Advanced monitoring methods:

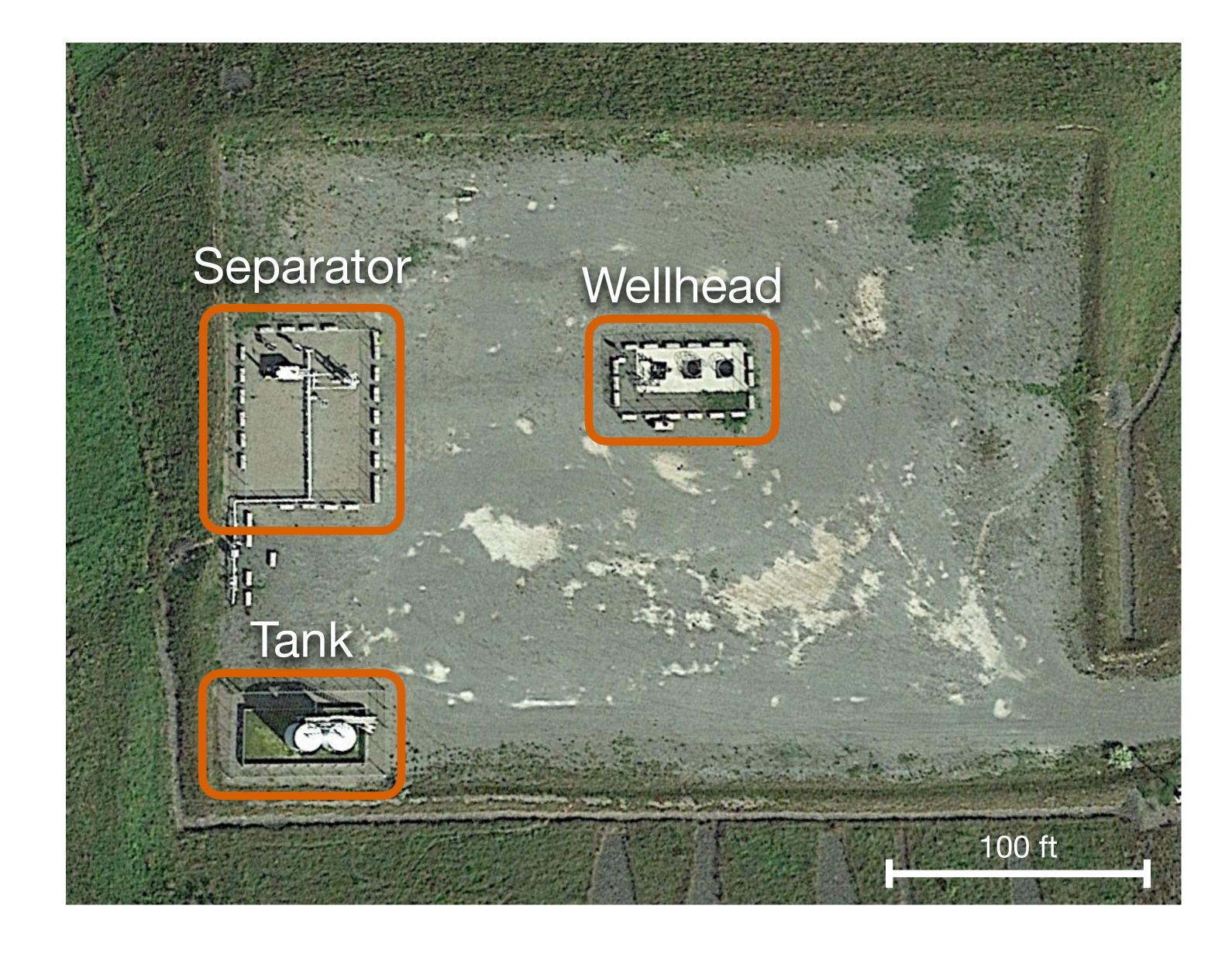
Estimating methane emission source and rate with continuous monitoring systems

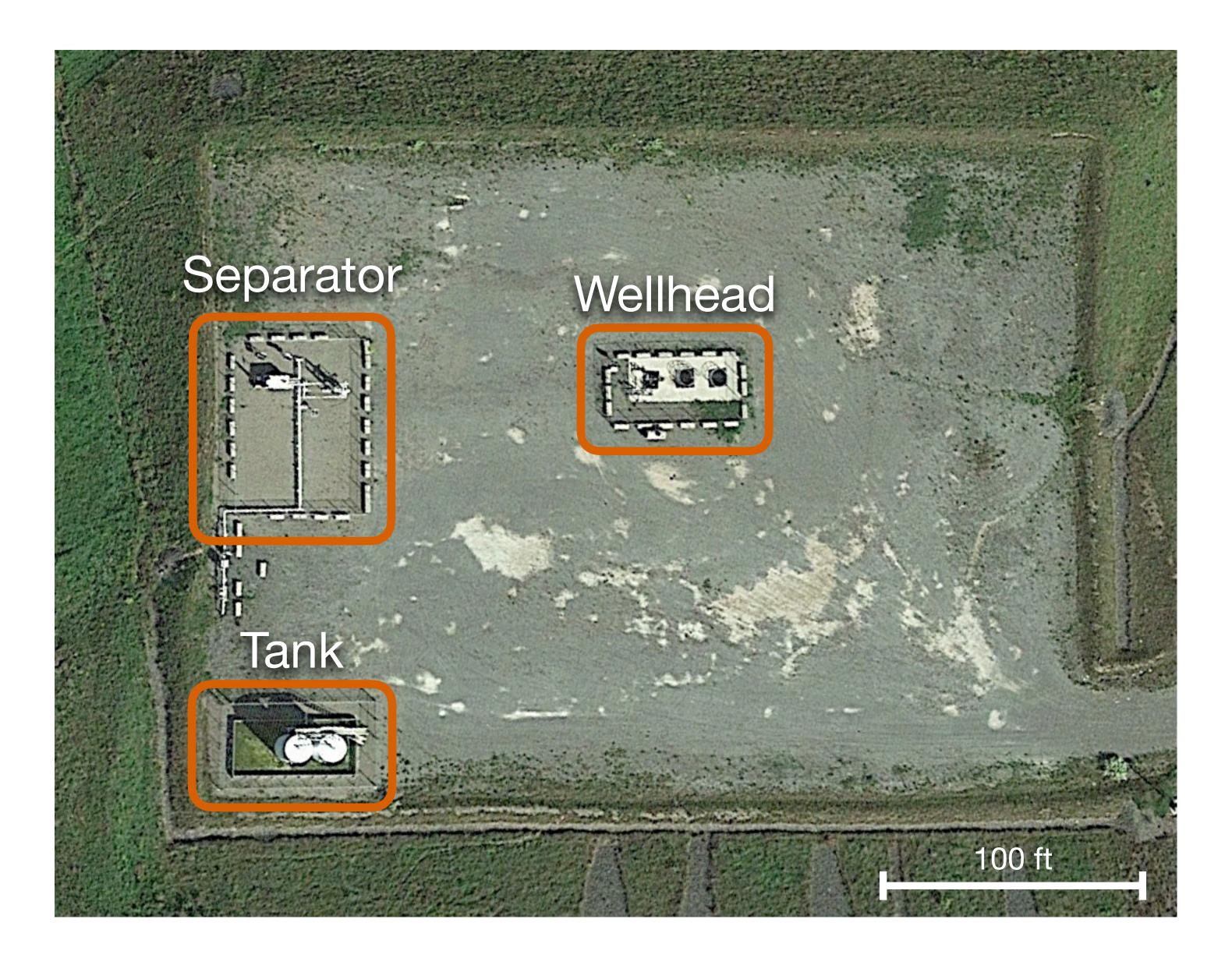
William Daniels and the Colorado School of Mines Team

Department of Applied Mathematics and Statistics



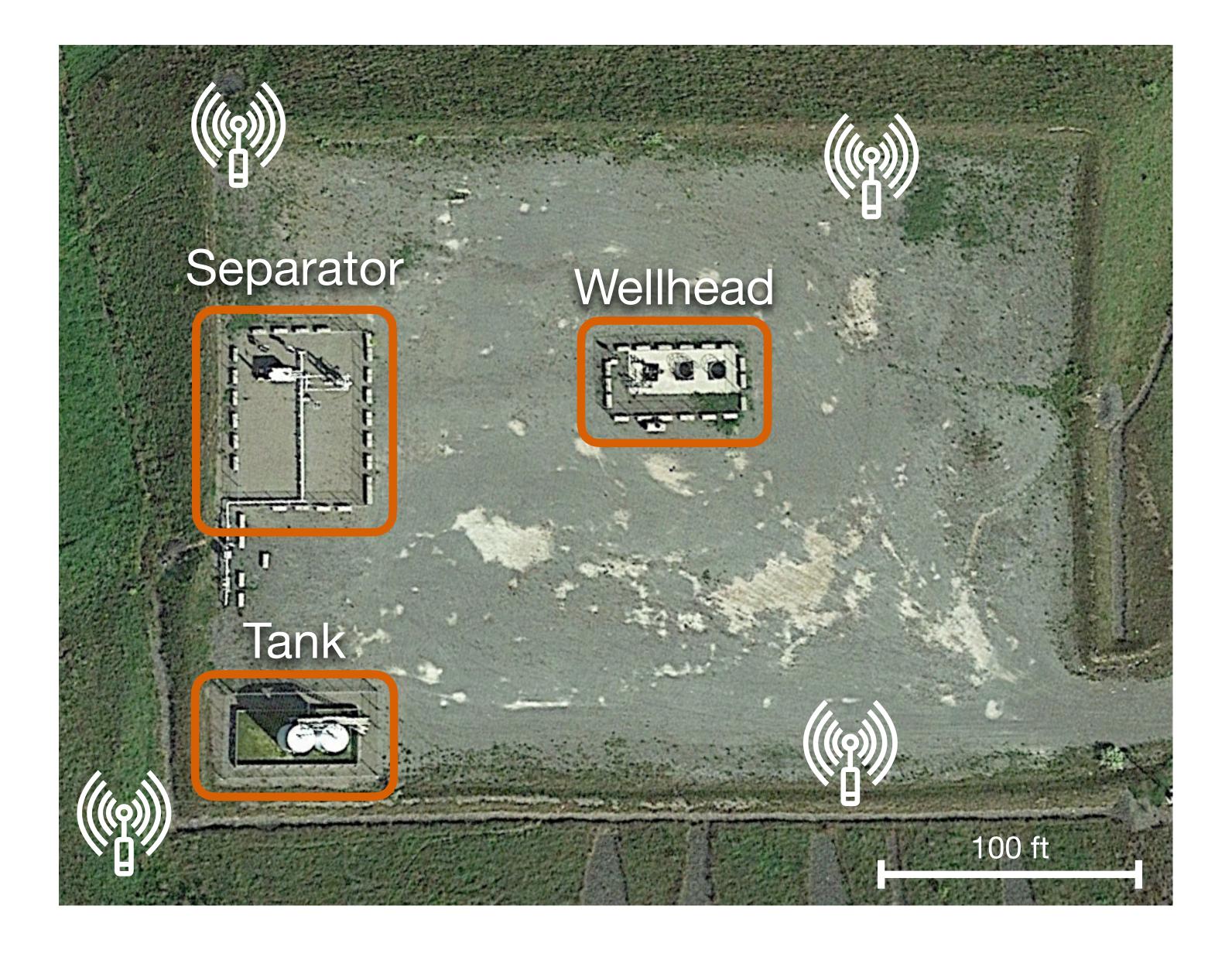






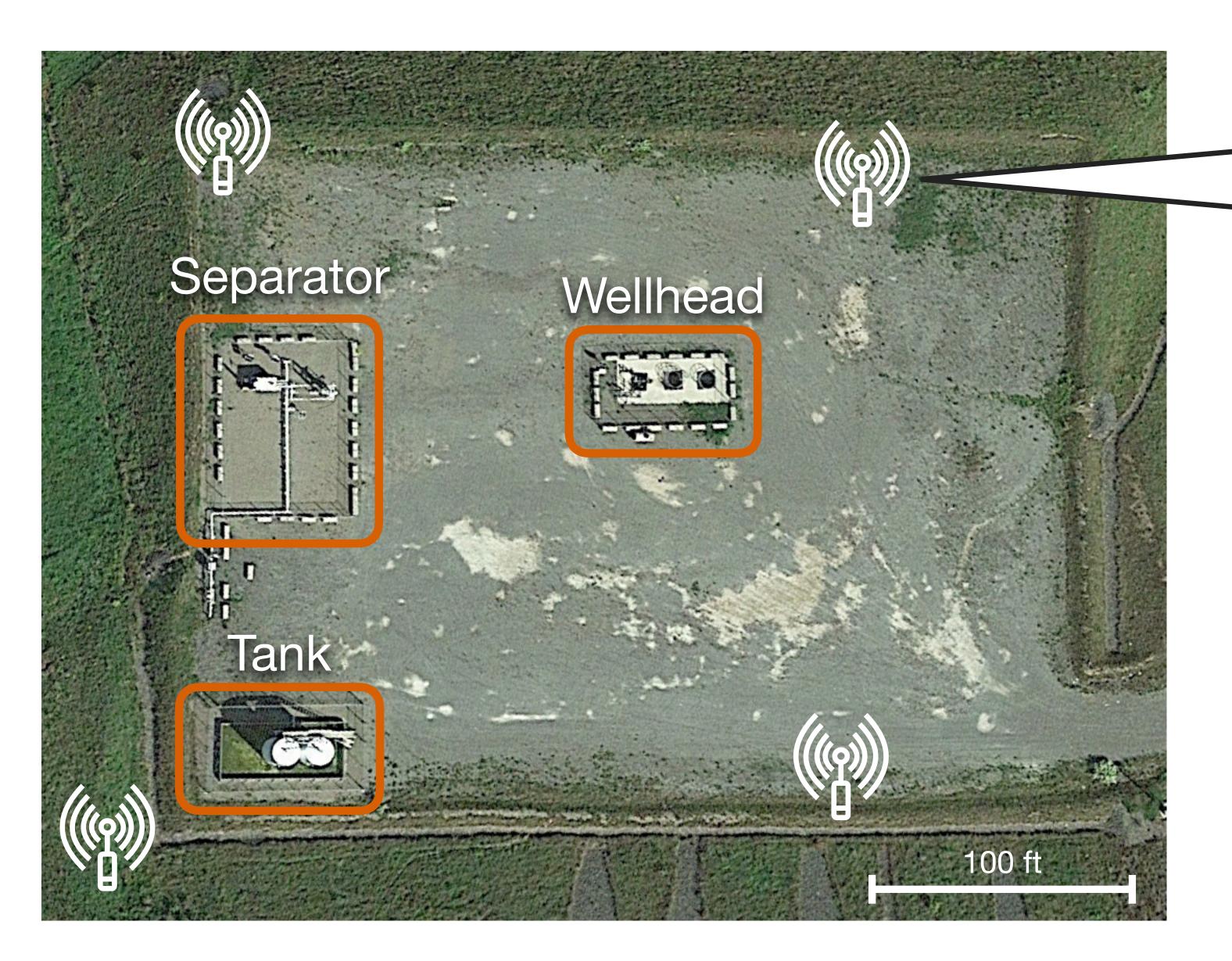
Continuous monitoring system (CMS)

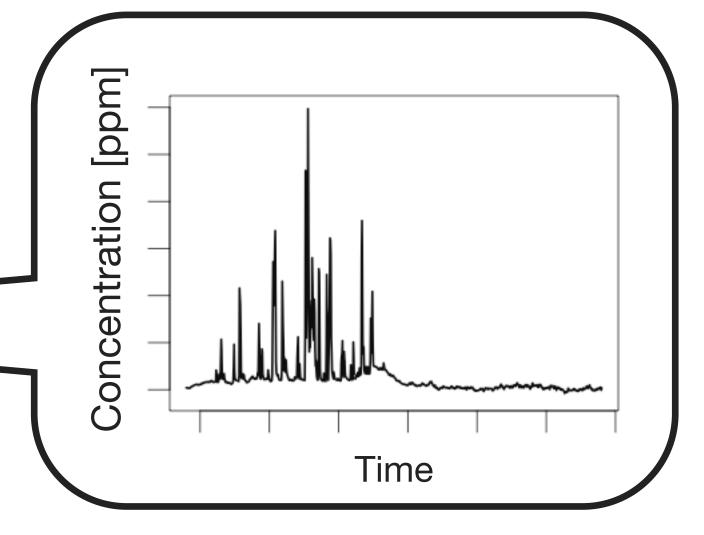


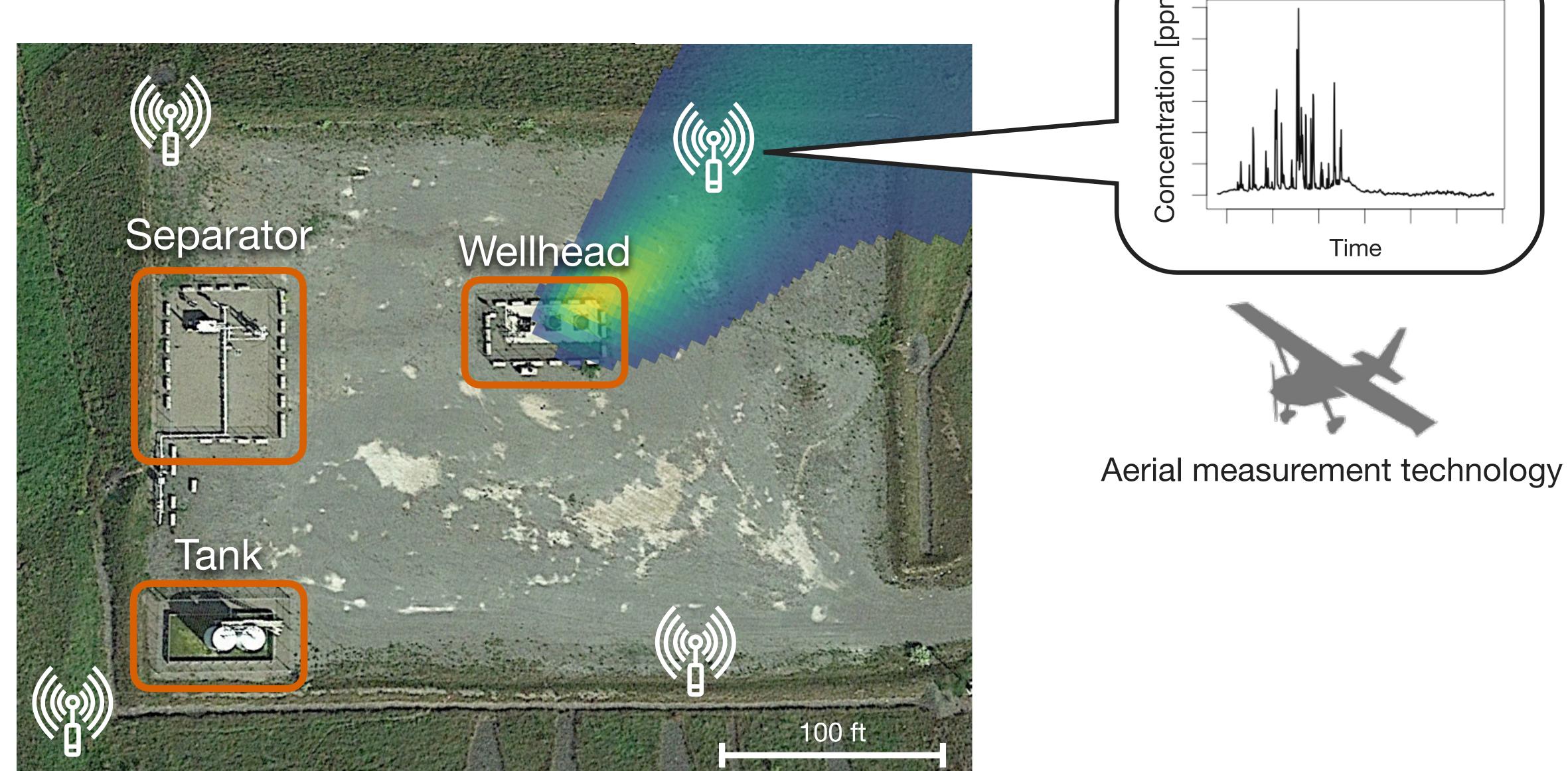


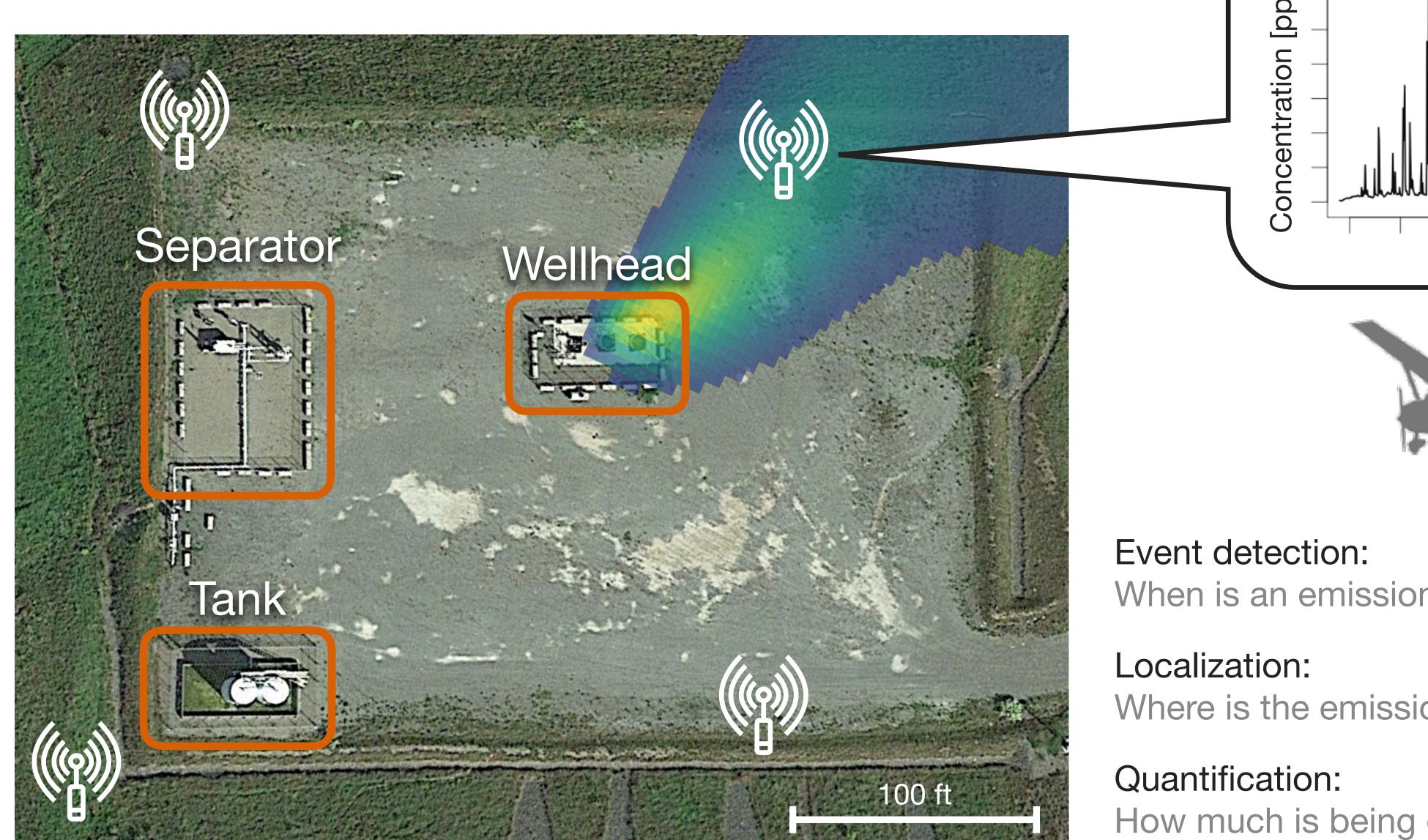
Continuous monitoring system (CMS)

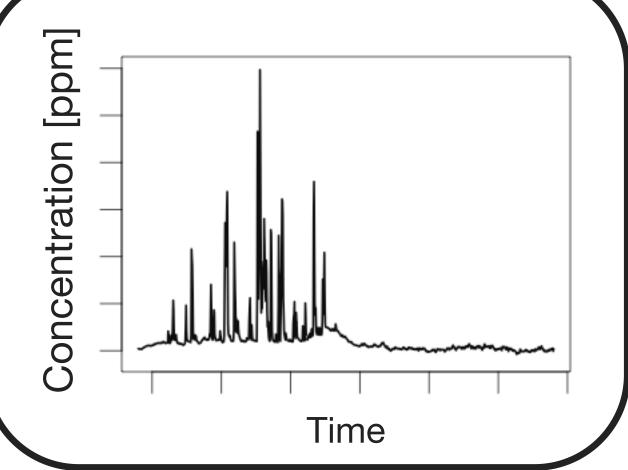








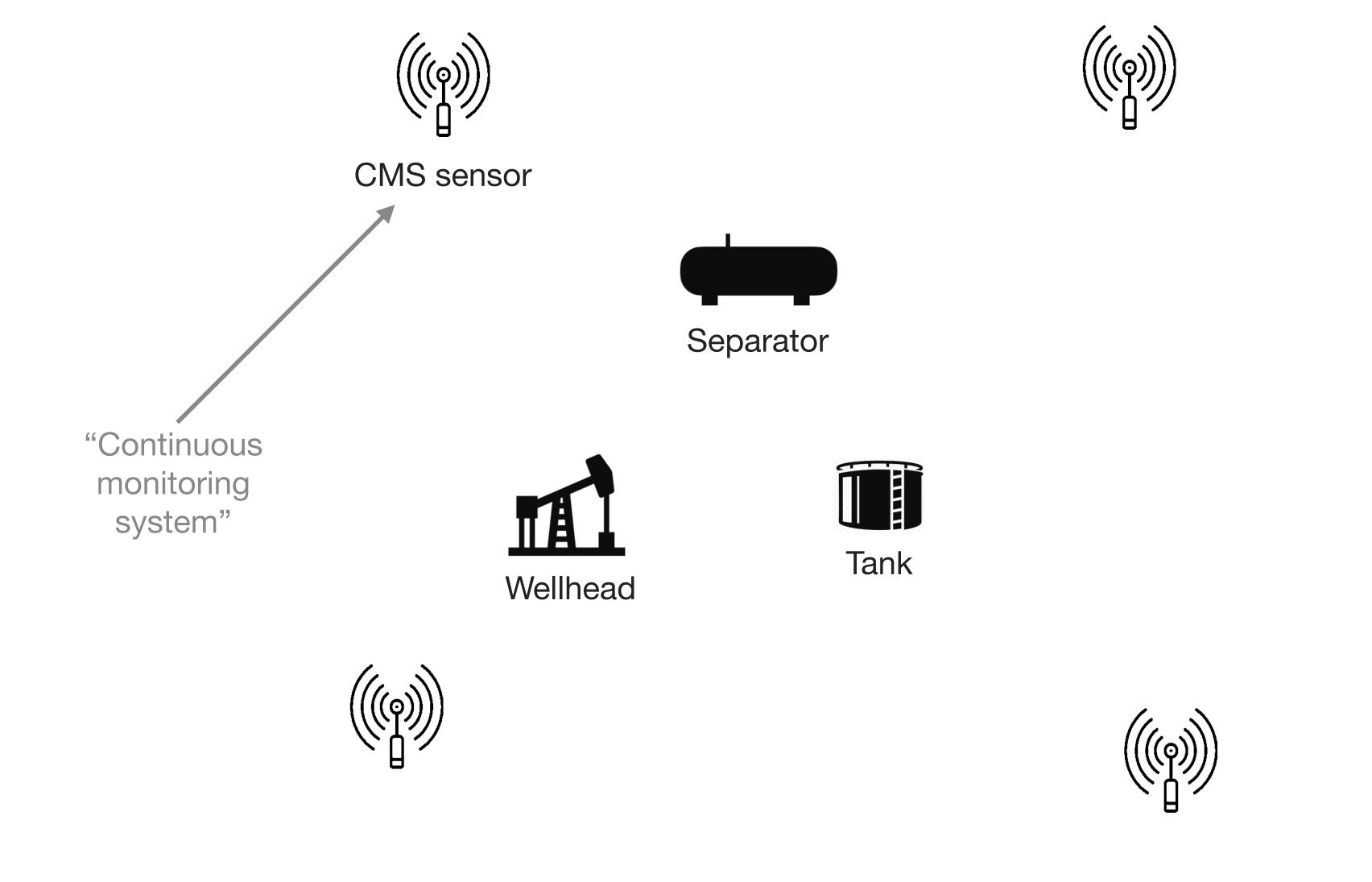




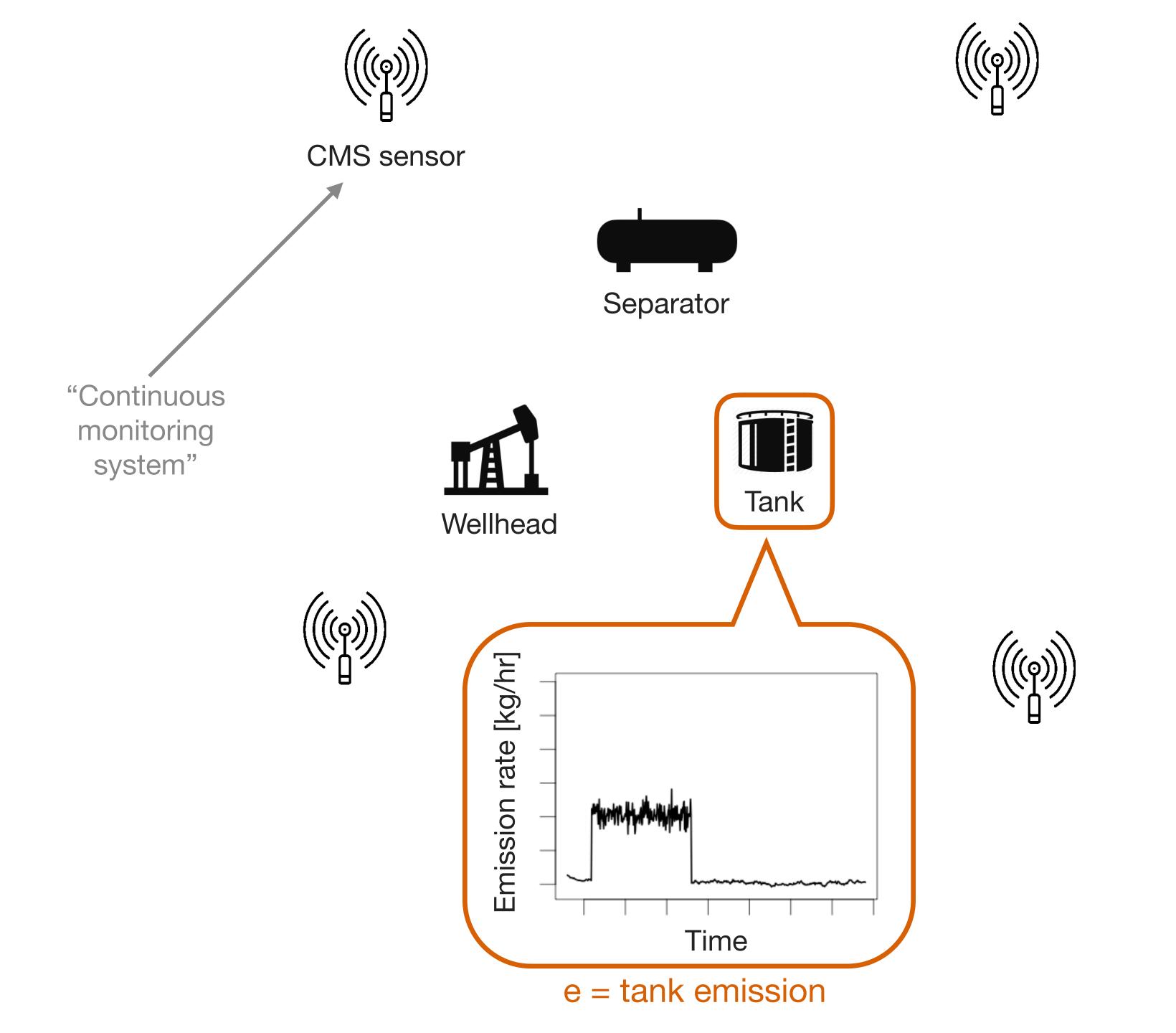
When is an emission happening?

