Developing fully transparent, site-level, measurement-based inventories using continuous monitoring data

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Department of Applied Mathematics and Statistics





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Fully transparent = all of the methods are open source!

#### site-level & measurement-based

Site-level = only measurements from the specific site used to build the inventory

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#### Advantages

- No assumptions about similar sites following similar distributions
- No potentially for underestimation to leak through from the inventory

#### site-level & measurement-based

Site-level = only measurements from the specific site used to build the inventory

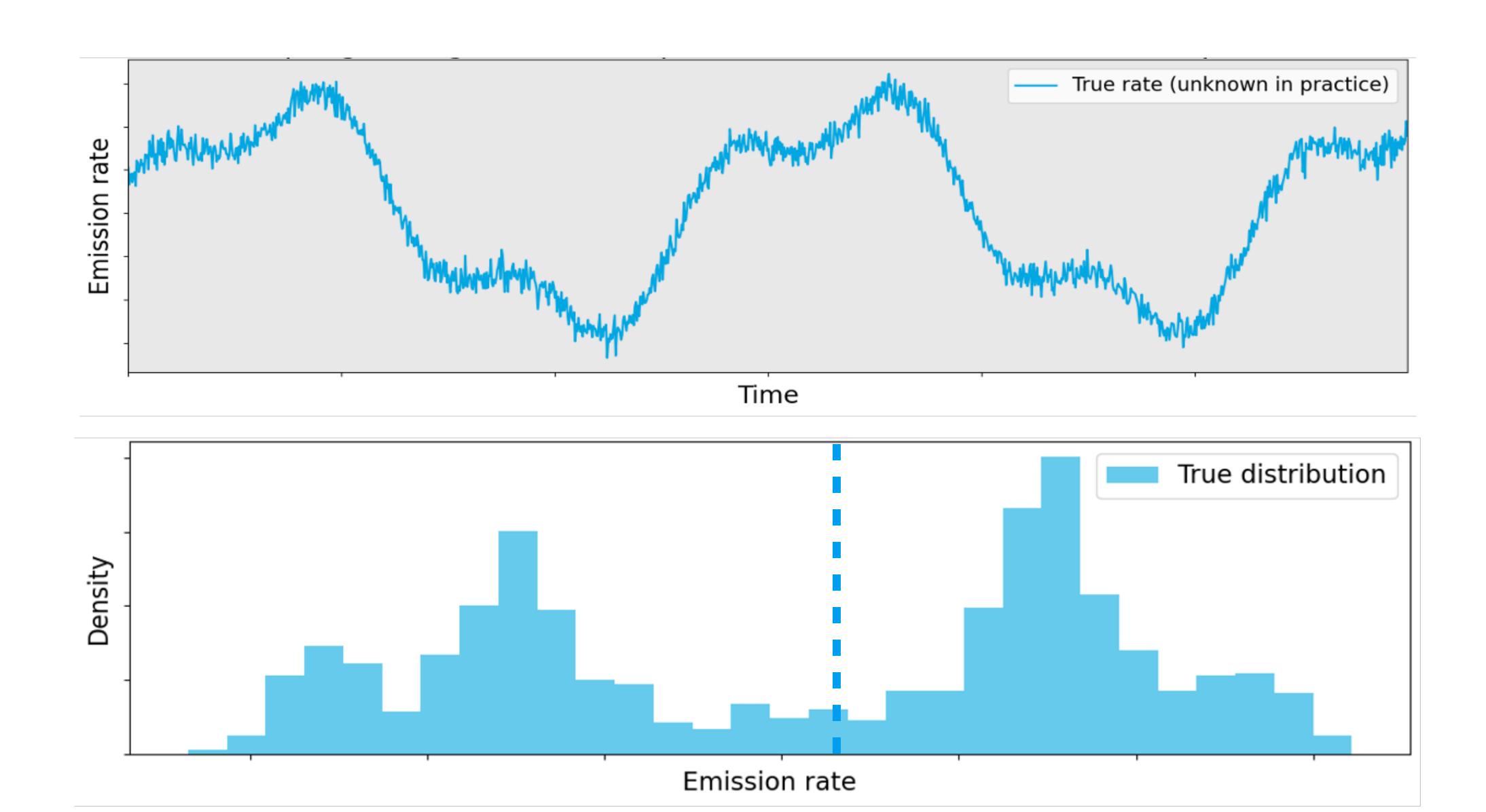
Measurement-based = only use measurement data to build the inventory

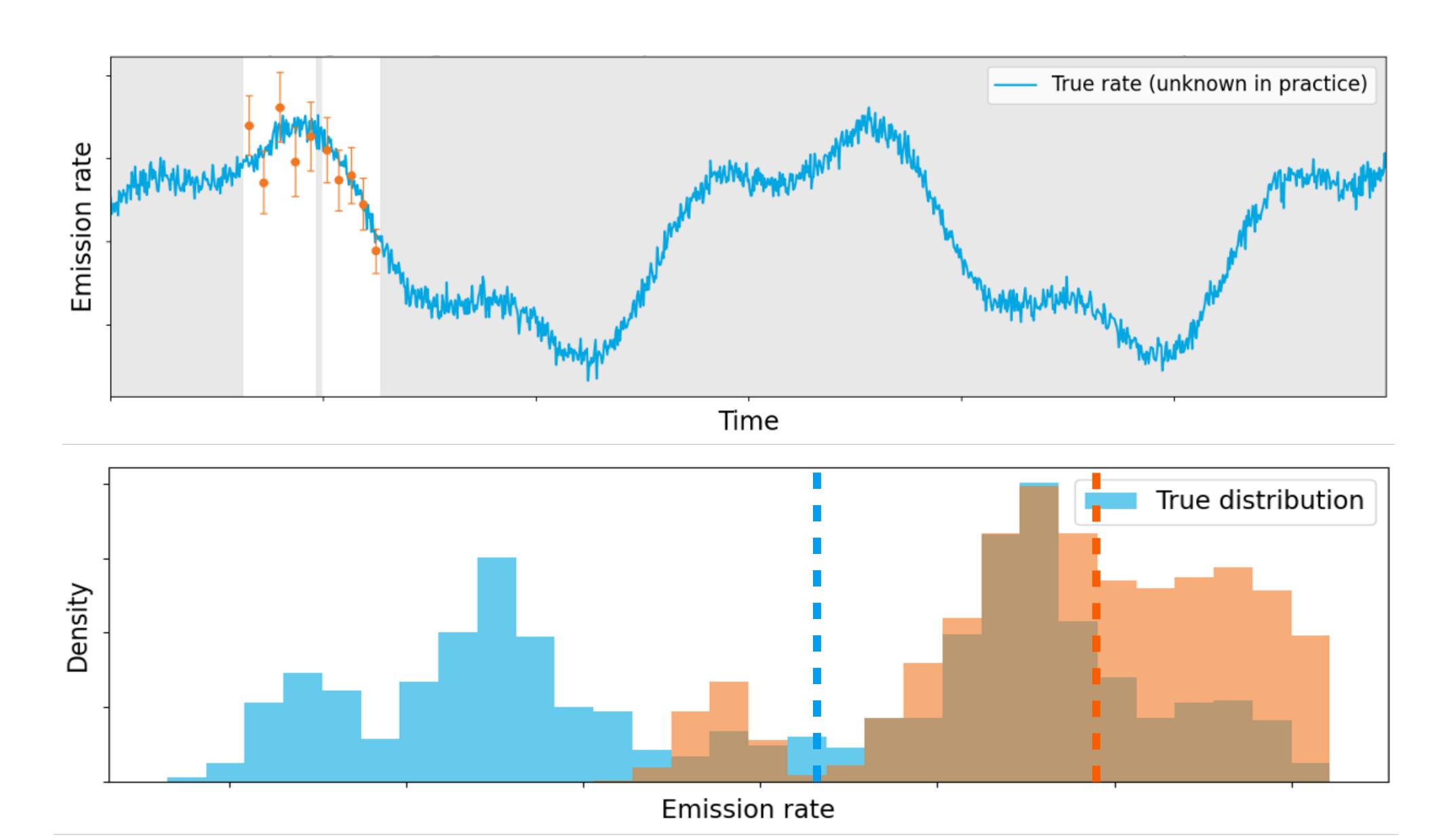
#### Advantages

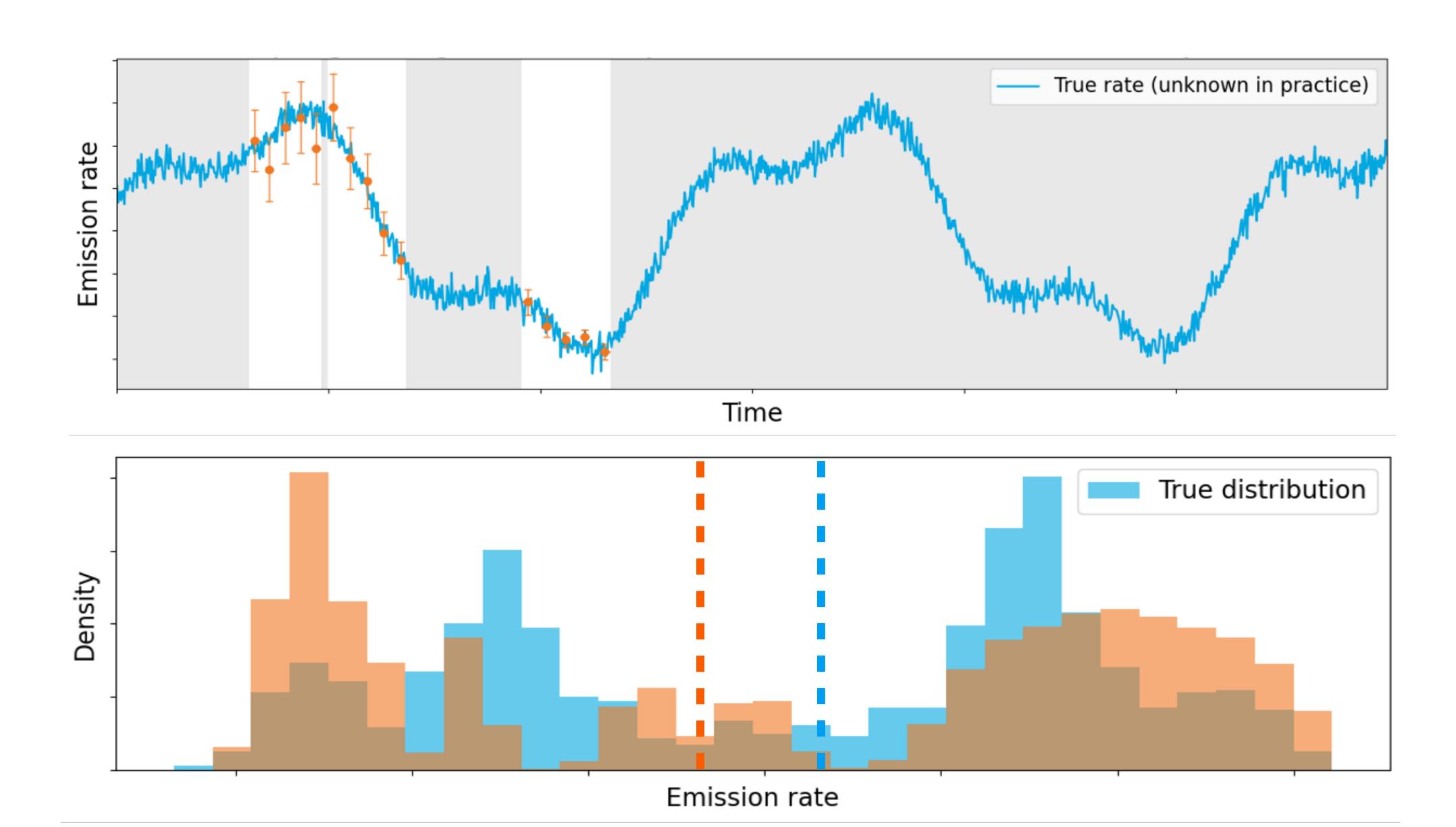
- No assumptions about similar sites following similar distributions
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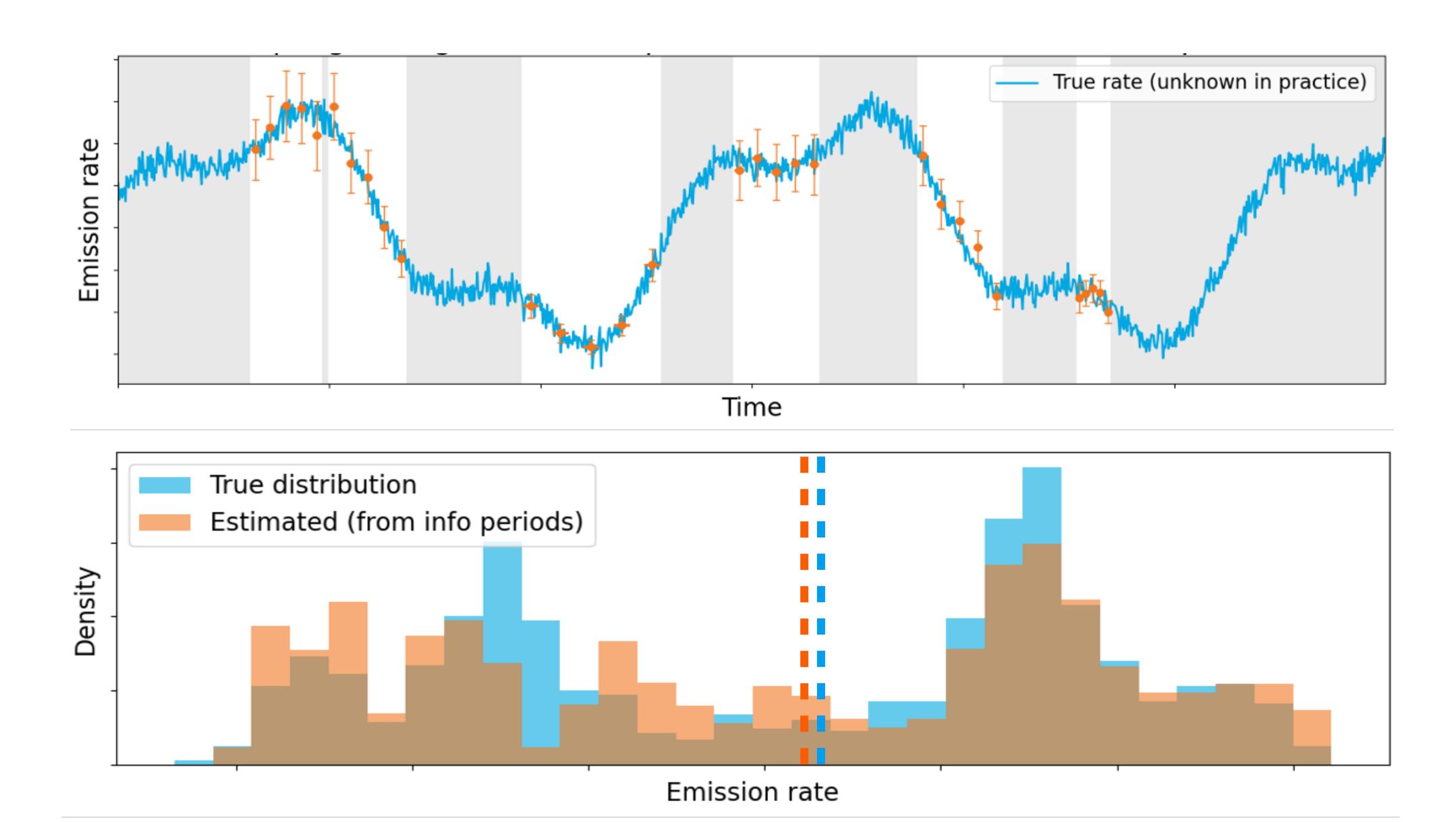
#### Challenges

- Source estimate does not necessarily equal root cause
- Need a lot of measurements on each site
- Scaling up requires lots of measurements on lots of sites

