Design and implementation of an

Environmental Decision Support System

for the control and management of

Drinking Water Treatment Plants

Industrial Doctoral Thesis | 5th November 2020

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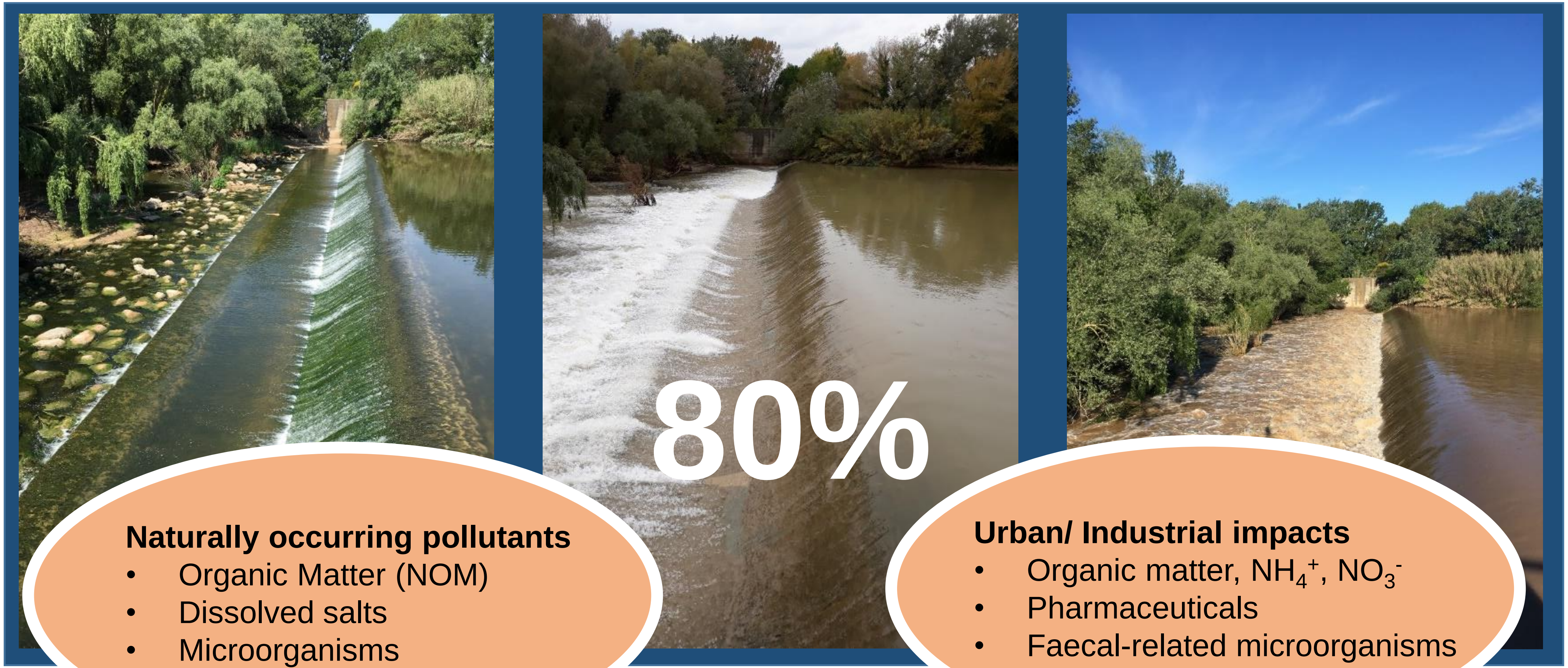
OUTLINE