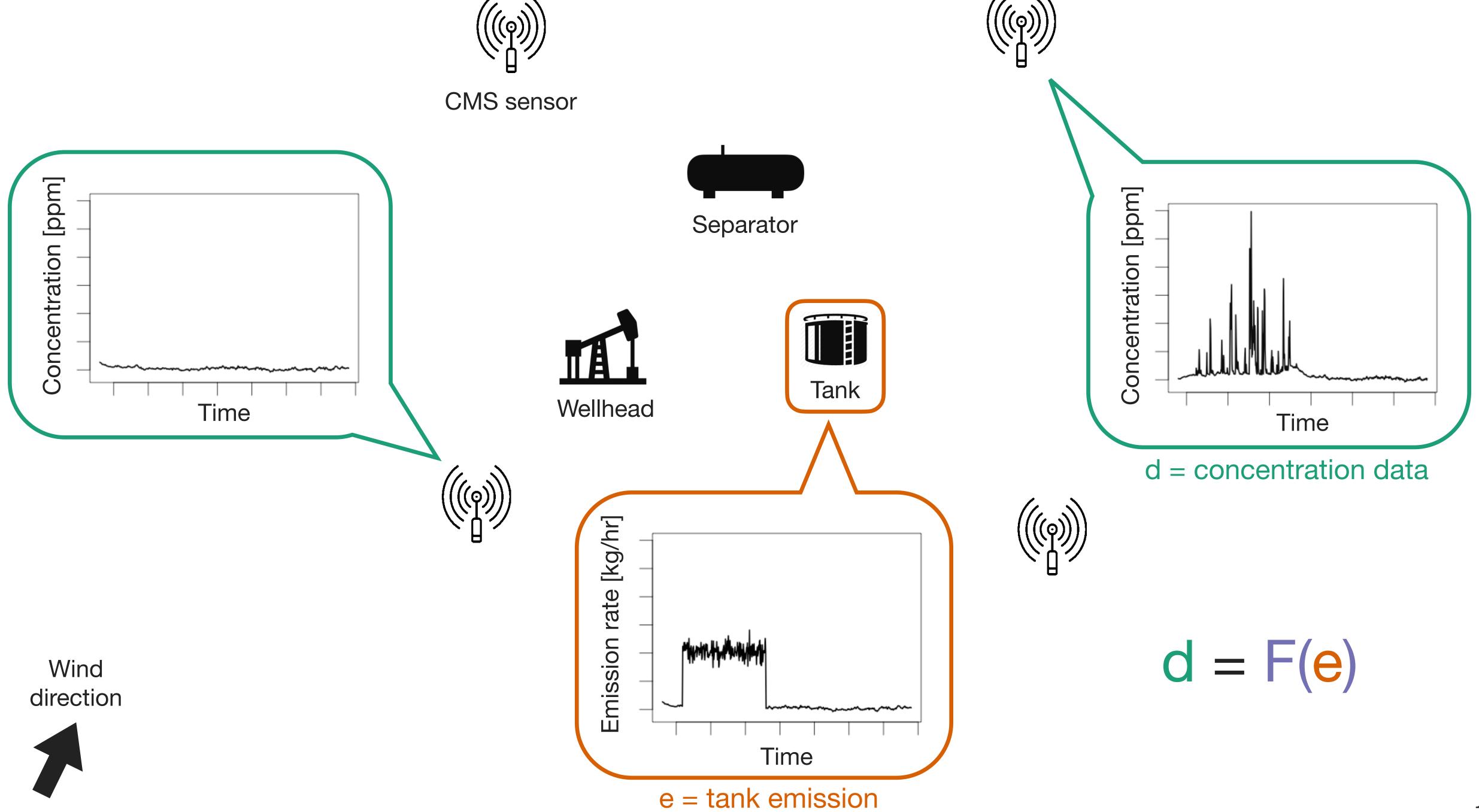
Where is the emission coming from?

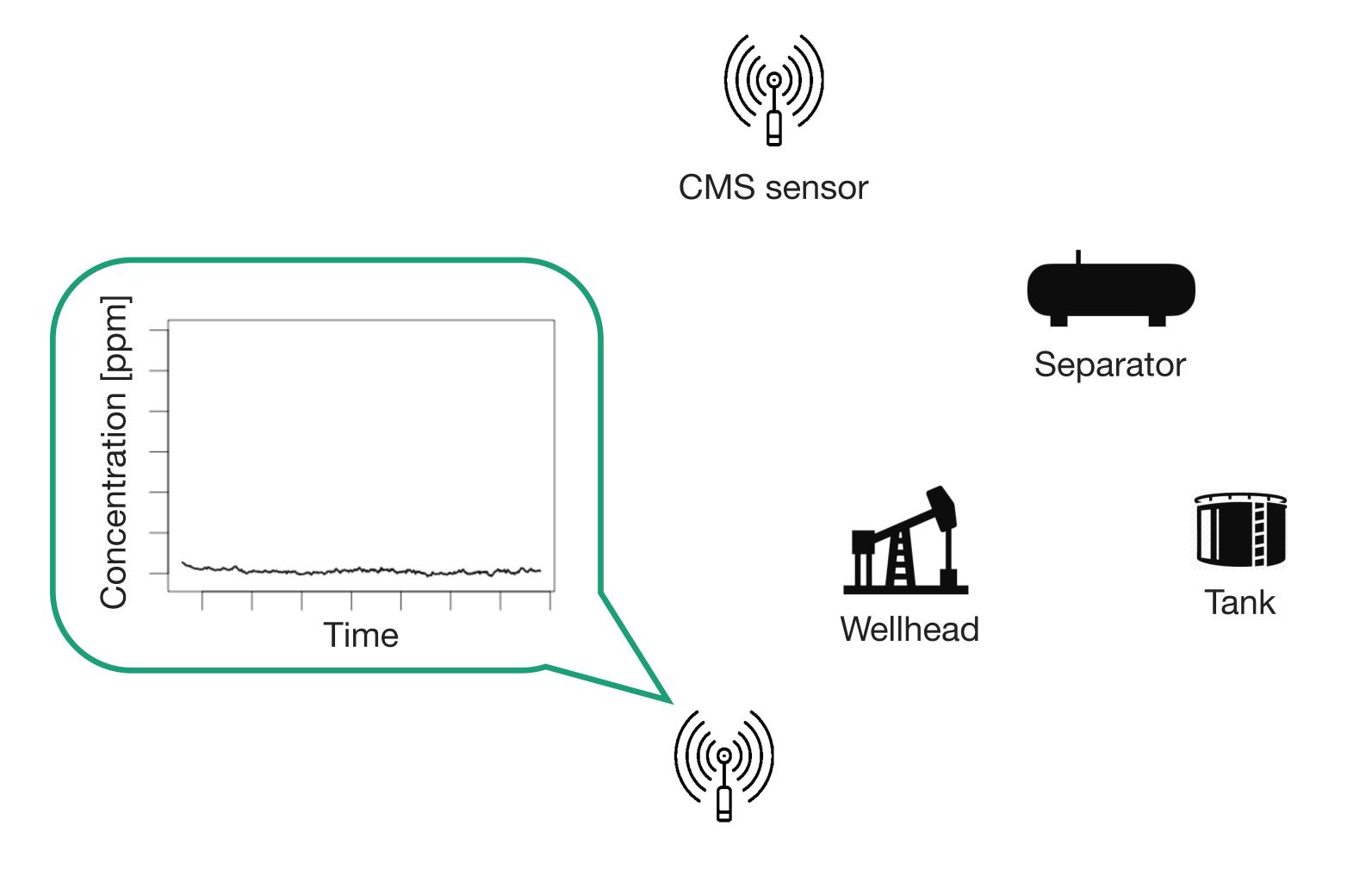
How much is being emitted?

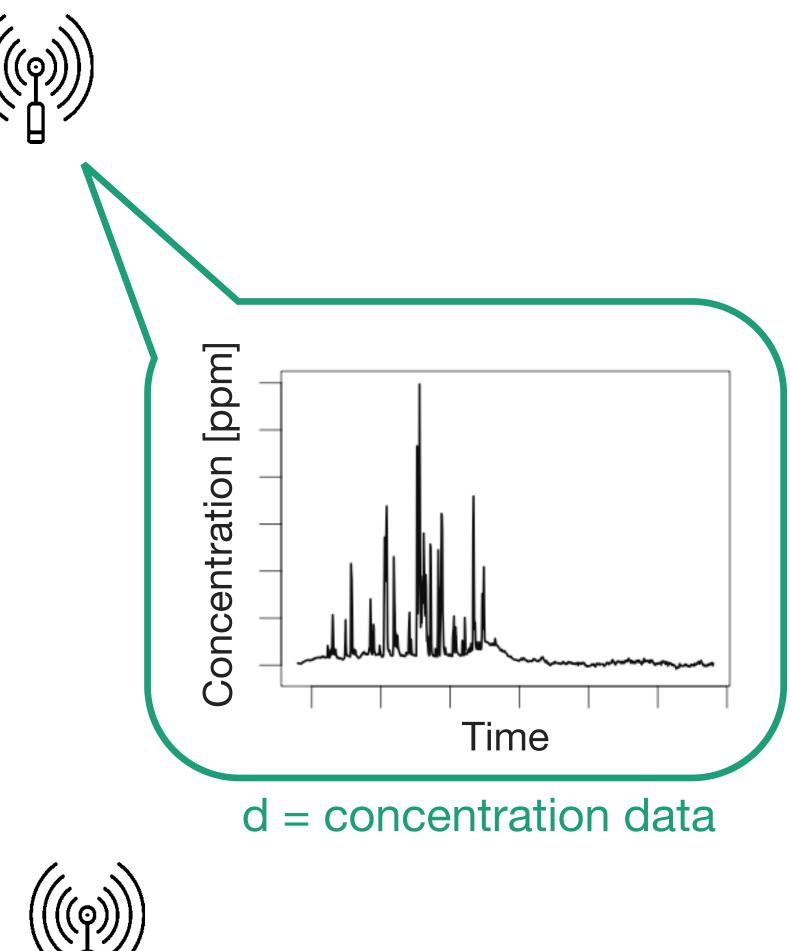


The single-source continuous monitoring inverse problem











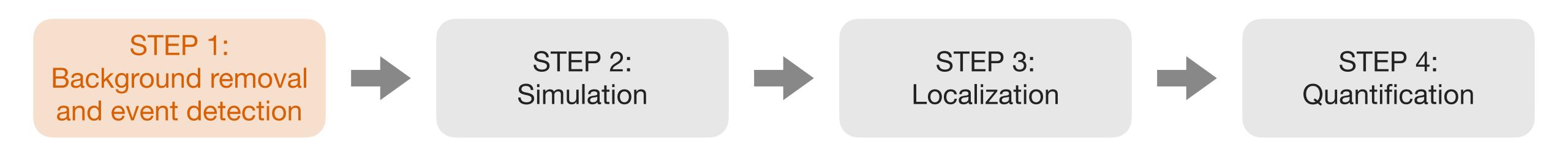
$$d = F(e)$$

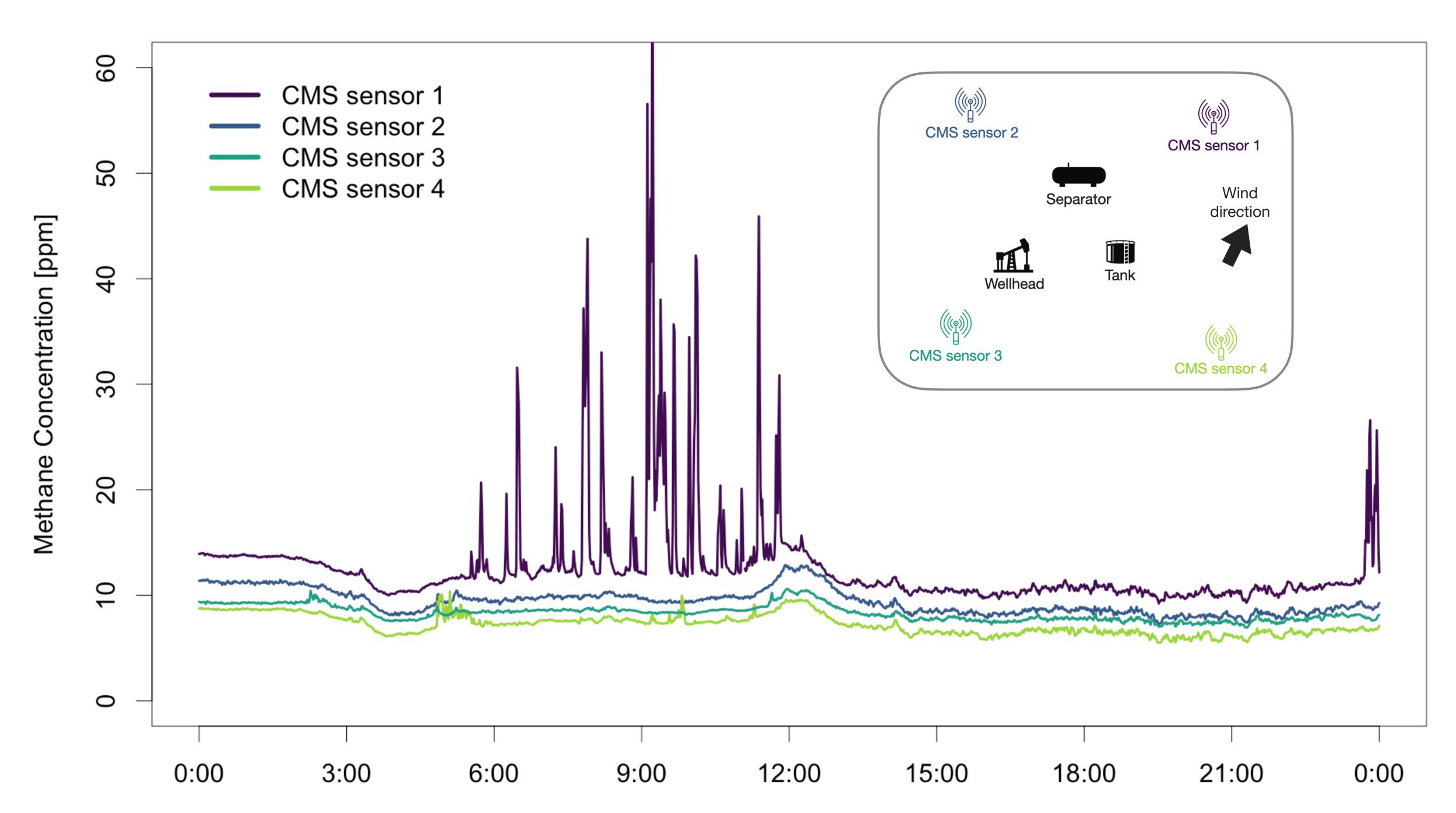
$$e = F^{-1}(d)$$

Wind direction

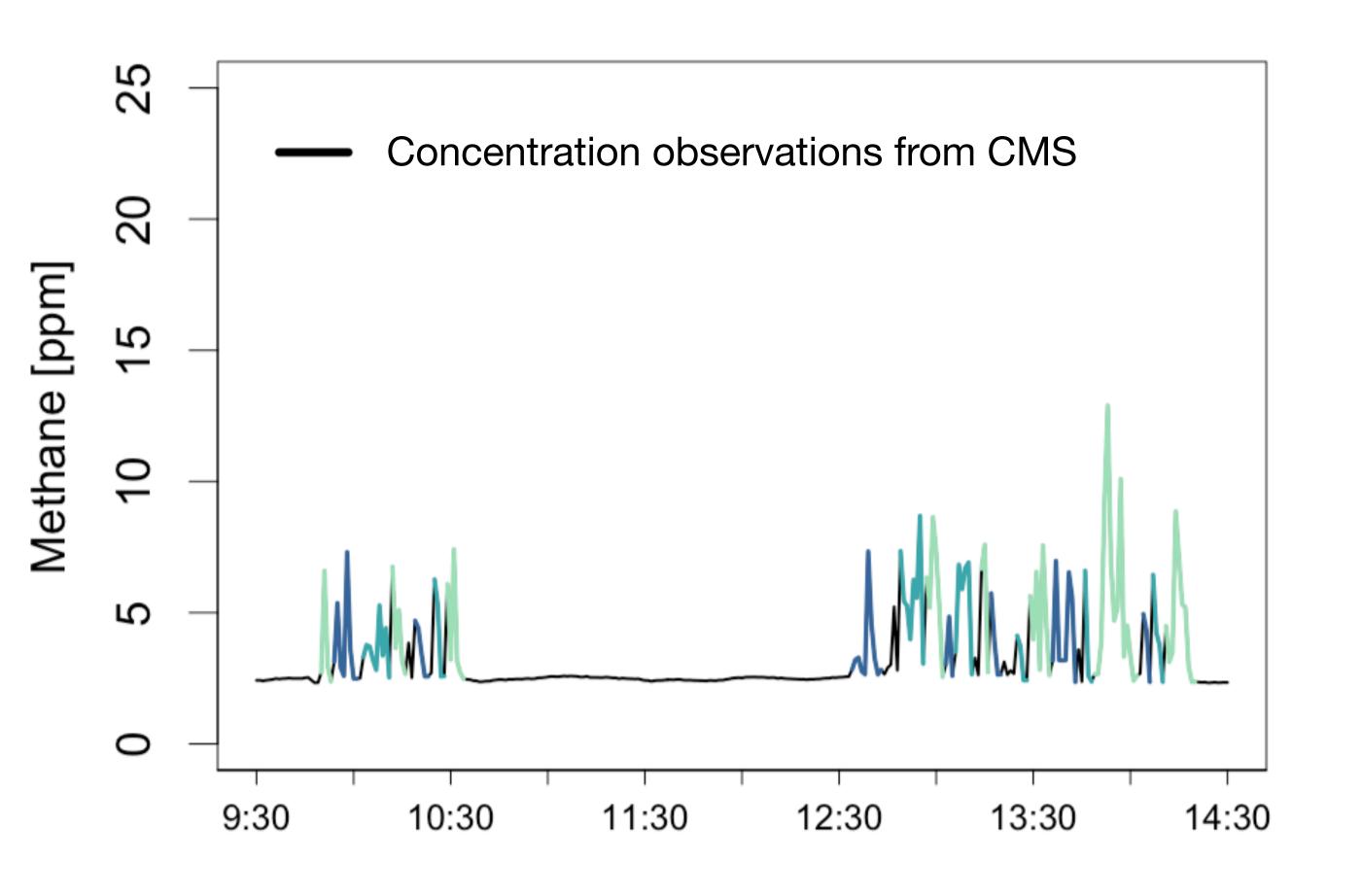


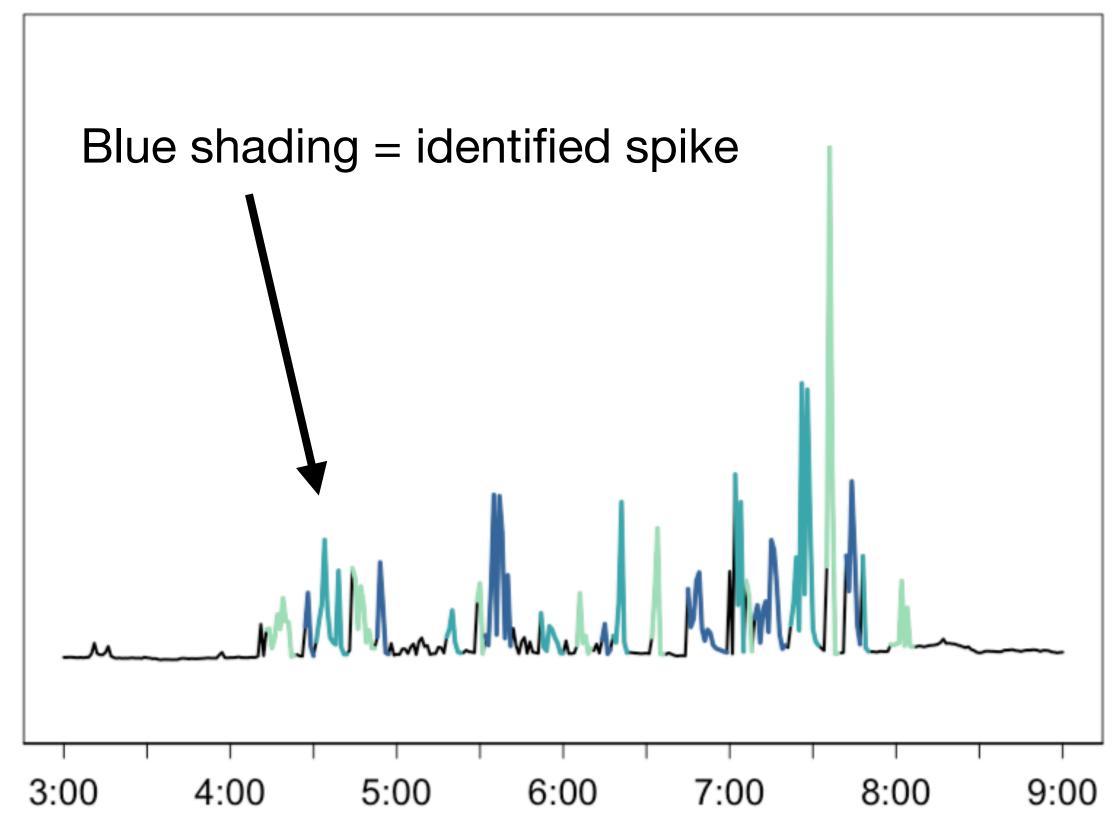
Open source framework for solving inverse problem