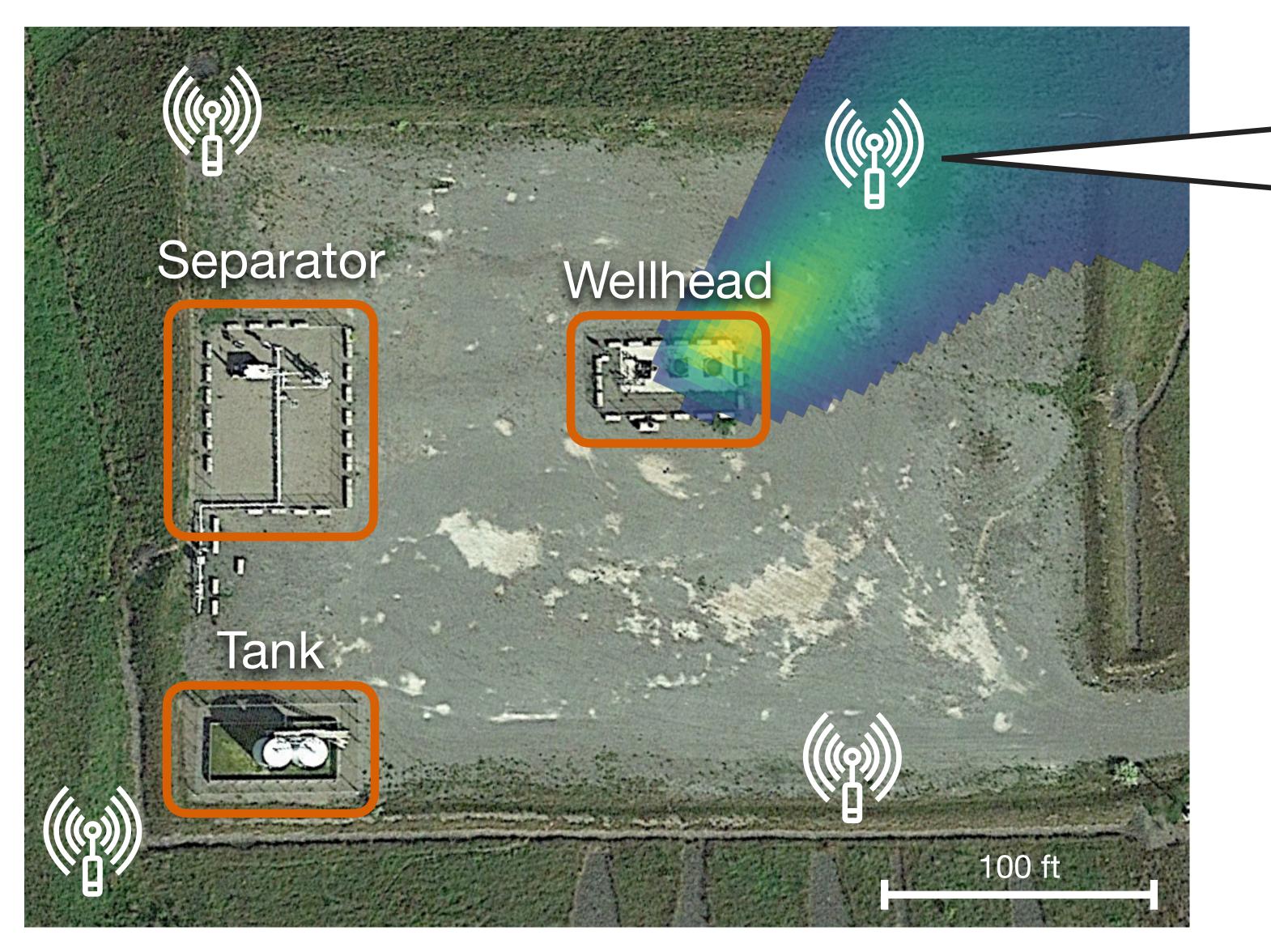


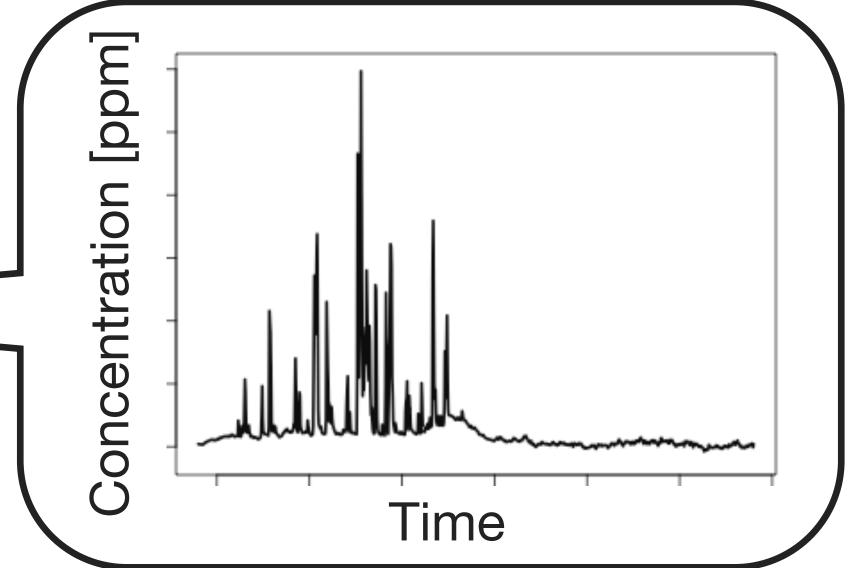






#### Continuous monitoring 101

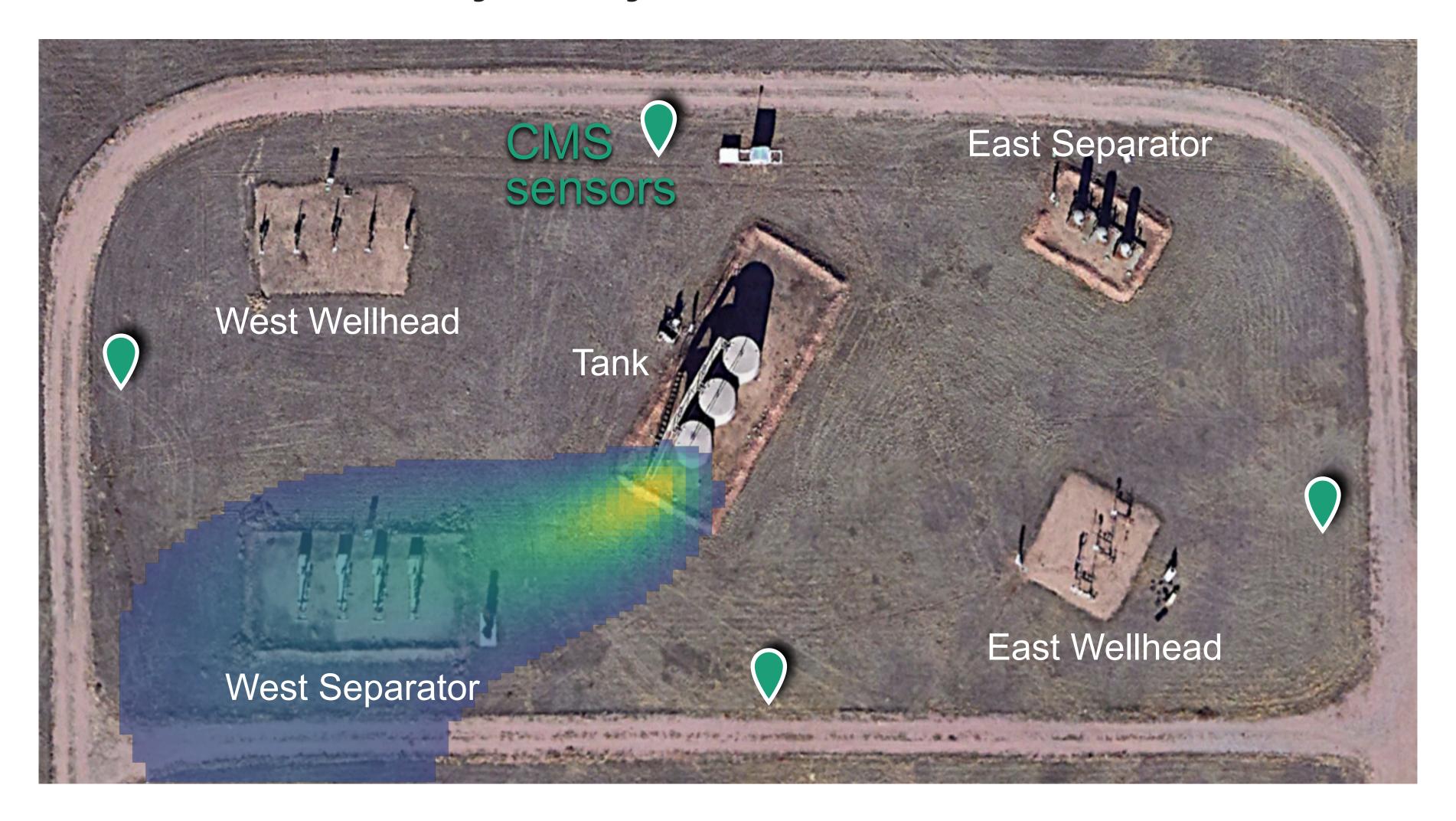






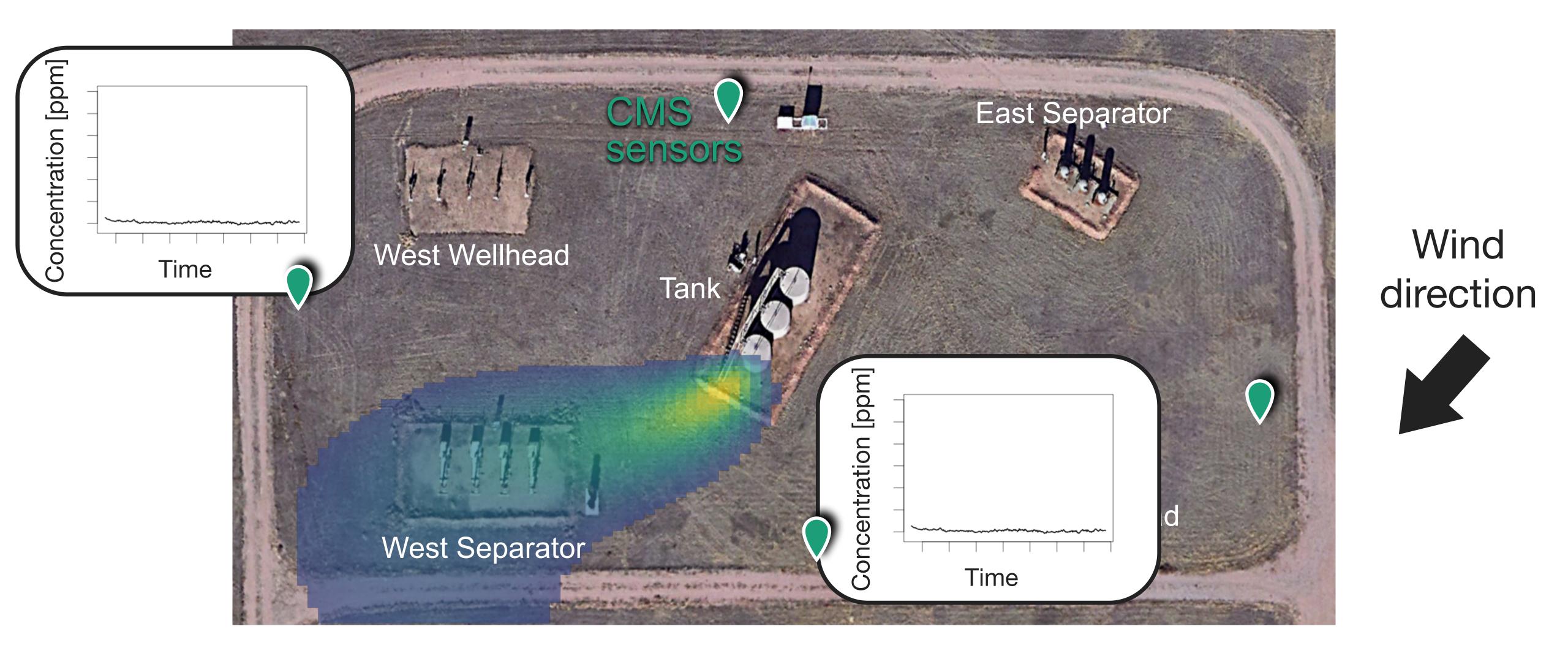
Aerial measurement technology



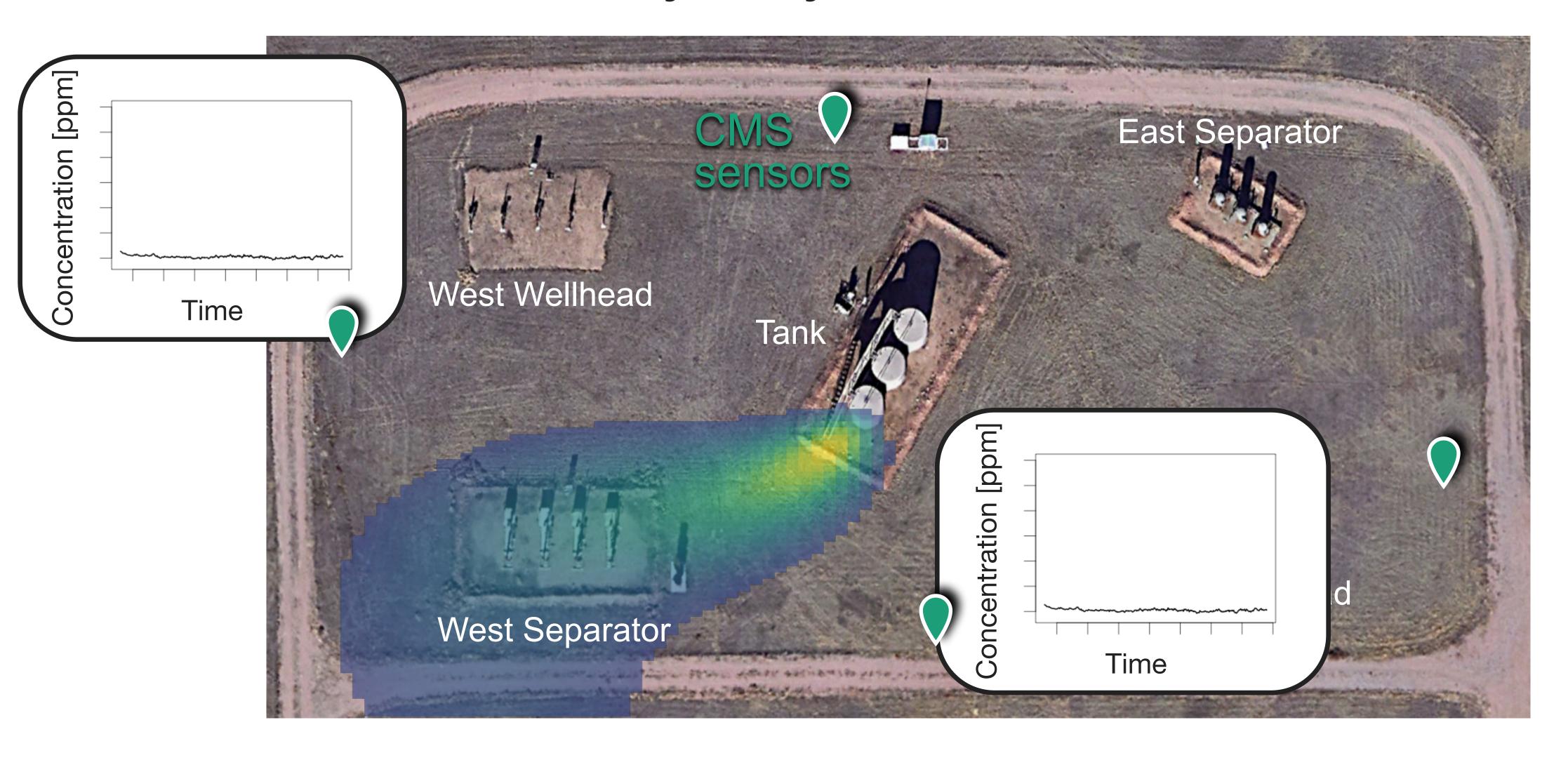


Wind direction





No emissions information when the wind blows between sensors

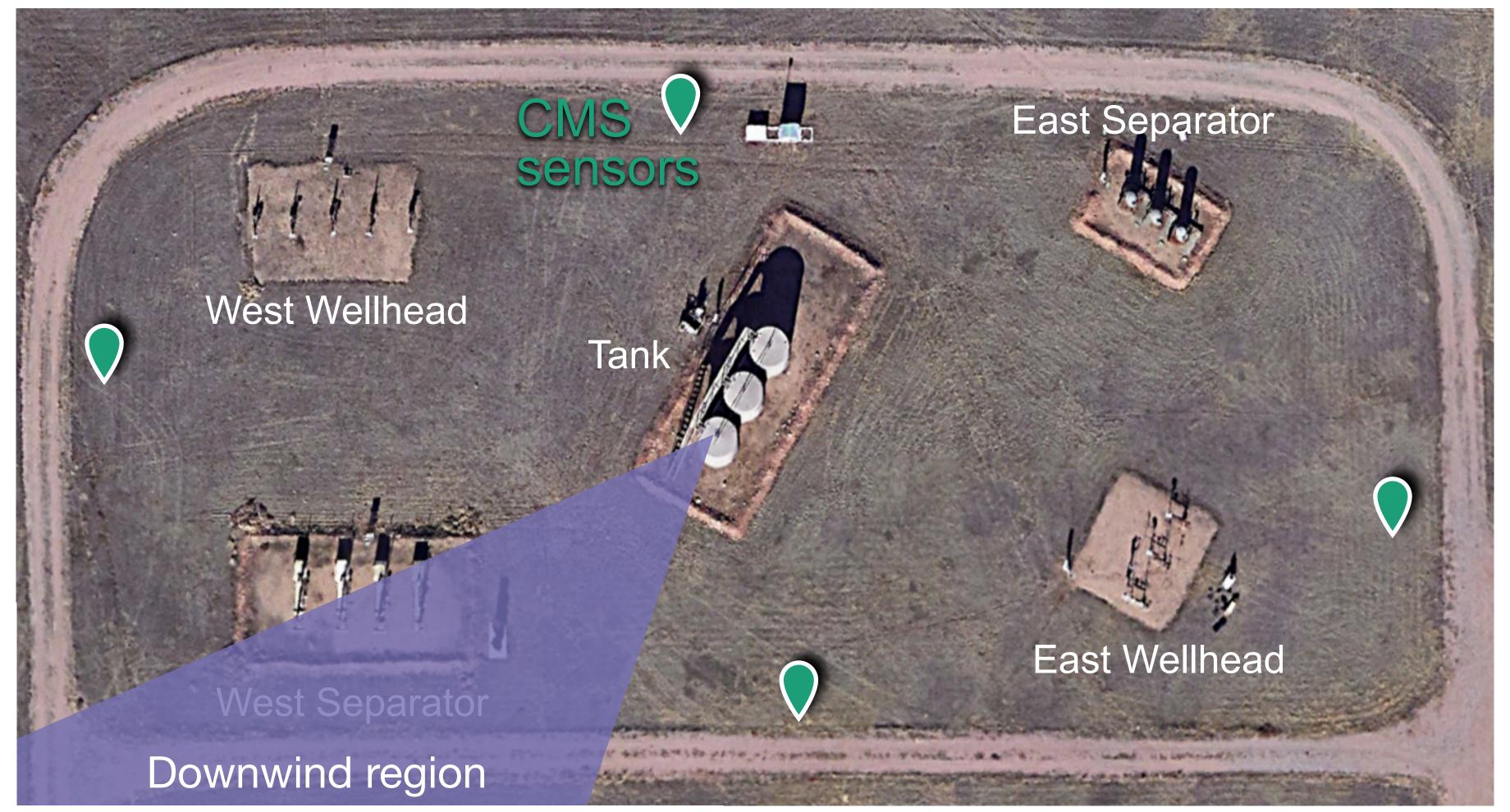


Wind direction



This cannot be interpreted as 0 kg/hr!

#### However... we can estimate when this happens!

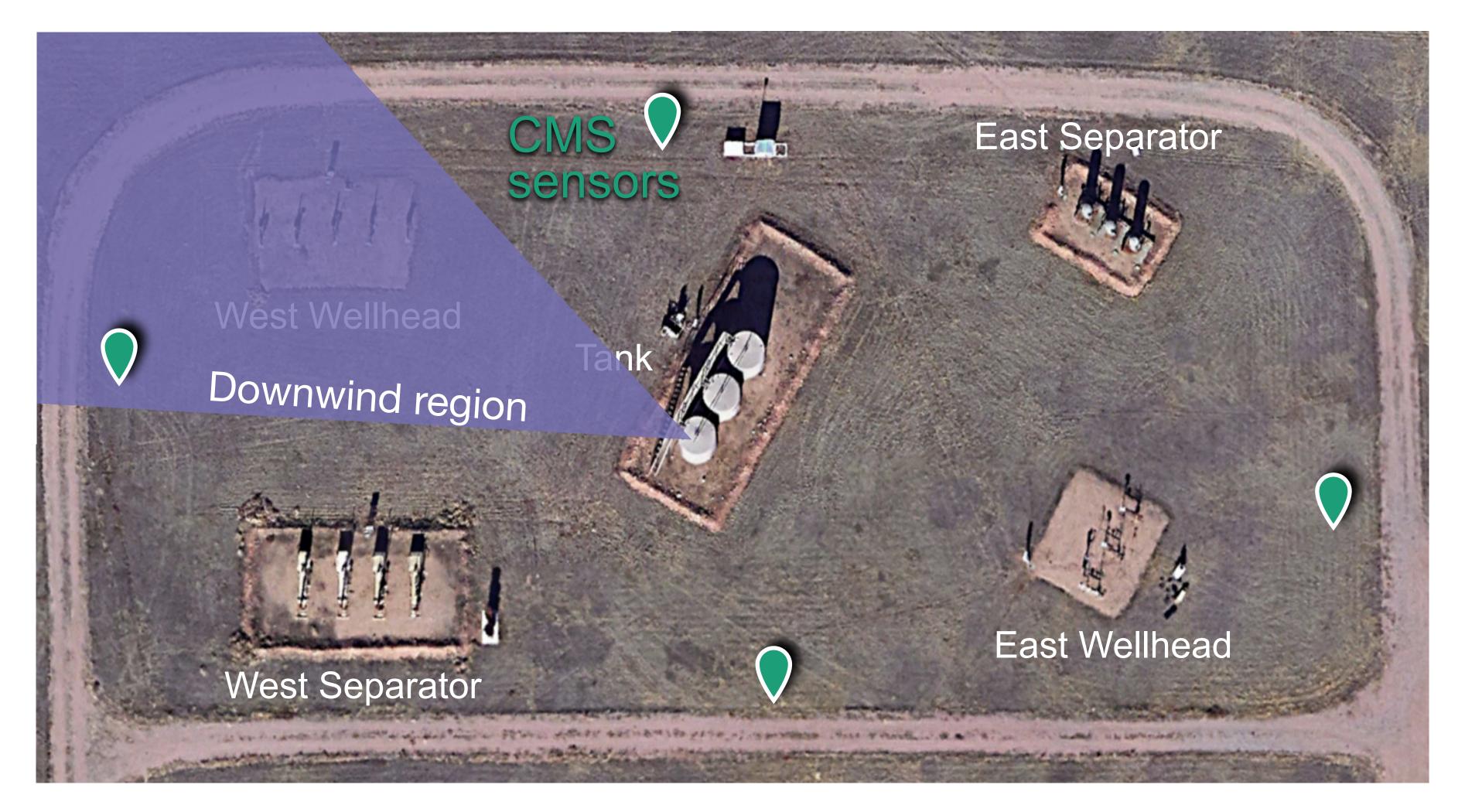


Downwind region **does not** overlap with CMS sensors = period of "no information"

Wind

direction

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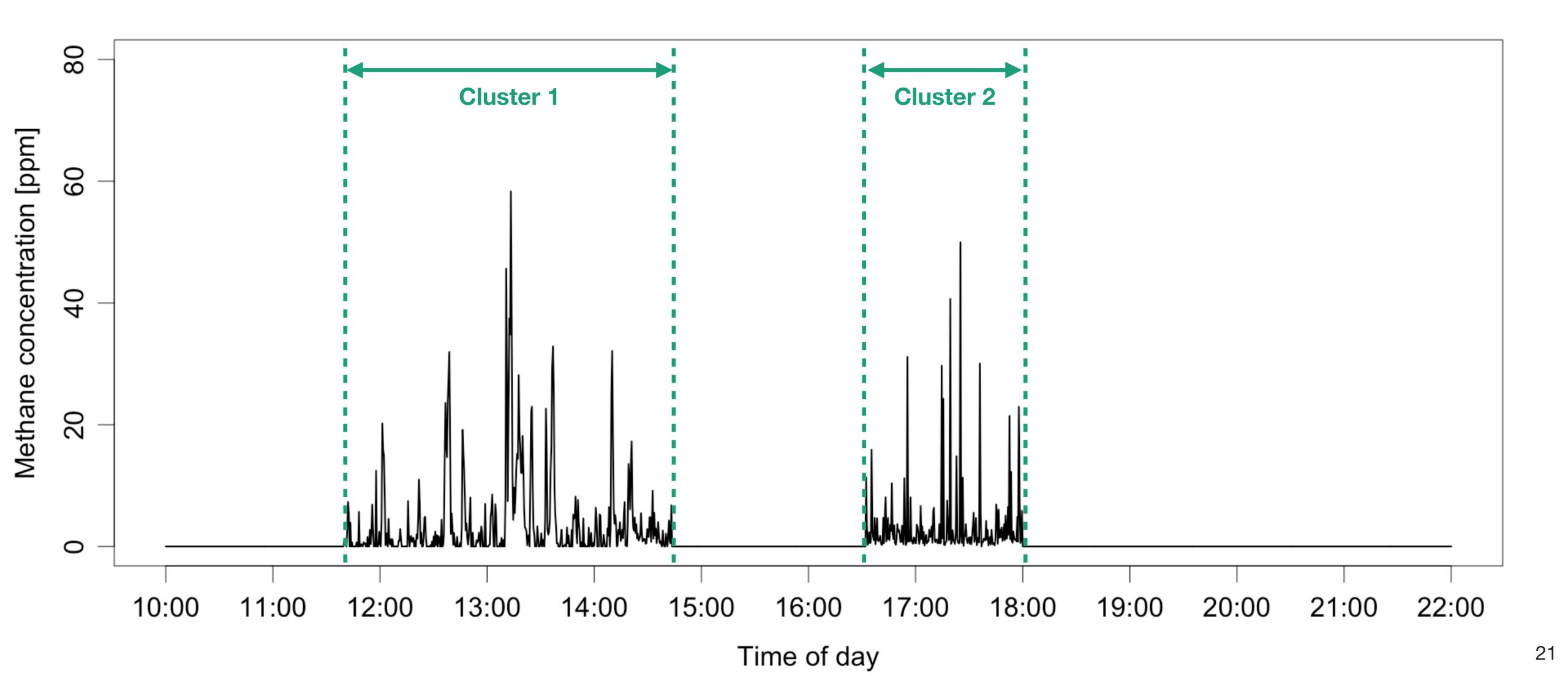


Downwind region **does** overlap with CMS sensors = period of "information"

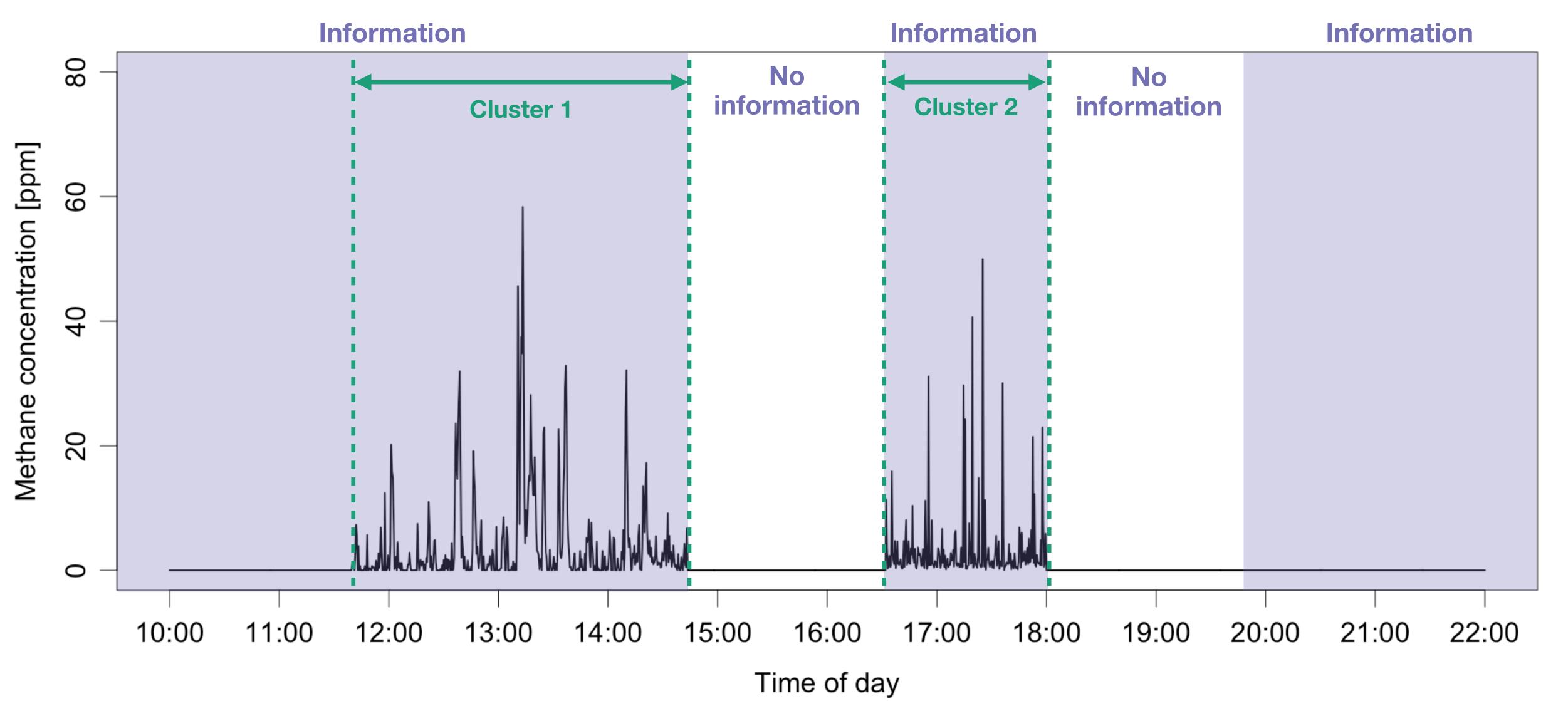
Wind

direction

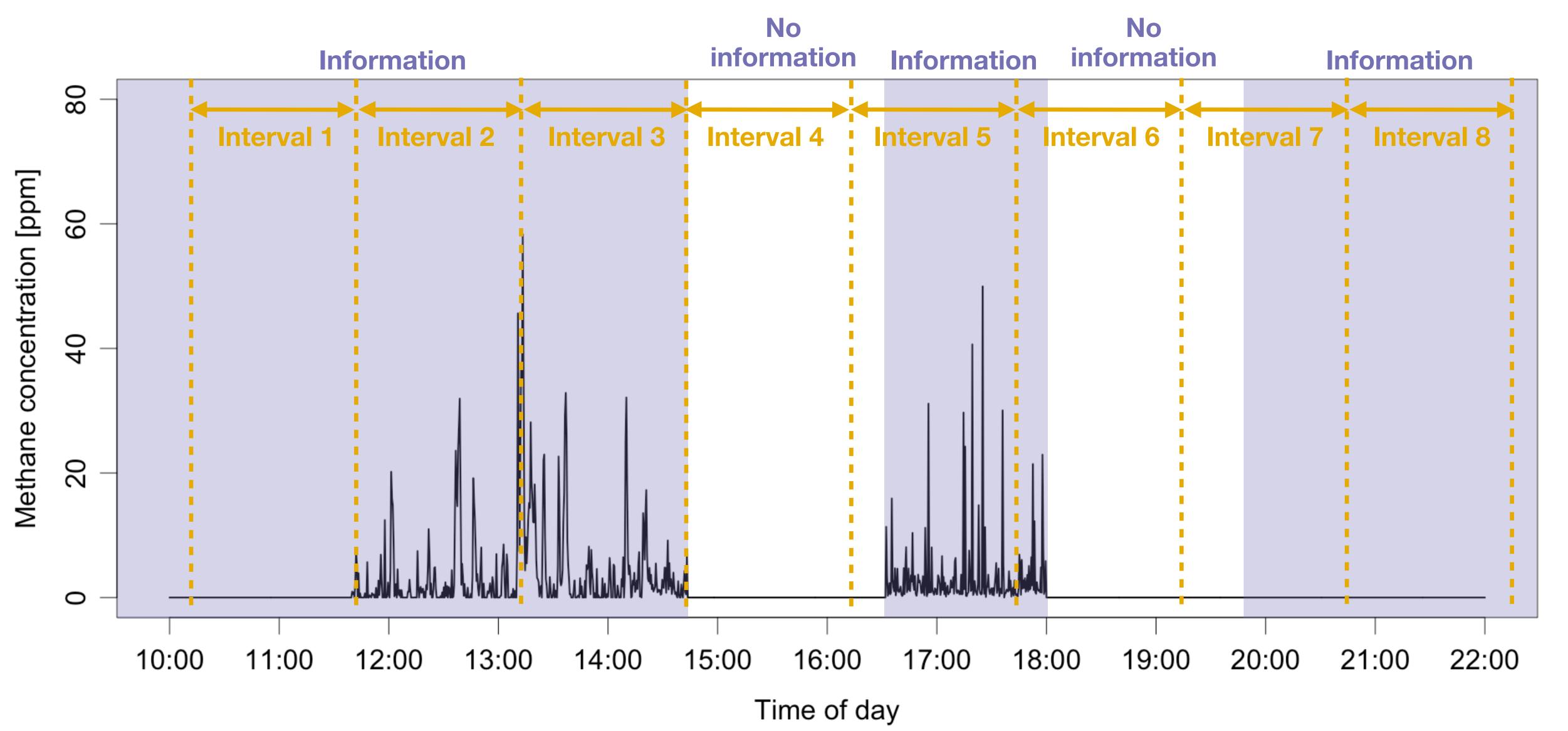
## How do periods of information and no information present themselves in the data?



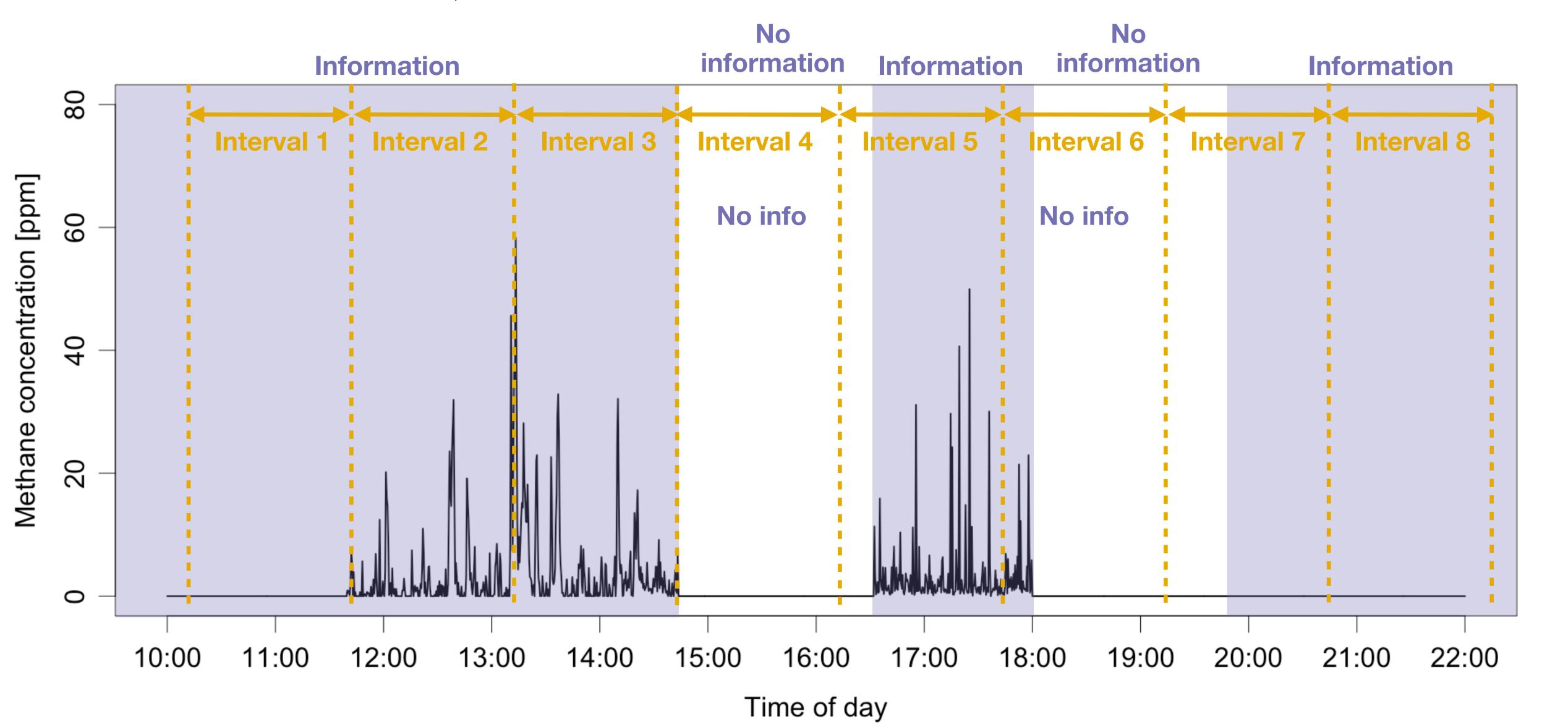
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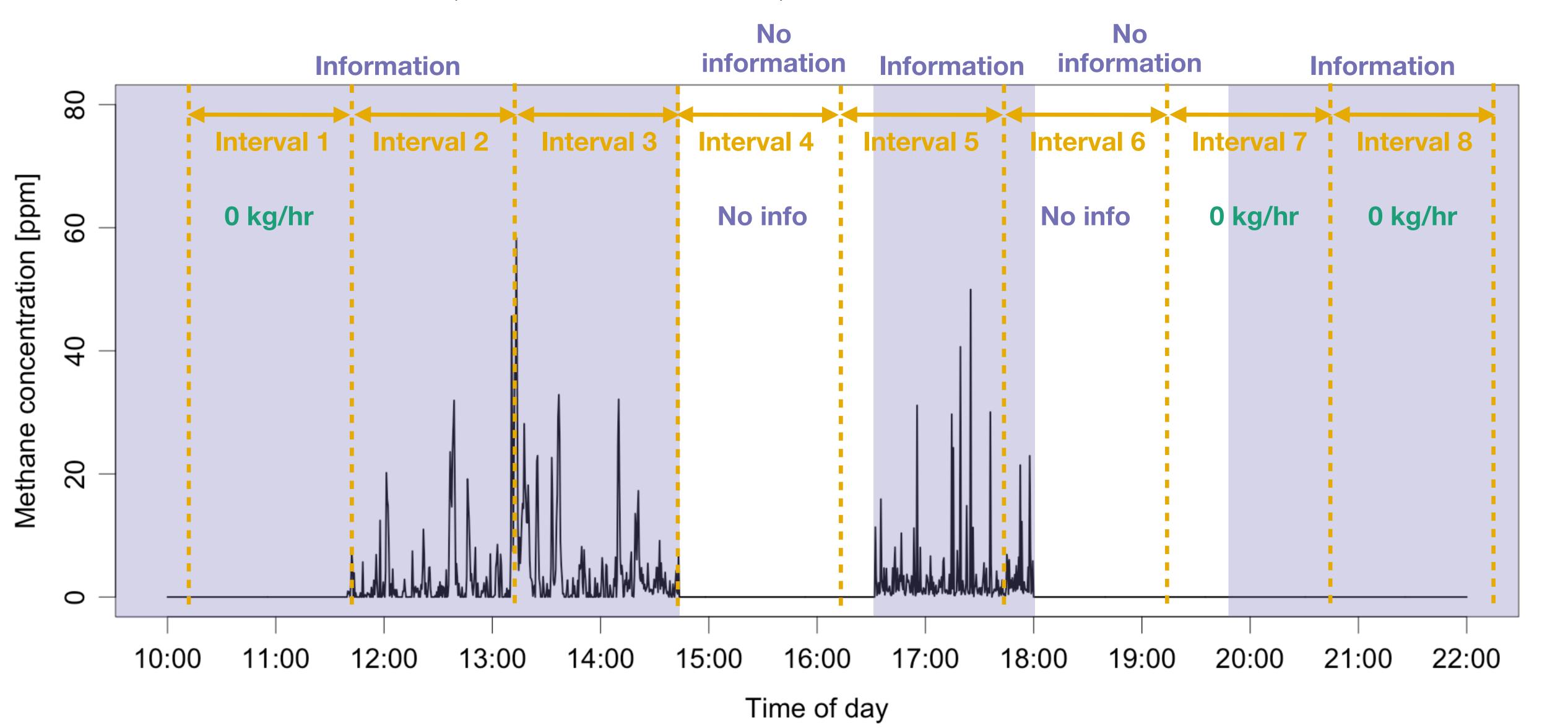
#### In practice, we estimate emissions on fixed fixed intervals



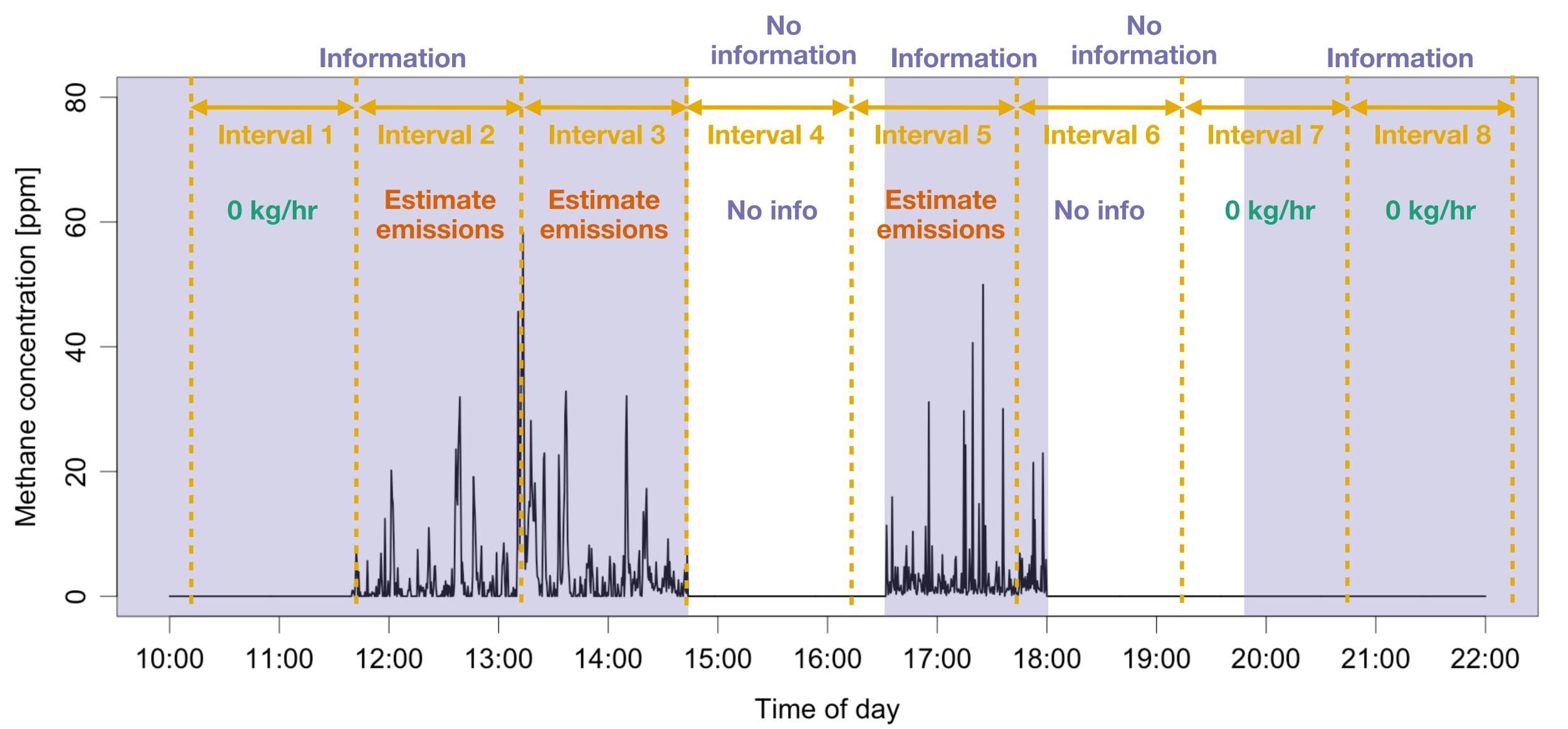
## Before building an inventory, we need to identify when an interval has no information,