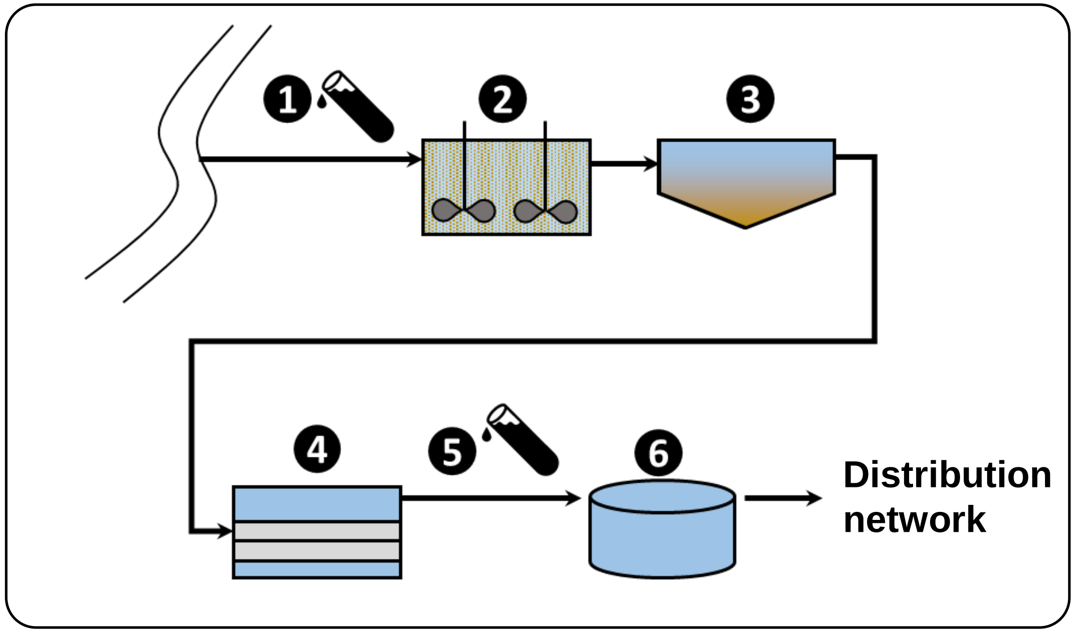


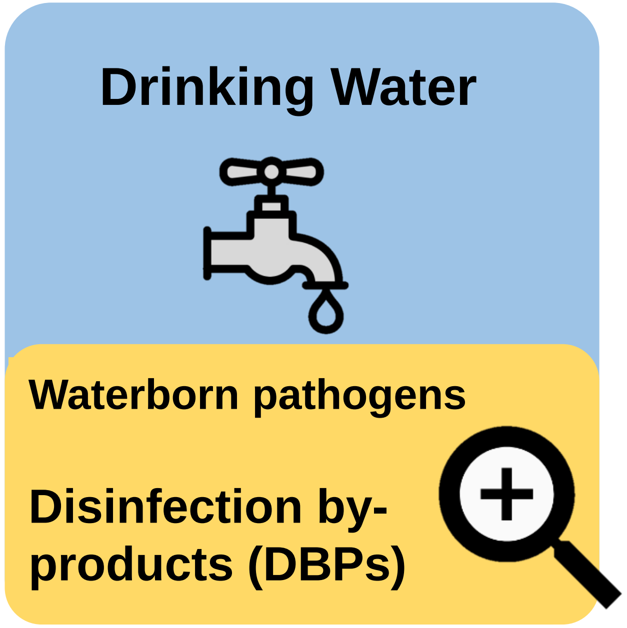
Naturally occurring pollutants
- Organic Matter (NOM)
- Dissolved salts
- Microorganisms

Urban/ Industrial impacts
- Organic matter, NH_4^+, NO_3^-
- Pharmaceuticals
- Faecal-related microorganisms

Introduction

Drinking water treatment plant (DWTP)





Introduction

Formation of disinfection by-products (DBPs)

DBPs Precursors

Natural Organic Matter

+ Inorganic ions
(Br^-, I^-, NO_2^-)

+

Disinfectant

Cl_2 NaOCl, ClO_2 NH_2Cl O_3

pH
Temperature
Time

Disinfection By-Products

Trihalomethanes (THMs)

($CHCl_3$, $CHBrCl_2$, $CHBr_2Cl$, $CHBr_3$)

Haloacetic acids (HAA5)

