



A probabilistic model for evaluating  
human health and environmental risks of  
chemicals in advanced treated water:  
the Montornès case study

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# An Early Warning Exposure Assessment Framework



## PROMISCES

Preventing Recalcitrant Organic Mobile Industrial chemicals  
for Circular Economy in the Soil-sediment-water system

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Article

### An Early Warning Exposure Assessment Framework (EWEX) for Health and Environmental Risk Evaluation Using PFAS in Indirect Potable Water Reuse Systems

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# What it is eurecat!



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Eurecat is one of Europe's leading technology centers for accelerating innovation in companies.

**2**

We work with businesses of all sizes and sectors across the entire R&D&I process.

**3**

Our multi-technology approach enables us to tackle complex challenges and address major industrial and social issues.

**4**

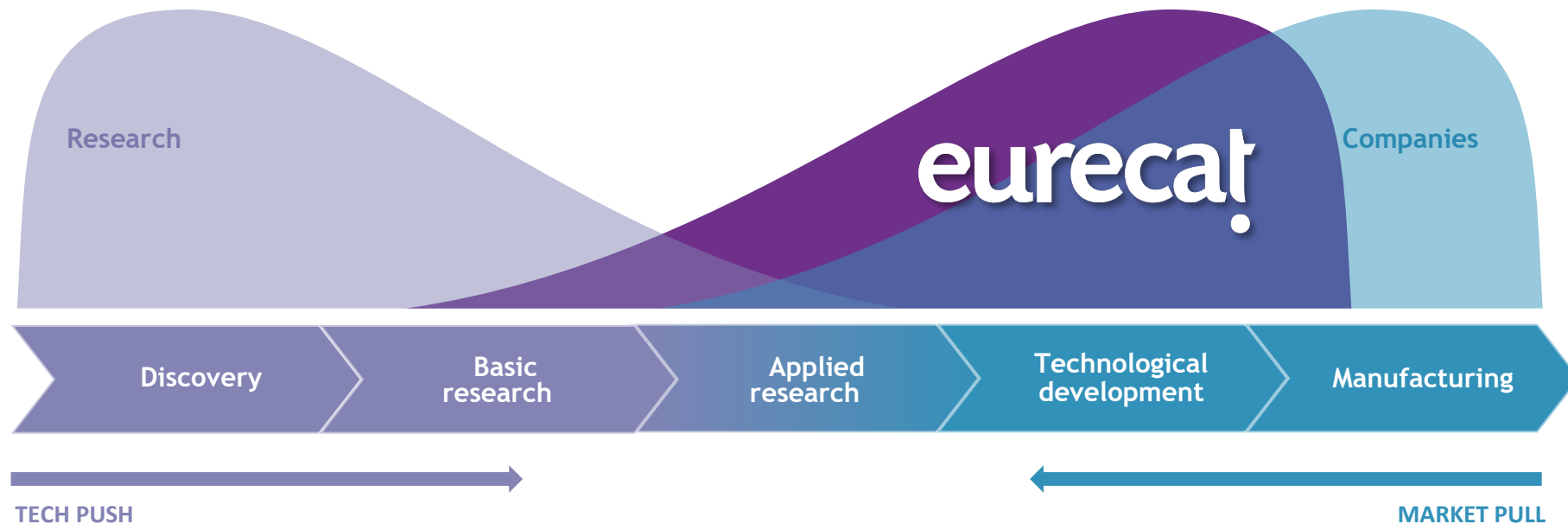
We have cutting-edge facilities and laboratories specialising in water technology, medical devices, personalised nutrition, embedded electronics, artificial intelligence in industrial environments, lightweight materials, cognitive robotics and more.

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technology development and  
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It's quite the challenge! ...  
which opens up great opportunities



# Why Do We Need a Probabilistic Exposure Assessment in Reclaimed Water?

## Challenges:

- Limited data
- Variable influent and effluent composition
- Complex treatment trains with variability (operational, analytical, seasonal, etc.)
- Interactions between co-contaminants
- ...



A **probabilistic approach** integrates uncertainty into reclaimed water risk assessment, moving beyond a simple compliant/non-compliant outcome to **quantify the reliability** of a treatment solution in meeting the required safety targets.



# Why Use a Probabilistic Approach?

## DETERMINISTIC MODEL

Input value



Treatment  
process

Output value



ONE RESULT

## PROBABILISTIC MODEL

Input distribution



Treatment  
process

Output distribution



RANGE OF POSSIBLE RESULTS



More reliable  
outcomes



# Bayesian Inference Applied to Removal Factors

“Today’s posterior is tomorrow’s prior.”