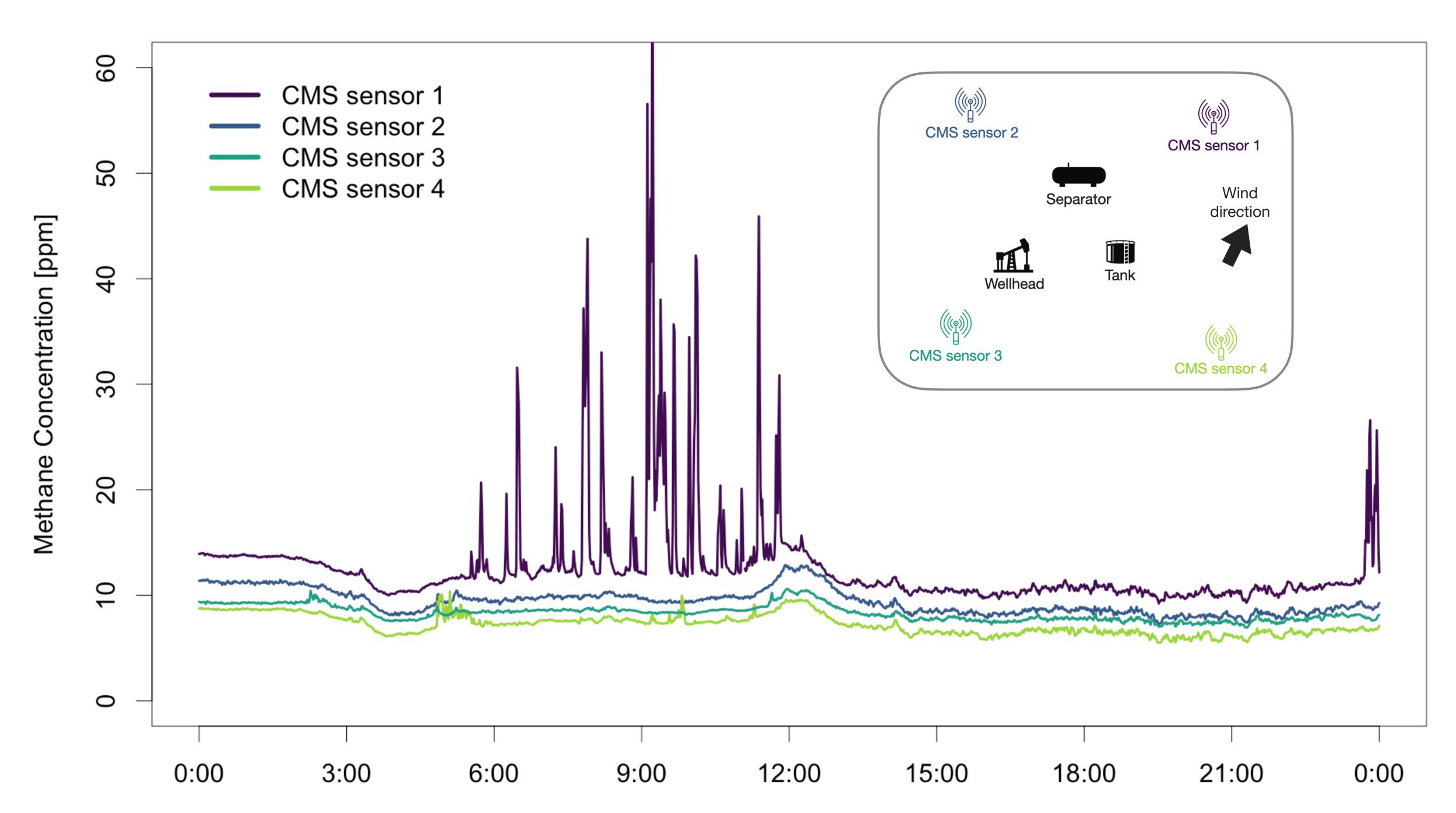


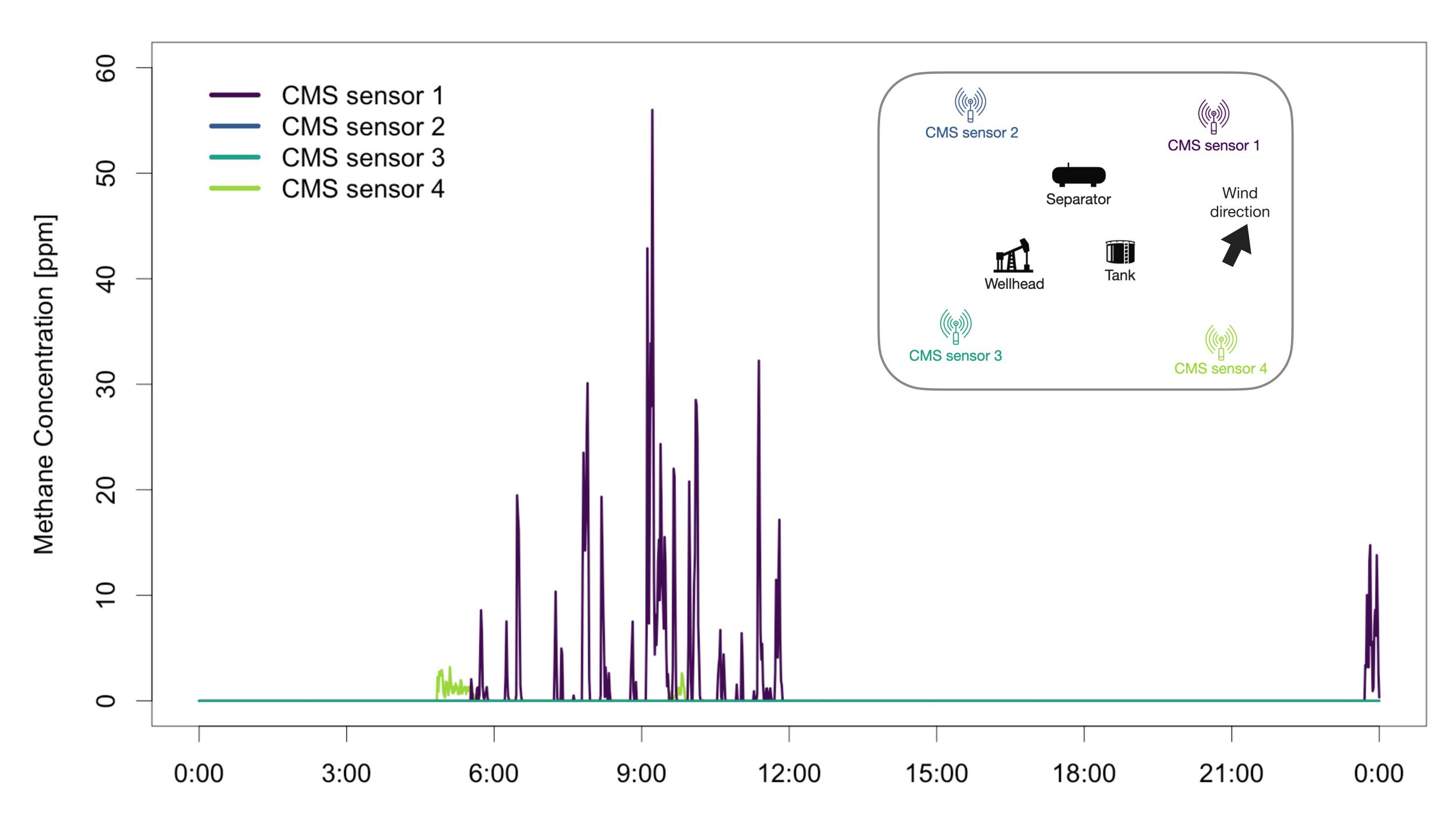


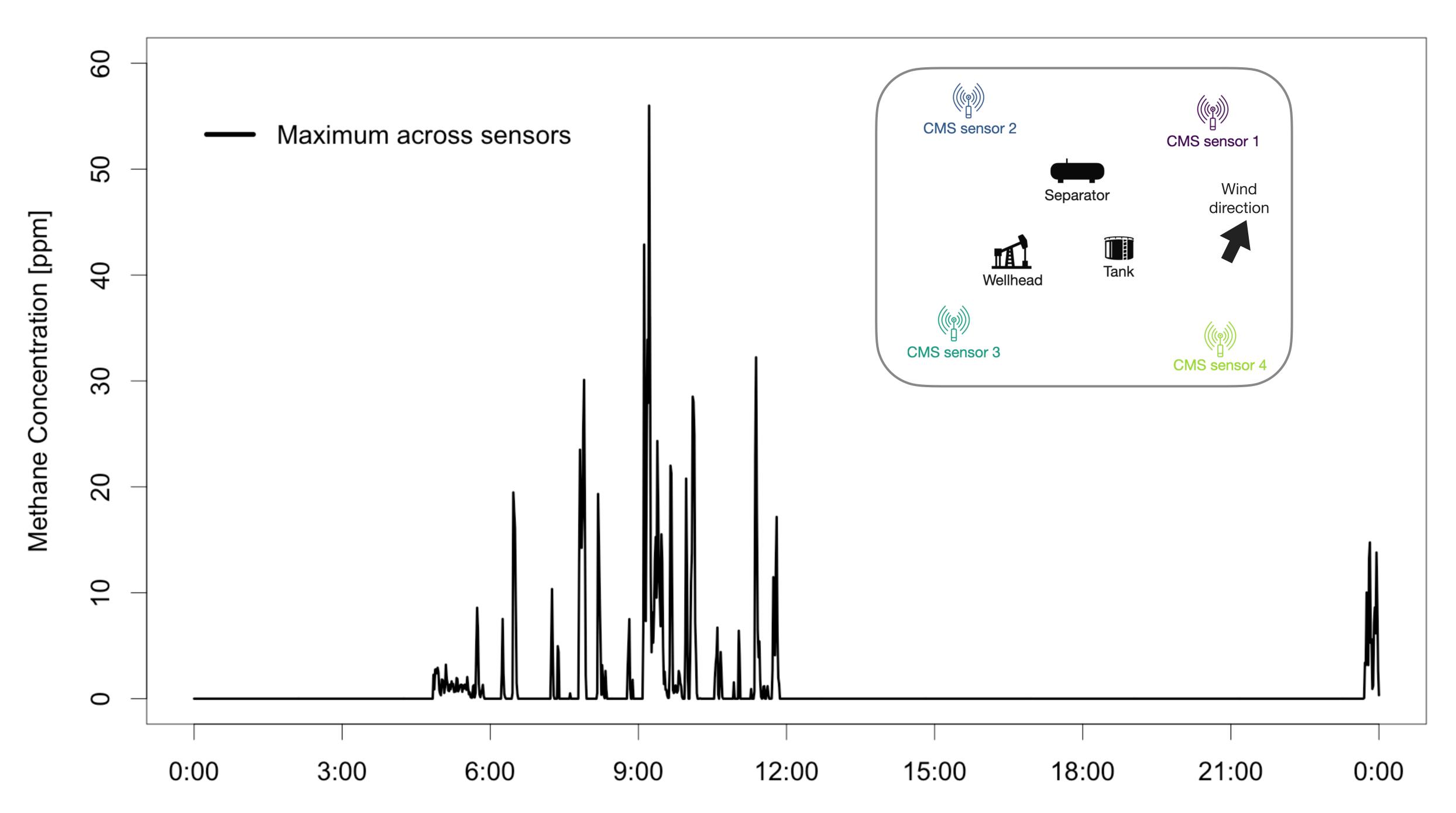
Spike detection algorithm examples

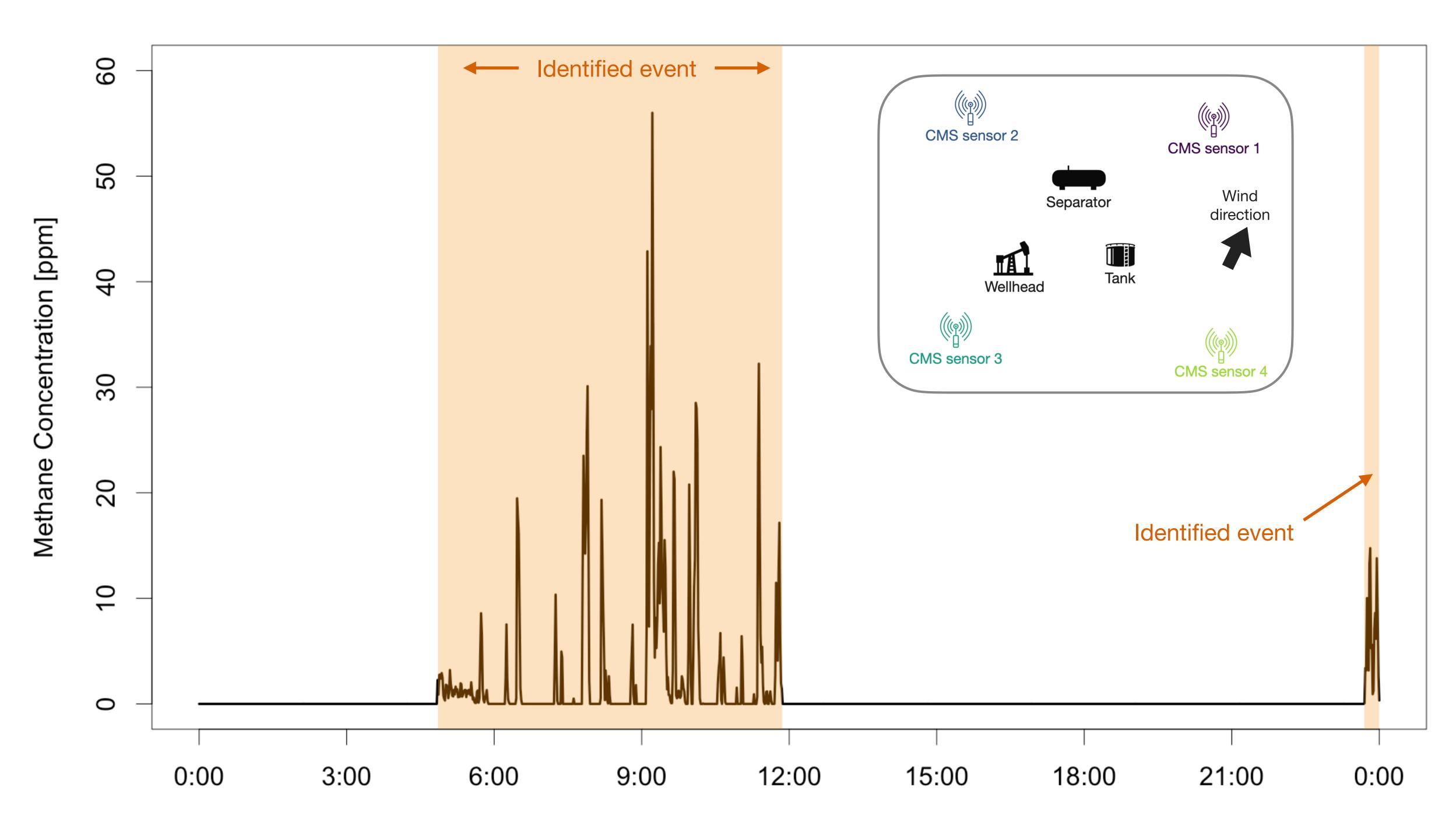


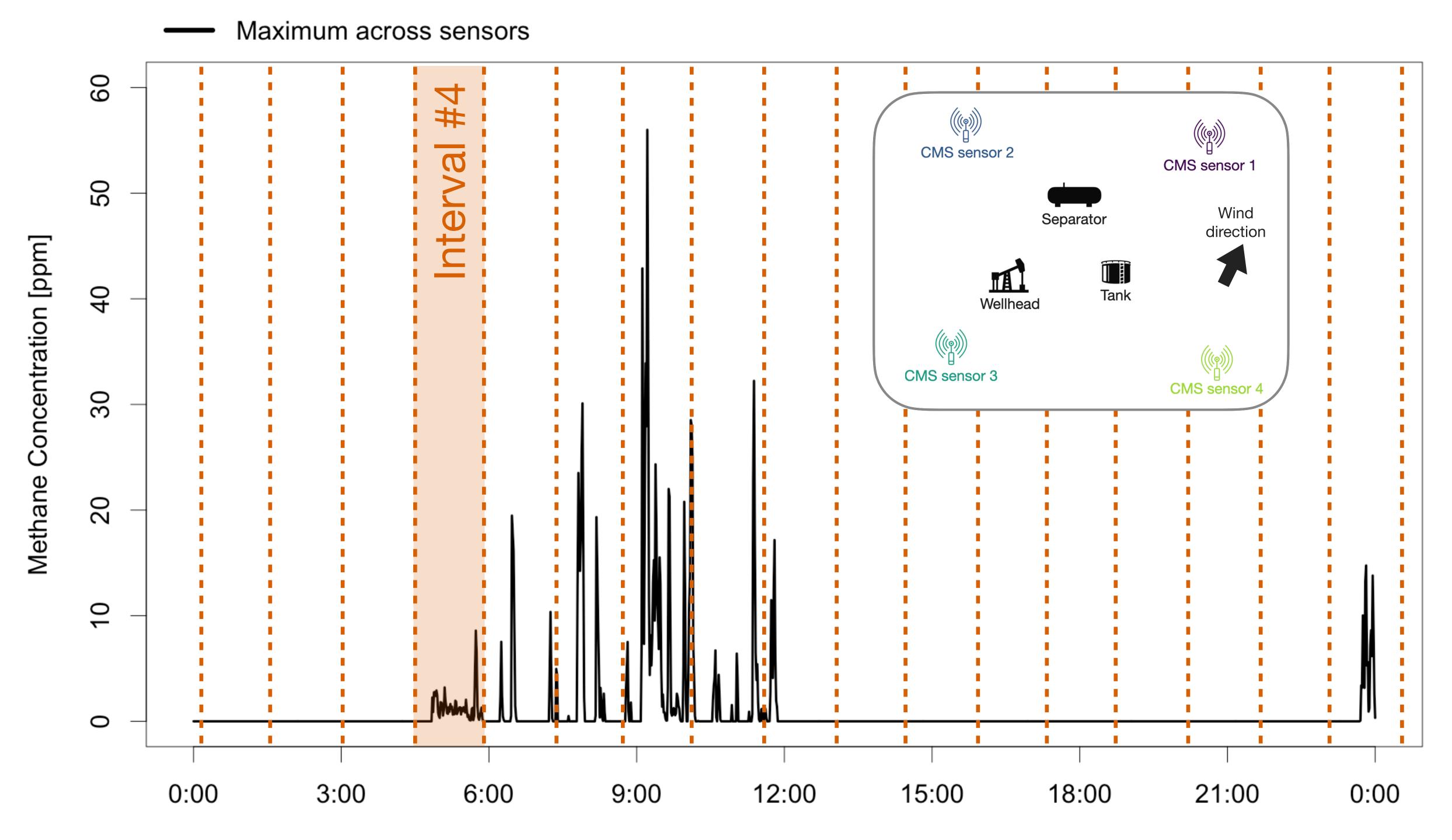




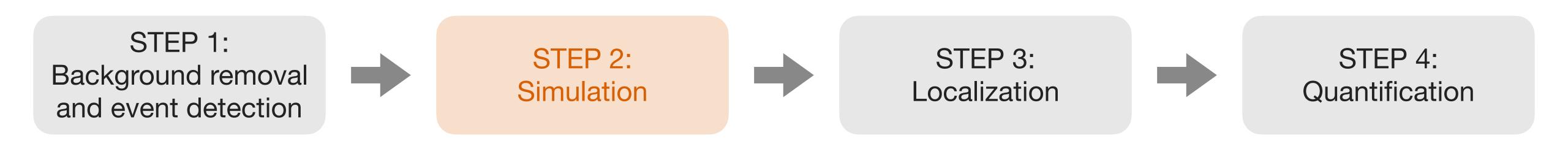








Open source framework for solving inverse problem



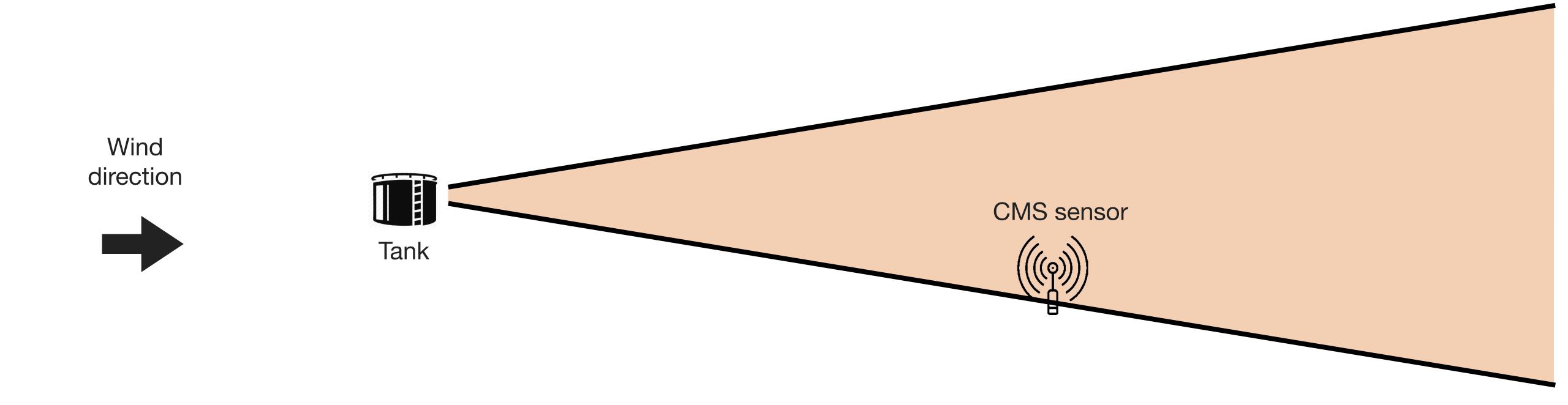
Gaussian plume model:

models the transport of methane by assuming that everything is steady state



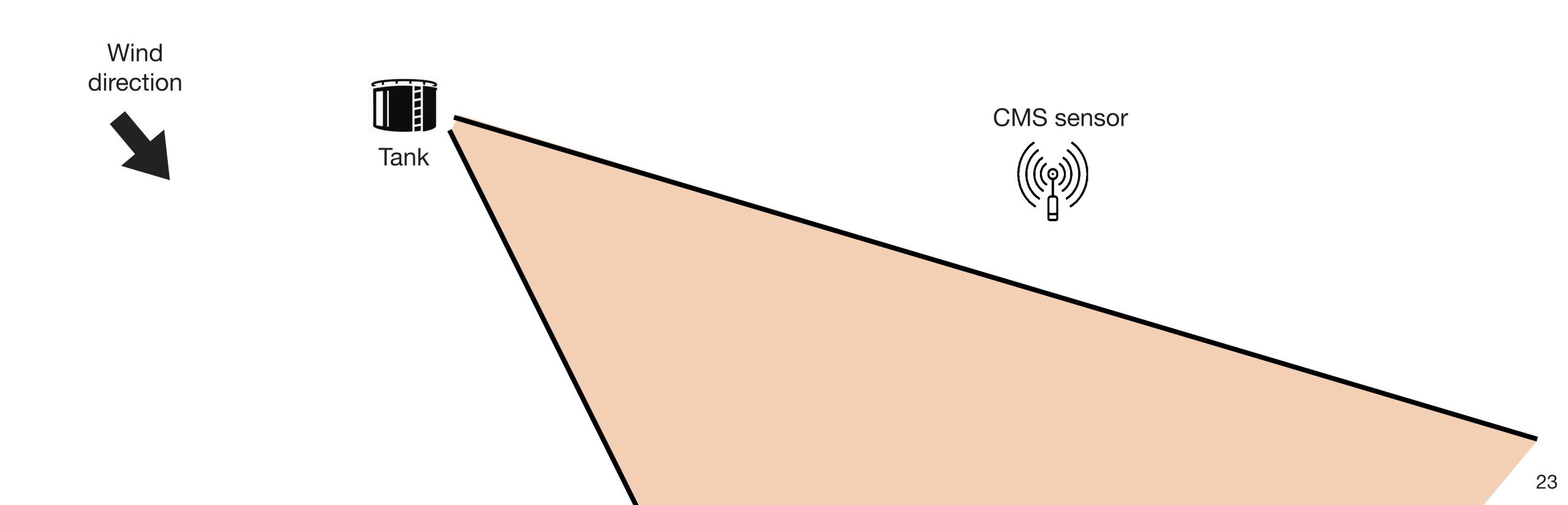
Gaussian plume model:

models the transport of methane by assuming that everything is steady state



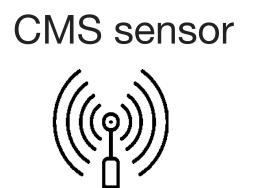
Gaussian plume model:

models the transport of methane by assuming that everything is steady state









approximates a continuous release of methane as a sum of many small "puffs"







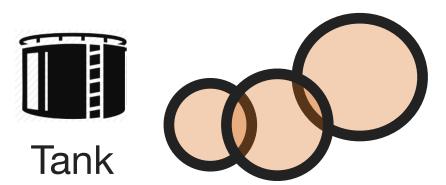


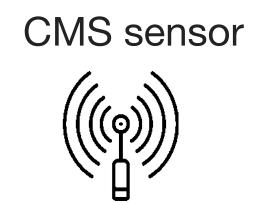
CMS sensor







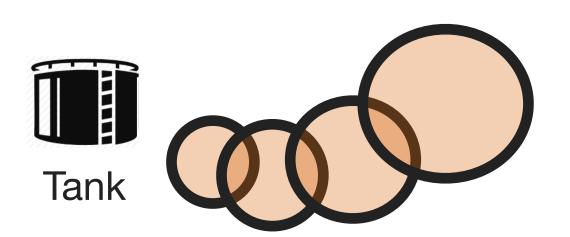




approximates a continuous release of methane as a sum of many small "puffs"

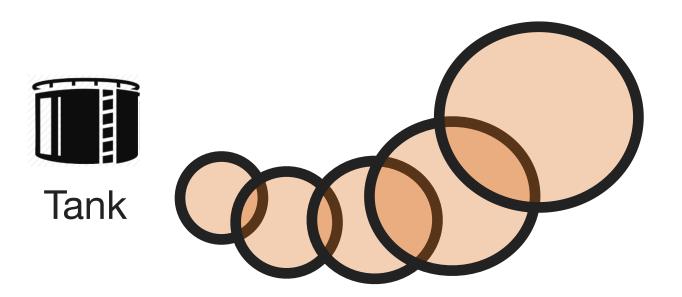


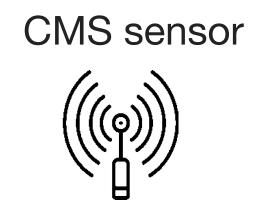


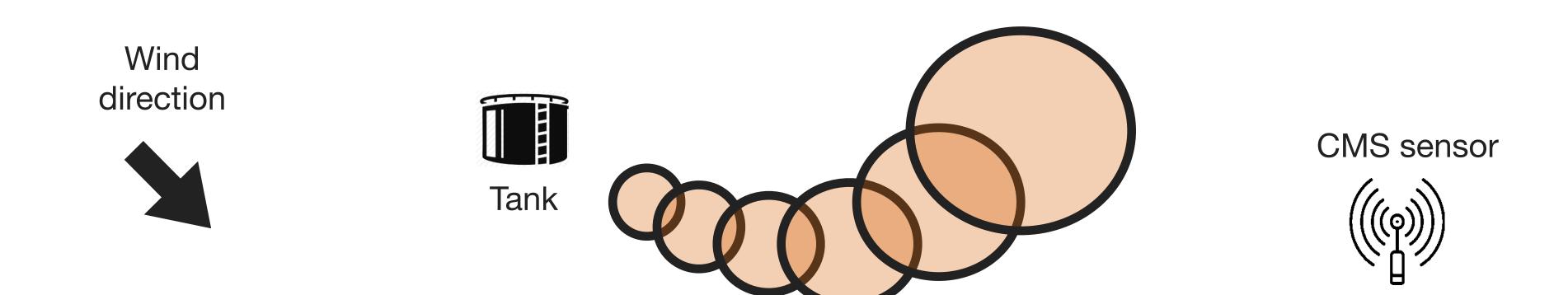


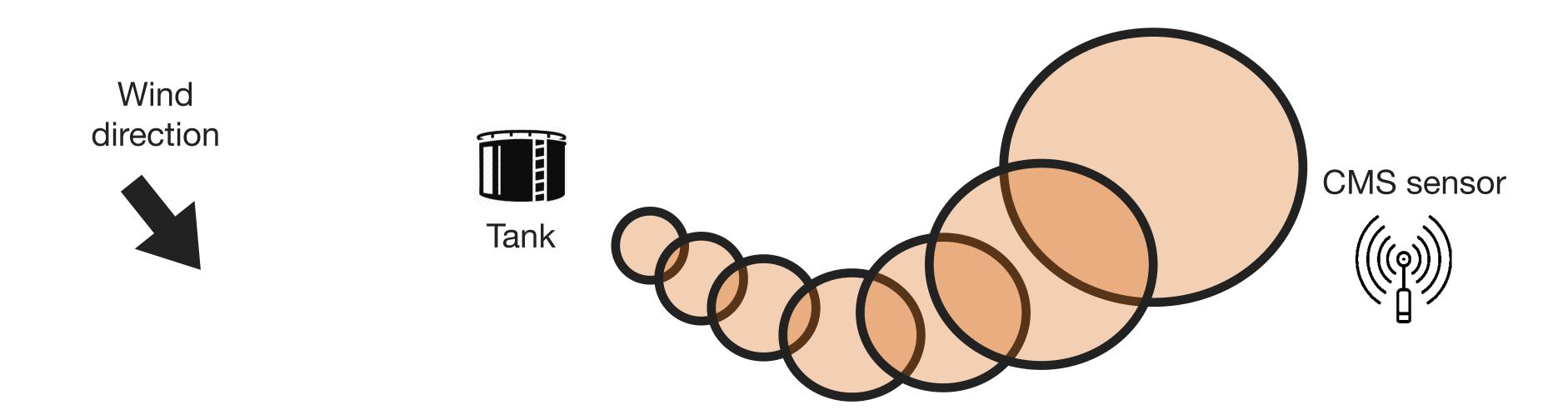
CMS sensor

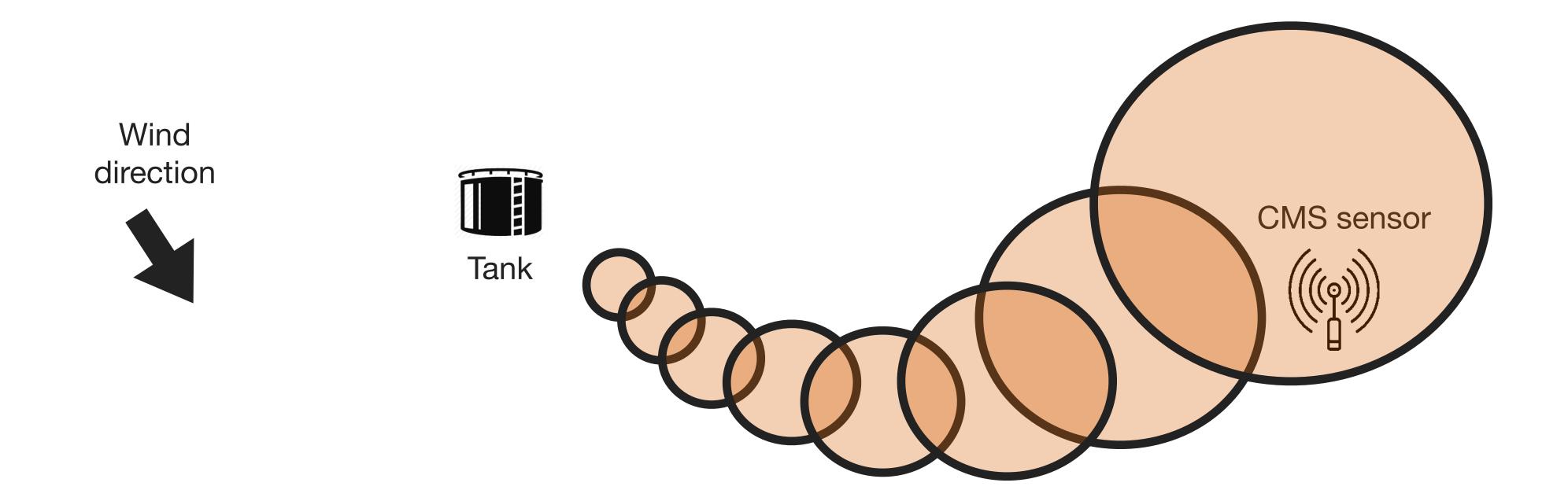




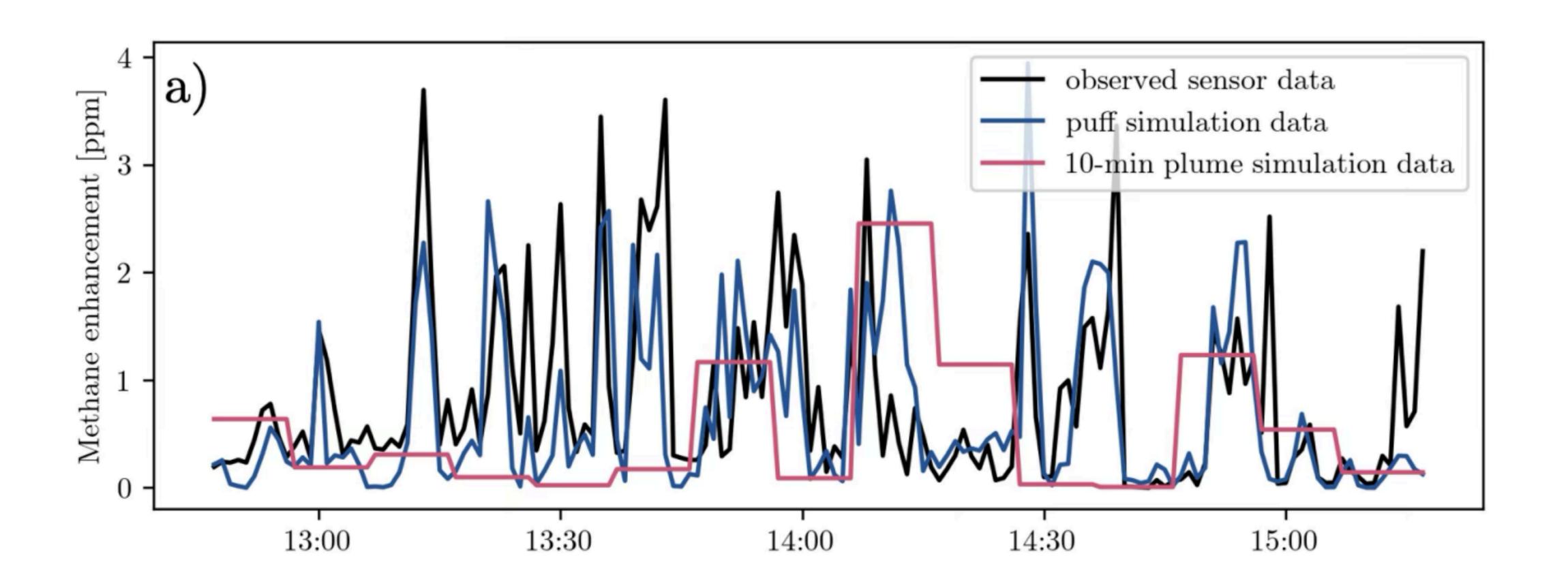






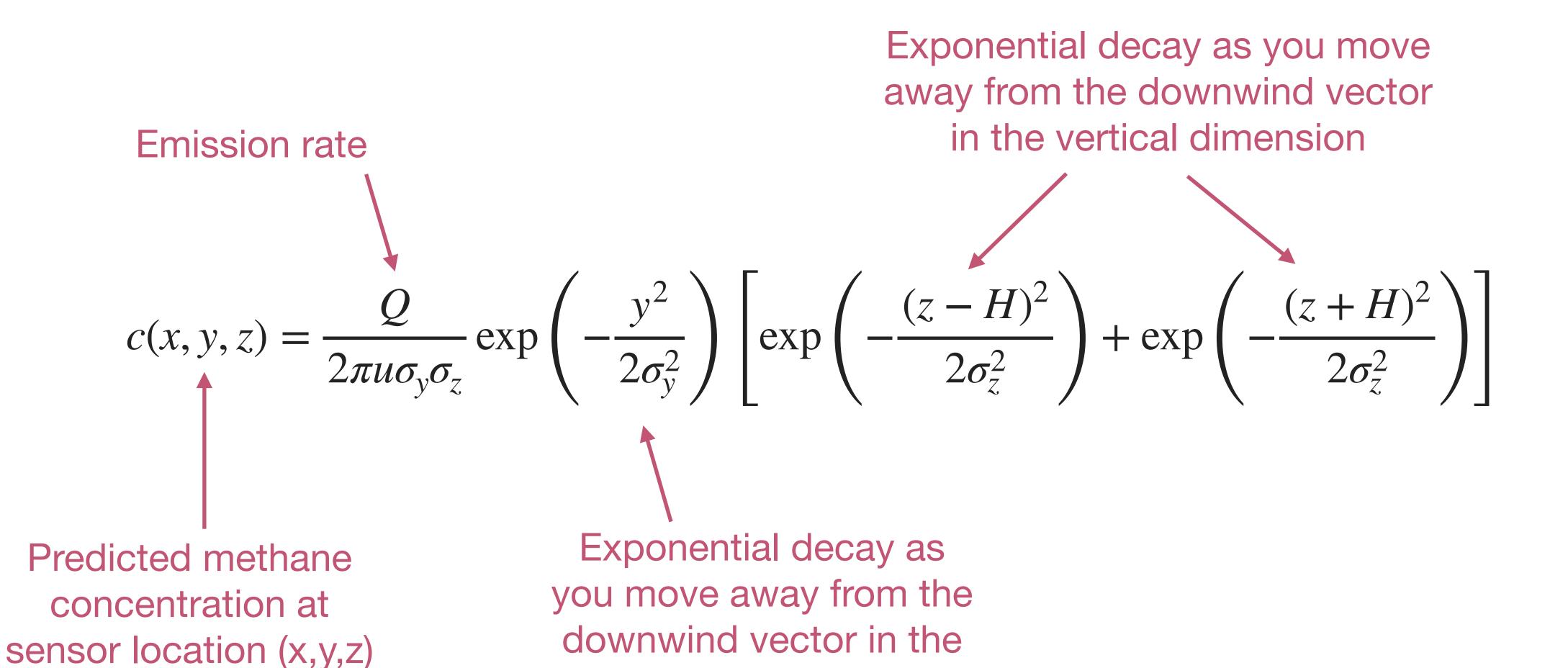


The Gaussian puff can leverage high frequency wind data, while the Gaussian plume requires a temporal average.