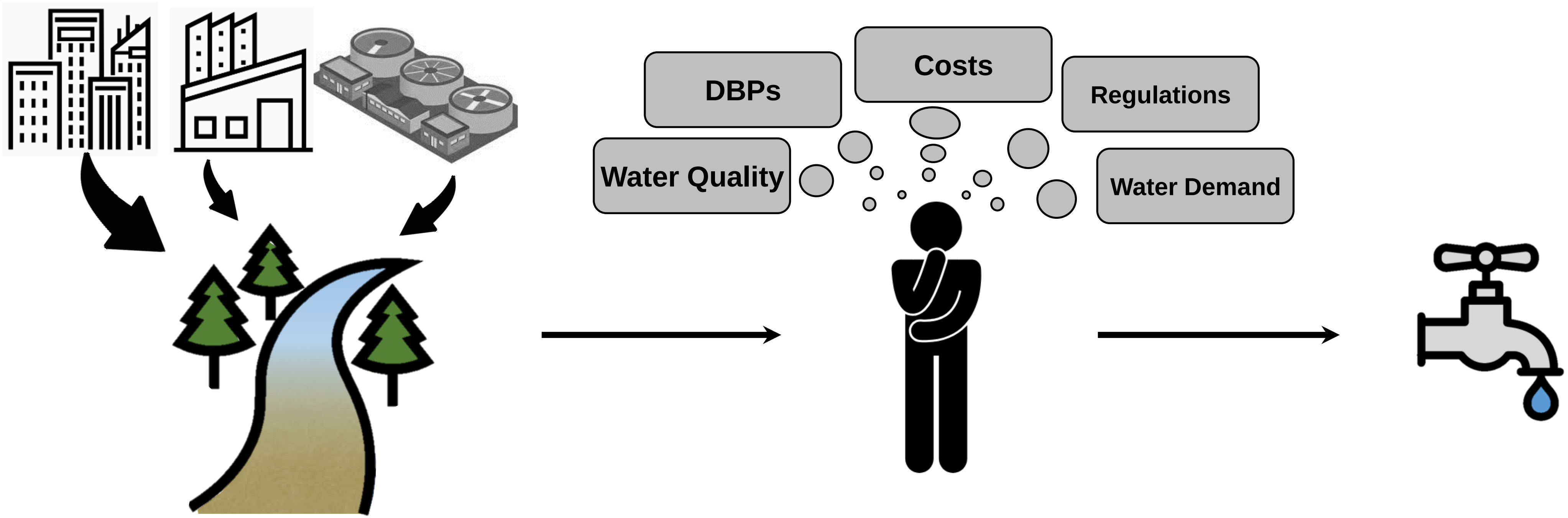
N-DBPs

EU - EC 98/1998
Spain - RD 140/2003

THMs < 100 µg·L^{-1}

HAA5 < 60 µg·L^{-1} ? (New)

Introduction

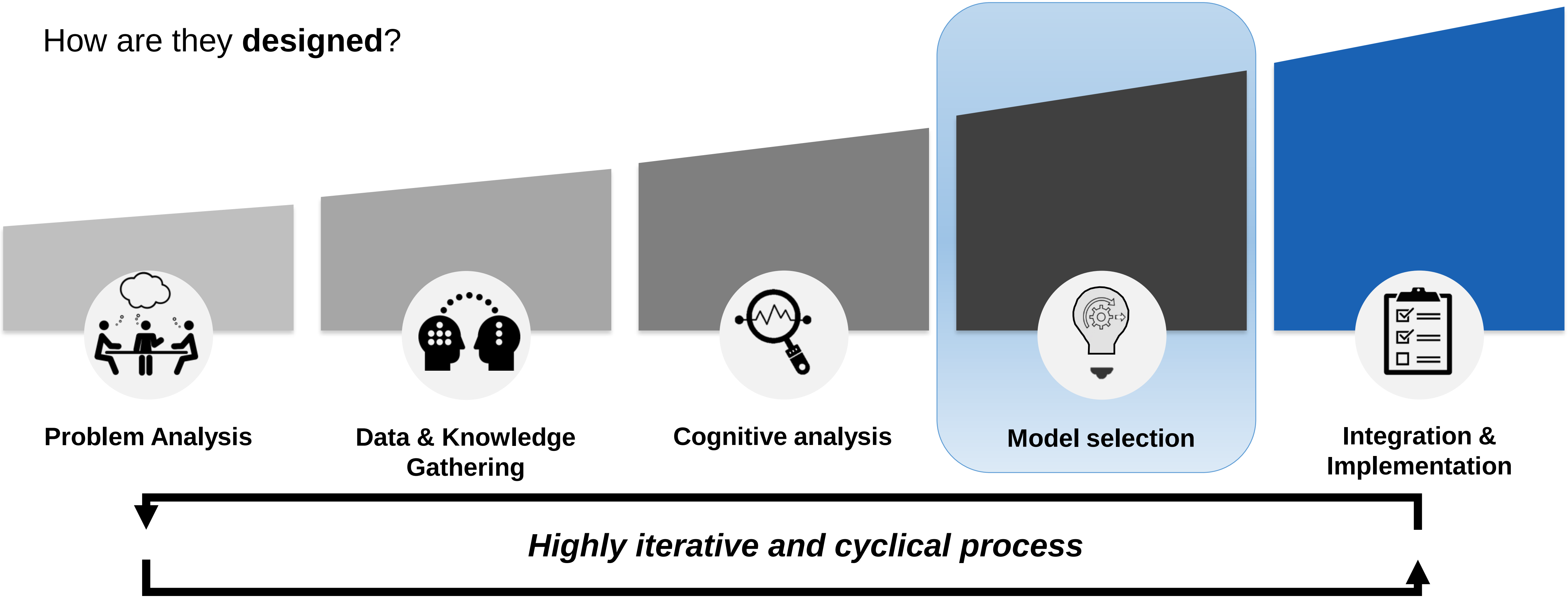


Environmental Decision Support Systems (EDSS)