*Dennis Lindley, professor of Statistics*

Bayes inference:

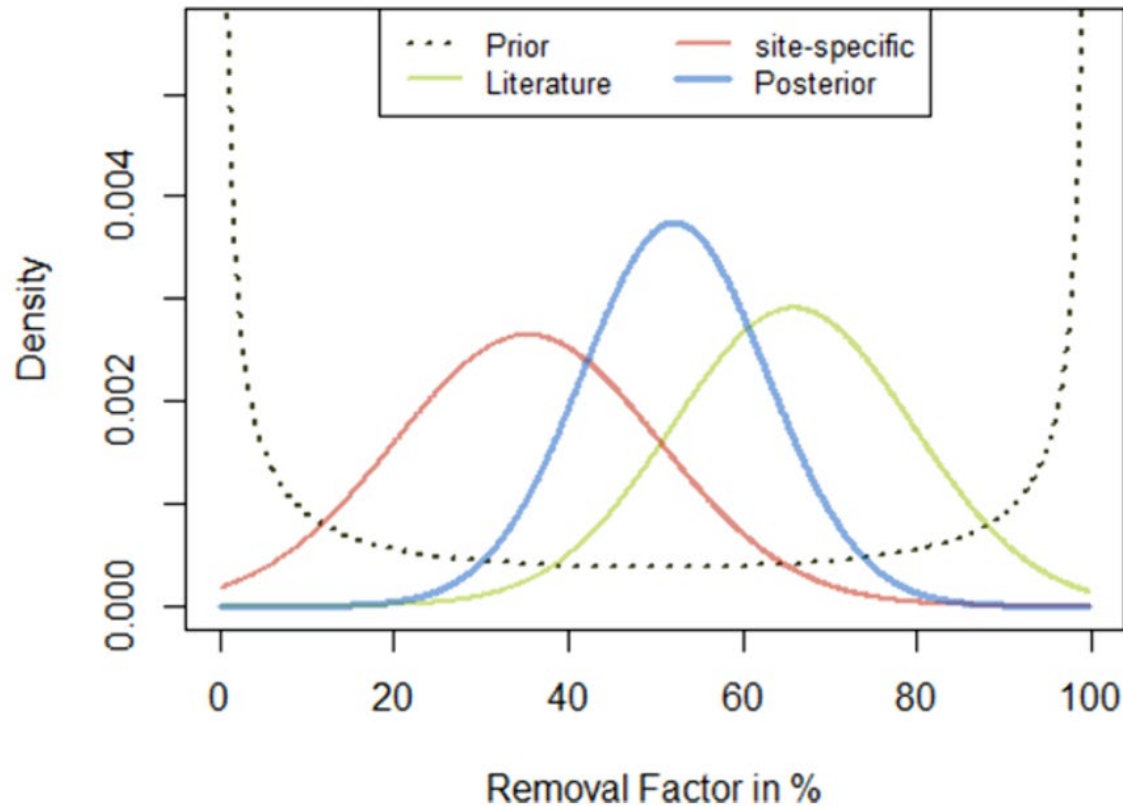
$$\underbrace{p(RF|D)}_{\text{posterior}} = \underbrace{p(RF)}_{\text{prior}} \cdot \underbrace{\frac{p(D|RF)}{\int_{\mathcal{R}} p(D|RF) \cdot p(RF) \cdot dRF}}_{\text{likelihood}}$$

Where...

- **Prior:** What we already know about treatment performance, before considering the new experimental data.
- **Likelihood:** What the new experimental data tell us.
- **Posterior:** Our updated knowledge after combining both. Probability distribution of the Removal Factor (RF) after observing the experimental data (D).