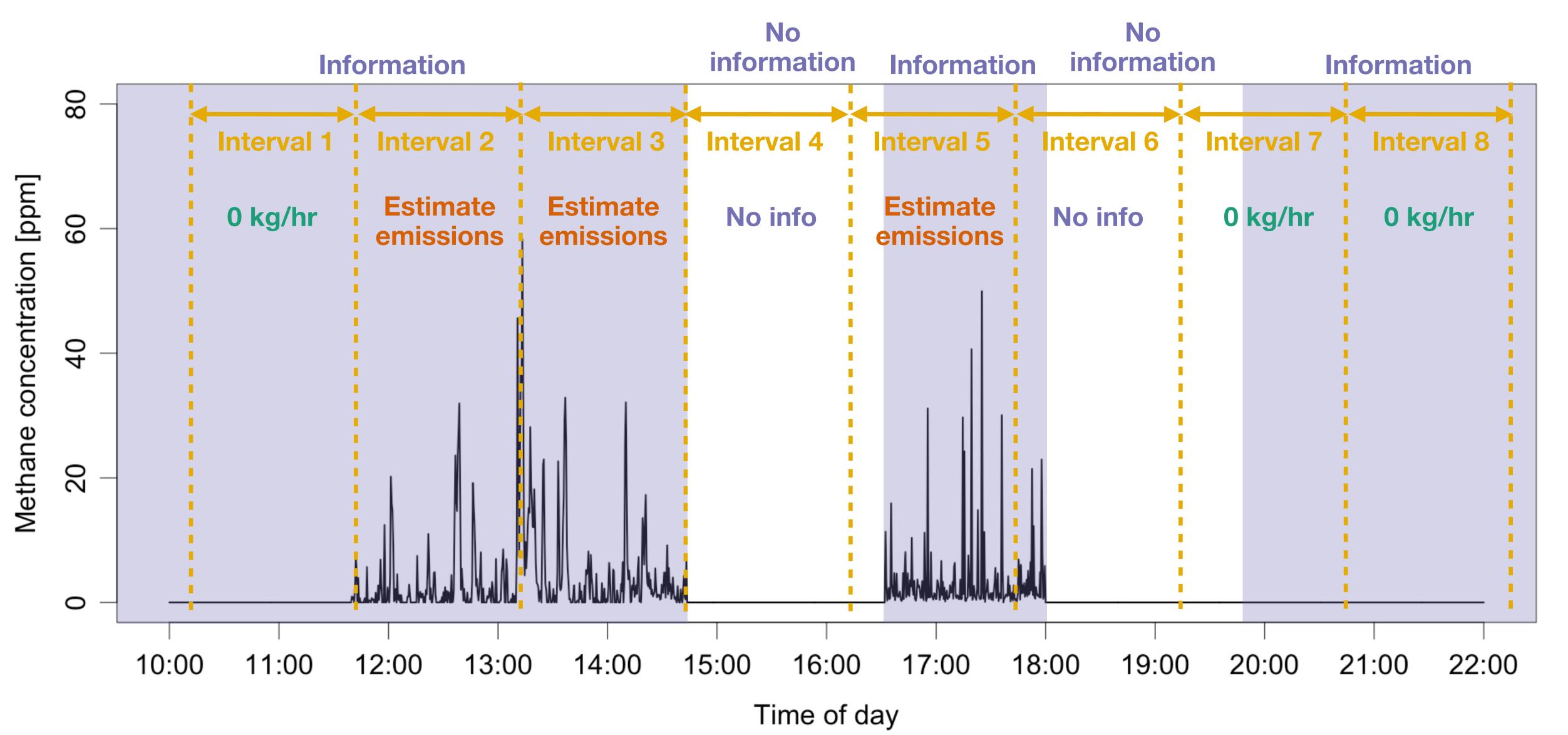
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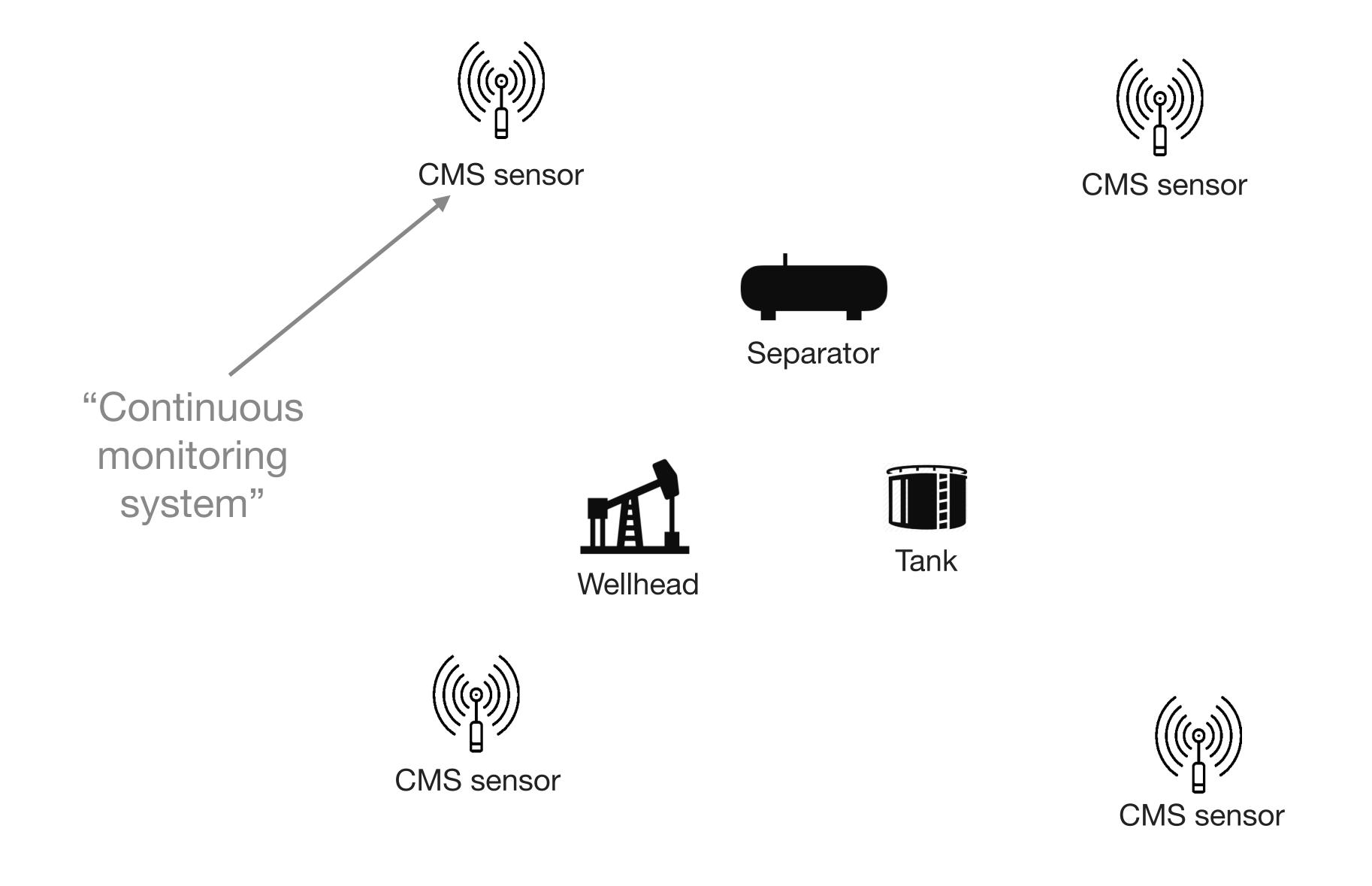


## Before building an inventory, we need to identify when an interval has no information, no emissions, or a non-zero emission

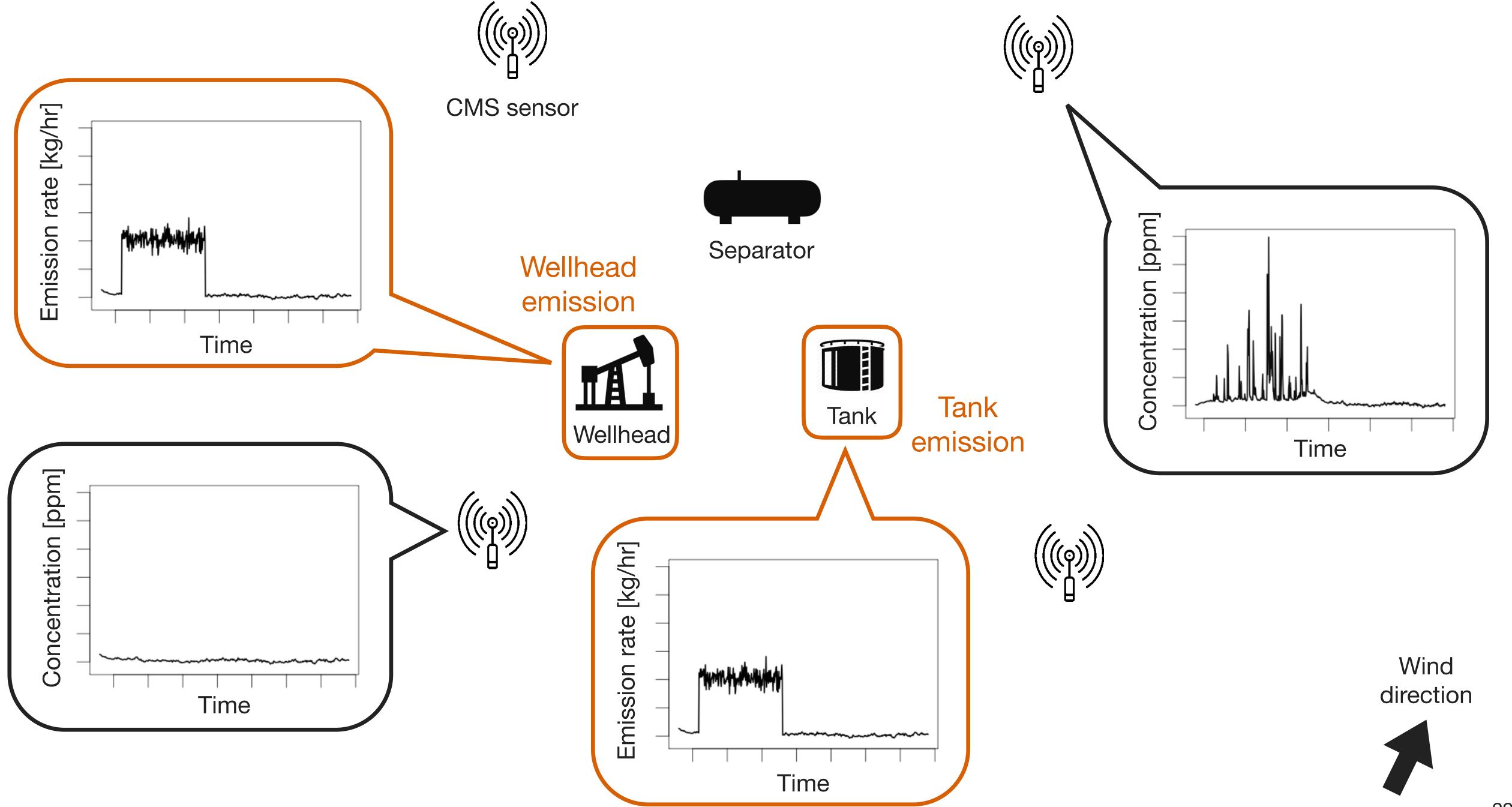


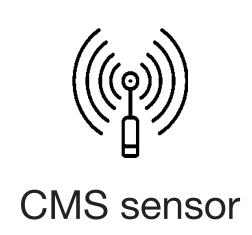
#### How do you get the inventory? We're almost there...





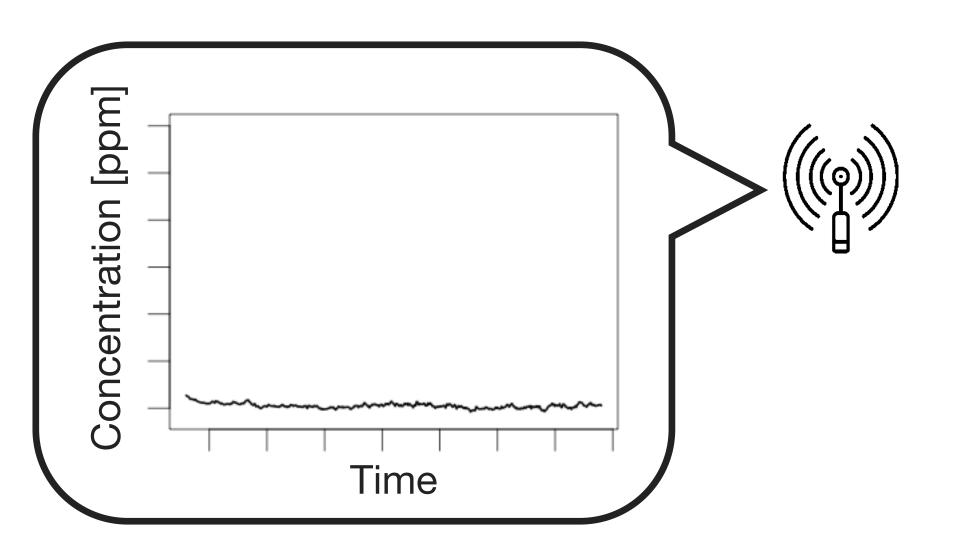
Estimating multi-source emissions with continuous monitors



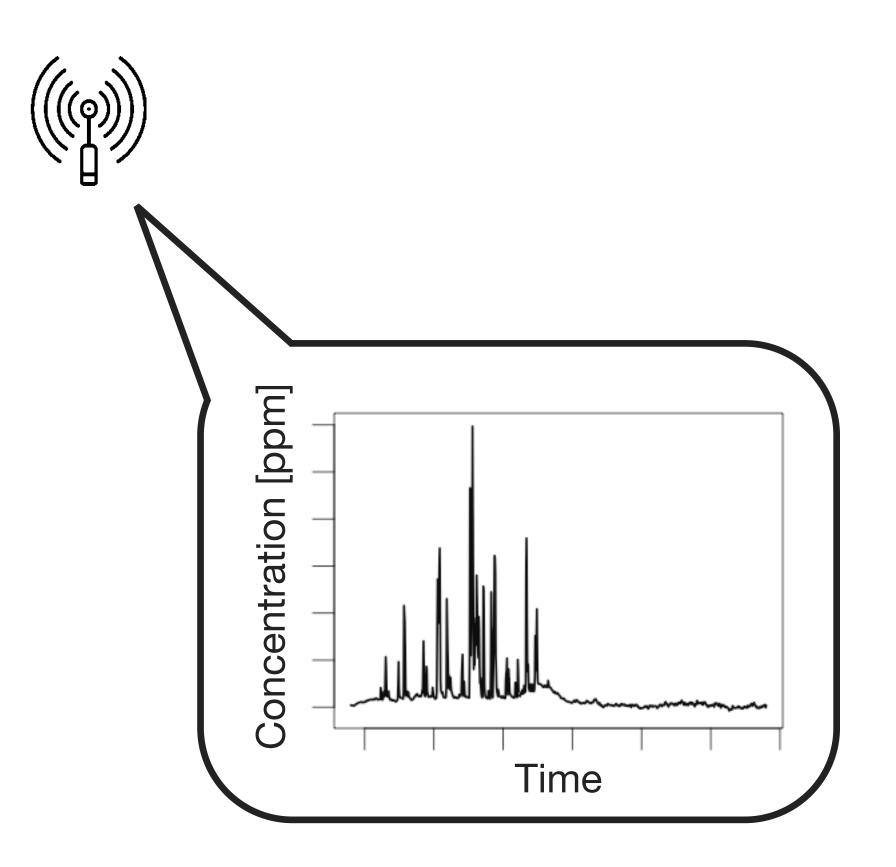














Wind direction

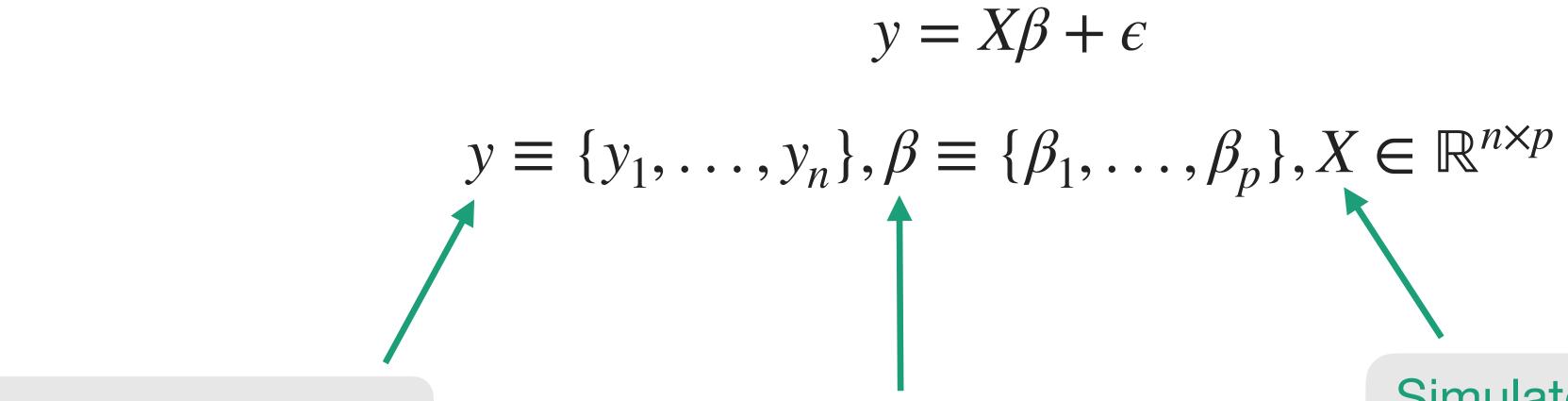


#### Multisource detection, localization, and quantification (MDLQ) model

Assume a multiple linear regression model at the data level

n = number of observations

p = number of potential sources



Concentration
observations
from CMS sensors

Emission rates for each source

Simulated concentrations from forward model, with each column assuming a different source

#### 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

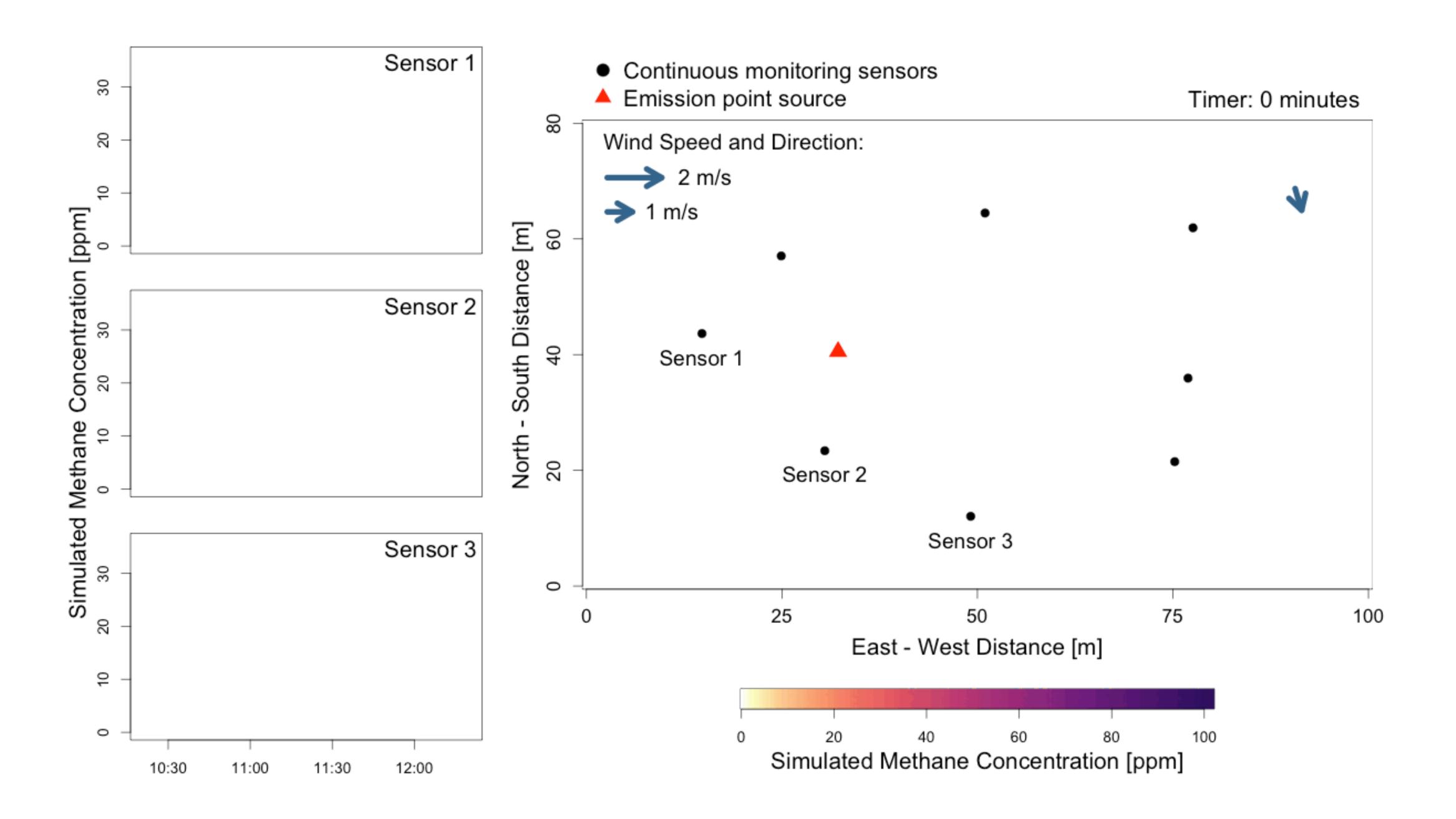
Total concentration 
$$c(x, y, z, t, Q) = \sum_{p=1}^{\infty} c_p(x, y, z, t, Q)$$
 at  $(x, y, z, t)$ 

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

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

Exponential decay in concentration in vertical dimension (z)



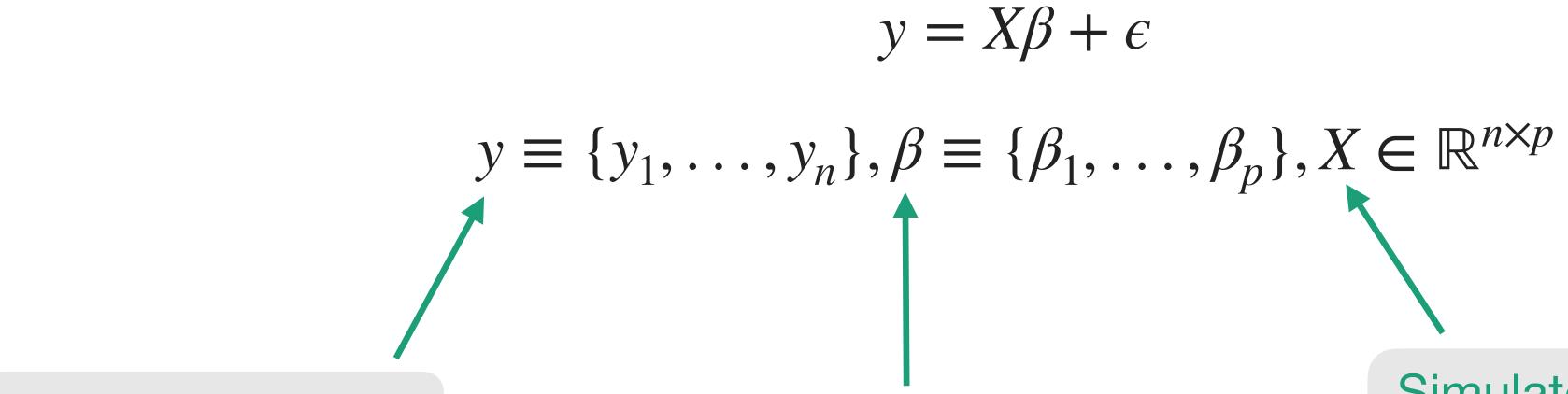


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Assume a multiple linear regression model at the data level

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

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

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

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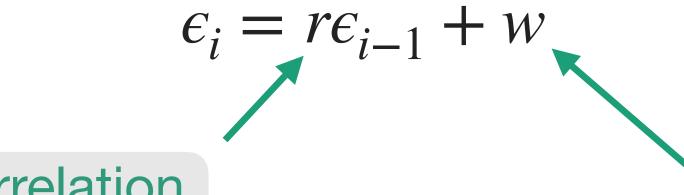
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Let the errors follow an AR(1) process such that



Autocorrelation coefficient

Gaussian white noise

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

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

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

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

 $y = X\beta + \epsilon$ Data-level:

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

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

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

$$z_i = 0$$

"Slab" component is non-negative

Proportion of samples where  $z_i = 1$  gives

posterior probability that source i is emitting

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

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

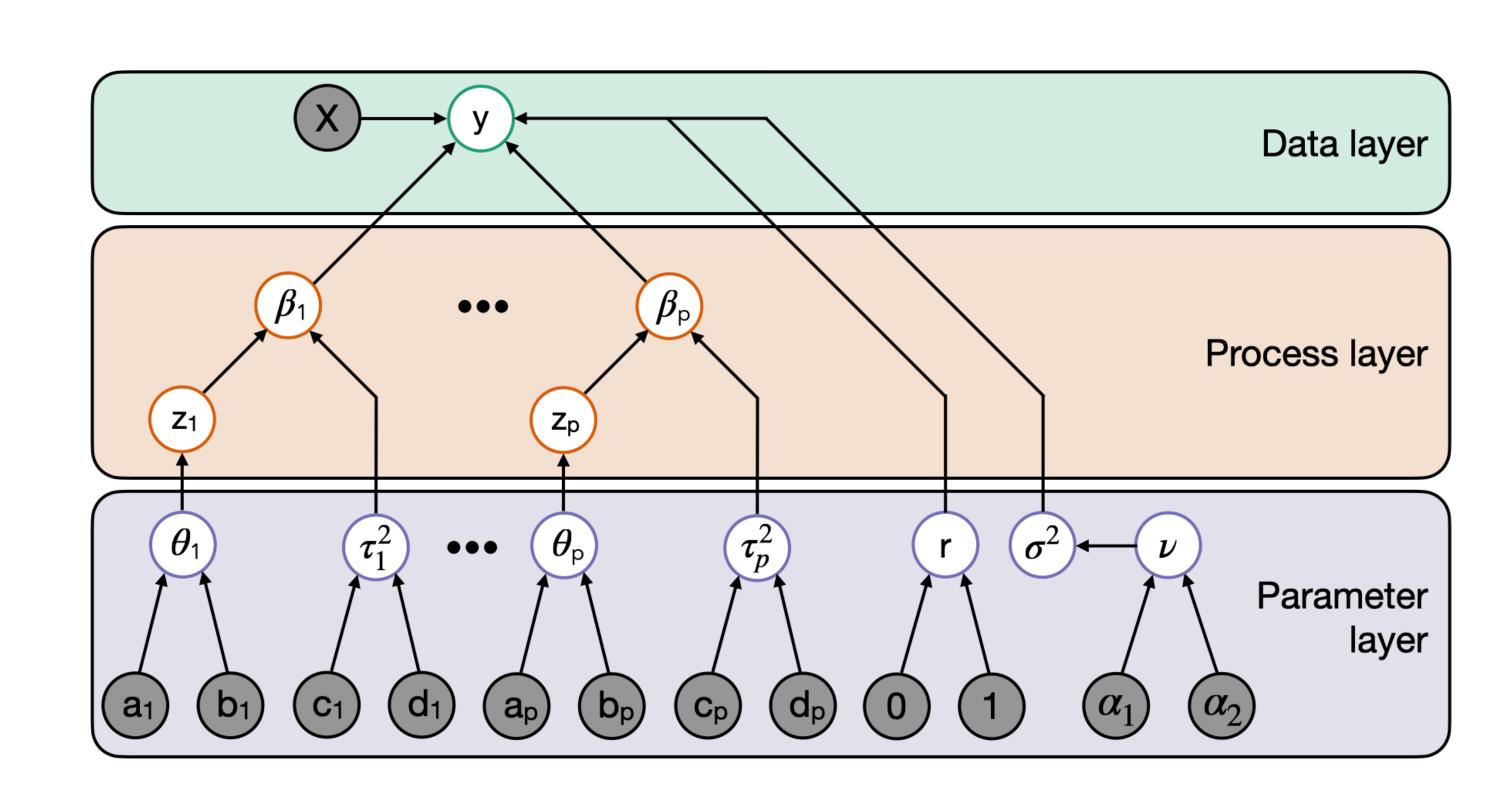
 $\sigma^2 \sim \text{Inv-Gamma}(\nu/2, \nu/2)$ 