Gaussian plume model: mathematical definition

Set up coordinate system so that source is at (0,0,H) and positive x-axis aligns with downwind vector



horizontal plane

Gaussian puff model: mathematical definition

Set up coordinate system so that source is at (0,0,H) and positive x-axis aligns with downwind vector



$$c_{p}(x, y, z, t, Q) = \frac{Q}{(2\pi)^{3/2} \sigma_{y}^{2} \sigma_{z}} \exp\left(-\frac{(x - ut)^{2} + y^{2}}{2\sigma_{y}^{2}}\right) \left[\exp\left(-\frac{(z - H)^{2}}{2\sigma_{z}^{2}}\right) + \exp\left(-\frac{(z + H)^{2}}{2\sigma_{z}^{2}}\right)\right]$$

Predicted methane concentration at sensor location (x,y,z) and time t from puff *p*

Exponential decay in concentration in horizontal plane (x, y)

Exponential decay in concentration in vertical dimension (z)

Gaussian puff model: mathematical definition

Set up coordinate system so that source is at (0,0,H) and positive x-axis aligns with downwind vector

Total volume of methane contained in puff p

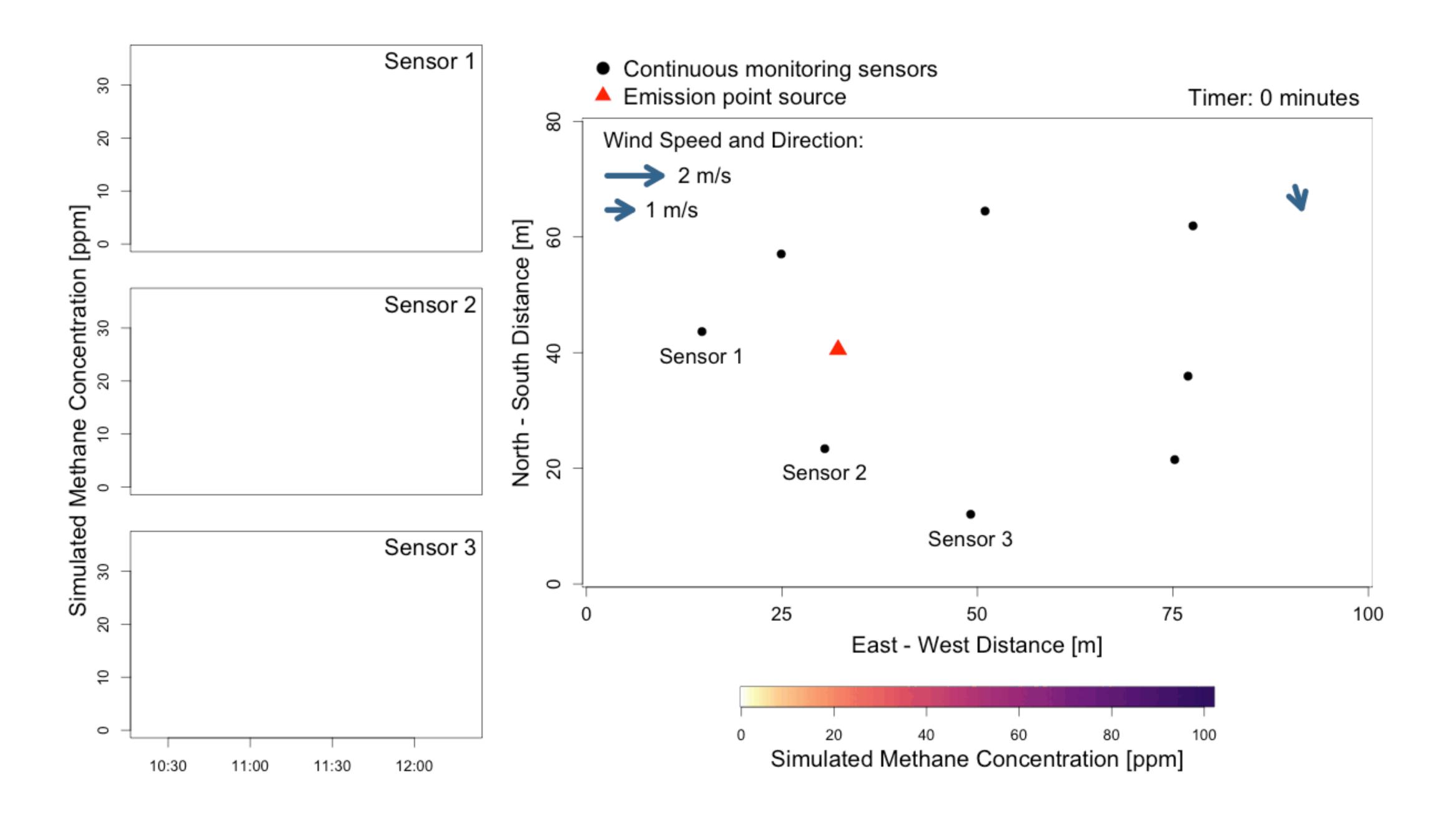
Total
$$c(x, y, z, t, Q) = \sum_{p=1}^{P} c_p(x, y, z, t, Q)$$
 at (x, y, z, t)

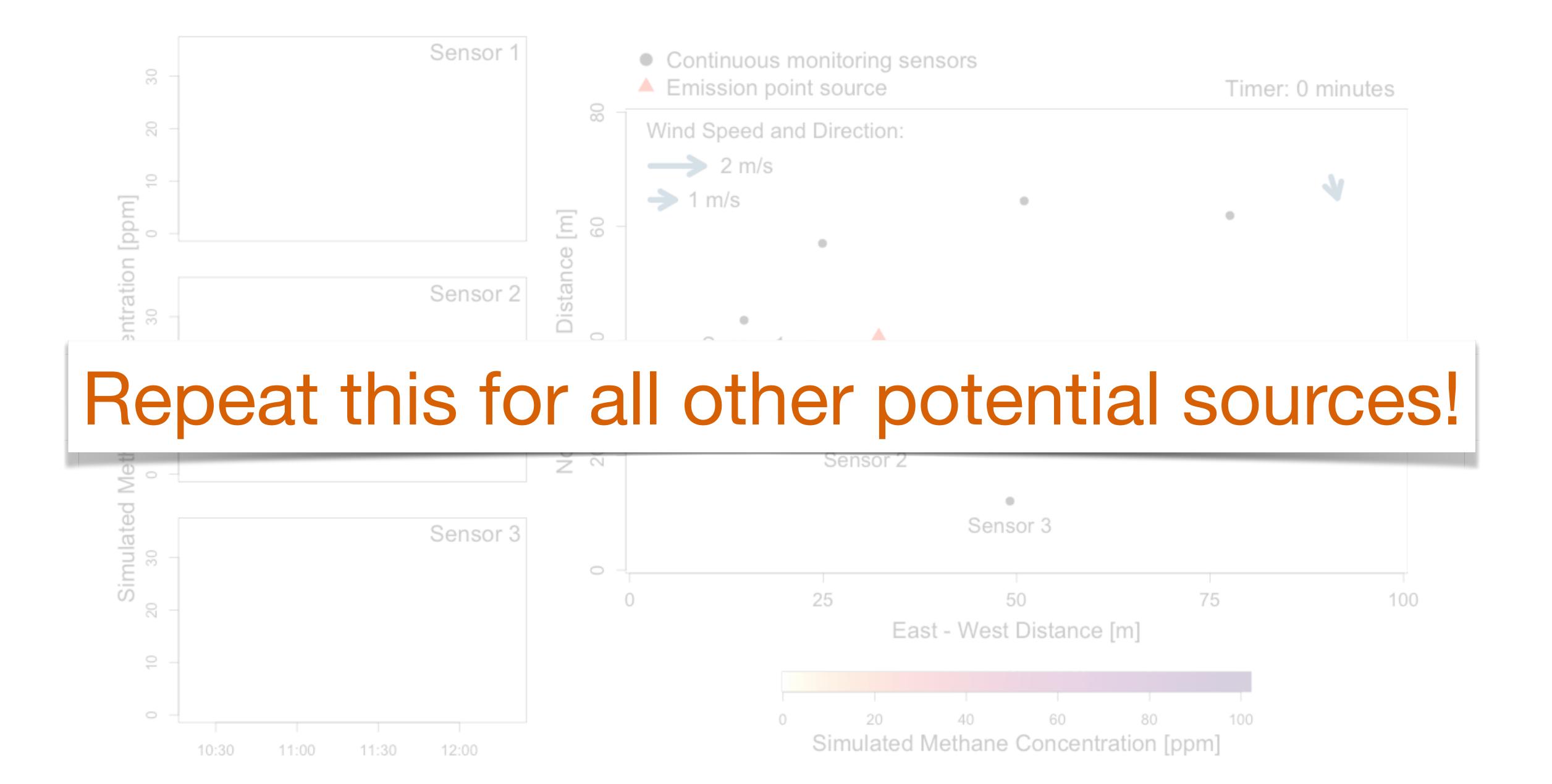
$$c_p(x, y, z, t, Q) = \frac{Q}{(2\pi)^{3/2} \sigma_y^2 \sigma_z} \exp\left(-\frac{(x - ut)^2 + y^2}{2\sigma_y^2}\right) \left[\exp\left(-\frac{(z - H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + H)^2}{2\sigma_z^2}\right)\right]$$

Predicted methane concentration at sensor location (x,y,z) and time t from puff *p*

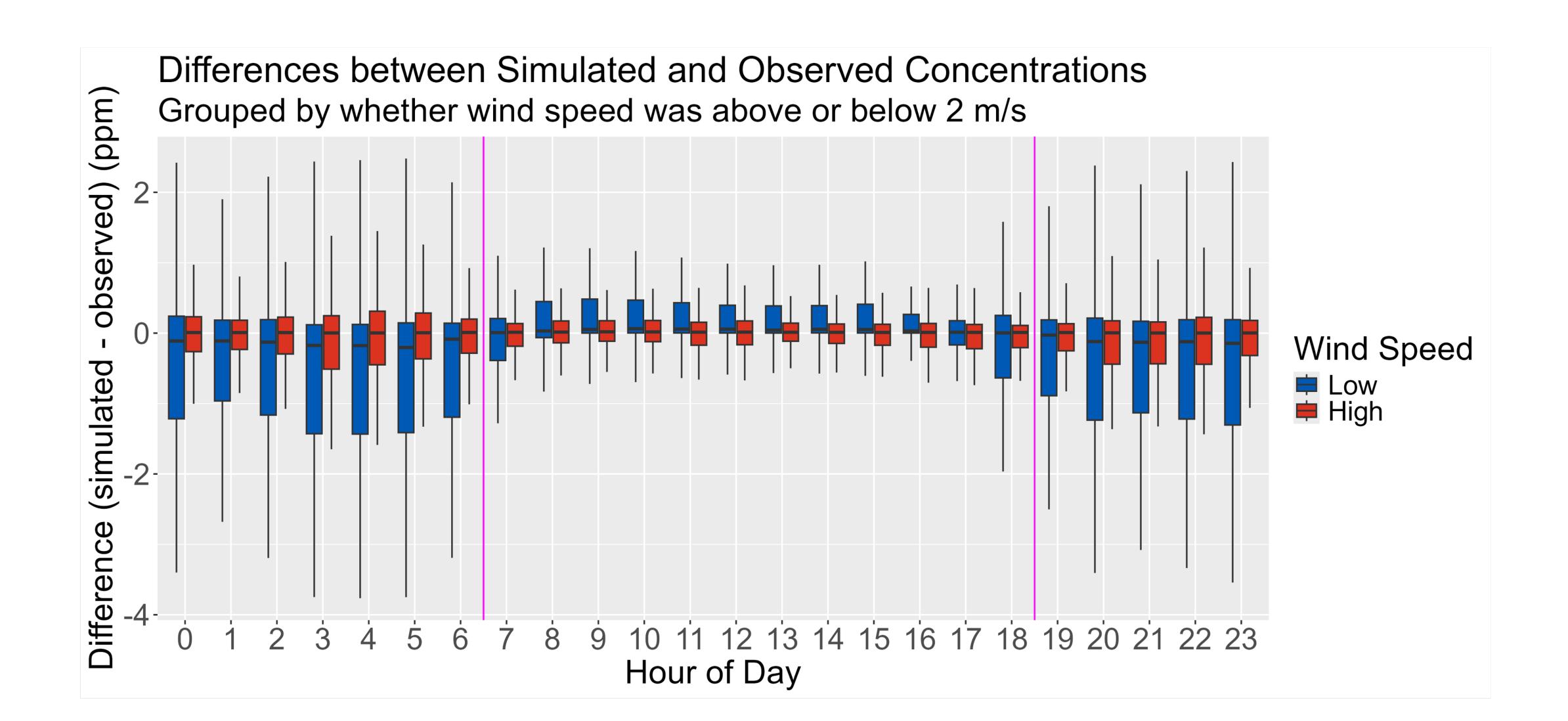
Exponential decay in concentration in horizontal plane (x, y)

Exponential decay in concentration in vertical dimension (z)

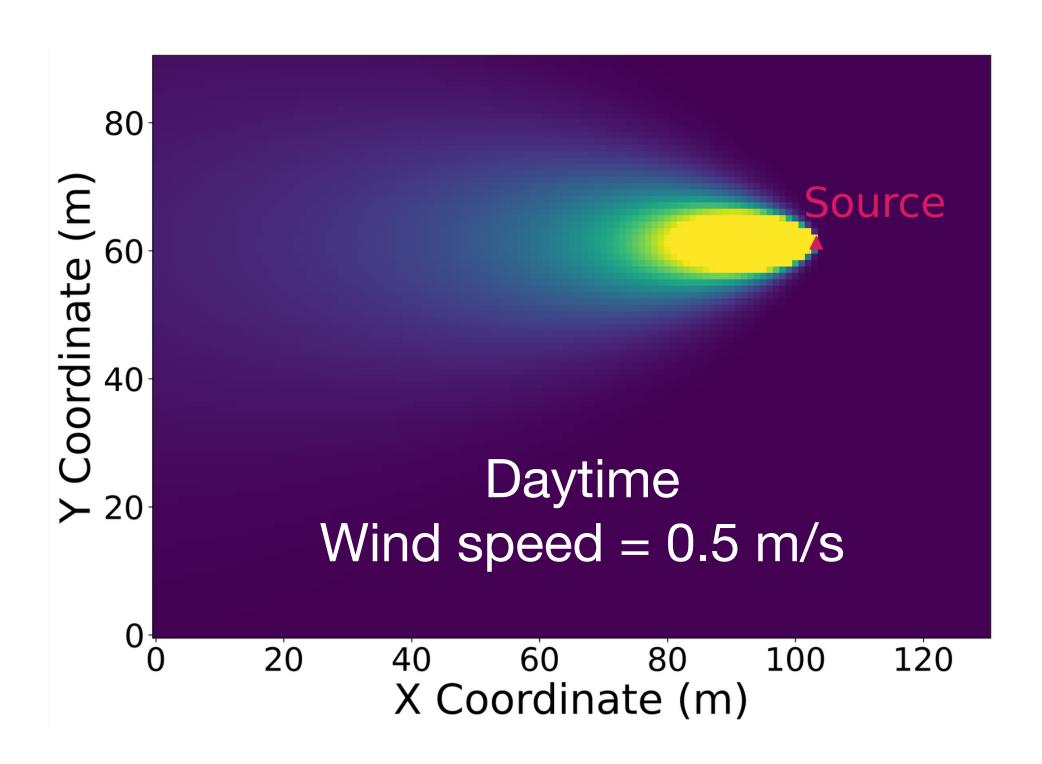


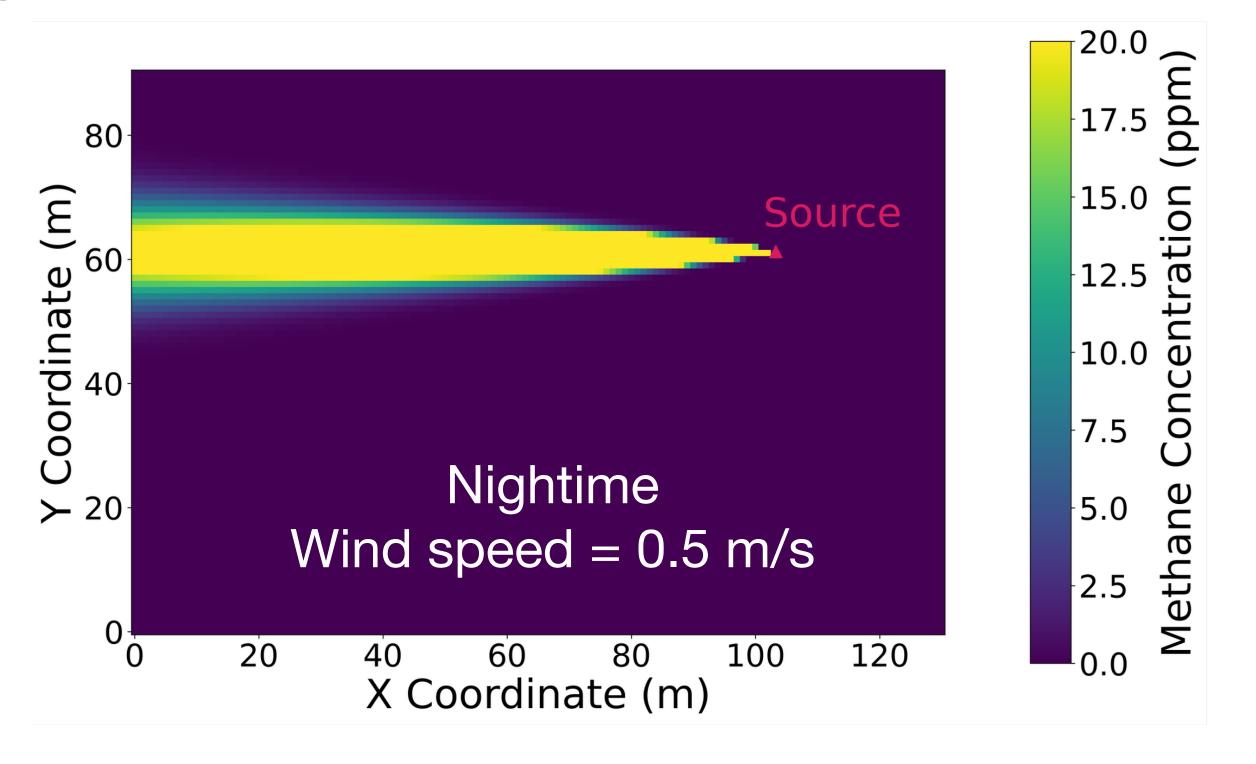


Direction #1: Better fidelity at low wind speeds

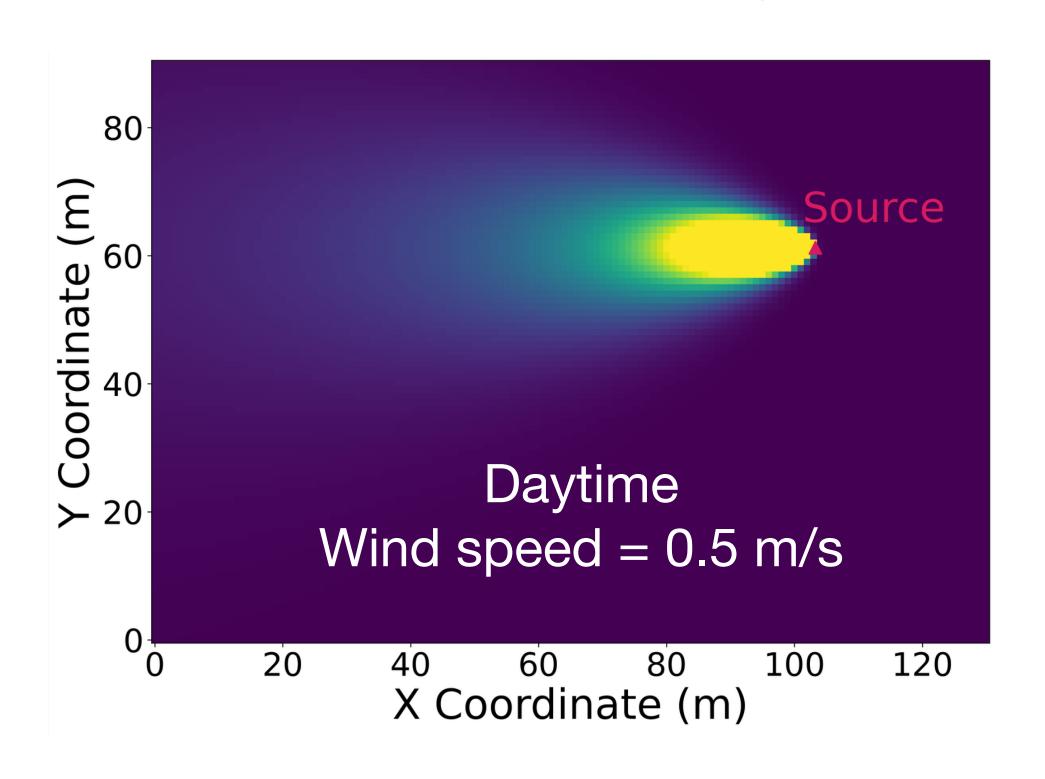


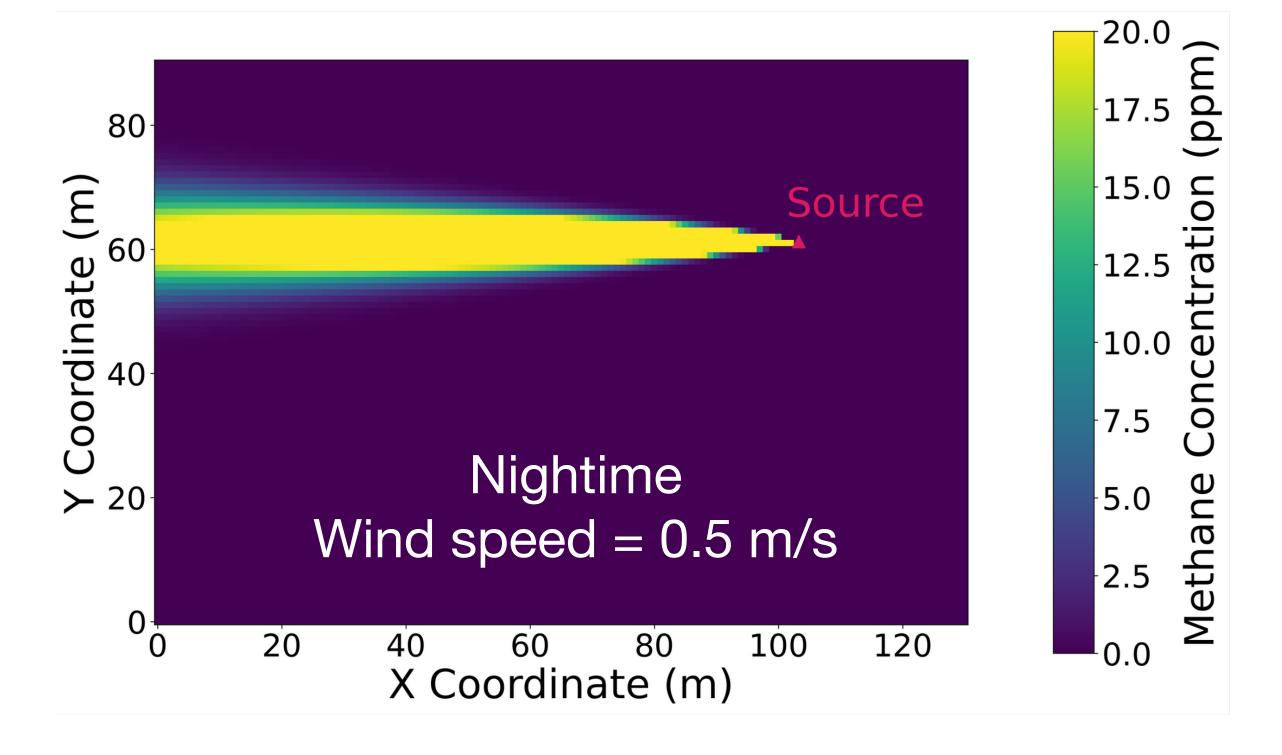
Direction #1: Better fidelity at low wind speeds





Direction #1: Better fidelity at low wind speeds



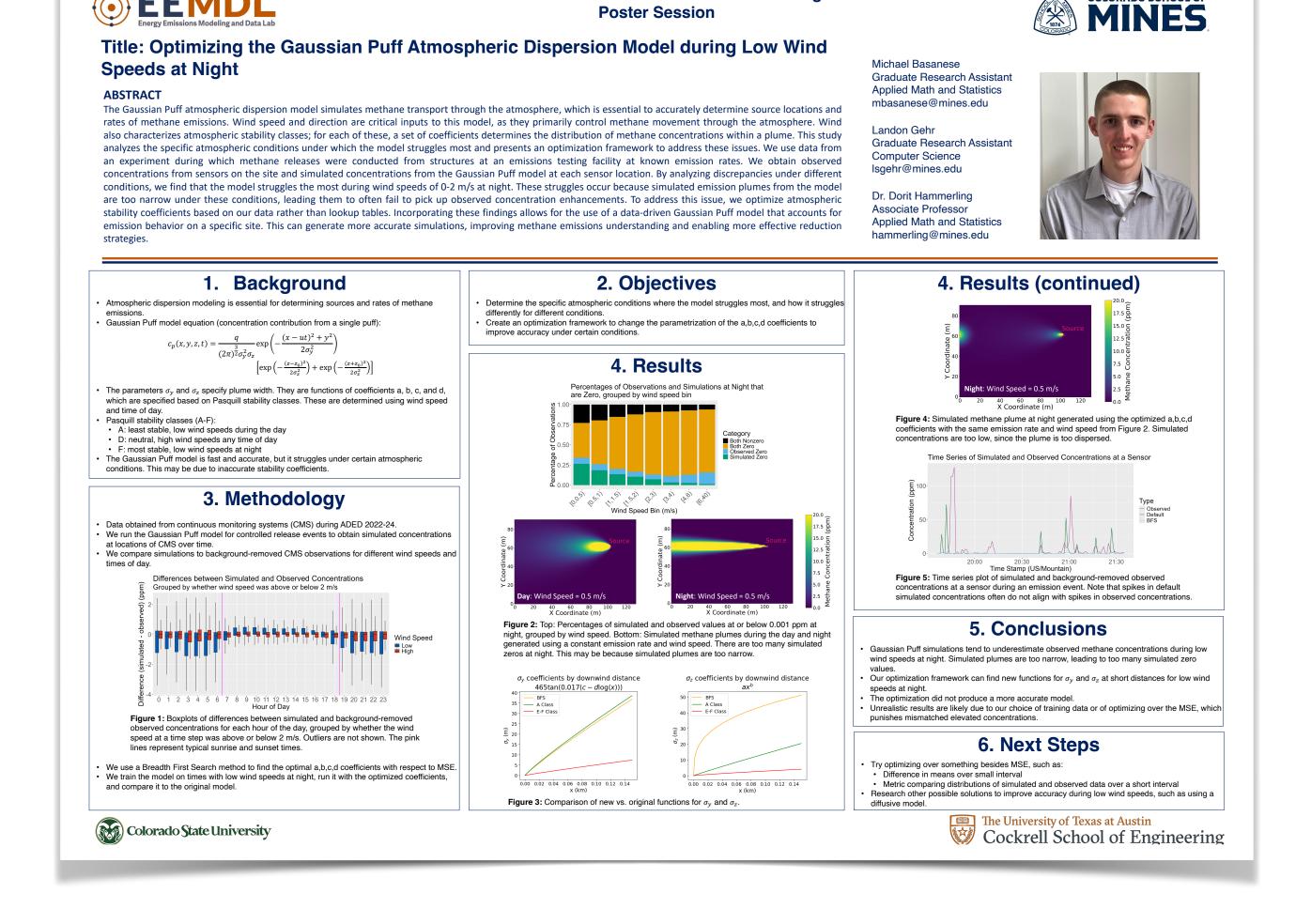


$$c_{p}(x, y, z, t, Q) = \frac{Q}{(2\pi)^{3/2} \sigma_{y}^{2} \sigma_{z}} \exp\left(-\frac{(x - ut)^{2} + y^{2}}{2\sigma_{y}^{2}}\right) \left[\exp\left(-\frac{(z - H)^{2}}{2\sigma_{z}^{2}}\right) + \exp\left(-\frac{(z + H)^{2}}{2\sigma_{z}^{2}}\right)\right]$$

Can we optimize the dispersion coefficients based on the data?

Direction #1: Better fidelity at low wind speeds

2025 EEMDL Annual Conference & Meeting



See Michael Basanese's poster for more details!

"Optimizing the Gaussian Puff Atmospheric Dispersion Model during Low Wind Speeds at Night"

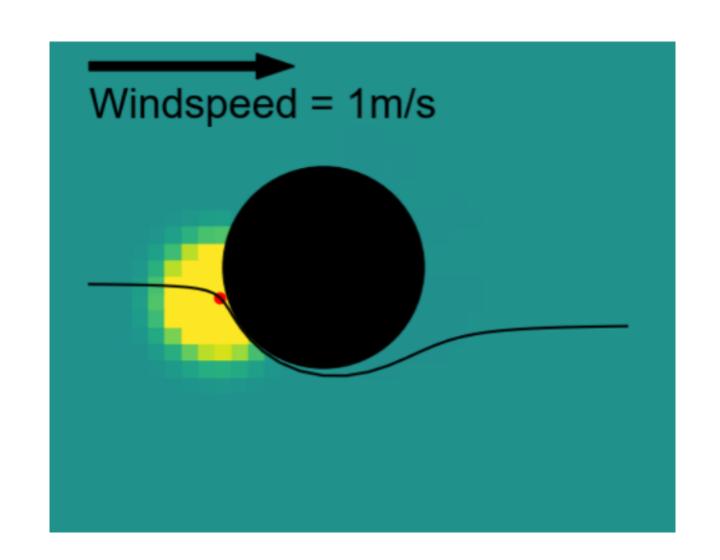
Direction #2: Account for obstacles

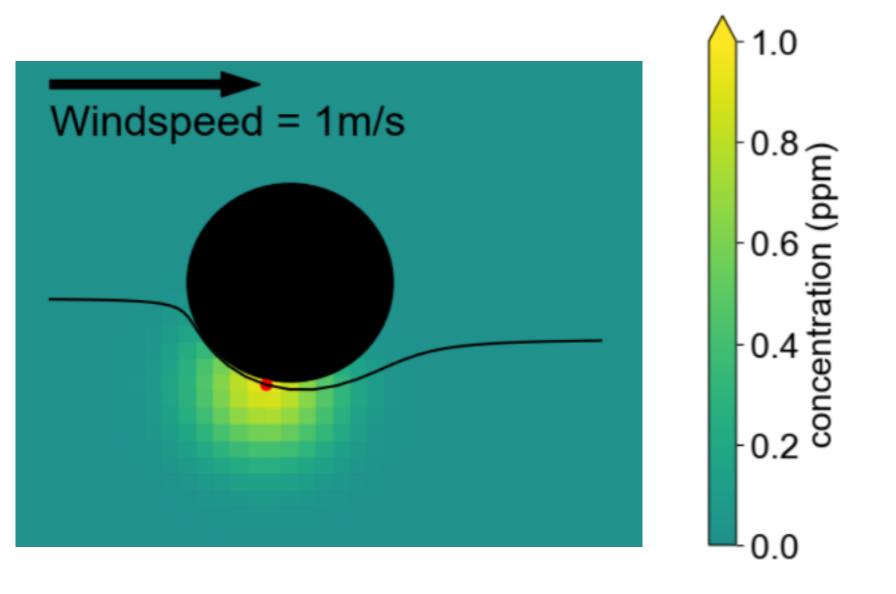
•The current Gaussian puff model is not aware of obstacles, like tanks or buildings.