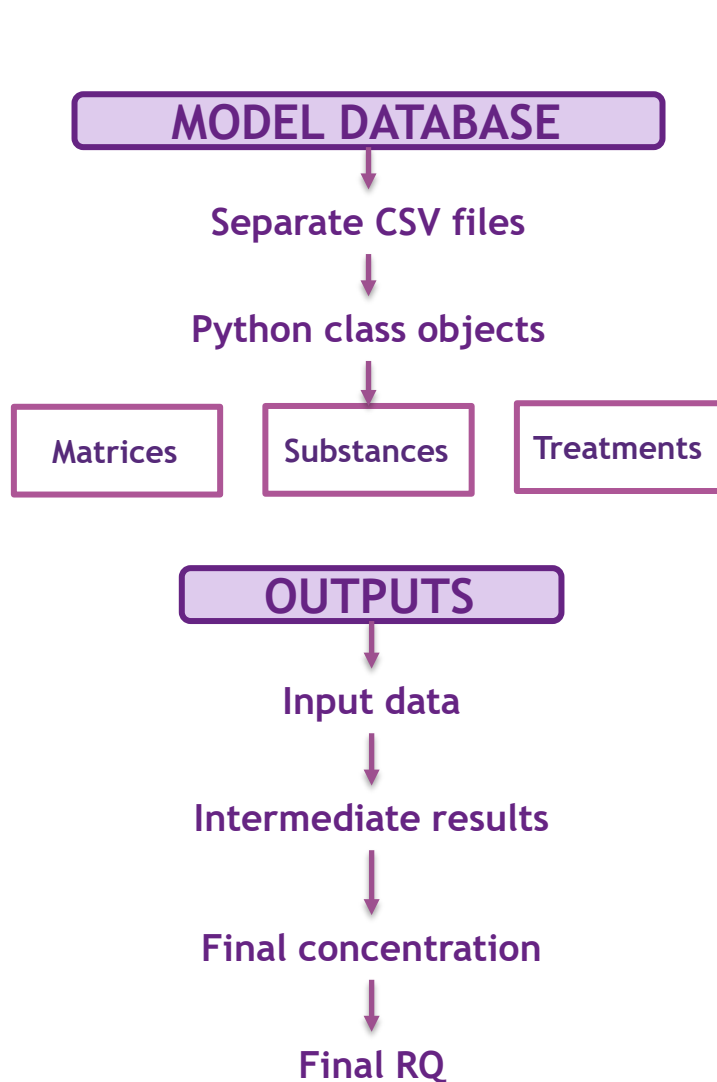
# Bayesian Inference Applied to Removal Factors



Bayesian inference allows us to update our previous knowledge with new experimental data, showing **which Removal Factors are most supported by the available evidence.**

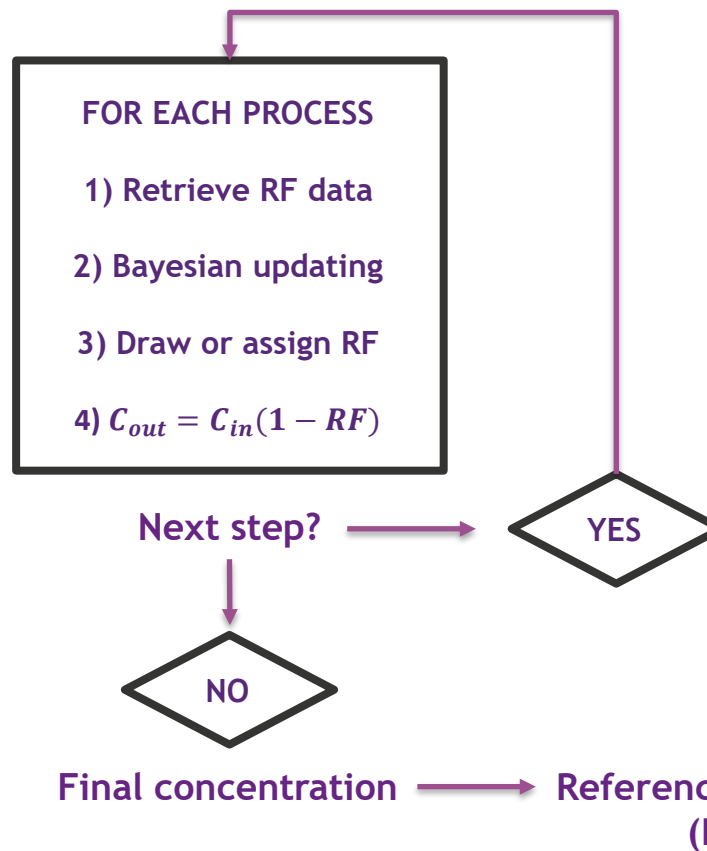


# Model Implementation



## SIMULATION WORKFLOW

Select matrix and target substance  
Define or retrieve starting concentration



## OPEN-SOURCE PYTHON MODEL

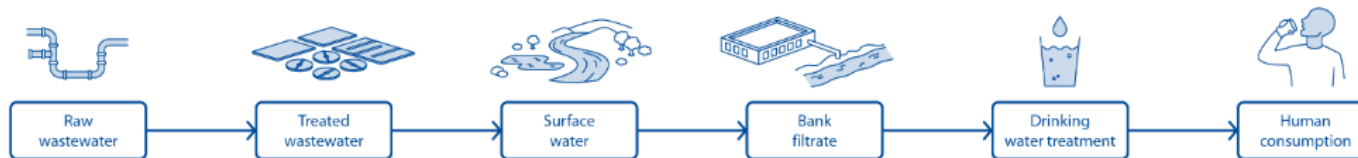
basic\_hhea.ipynb

[github.com/KWB-R/promiscues.hhea](https://github.com/KWB-R/promiscues.hhea)