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

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

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  $\nu$ .

$$\theta_{i}|\xi \sim \text{Beta}(z_{i} + a_{i}, 1 - z_{i} + b_{i})$$

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

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

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

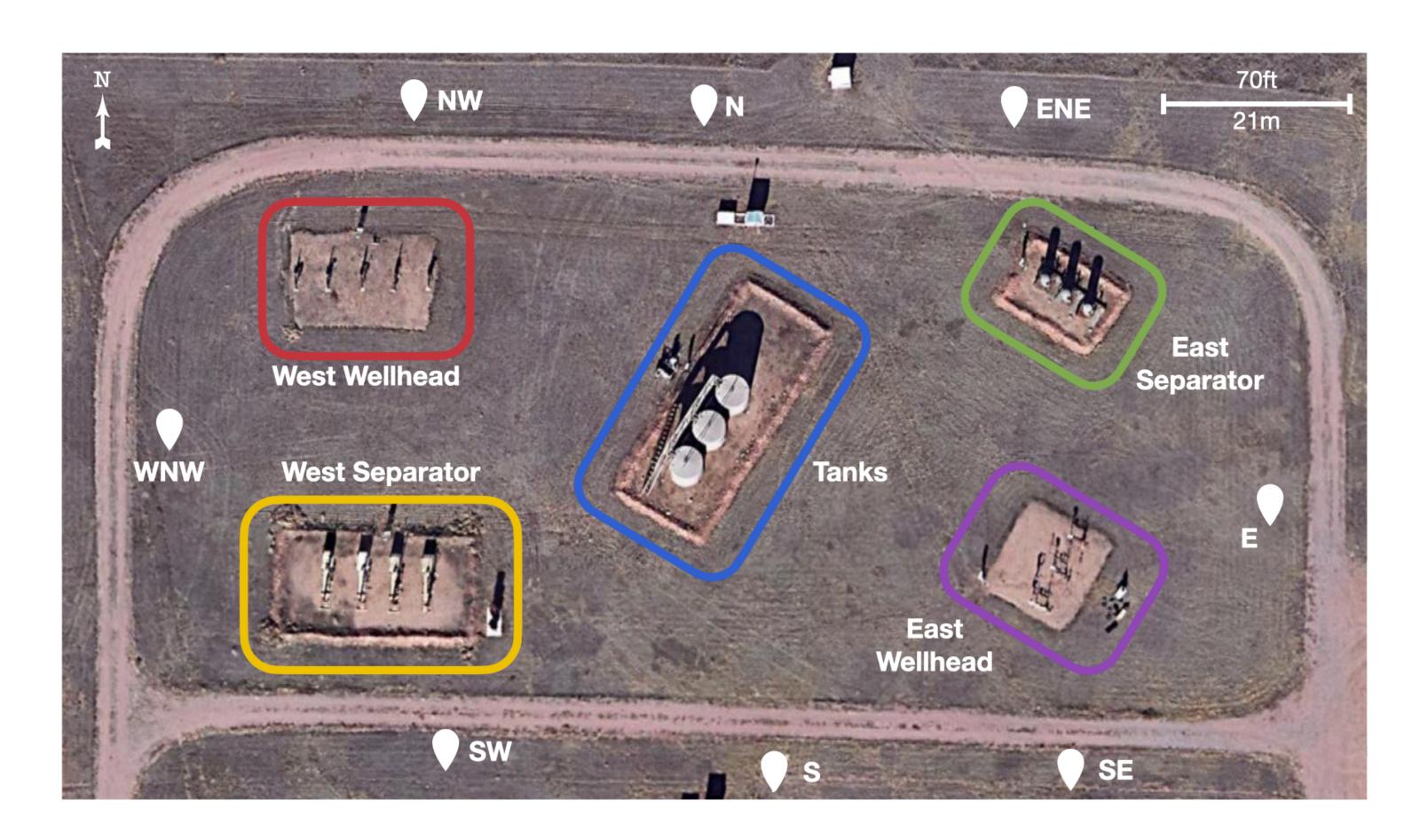
$$\beta_i | \xi \sim \begin{cases} 0 & z_i = 0 \\ \mathcal{N} \left( \left( \frac{X^T R^{-1} X}{\sigma^2} \right)^{-1} \left( \frac{X^T R^{-1} y}{\sigma^2} - \frac{e_i}{\tau_i^2 \sigma^2} \right), \left( \frac{X^T R^{-1} X}{\sigma^2} \right)^{-1} \right) & z_i = 1 \end{cases}$$

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

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

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

#### Model evaluation on multi-source controlled release data



Methane Emissions Technology Evaluation Center (METEC)

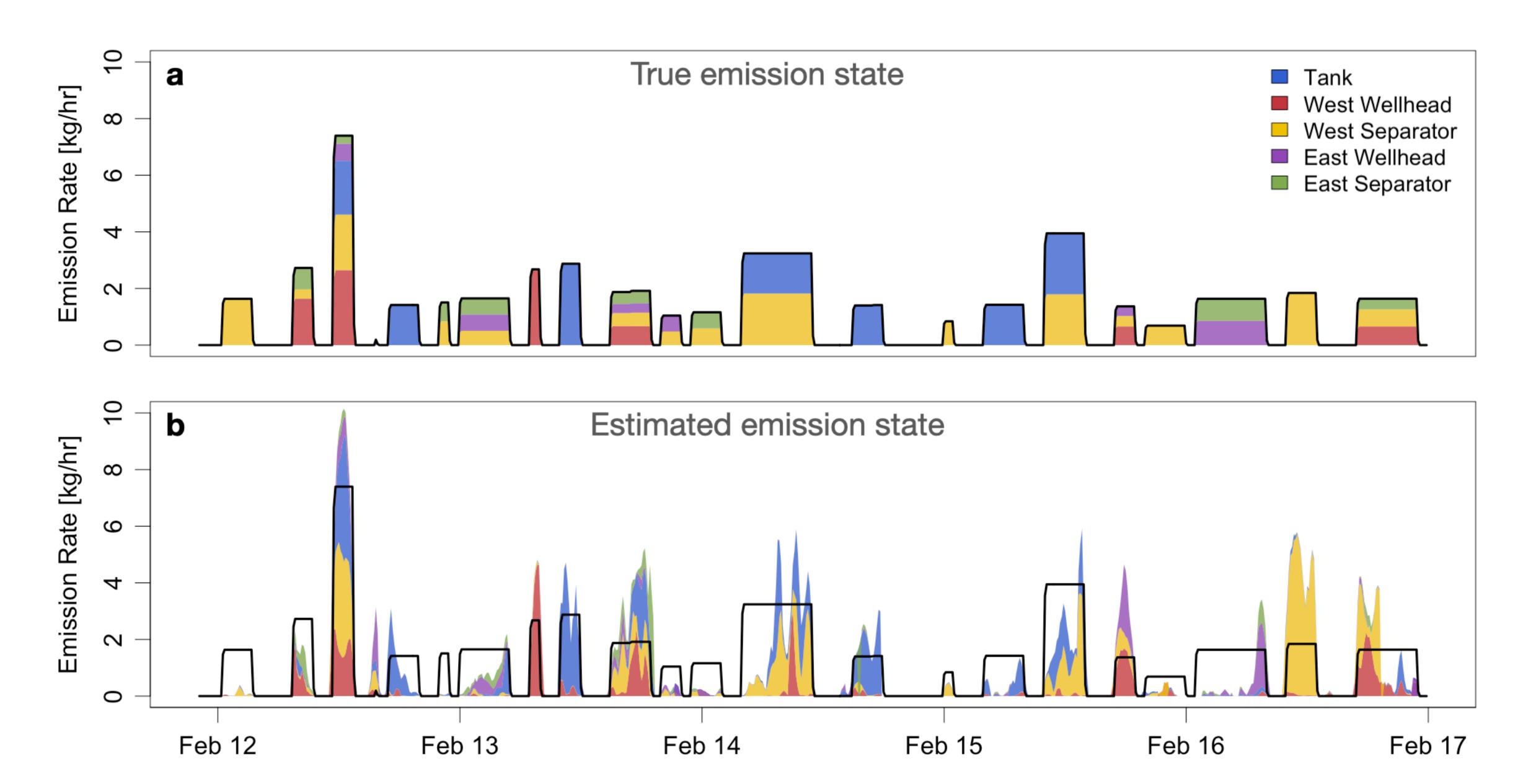
337 controlled releases:

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

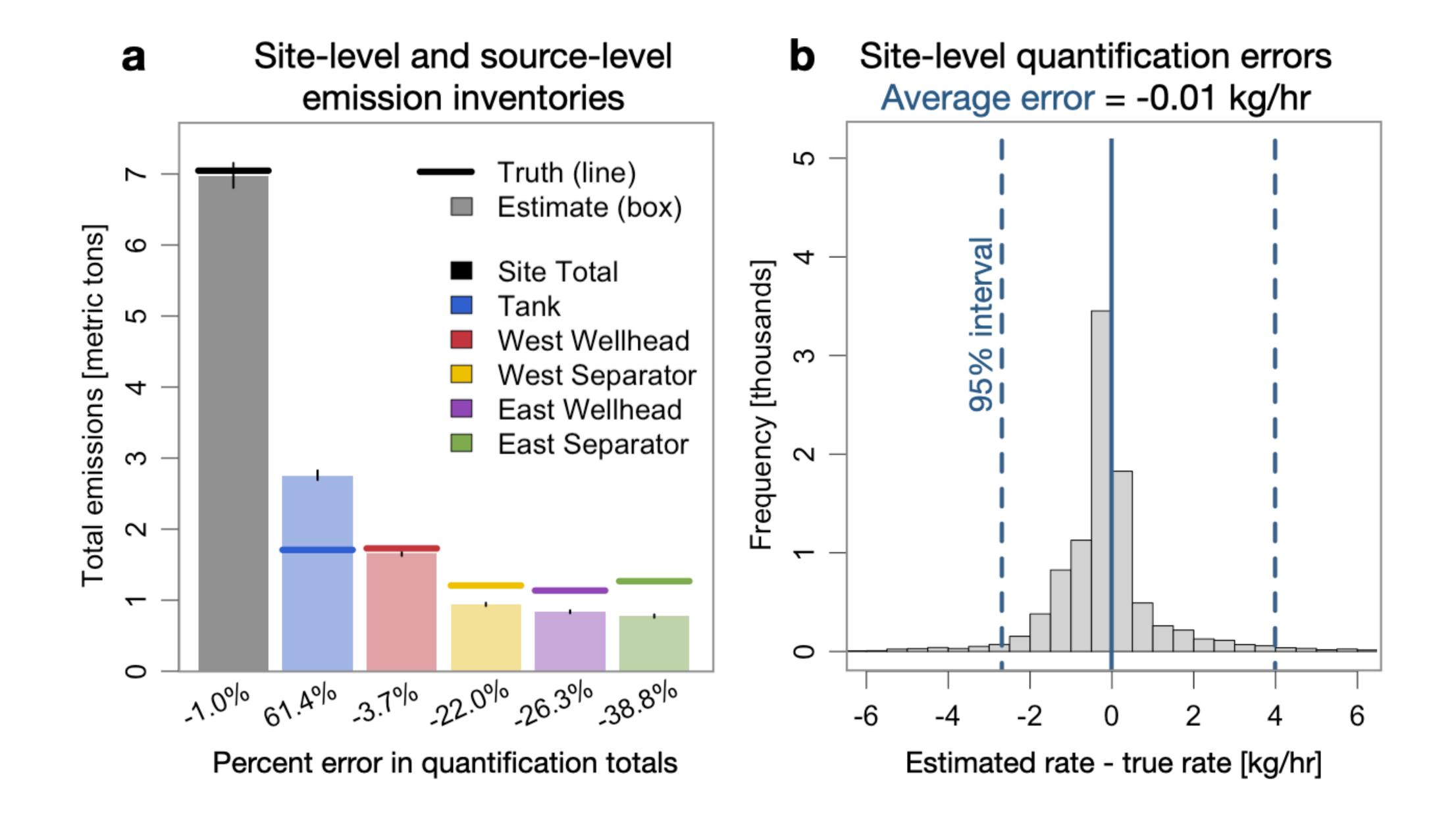
Emission rates range from **0.08** to **7.2** kg/hr

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

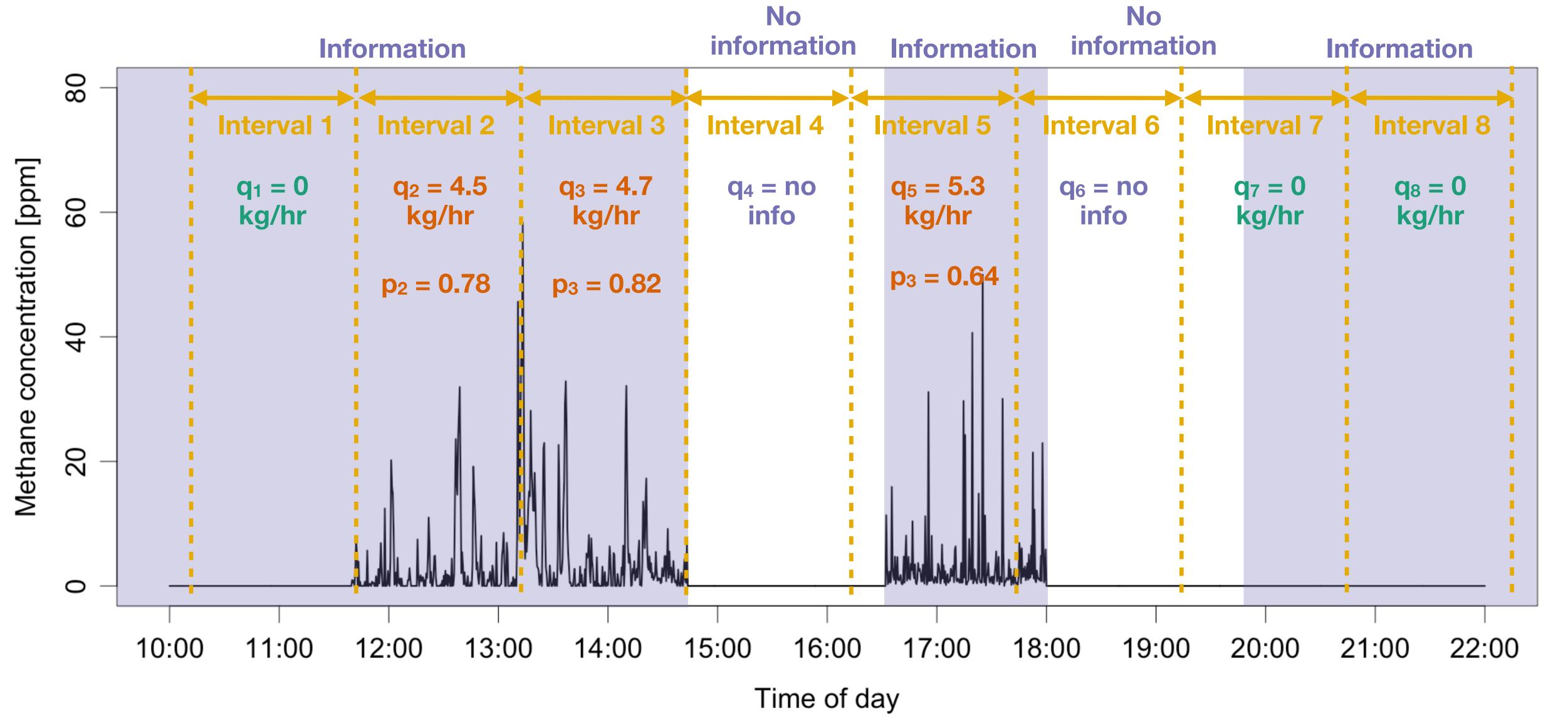
#### Model evaluation on multi-source controlled release data



#### Model evaluation on multi-source controlled release data



## Need to identify when an interval is no information, no emissions, or a non-zero emission



# Measurement-based inventory results for the Appalachian Methane Initiative (AMI)

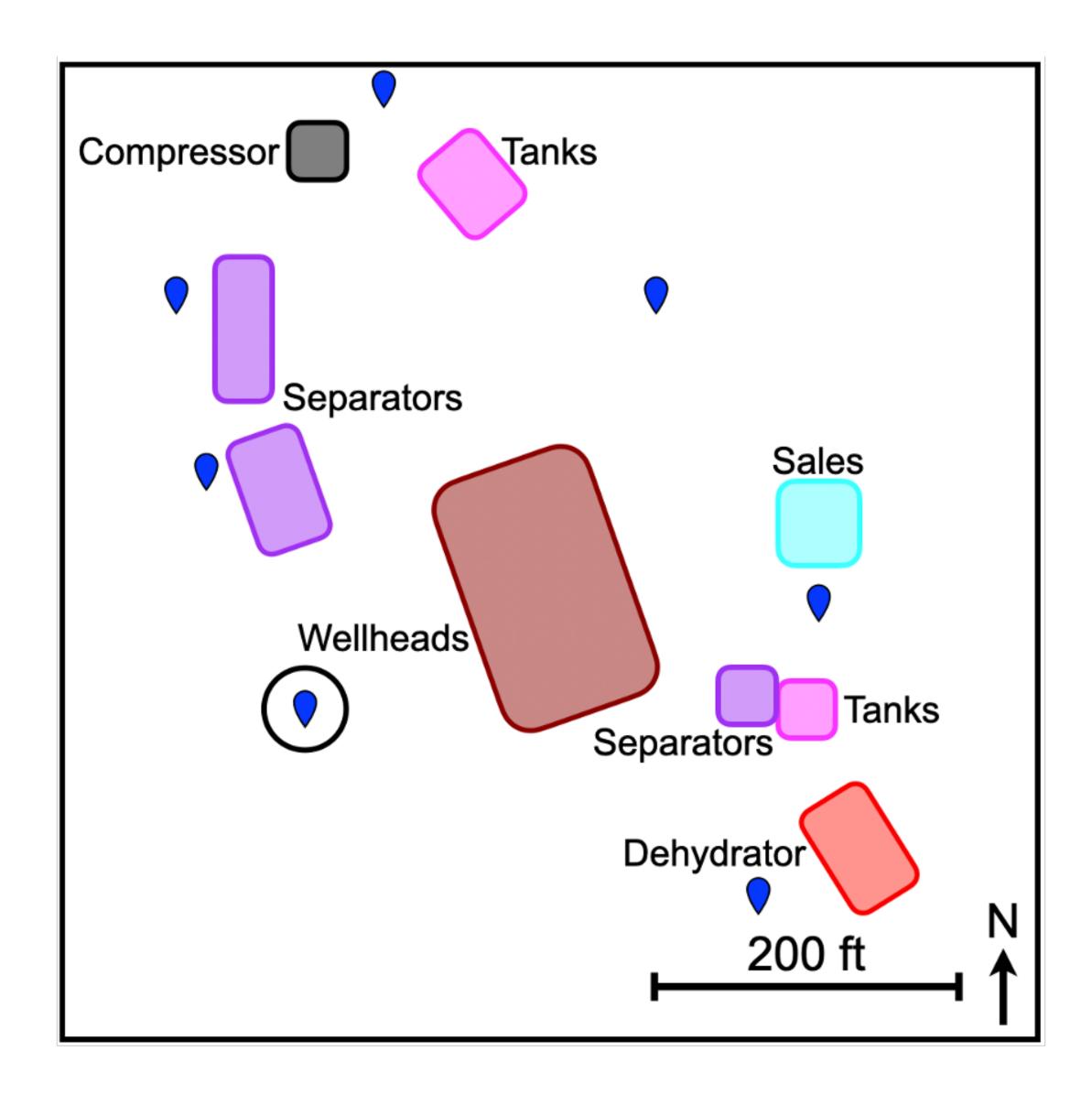
#### We have data from 26 production sites

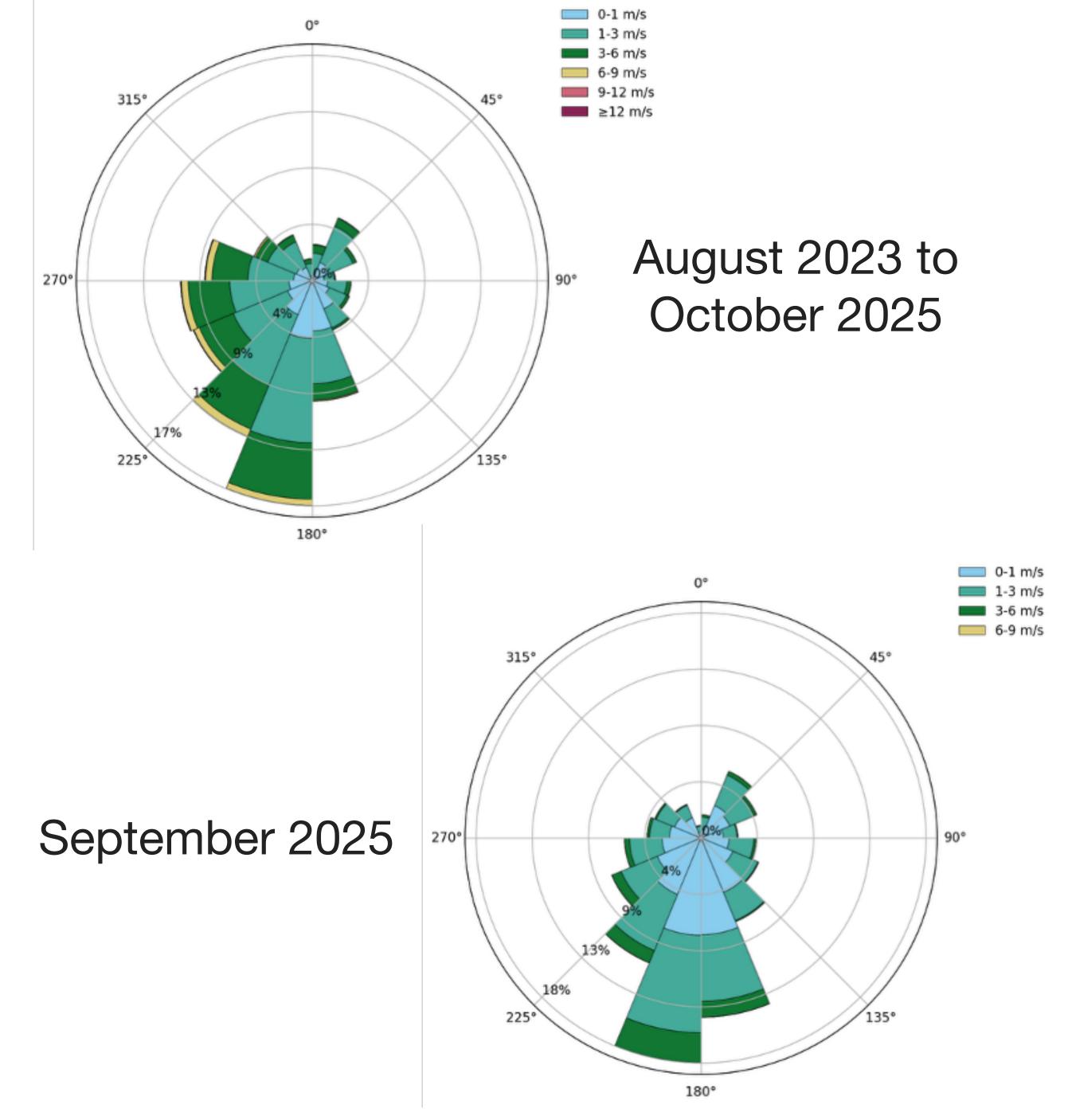
- All are equipped with high-end continuous monitoring point sensors
- Number of sensors per site varies from 3 to 7

#### 57.82 total years of data

Average of 2.22 years per site

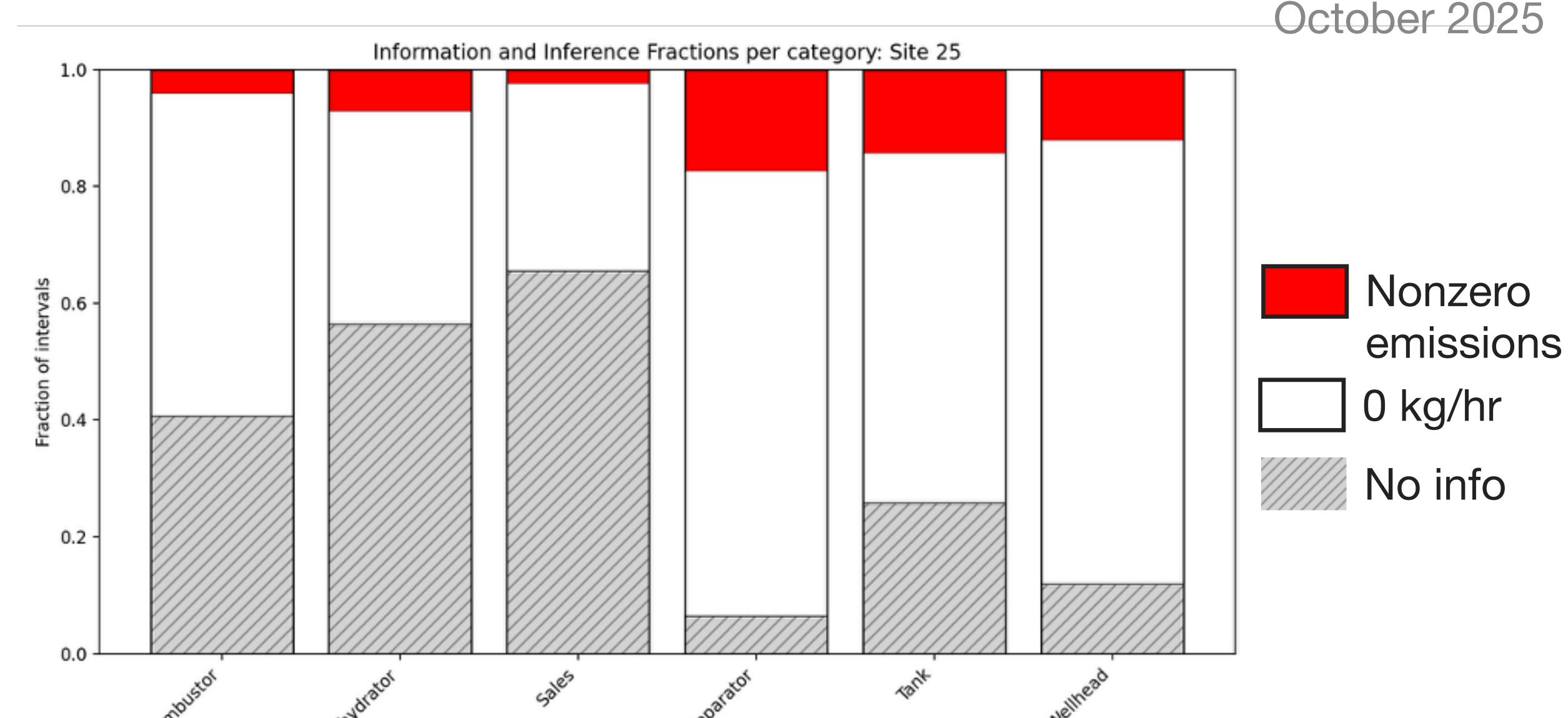
## Example: Site 25





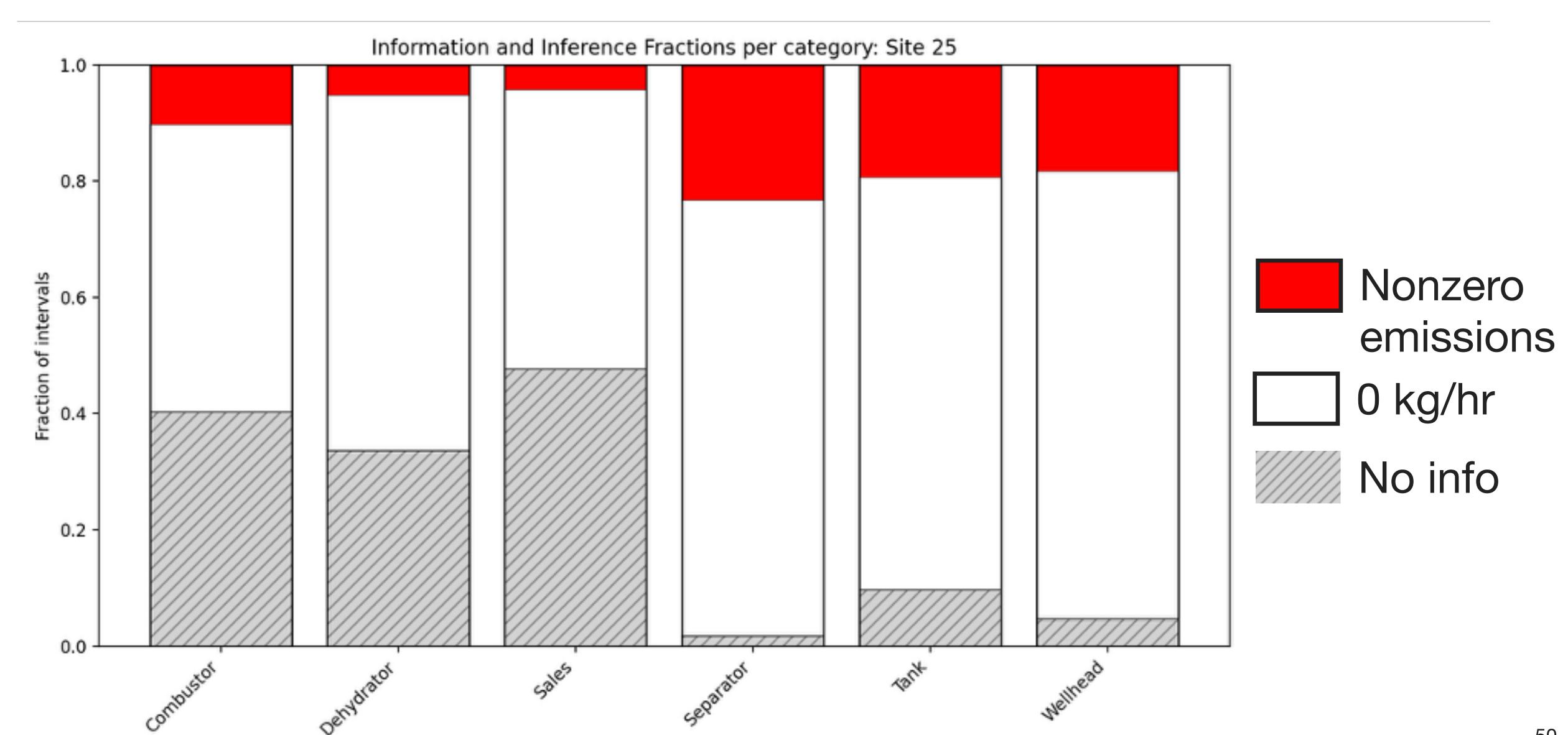
#### Ratio of no information to information

