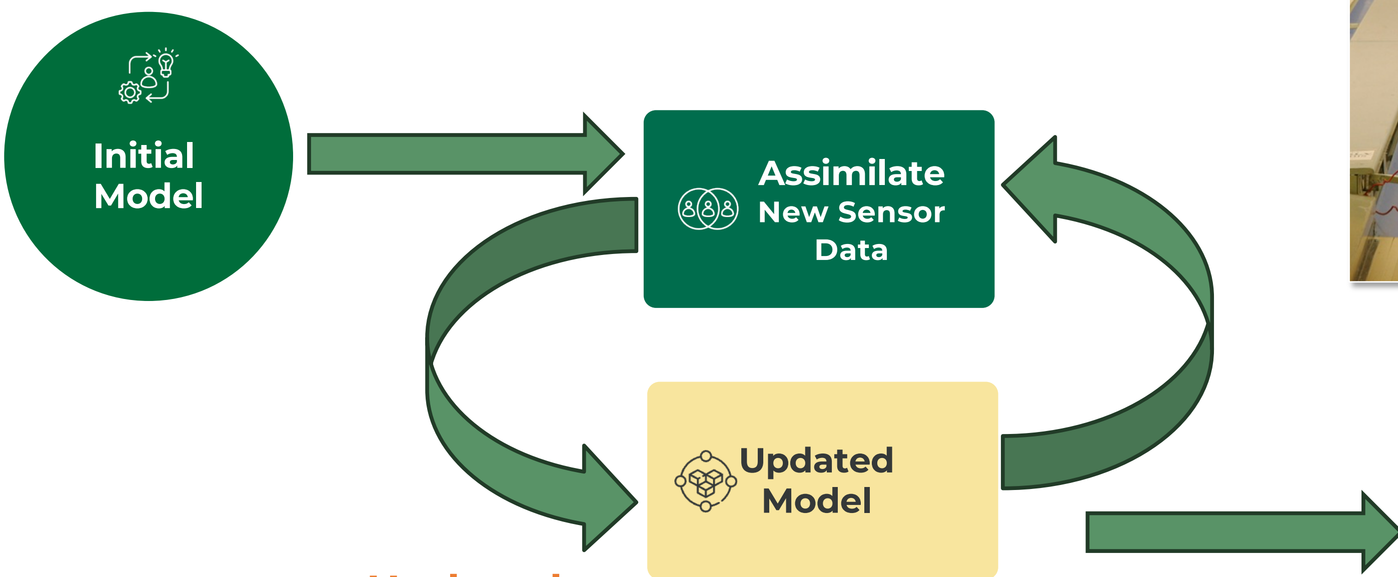
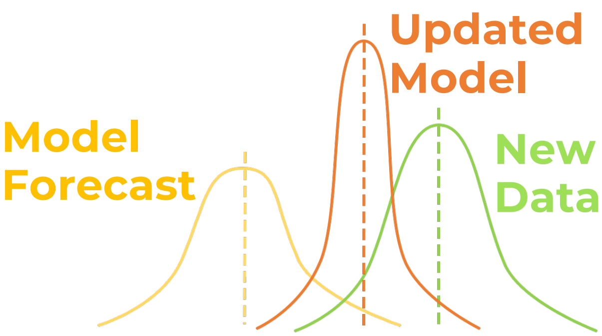
Site insights for
a better world.

Why Autonomous Sensors?

Continuously Monitor and Update Decision Critical Predictions



Improve **Decision** Confidence



Risk/Liability continuously updated:

- ✓ Plume Stability
- ✓ Natural depletion (NSZD)
- ✓ Is applied remediation effective?

Why EMS?

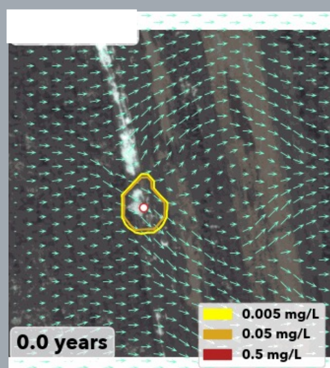
Increased Data at Reduced Cost

	Traditional Annual Sampling	EMS Autonomous Sensor Direct Measurement
# Monitoring Wells	6	6
Sample Frequency	Twice a year or Annually (depending on Regulations)	Every 30 minutes
Field Work	Pull sample, send to lab, wait for report	None after sensor install into existing monitoring wells/easy removal
Analysis	Single point in time sample 10 mL of 250 mL / 1L water One report	Continuously updated, online visual trends predict risks, fast decisions, assess more sites
Data Points per well each sampling event (e.g., annual)	1-2	17,520
Time to Risk Understanding	**~ 3 Years**	**~ 3 to 6 months**
Cost	$30,000 - $60,000	$14,500 or $29,000 / year
Cost/data point	**$5,000.00 - $10,000.00 each**	**$0.80 - $1.60 each**