Introduction

Environmental decision support systems

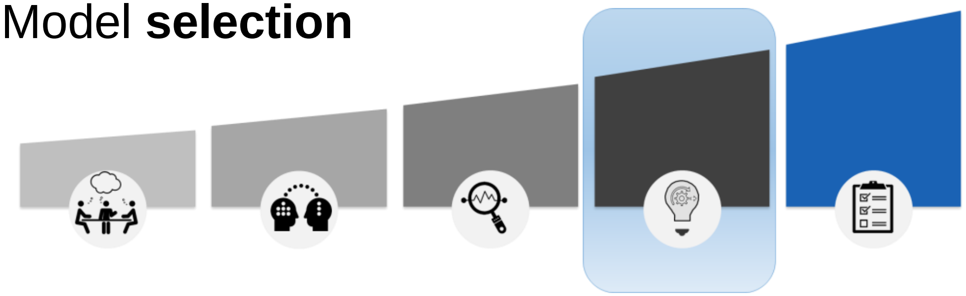
How are they **designed**?



Cortés et al. (2000)
Poch et al. (2004)
Hamouda et al. (2009)

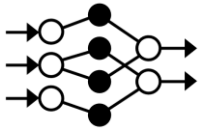
Environmental decision support systems

Model **selection**

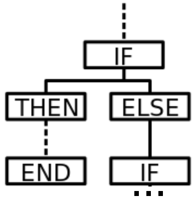


- **Mechanistic models** $\frac{dX}{dt} = \frac{\mu_m \cdot S}{K_s \cdot S} \cdot X$