Direction #2: Account for obstacles

- •The current Gaussian puff model is not aware of obstacles, like tanks or buildings.
- •Use the Method of Fundamental Solutions (MFS) to approximate the wind field, $\mu(x)$, around an obstacle

$$u(x) = \nabla \phi(x) + u_{\infty}$$
$$\phi(x) = \sum_{i=1}^{N_1} \alpha_i G_{x_i}(x)$$





Direction #2: Account for obstacles



2025 EEMDL Annual Conference & Meeting Poster Session

Title: Obstacle-aware Gaussian Atmospheric Dispersion Model

Due to environmental concerns, there is a pressing need for accurate and fast atmospheric dispersion models. The Gaussian Puff model is a model for estimating the dispersion of trace gases such as methane. The Puff model estimates methane concentrations analytically by modeling the emission source as a series of discrete and instantaneous "puffs". This allows the model to be very fast and lightweight. However, the current version of the Puff model fails to account for impenetrable obstacles on the domain, which can lead to highly inaccurate results, especially on industrial facilities which have large buildings and equipment downwind of the emission source. This research proposes an obstacle-aware implementation of the Gaussian Puff model. The obstacle-aware version will dynamically estimate the windfield accounting for obstacles on the domain, leading to more accurate modeling for the advection of each "puff" of methane. Additionally, each puff will follow a modified Gaussian equation designed to satisfy the no-penetration condition near the border of an impenetrable obstacle. Importantly, this model is completely grid-free, which allows for fast computation which is in turn crucial for real-time inference and broad applicability.

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Dr. Dorit Hammerling
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1. Background

- Fast and accurate methane dispersion models are needed to estimate emissions on industrial facilities.
- The Gaussian Puff model is accurate and very fast. However, it fails in situations with large obstacles.
- We propose an obstacle-aware version.

3. Methodology

• We use the Method of Fundamental Solutions (MFS) to approximate the windfield u(x) around an obstacle:

$$u(x) = \nabla \phi(x) + u_{\infty}$$

- The functions G_{x_i} satisfy a continuity equation, and the coefficients α are chosen to minimize penetration of wind into the surface of the obstacle. u_{∞} is a constant which
- Additionally, the Method of Fundamental Solutions is used to modify every puff at each timestep.

$$c_{MFS}(\mathbf{x}, t) = c(\mathbf{x}, t) + \sum_{i=1}^{N_1} \alpha_i f_{\mathbf{x_i}}(\mathbf{x}, t)$$

represents the windspeed coming from a point at infinity.

• Here c (in ppm) is the original Gaussian puff equation, and f_{∞} are functions which also take a Gaussian form.

2. Objectives

- Model the windfield around an arbitrarily shaped impenetrable obstacle.
 Modify the dispersion of methane to account for the dispersion of the dispersion of methane to account for the dispersion of methane to account for the dispersion of the dispersi
- Modify the dispersion of methane to account for the obstacle.

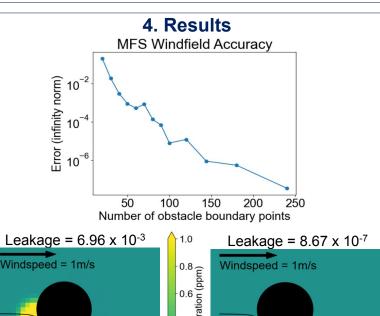


Figure 1: Accuracy and leakage. Top: accuracy of the MFS solution for windfield compared to an analytic solution. Bottom: 2D slice of methane concentration field for a single puff, at 2 different timesteps. Black lines represent the path of the puff.

5. Conclusions

- This framework can analytically estimate methane concentration from a single puff as a function of space and time
- Accuracy can be improved by increasing the number of source points, which comes at the cost of computational complexity
- This method never calculates 3-D integrals, only 1-D and 2-D. This results in very fast computation times.

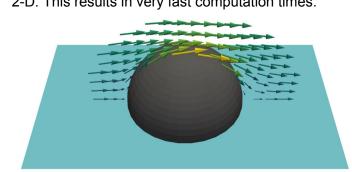


Figure 2: Wind speed and direction at points around a spherical obstacle, estimated using the MFS.

6. Next Steps

- The methodology here works for a single puff, we still need an algorithm for integrating over many puffs to form a complete dispersion model.
- Accuracy of the model will be evaluated by comparing to real observations at testing centers and operational facilities

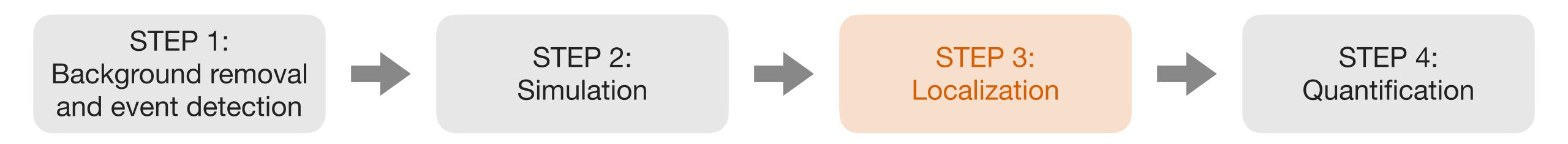


See Andres Pruet's poster for more details! (presented by Michael)

"Obstacle-aware Gaussian Atmospheric Dispersion Model"



Open source framework for solving inverse problem









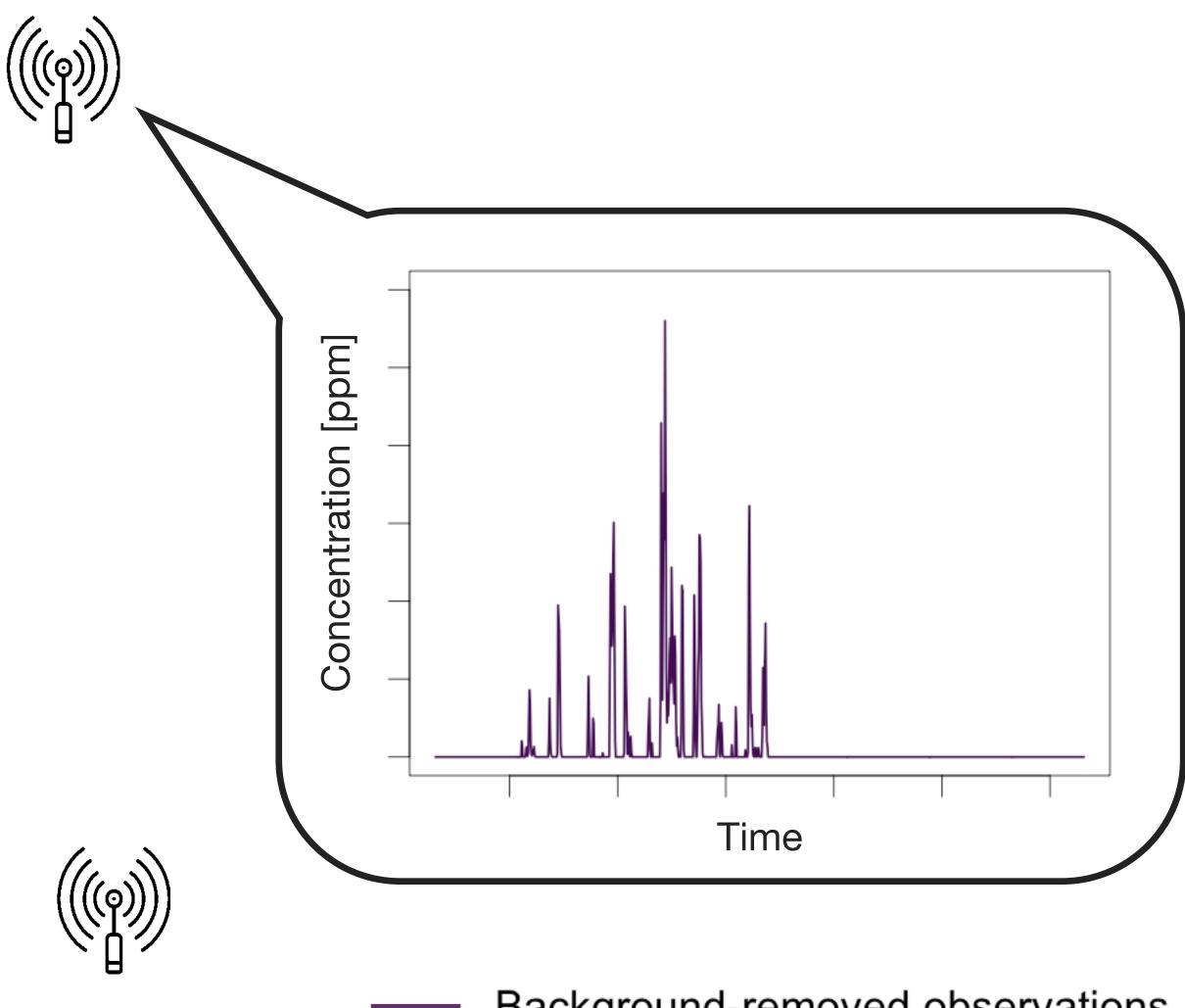




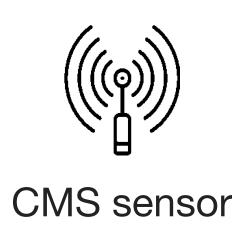




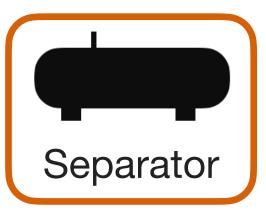




Background-removed observations



Simulation emission source





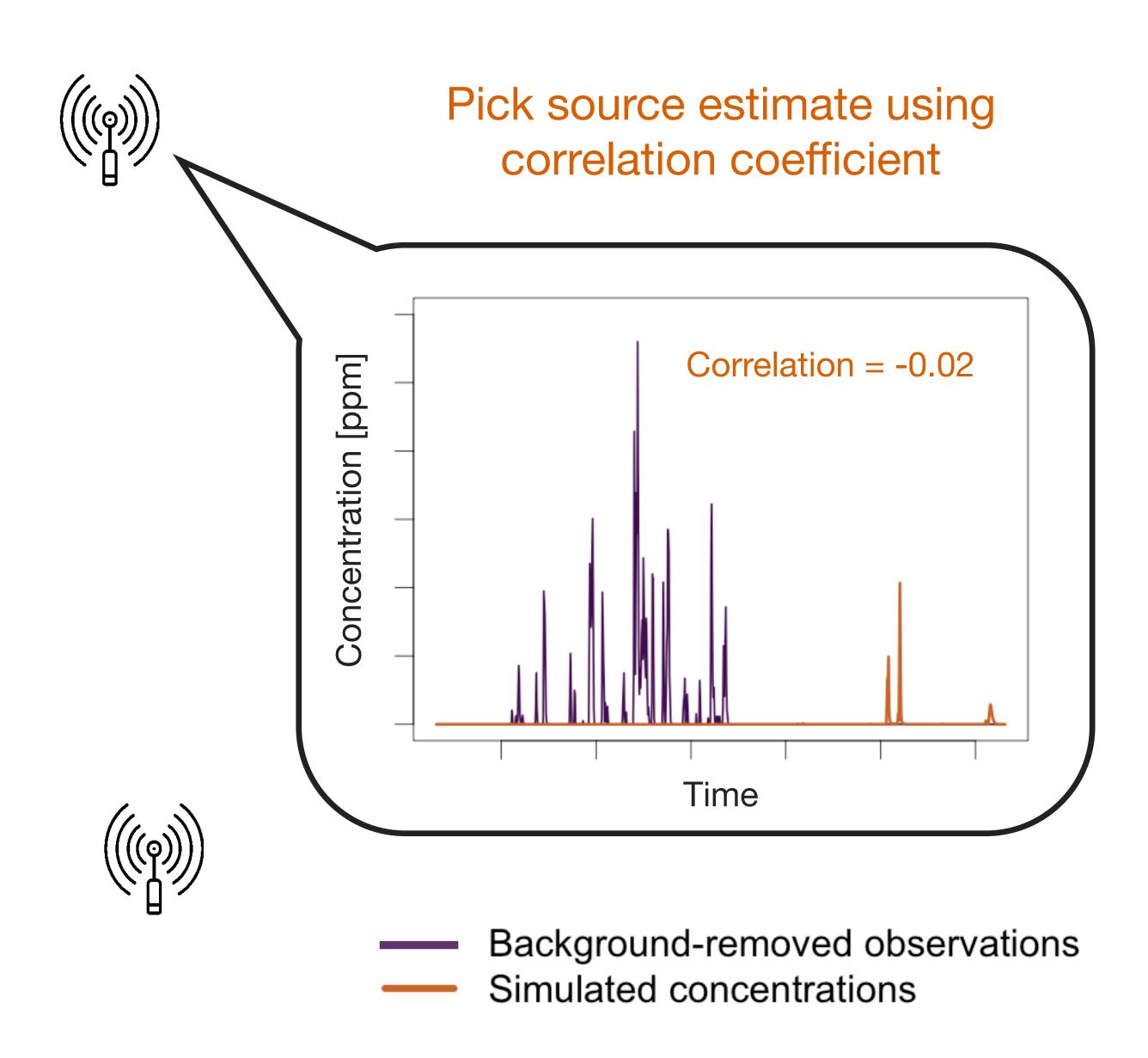




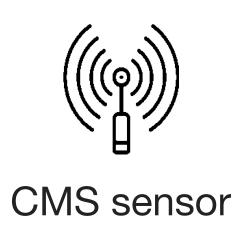








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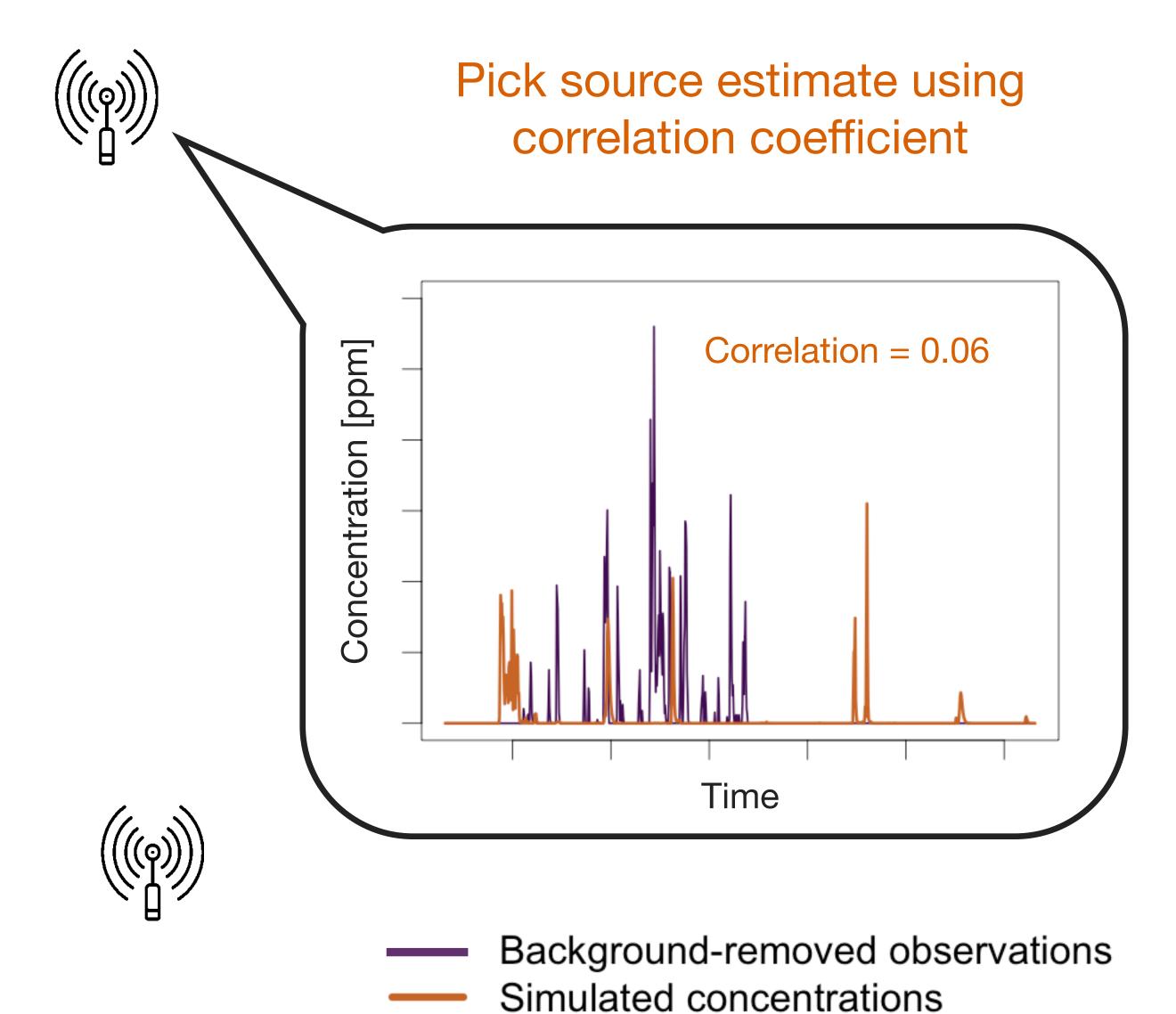






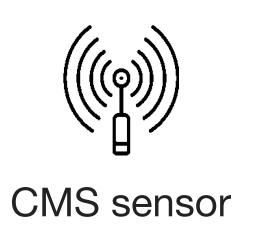


Simulation emission source



Wind direction







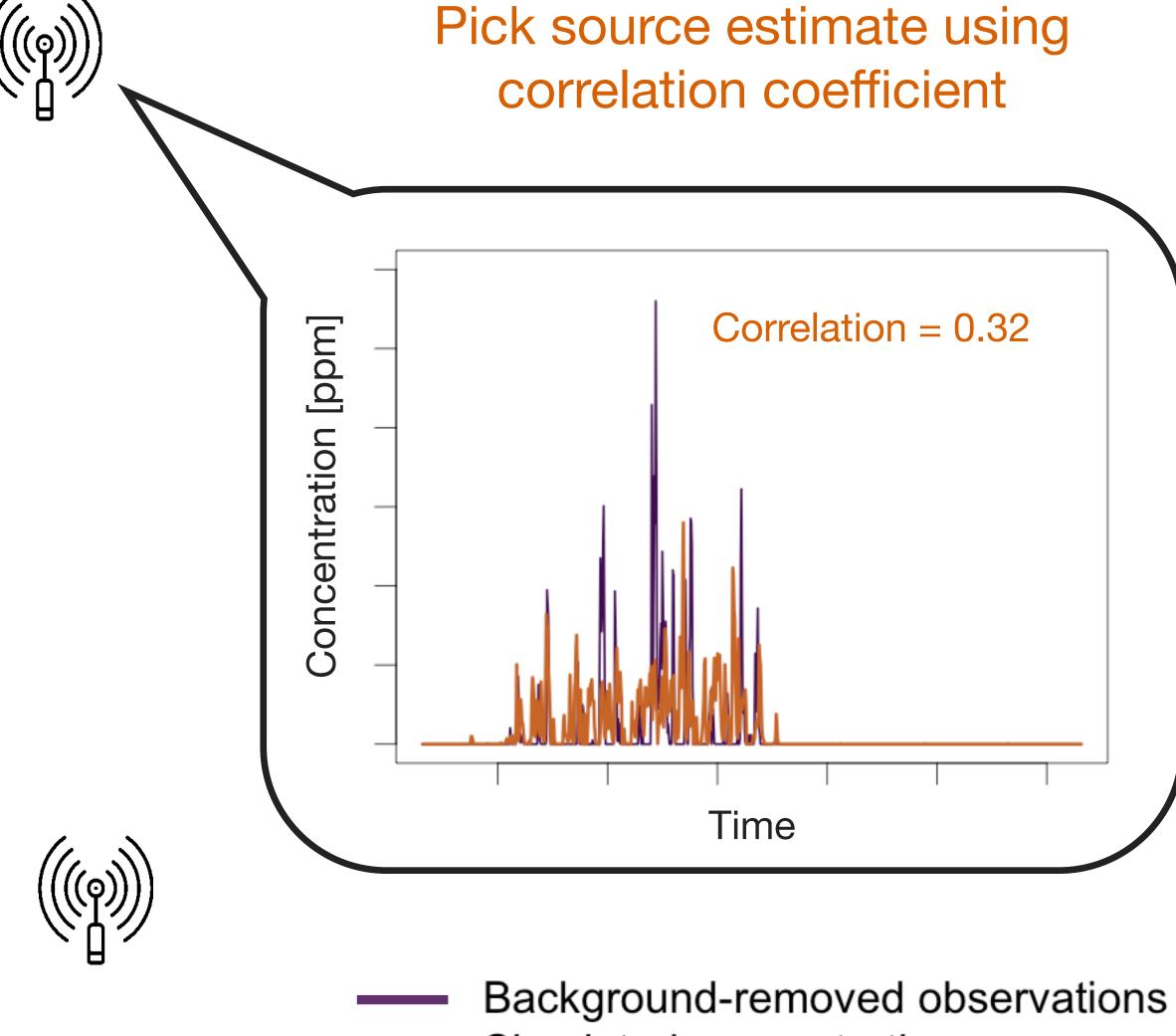




Simulation emission source





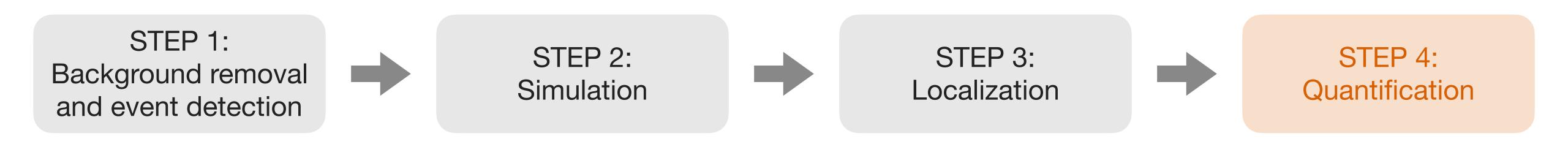


Wind direction



Simulated concentrations

Open source framework for solving inverse problem



Simulation is a linear function of emission rate

Volume of methane contained in puff *p*

$$c_{p}(x, y, z, t, Q) = Q \frac{1}{(2\pi)^{3/2} \sigma_{y}^{2} \sigma_{z}} \exp\left(-\frac{(x - ut)^{2} + y^{2}}{2\sigma_{y}^{2}}\right) \left[\exp\left(-\frac{(z - H)^{2}}{2\sigma_{z}^{2}}\right) + \exp\left(-\frac{(z + H)^{2}}{2\sigma_{z}^{2}}\right)\right]$$

Concentration contribution of puff p

$$c(x, y, z, t, Q) = \sum_{p=1}^{P} c_p(x, y, z, t, Q)$$

Total concentration at (x, y, z, t)

Simulation is a linear function of emission rate

Volume of methane contained in puff p

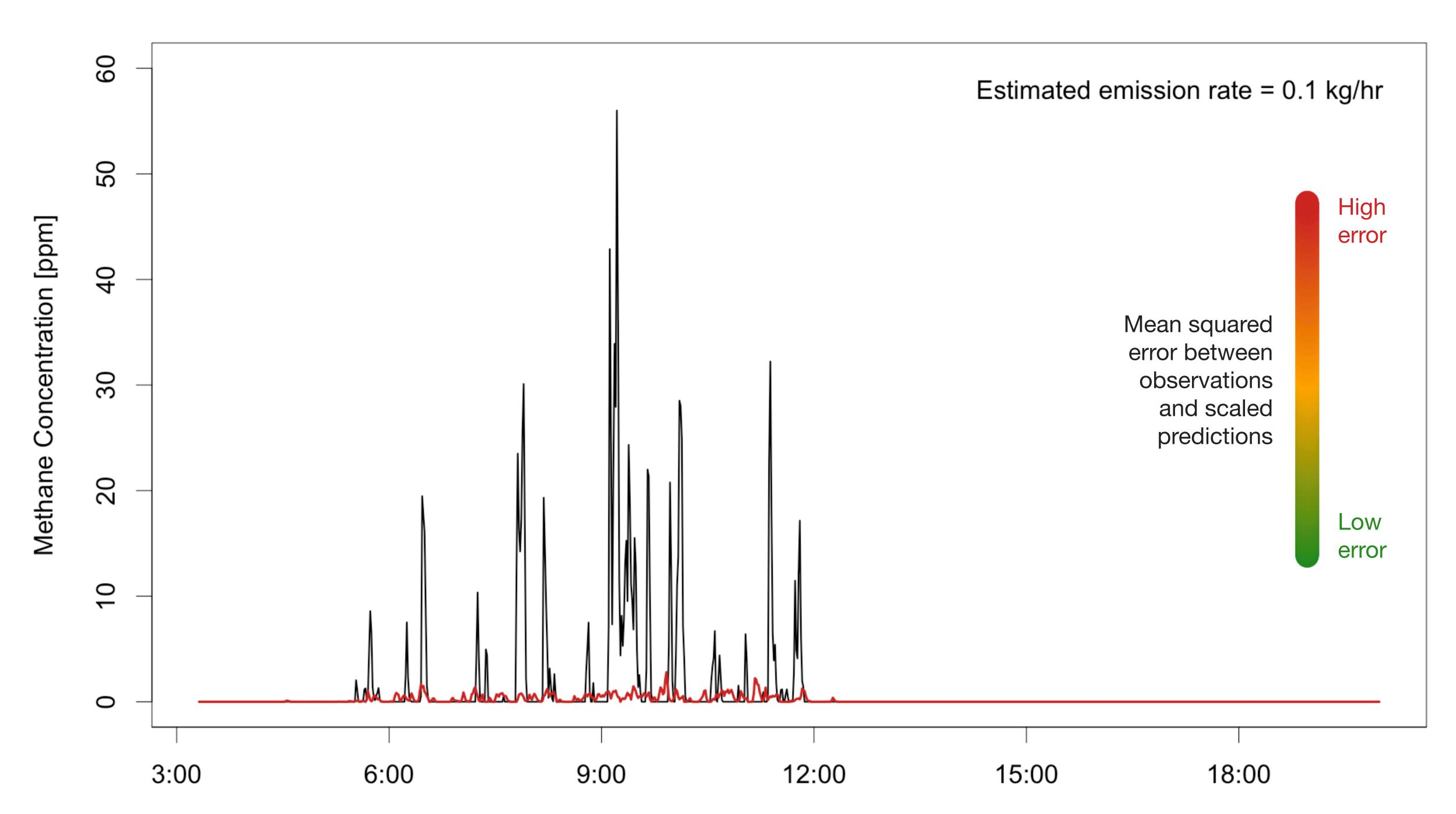
$$c_{p}(x, y, z, t, Q) = Q \frac{1}{(2\pi)^{3/2} \sigma_{y}^{2} \sigma_{z}} \exp\left(-\frac{(x - ut)^{2} + y^{2}}{2\sigma_{y}^{2}}\right) \left[\exp\left(-\frac{(z - H)^{2}}{2\sigma_{z}^{2}}\right) + \exp\left(-\frac{(z + H)^{2}}{2\sigma_{z}^{2}}\right)\right]$$