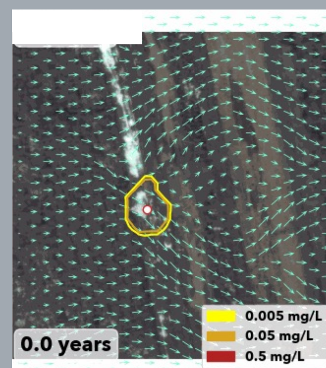
Why PlumeFutures?

Scenario Planning

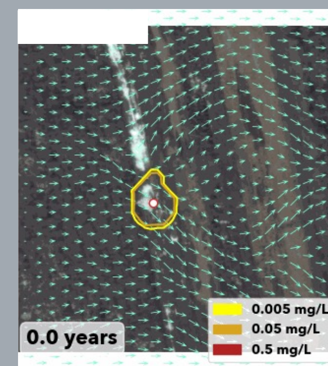
Baseline

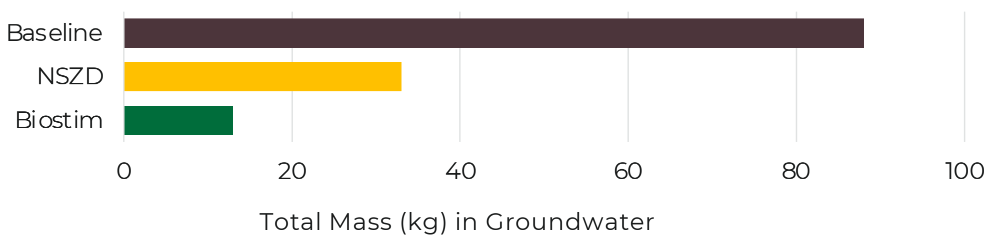


NSZD



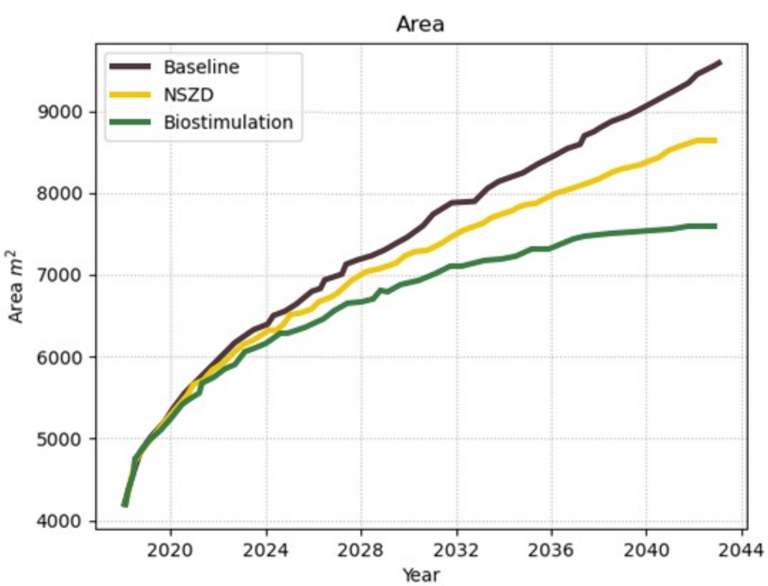
Biostim

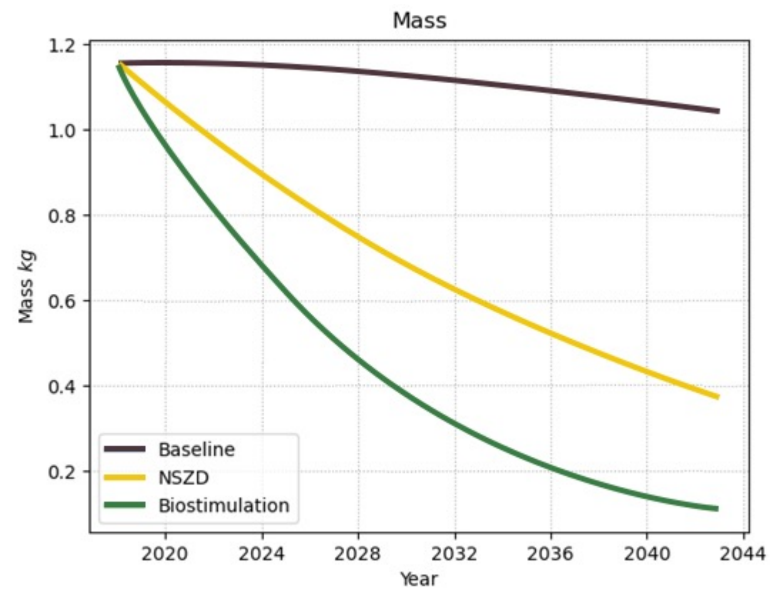




Why PlumeFutures?