August 2023 to

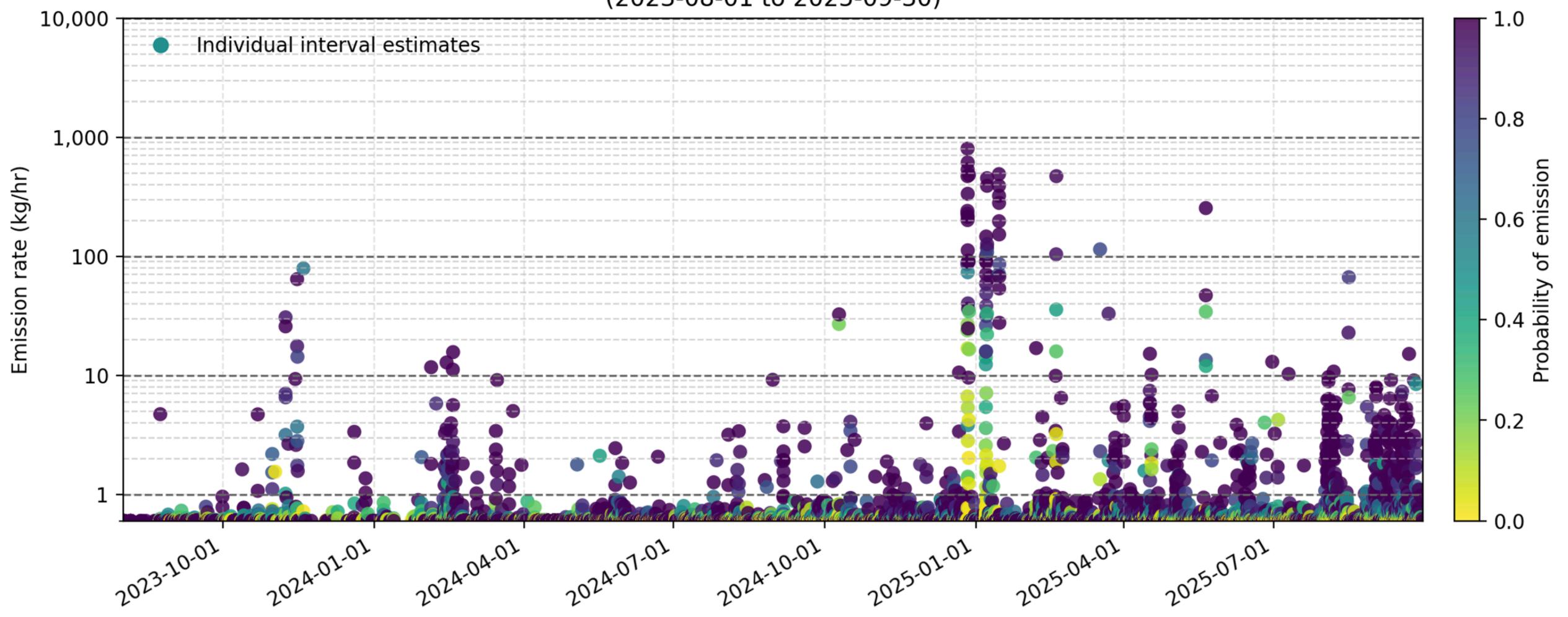


## Ratio of no information to information

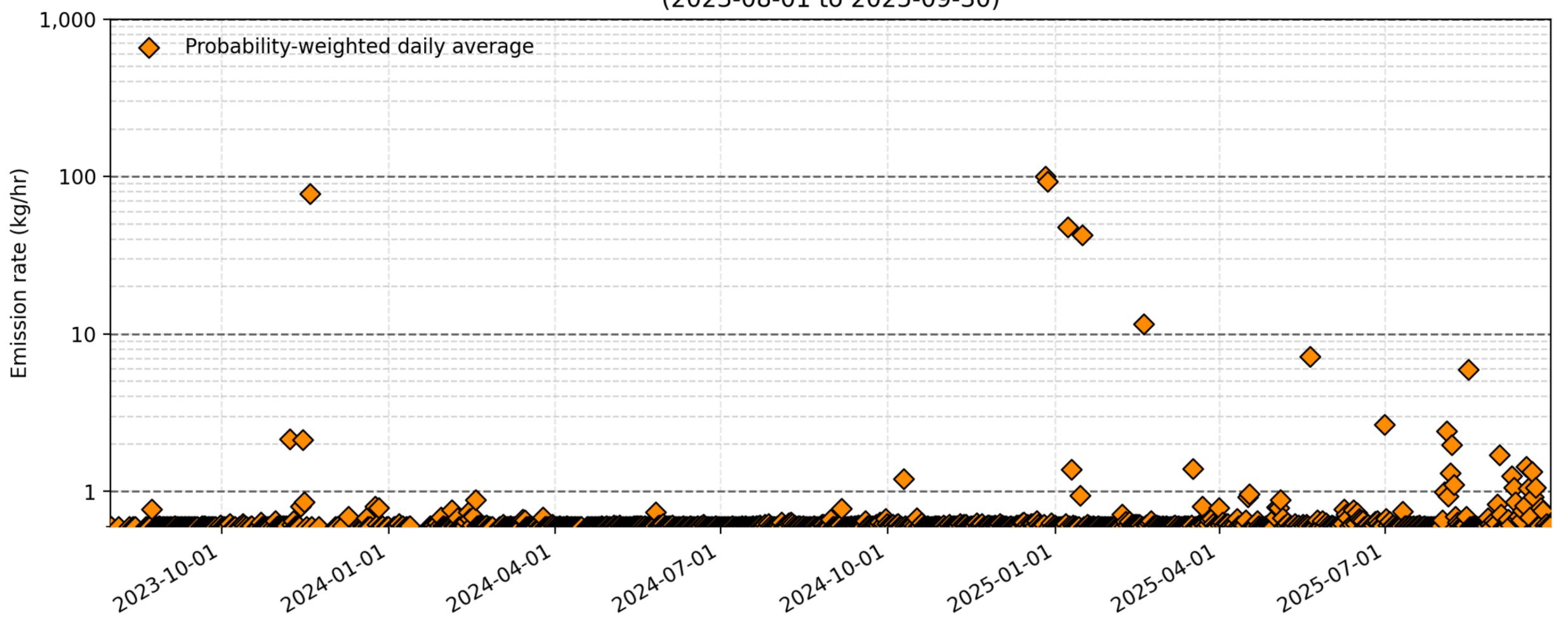
September 2025

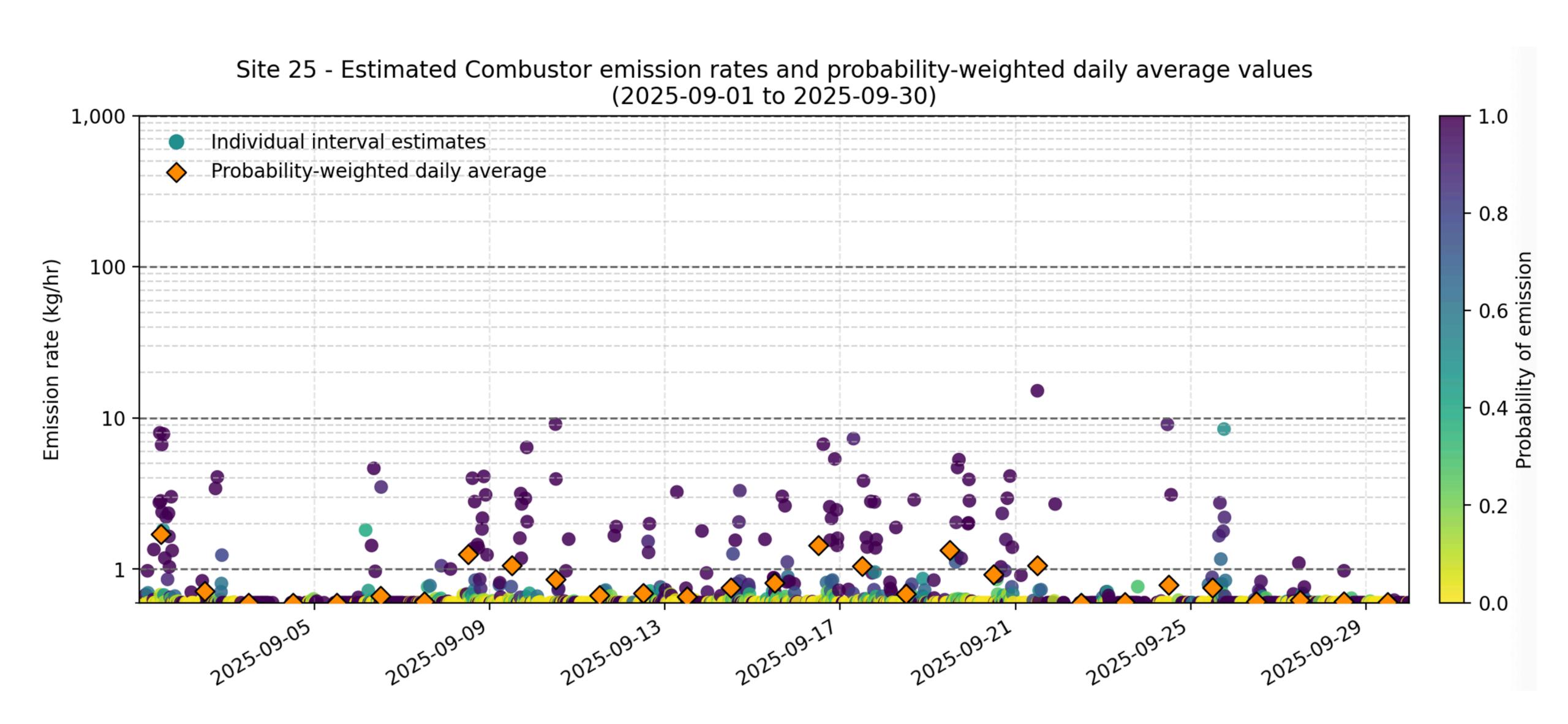


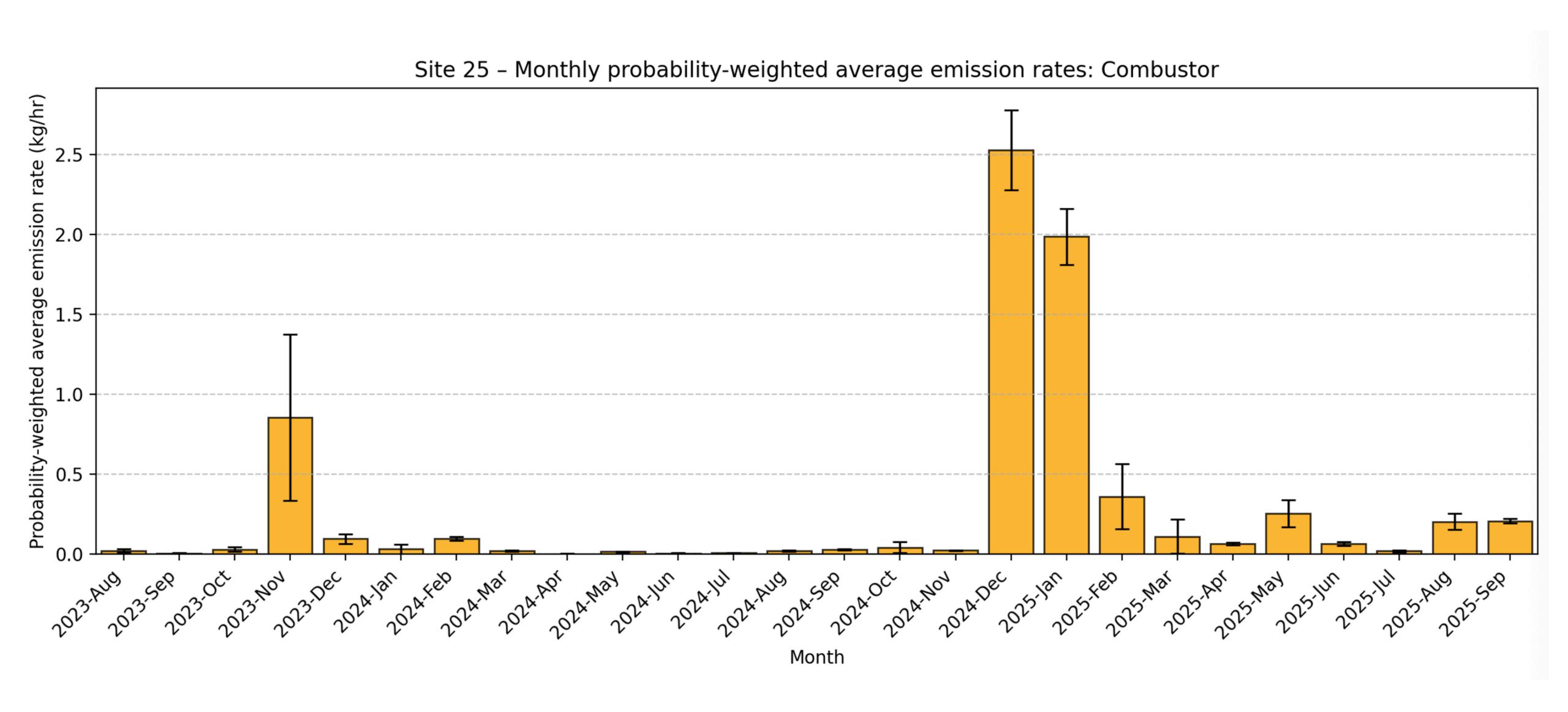
Site 25 - Estimated Combustor emission rates (2023-08-01 to 2025-09-30)

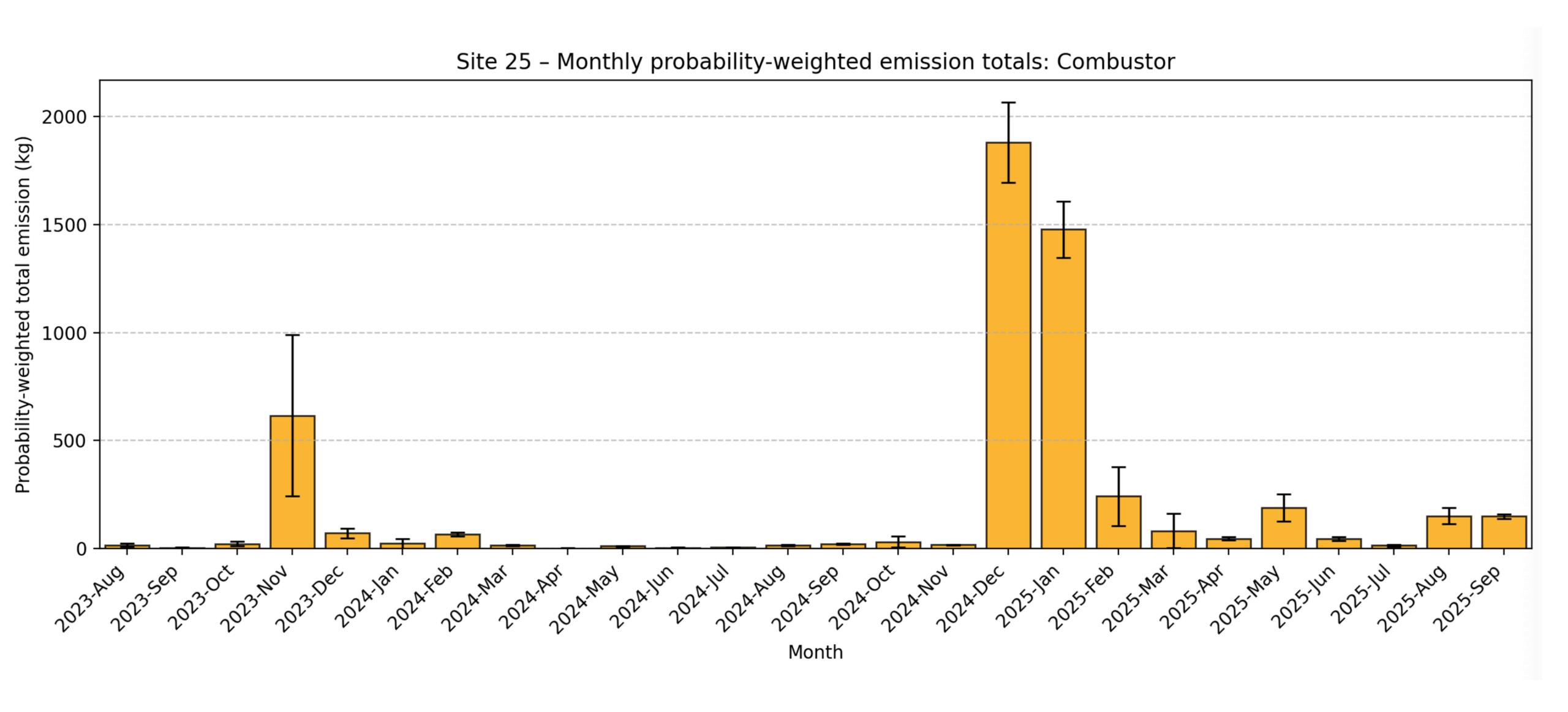


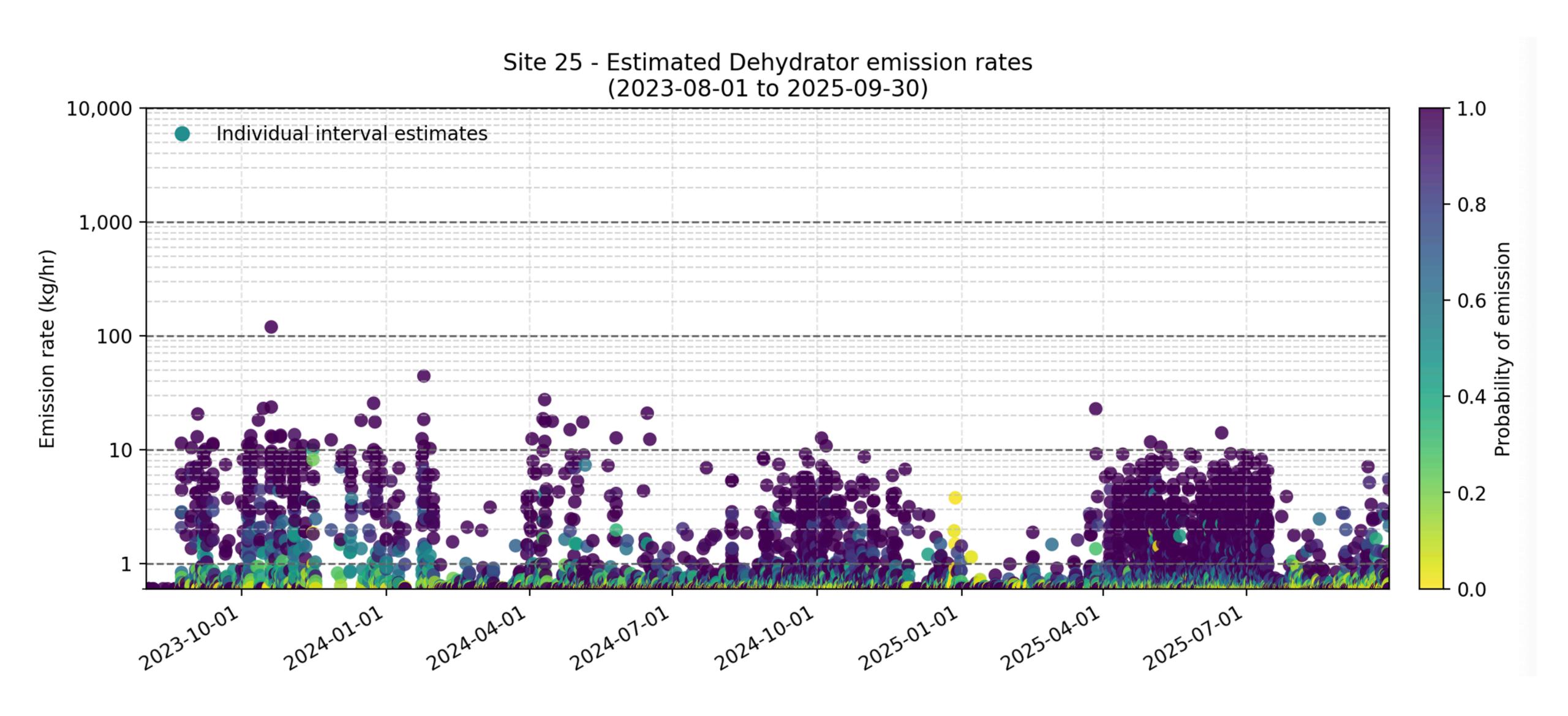
Site 25 - Estimated Combustor probability-weighted daily average values (2023-08-01 to 2025-09-30)