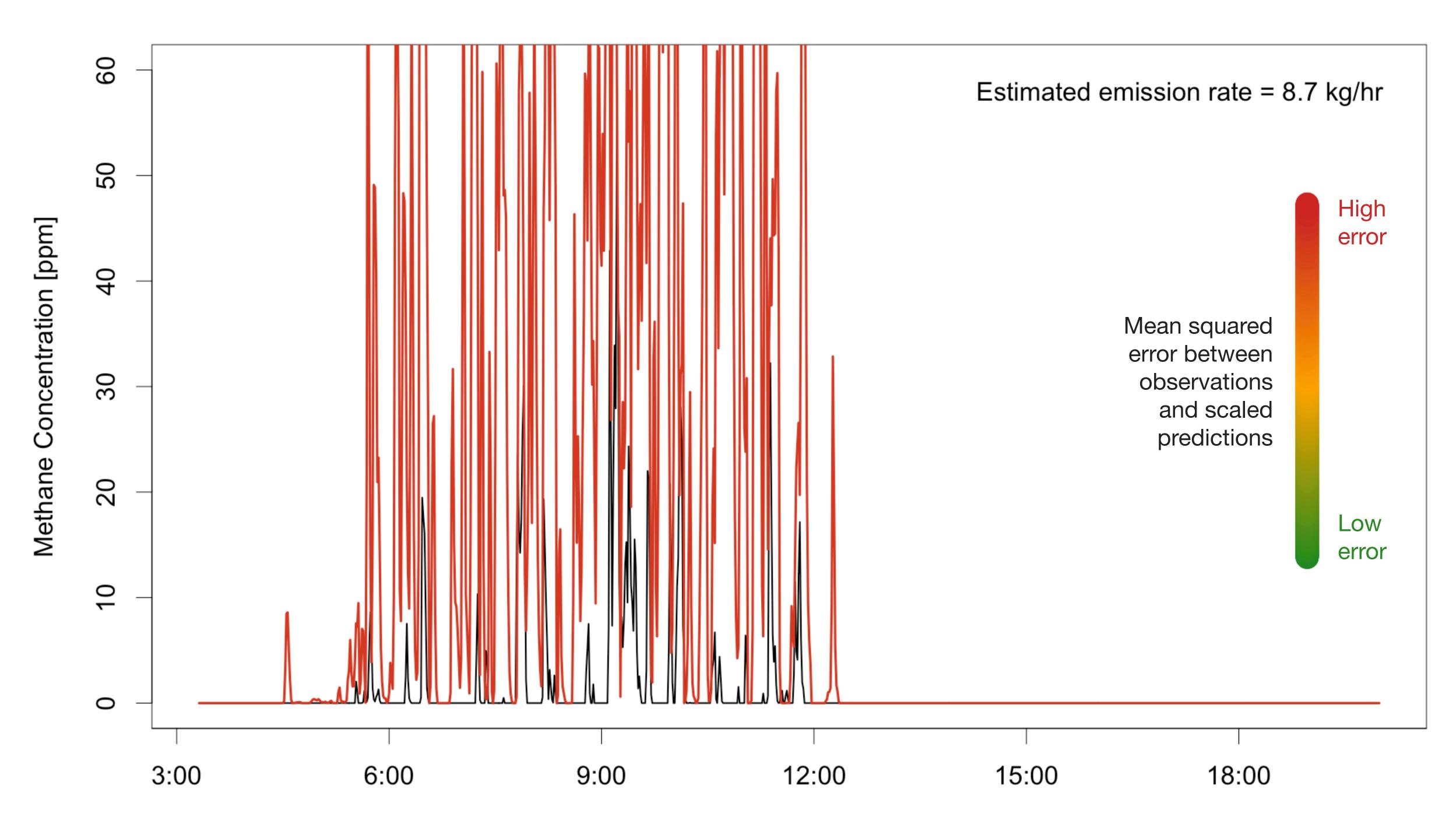
Concentration contribution of puff p

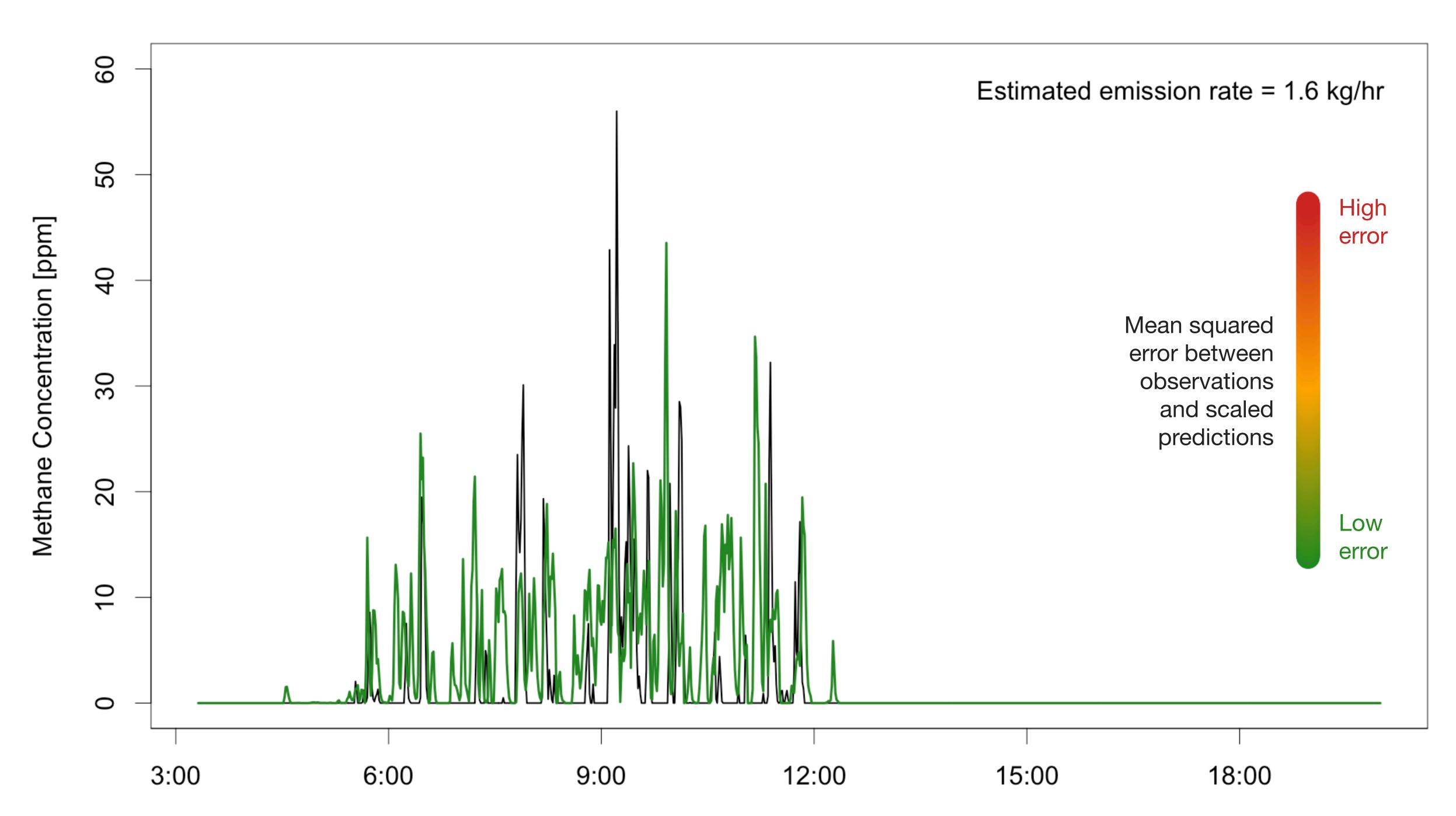
at (x, y, z, t)

$$c(x,y,z,t,Q) = \sum_{p=1}^{P} c_p(x,y,z,t,Q)$$
 Total concentration

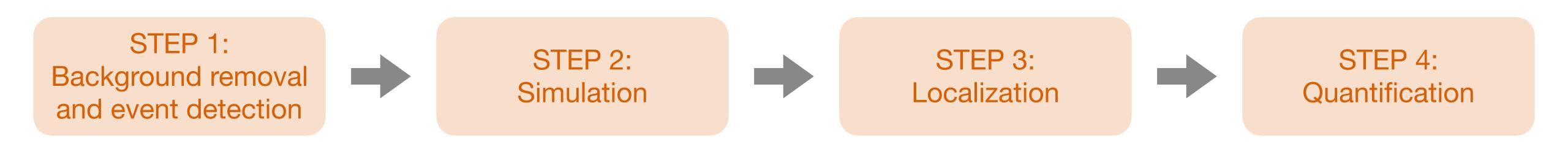
Concentration data $c(x, y, z, t, Q) = \sum_{p=1}^{P} c_p(x, y, z, t, Q)$ $\hat{Q} = \underset{Q}{\operatorname{argmin}} \left\{ \frac{1}{n} \sum_{t=1}^{n} \left(d(x, y, z, t) - c(x, y, z, t, Q) \right)^2 \right\}$ Simulated **Emission rate** concentrations estimate



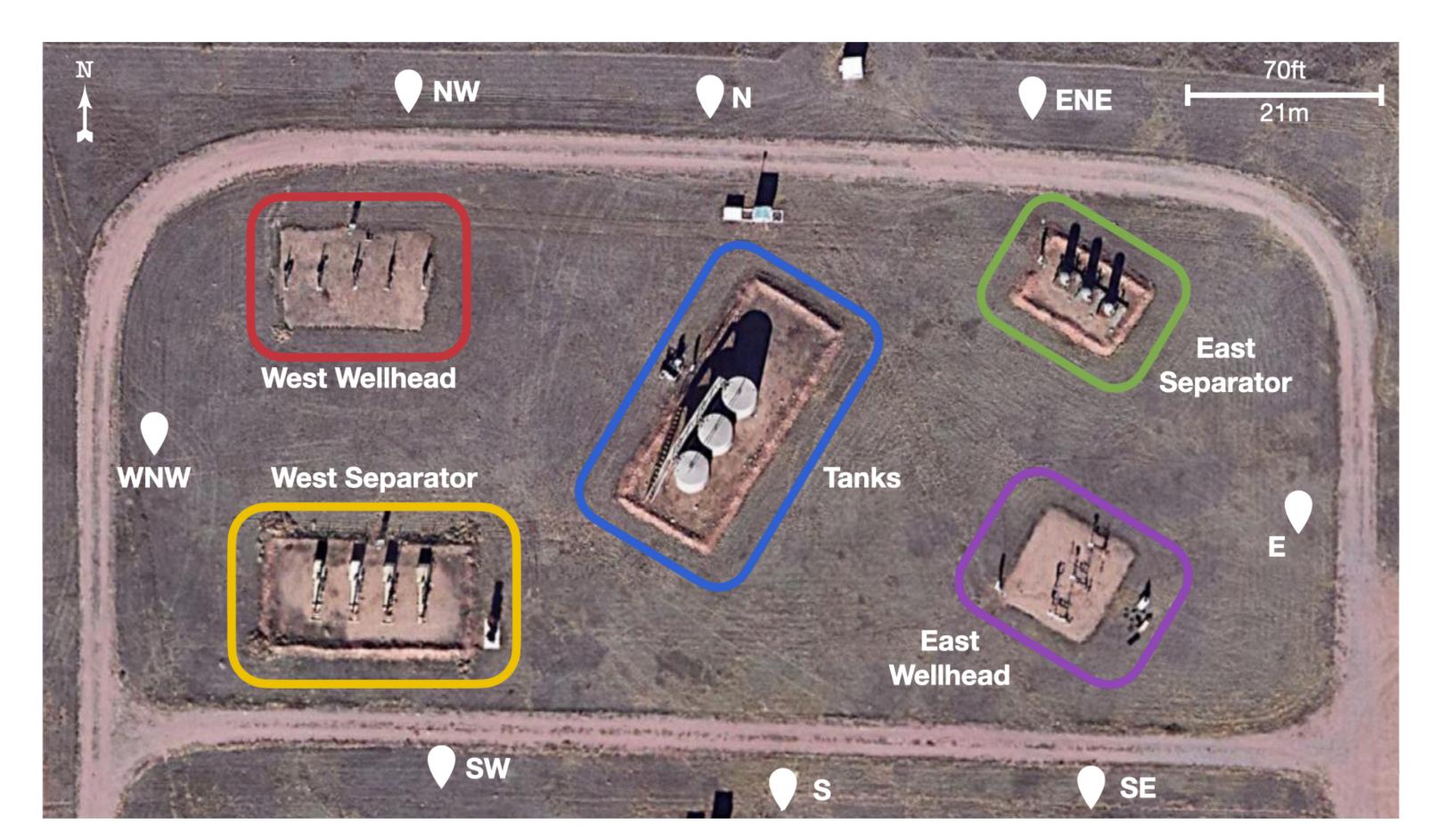




Open source framework for solving inverse problem



Evaluation on single-source controlled releases



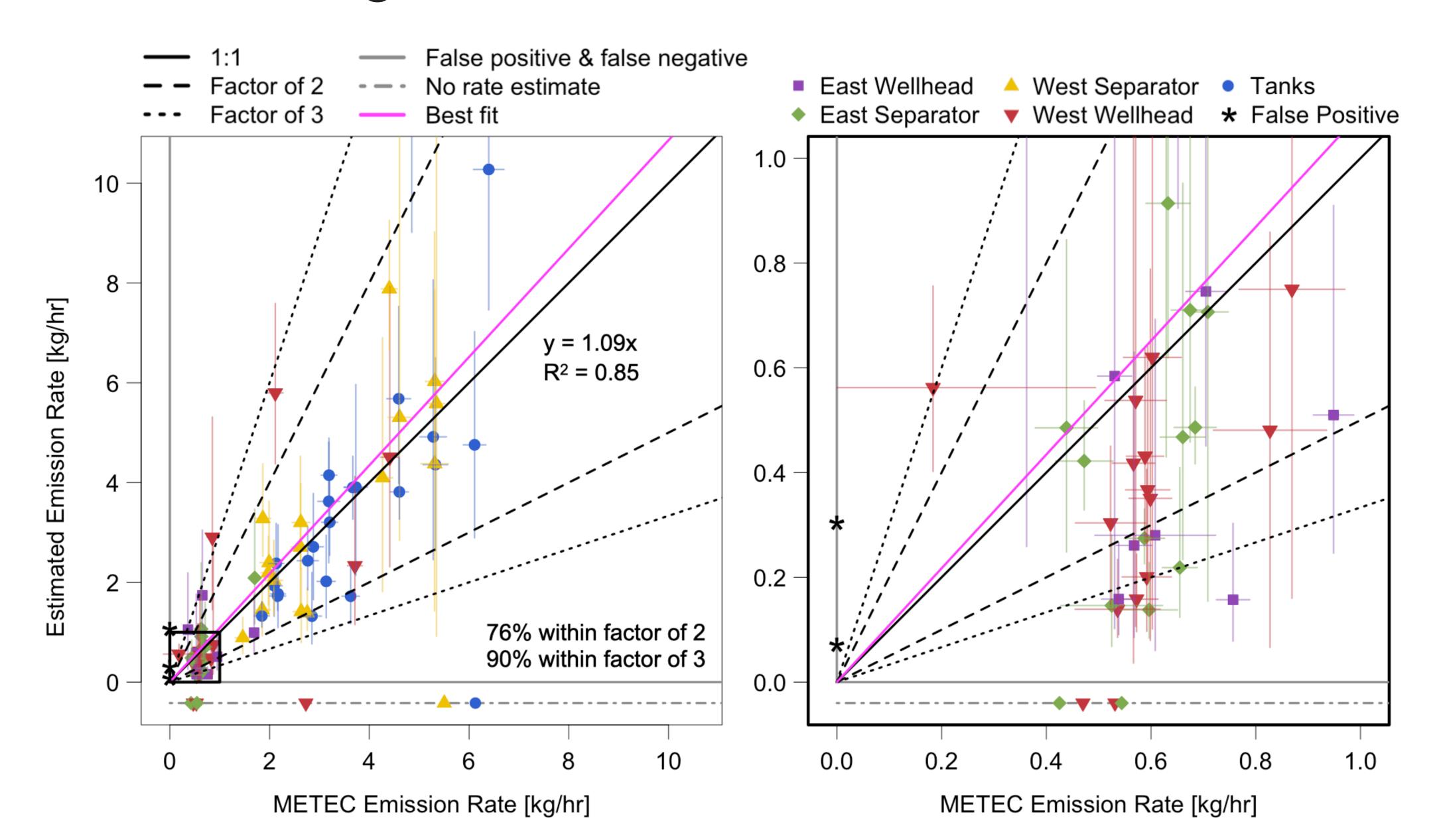
Methane Emissions Technology Evaluation Center (METEC)

85 single-source controlled releases

Emission rates range from **0.2** to **6.4** kg/hr

Emission durations range from **0.5** to **8.25** hours

Evaluation on single-source controlled releases



Part 1: Single-source emission detection, localization, and quantification

Detection, localization, and quantification of single-source methane emissions on oil and gas production sites using point-in-space continuous monitoring systems.

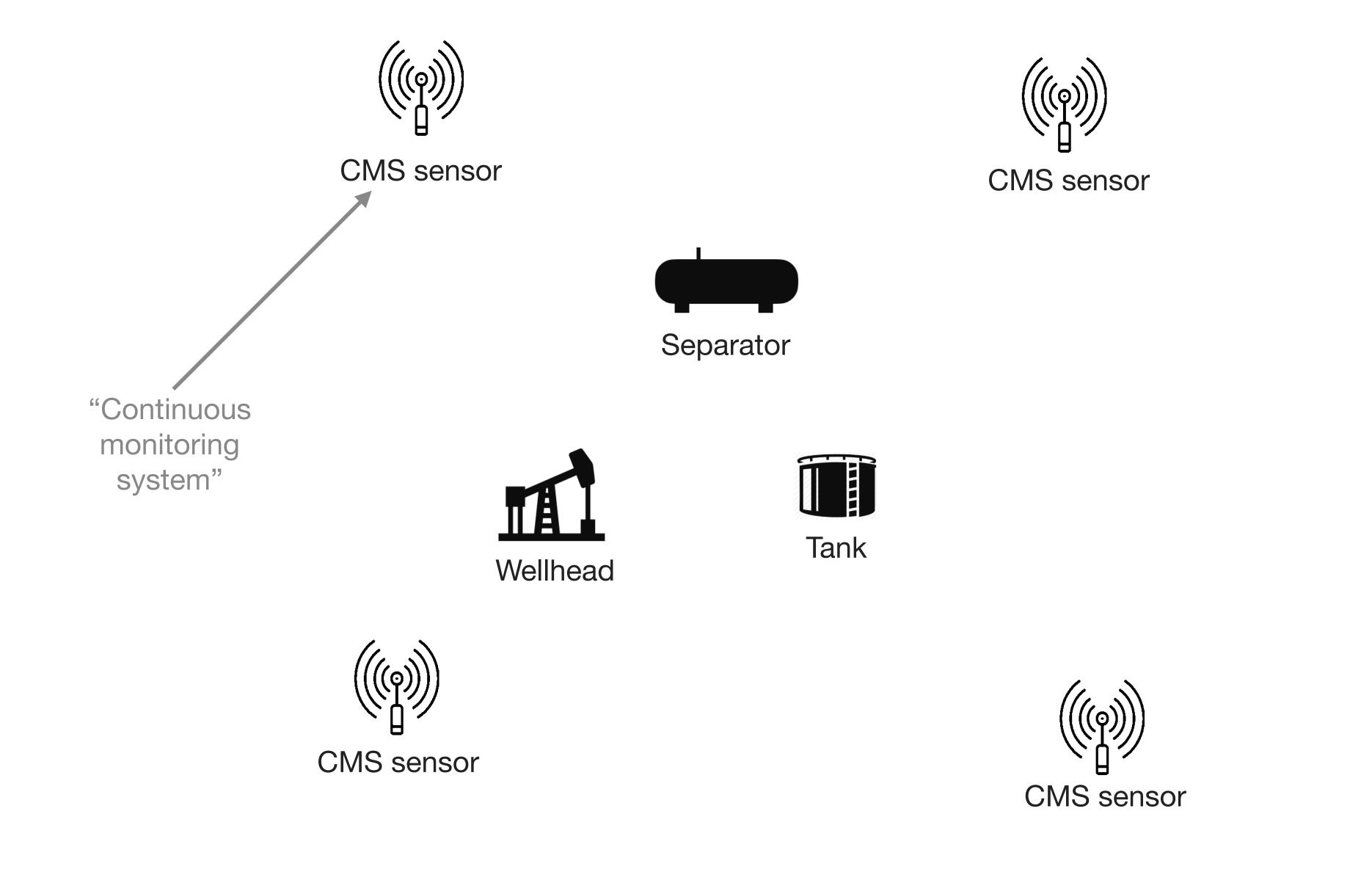
William Daniels, Meng Jia, Dorit Hammerling. *Elementa: Science of the Anthropocene*, 12(1), 00110, (2024).



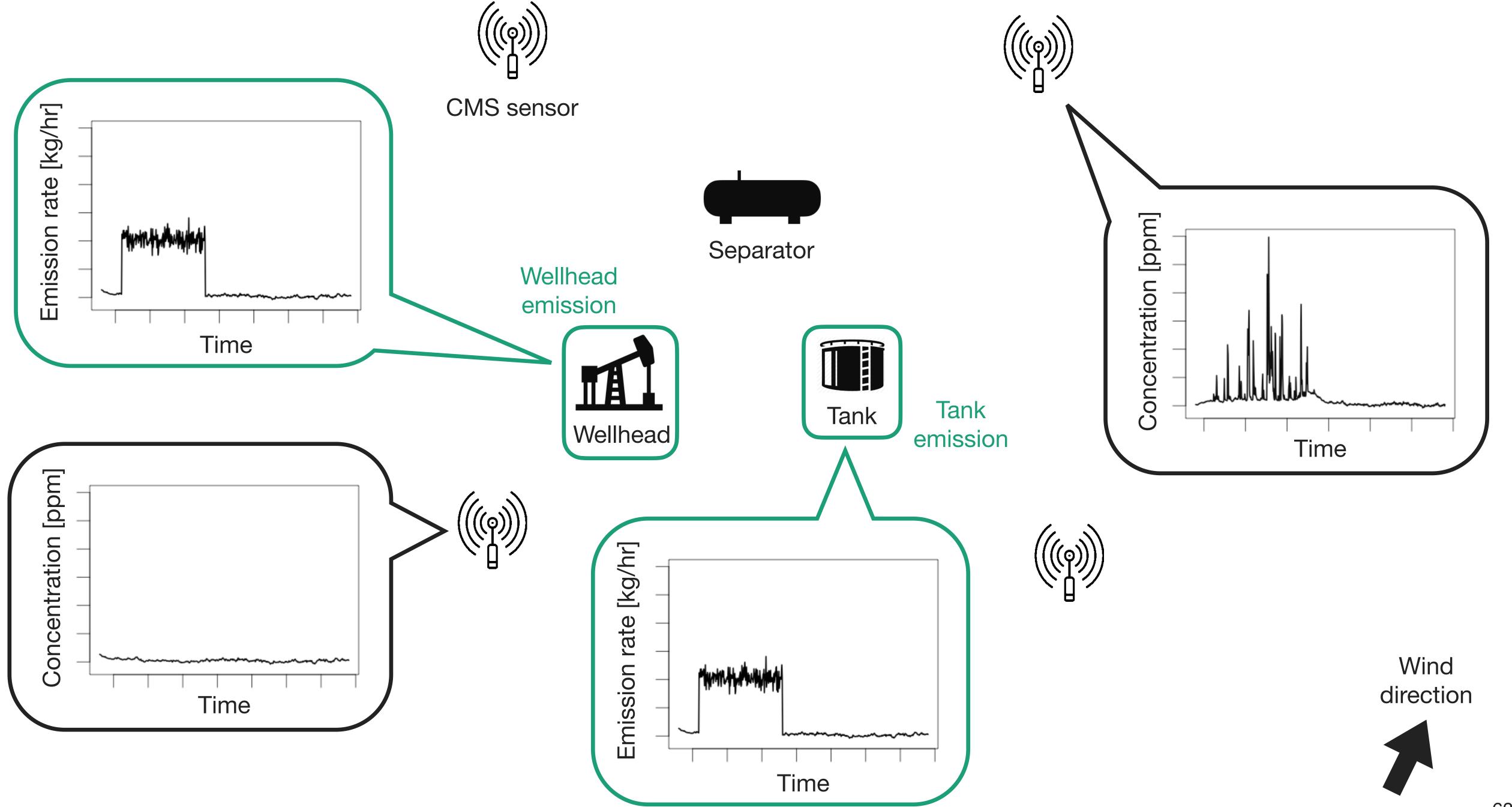


A fast and lightweight implementation of the Gaussian puff model for near-field atmospheric transport of trace gasses.

Meng Jia, Ryker Fish, William Daniels, Brennan Sprinkle, Dorit Hammerling. *Scientific Reports*, 15, 18710 (2025).



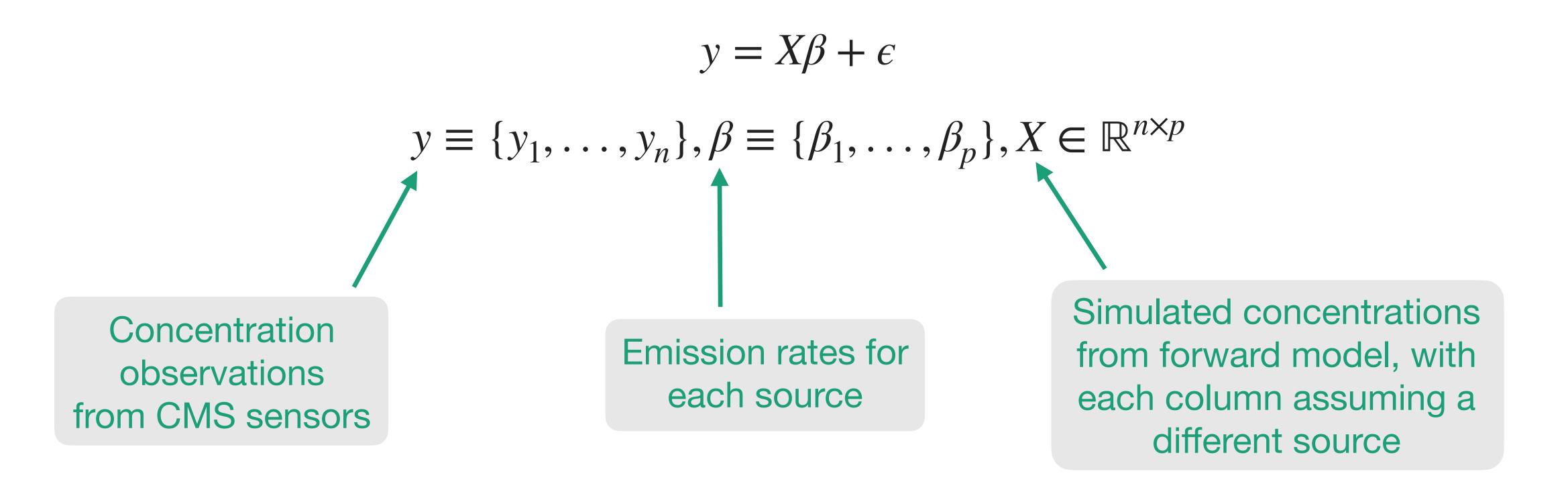
The multi-source continuous monitoring inverse problem



Assume a multiple linear regression model at the data level

n = number of observations

p = number of potential sources



n = number of observationsp = number of potential sources

Assume a multiple linear regression model at the data level

$$y = X\beta + \epsilon$$

$$y \equiv \{y_1, \dots, y_n\}, \beta \equiv \{\beta_1, \dots, \beta_p\}, X \in \mathbb{R}^{n \times p}$$

Assume that the errors $\epsilon \equiv \{\epsilon_1, \dots, \epsilon_n\}$ are are identically distributed, Gaussian, and autocorrelated such that

$$\epsilon \sim N(0, \sigma^2 R)$$

n = number of observations

Assume a multiple linear regression model at the data level

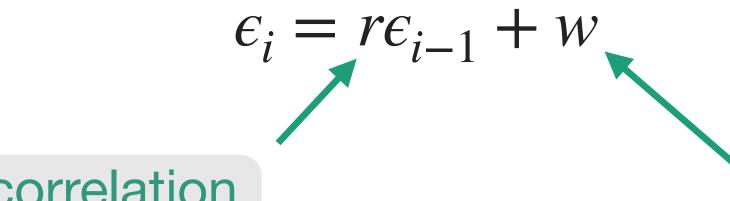
p = number of potential sources

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$$y \equiv \{y_1, \dots, y_n\}, \beta \equiv \{\beta_1, \dots, \beta_p\}, X \in \mathbb{R}^{n \times p}$$

Assume that the errors $\epsilon \equiv \{\epsilon_1, \dots, \epsilon_n\}$ are are identically distributed, Gaussian, and autocorrelated such that

$$\epsilon \sim N(0, \sigma^2 R)$$

Let the errors follow an AR(1) process such that



Autocorrelation coefficient

Gaussian white noise

n = number of observations

p = number of potential sources

Assume a multiple linear regression model at the data level

$$y = X\beta + \epsilon$$
$$y \equiv \{y_1, \dots, y_n\}, \beta \equiv \{\beta_1, \dots, \beta_p\}, X \in \mathbb{R}^{n \times p}$$

Assume that the errors $\epsilon \equiv \{\epsilon_1, \dots, \epsilon_n\}$ are are identically distributed, Gaussian, and autocorrelated such that

$$\epsilon \sim N(0, \sigma^2 R)$$

Let the errors follow an AR(1) process such that

$$\epsilon_i = r\epsilon_{i-1} + w$$

This gives us: $y \sim N(X\beta, \sigma^2 R)$

Given an AR(1) process for ϵ , the correlation matrix is

$$R = \begin{bmatrix} 1 & r & r^2 & \dots & r^{n-1} \\ r & 1 & r & \dots & \vdots \\ r^2 & r & 1 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ r^{n-1} & \dots & \dots & 1 \end{bmatrix}$$

n = number of observations

p = number of potential sources

Given an AR(1) process for ϵ , the correlation matrix is

n = number of observationsp = number of potential sources

$$R = \begin{bmatrix} 1 & r & r^2 & \dots & r^{n-1} \\ r & 1 & r & \dots & \vdots \\ r^2 & r & 1 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ r^{n-1} & \dots & \dots & 1 \end{bmatrix}$$

which has closed form expressions for the inverse and determinant:

$$R^{-1} = \frac{1}{(1-r^2)} \begin{bmatrix} 1 & -r & 0 & \dots & 0 \\ -r & 1+r^2 & -r & \dots & \vdots \\ 0 & -r & 1+r^2 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & 1 \end{bmatrix}$$
 and
$$|R| = (1-r^2)^{n-1}$$

Data-level: $y = X\beta + \epsilon$ $\epsilon \sim N(0, \sigma^2 R)$

$$\epsilon \sim N(0, \sigma^2 R)$$

n = number of observations p = number of potential sources

The remainder of the hierarchy takes the following form

Spike-and-slab prior allows samples to be identically zero

 $lacksquare eta_i \sim egin{cases} 0, & z_i = 0 \ \exp(au_i^2 \sigma^2), & z_i = 1 \end{pmatrix}$

 $z_i \sim \text{Bernoulli}(\theta_i)$

$$z_i = 0$$

"Slab" component is non-negative

Proportion of samples where $z_i = 1$ gives posterior probability that

source i is

emitting

 $\theta_i \sim \text{Beta}(a_i, b_i) \blacktriangleleft$

 $\tau_i^2 \sim \text{Inv-Gamma}(c_i, d_i) \blacktriangleleft$

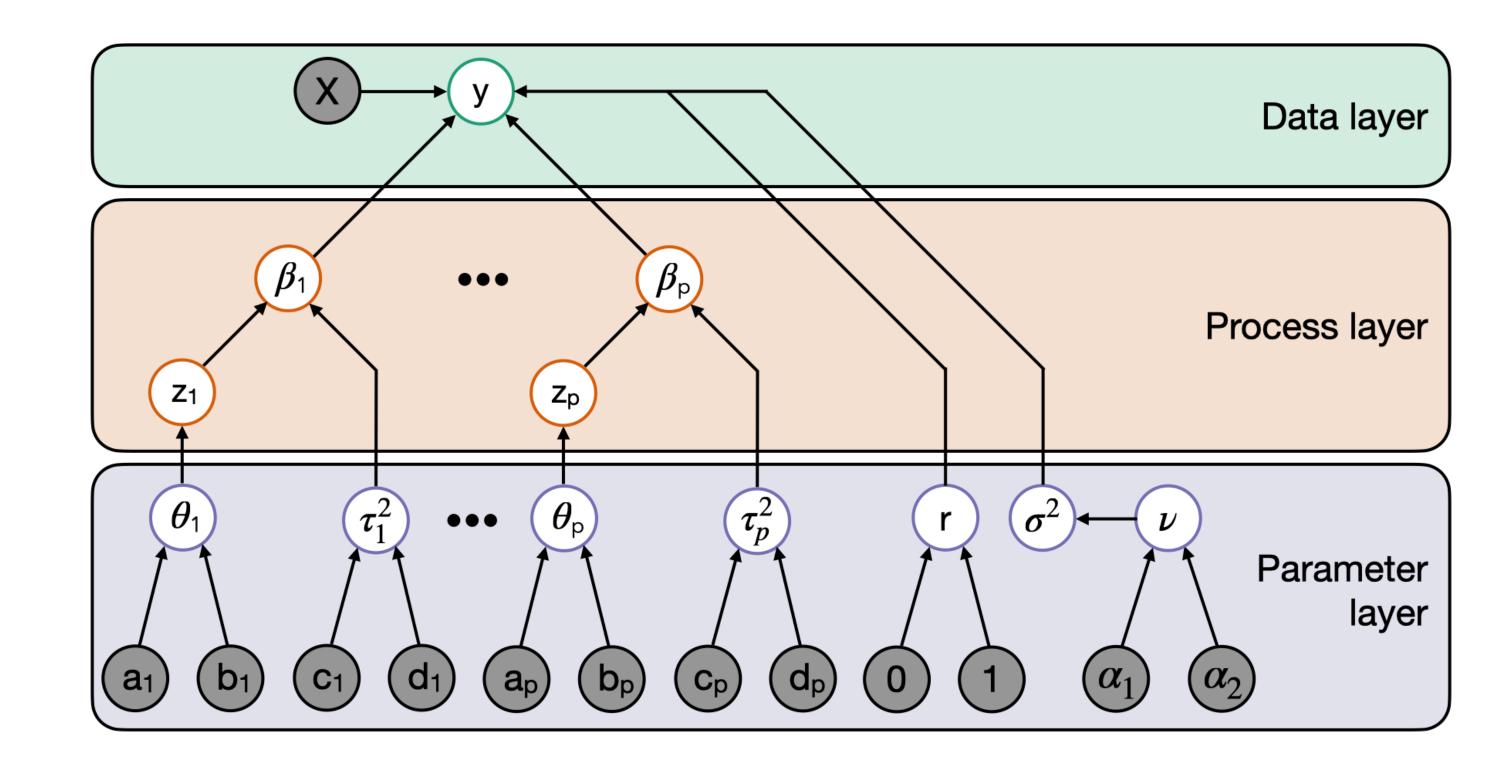
 $\sigma^2 \sim \text{Inv-Gamma}(\nu/2, \nu/2)$