- **Data-driven models**



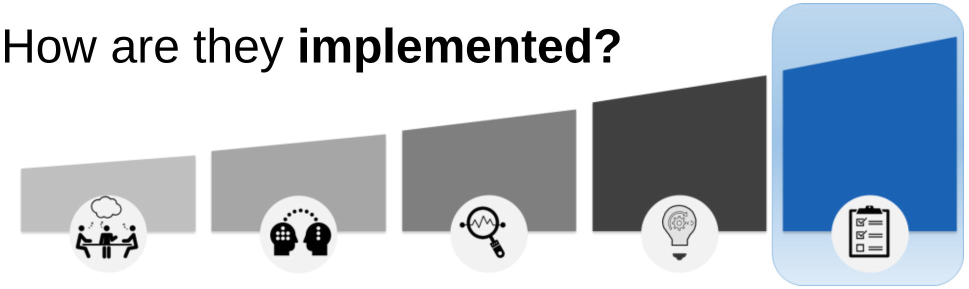
- **Knowledge-based models**

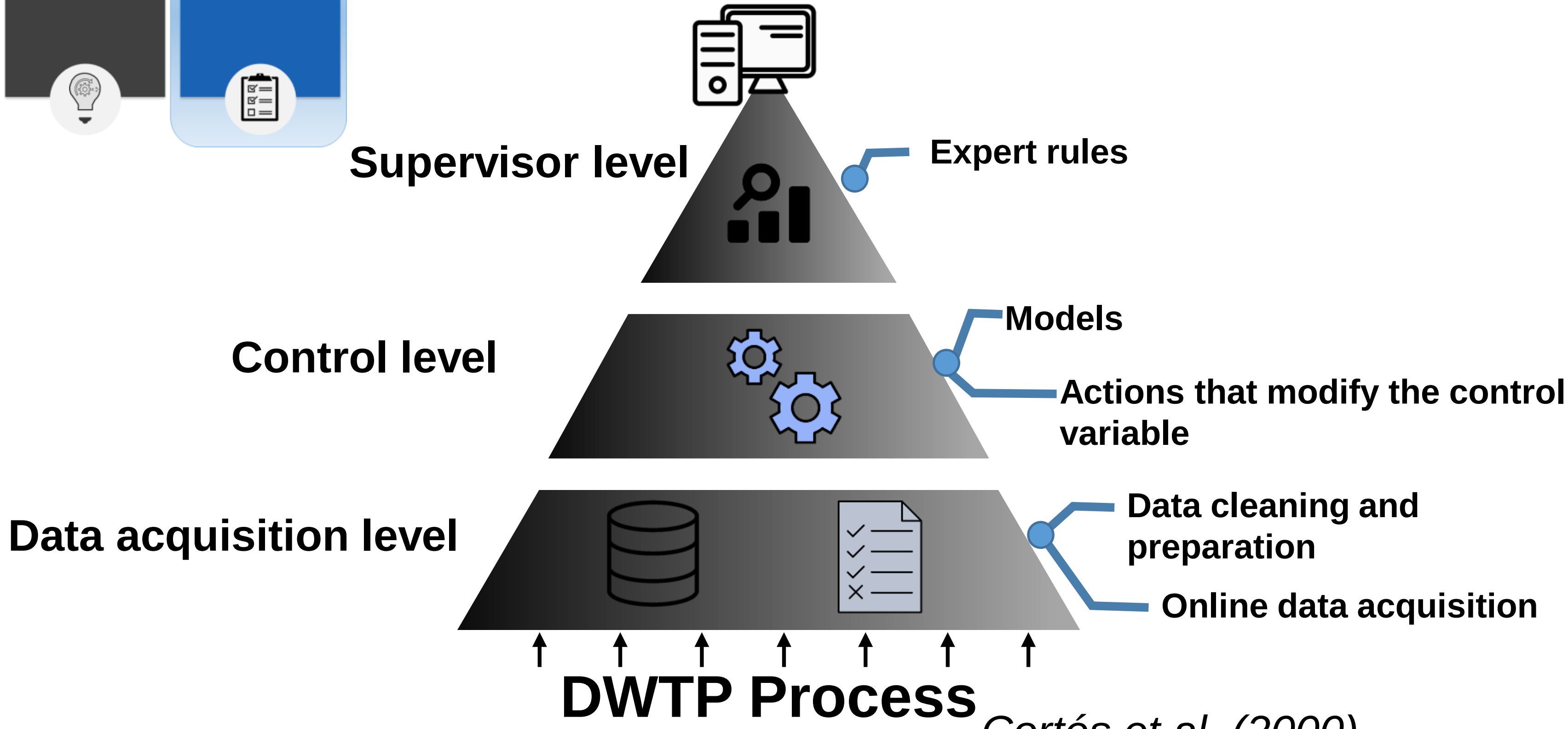


- **Hybrid models**

Environmental decision support systems

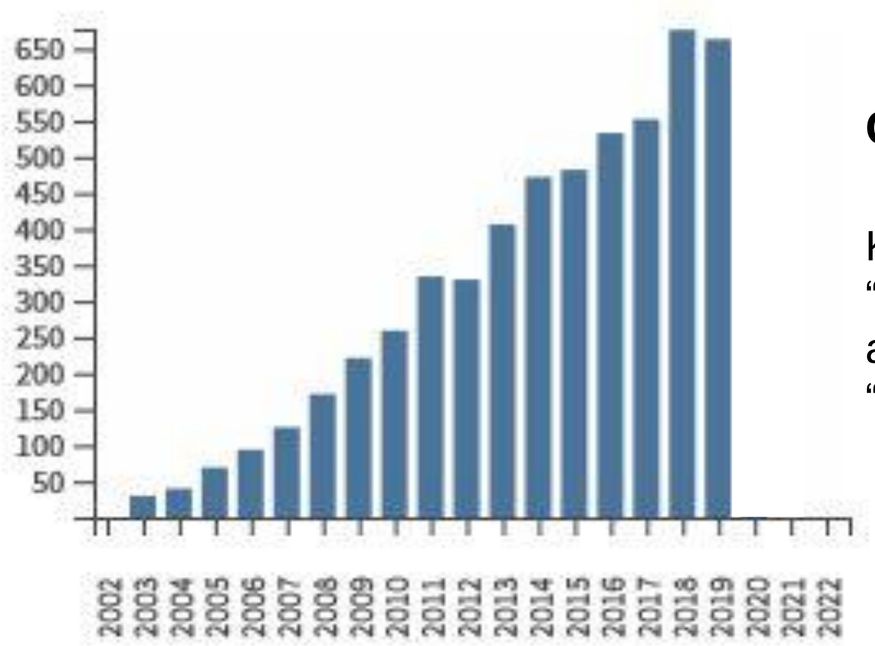
How are they **implemented?**





Cortés et al. (2000)
Poch et al. (2004)

Environmental decision support systems



Citations per year (Web of Science)

Keywords:
“**Environmental decision support system**”
and
“**Water**”