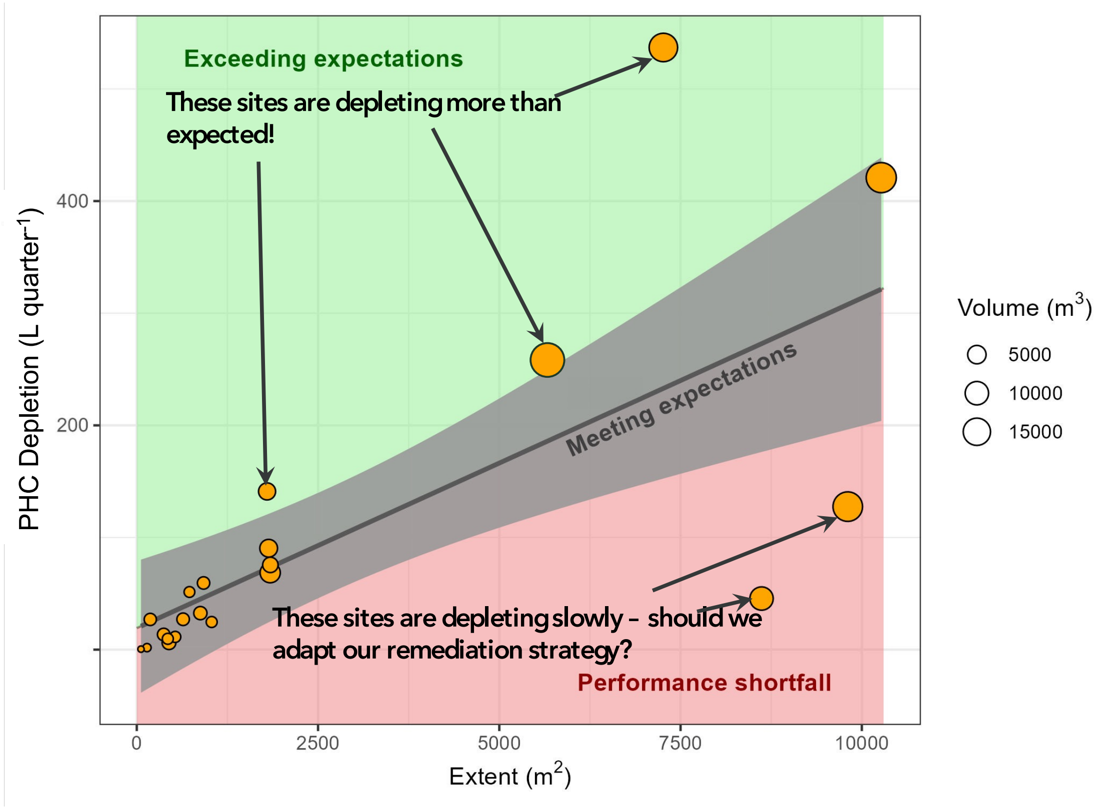
Scenario Planning



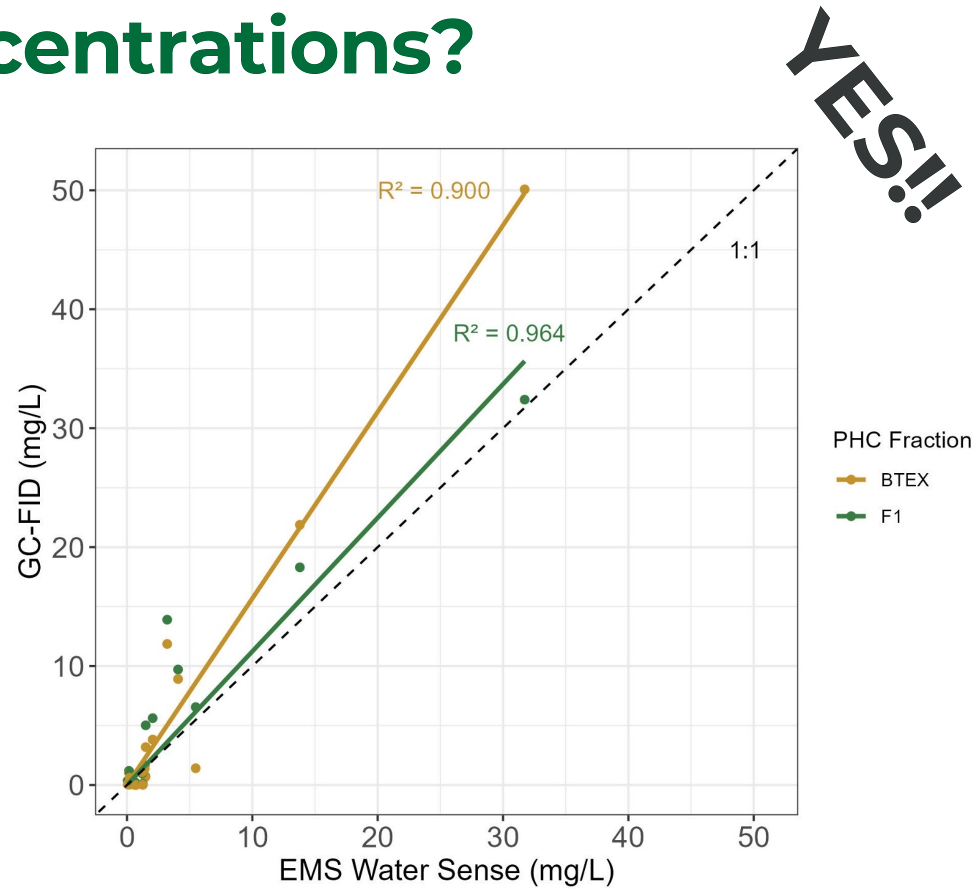


