Implementing the Gaussian puff atmospheric dispersion model and using it to estimate methane emission rates

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COLORADO SCHOOL OF MINES

Agenda

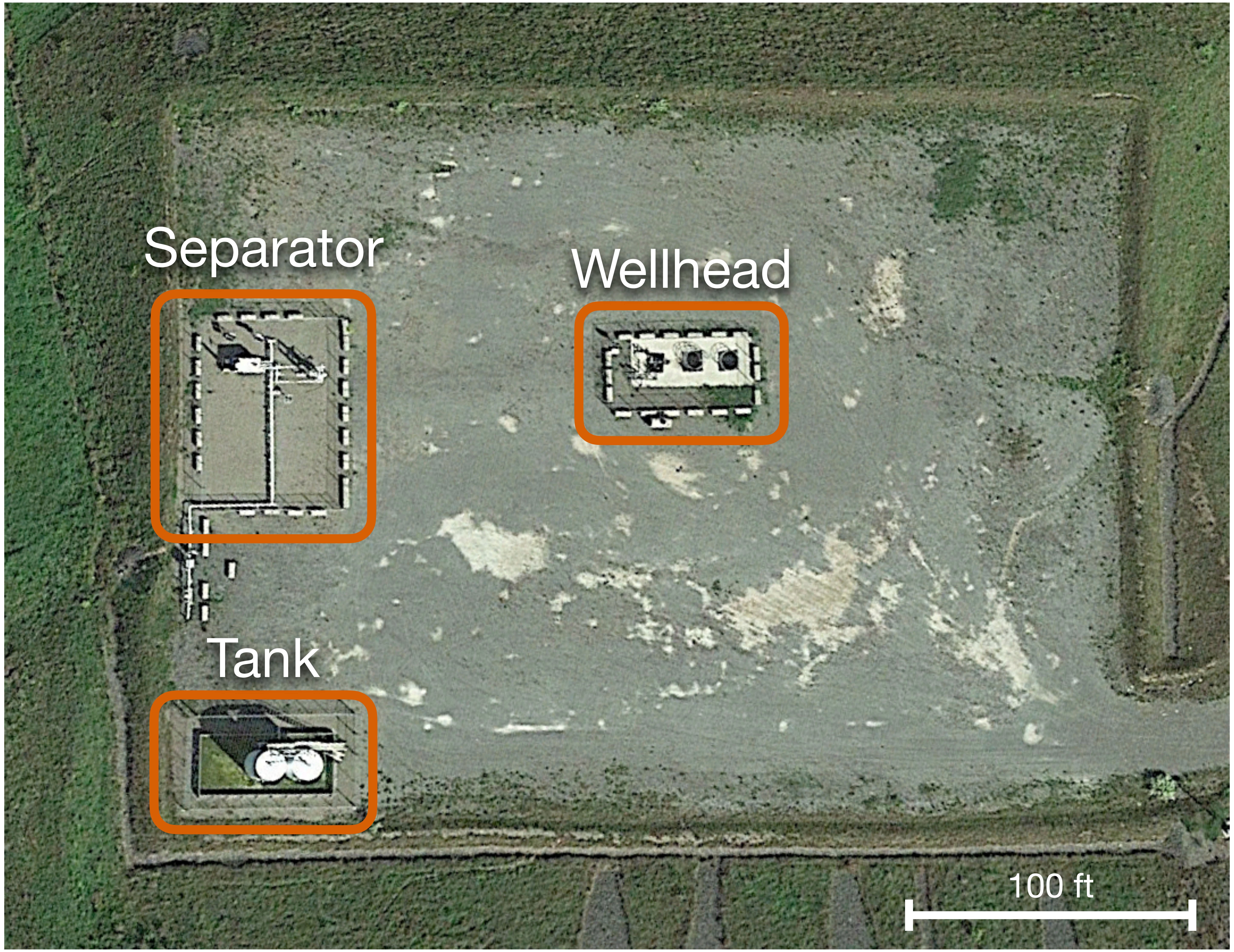
Talk (~30 min):

- Overview of the Gaussian plume and Gaussian puff models
- Mathematical relationship between the Gaussian plume and puff models
- Using the Gaussian puff model to estimate emission source and rate
- Fast implementation of the Gaussian puff model

Workshop (~60 min):

- Running the Gaussian puff
- Running the inversion to estimate source and rate
- Work time and questions

Overview



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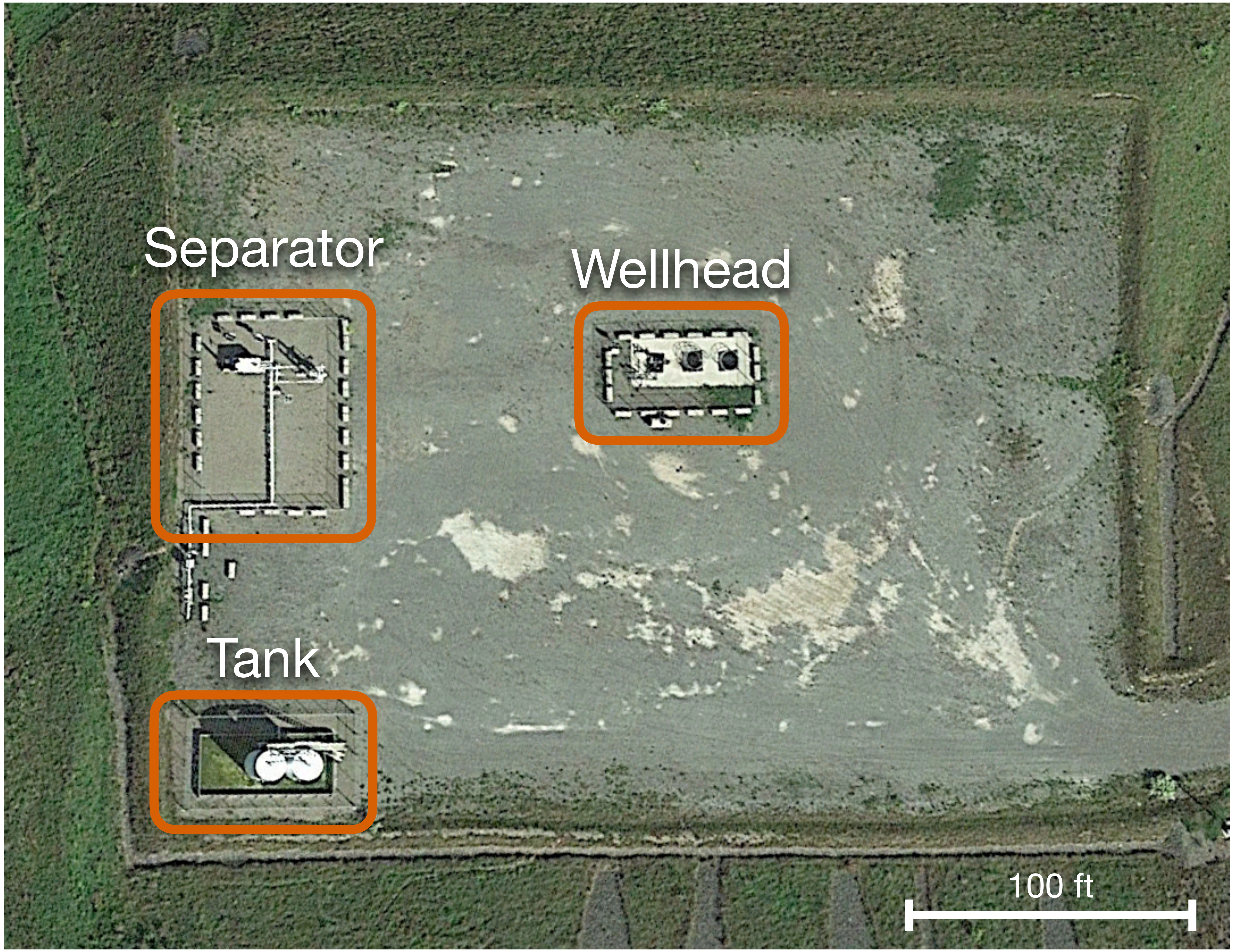
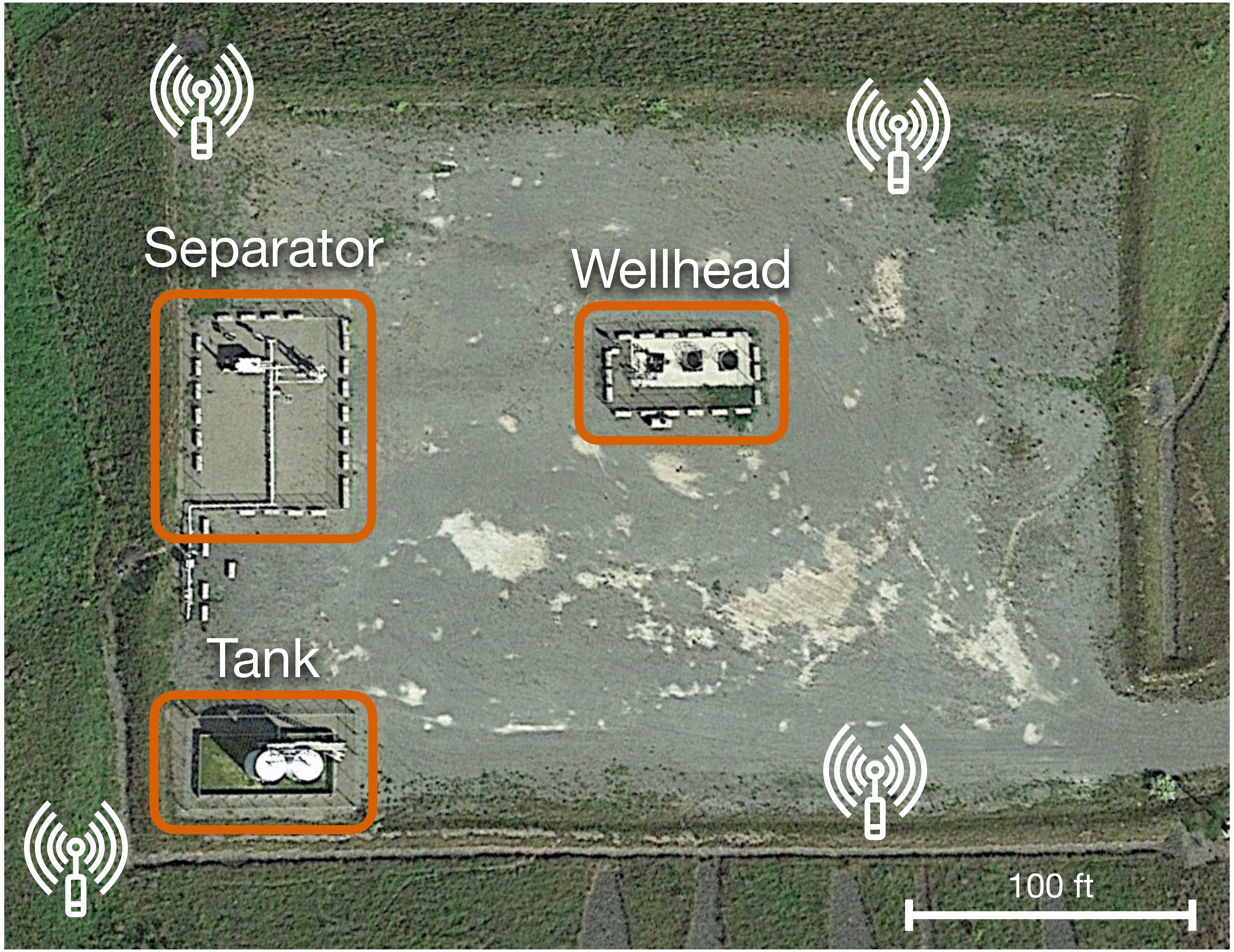


Continuous monitoring system (CMS)

Overview



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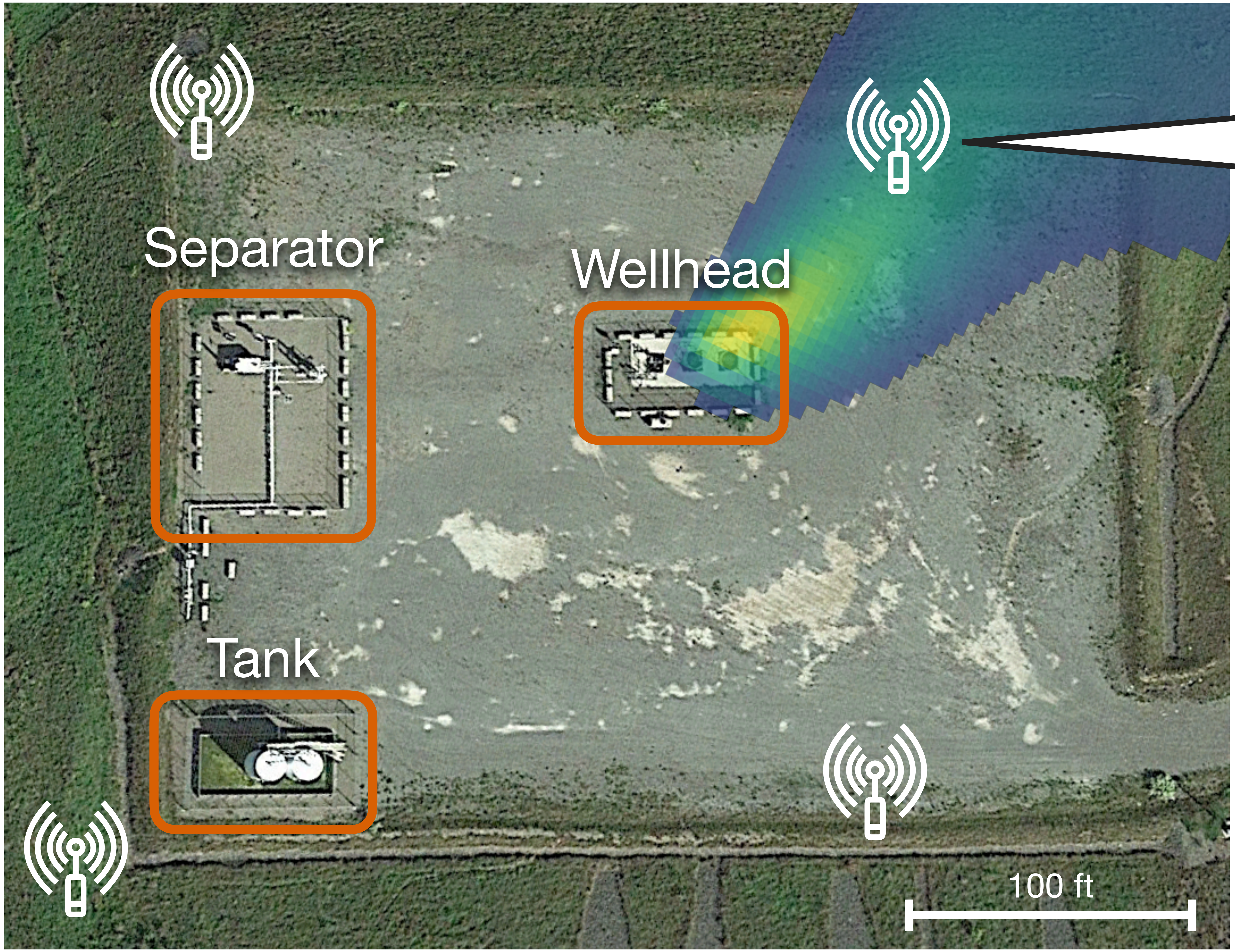

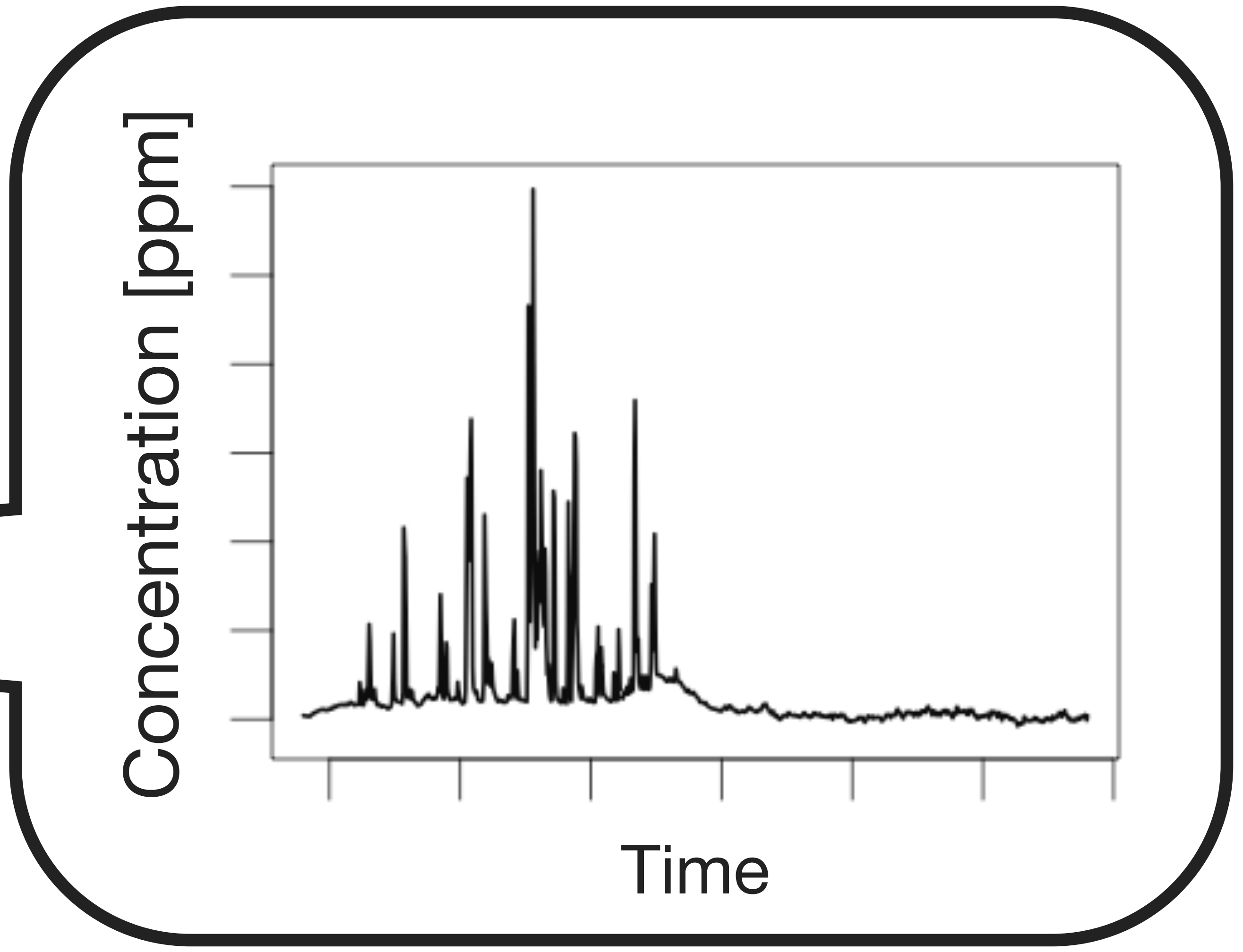

Atmospheric transport models (like the Gaussian puff) simulate the transport of a trace gas (like methane) from a source to a receptor

Gaussian plume model:

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

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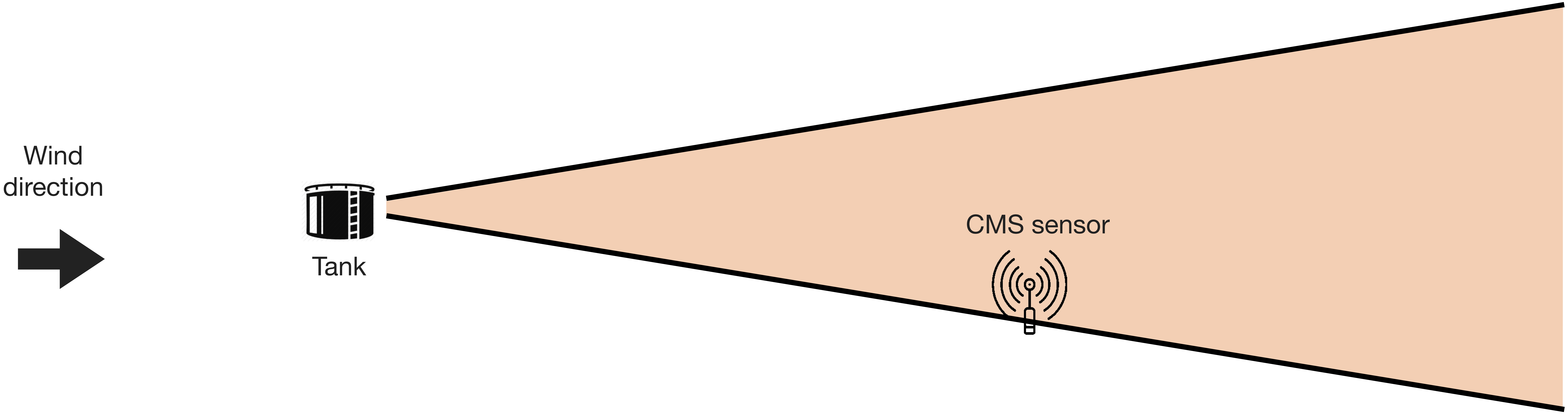

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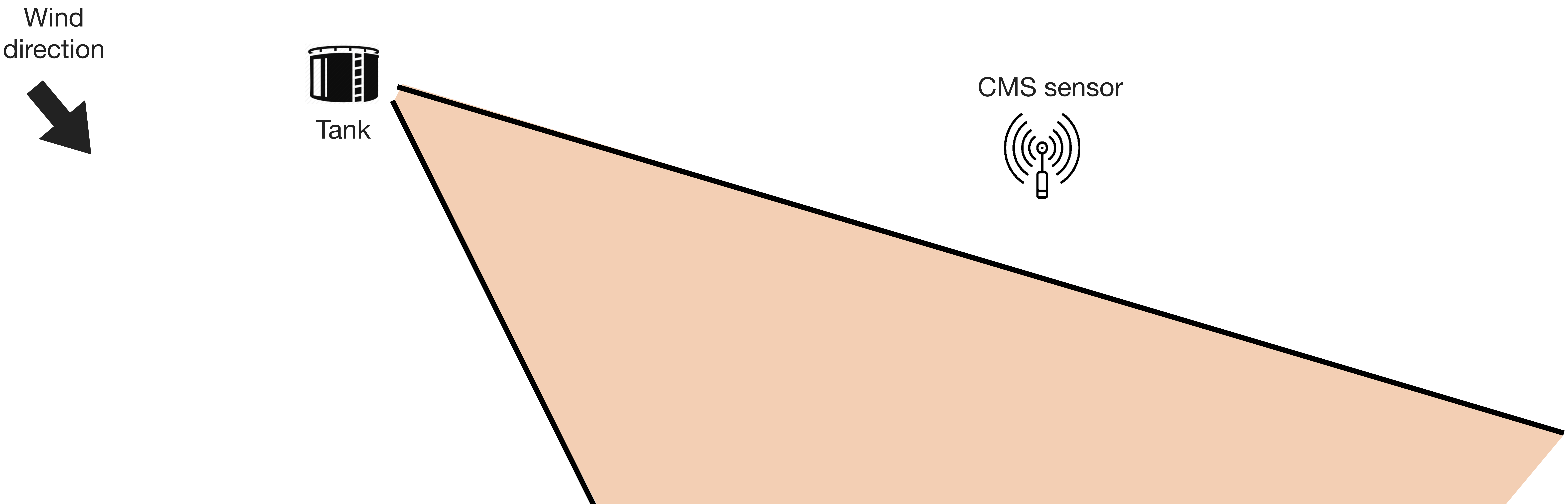