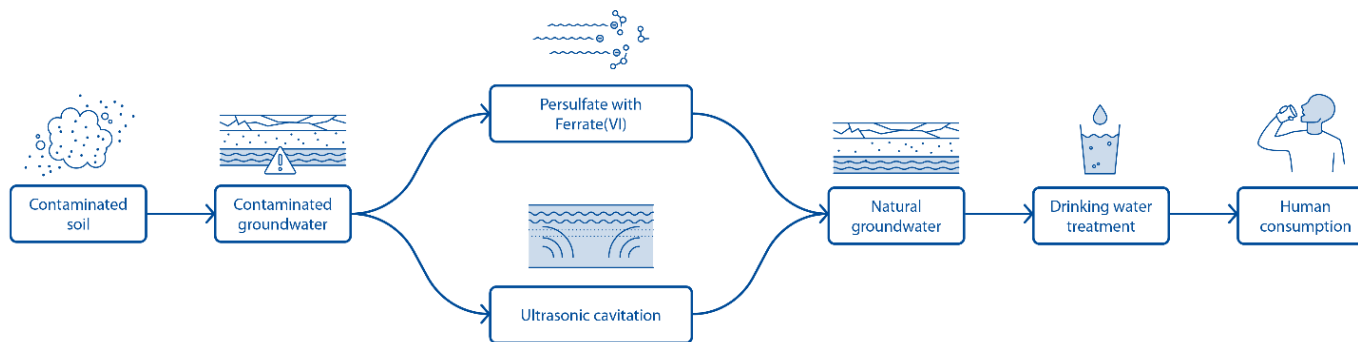
# Exposure Routes Assessed in PROMISCES

1)



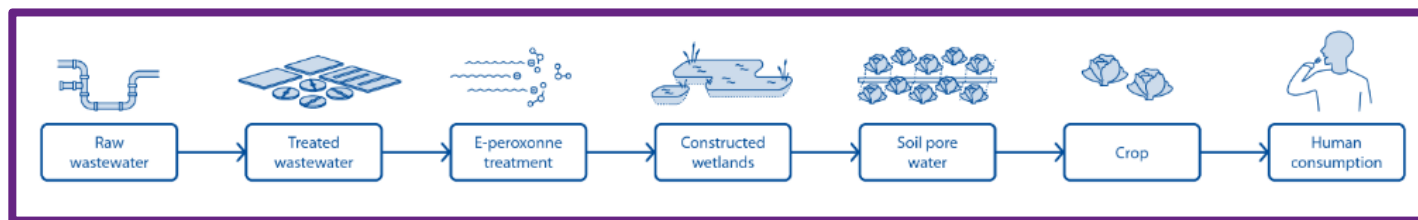
Semi-closed water cycle

2)



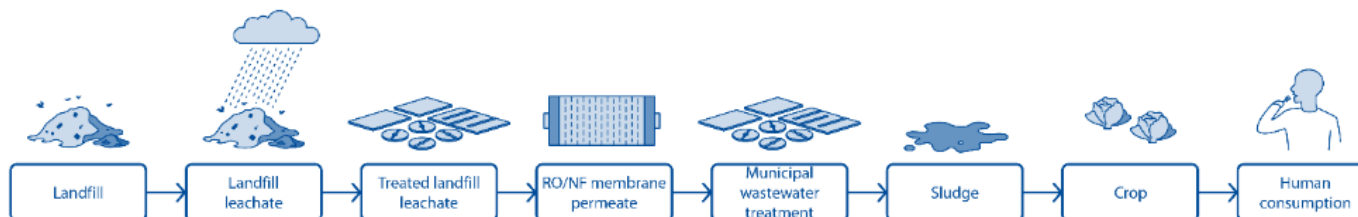
Groundwater remediation

3)