Implementation of EDSS at full-scale DWTPs: Challenges

Lack of generic EDSS

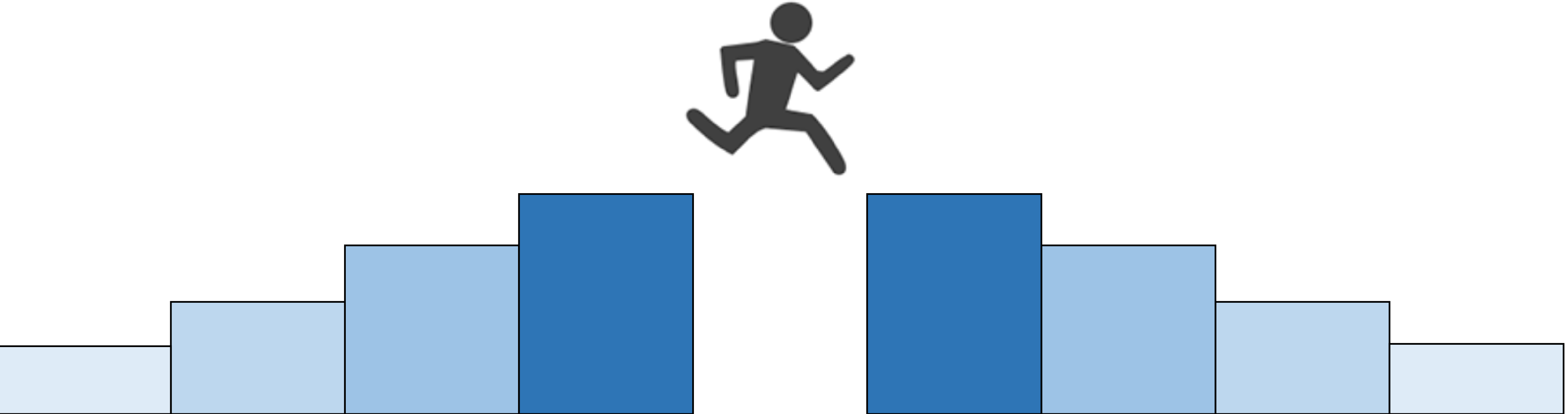
(Hamouda et al., 2009)

Reflect practical needs

(Hamouda et al., 2009; McIntosh et al., 2011; Raseman et al. 2017)

Incorporation of uncertainty

(Raseman et al., 2017, Humphrey et al., 2017)



Introduction

Motivation

- Challenges in operation of DWTPs
- Digitalisation of industry
- High amount of literature in wastewater treatment, fewer on drinking water.

Hypothesis

New models should be developed upon available knowledge and data from full-scale plants to address operational challenges

Objectives

Main Objective

- To develop an EDSS to help DWTP managers in setting the most adequate operational set-points in real-time

Secondary objectives

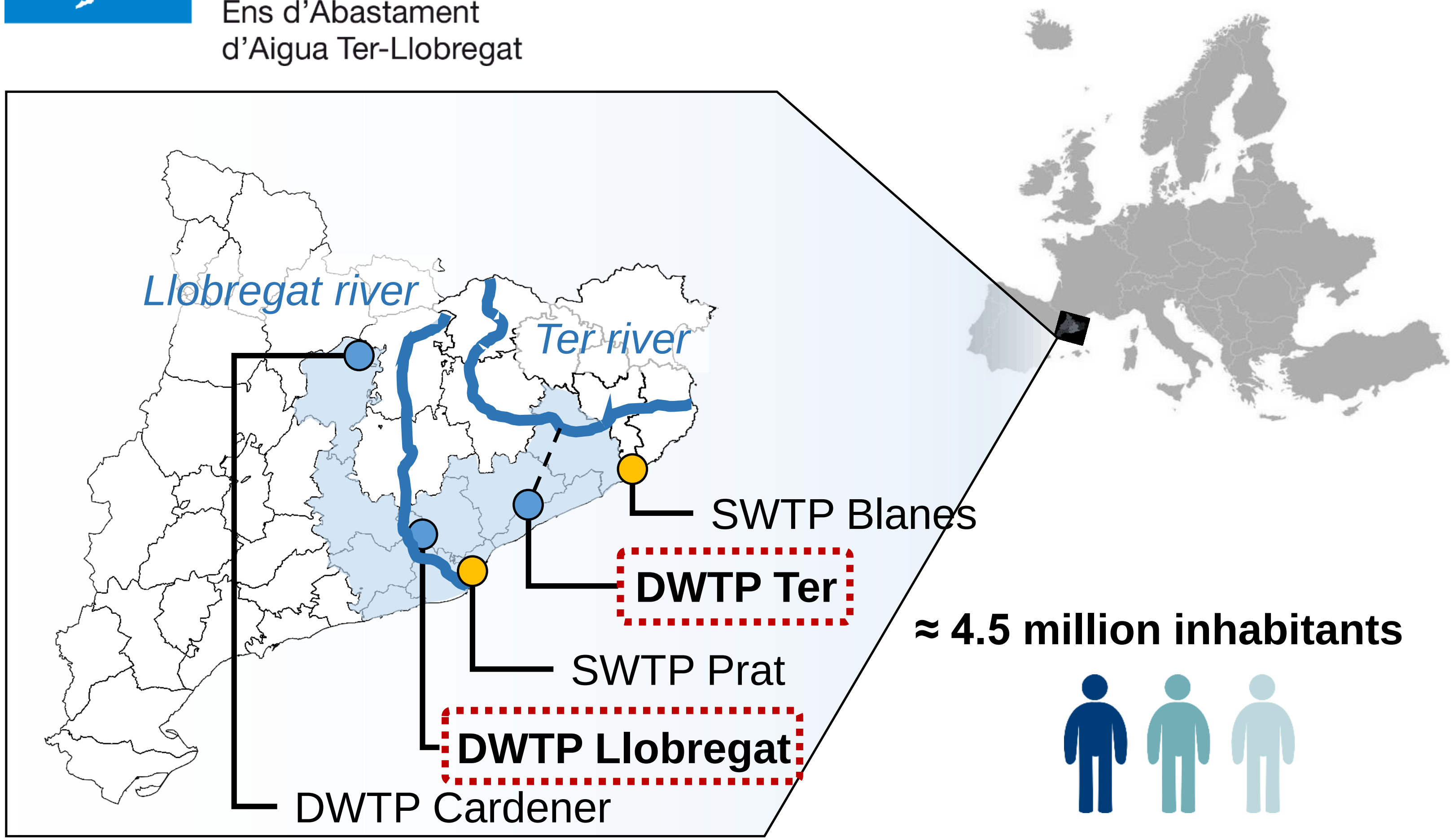
- Preoxidation process
- DBPs formation through predictive models
- Supervision of the microbiological safety