Gaussian puff model:

approximates a continuous release of methane as a sum of many small “puffs”

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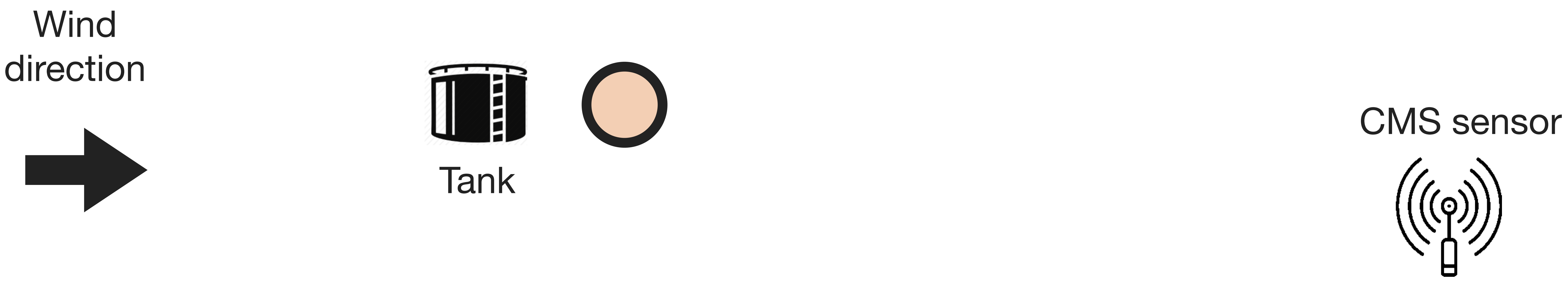

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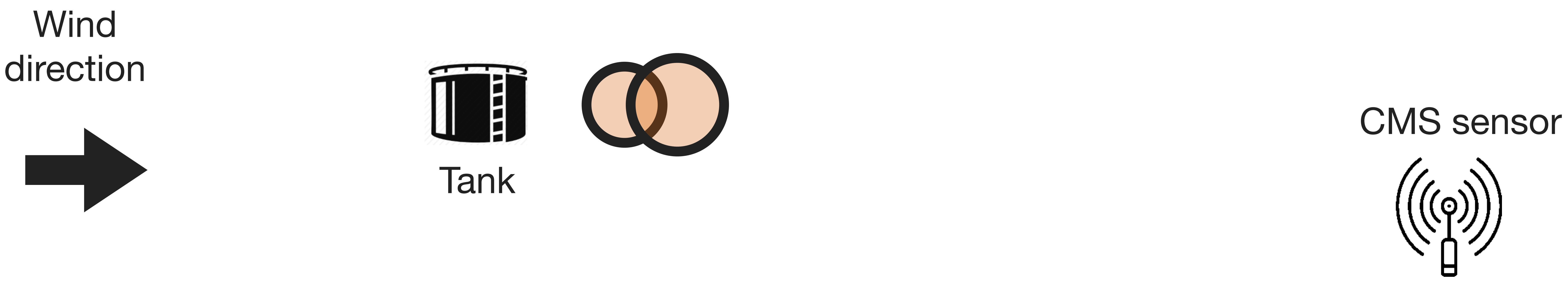

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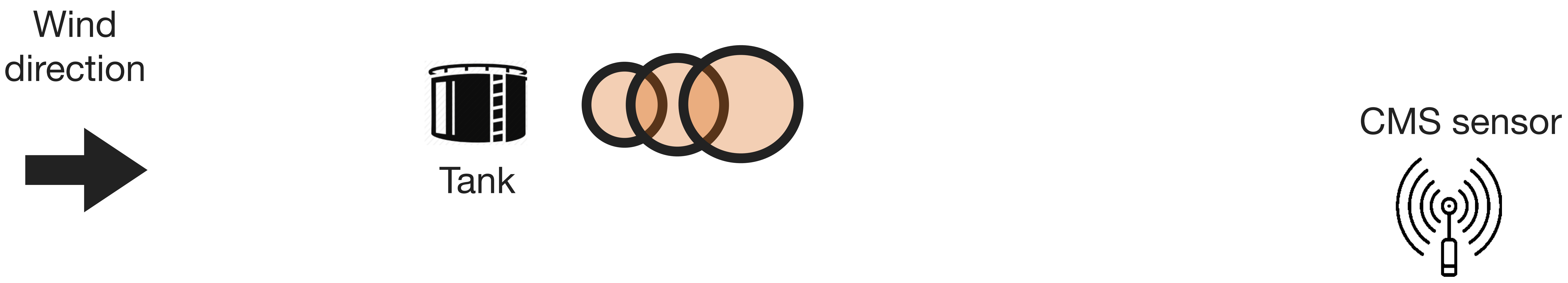

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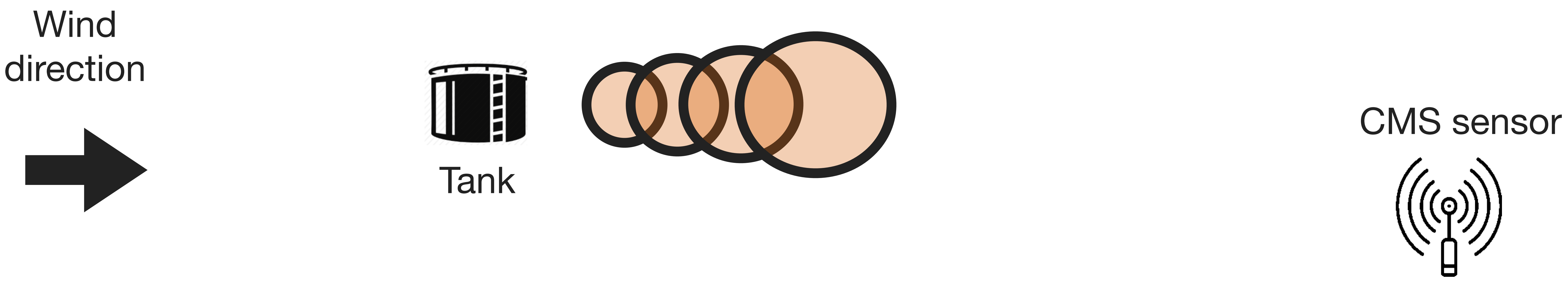

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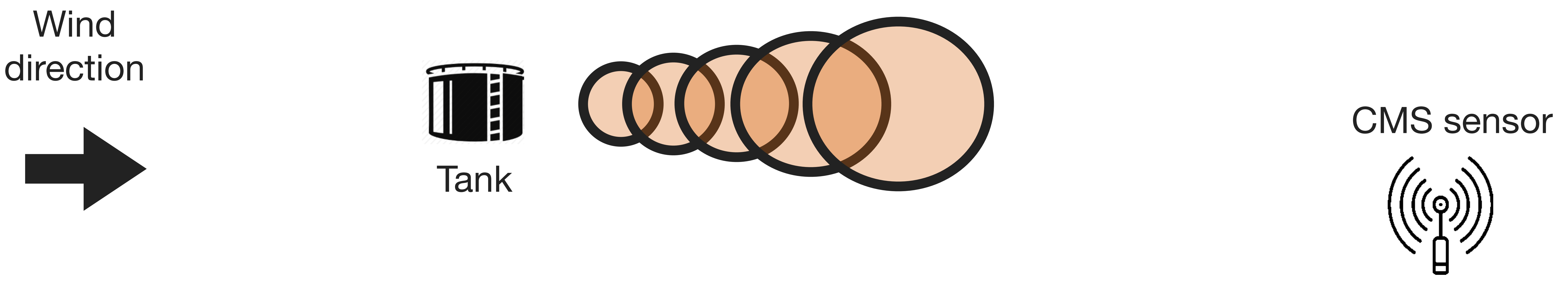

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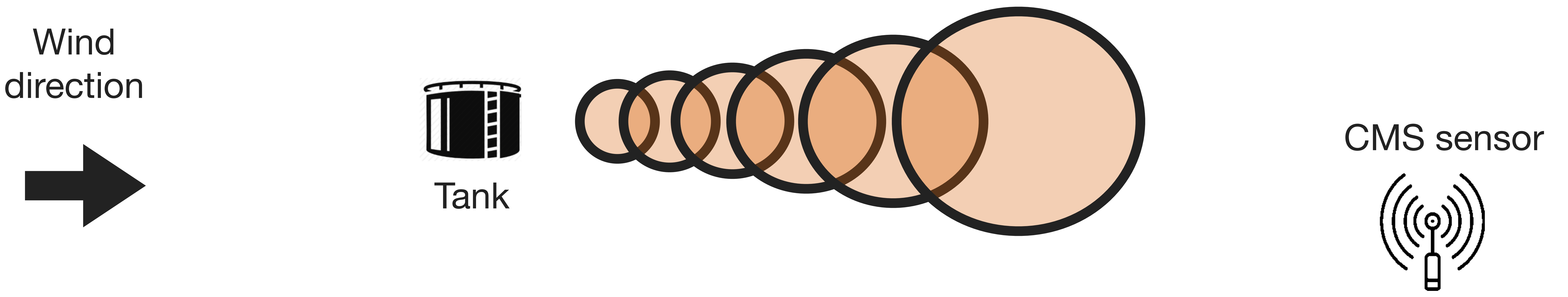

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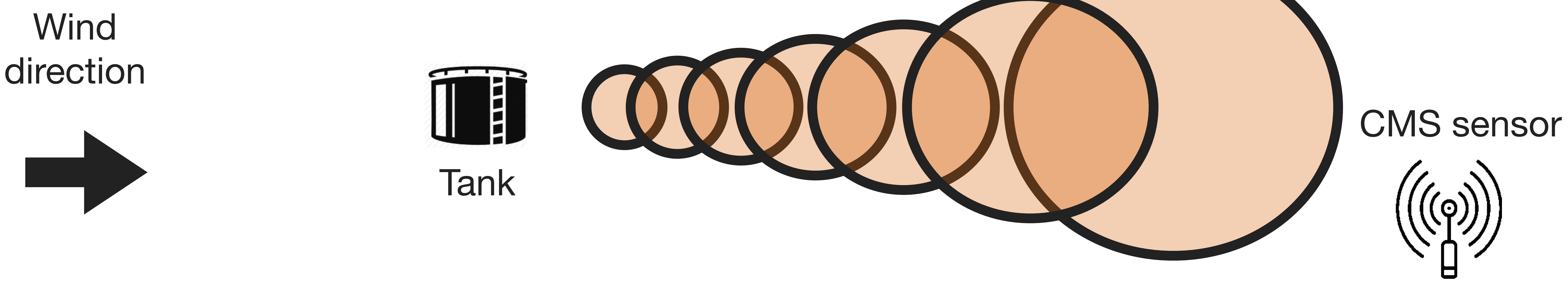

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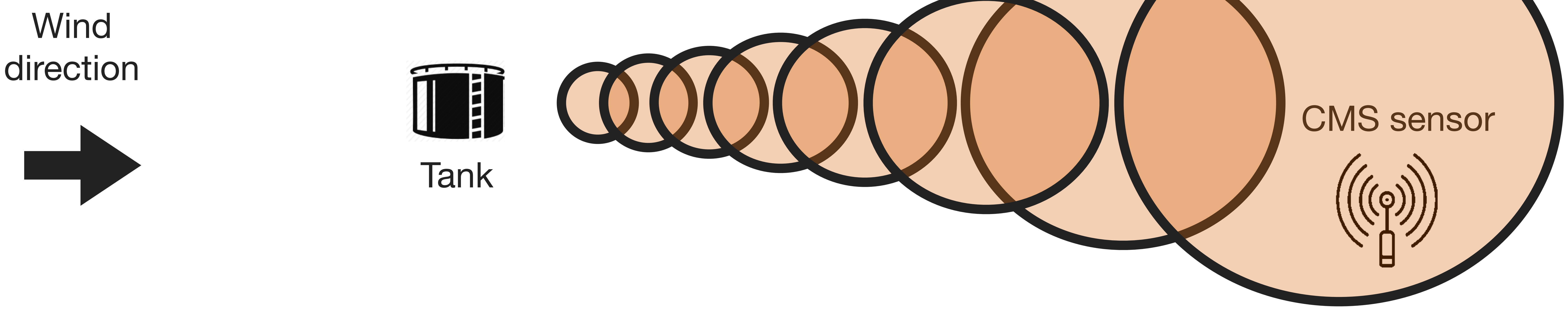

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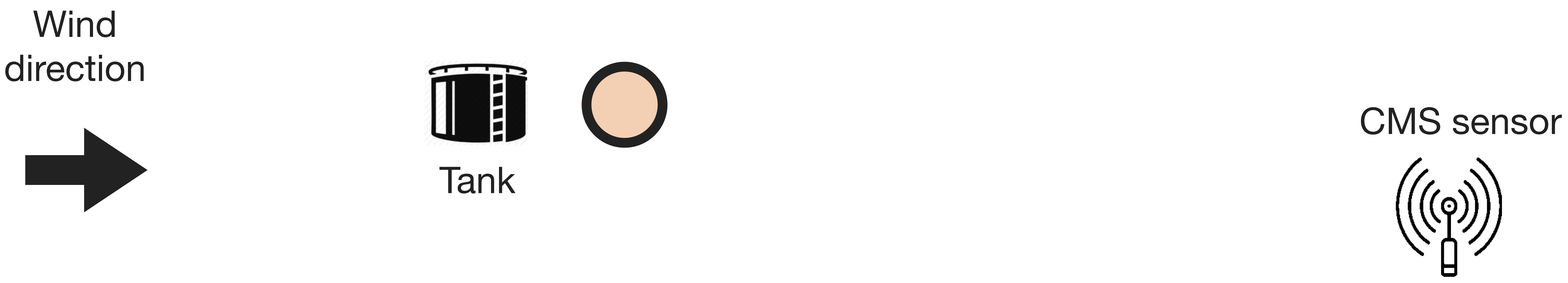

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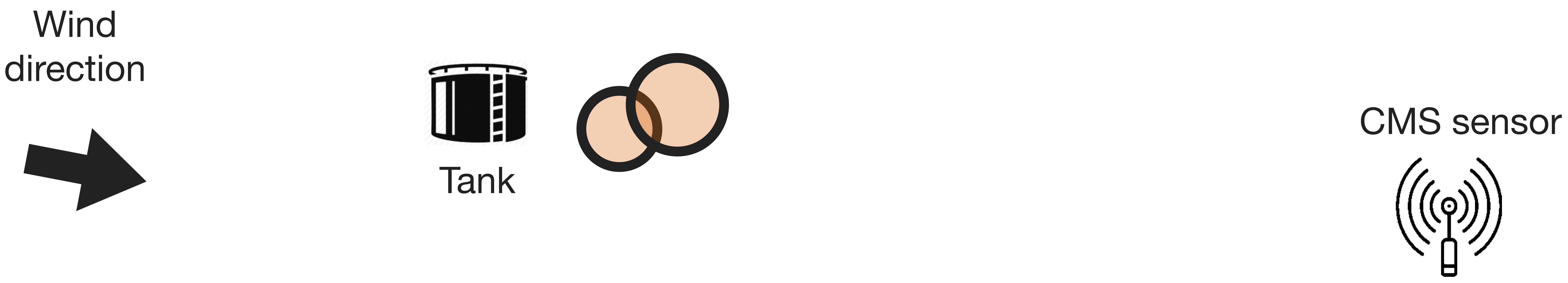

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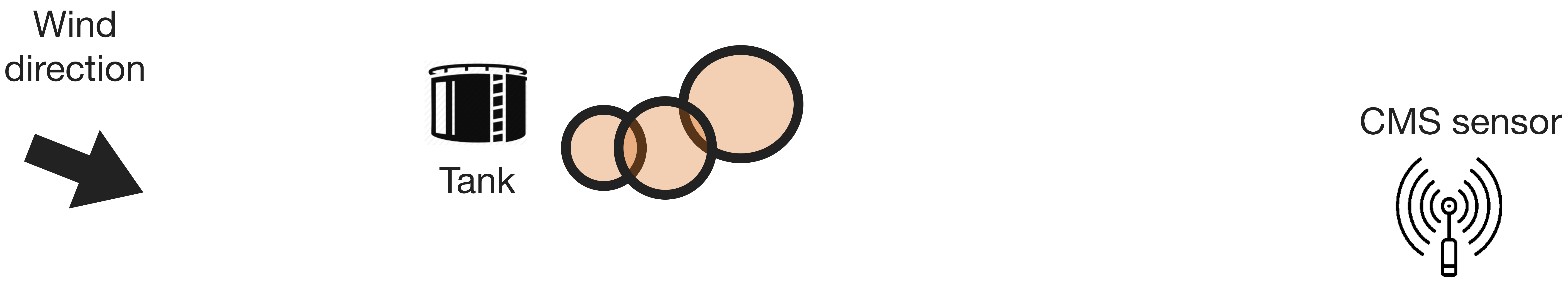

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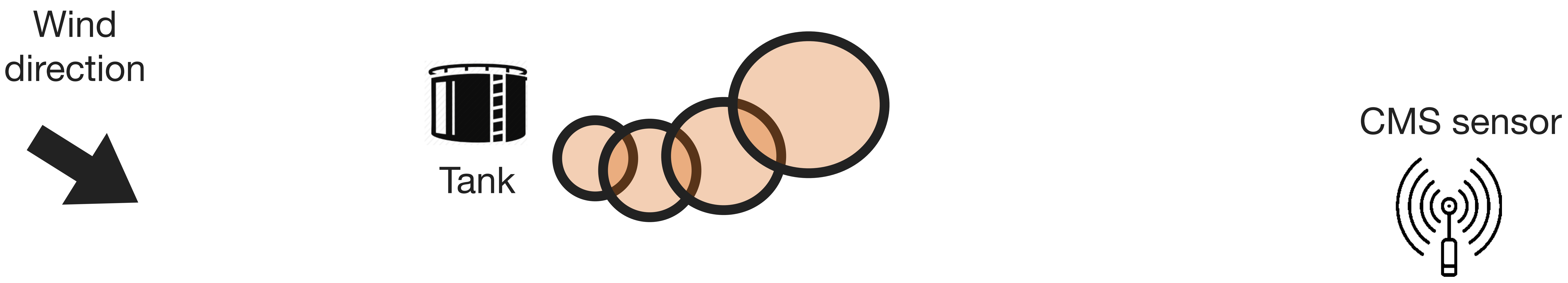

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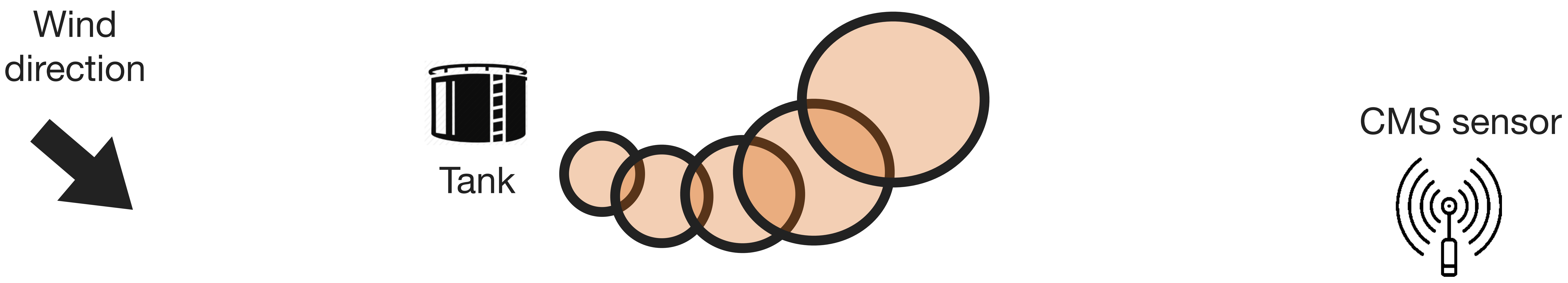

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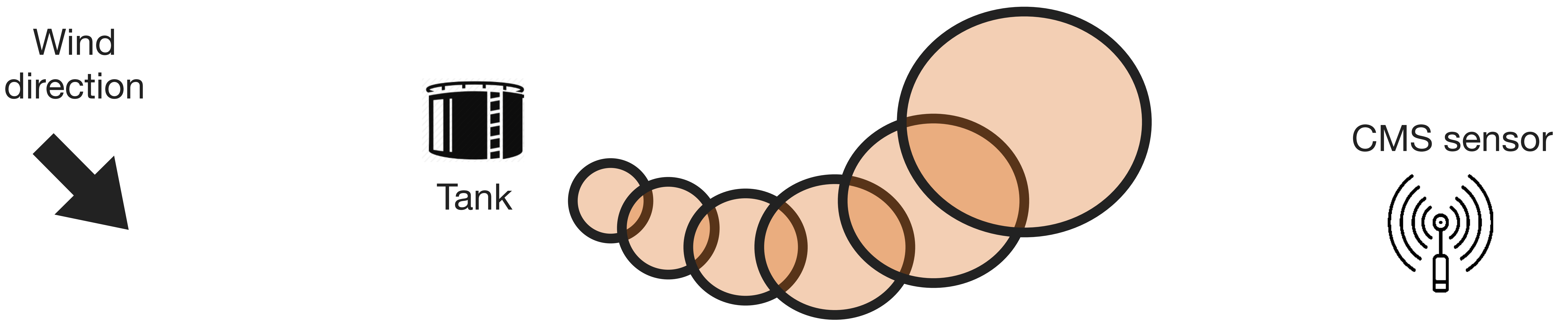