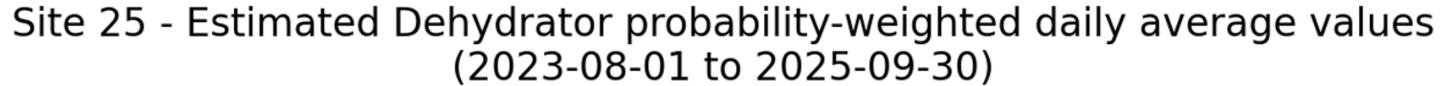


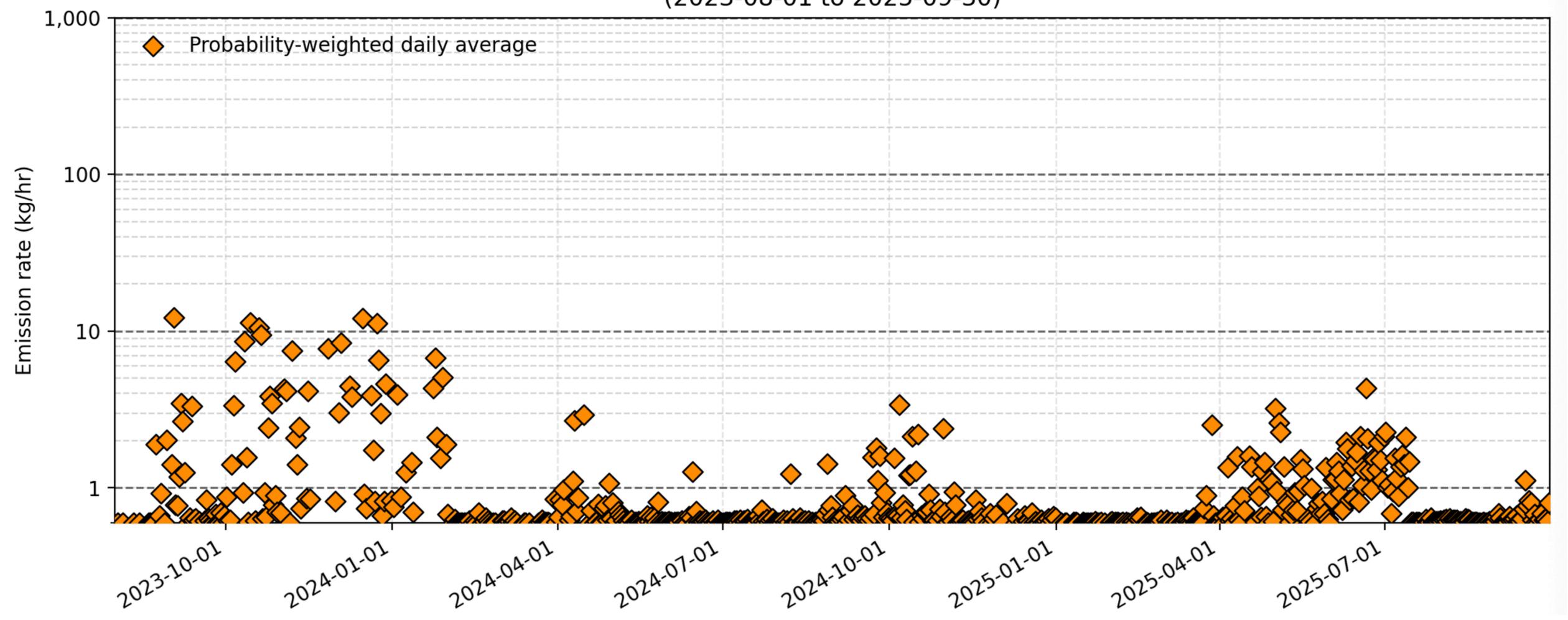




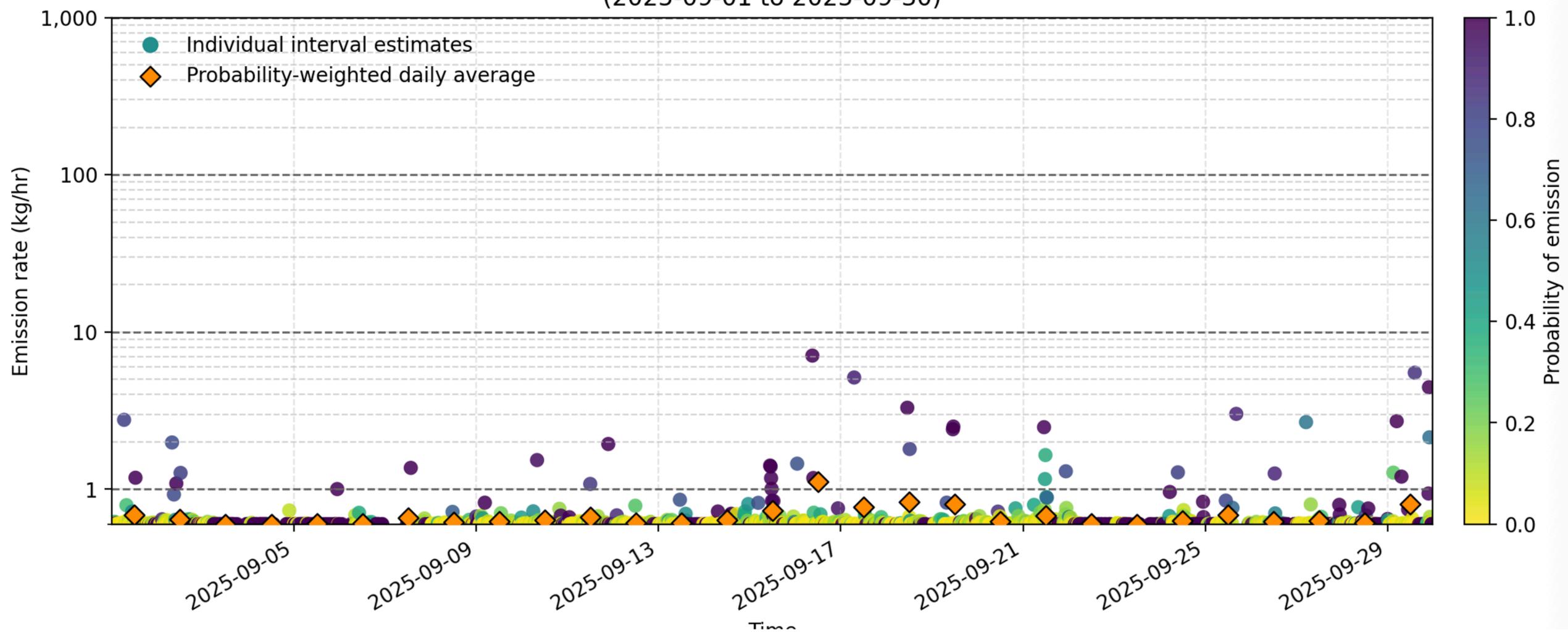


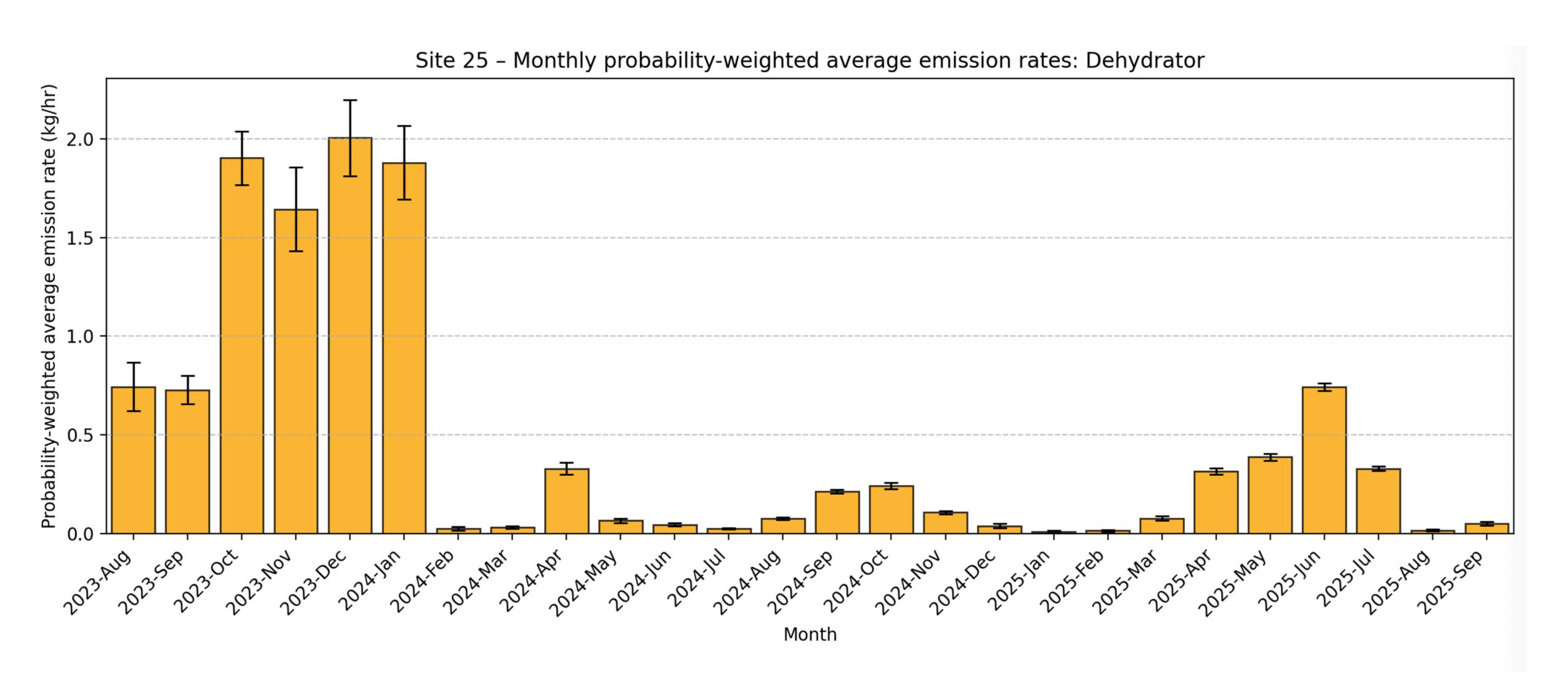


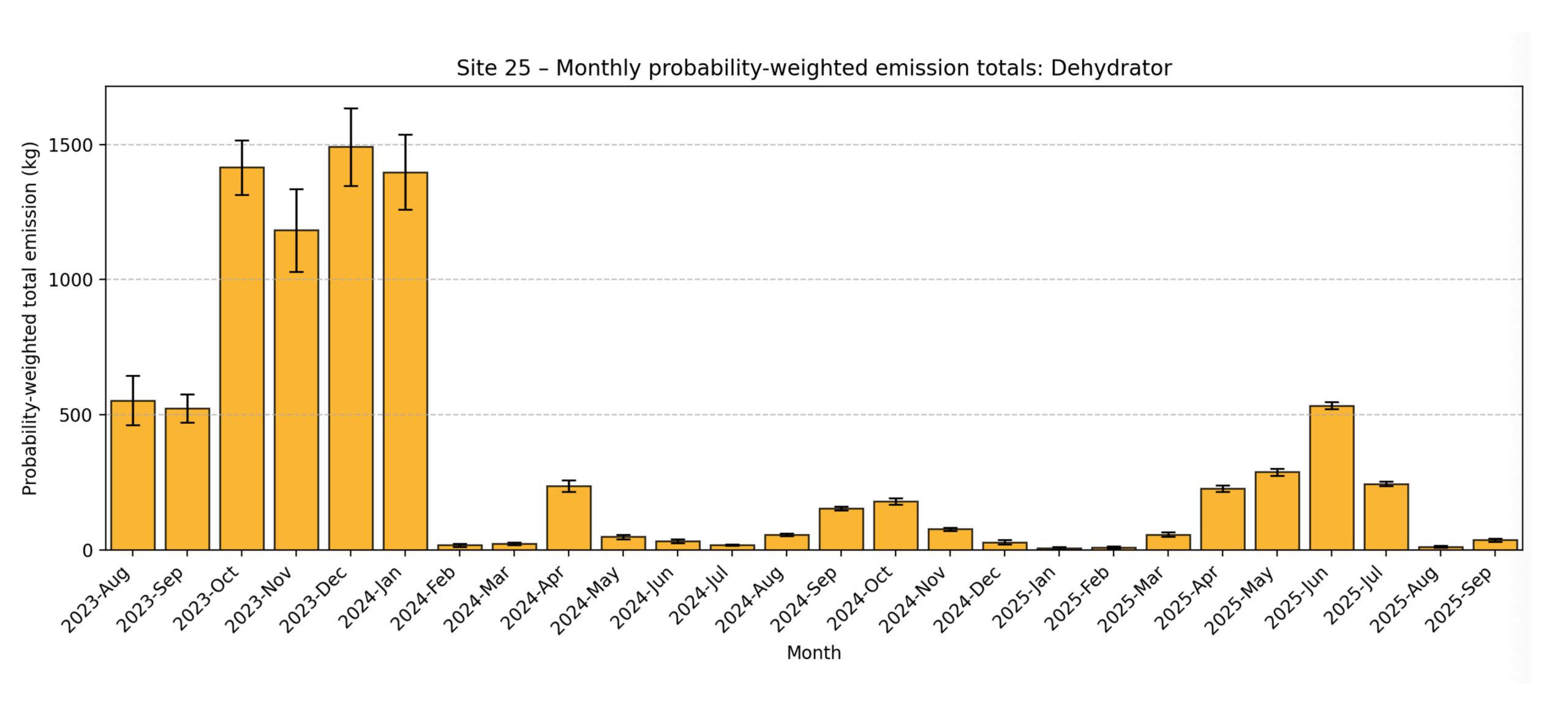


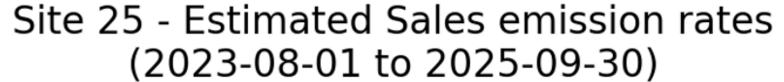


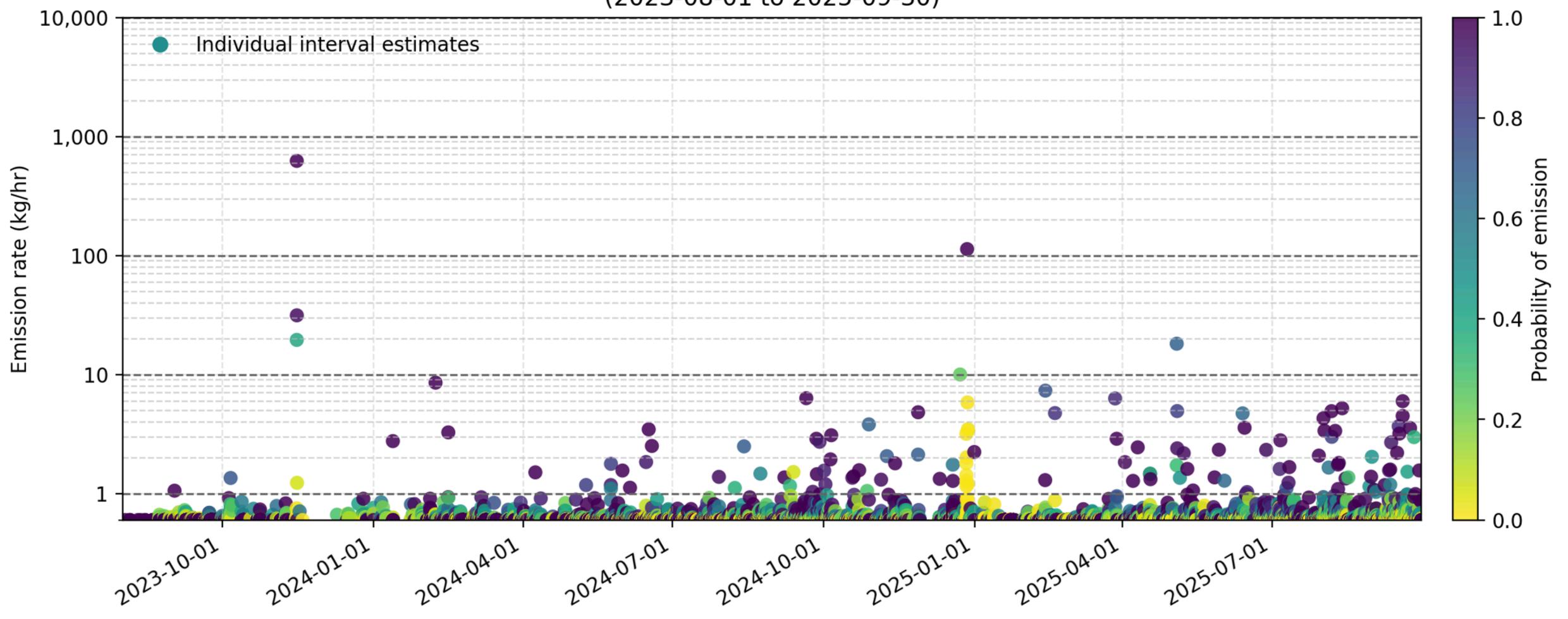
Site 25 - Estimated Dehydrator emission rates and probability-weighted daily average values (2025-09-01 to 2025-09-30)



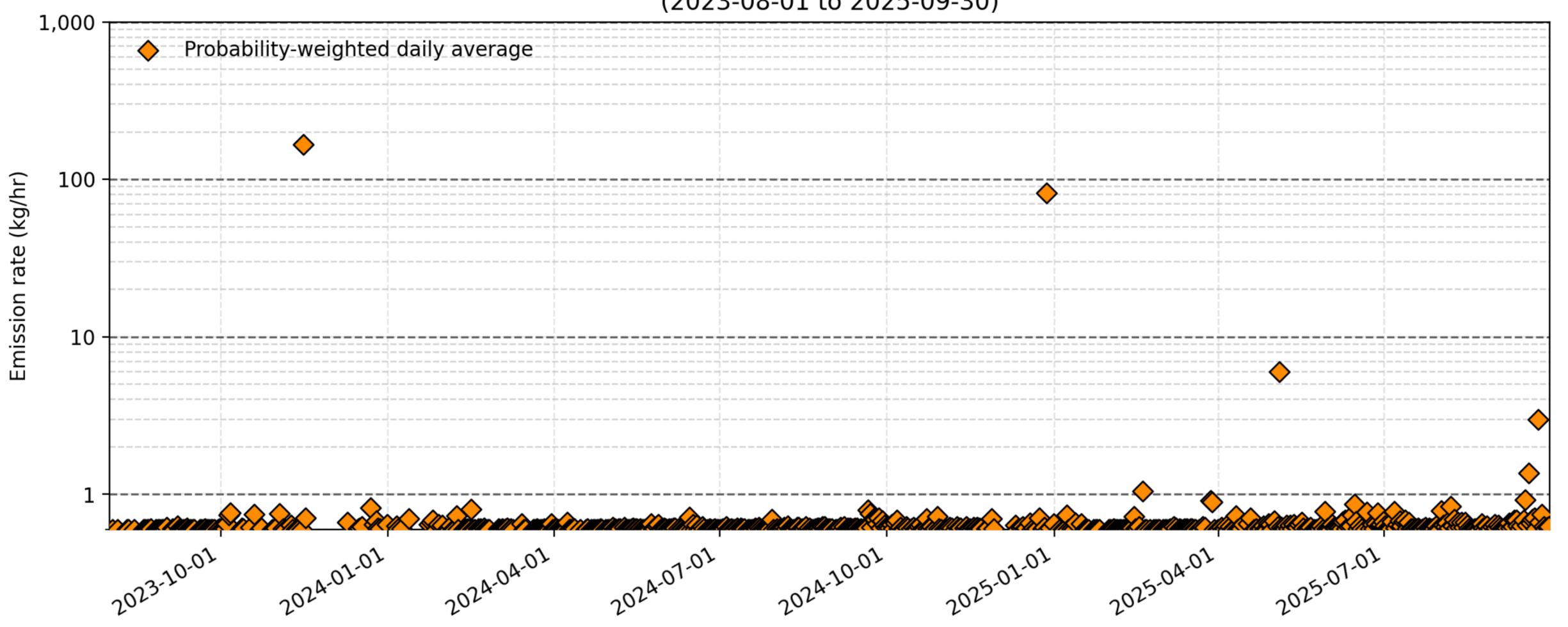


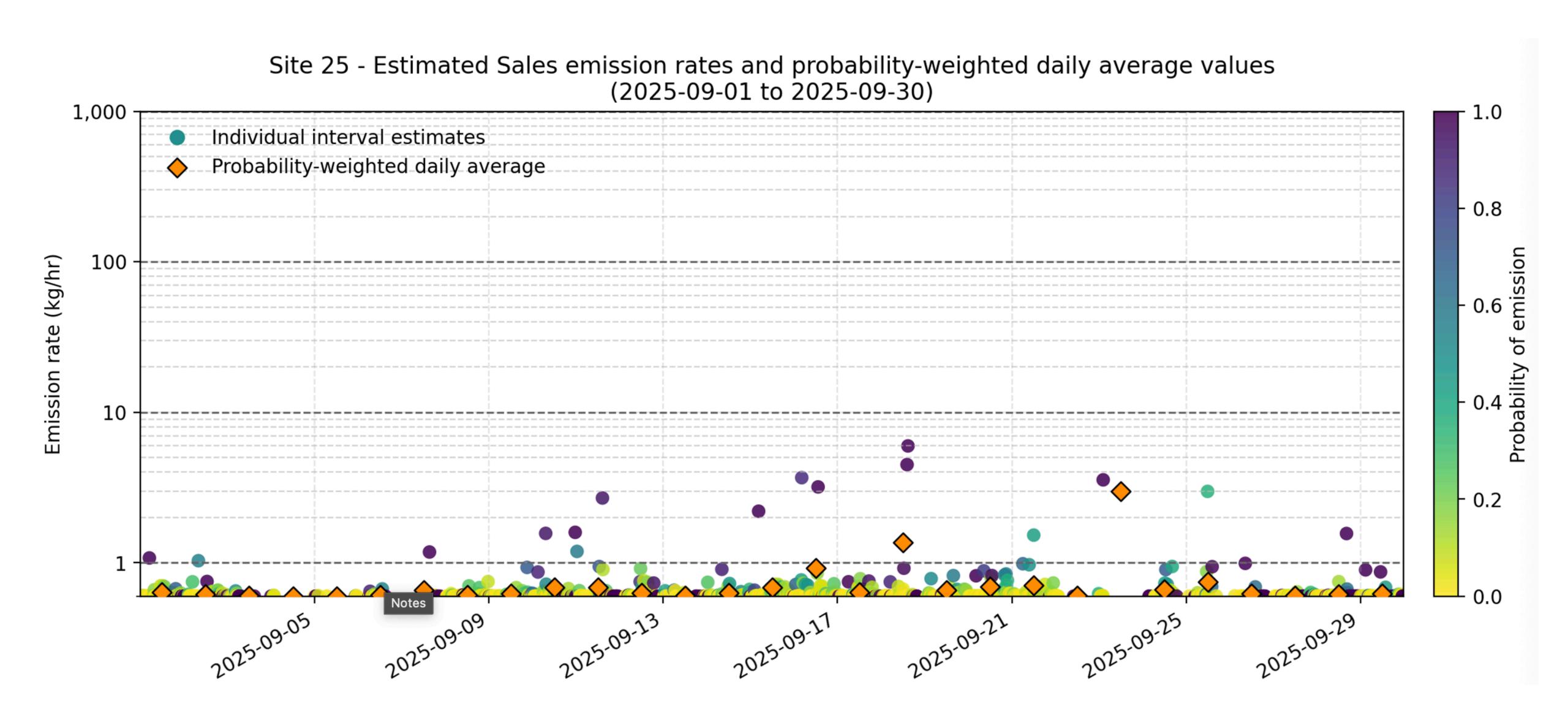


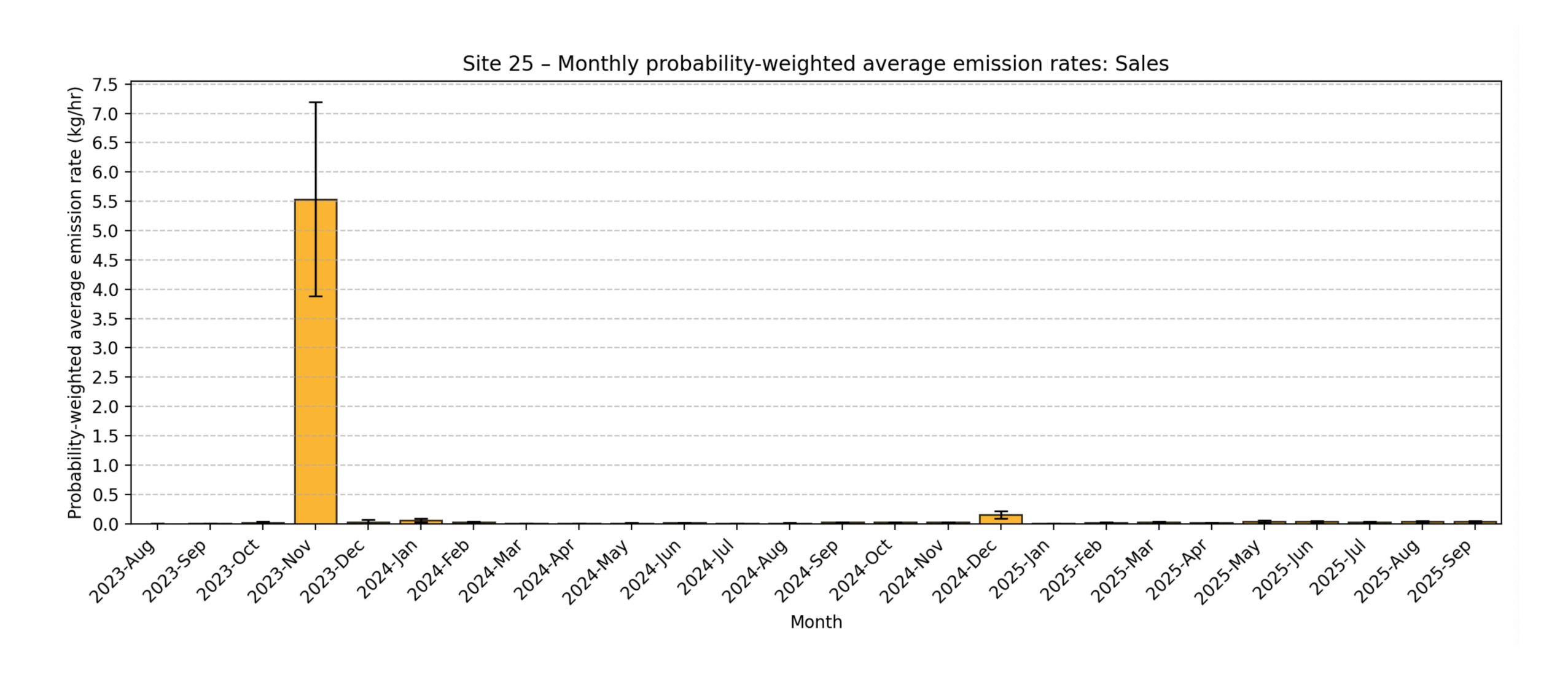


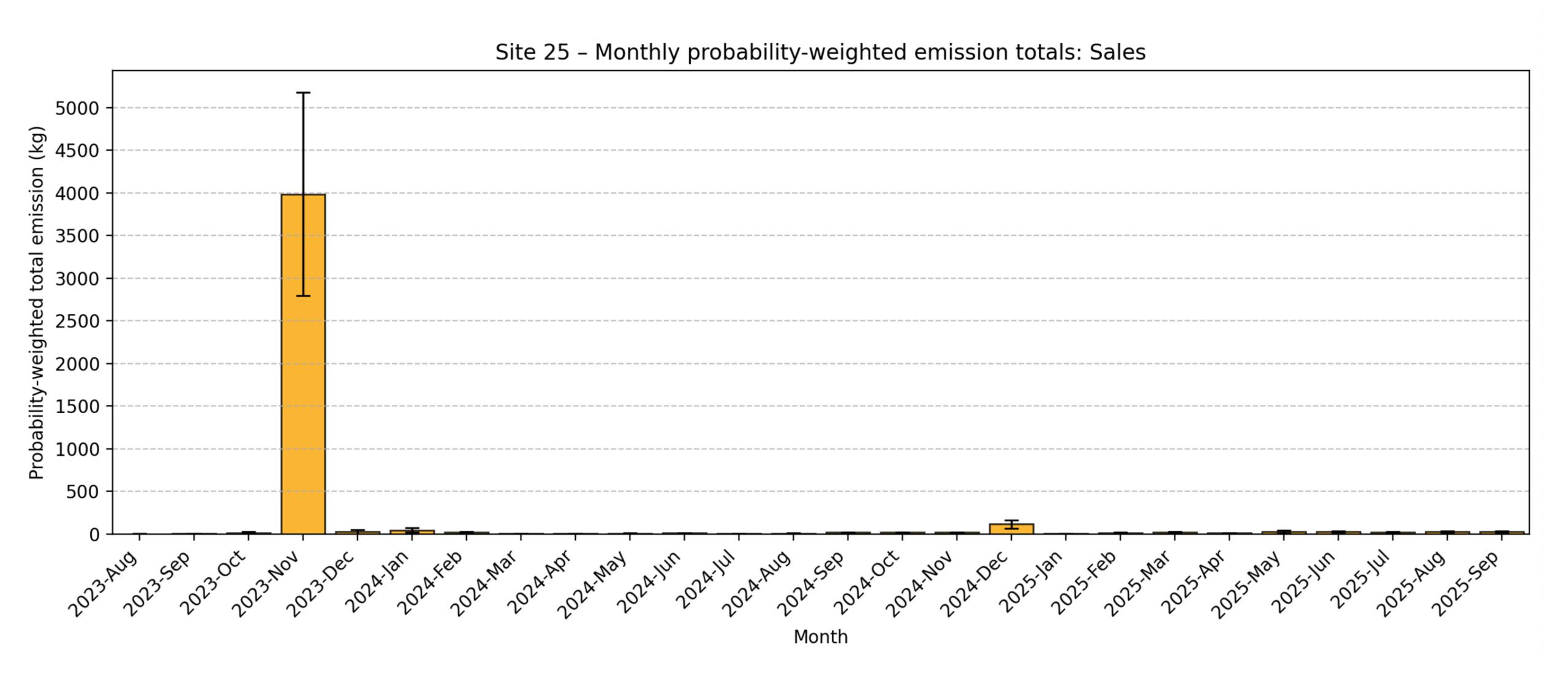


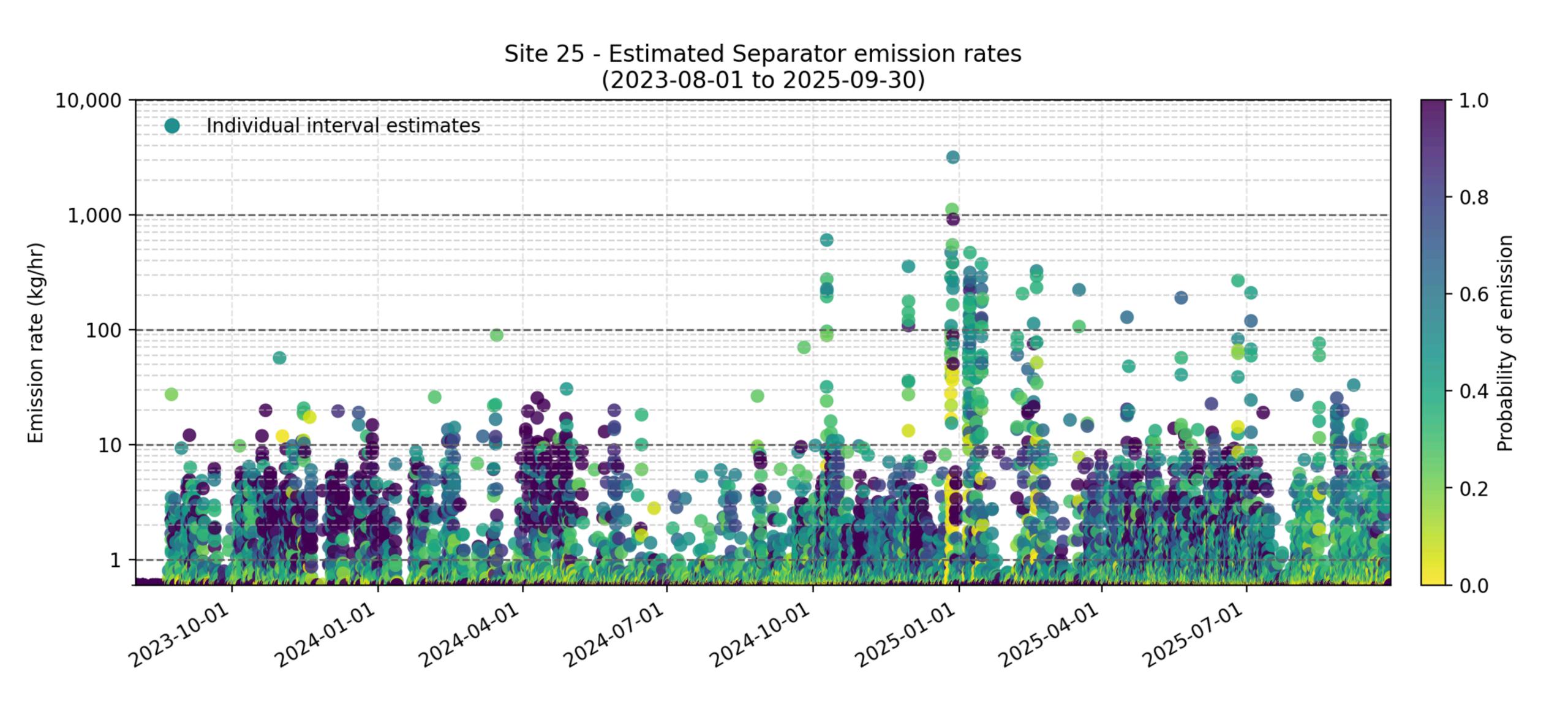
Site 25 - Estimated Sales probability-weighted daily average values (2023-08-01 to 2025-09-30)