Montornès case study:  
Water reuse for agricultural irrigation

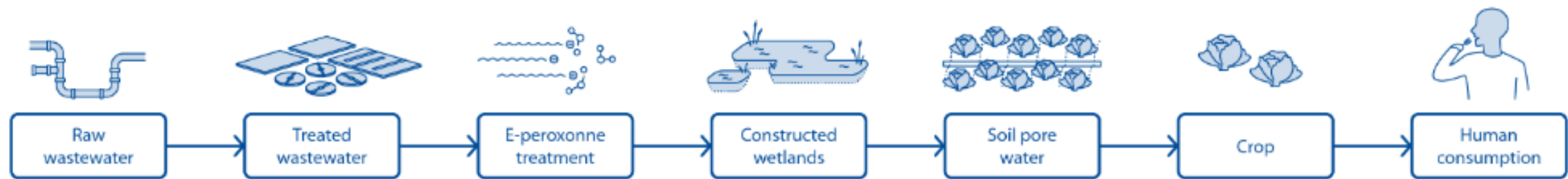
4)



Nutrient recovery



# Montornès Water Reuse Exposure Route



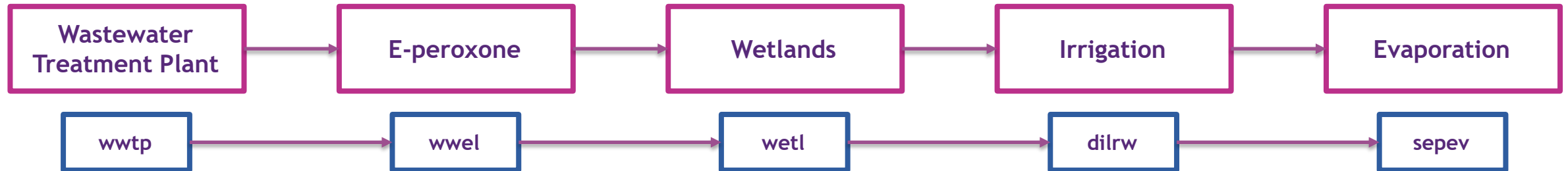
## Assessment scope:

- 10 PFAS
- 4 iPMT compounds
- Final modelled matrix: soil porewater
- Theoretical endpoint: lettuce consumption

| PFAS  |                               | iPMT   |                   |
|-------|-------------------------------|--------|-------------------|
| PFHxA | Perfluorohexanoic acid        | DEP    | Diethyl phthalate |
| PFPeA | Perfluoropentanoic acid       | DBP    | Dibutyl phthalate |
| PFBS  | Perfluorobutane sulfonic acid | CBZ    | Carbamazepine     |
| PFBA  | Perfluorobutanoic acid        | Diuron | Diuron            |
| PFDA  | Perfluorodecanoic acid        |        |                   |
| PFNA  | Perfluorononanoic acid        |        |                   |
| PFOS  | Perfluorooctane sulfonic acid |        |                   |
| PFOA  | Perfluorooctanoic acid        |        |                   |
| PFHpA | Perfluoroheptanoic acid       |        |                   |
| PFHxS | Perfluorohexane sulfonic acid |        |                   |