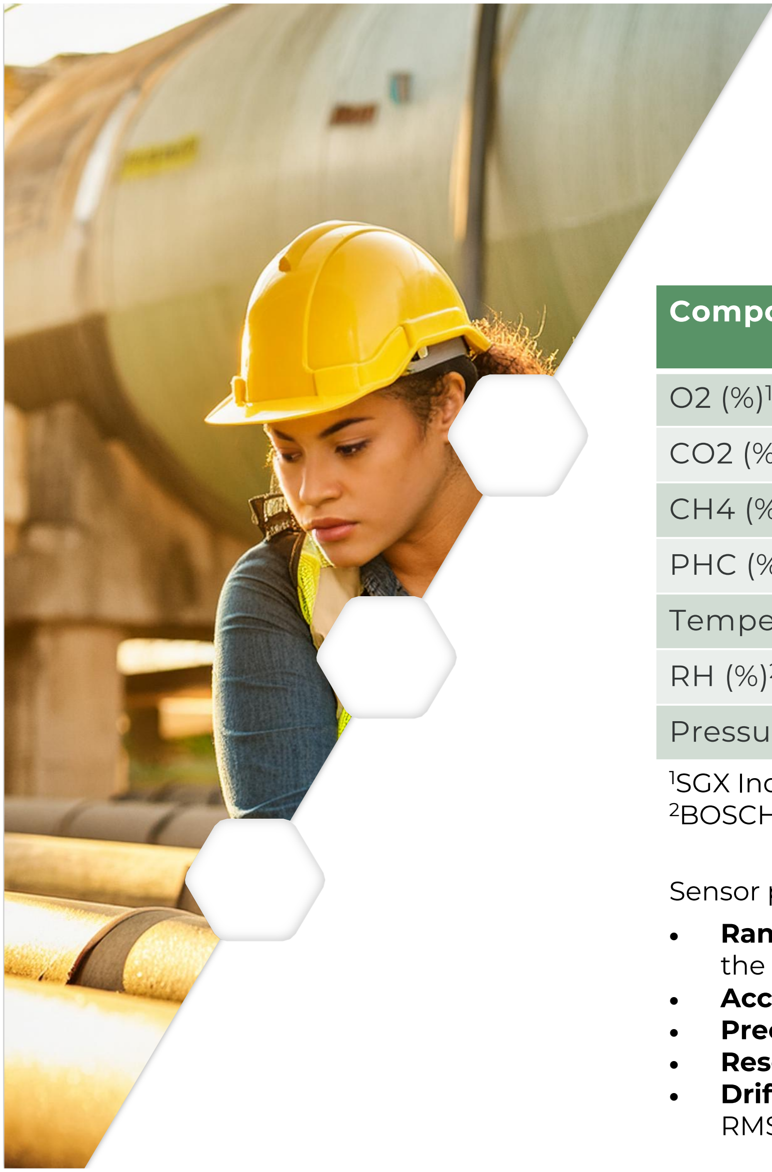
Why PlumeFutures?

Site Triage



But can WaterSense really estimate GW PHC concentrations?