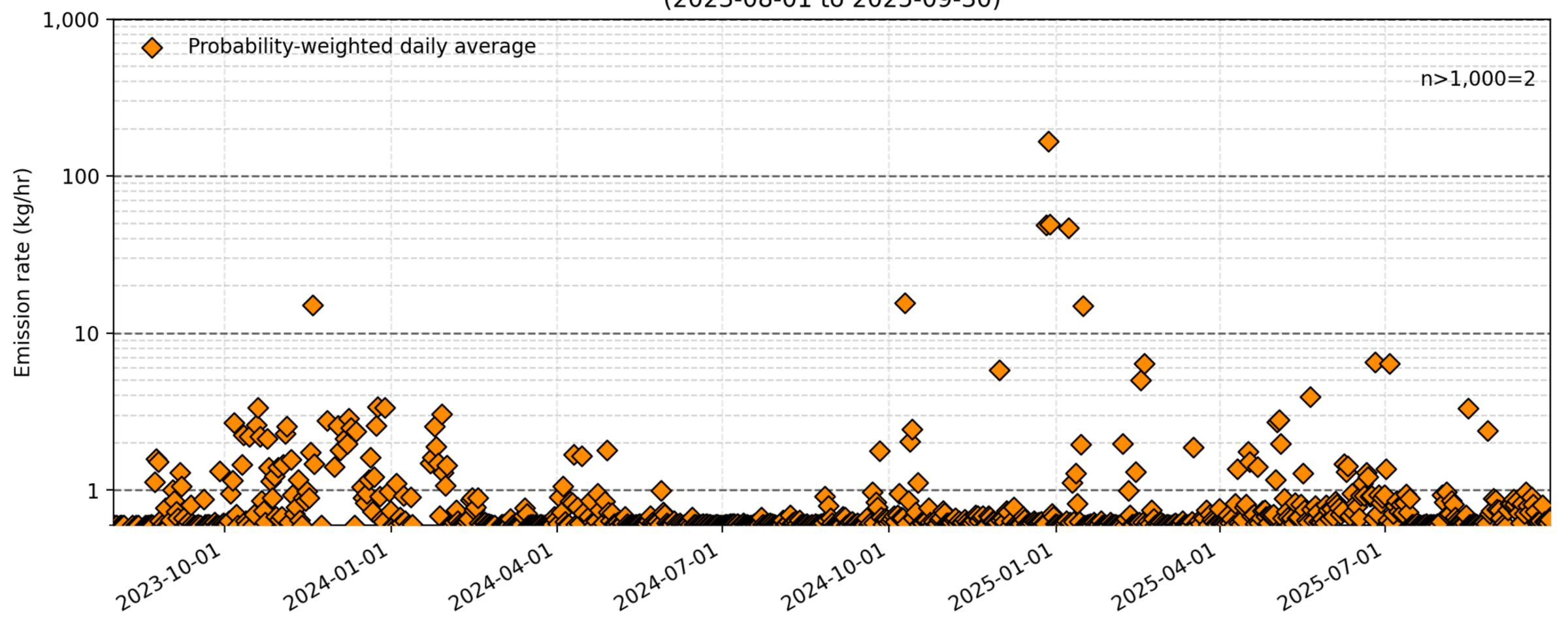


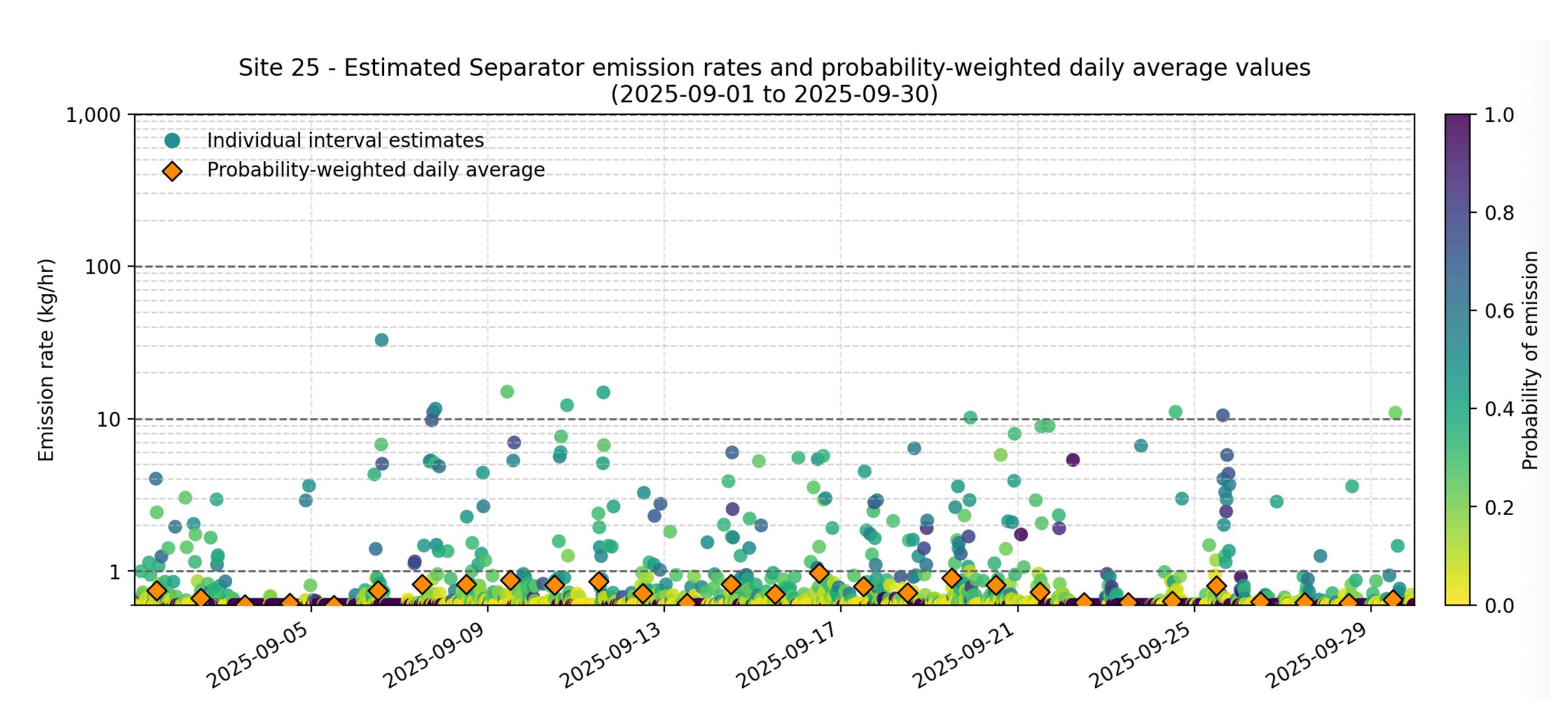


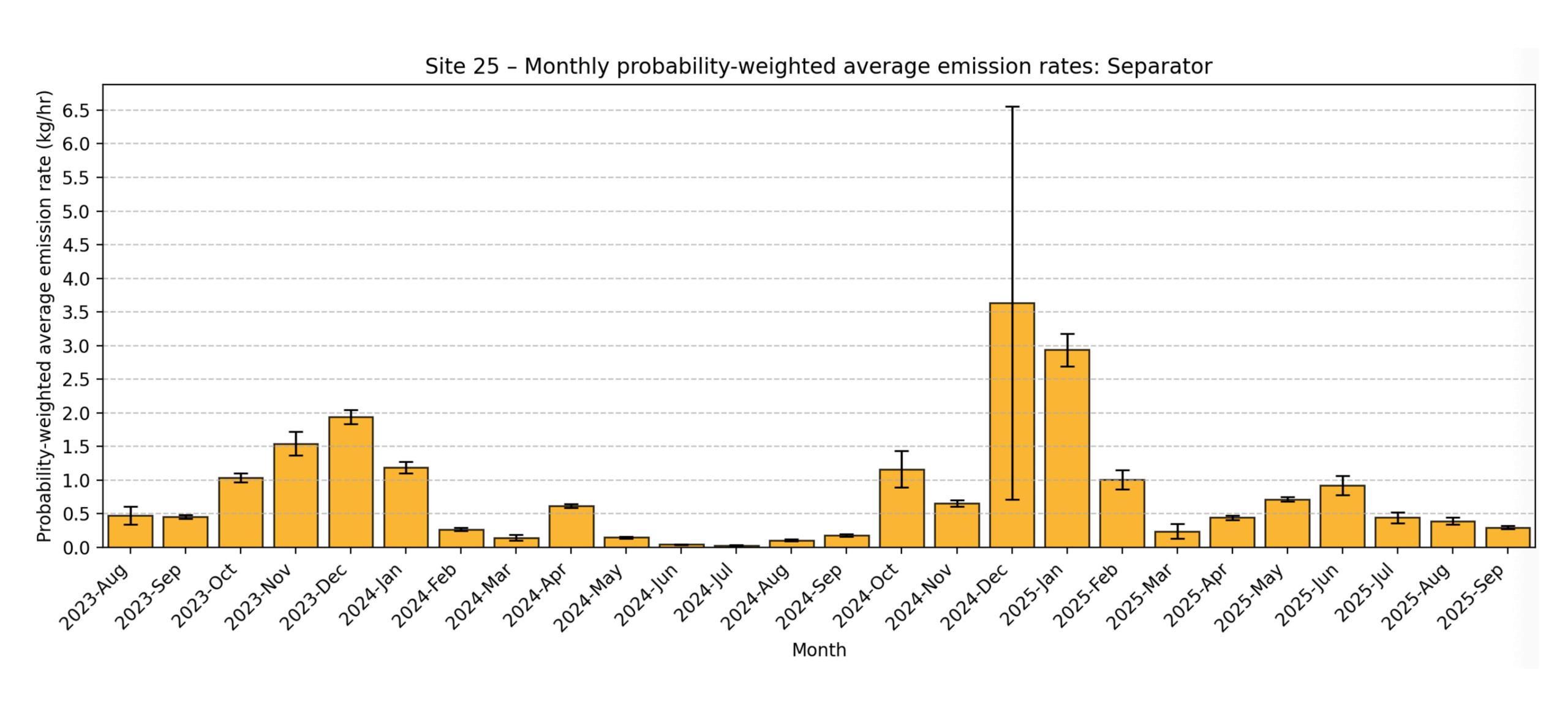


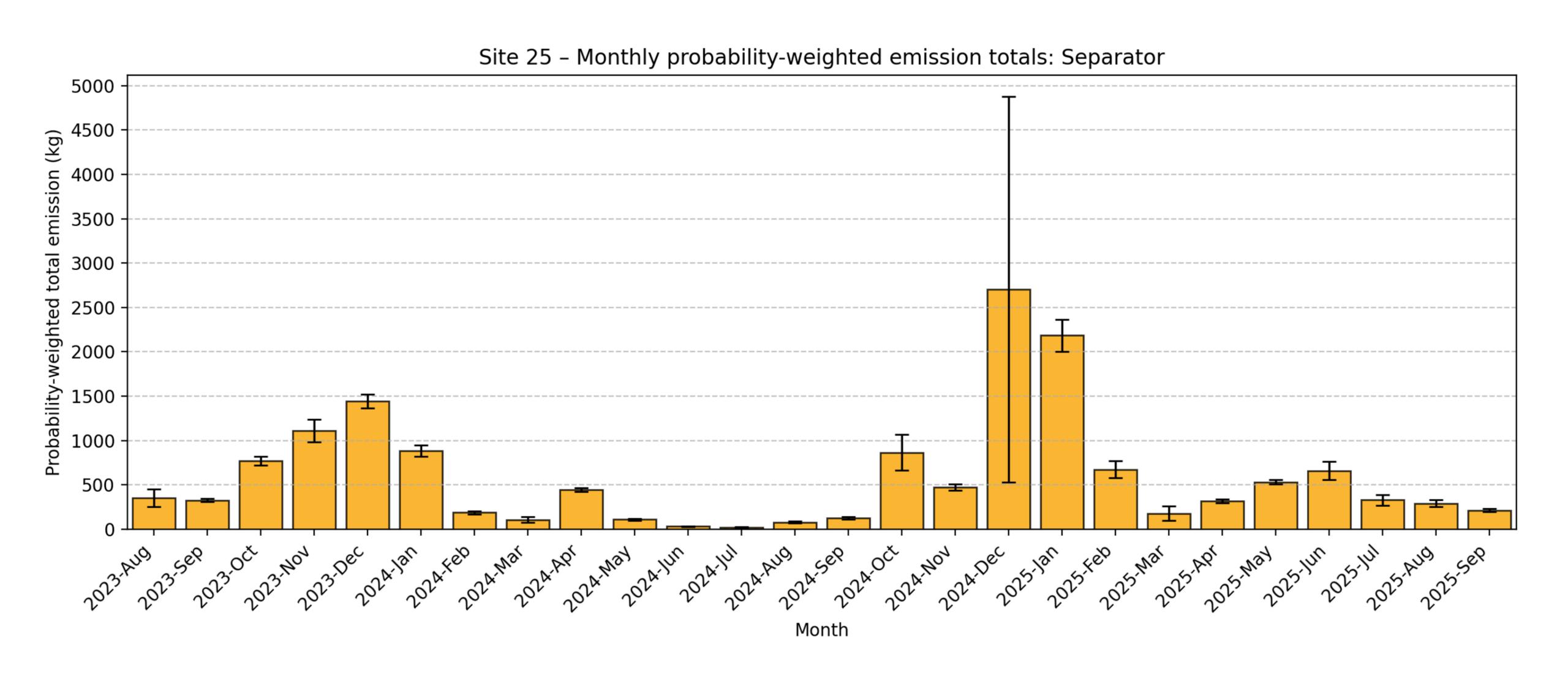


Site 25 - Estimated Separator probability-weighted daily average values (2023-08-01 to 2025-09-30)

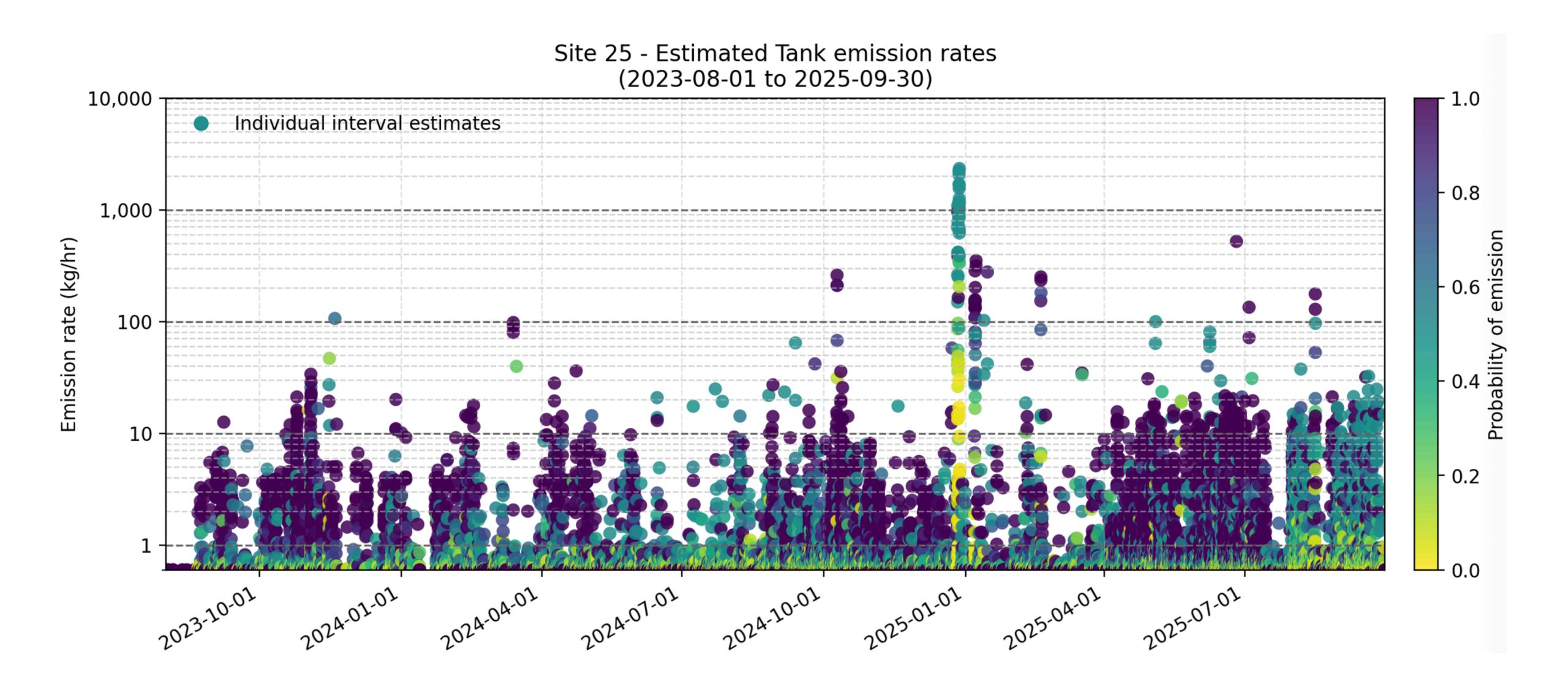




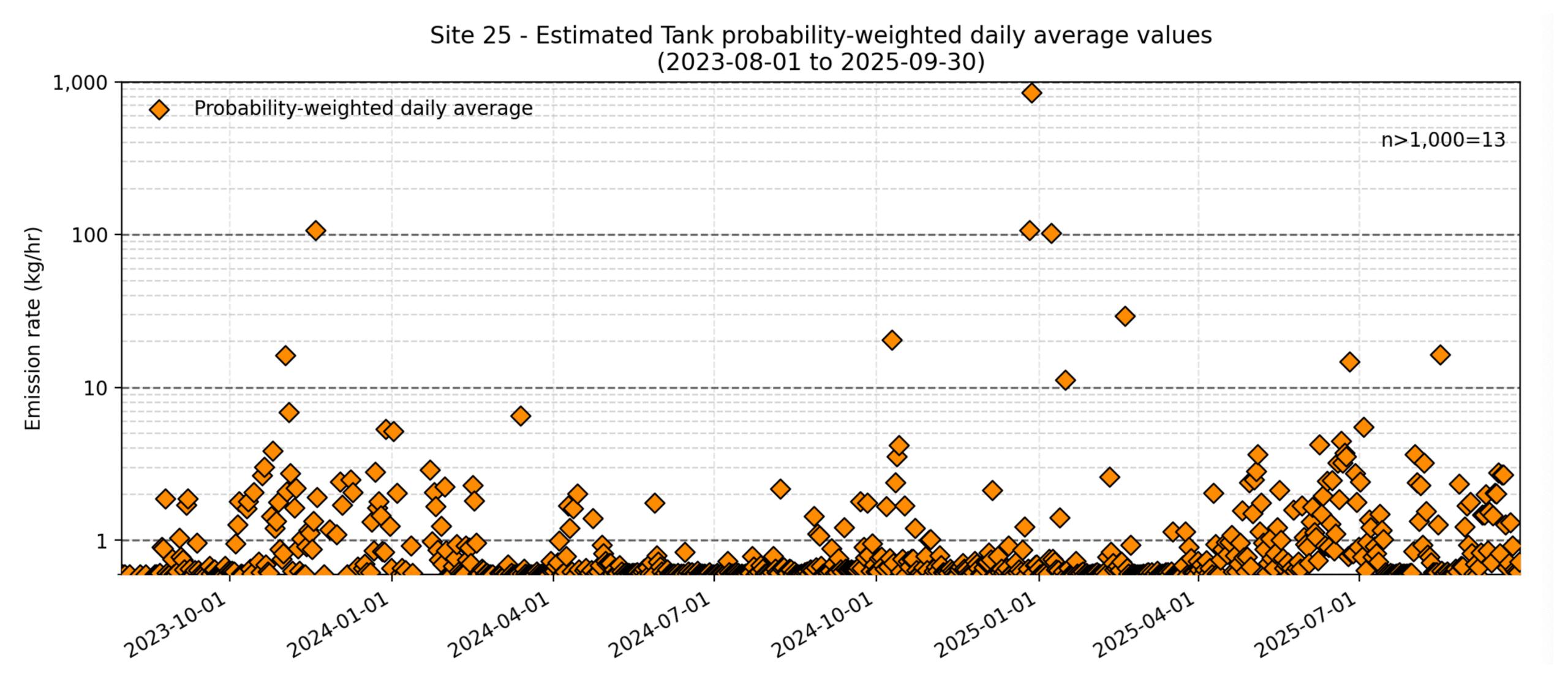




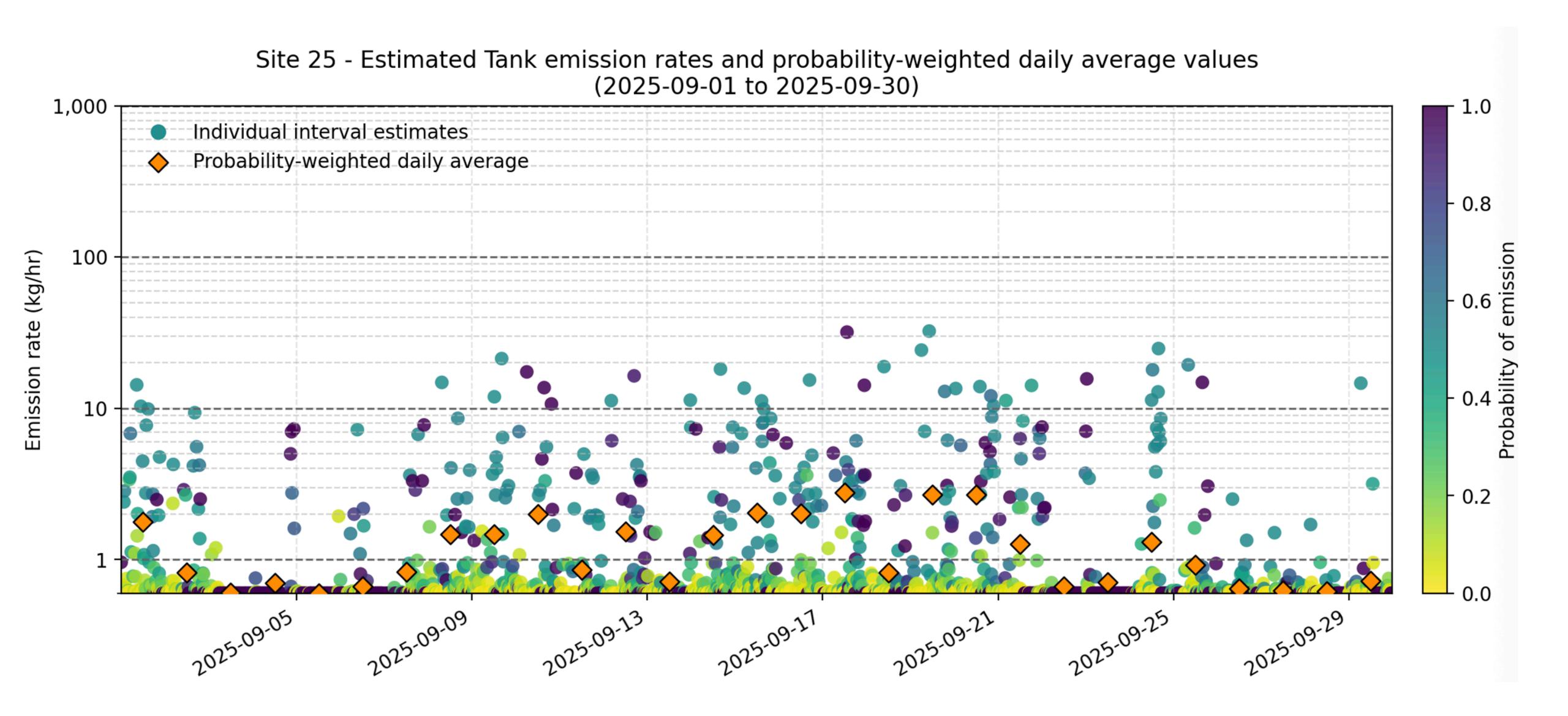
#### Tank emission rate estimates over time



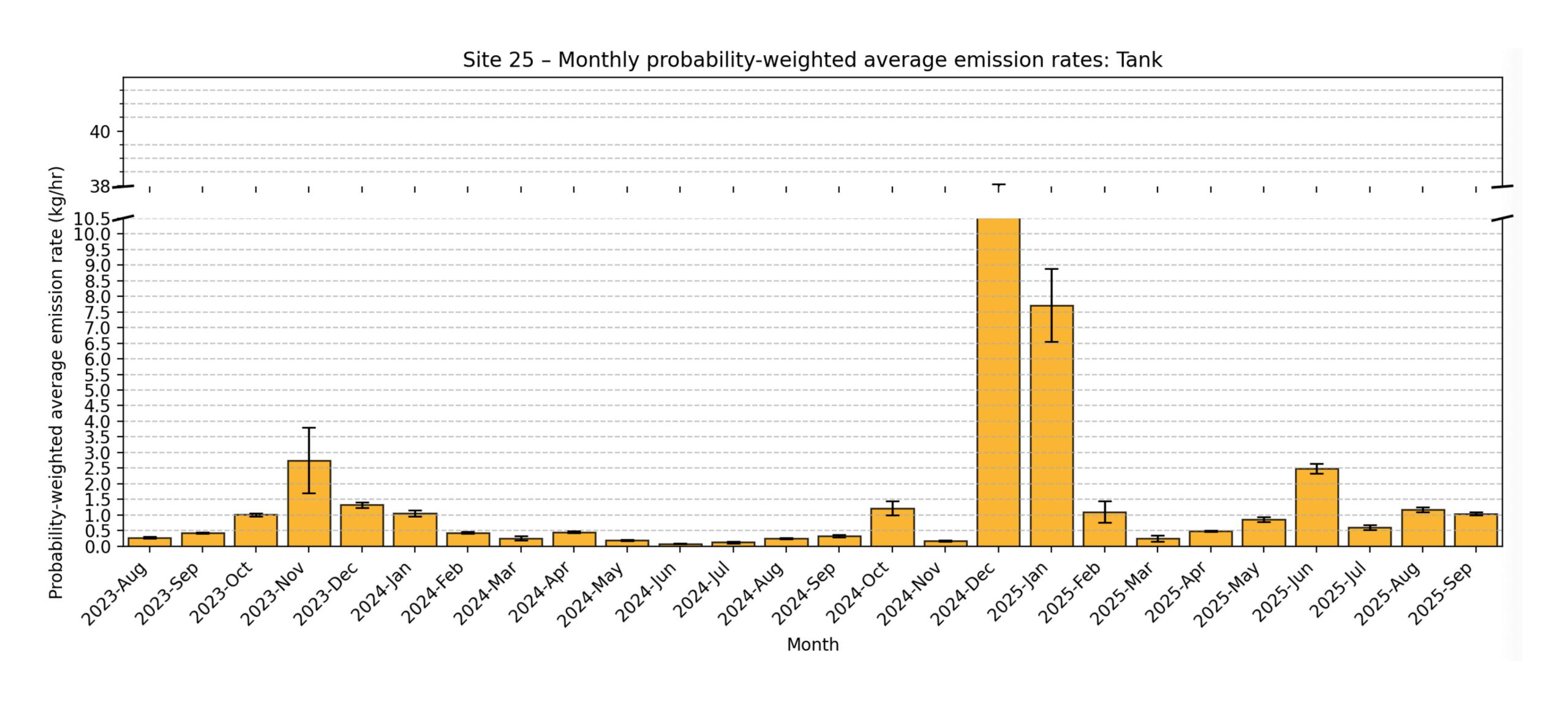
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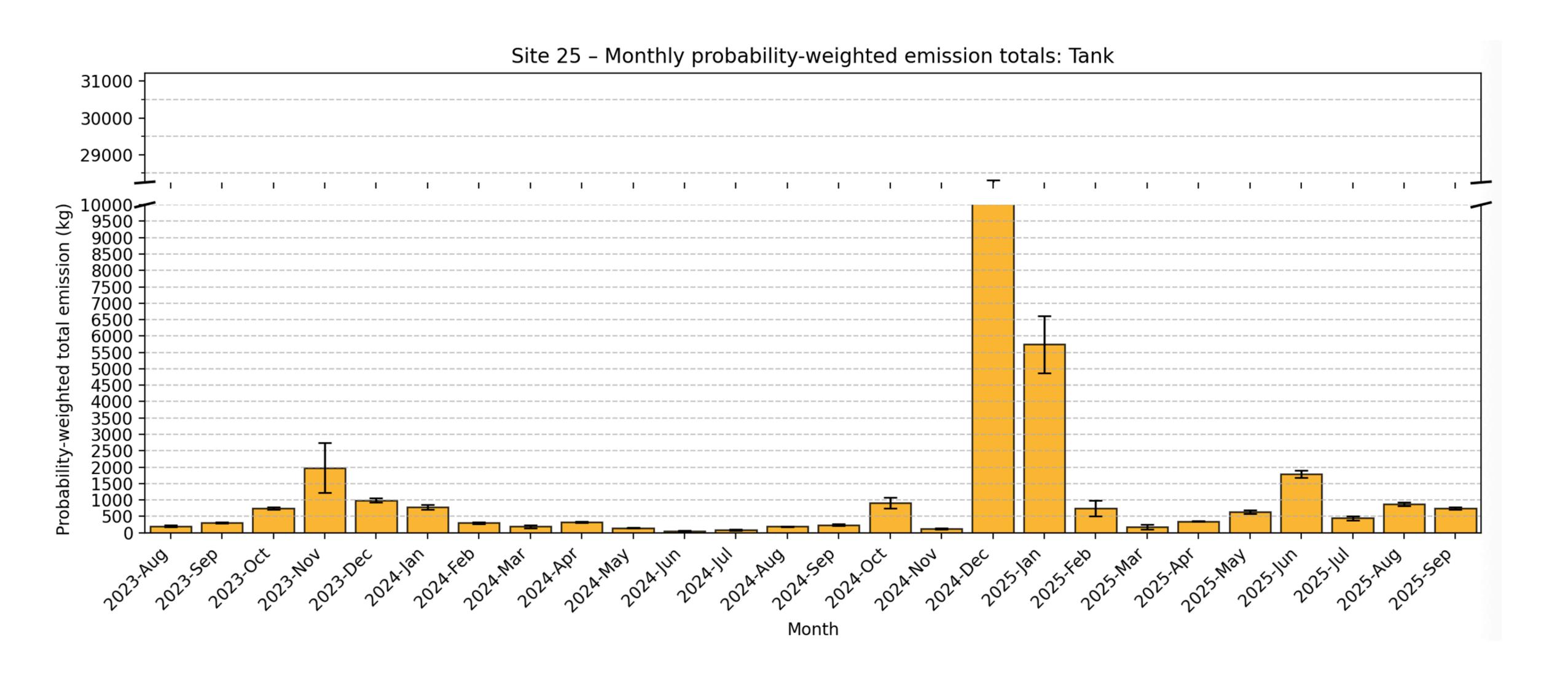
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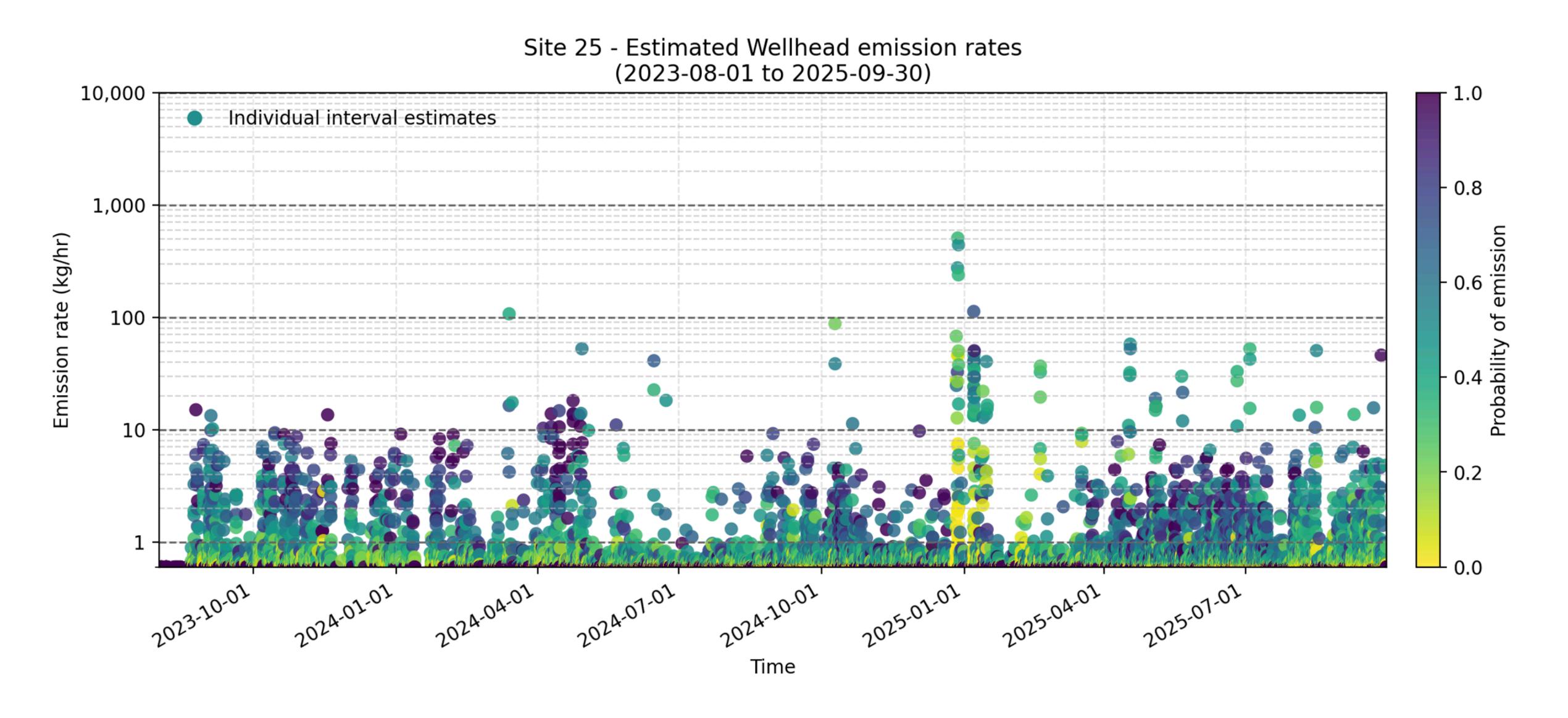