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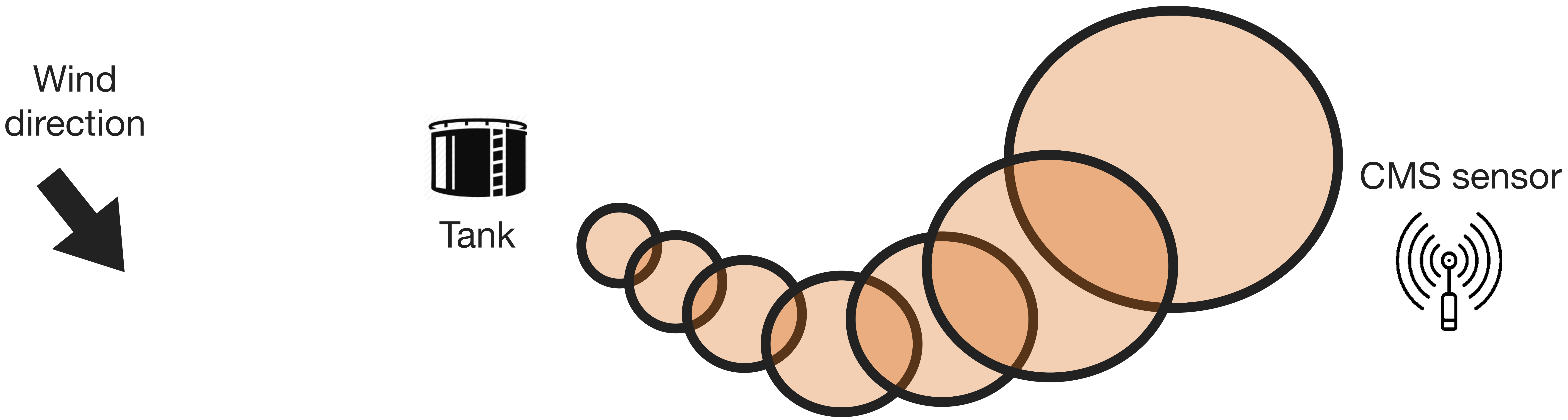

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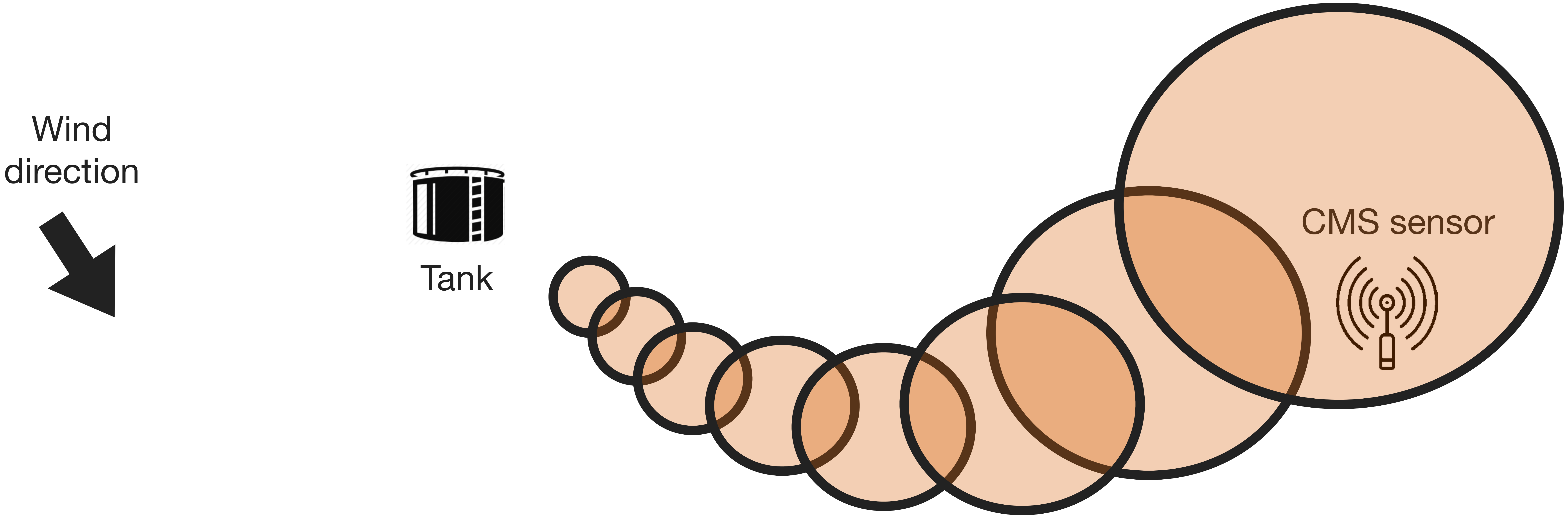
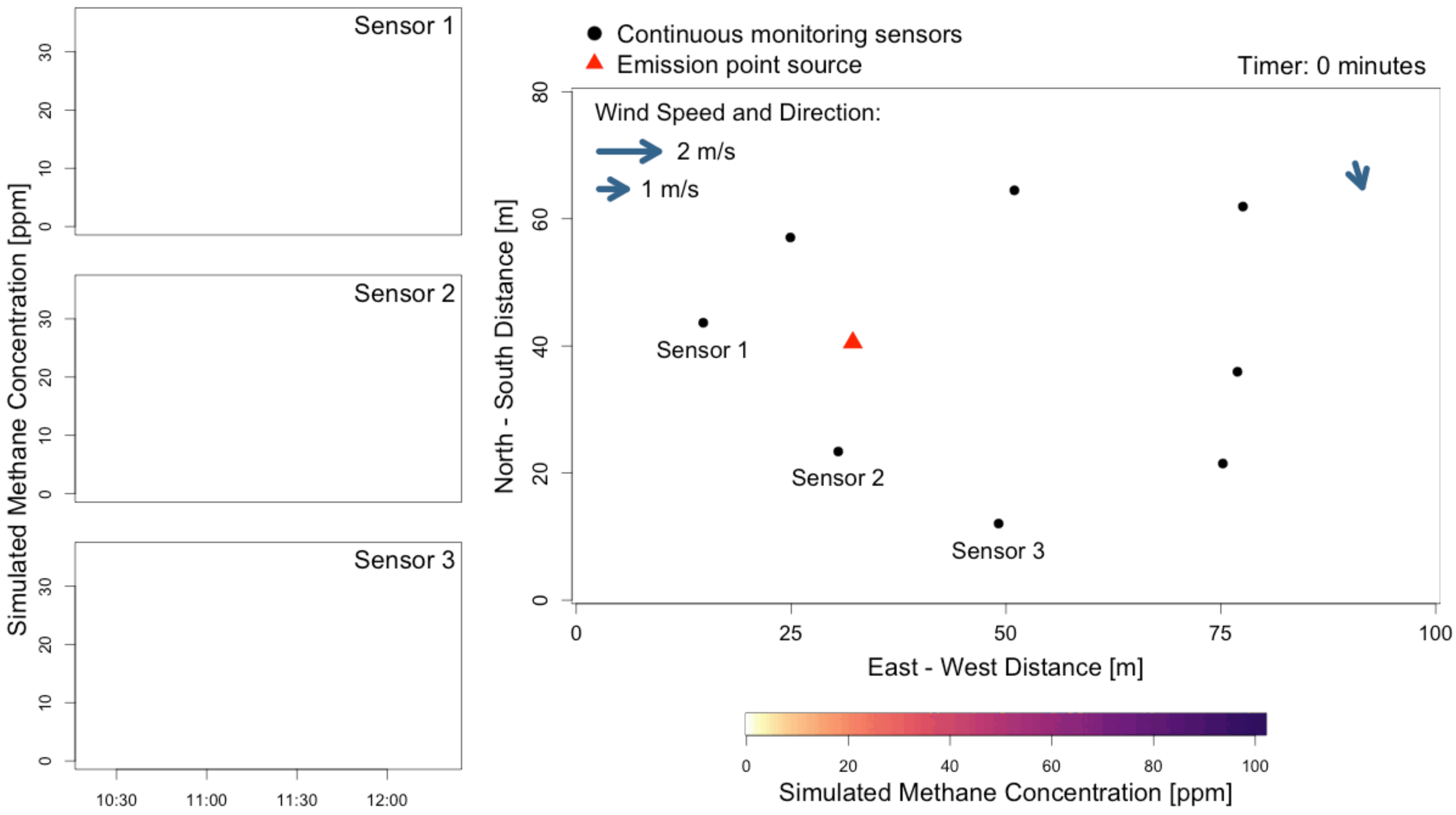
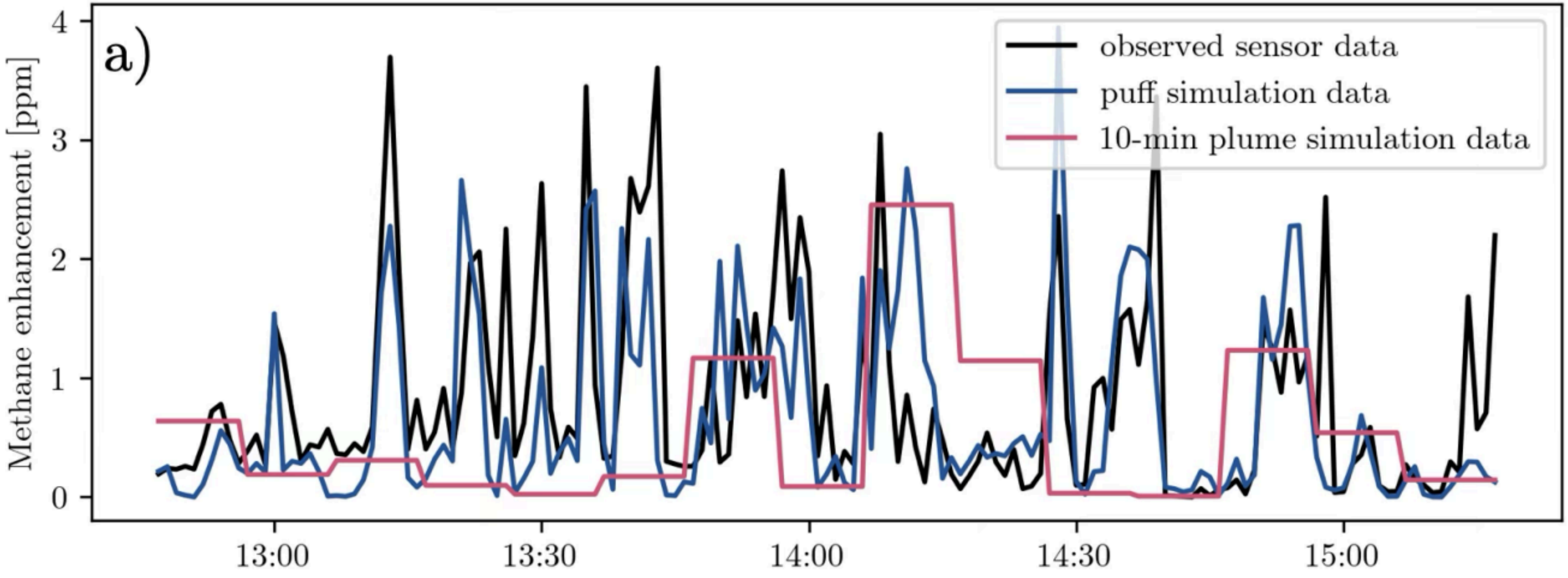



Sensor 1
Sensor 2
Sensor 3
Simulated Methane Concentration [ppm]
10:30
11:00
11:30
12:00
Continuous monitoring sensors
Emission point source
Timer: 0 minutes
Wind Speed and Direction:
2 m/s
1 m/s
North - South Distance [m]
East - West Distance [m]
Simulated Methane Concentration [ppm]

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



Meng Jia, Ryker Fish, et al. A fast and lightweight implementation of the Gaussian puff model for near-field atmospheric transport of trace gasses. *Scientific Reports (in press)*, 2025.

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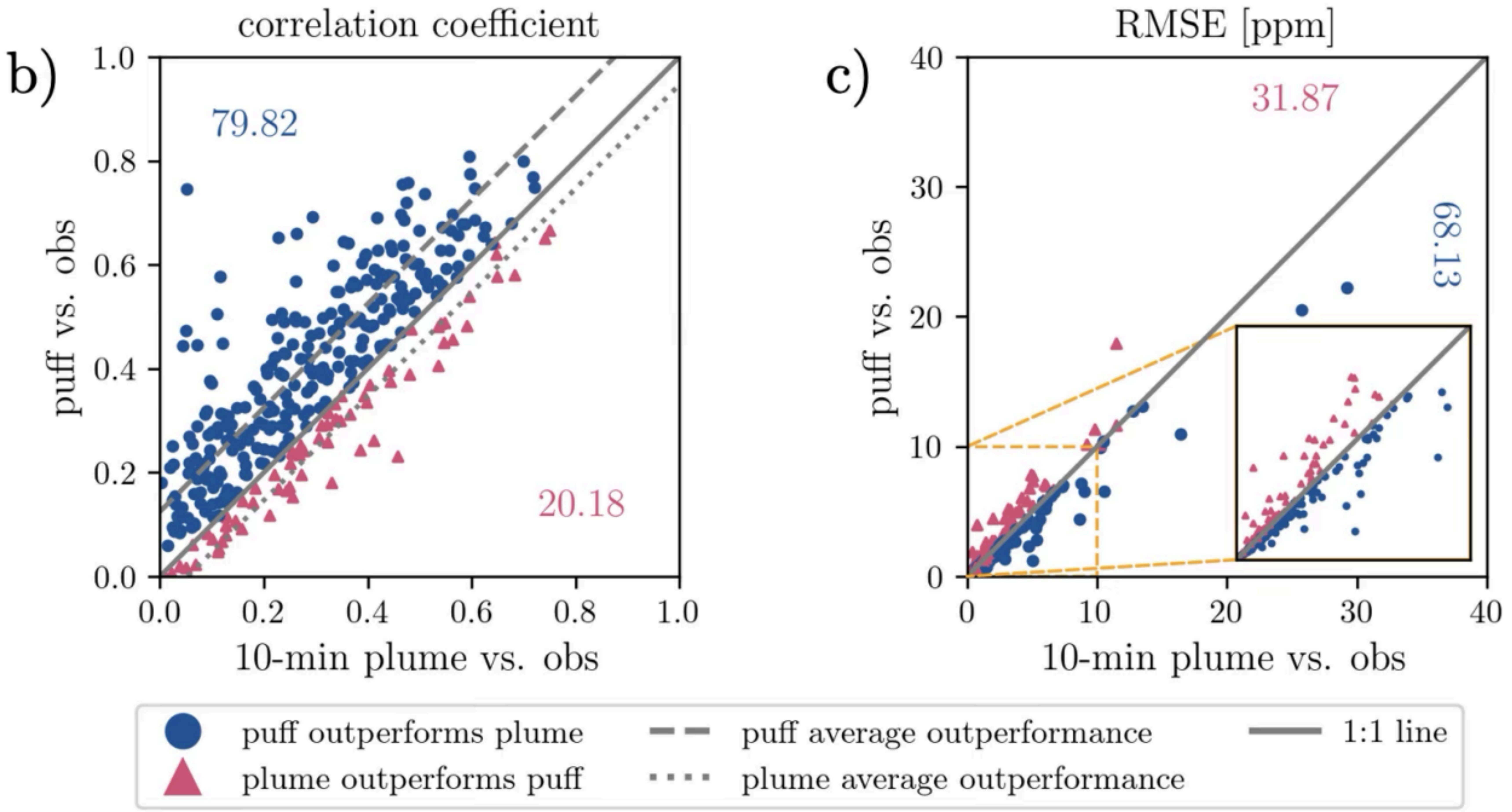

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Gaussian plume model: mathematical definition

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

Exponential decay as you move away from the downwind vector in the vertical dimension

Emission rate

$$c(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right]$$

Predicted methane concentration at sensor location (x,y,z)

Exponential decay as you move away from the downwind vector in the 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

Total volume of methane contained in puff p

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

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 concentration at (x, y, z, t)

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

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Exponential decay in concentration in vertical dimension (z)

Agenda

Talk (~30 min):

- ~~Overview of the Gaussian plume and Gaussian puff models~~
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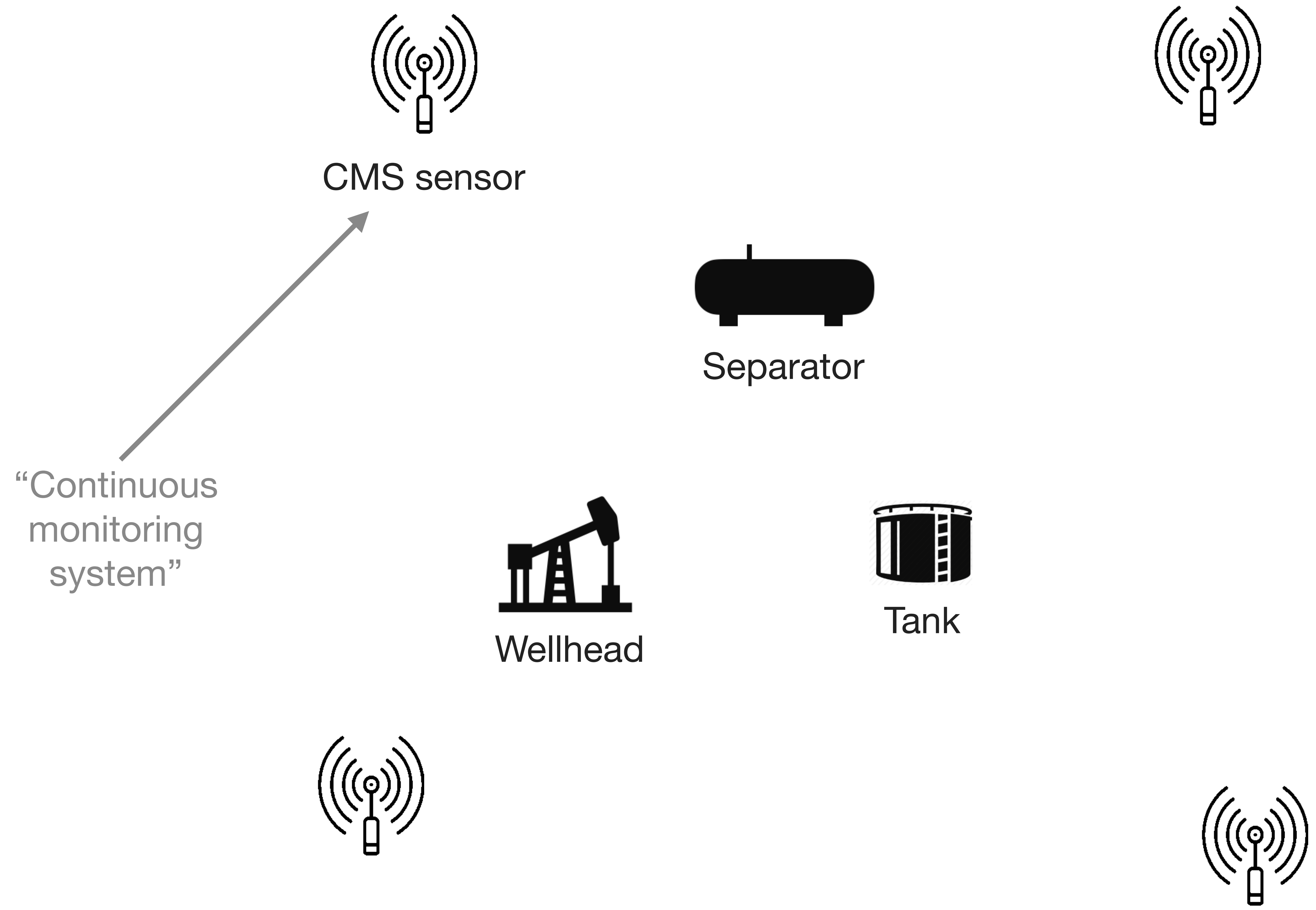
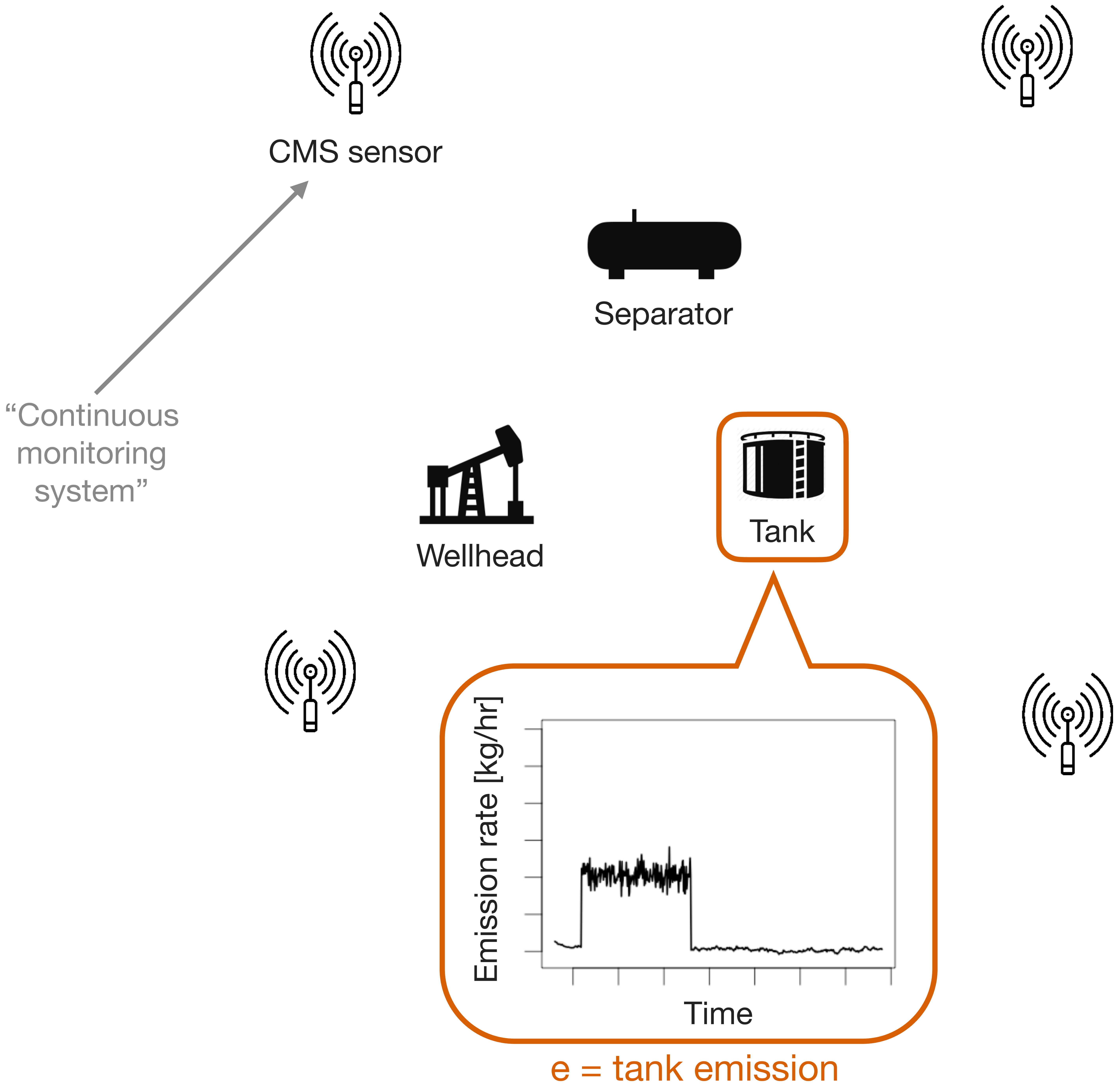
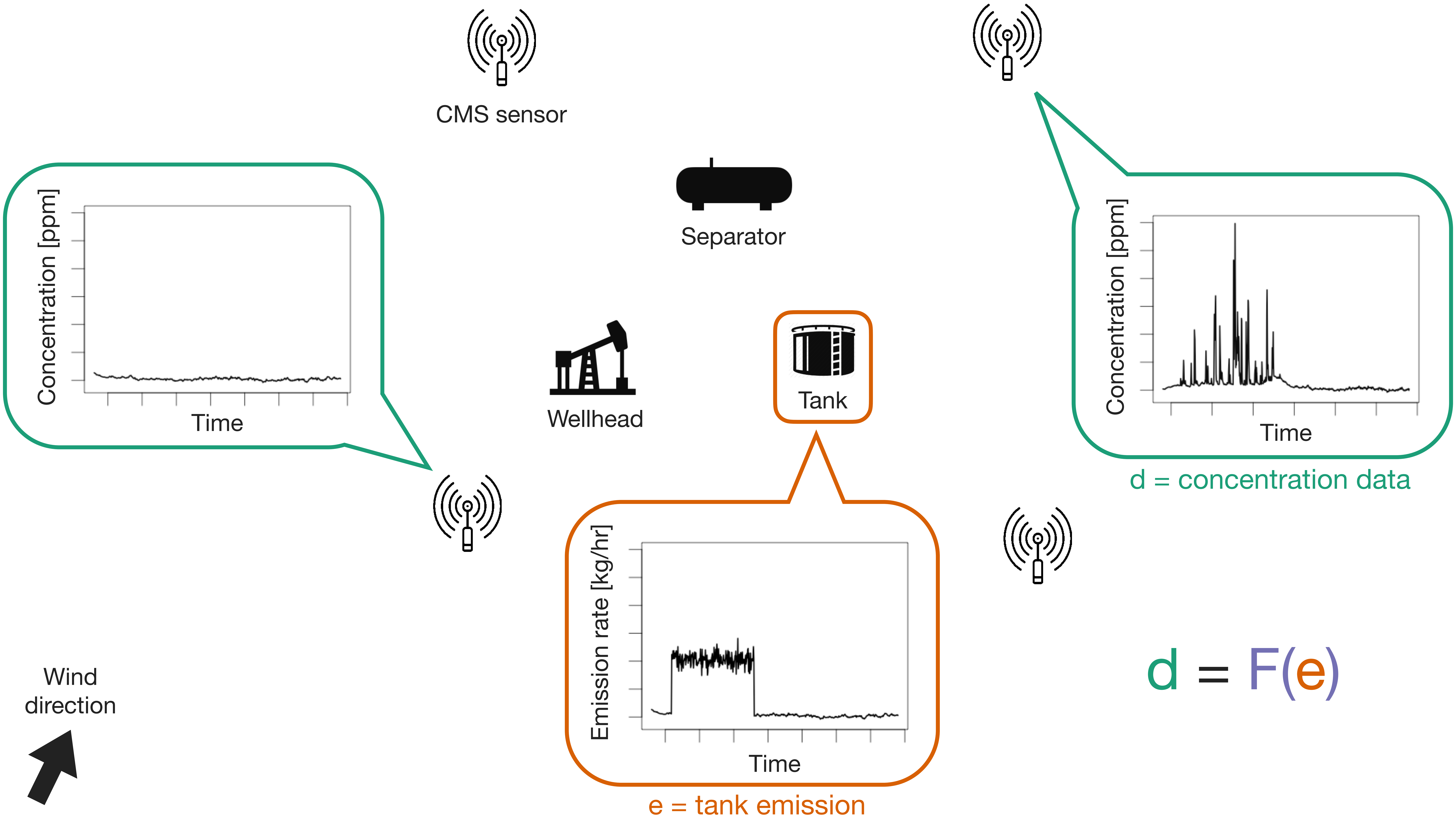
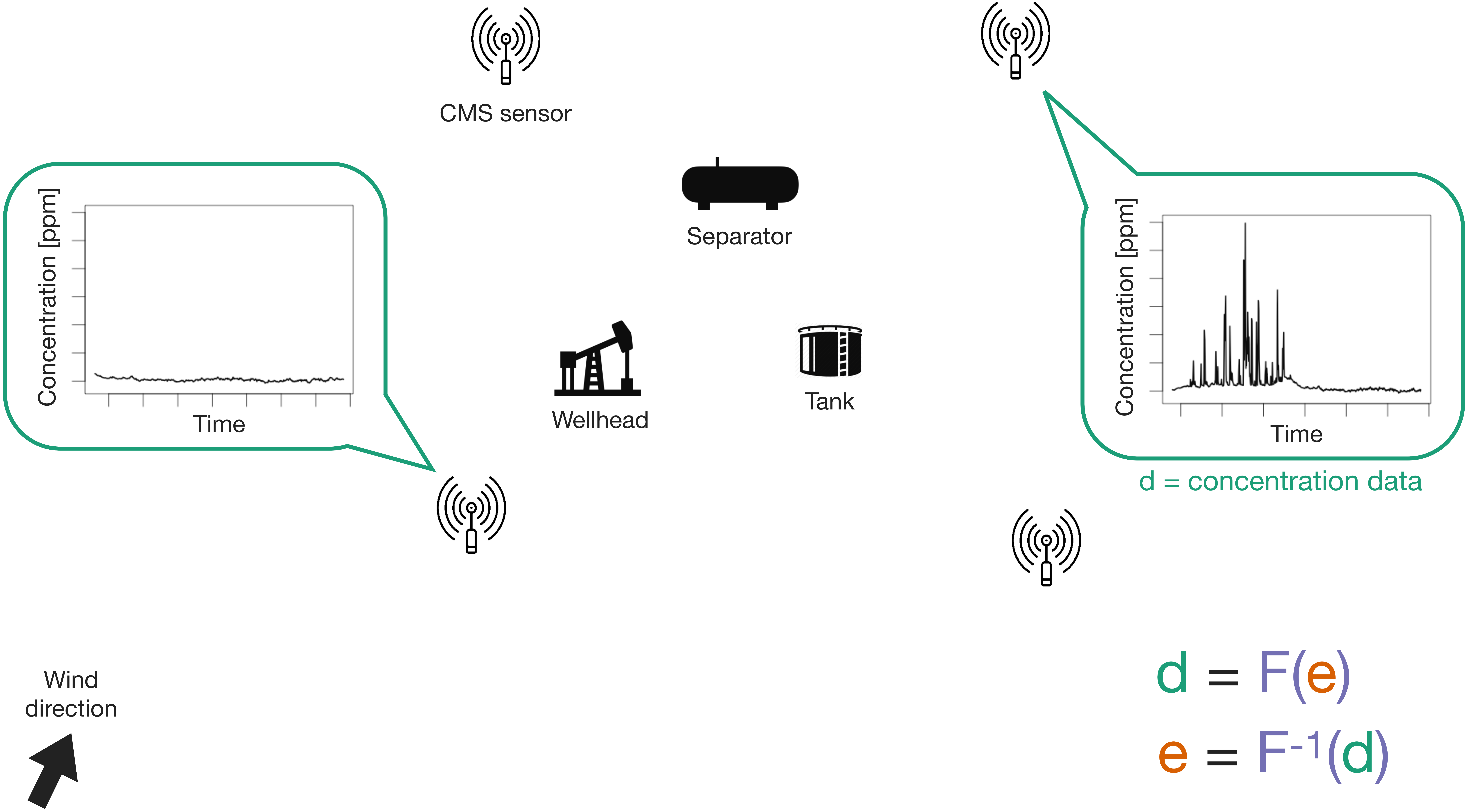