 $\nu \sim \text{Inv-Gamma}(\alpha_1, \alpha_2)$

 $r \sim \text{Uniform}(0,1)$

ai, bi, ci, di can contain operator insight

$$eta_i \sim egin{cases} 0, & z_i = 0 \ \operatorname{Exp}(au_i^2 \sigma^2), & z_i = 1 \end{cases}$$
 $z_i \sim \operatorname{Bernoulli}(heta_i)$
 $heta_i \sim \operatorname{Beta}(a_i, b_i)$
 $au_i^2 \sim \operatorname{Inv-Gamma}(c_i, d_i)$
 $\sigma^2 \sim \operatorname{Inv-Gamma}(
u/2,
u/2)$
 $u \sim \operatorname{Inv-Gamma}(\alpha_1, \alpha_2)$
 $u \sim \operatorname{Uniform}(0, 1)$



Sampling from the posterior

We can derive Gibbs updates for all parameters except ν .

$$\theta_i | \xi \sim \text{Beta}(z_i + a_i, 1 - z_i + b_i)$$

$$\sigma^2 | \xi \sim \text{Inv-Gamma}\left(\frac{\nu}{2} + \frac{n}{2}, \frac{\nu}{2} + \frac{1}{2}(y - X\beta)^T R^{-1}(y - X\beta)\right)$$

$$r | \xi \sim \begin{cases} \mathcal{N}(X\beta, \sigma^2 R) & 0 < r < 1\\ 0 & \text{otherwise} \end{cases}$$

$$\tau_i^2 | \xi \sim \text{Inv-Gamma}\left(z_i + c_i, \frac{\beta_i}{\sigma^2} + d_i\right)$$

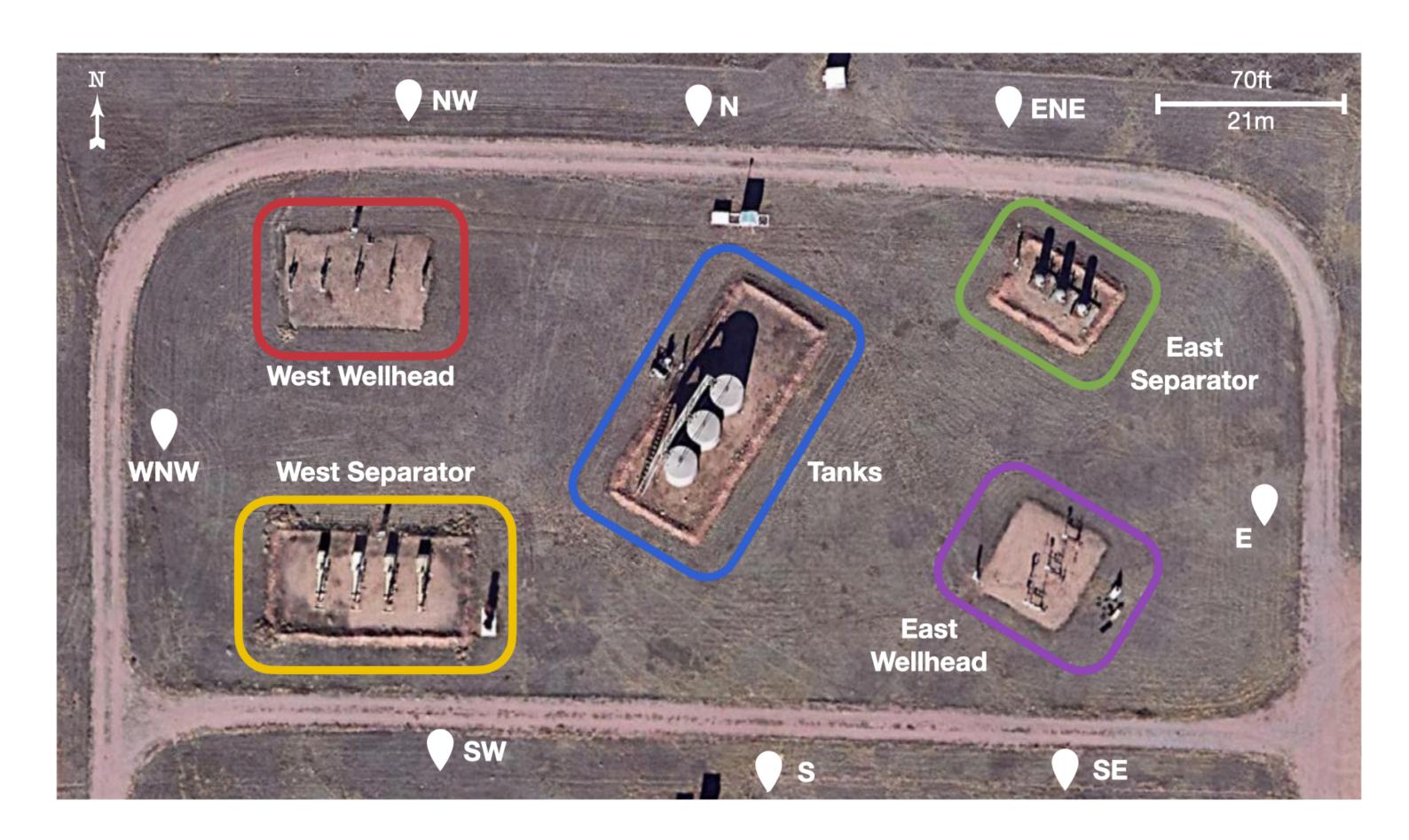
Iterative samples from each full conditional gives you samples from the joint posterior!

$$\beta_i | \xi \sim \begin{cases} 0 & z_i = 0 \\ \mathcal{N} \left(\left(\frac{X^T R^{-1} X}{\sigma^2} \right)^{-1} \left(\frac{X^T R^{-1} y}{\sigma^2} - \frac{e_i}{\tau_i^2 \sigma^2} \right), \left(\frac{X^T R^{-1} X}{\sigma^2} \right)^{-1} \right) & z_i = 1 \end{cases}$$

$$z_{i} | \xi \sim \text{Bernoulli} \left(1 - \frac{1 - \theta_{i}}{(1 - \theta_{i}) + \theta_{i} \left(\frac{1}{\tau_{i}^{2} \sigma^{2}} \right) \exp \left(\frac{\left(\sum_{j=1}^{n} (w_{j} X_{j,i}^{*} + w_{j}^{*} X_{j,i}) - \frac{2}{\tau_{i}^{2}} \right)^{2}}{4\sigma^{2} \sum_{j=1}^{n} X_{j,i} X_{j,i}^{*}} \right) \left(\frac{2\sigma^{2} \pi}{\sum_{j=1}^{n} X_{j,i} X_{j,i}^{*}} \right)^{1/2} \left(\frac{1}{2} \right) \right)$$

 $\nu | \xi \sim ?$ (Use a Metropolis-Hastings step)

Model evaluation on multi-source controlled release data



Methane Emissions Technology Evaluation Center (METEC)

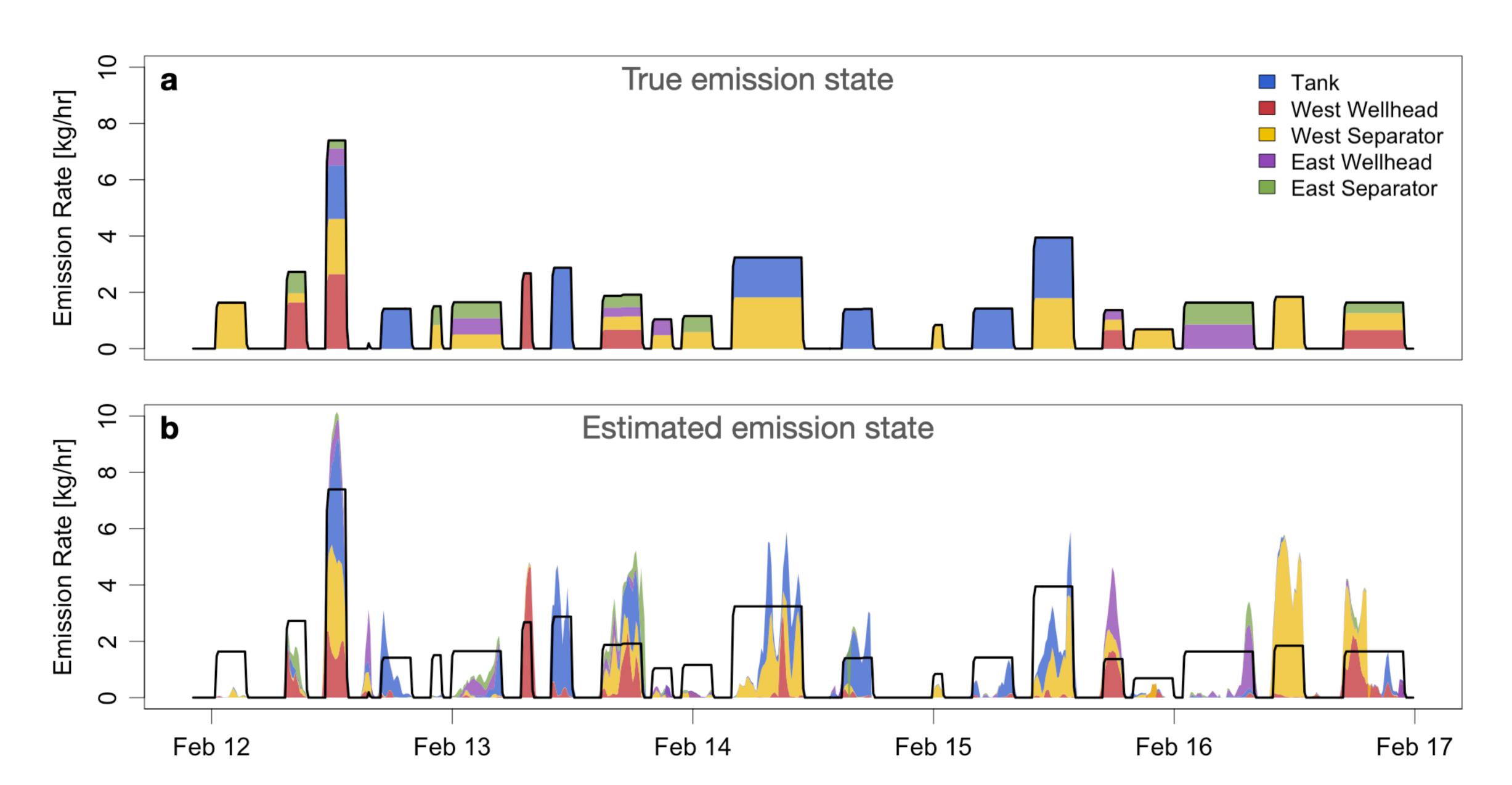
337 controlled releases:

- 99 (29%) single-source
- 238 (71%) multi-source

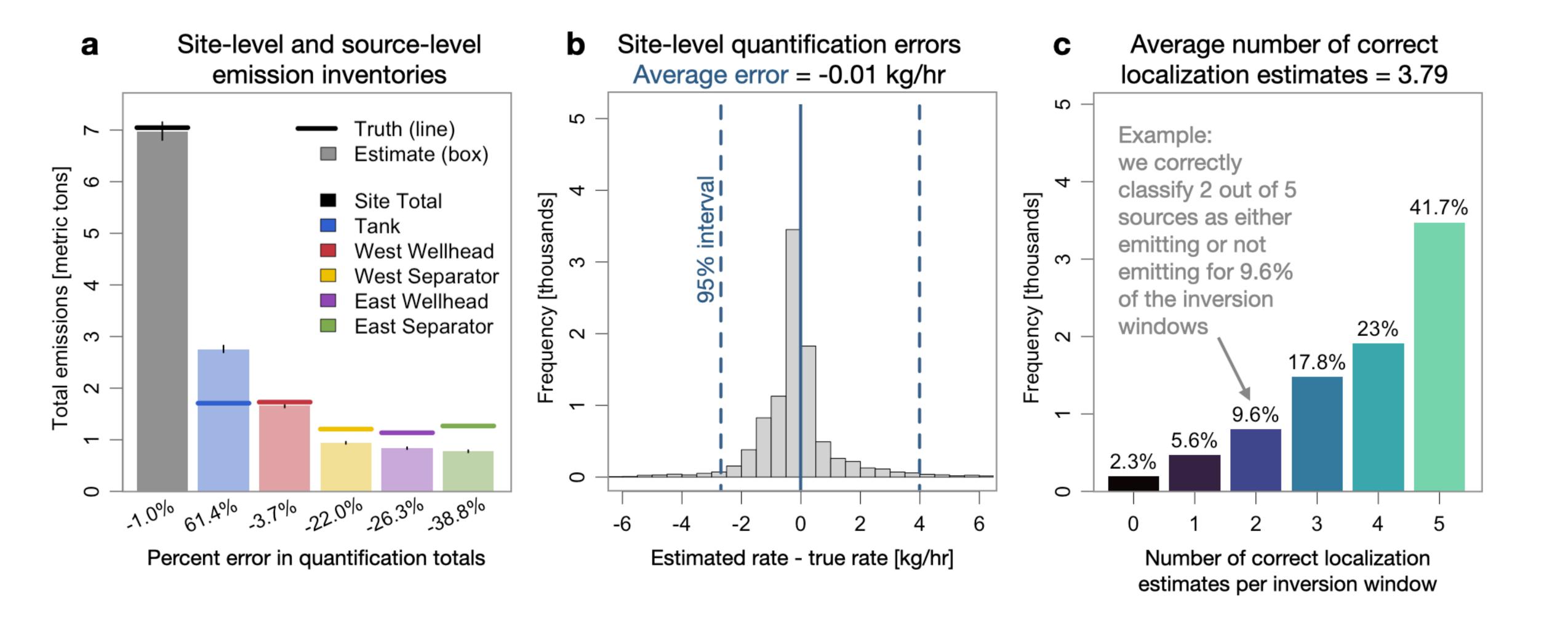
Emission rates range from **0.08** to **7.2** kg/hr

Emission durations range from **0.5** to **8** hours

Model evaluation on multi-source controlled release data



Model evaluation on multi-source controlled release data



Part 2: Multi-source emission detection, localization, and quantification

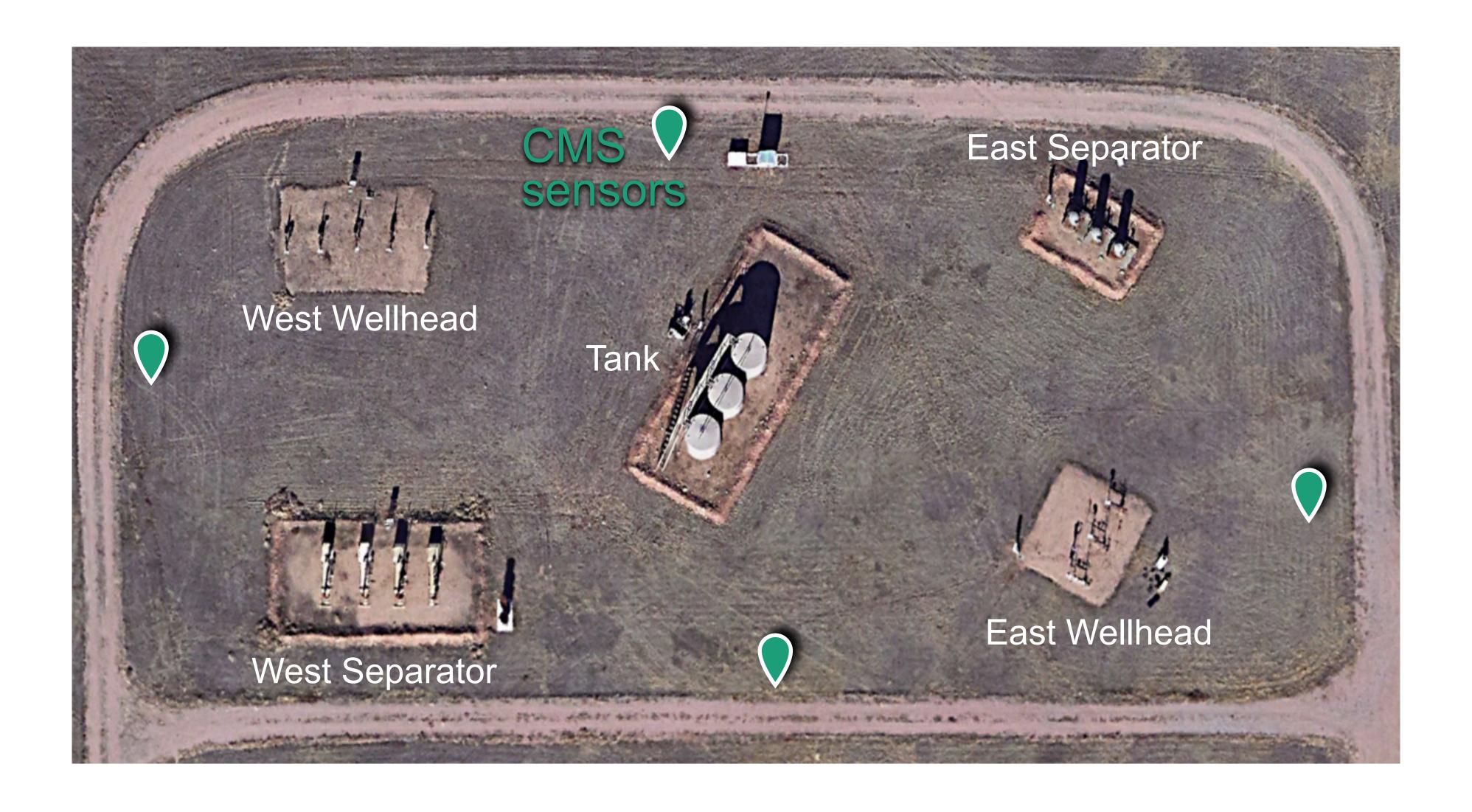


A Bayesian hierarchical model for methane emission source apportionment.

William Daniels, Douglas Nychka, Dorit Hammerling.

Annals of Applied Statistics, submitted, (2025).

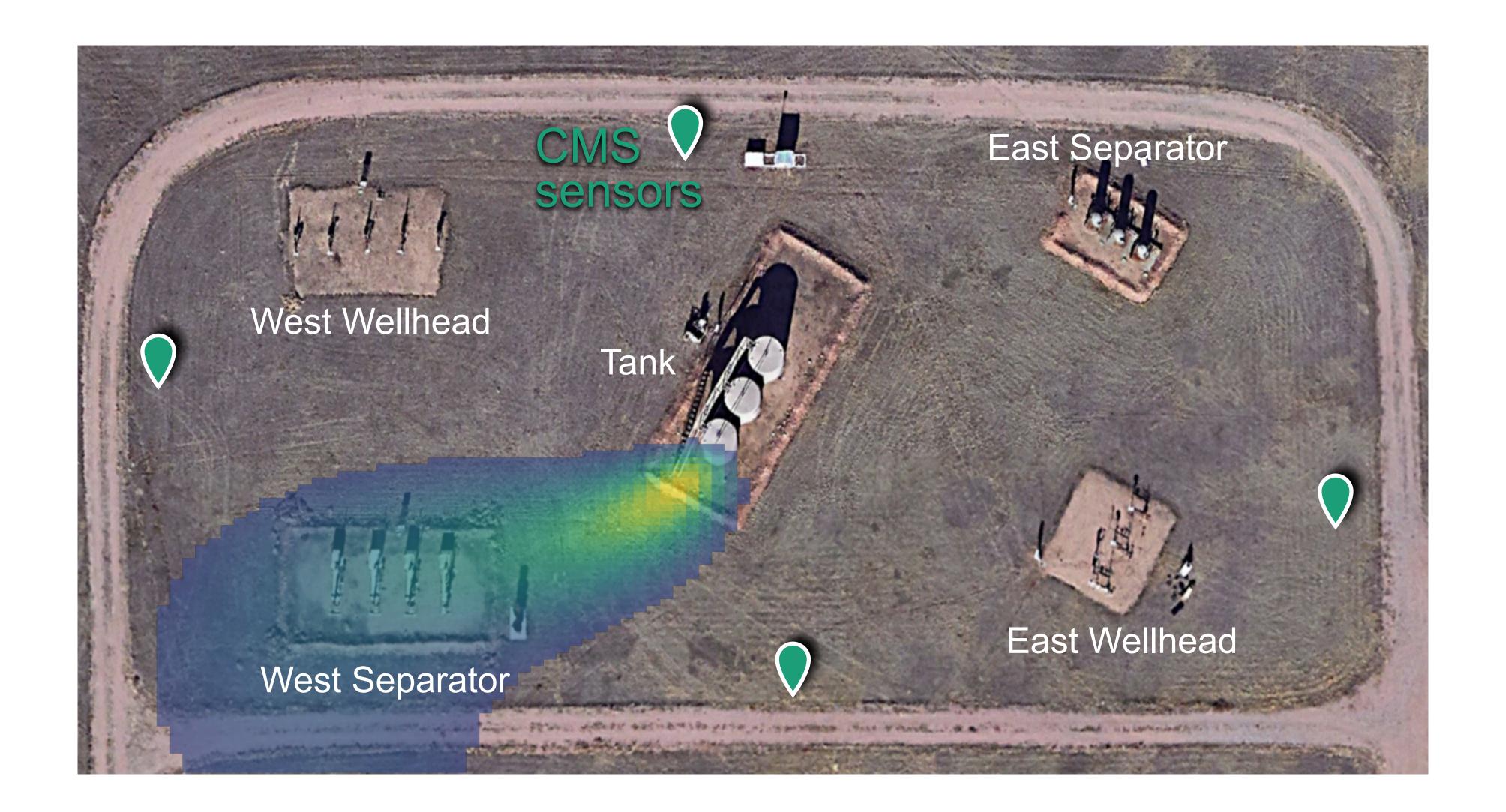
One problem... incomplete sensor coverage



Wind direction



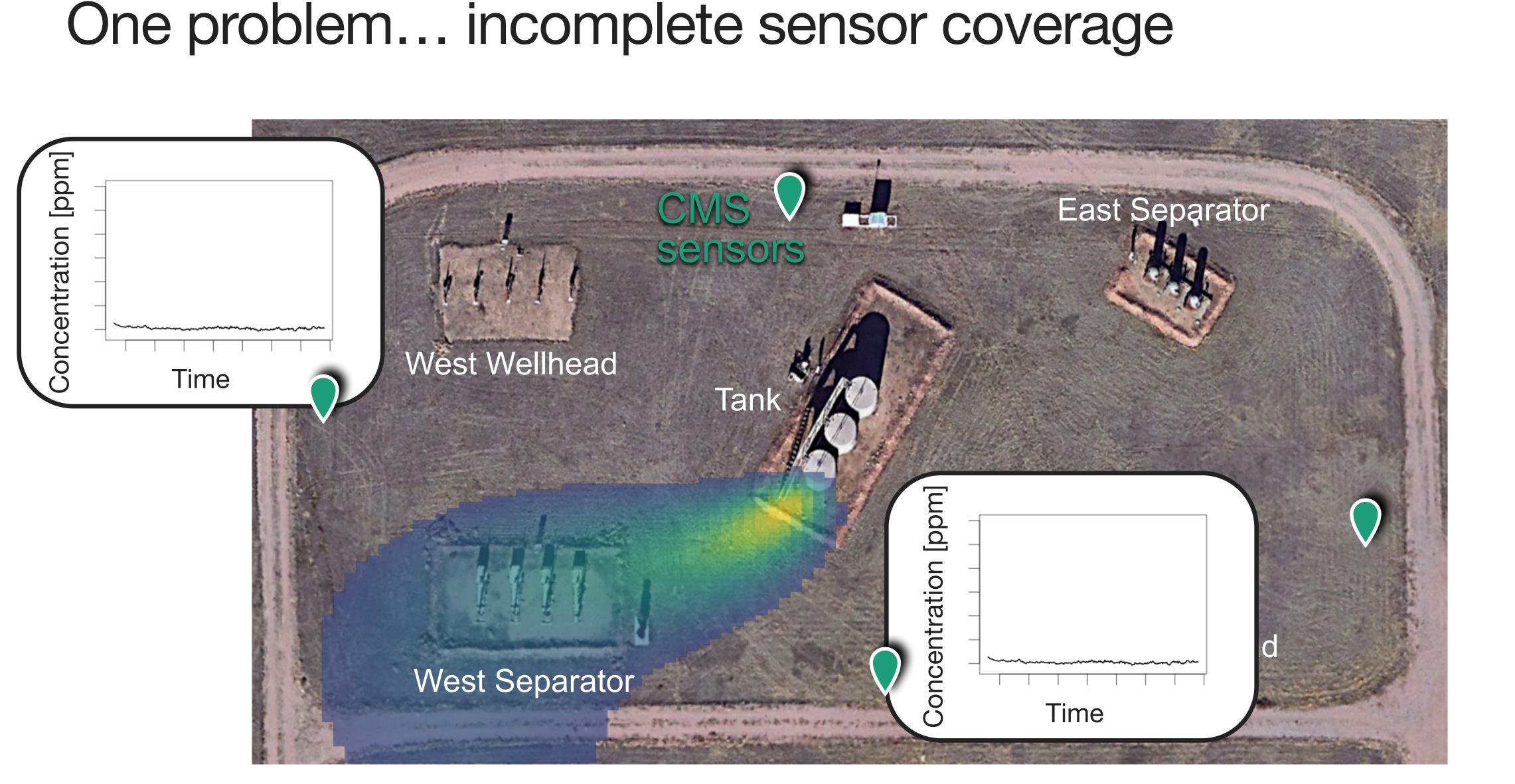
One problem... incomplete sensor coverage



Wind

direction





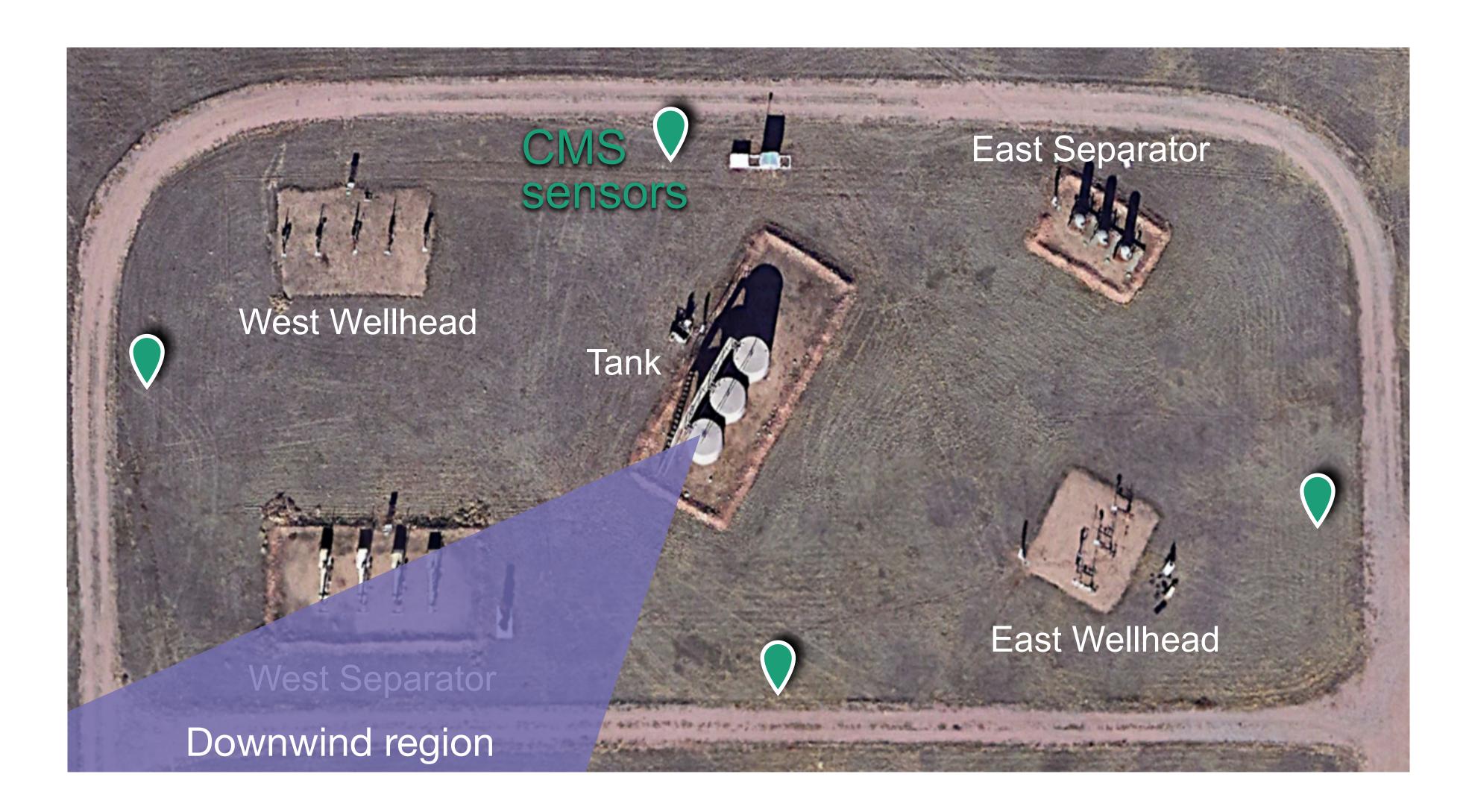
CMS do not provide emission information when the wind blows between sensors

Wind

direction



However, we can estimate when this happens!