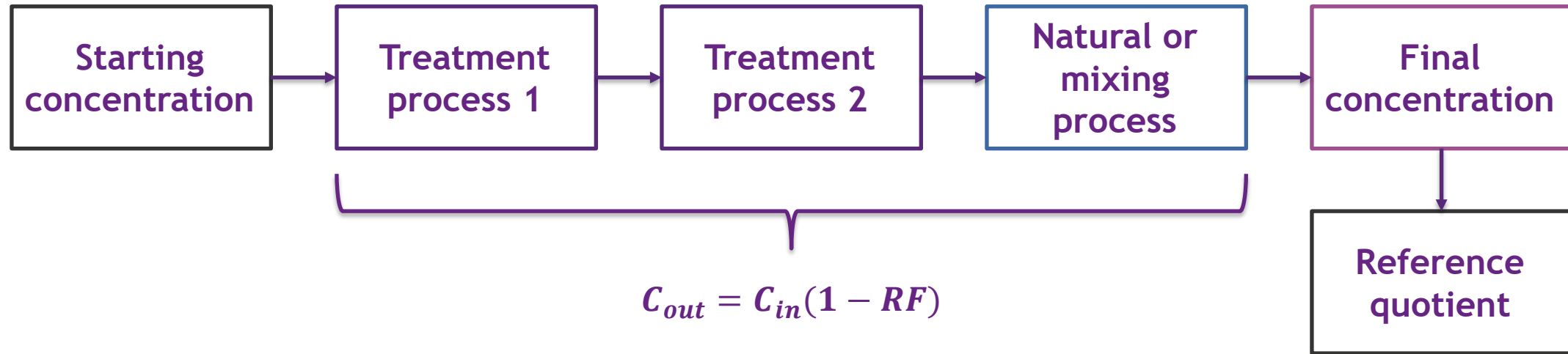
# Model Inputs and Baseline Assumptions



| Variable                  | Value                                              |
|---------------------------|----------------------------------------------------|
| treatment_train           | ["wwtp", "wwel", "wetl", "dilrw", "sepev"]         |
| substance                 | "pfoa"                                             |
| case_study_name           | "water reuse"                                      |
| scenario_name             | "standard"                                         |
| input_matrix              | rw (raw waste water)                               |
| n_runs                    | 10 000                                             |
| removal_factor_resolution | 1000 (--> resolution of 0.1% removal factor steps) |



# From Initial Concentration to Final Exposure Risk



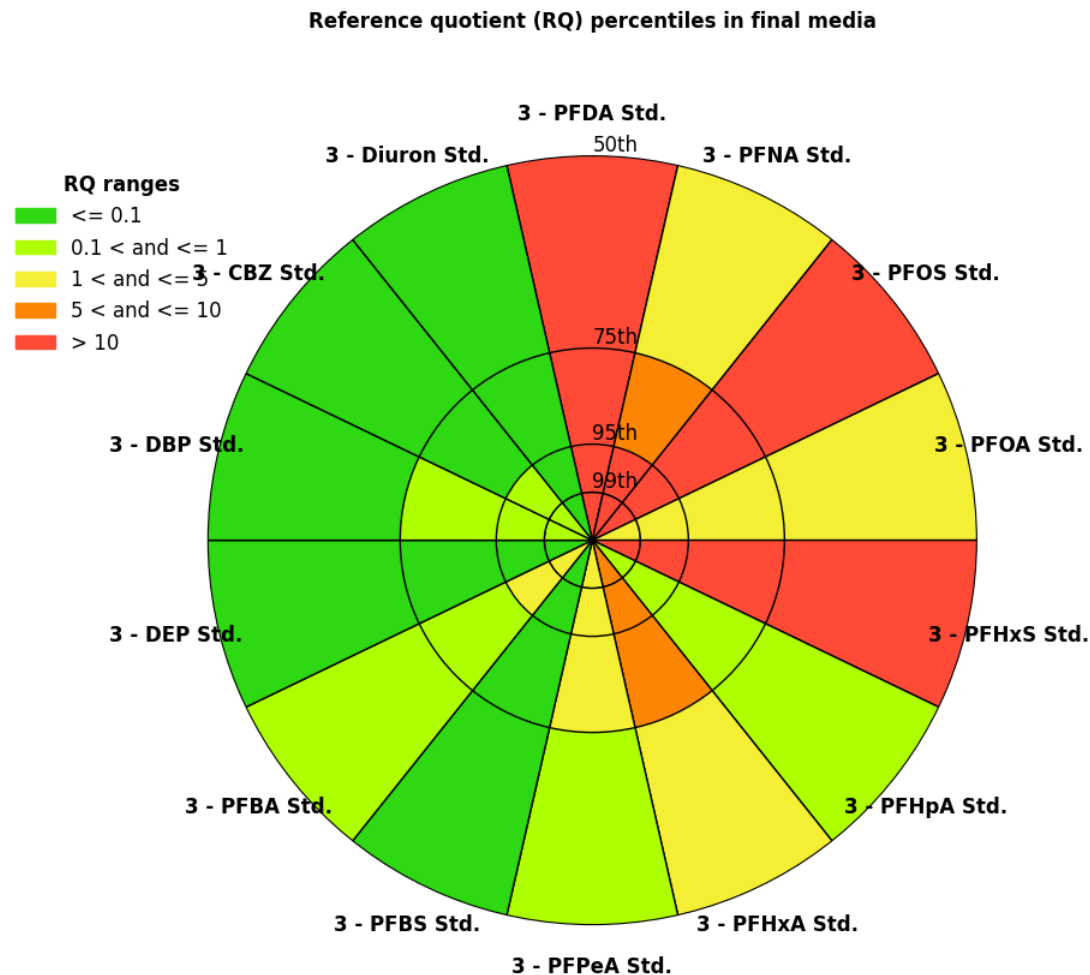
## Where:

- $C_{in}$  is the input concentration
- $RF$  is the removal factor, (0-1) or (0-100%)
- $C_{out}$  is the output concentration
- **Reference value** is the threshold value applicable to the compound
  - If  $RQ < 1$ , output concentration below **Reference value**
  - If  $RQ = 1$ , output concentration equal **Reference value**
  - If  $RQ > 1$ , output concentration exceeds **Reference value**

$$RQ = \frac{C_{out} \text{ distribution}}{\text{Reference value}}$$



# Baseline Risk Screening of the 14 Compounds



Highest concern in most samples:

PFDA  
PFOS  
PFOA  
PFHxS...