The continuous monitoring inverse problem


CMS sensor
Separator
"Continuous monitoring system"
Wellhead
Tank
Emission rate [kg/hr]
Time
e = tank emission


CMS sensor
Separator
Concentration [ppm]
Time
Wellhead
Tank
Concentration [ppm]
Time
d = concentration data
Emission rate [kg/hr]
Time
e = tank emission
Wind
direction
d = F(e)


CMS sensor
Concentration [ppm]
Time
Separator
Wellhead
Tank
Concentration [ppm]
Time
d = concentration data
Wind
direction

$$d = F(e)$$

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

Open source framework for solving inverse problem

STEP 1:
Background removal
and event detection

→

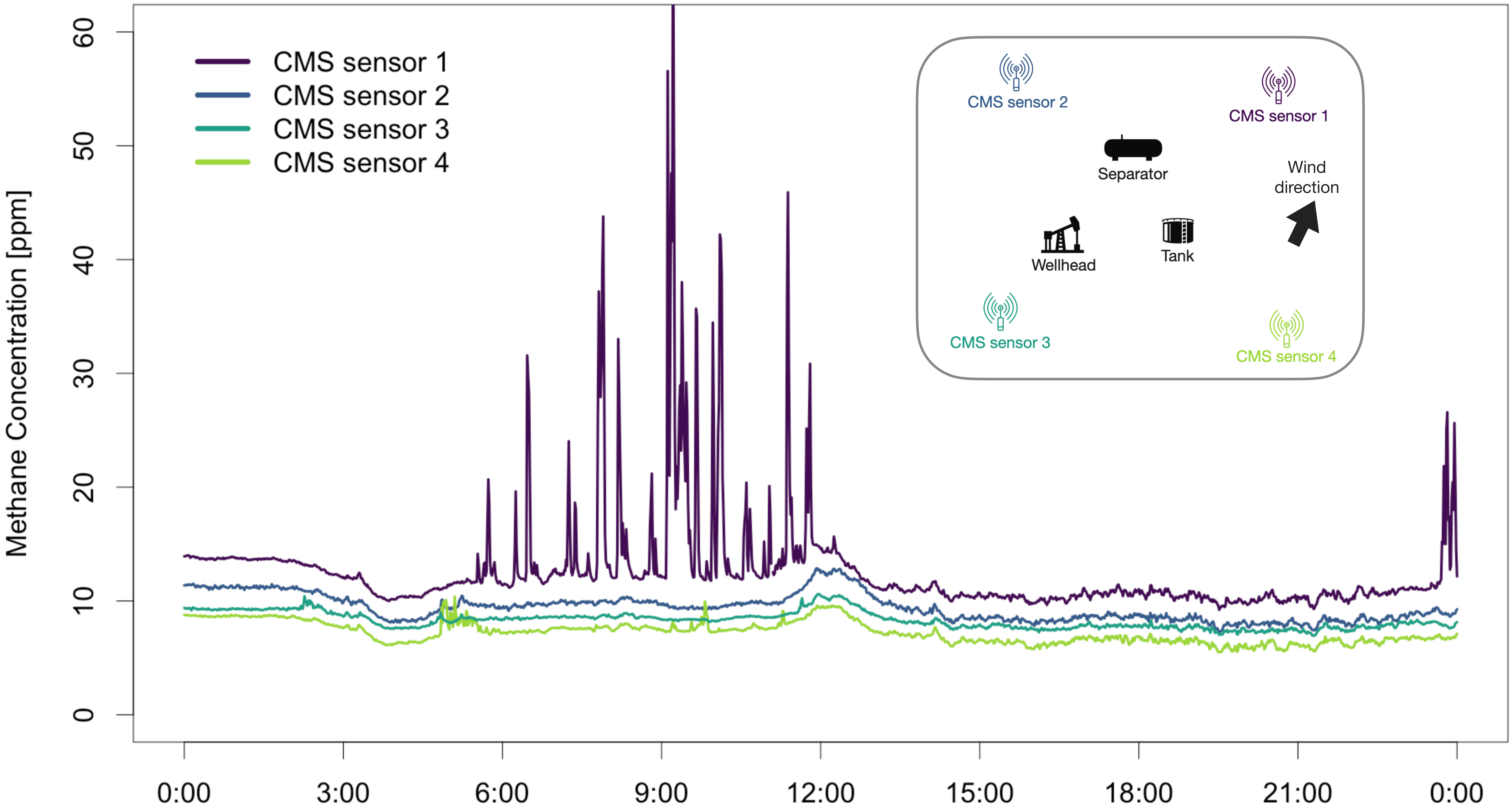
STEP 2:
Simulation

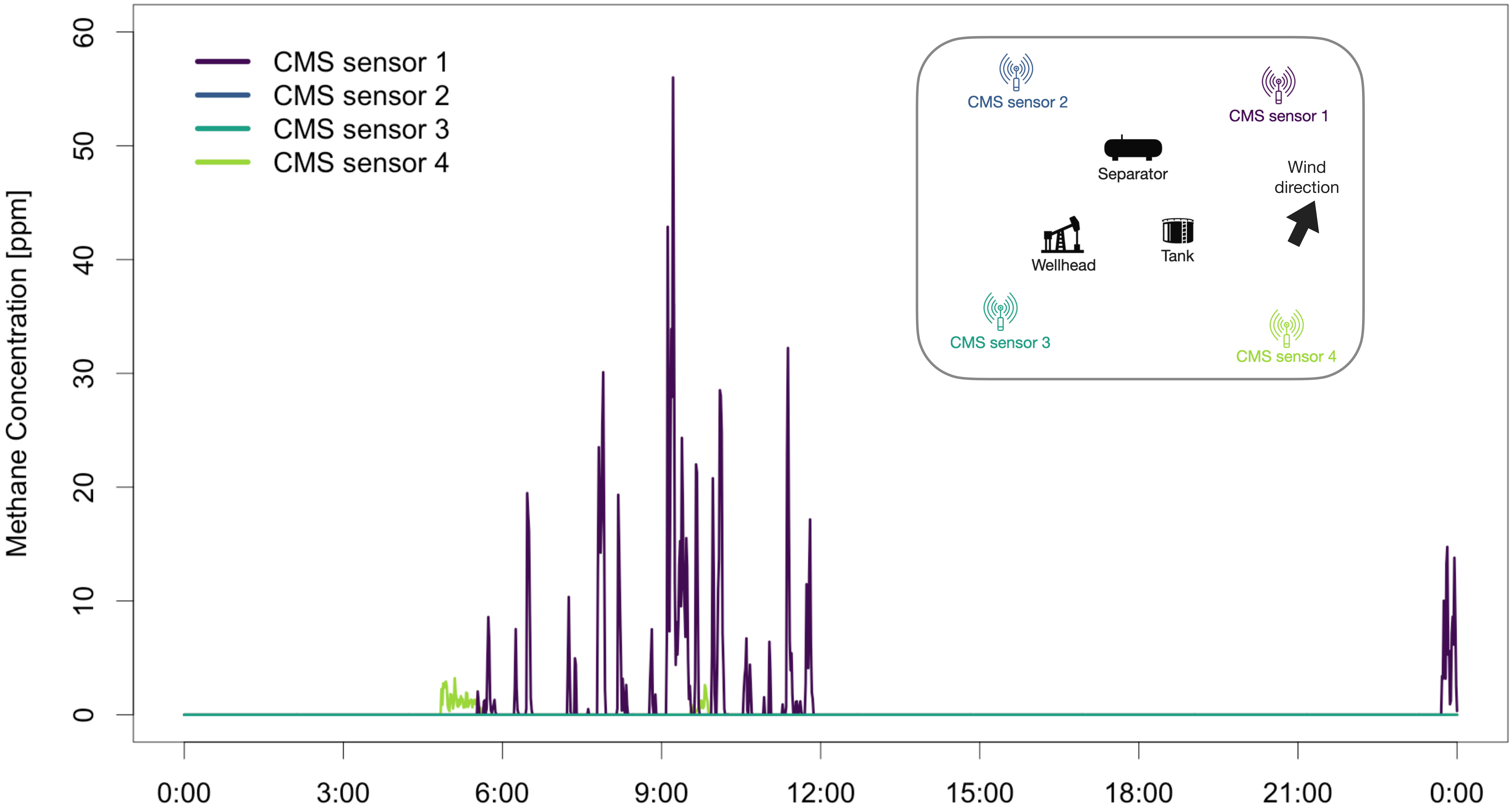
→

STEP 3:
Localization

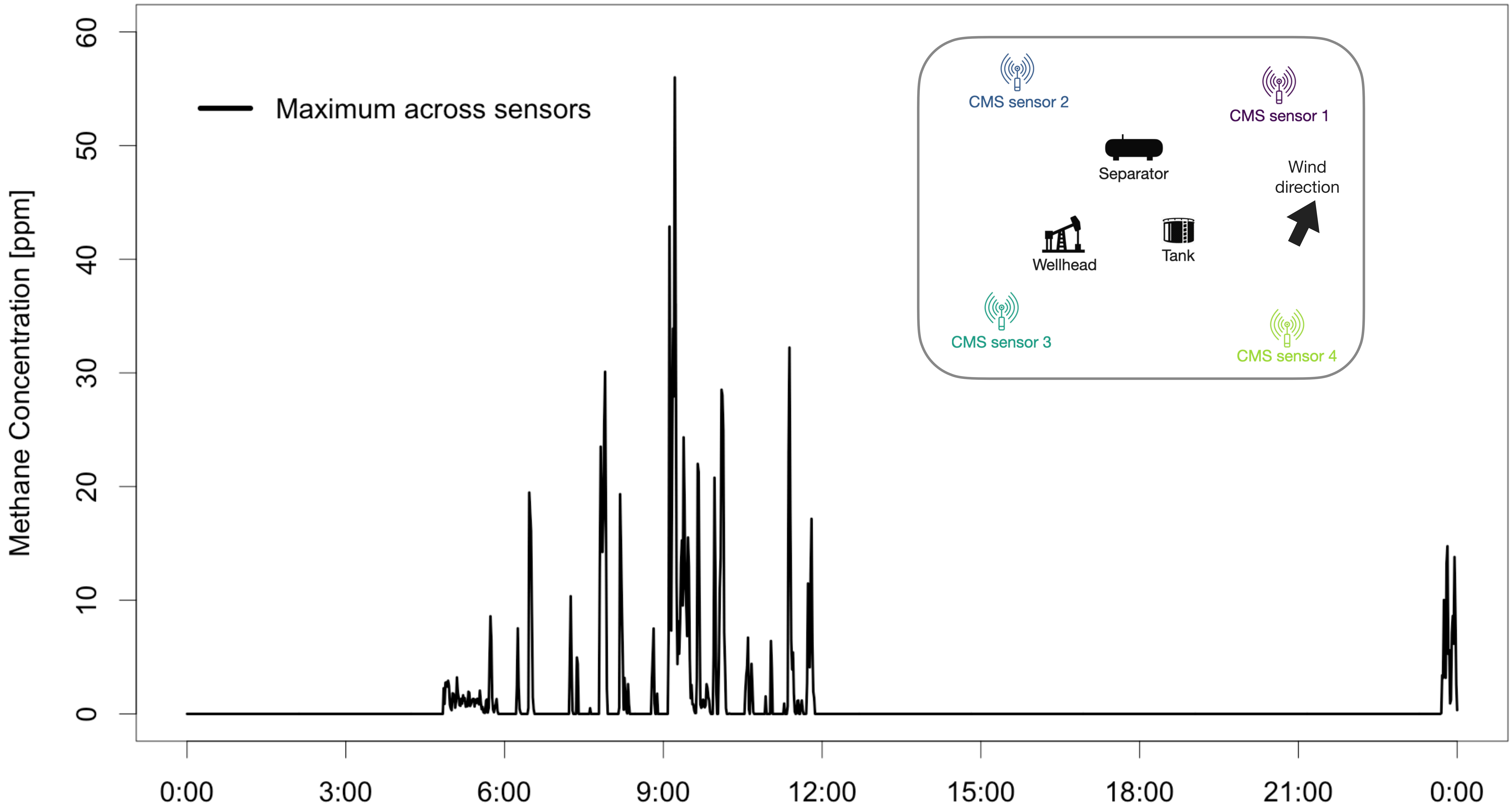
→

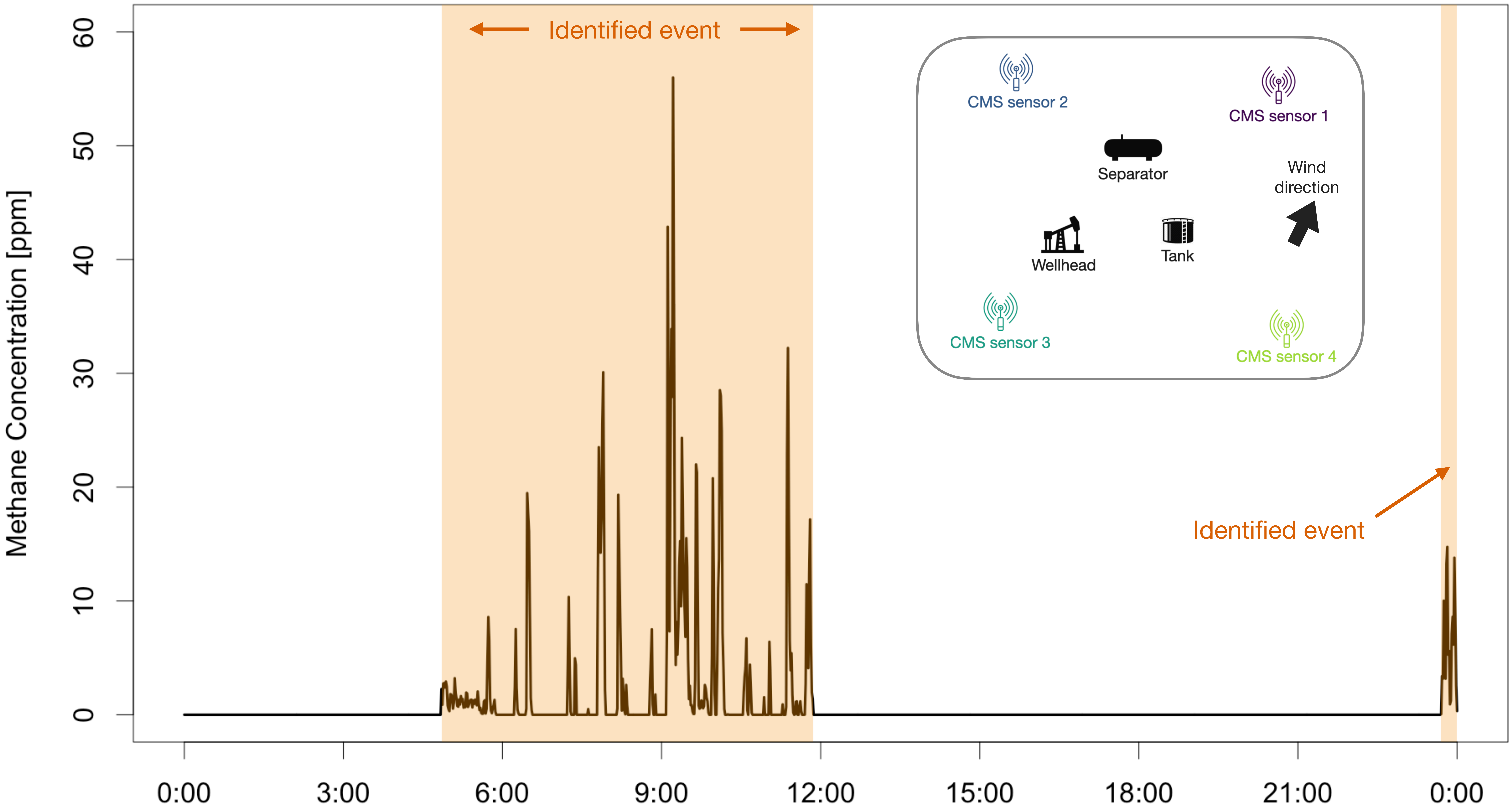
STEP 4:
Quantification


CMS sensor 1
CMS sensor 2
CMS sensor 3
CMS sensor 4
Methane Concentration [ppm]
0
10
20
30
40
50
60
0:00
3:00
6:00
9:00
12:00
15:00
18:00
21:00
0:00
CMS sensor 2
CMS sensor 1
Separator
Wind direction
Wellhead
Tank
CMS sensor 3
CMS sensor 4