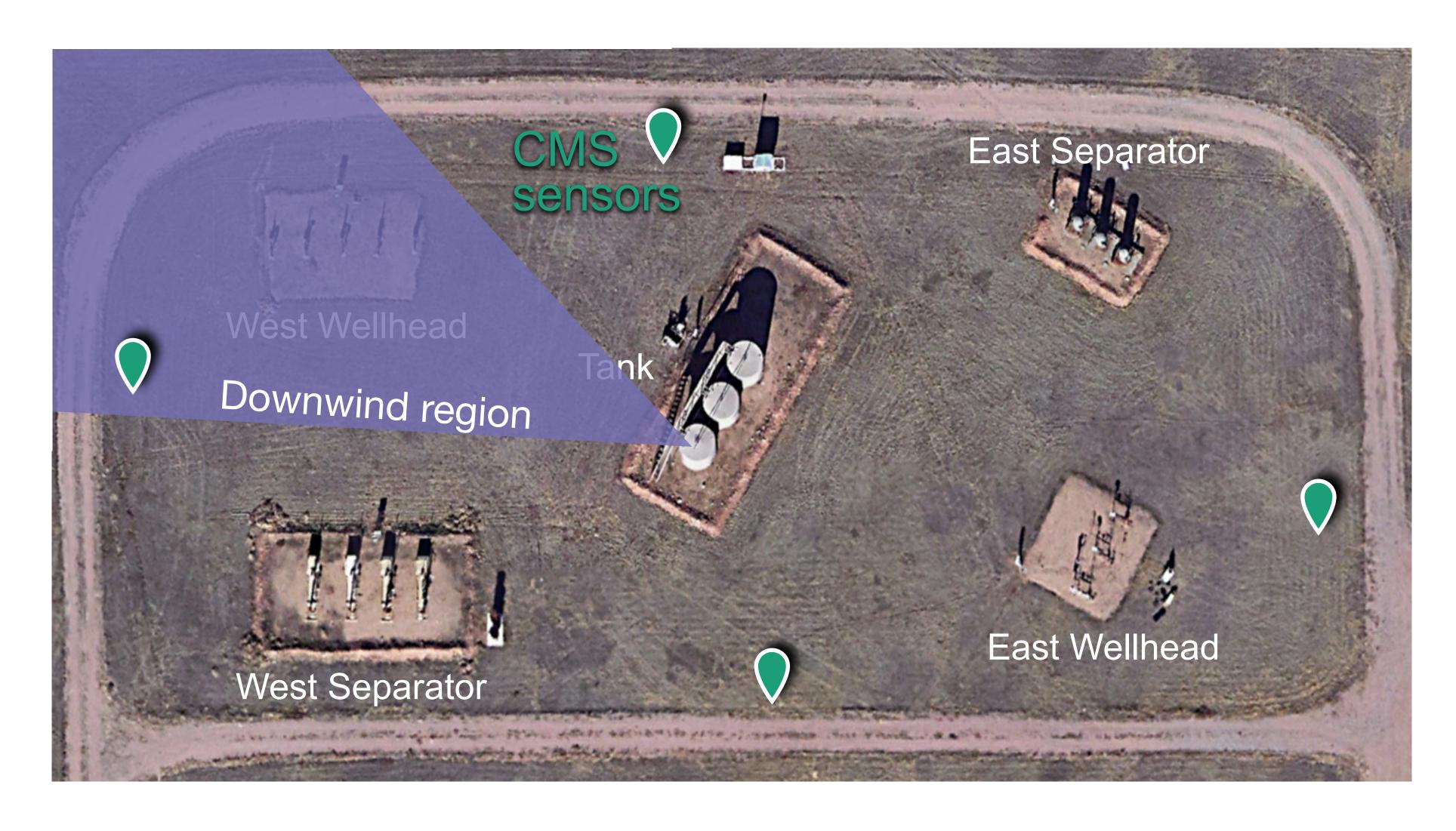


Downwind region does not overlap with CMS sensors = period of "no information"

Wind direction

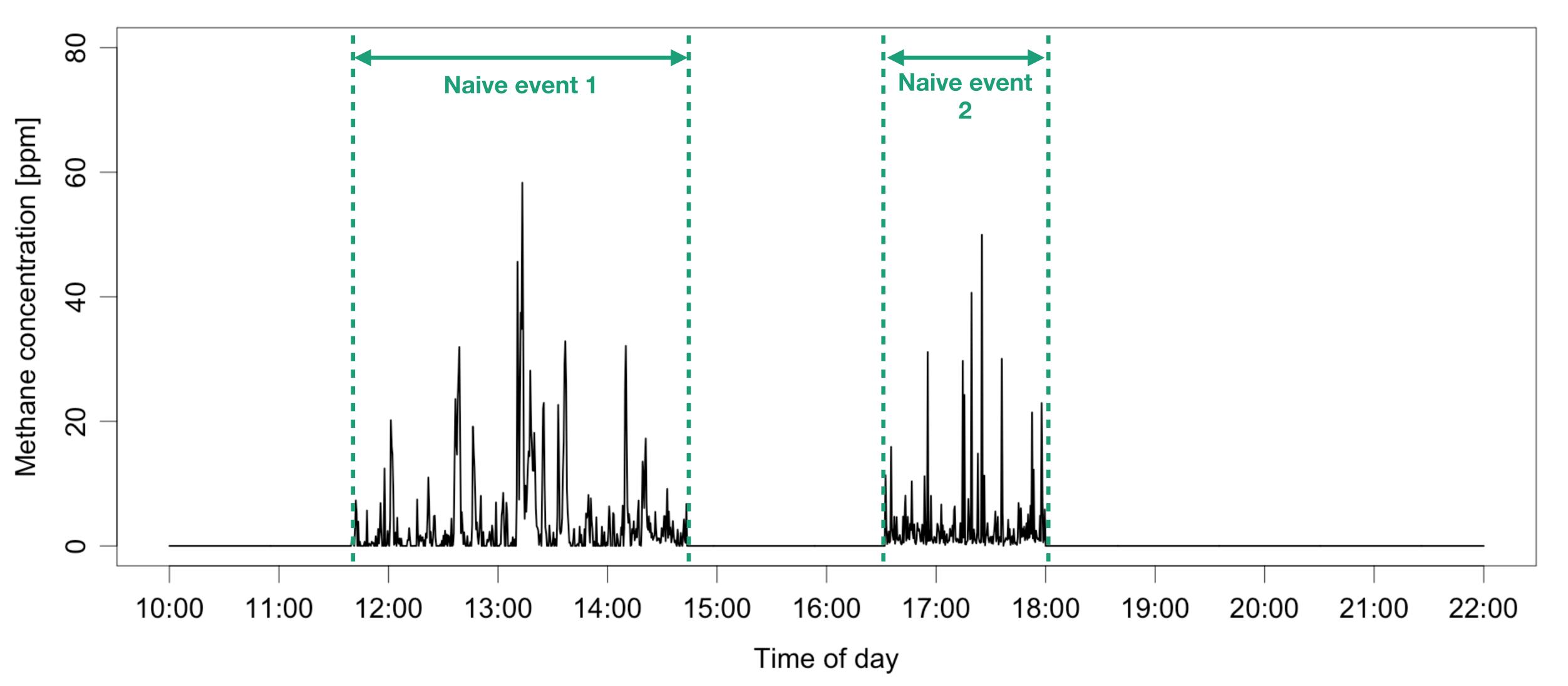
However, we can estimate when this happens!



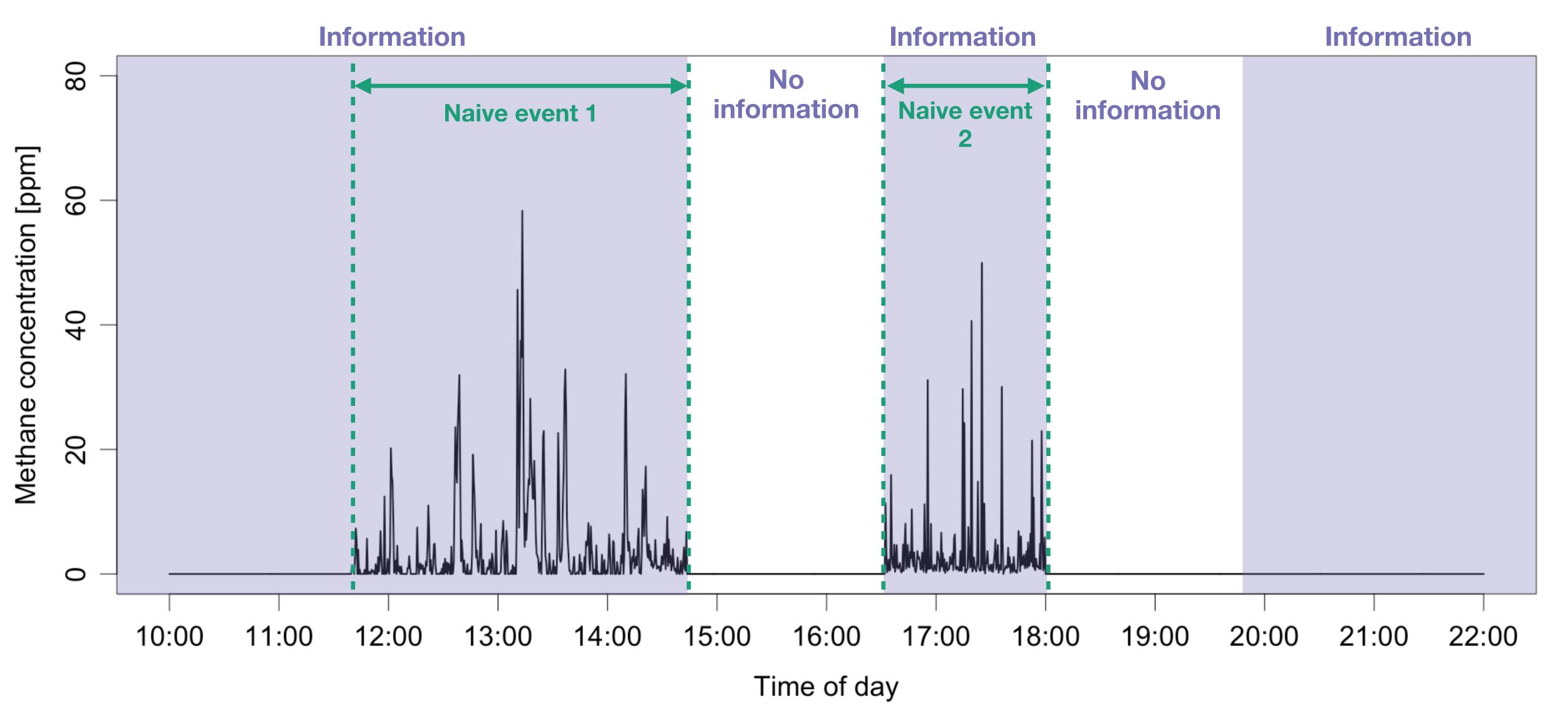


Downwind region does overlap with CMS sensors = period of "information"

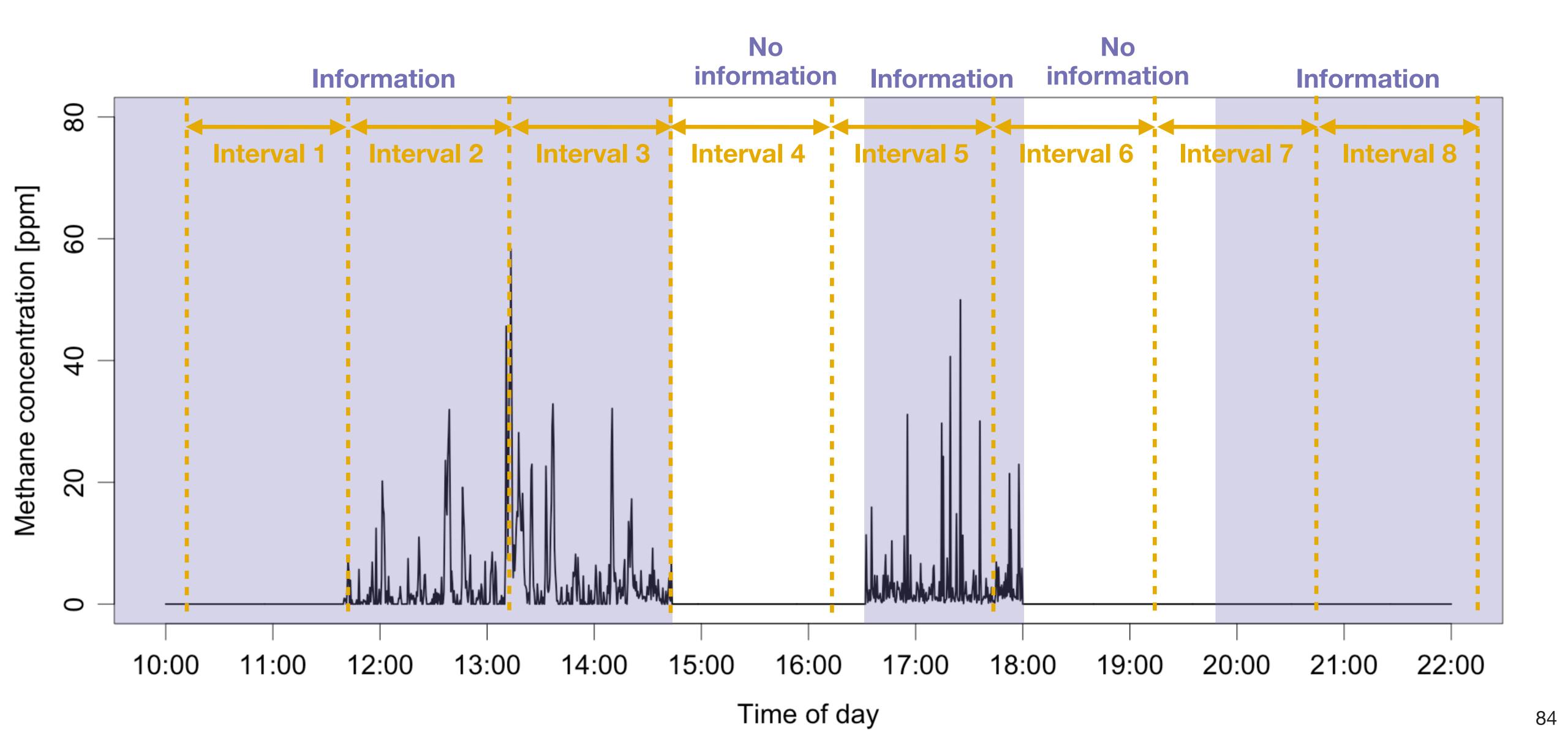
How do periods of information and no information present themselves in the data?



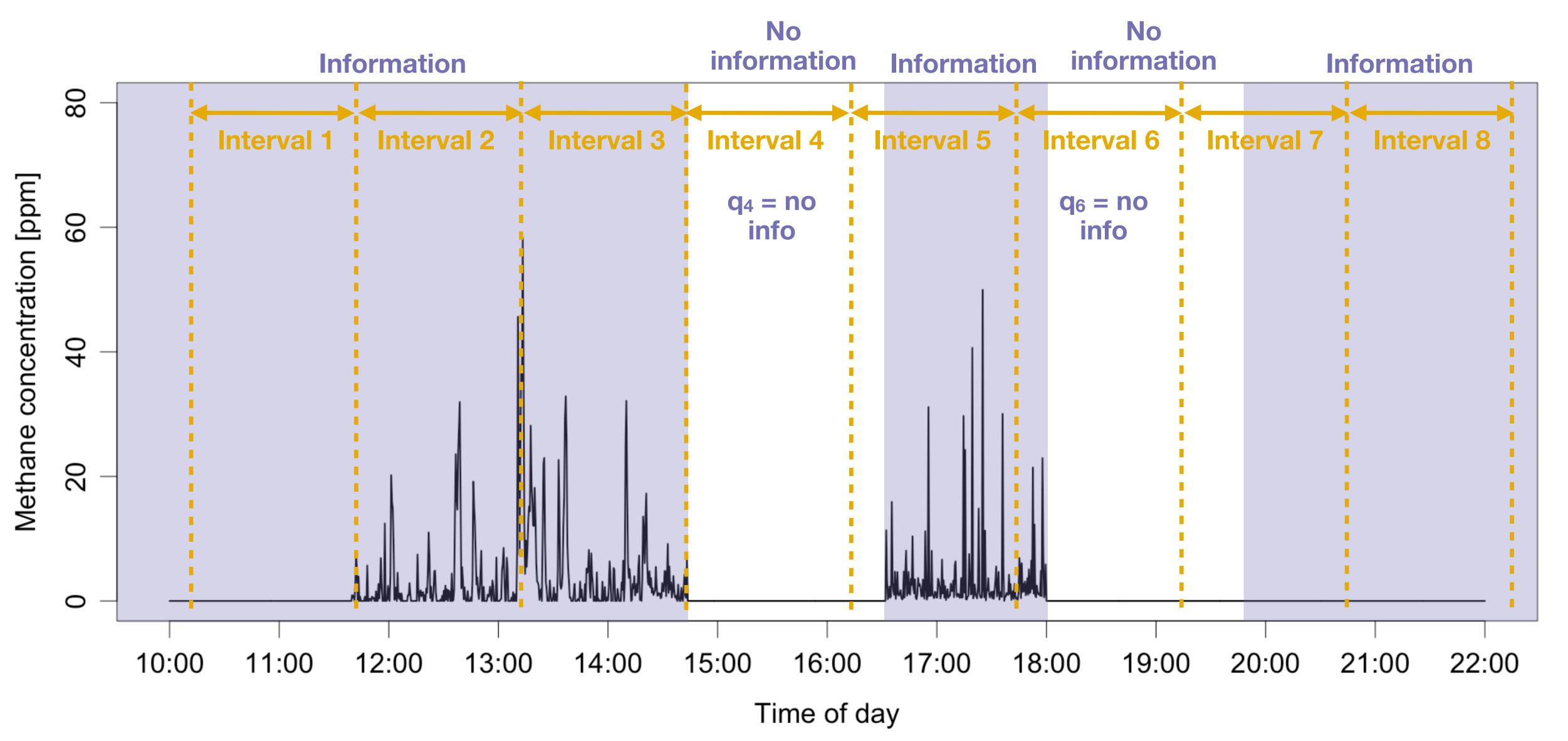
How do periods of information and no information present themselves in the data?



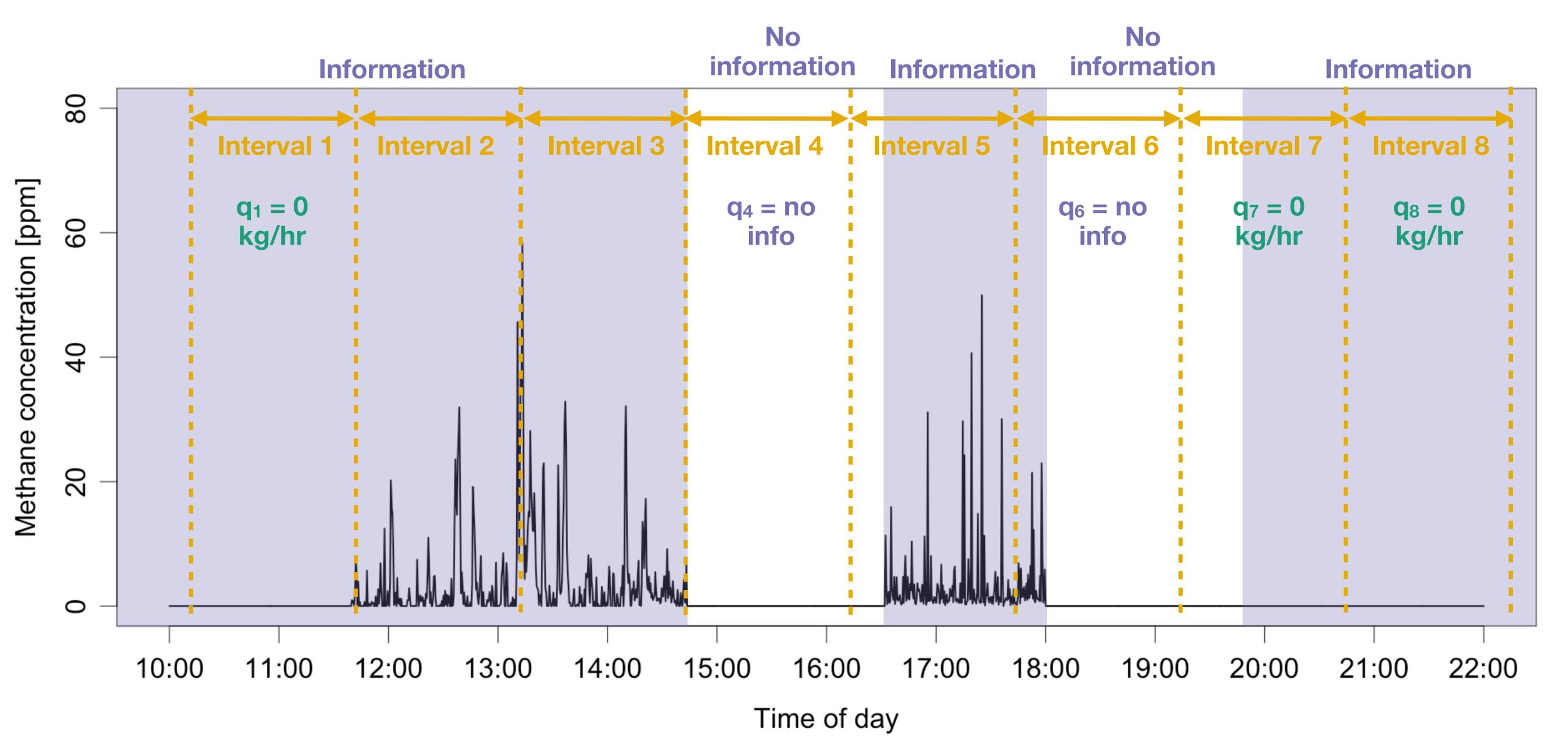
In practice, run the MDLQ (or DLQ) model on fixed intervals



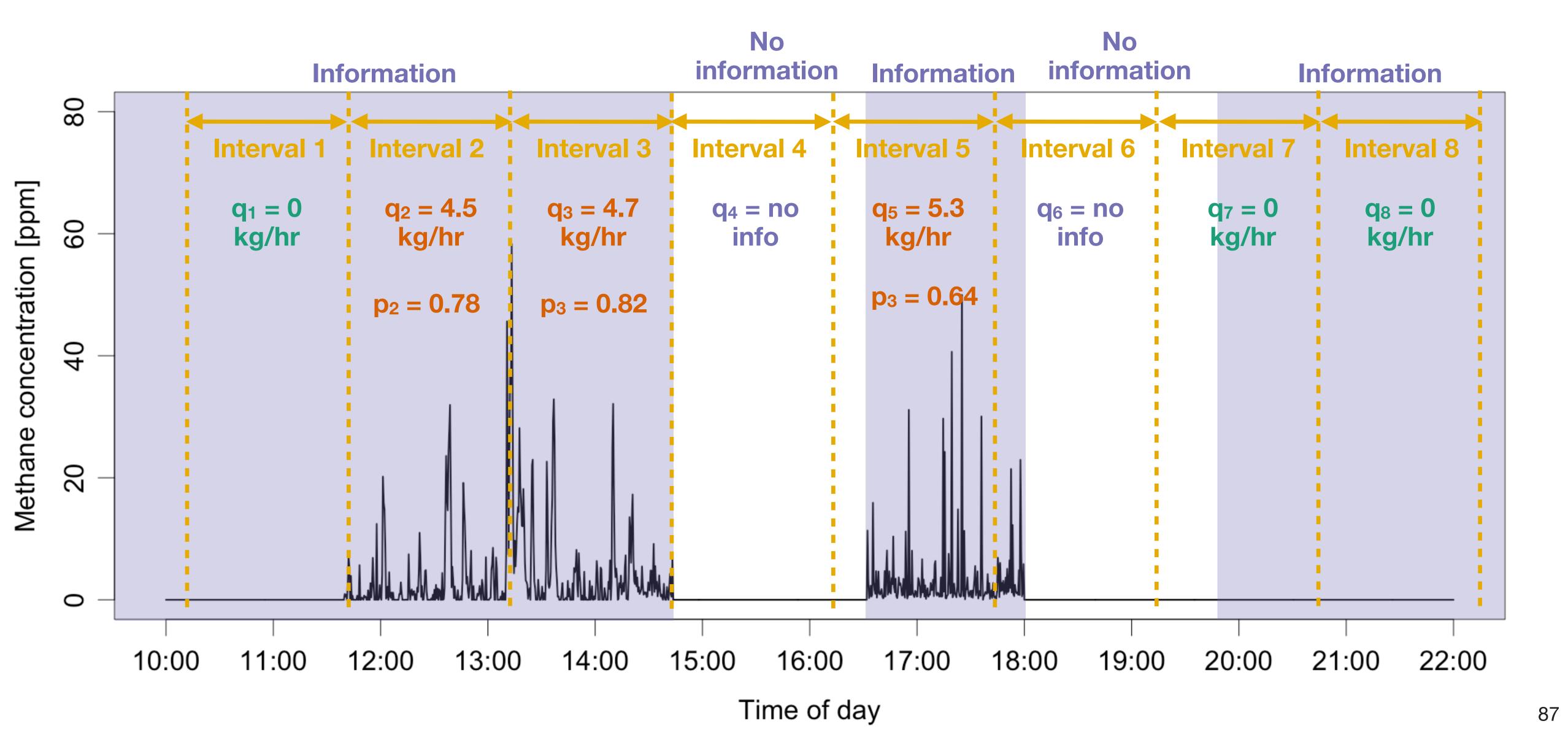
Whether an interval is no information,



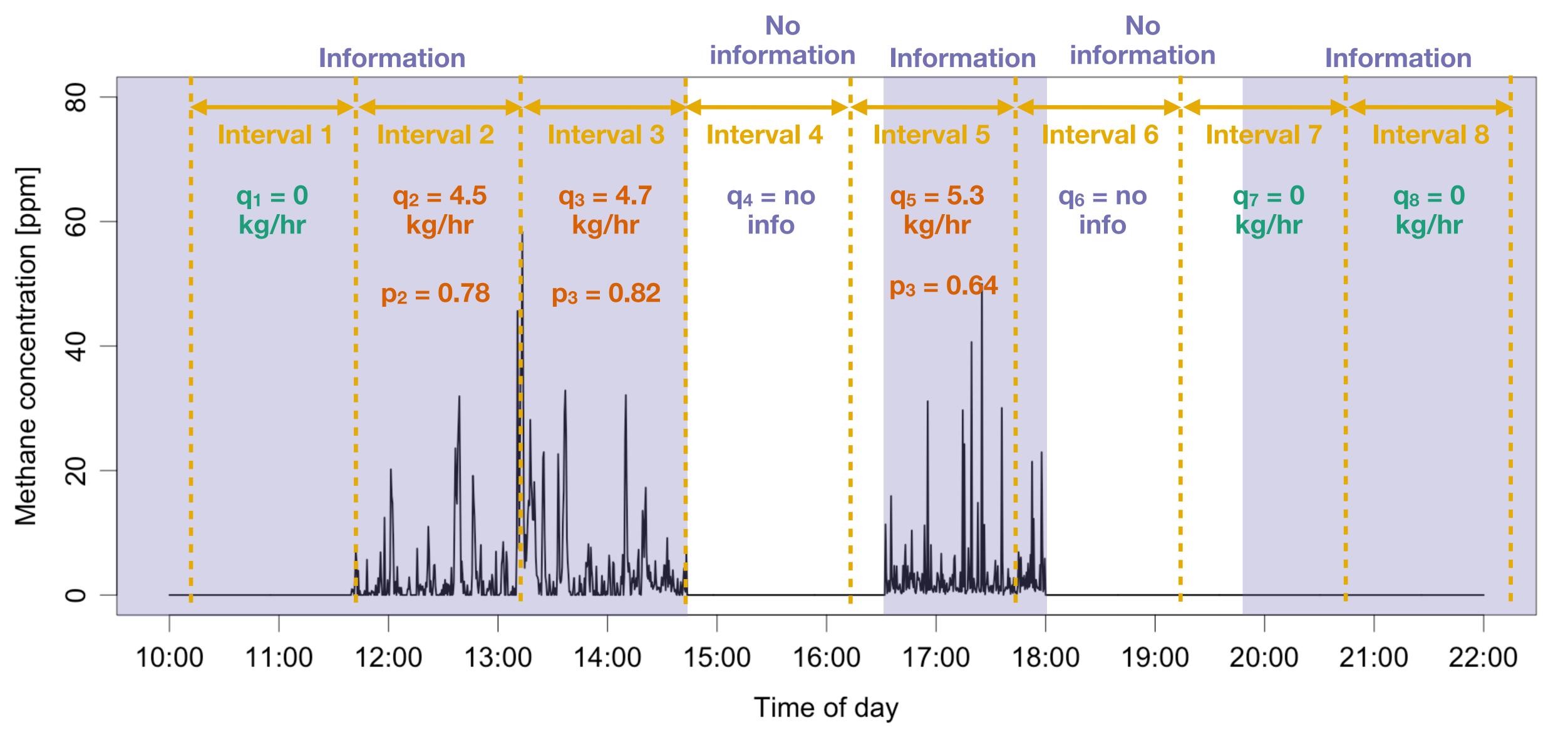
Whether an interval is no information, zero emission rate,



Whether an interval is no information, zero emission rate, or non-zero emission rate depends on the data.

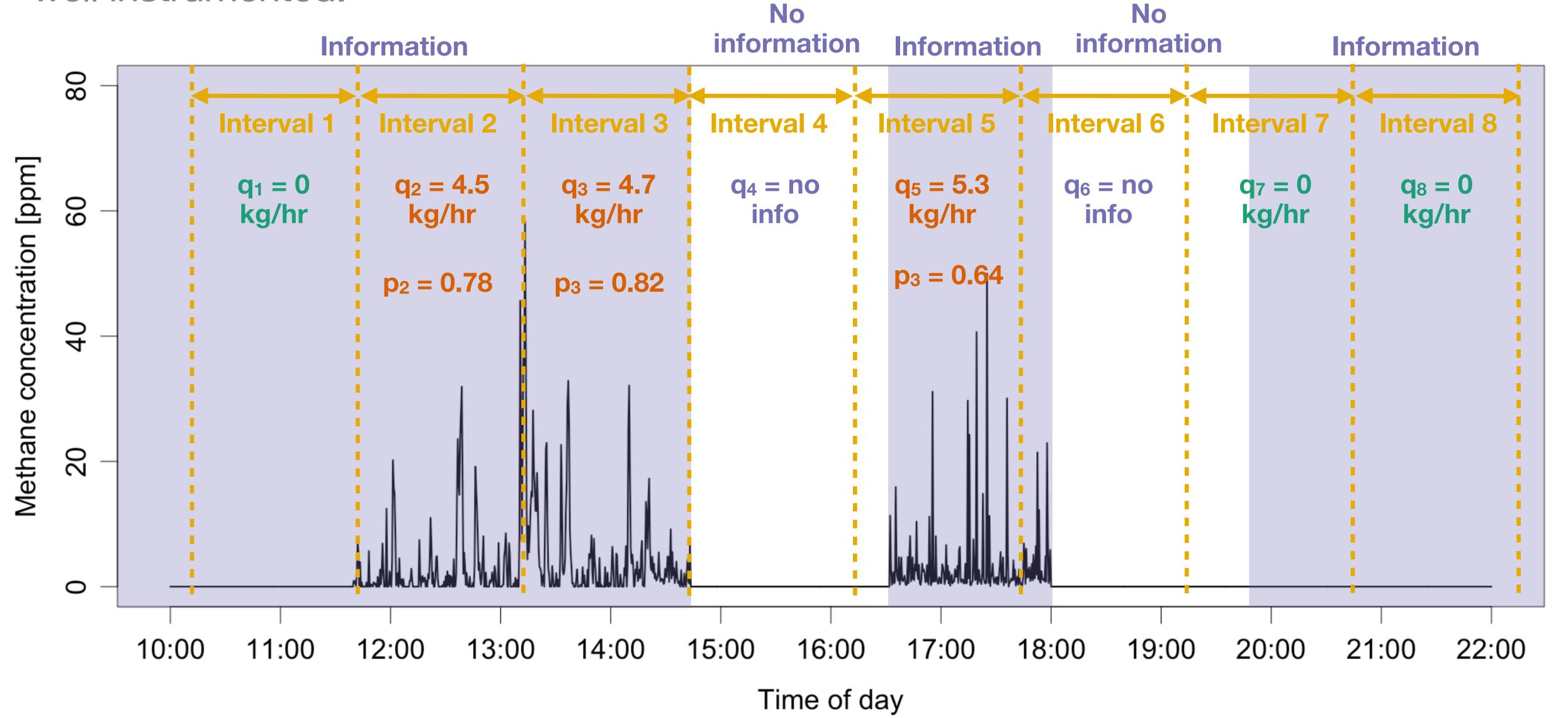


How do you turn these estimates into a measurement-derived inventory?



How do you turn these estimates into a measurement-derived inventory?

One option: run it long enough to build stable distributions. How long? Depends on how well instrumented.



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Thank you!