OUTLINE

1. Introduction
2. Objectives
3. **Materials and methods**
4. Results
   1. Results I
   2. Results II
   3. Results III
   4. Results IV
5. Discussion
6. General conclusions

Materials and Methods

ATL
Ens d'Abastament
d'Aigua Ter-Llobregat



Llobregat river
- Mediterranean river
- Irregular flow
- Anthropogenic impact
- Organic matter ↑
- Bromides↑

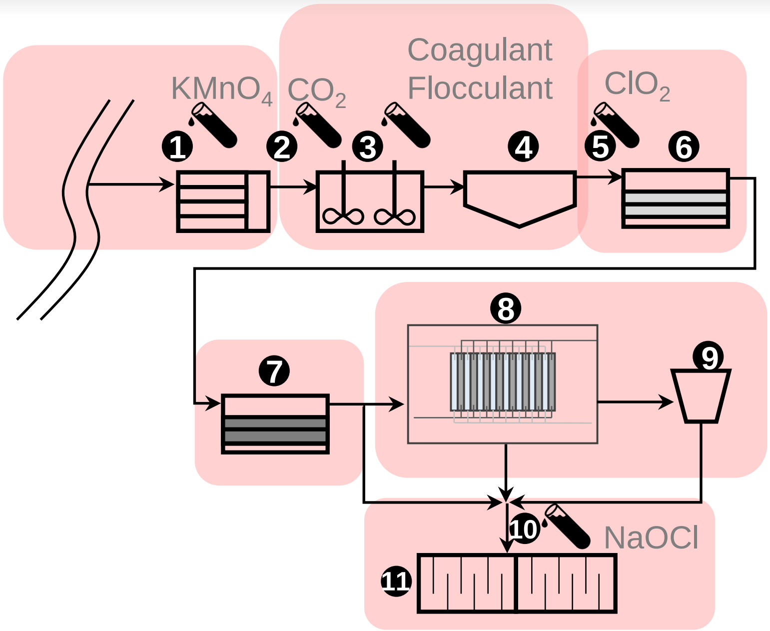
Ter river
- Taken from reservoirs systems
- Low turbidity

Materials and Methods

Llobregat DWTP

Capacity: 3.2 $m^3 \cdot s^{-1}$

1. Preoxidation
2. pH adjustment
3. Coagulation/focculation
4. Settling
5. Primary disinfection
6. Filtration
7. GAC filtration
8. Electrodialysis Reversal
9. Remineralisation
10. Secondary disinfection
11. Storage