Methane Concentration [ppm]
0
10
20
30
40
50
60
0:00
3:00
6:00
9:00
12:00
15:00
18:00
21:00
0:00
CMS sensor 1
CMS sensor 2
CMS sensor 3
CMS sensor 4
CMS sensor 2
CMS sensor 1
Separator
Wind direction
Wellhead
Tank
CMS sensor 3
CMS sensor 4


Maximum across sensors
CMS sensor 2
CMS sensor 1
Separator
Wind direction
Wellhead
Tank
CMS sensor 3
CMS sensor 4
Methane Concentration [ppm]
0
10
20
30
40
50
60
0:00
3:00
6:00
9:00
12:00
15:00
18:00
21:00
0:00



Identified event
CMS sensor 2
CMS sensor 1
Separator
Wind direction
Wellhead
Tank
CMS sensor 3
CMS sensor 4
Identified event
Methane Concentration [ppm]
0
10
20
30
40
50
60
0:00
3:00
6:00
9:00
12:00
15:00
18:00
21:00
0:00

Open source framework for solving inverse problem

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Gaussian puff atmospheric dispersion model

Total volume of methane contained in puff p

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

Concentration contribution of puff p

Decay in puff concentration in horizontal plane (x, y)

Decay in puff concentration in vertical dimension (z)

Gaussian puff atmospheric dispersion model

Total volume of methane contained in puff p

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

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

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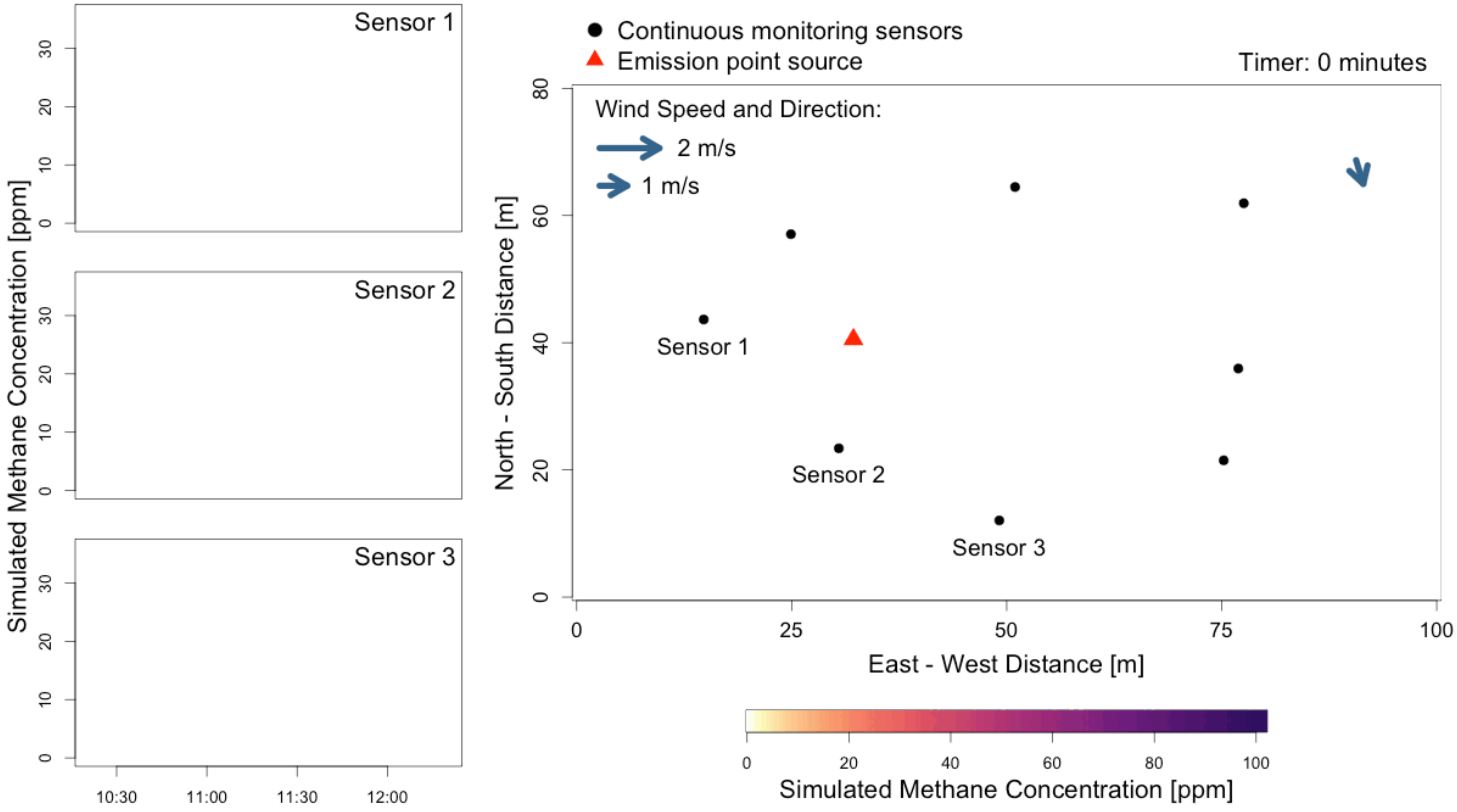
Sensor 1
Sensor 2
Sensor 3
Simulated Methane Concentration [ppm]
0
10
20
30
10:30
11:00
11:30
12:00
Continuous monitoring sensors
Emission point source
Timer: 0 minutes
Wind Speed and Direction:
2 m/s
1 m/s
North - South Distance [m]
East - West Distance [m]
0
20
40
60
80
25
50
75
100
Simulated Methane Concentration [ppm]

Repeat this for all other potential sources!

Open source framework for solving inverse problem

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Background removal
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→

STEP 2:
Simulation

→

STEP 3:
Localization

→

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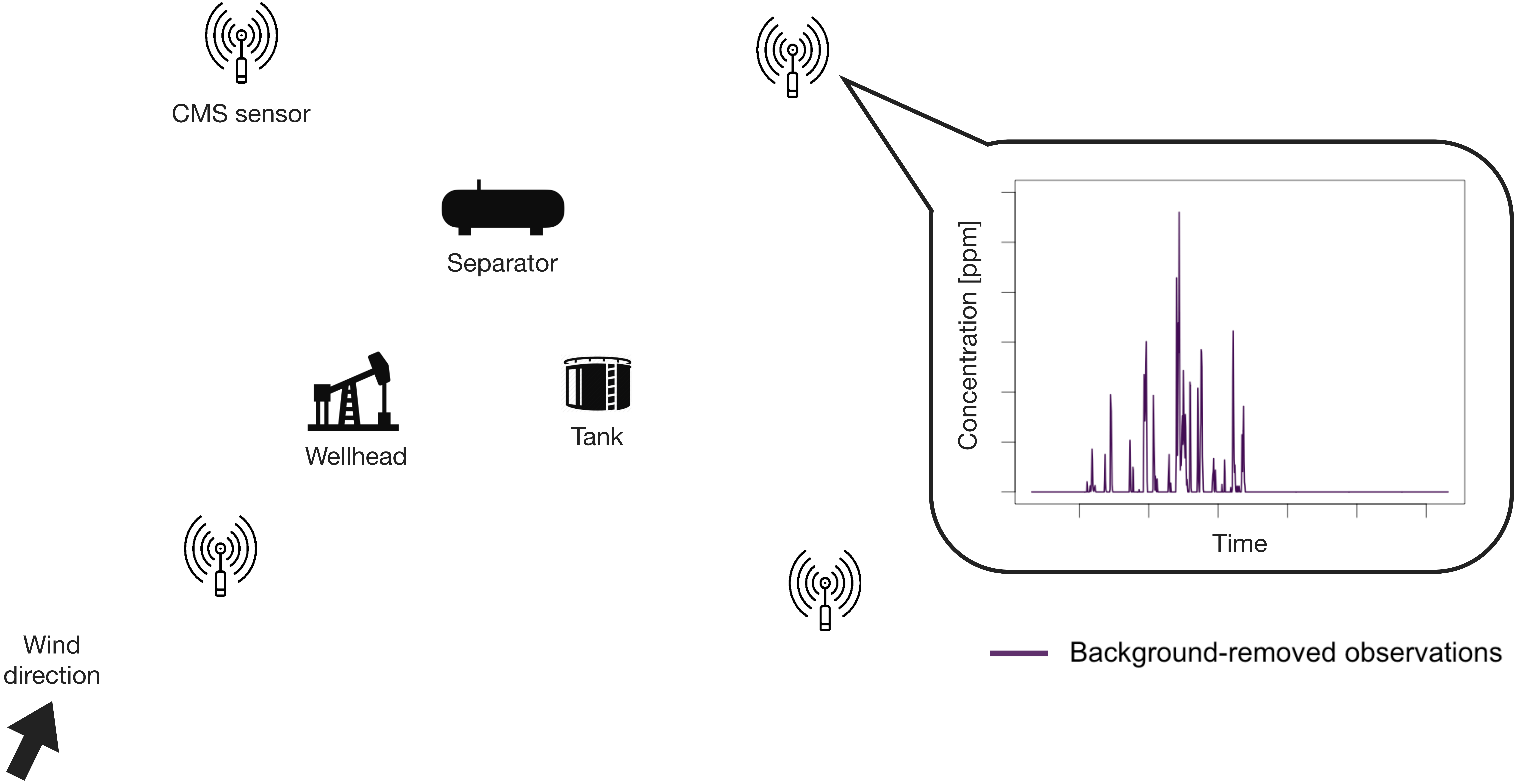
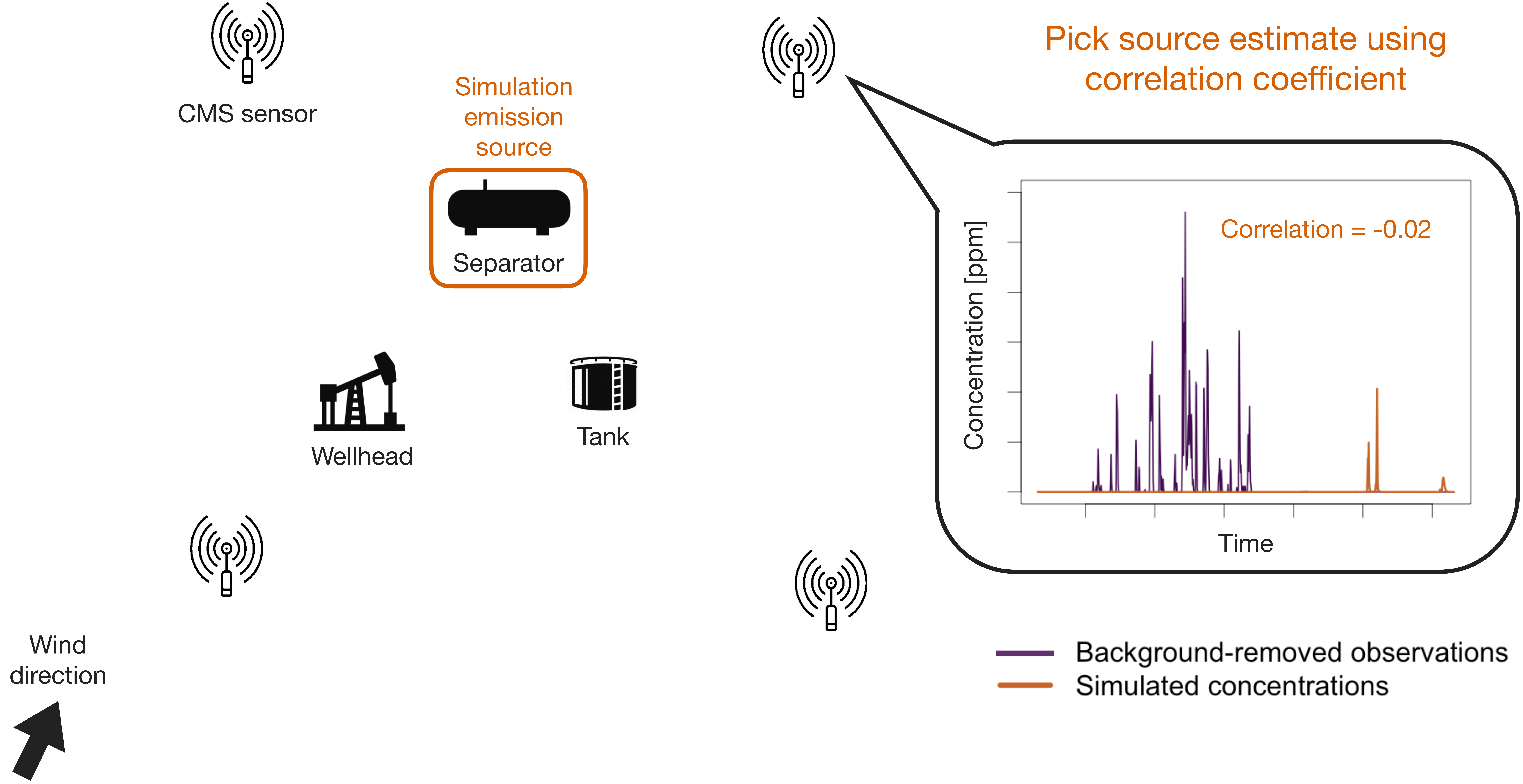
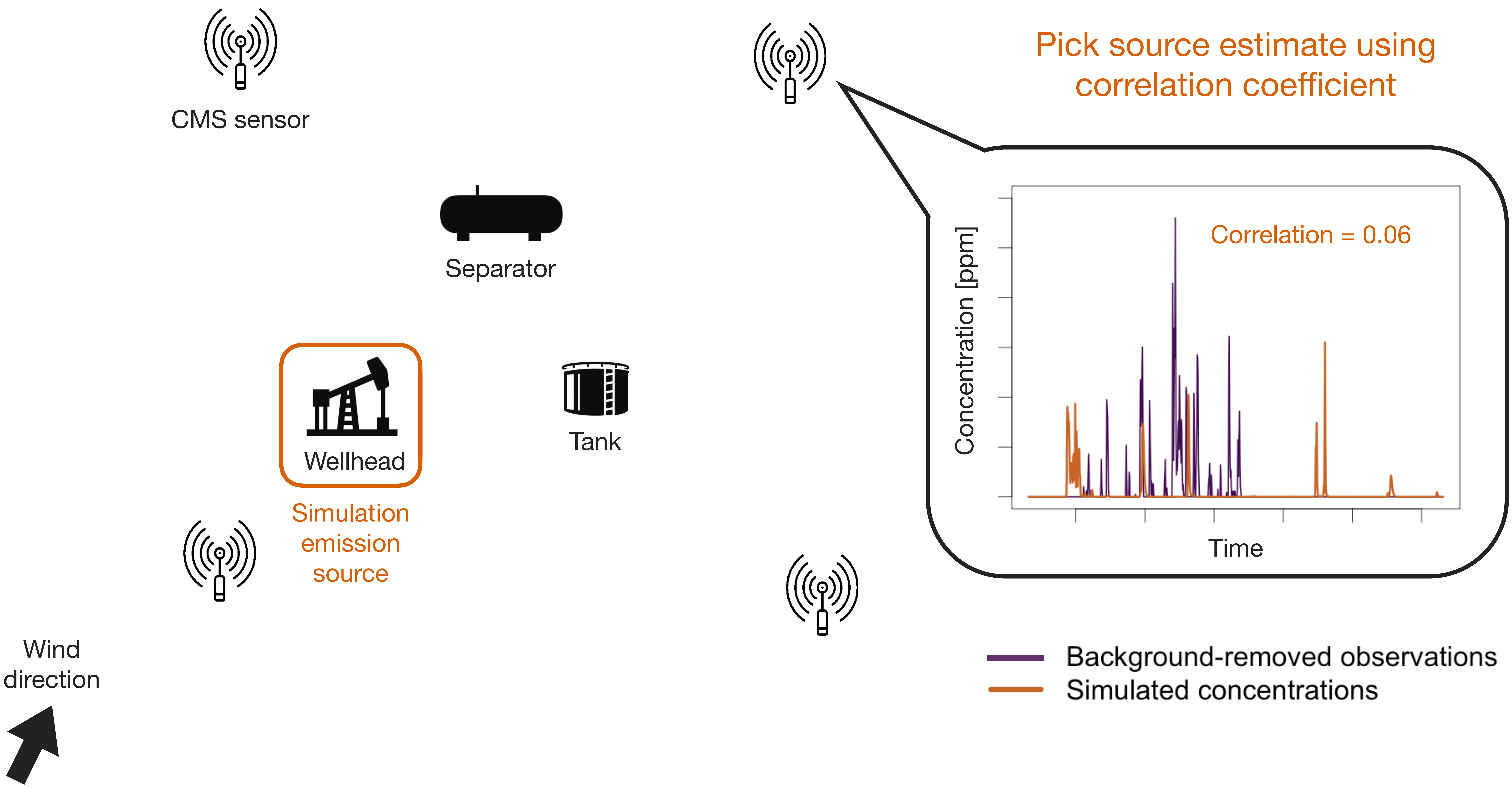
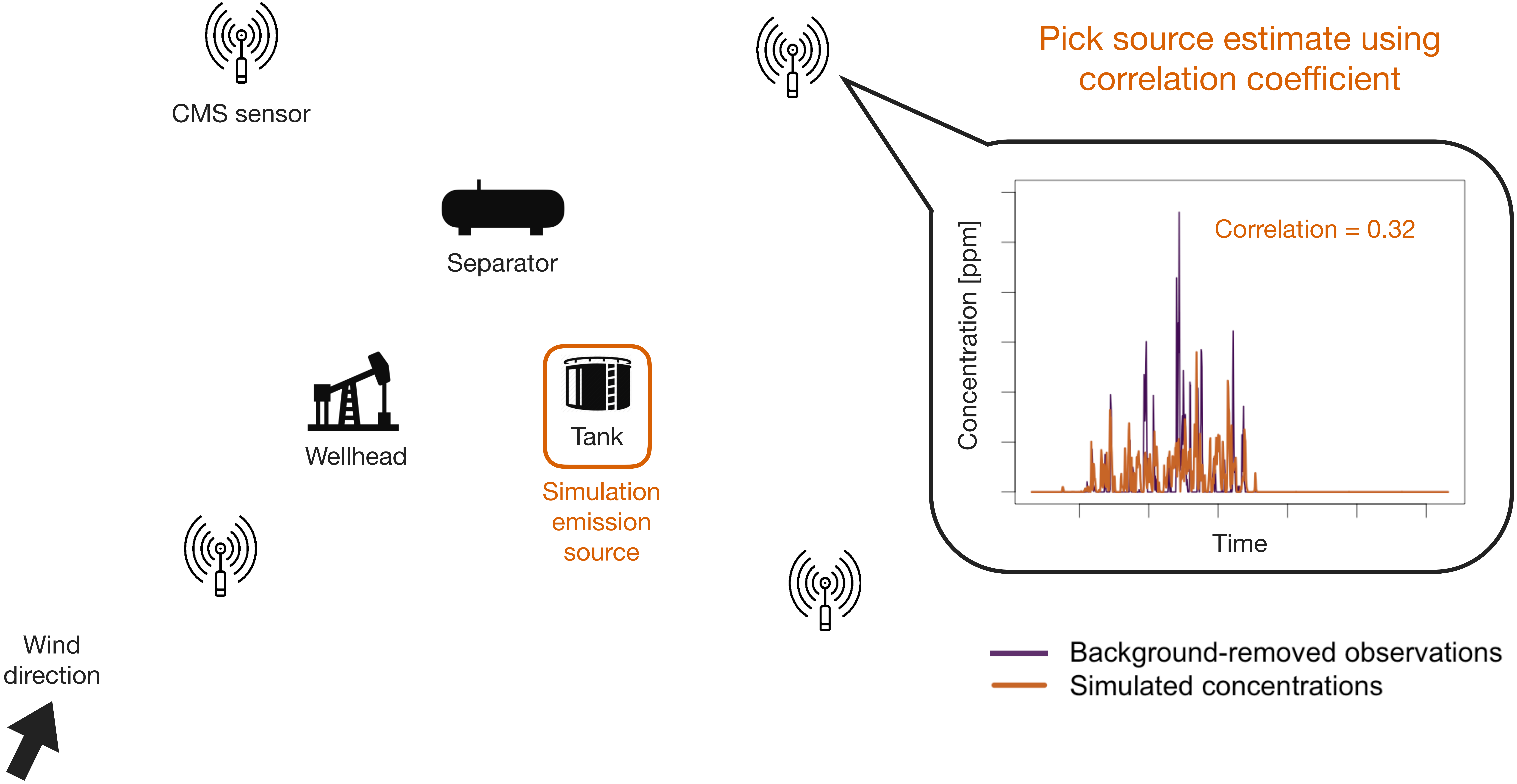

CMS sensor
Separator
Wellhead
Tank
Wind
direction
Concentration [ppm]
Time
Background-removed observations

Pick source estimate using correlation coefficient





CMS sensor
Separator
Wellhead
Tank
Simulation emission source
Wind direction
Pick source estimate using correlation coefficient
Correlation = 0.06
Concentration [ppm]
Time
Background-removed observations
Simulated concentrations



Pick source estimate using correlation coefficient
CMS sensor
Separator
Wellhead
Tank
Simulation emission source
Wind direction
Correlation = 0.32
Concentration [ppm]
Time
Background-removed observations
Simulated concentrations

Open source framework for solving inverse problem

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Background removal
and event detection

STEP 2:
Simulation

STEP 3:
Localization

STEP 4:
Quantification

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

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Concentration contribution of puff p