PFOA and PFOS selected  
for scenario analysis



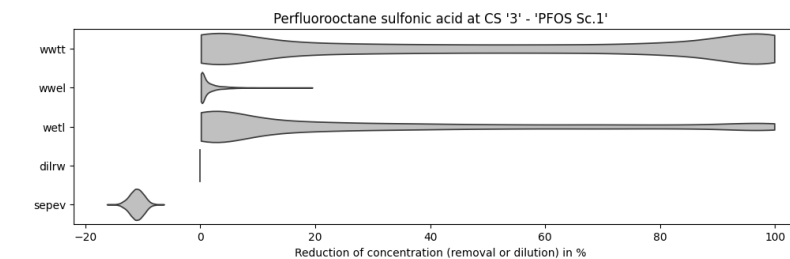
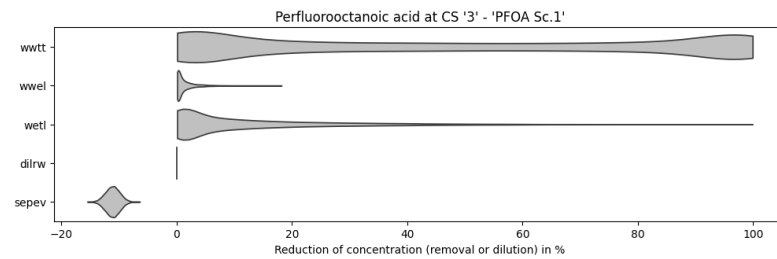
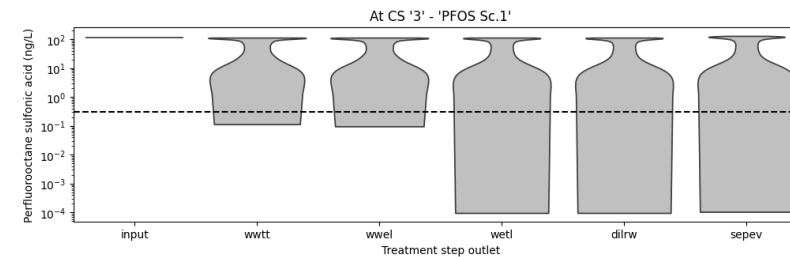
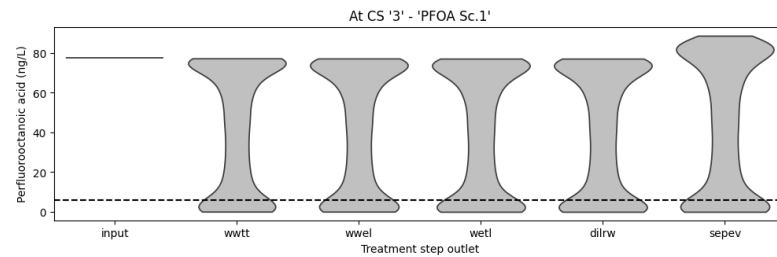
# Scenario Results: Main Risk Drivers

4 scenarios for PFOS and PFOA: alternative conditions.