Specifications

Component	Range	Resolution	Accuracy (+/-)	Precision	Drift (yr^{-1})
O_2 (%)[1]	0 – 25	0.01	0.6	0.3	<5
CO_2 (%)	0 – 10	0.002	0.002	0.03	0.05
CH_4 (%)	0 – 50	0.0004	0.006	0.17	0.05
PHC (%)	0 – 2.1	0.001	0.003	0.0007	0.025
Temperature (°C)[2]	-40 – 85	0.01	1.0	0.1	0.02
RH (%)[2]	0 – 100	0.008	3.0	0.02	0.5
Pressure (mb)[2]	300 – 1,100	0.0018	1.0	0.013	1.0

[1]SGX Industrial Oxygen Sensor (SGX-4Ox-EL)
[2]BOSCH Combined Temperature, Humidity, and Pressure Sensor (BME280)

Sensor performance is reported according to the following definitions:

- **Range** – Reported in absolute units as the minimum and maximum values of the range the sensor detects.
- **Accuracy*** – Reported in absolute units as the Root Mean Squared Error (RMSE).
- **Precision*** – Reported in absolute units as the standard deviation.
- **Resolution** – Reported in absolute units as the smallest detectable change.
- **Drift** – Reported as the difference between RMSE at 1 year after calibration and RMSE at calibration.

PlumeFutures

MODFLOW is a widely used groundwater modeling software developed by the United States Geological Survey (USGS). Here's what it does:

1. **Groundwater Flow Simulation**: MODFLOW simulates the flow of groundwater through aquifers. It can model how water moves underground, which is essential for understanding and managing water resources.
2. **Grid-Based Model**: The area being studied is divided into a grid of cells. Each cell represents a specific volume of the aquifer. The model calculates the water flow between these cells over time.
3. **Input Parameters**: Users provide various inputs like hydraulic conductivity, recharge rates (**HYDRUS**), pumping rates, and boundary conditions. These parameters define how water moves through the aquifer.
4. **Applications**: MODFLOW is used for water supply planning, contamination assessment, and managing groundwater resources. It helps in predicting how groundwater levels change in response to natural and human activities.

PEST++ is an advanced version of the PEST (Parameter ESTimation) software, which is used for model calibration and uncertainty analysis. Here's what it does:

1. **Model Calibration**: PEST++ adjusts the input parameters of a model (like MODFLOW) to match observed data (e.g., water levels, flow rates). This process ensures that the model accurately represents the real-world system.
2. **Optimization**: PEST++ uses optimization algorithms to find the best set of parameters that minimize the difference between observed data and model predictions.
3. **Uncertainty Analysis**: It also quantifies the uncertainty in model predictions. This means it helps in understanding how certain or uncertain the model outputs are, given the possible variations in input parameters.
4. **Automation and Efficiency**: PEST++ is designed to be more efficient and capable of handling large and complex models compared to the original PEST. It can automate many of the calibration tasks, making it faster and more reliable.

How They Work Together

When used together, MODFLOW and PEST++ provide a powerful toolkit for groundwater modeling:

•**MODFLOW** creates a detailed simulation of groundwater flow.

•**PEST++** calibrates the MODFLOW model to ensure it accurately reflects observed data and assesses the uncertainty in the model predictions.

This combination is essential for making informed decisions about groundwater management and ensuring that models are reliable and useful for planning and analysis.

PlumeFutures

Workflow Example

1. **Initial Setup**: Develop HYDRUS and MODFLOW models for your study area. Define the soil properties, boundary conditions, and initial conditions for HYDRUS. Define the aquifer properties and boundary conditions for MODFLOW.
2. **HYDRUS Simulation**: Run HYDRUS to simulate soil moisture dynamics and calculate recharge rates based on precipitation, evapotranspiration, and soil properties.
3. **MODFLOW Simulation**: Use the recharge rates from HYDRUS as input for MODFLOW. Run MODFLOW to simulate groundwater flow and levels.
4. **Calibration with PEST++**: Use observed data (e.g., soil moisture content, groundwater levels) to calibrate both models. PEST++ will adjust the parameters in HYDRUS and MODFLOW to minimize the differences between observed and simulated values.
5. **Iterate and Refine**: Iterate the process, running HYDRUS and MODFLOW simulations, and recalibrating with PEST++ until the models are well-calibrated and accurately reflect the observed data.
6. **Uncertainty Analysis**: Use PEST++ to perform uncertainty analysis, providing insights into the reliability of the model predictions.