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

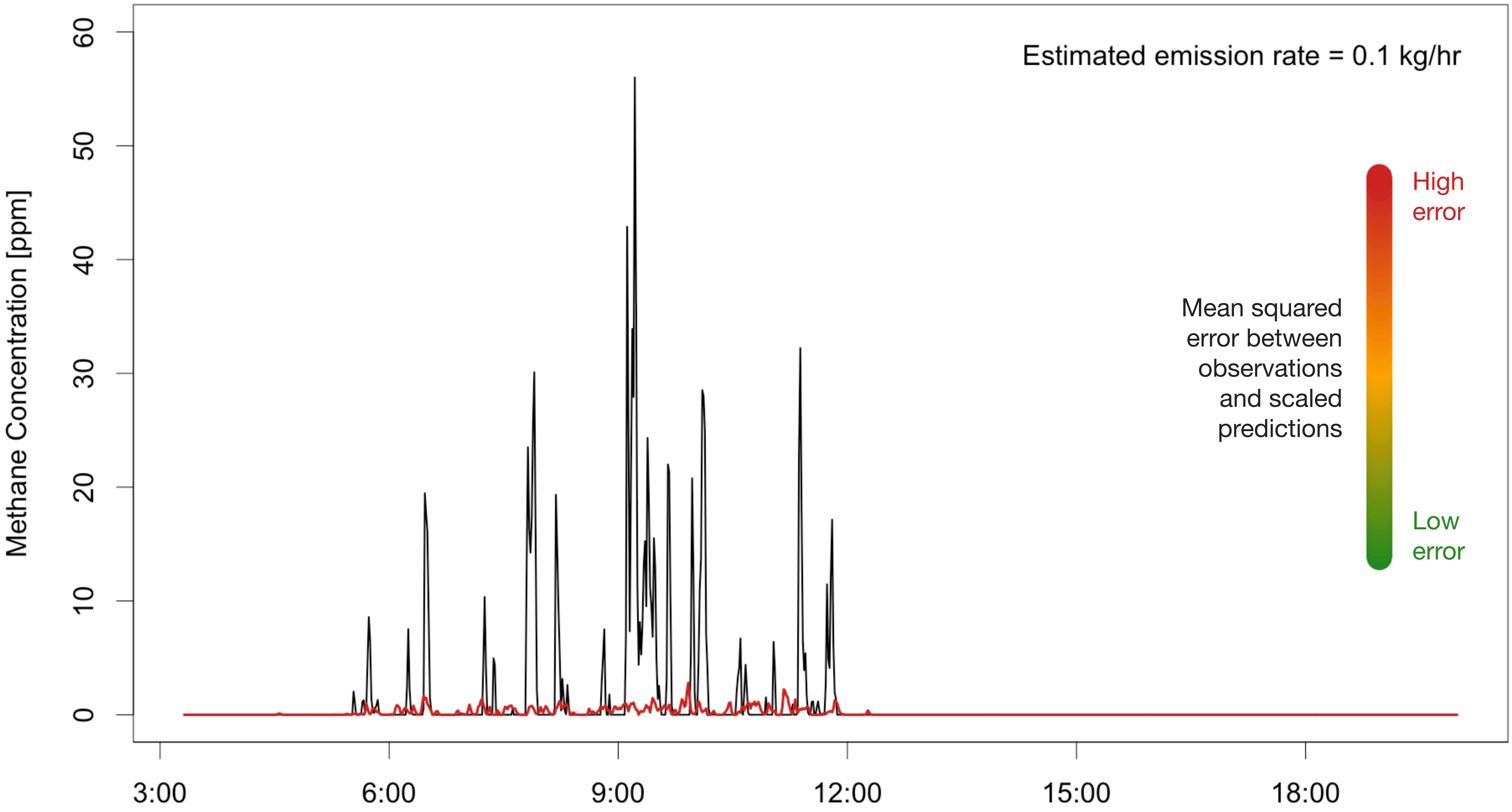
Total concentration at (x, y, z, t)

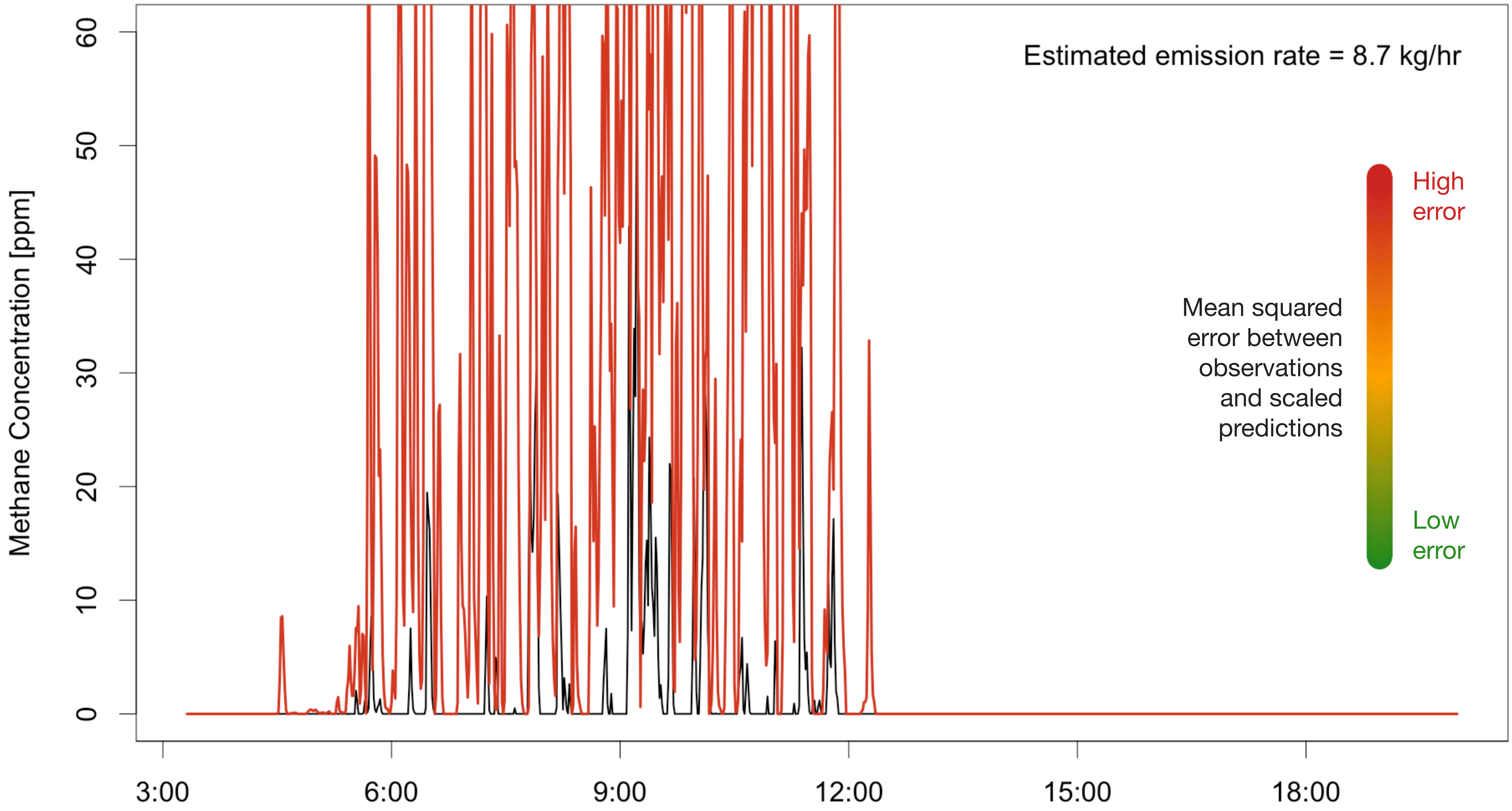
Concentration data

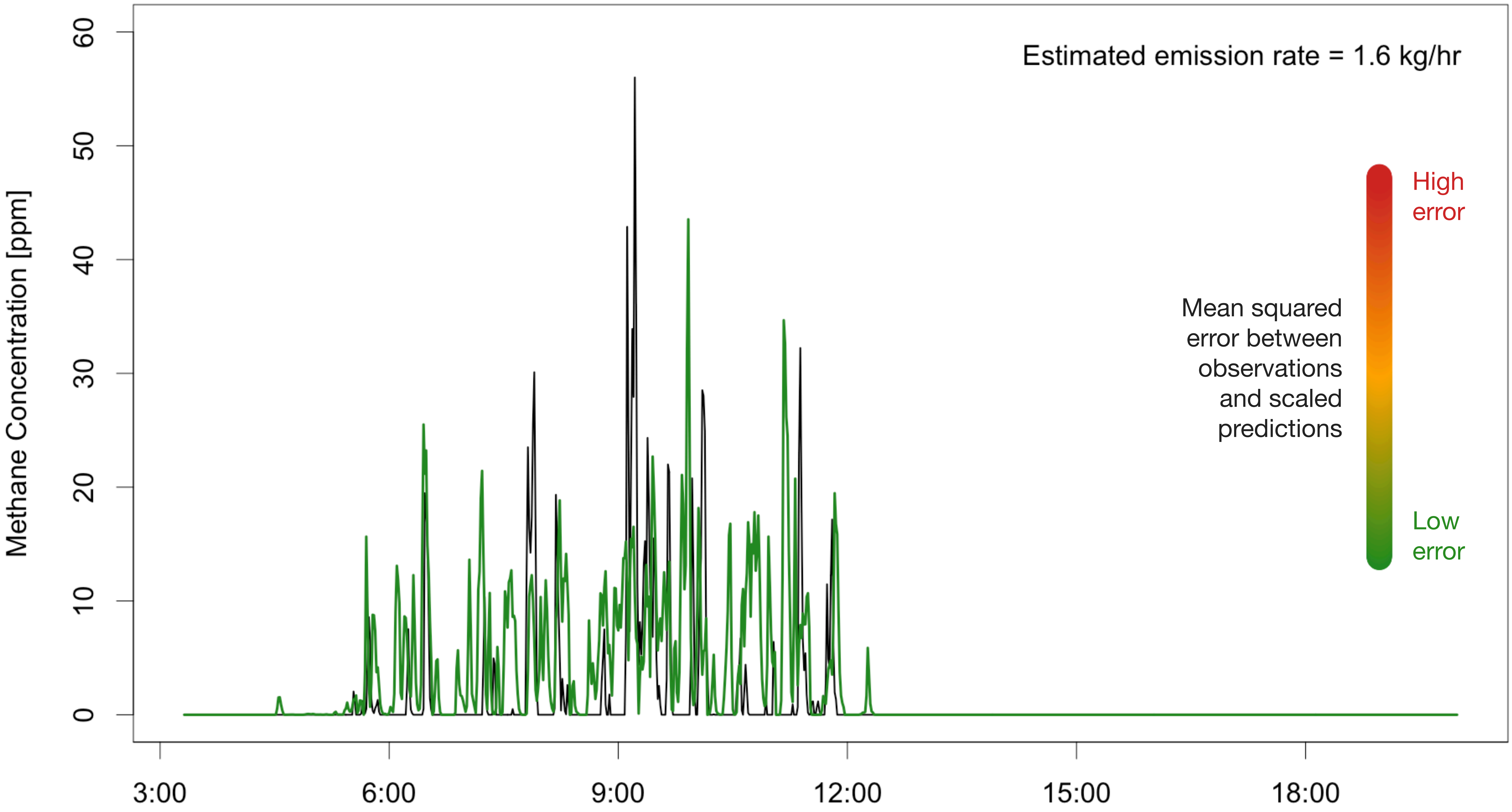
$$\hat{Q} = \underset{Q}{\operatorname{argmin}} \left\{ \frac{1}{n} \sum_{t=1}^{n} \big(d(x, y, z, t) - c(x, y, z, t, Q)\big)^2 \right\}$$

Emission rate estimate

Simulated concentrations

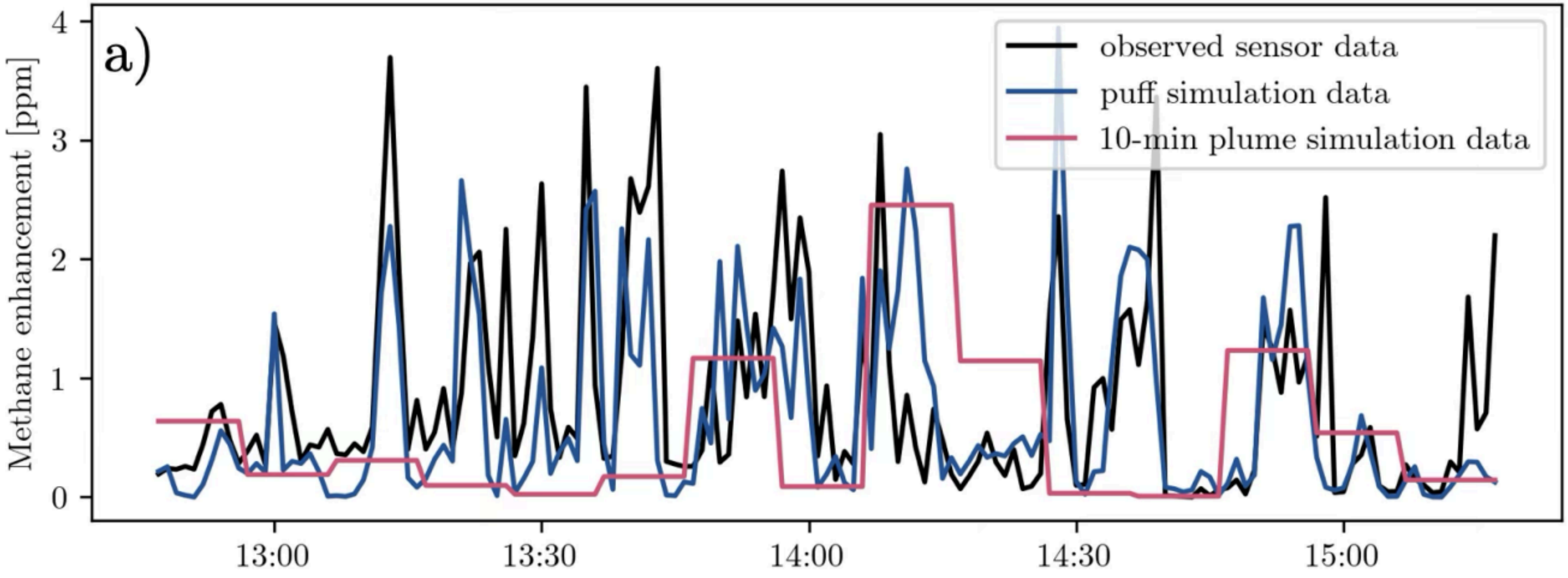

Estimated emission rate = 0.1 kg/hr
Methane Concentration [ppm]
0
10
20
30
40
50
60
3:00
6:00
9:00
12:00
15:00
18:00
Mean squared error between observations and scaled predictions
High error
Low error


Estimated emission rate = 8.7 kg/hr
Methane Concentration [ppm]
0
10
20
30
40
50
60
3:00
6:00
9:00
12:00
15:00
18:00
Mean squared error between observations and scaled predictions
High error
Low error



Estimated emission rate = 1.6 kg/hr
Methane Concentration [ppm]
0
10
20
30
40
50
60
3:00
6:00
9:00
12:00
15:00
18:00
Mean squared error between observations and scaled predictions
High error
Low error

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



Meng Jia, Ryker Fish, et al. A fast and lightweight implementation of the Gaussian puff model for near-field atmospheric transport of trace gasses. *Scientific Reports (in press)*, 2025.

Agenda

Talk (~30 min):

- ~~Overview of the Gaussian puff model~~
- ~~Relationship between the Gaussian puff and the Gaussian plume models~~
- ~~Using the Gaussian puff model to estimate emission source and rate~~
- Fast implementation of the Gaussian puff model

Workshop (~60 min):

- Code overview
- Running the Gaussian puff
- Running the inversion to estimate source and rate
- Work time and questions

FastGaussianPuff implementation

Ryker Fish and William Daniels

Gaussian Puff Model

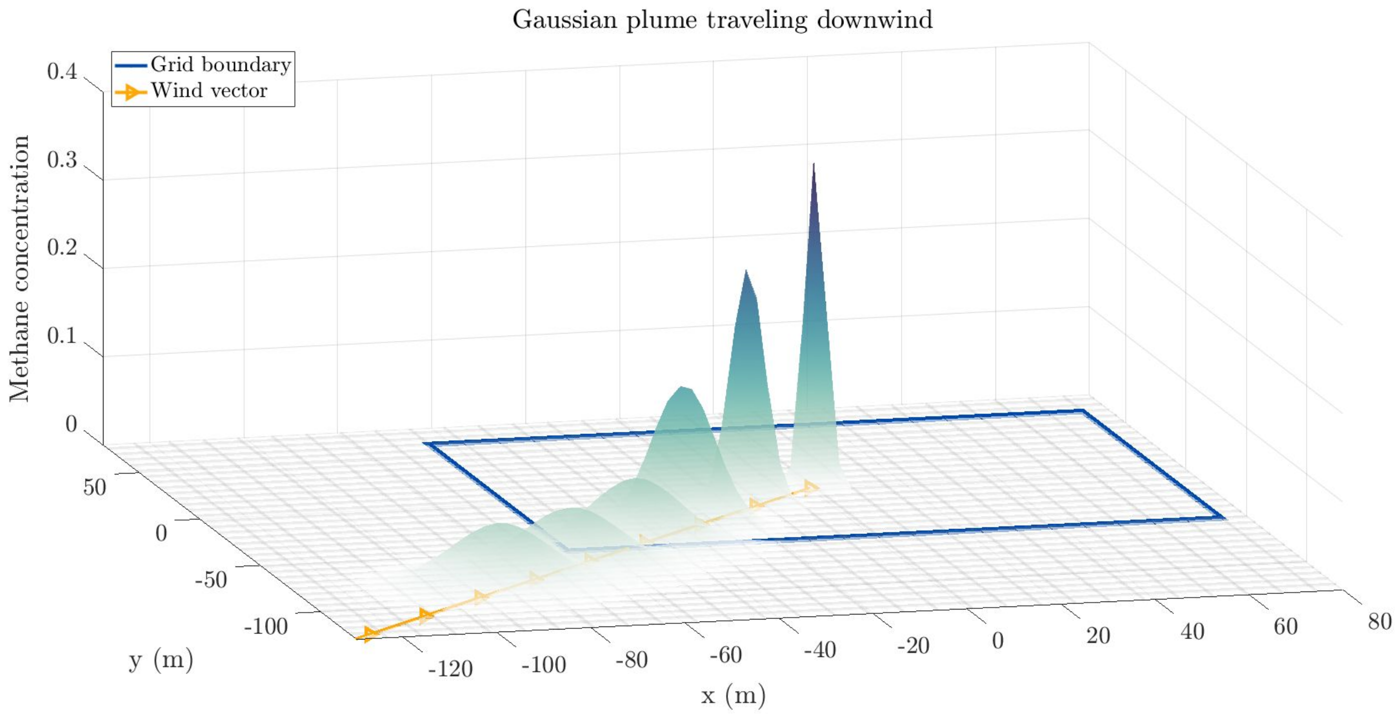
Concentration per puff:

$$c_p(x,y,z,t) = \frac{Q}{(2\pi)^{3/2}\sigma_y^2\sigma_z} \exp\left(-\frac{(x-ut)^2+y^2}{2\sigma_y^2}\right)\left[\exp\left(-\frac{(z-H_0)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{(z+H_0)^2}{2\sigma_z^2}\right)\right]$$

Overall concentration:

$$c(x,y,z,t) = \sum_{p\in\mathcal{S}_t} c_p(x,y,z,t)$$

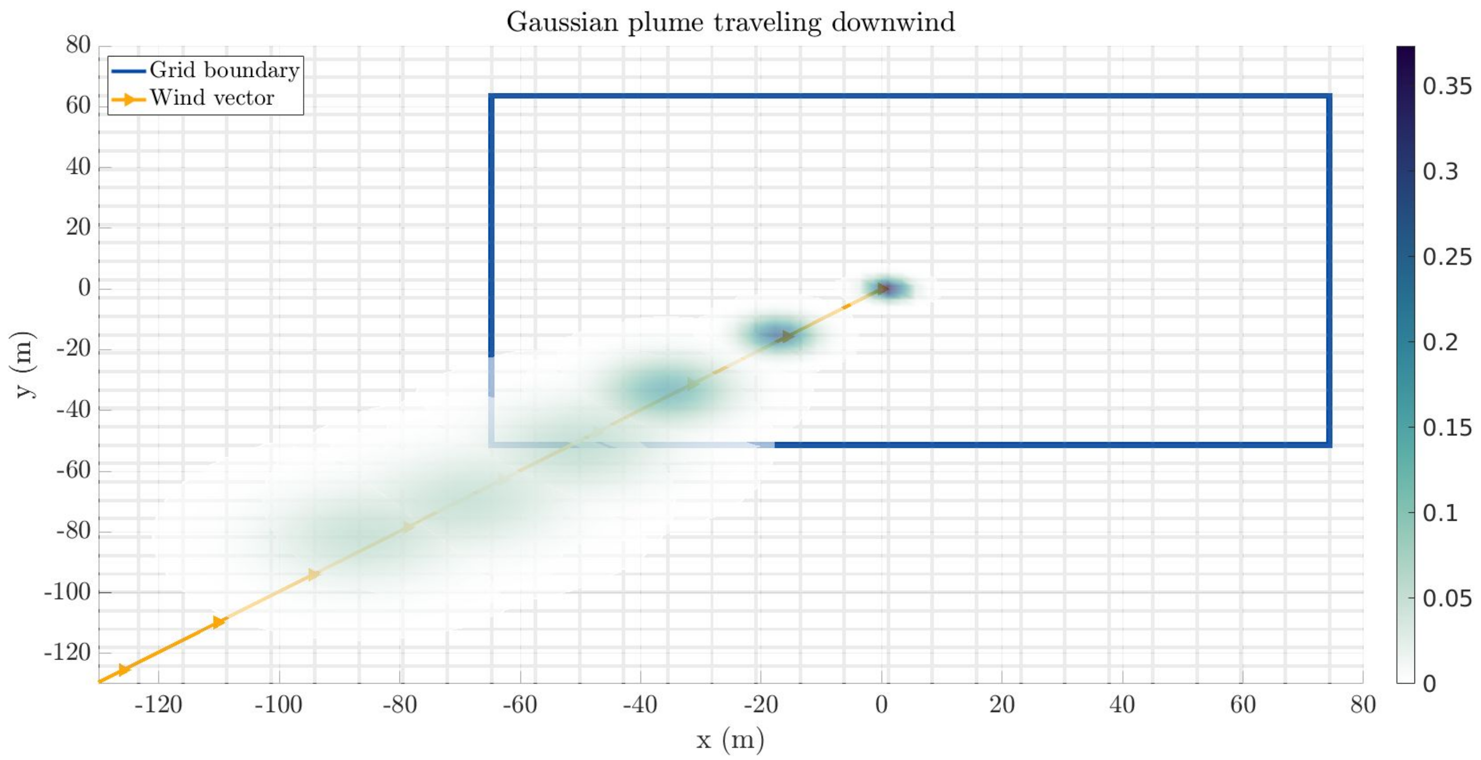
Goal: have model that can be run quickly on 3D grids or for long times on sparse sensor locations