## Tank emission rate estimates over time

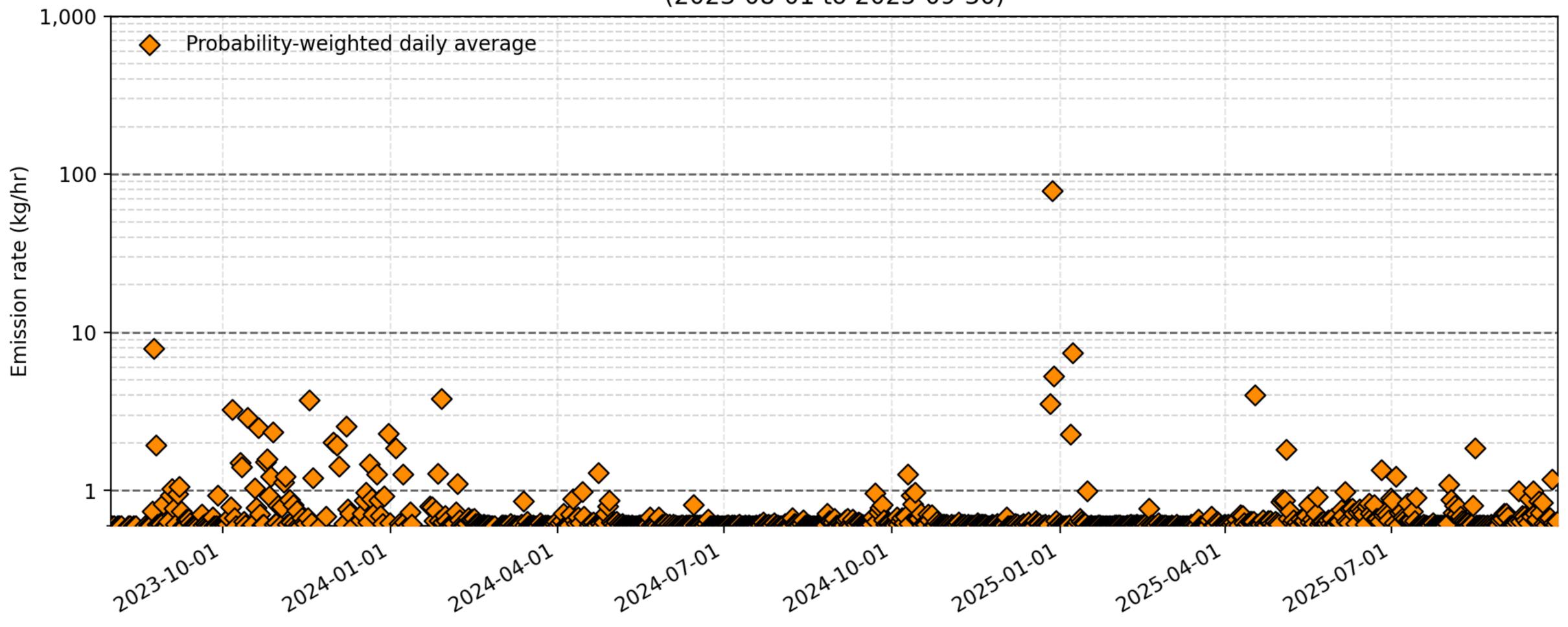


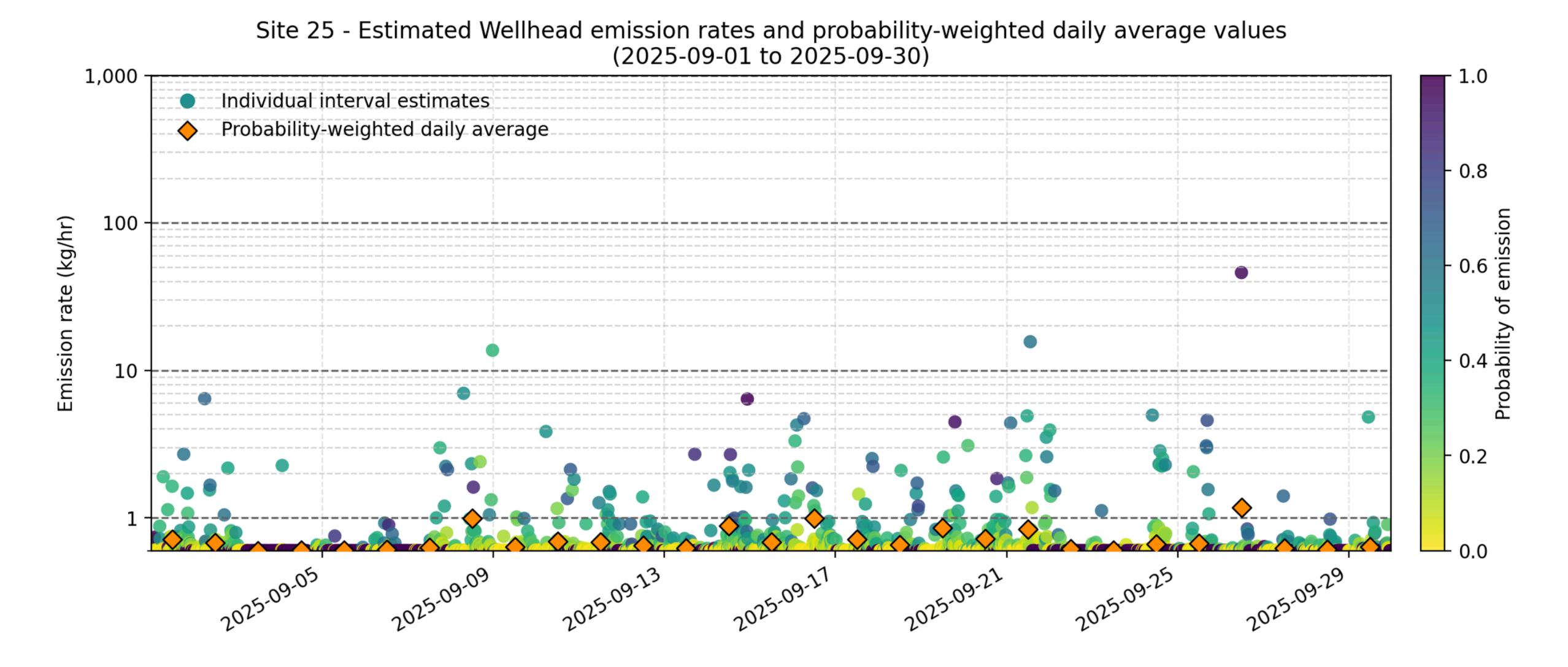
## Tank emission rate estimates over time

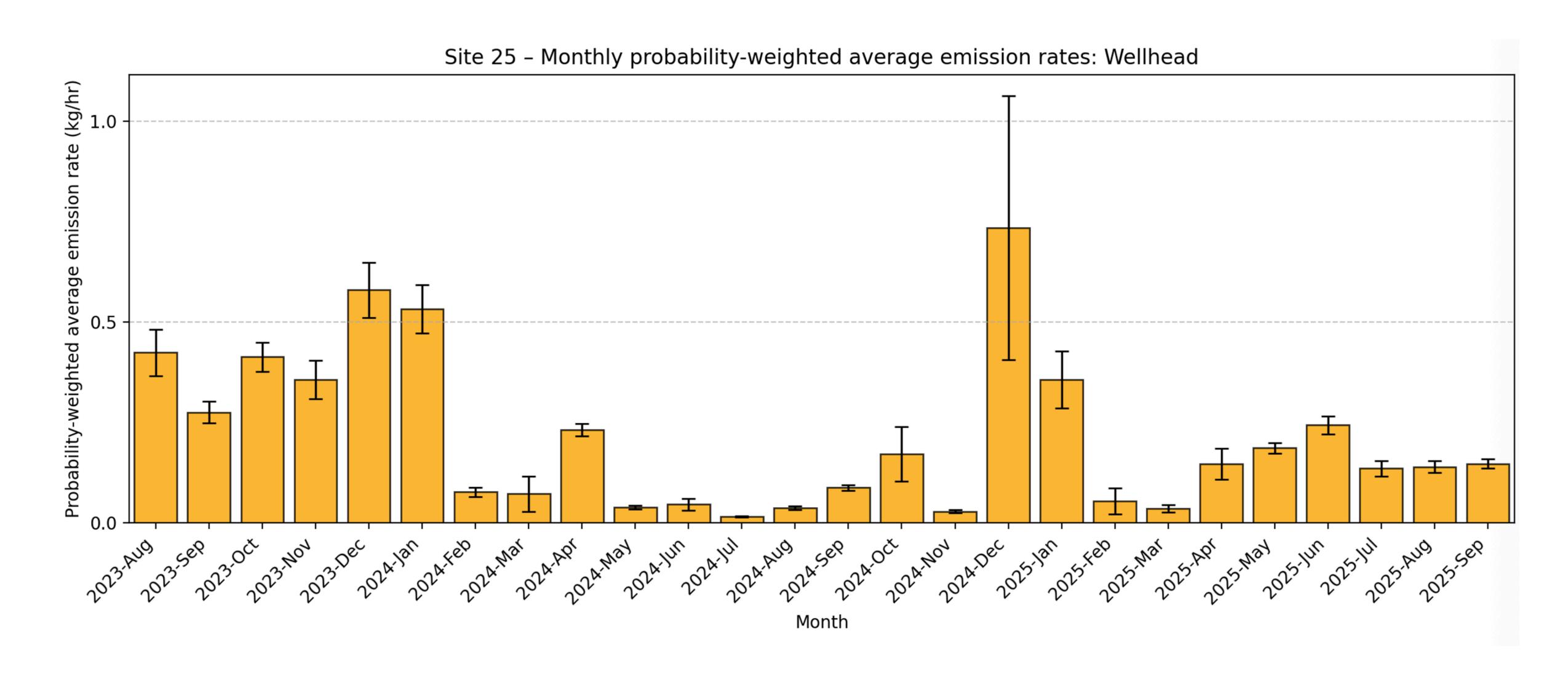


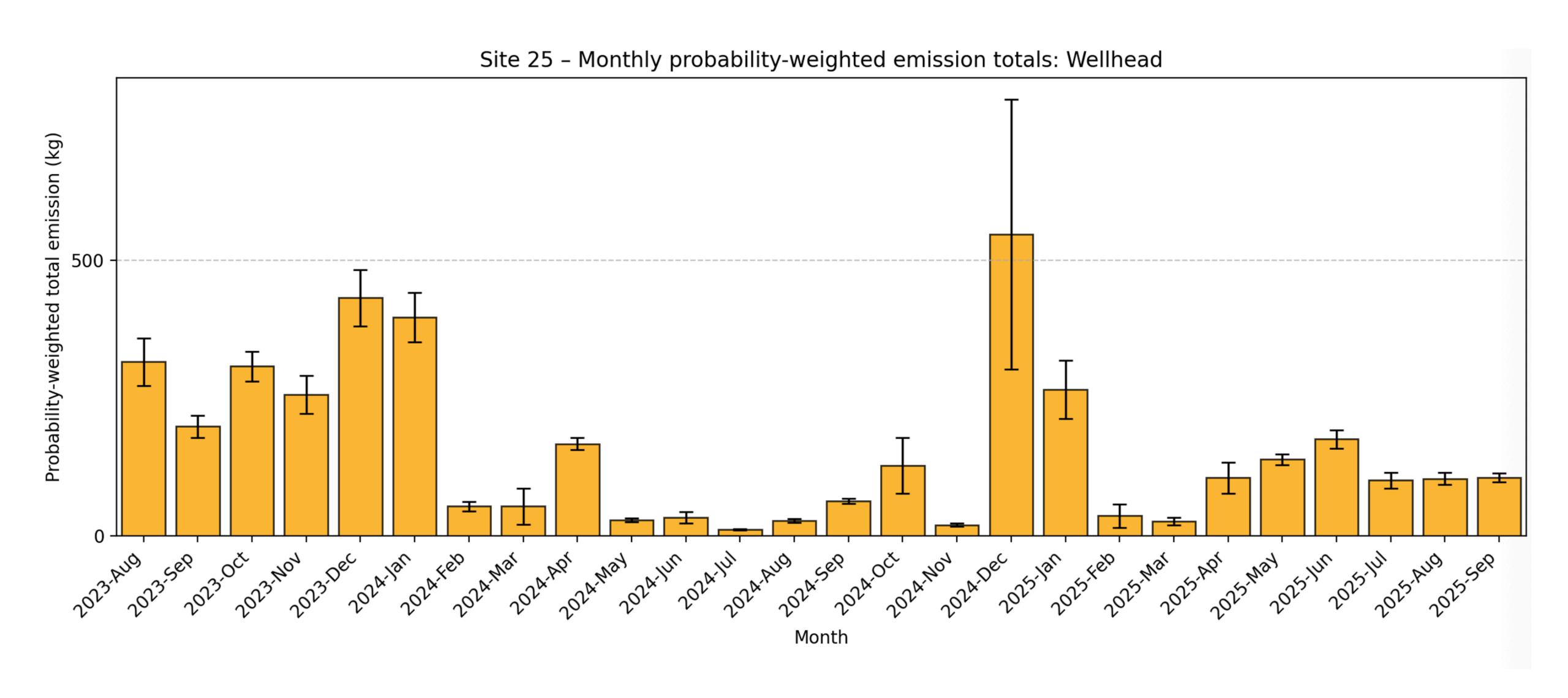


Site 25 - Estimated Wellhead probability-weighted daily average values (2023-08-01 to 2025-09-30)



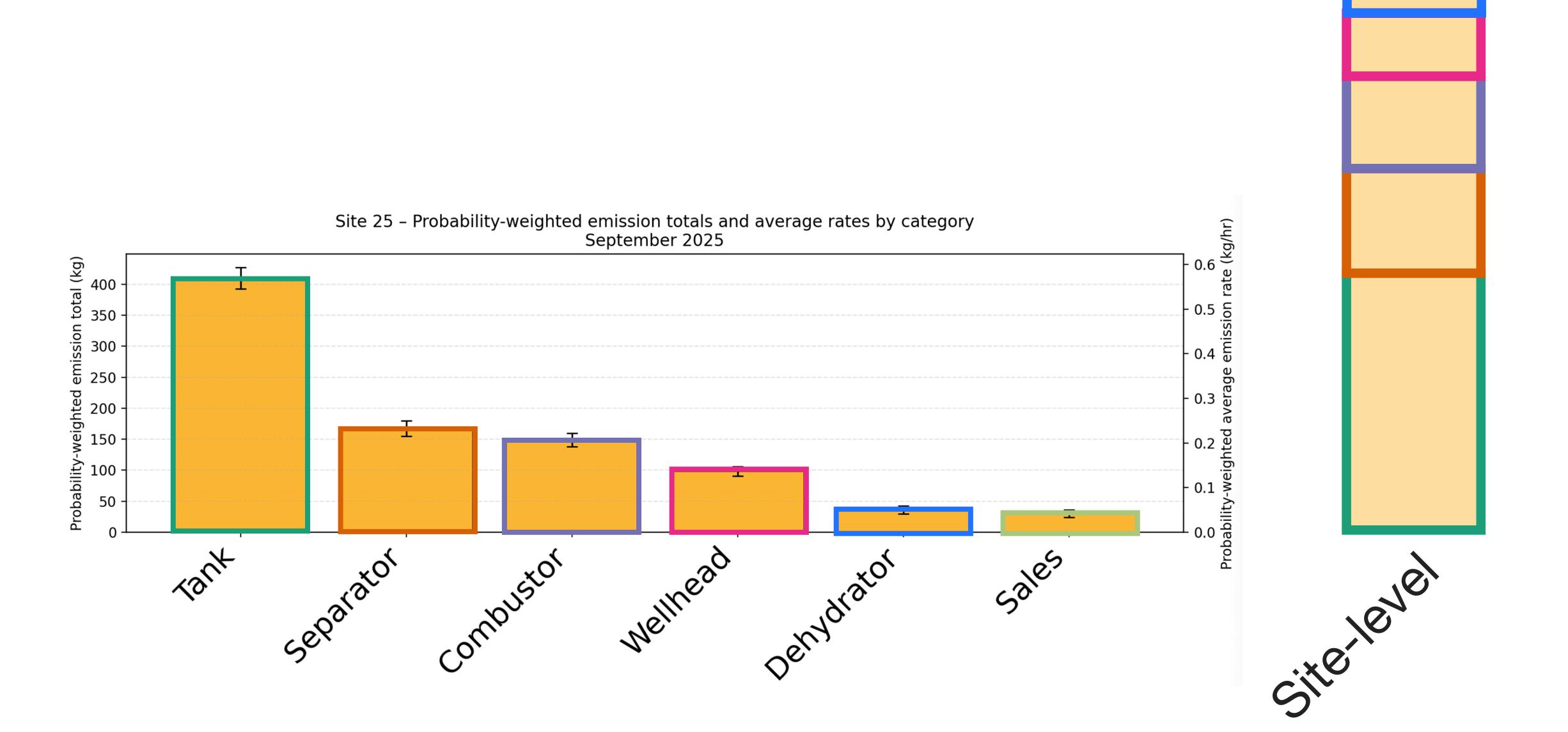




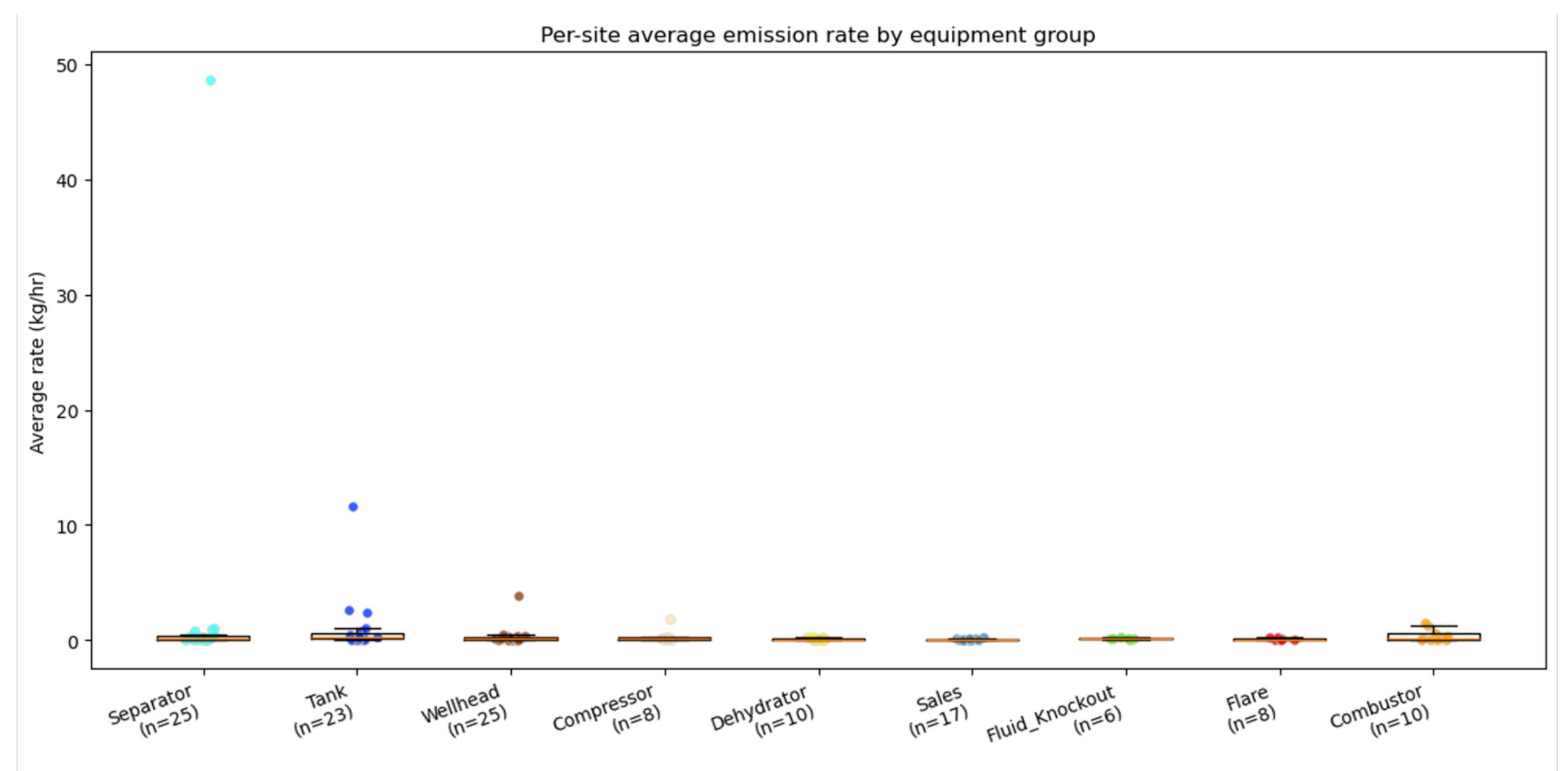


## Site 25: September 2025 inventory

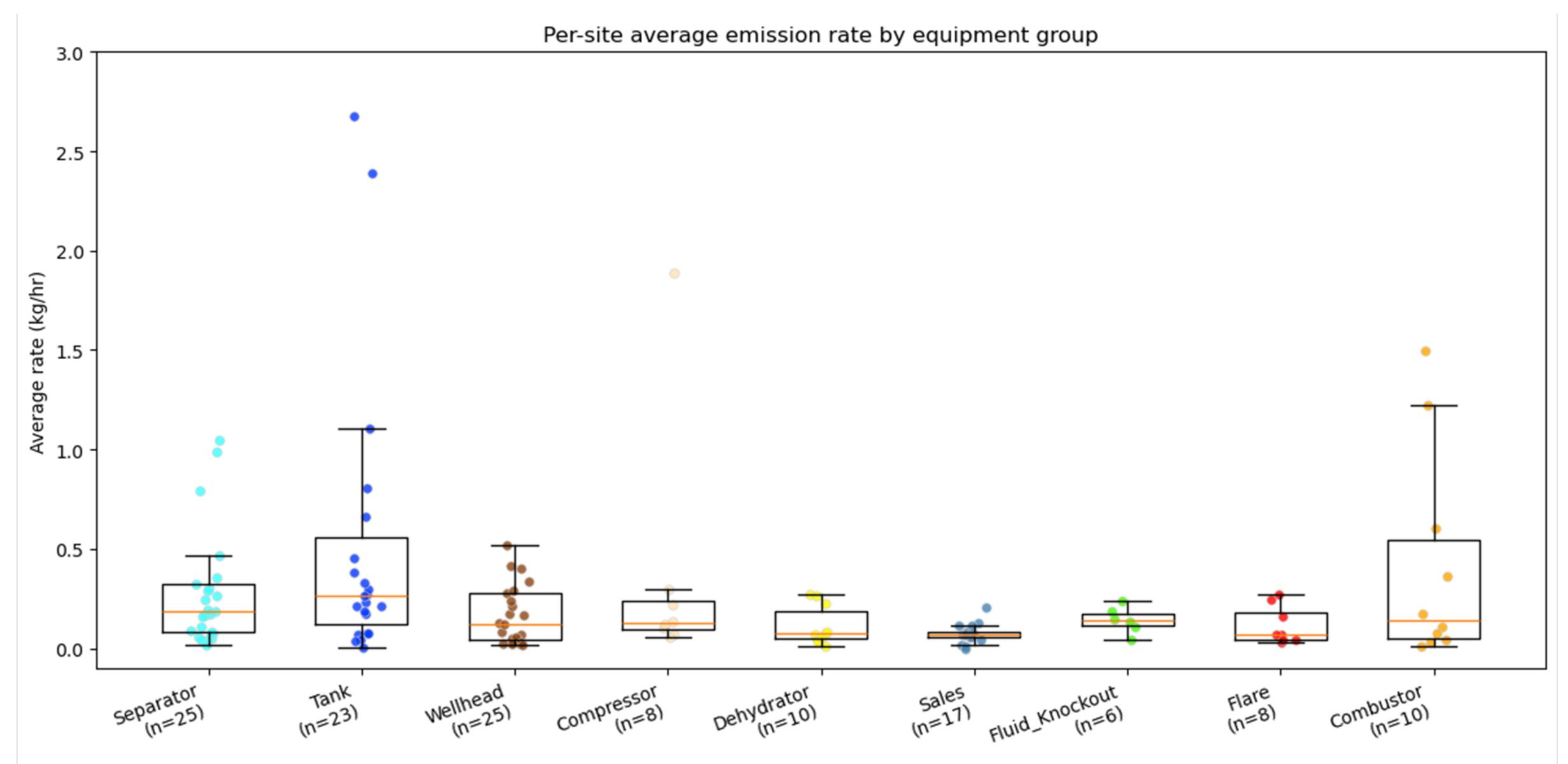
#### 890 [830, 951] kg



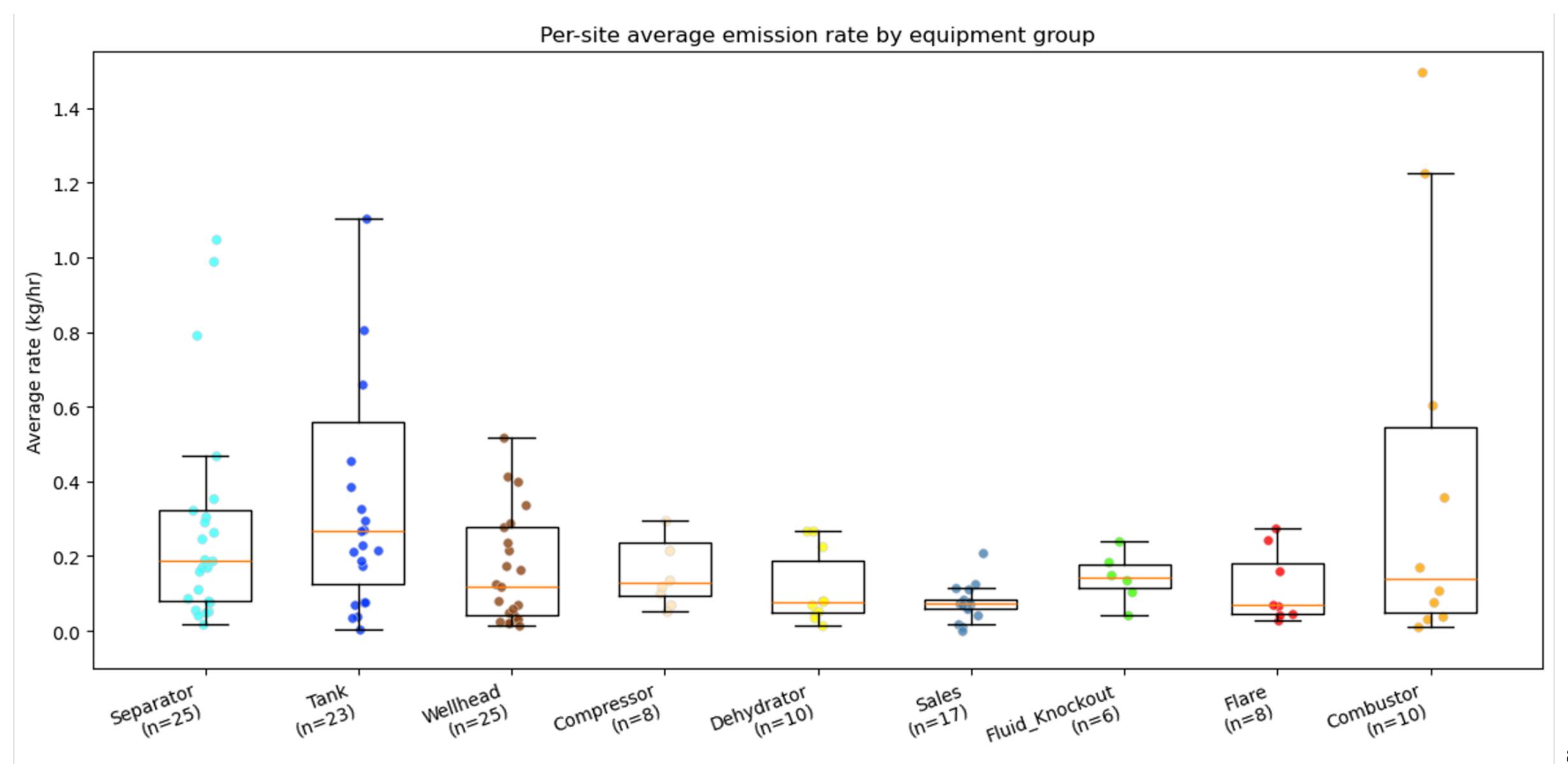
## Summary across all 26 sites



## Summary across all 26 sites



## Summary across all 26 sites



#### Concluding thought:

- CMS provide enough measurements to create fully measurement-based inventories at the site-level... IF
  - You account for periods of no information
  - You have an unbiased inverse model (or know how to correct for the bias)
- There's a lot of information in the CMS-based emission rates, and we are just getting started analyzing it

#### Next steps:

- Compare to other inventory methods (UT MII, CSU MAES, GHGRP)
  - We have already done this on 5 sites for the COBE project in Colorado
- Use CMS-based emission rate estimates to inform "prototypical sites" or subsets of sites where distributions are similar
  - E.g. conventional wells

# Thank you! Questions?

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