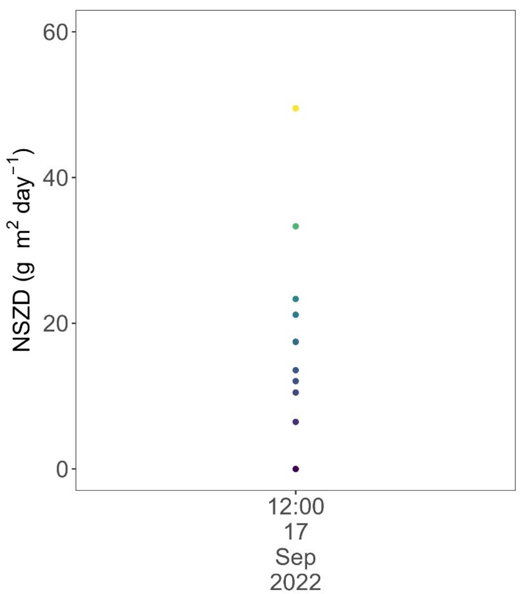
By integrating HYDRUS with MODFLOW and using PEST++ for calibration, you can create a robust and accurate modeling framework that covers the entire hydrological cycle from the unsaturated zone to the groundwater system. This integrated approach is valuable for various applications, including water resource management, agricultural planning, and contaminant transport studies.

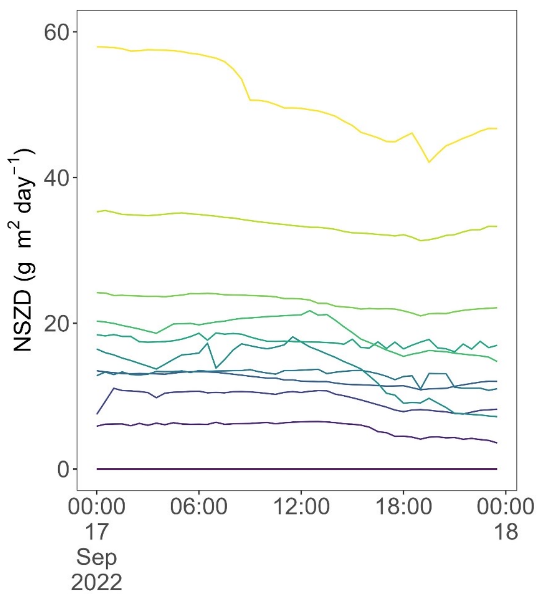
The Challenge of Point-in-time Sampling to Assess Risks