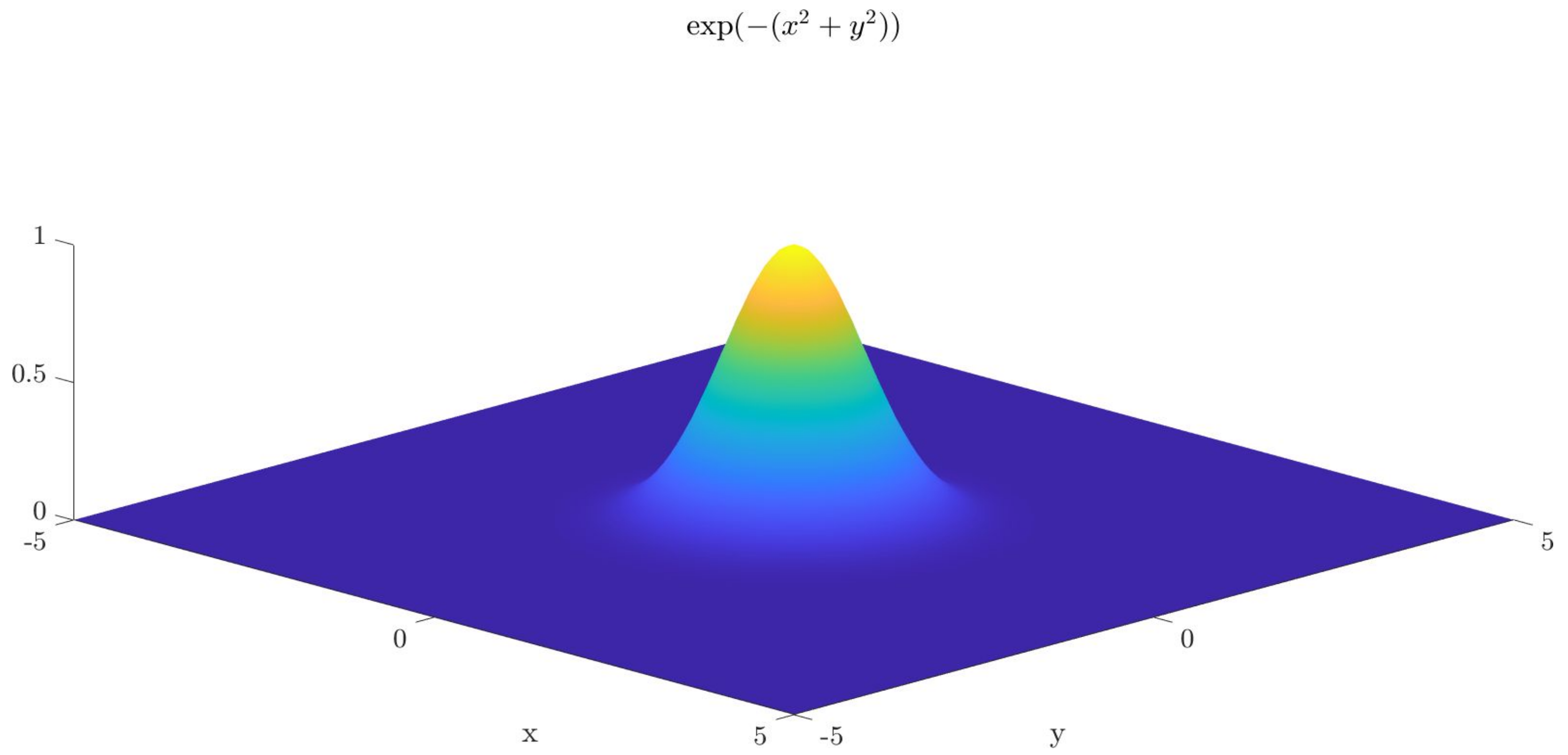
Gaussian Puff Model: Assumptions

1. Wind speed and direction are constant for each puff's lifetime

2. Diffusion coefficients are a function of downwind distance



Spatial Thresholding



- Gaussians decay quickly away from their center
- Idea: only evaluate Gaussians close to their mean
    - What counts as “close” is determined by their variance

Spatial Thresholding

$$c_p(x, y, z, t) \leq \epsilon$$

$$q_{yz} \exp\left(-\frac{(x - wt)^2}{2\sigma_y^2}\right) \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \left[\exp\left(-\frac{(z - z_0)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + z_0)^2}{2\sigma_z^2}\right)\right] \leq \epsilon$$

$$q_{yz} \exp\left(-\frac{(x - wt)^2}{2\sigma_y^2}\right) \leq \epsilon$$

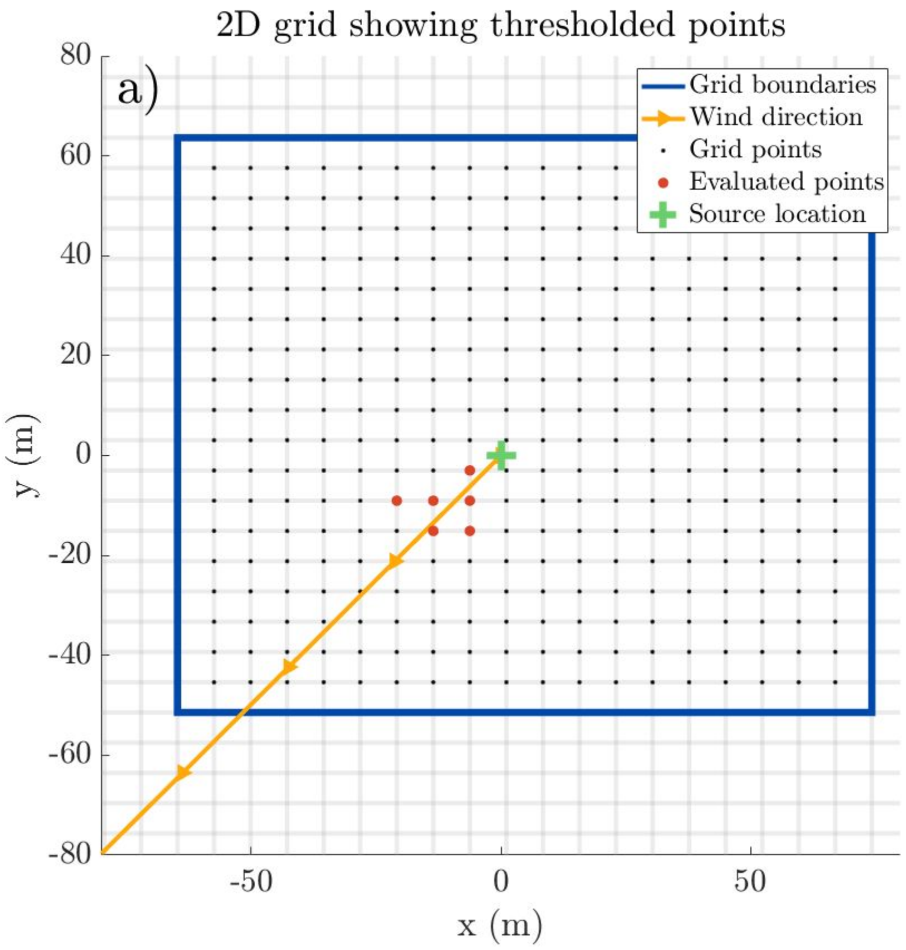
$$q_{yz} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \leq \epsilon$$

$$q_{yz} \left[\exp\left(-\frac{(z - z_0)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + z_0)^2}{2\sigma_z^2}\right)\right] \leq \epsilon$$

Spatial thresholding: Result

- Only points in red contribute significantly to the concentration, skip all other points

- Still need to check threshold conditions on each black point



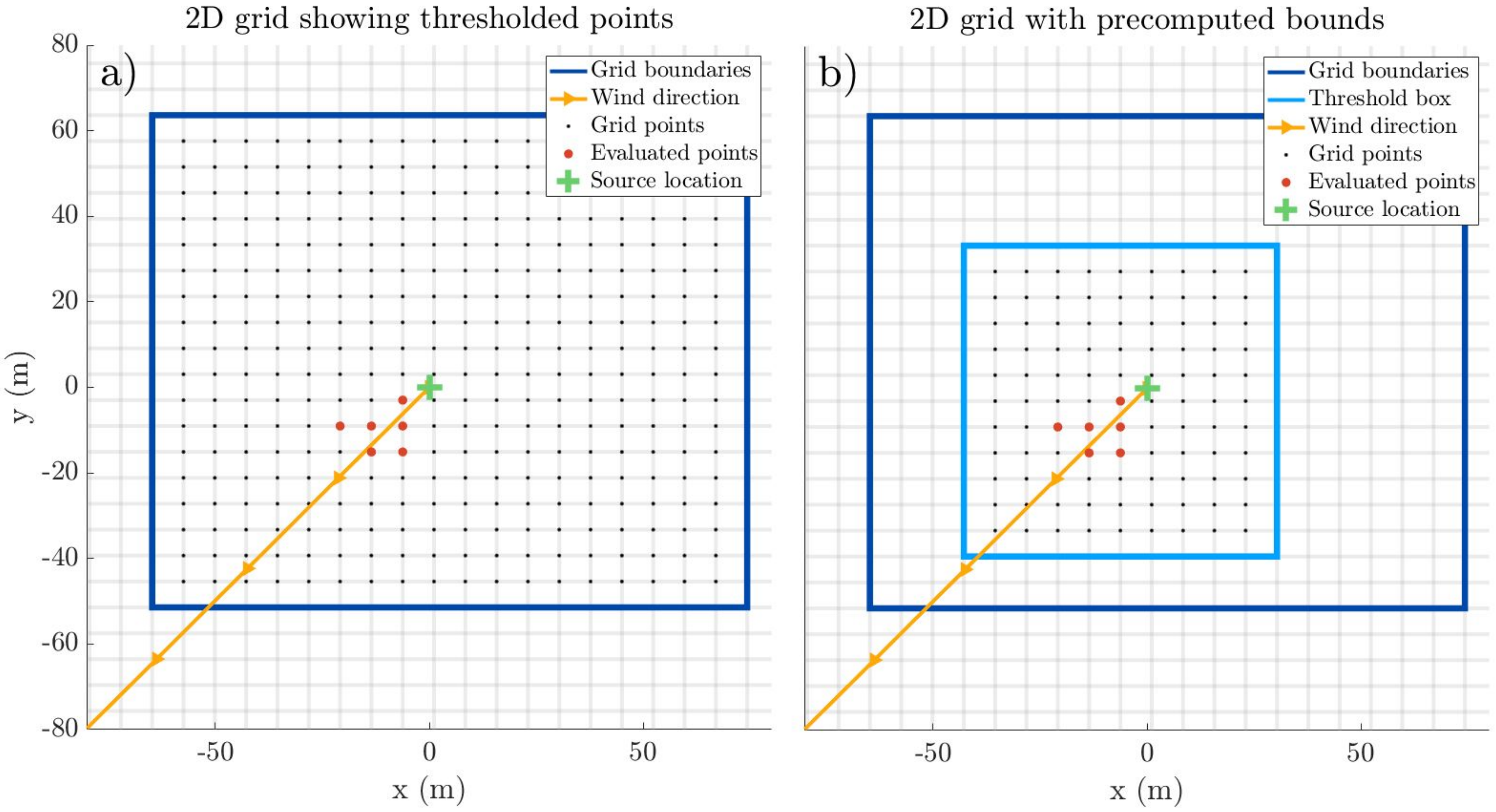
Precomputed Threshold: Result

- Solving for i, j, and k gives upper and lower limits for where to check on the grid (light blue box)

- Ex.

$$\frac{-\mathbf{x}_0^{rt} \cdot \hat{\mathbf{v}} - t_{xy}^{\max}}{\Delta x} < i < \frac{-\mathbf{x}_0^{rt} \cdot \hat{\mathbf{v}} + t_{xy}^{\max}}{\Delta x}$$

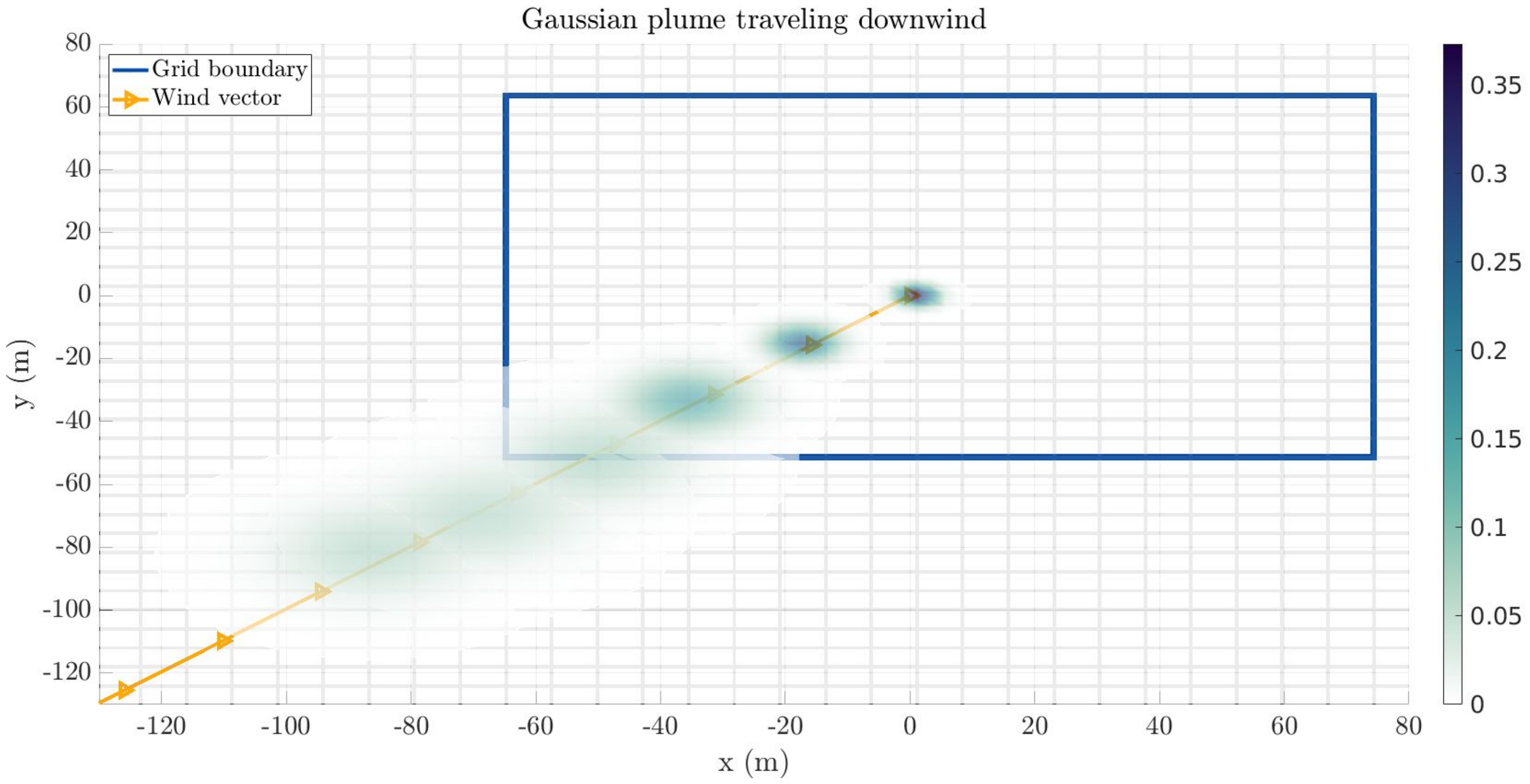
- Bounds computed with largest possible dispersion coefficients



Temporal Thresholding

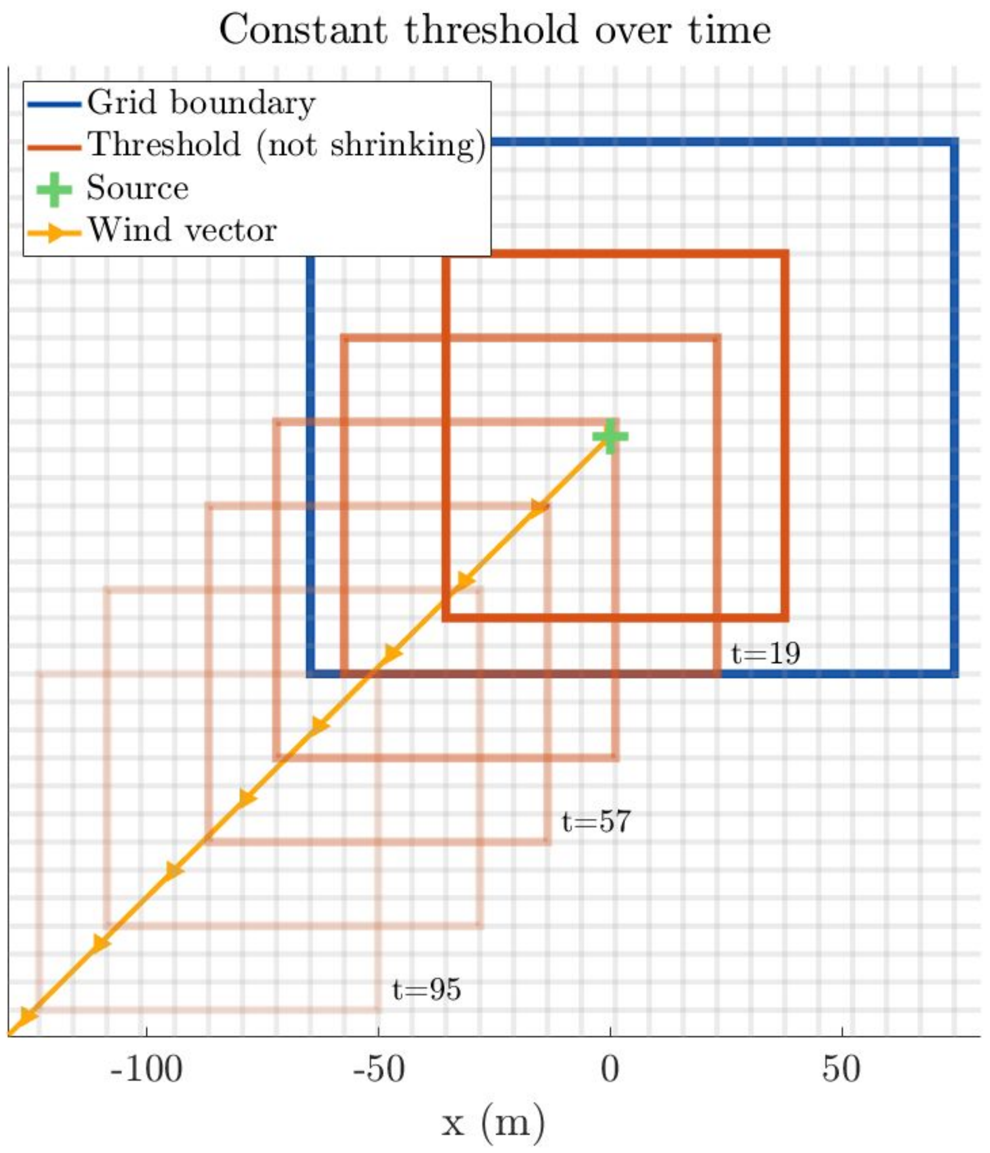
- Model assumption: wind direction and speed is constant for a puff's lifetime

- In simulation: a puff will eventually travel off grid and not return



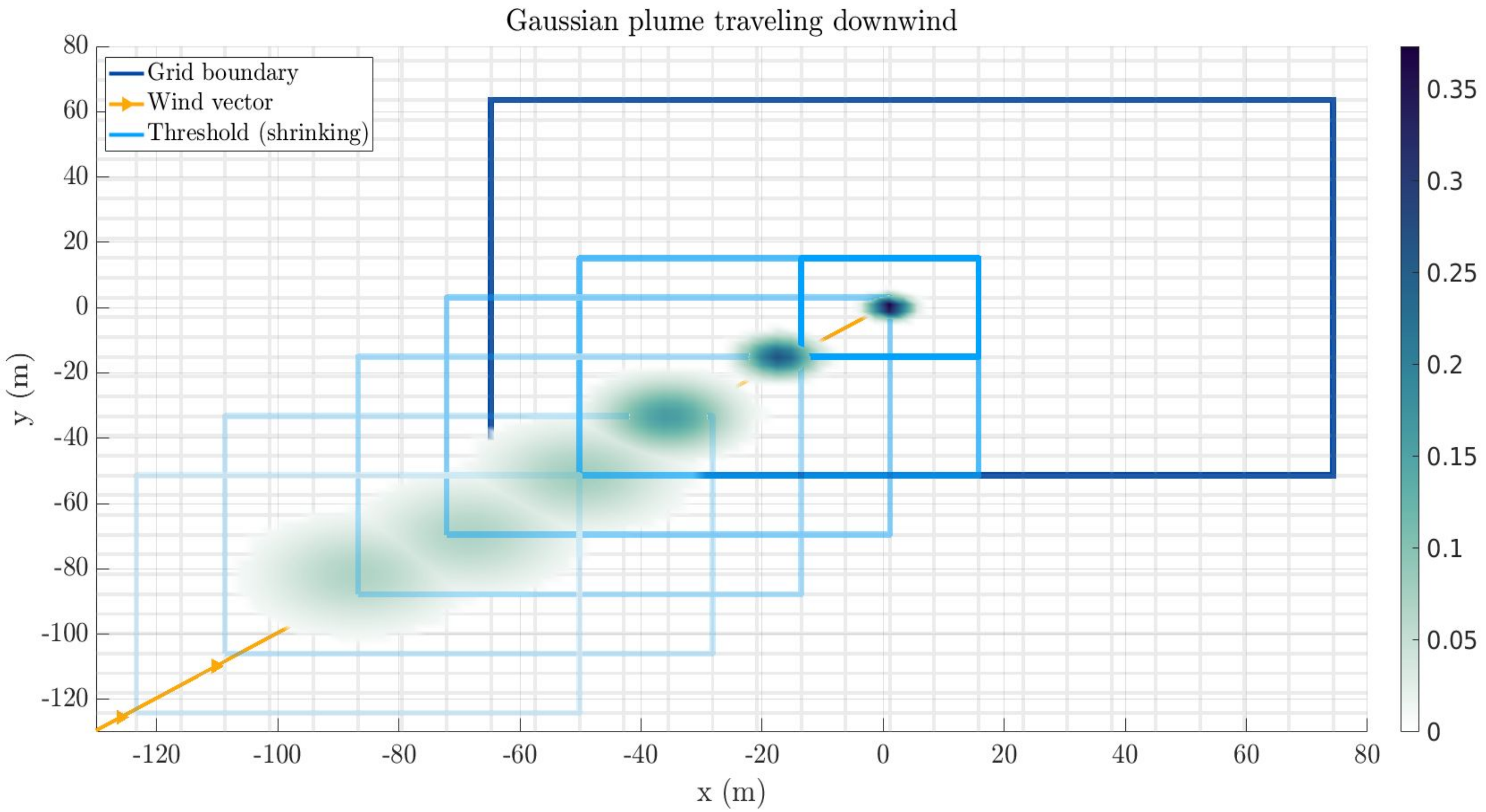
Temporal Thresholding

- Using the largest bounding box and the wind speed gives an estimate of travel time for the puff.