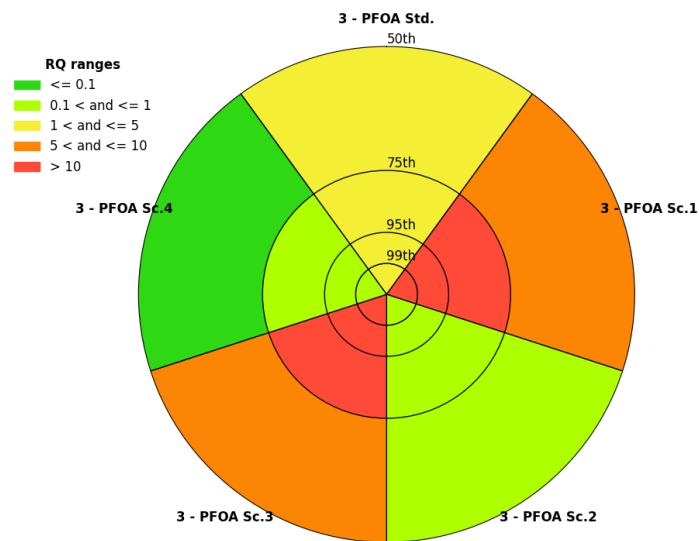
|                                                         | PFOA |          | PFOS  |          | Comments                                         |
|---------------------------------------------------------|------|----------|-------|----------|--------------------------------------------------|
|                                                         | Mean | $\sigma$ | Mean  | $\sigma$ |                                                  |
| Standard                                                |      |          |       |          |                                                  |
| Raw wastewater concentration (ng/L)                     | 26.7 | 75.2     | 61.7  | 78.9     | All literature and site data considered.         |
| E-peroxone removal rate (wwel) (%)                      | 28.4 | 41.3     | 14.2  | 60.3     | All literature and site data considered.         |
| Scenario 1: Poor performance, High inlet concentrations |      |          |       |          |                                                  |
| Raw wastewater concentration (ng/L)                     | 77.4 |          | 114.9 |          | Value = 75% normal distribution.                 |
| E-peroxone removal rate (wwel) (%)                      | 0.6  |          | -26.5 |          | Value = 25% normal distribution.                 |
| Scenario 2: Poor performance, Low inlet concentrations  |      |          |       |          |                                                  |
| Raw wastewater concentration (ng/L)                     | 1.0  |          | 8.5   |          | Value = 25% normal distribution (minimum 1 ng/L) |
| E-peroxone removal rate (wwel) (%)                      | 0.6  |          | -26.5 |          | Value = 25% normal distribution.                 |
| Scenario 3: Good performance, High inlet concentrations |      |          |       |          |                                                  |
| Raw wastewater concentration (ng/L)                     | 77.4 |          | 114.9 |          | Value = 75% normal distribution.                 |
| E-peroxone removal rate (wwel) (%)                      | 56.3 |          | 54.9  |          | Value = 75% normal distribution.                 |
| Scenario 4: Good performance, Low inlet concentrations  |      |          |       |          |                                                  |
| Raw wastewater concentration (ng/L)                     | 1.0  |          | 8.5   |          | Value = 25% normal distribution (minimum 1 ng/L) |
| E-peroxone removal rate (wwel) (%)                      | 56.3 |          | 54.9  |          | Value = 75% normal distribution.                 |



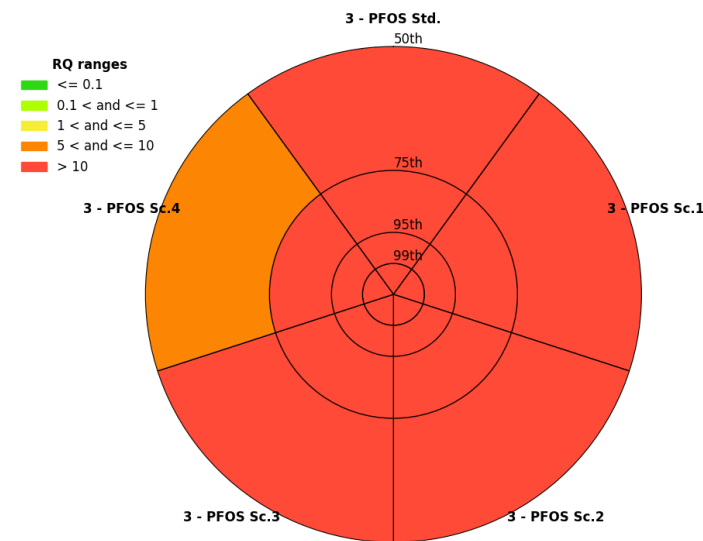
# Scenario Results: Main Risk Drivers



Reference quotient (RQ) percentiles in final media



Reference quotient (RQ) percentiles in final media





# Conclusions

- 1) The EWEX tool successfully propagates and visualizes uncertainty throughout the treatment train.
- 2) At the Montornès WWTP, risk-based assessment identified priority compounds among the 10 PFAS and 4 iPMTs evaluated.
- 3) Six PFAS showed  $RQ > 1$  in  $>50\%$  of simulated events at Montornès WWTP.
- 4) High inlet concentrations had a stronger influence on risk than E-peroxone performance.
- 5) The EWEX tool provides water managers with a decision-support framework to assess the probability of non-compliance in water quality.

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# Thank you

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