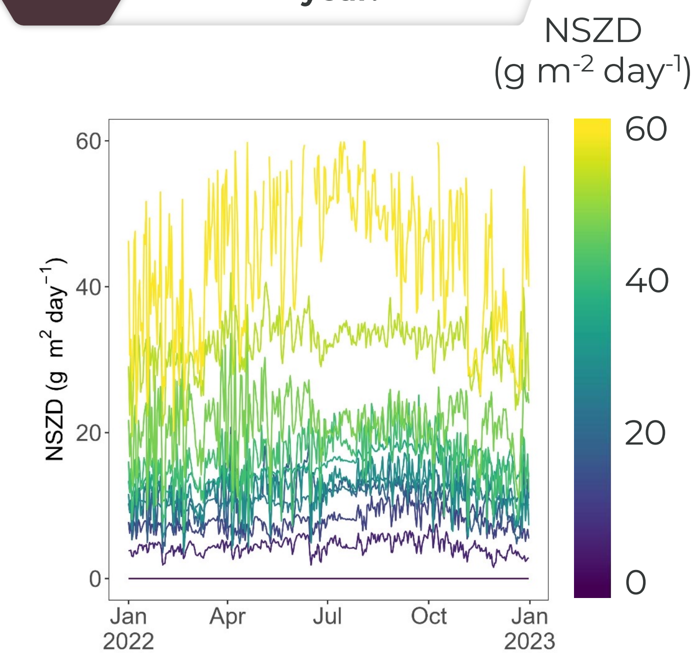
Traditional: various samples at a site

48 measurements show sample variability over 1 day

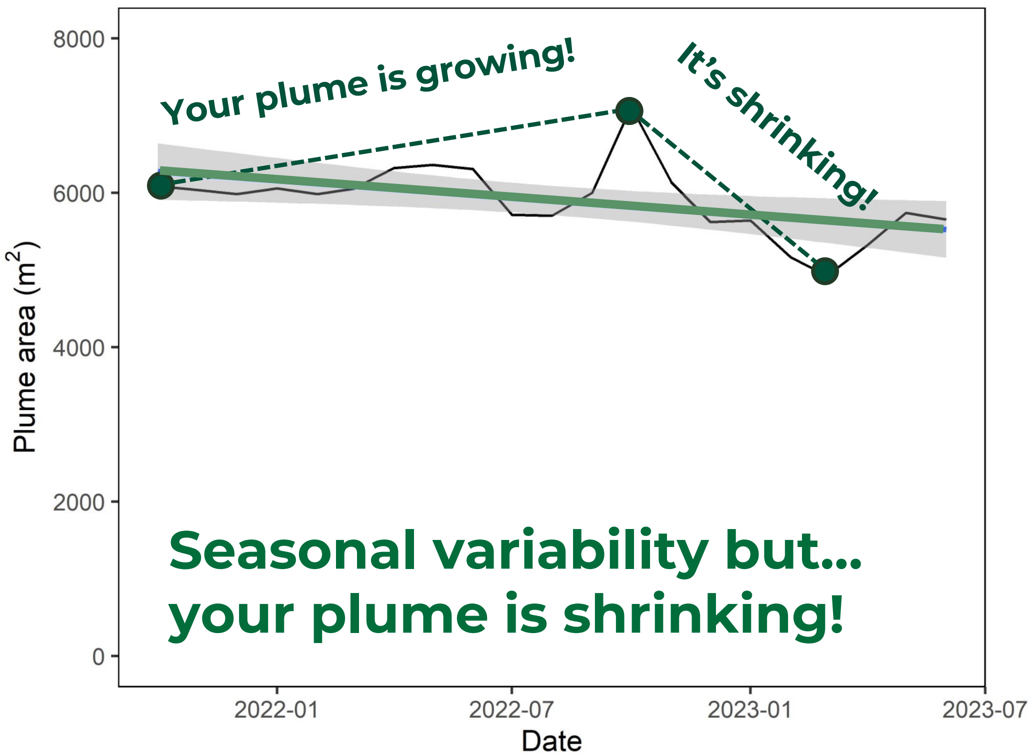
17,520 measurements show variability over 1 year!







The Challenge of Point-in-time Sampling to Assess Risks



- Typically, 5-10 sensors/site
- 30 min resolution.

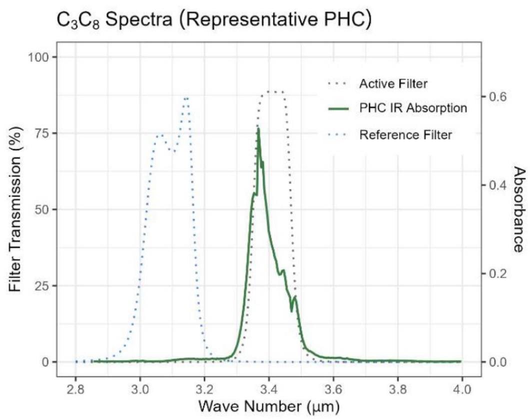
Plume area through time

Trend line

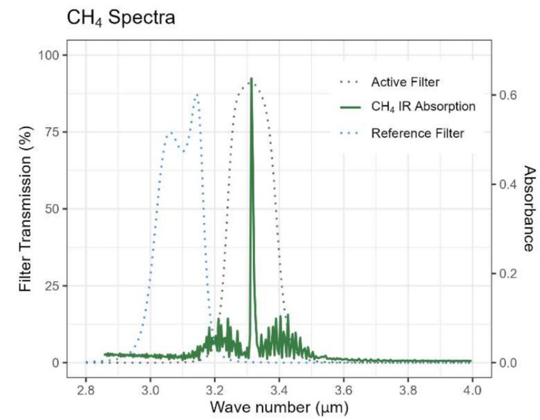
NDIR

Gas Absorption: Different gases absorb infrared light at specific wavelengths. For PHCs, CH_4, and CO_2, this absorption can be detected and measured. Here are the details about the 4-channel NDIR detector:

- Channel 1 (reference): 3.1 µm
- Channel 2 (CH_4): 3.3 µm
- Channel 3 (PHC): 3.4 µm
- Channel 4 (CO_2): 4.2 µm



EMS 4-channel NDIR sensor measure IR absorbances from 3.2 to 3.5 µm (C-H stretching) and 4.2-4.3 µm (O=C=O stretching). Above highlights how PHCs (propane (C_3C_8) is used as a representative PHC) are determined relative to a reference channel.



Above highlights how CH_4 is determined relative to a reference channel.