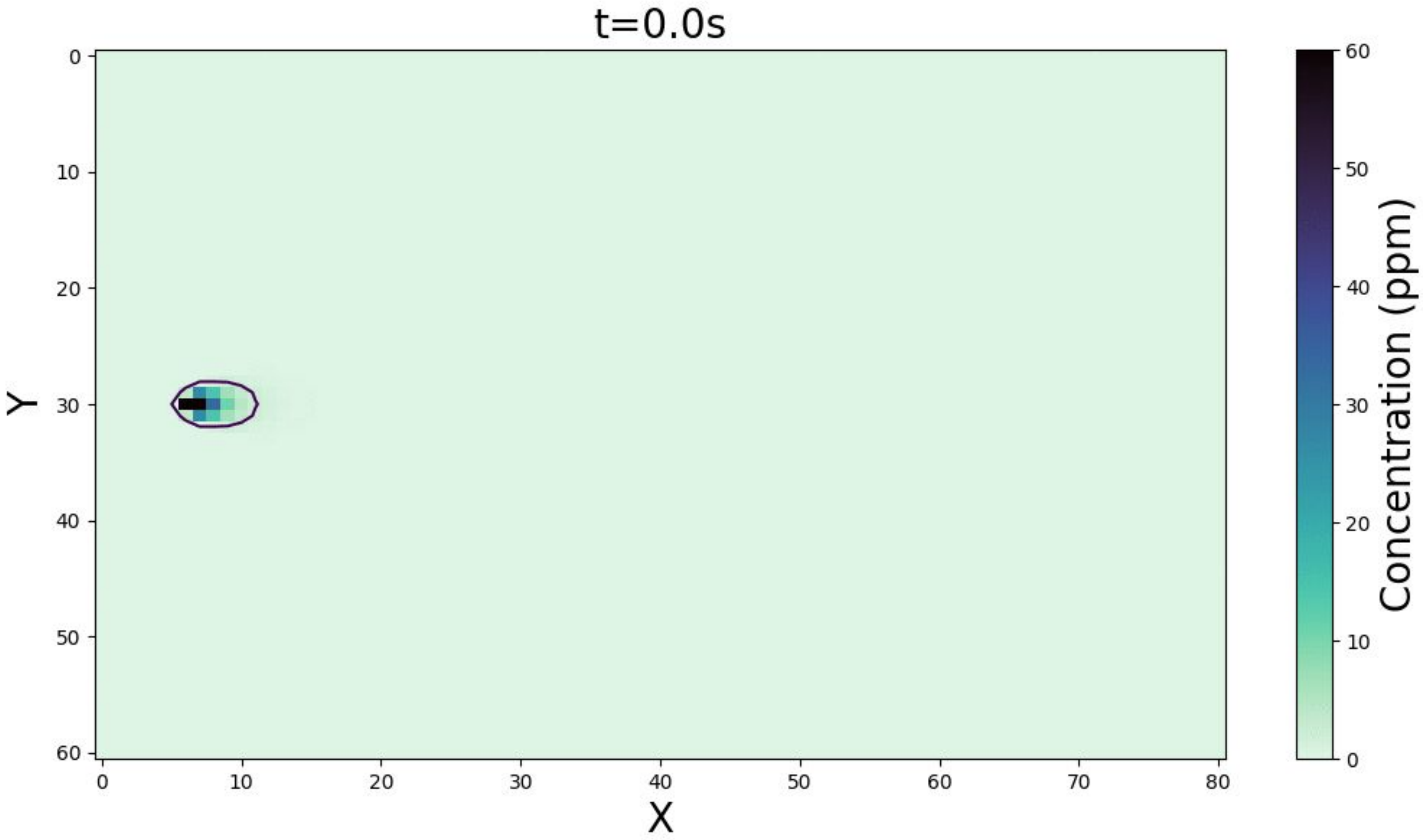


Dynamic Spatial Threshold

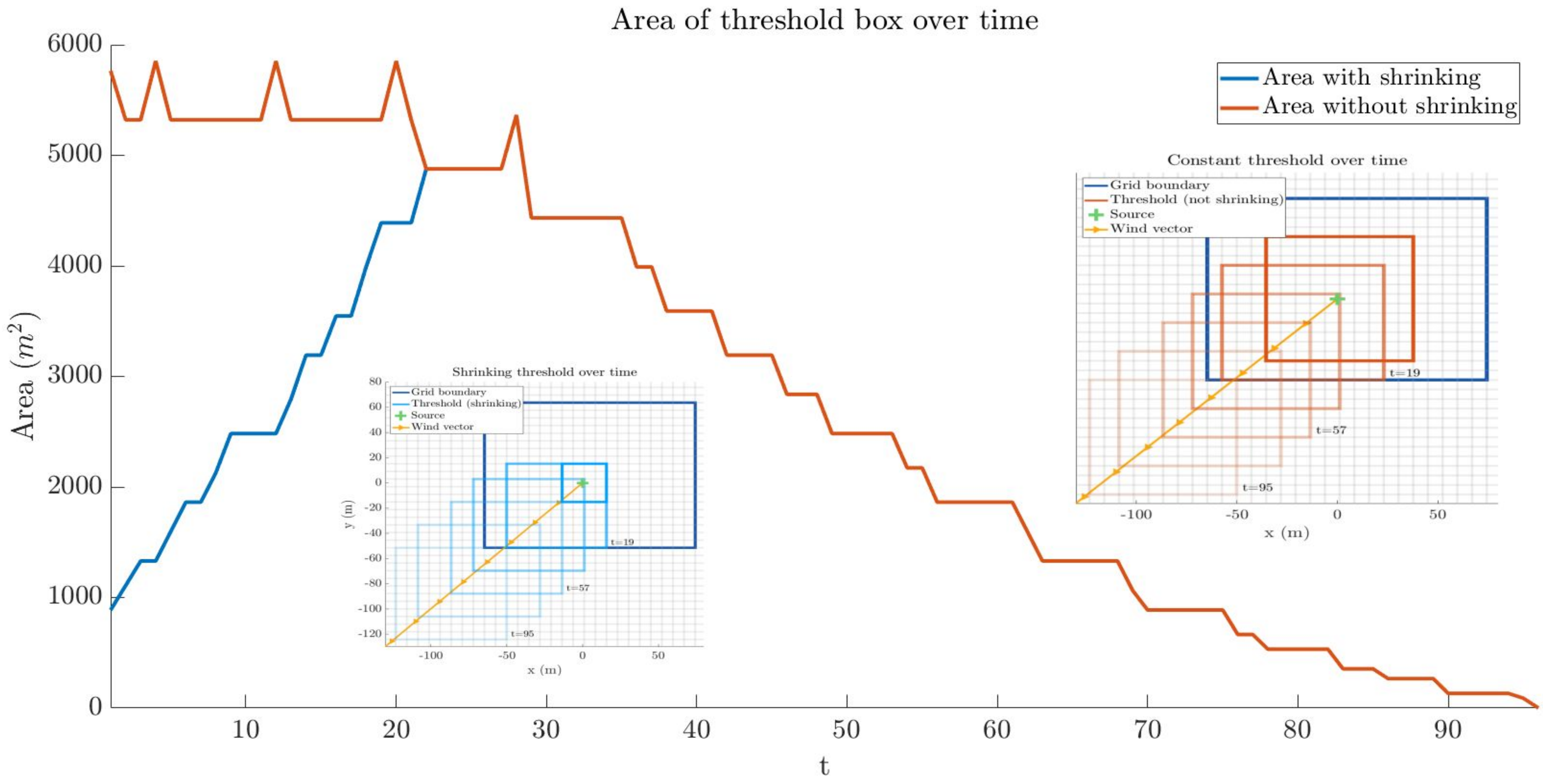
- Dispersion coefficients grow monotonically moving downwind
- Can create a smaller threshold box by carefully using smaller dispersion coefficients closer to the source



Dynamic Spatial Threshold



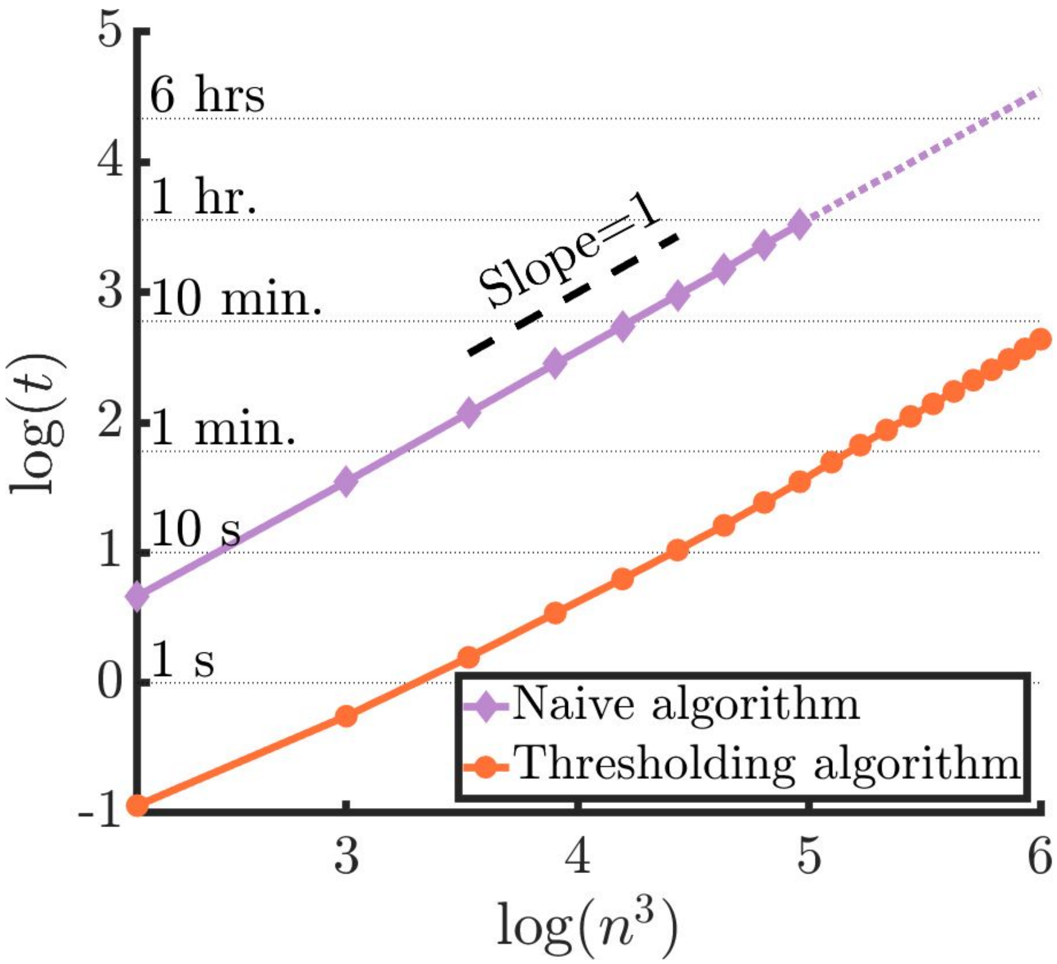
Temporal Thresholding: Shrinking

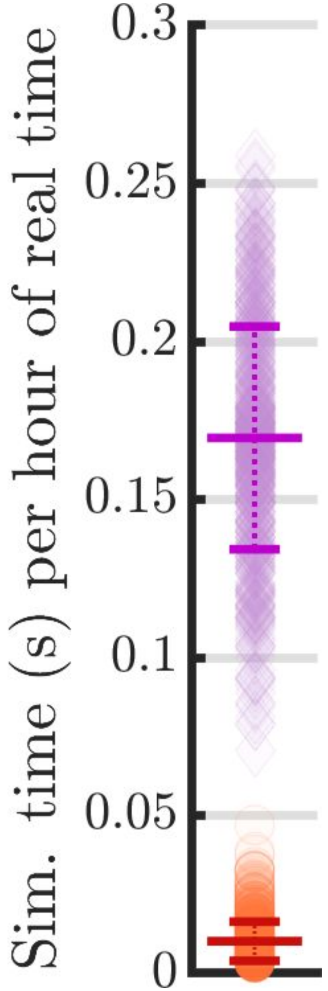


Timings

Left: runtime of the grid version versus grid size.

Right: runtime of the sensor version across the ADED 2022 campaign.

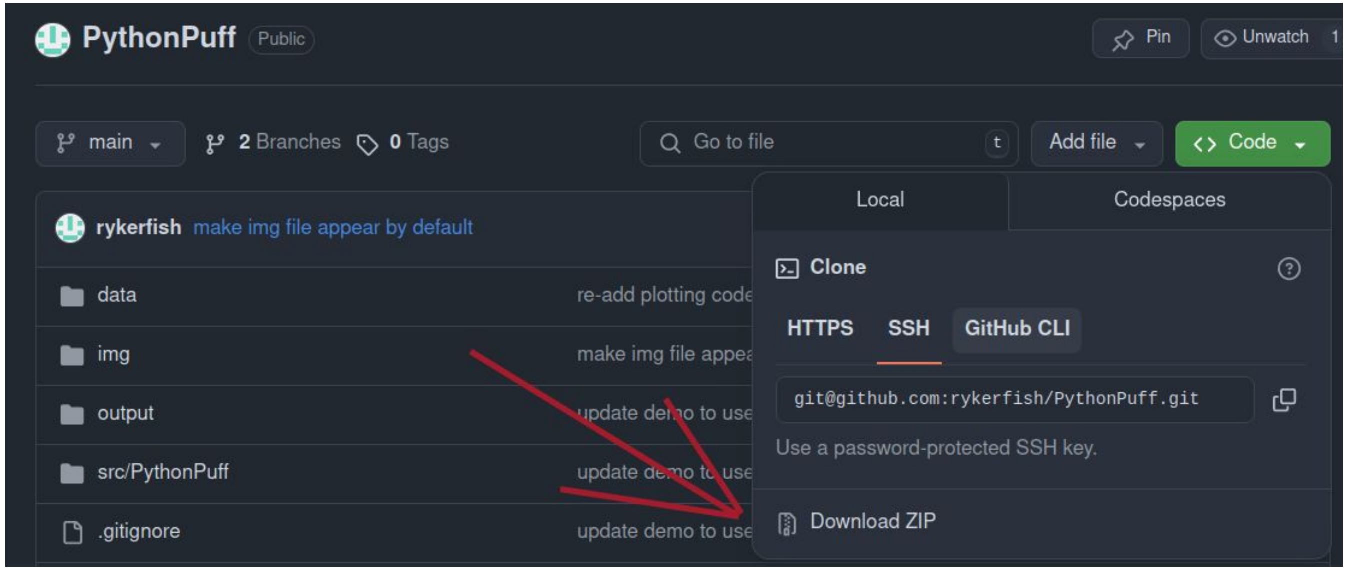




Demo

github.com/rykerfish/PythonPuff

Either clone the repository or download the ZIP file



Install

1. Open the PythonPuff folder in a VSCode, a terminal, or your preferred editor

2. Create and activate conda environment:
    a. *conda env create -f environment.yml*
    b. *conda activate pygp*

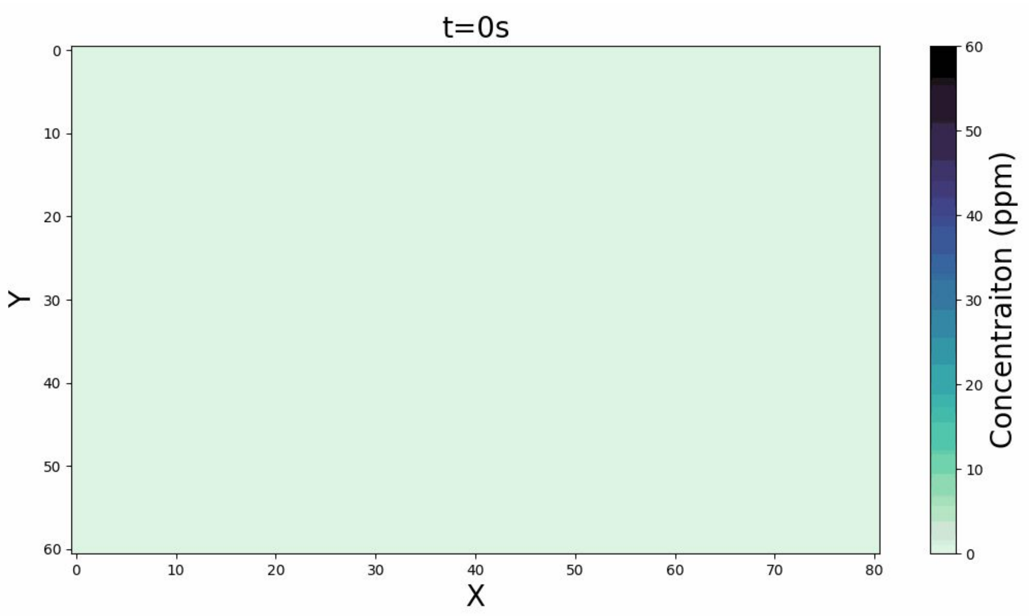
Alternative: install **pandas, numpy, numba,** and **matplotlib** using pip

3. Install the code so it is available everywhere in the conda environment
    a. *pip install .* (from inside the PythonPuff directory)

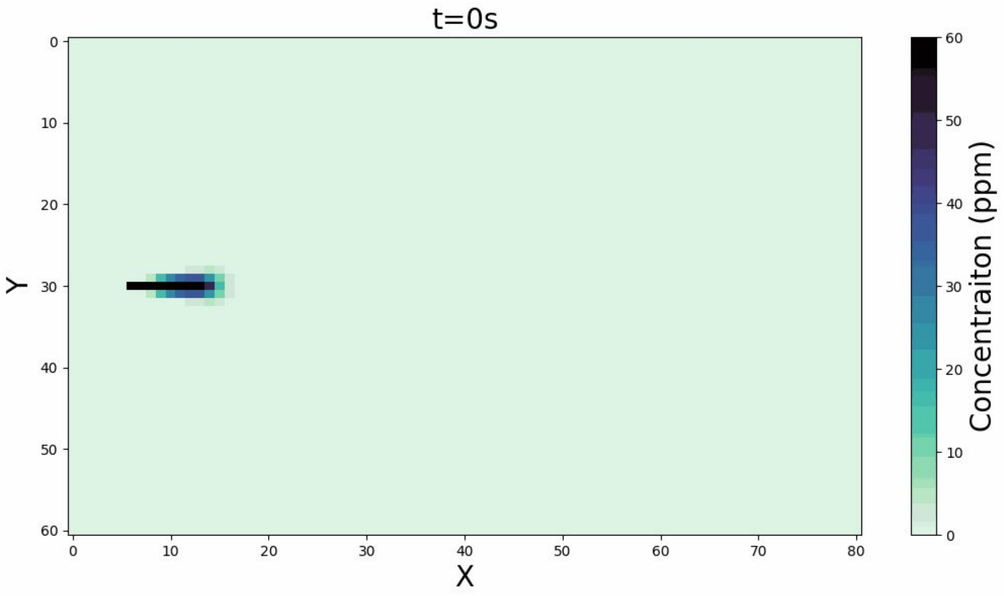
4. Run the demo!
    a. *python demo.py*

Timestep parameters

Simulation timestep, **sim_dt:** how frequently the simulation evaluates a puff so that it travels smoothly



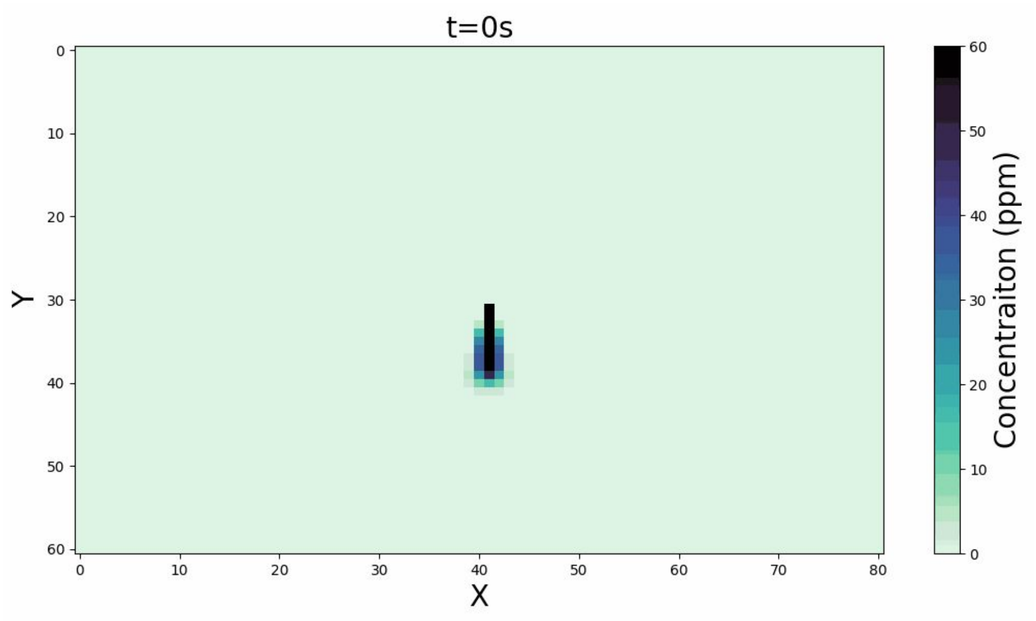
sim_dt being too low causes skipping



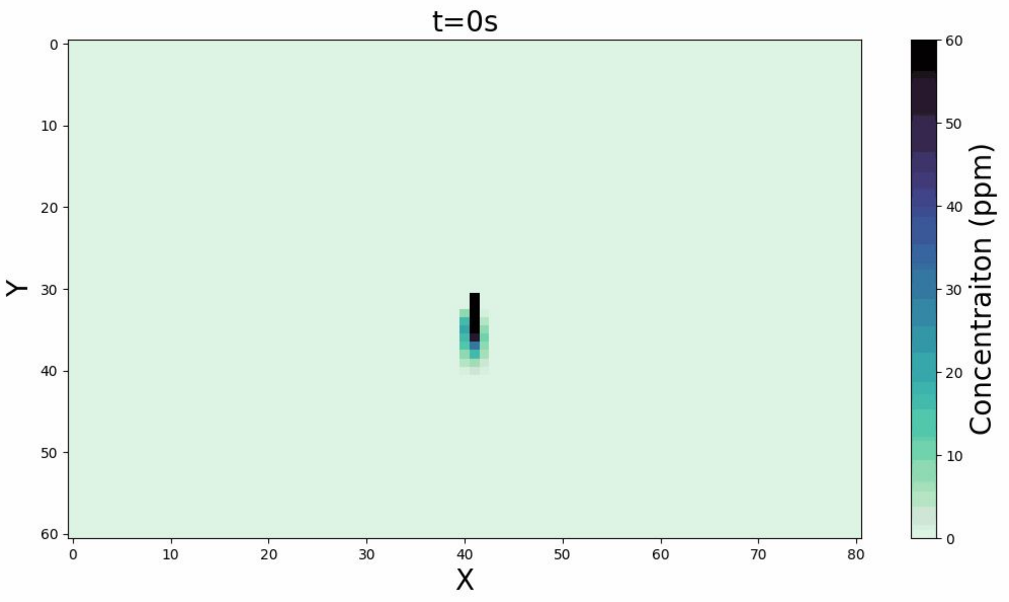
When sim_dt is right, resulting plume will be smooth

Timestep parameters

Puff creation timestep, **puff_dt:** how frequently puffs are created so that a plume is well-resolved.



puff_dt being too low creates a patchy plume



When sim_dt is right, resulting plume will be smooth

Gaussian puff code:

https://github.com/rykerfish/PythonPuff

Inversion code:

https://github.com/wsdaniels/DLQ

Thank you!

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