Beer-Lambert

At its core, the Beer-Lambert Law postulates that light absorbance (A) is directly proportional to the concentration (C) of the sample:

$$A = -ln\left(\frac{I_0}{I}\right) = \epsilon l C \qquad (1)$$

Where:
I_0 = incident intensity (dimensionless)
I = transmitted intensity (dimensionless)
l = length of the solution the light passes through (distance between IR emitter and detector; cm)
ϵ = molar absorption coefficient ($M^{-1}cm^{-1}$)

Practical considerations in the NDIR implementation require modifications to the Beer-Lambert Law, as follows, to obtain accurate readings:

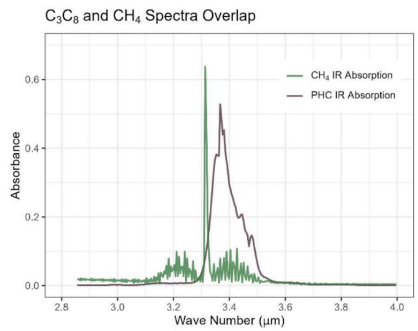
$$A = SPAN\left(1 - e^{-bC^{c}}\right) \qquad (2)$$

Where:
$SPAN$ = scaling factor that accounts for non-idealities in the measurement system (dimensionless)
b = slope correction factor non-linear increases in absorption with concentration (dimensionless)
C = concentration (as above)
c = molar absorption coefficient ($M^{-1}cm^{-1}$)

The $SPAN$ factor is introduced because not all the IR radiation that impinges upon the active detector is absorbed by the gas, even at high concentrations.

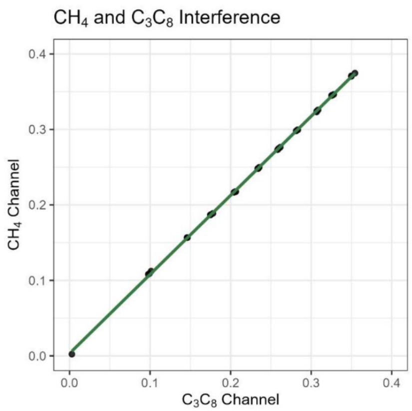
CH_4 and PHC Interference

There is overlap between IR CH_4 and other low molecular weight PHC absorption frequencies (e.g., C_3H_8):



Note the overlap between CH_4 and PHC spectra.

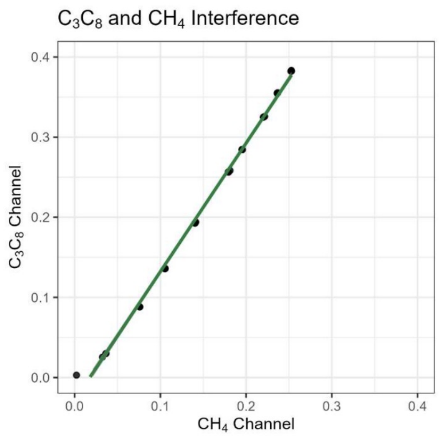
So PHC will be detected on the CH_4 channel:



Above highlights how PHC registers on the CH_4 channel.

CH_4 and PHC Interference

And CH_4 will be detected on the PHC channel:



Above highlights how CH_4 registers on the PHC channel.

To account for this, EMS uses absorption cross-interference algorithms[7] to determine PHC and methane concentrations in mixtures.

$$NA^{i}_{CH_4} = \frac{NA_{CH_4} - NA_{C_3H_8}K_{C_3H_8}}{1 - K_{CH_4}K_{C_3H_8}} \tag{8}$$

Where:
$NA^{i}_{CH_4}$ = interference corrected CH_4 normalized absorbance (dimensionless)
NA = uncorrected normalized absorbance for the corresponding gas (dimensionless)
K = interference correction constant for the corresponding gas (dimensionless)

Water Sense

Henry's Law:
The amount of dissolved gas in a liquid is proportional to its partial pressure above the liquid.

Raoult's Law:
The partial pressure of each component of an ideal mixture of liquids is equal to the vapour pressure of the pure component multiplied by its mole fraction in the mixture.

Water Sense

$$C_a = C_g P K_H^0 exp\left\{\delta\left[\frac{1}{T} - \frac{1}{T^0}\right]\right\} M_B \rho_w$$

C_a = Aqueous concentration

C_g = Gaseous concentration

P = Pressure

K_H^0 = Henry's constant for solubility in water

δ = Temperature dependence constant

T = Measured temperature

T^0 = Standard temperature

M_B = Benzene molar mass

ρ_w = Water density

Water Sense

$$C_a = C_g P K_H^0 exp\left\{\delta\left[\frac{1}{T} - \frac{1}{T^0}\right]\right\} M_B \rho_w$$

$C_a =$ Aqueous concentration

What we want

$C_g =$ Gaseous concentration

$P =$ Pressure

$T =$ Measured temperature

What we measure

$K_H^0 =$ Henry's constant for solubility in water

$\delta =$ Temperature dependence constant

$T^0 =$ Standard temperature

$M_B =$ Benzene molar mass

$\rho_w =$ Water density

Constants