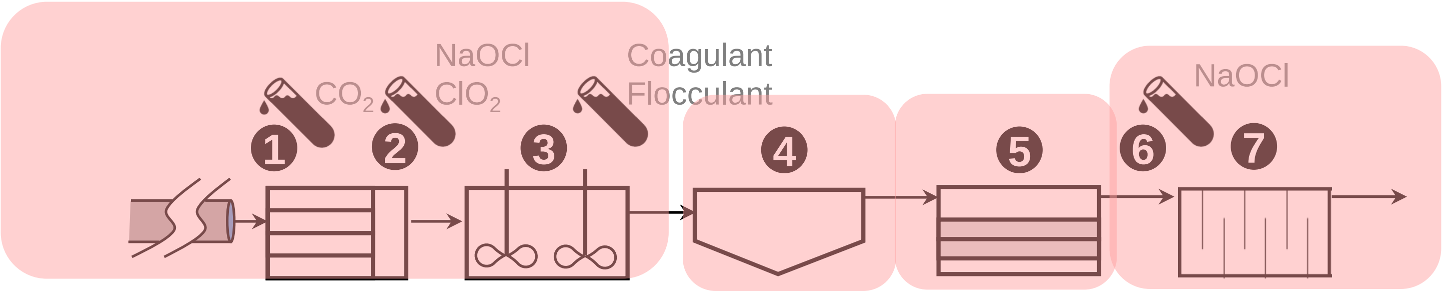


ATL
Ens d'Abastament d'Aigua Ter-Llobregat

Materials and Methods

Ter DWTP

Capacity: $8\ m^3 \cdot s^{-1}$



1. **pH adjustment**
2. **Primary disinfection**
3. **Coagulation/focculation**
4. **Settling**
5. **GAC filtration**
6. **Secondary disinfection**
7. **Storage**

ATL
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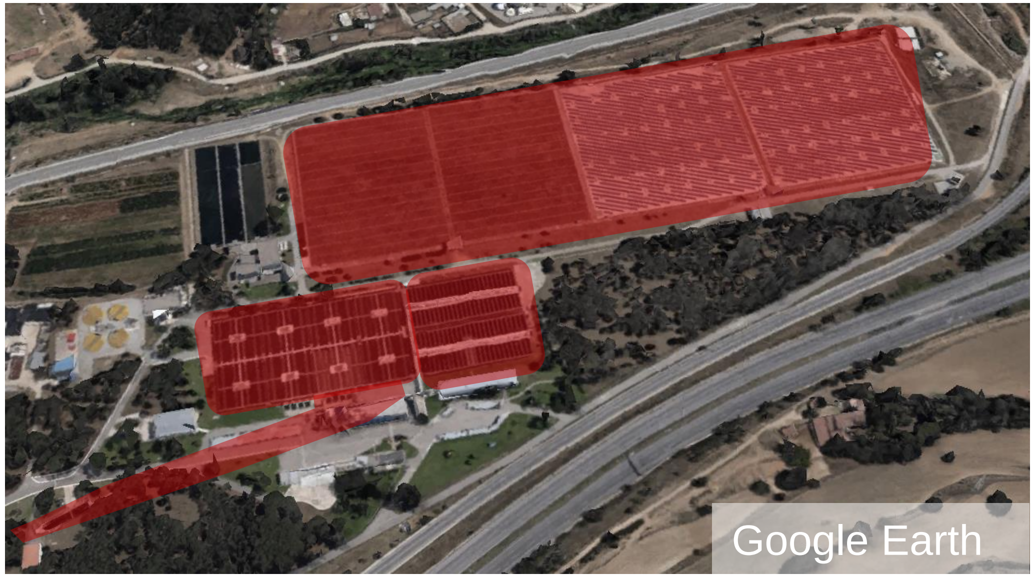
d'Aigua Ter-Llobregat



Materials and Methods

Data sources

ATL
Ens d'Abastament
d'Aigua Ter-Llobregat

- Routine laboratory analysis
- Sensor data
- Operational data

Software

MATLAB

- Data acquisition
- Data cleaning
- Model development
- Graphical user interfaces

OUTLINE

1. Introduction
2. Objectives
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4. **Results**
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    2. Results II
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    4. Results IV
5. Discussion
6. General conclusions

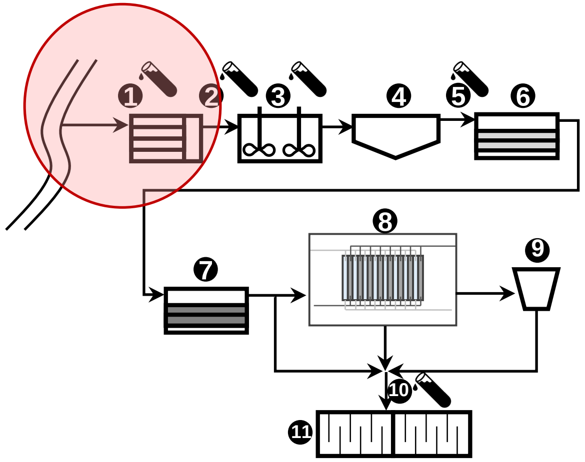
Results I

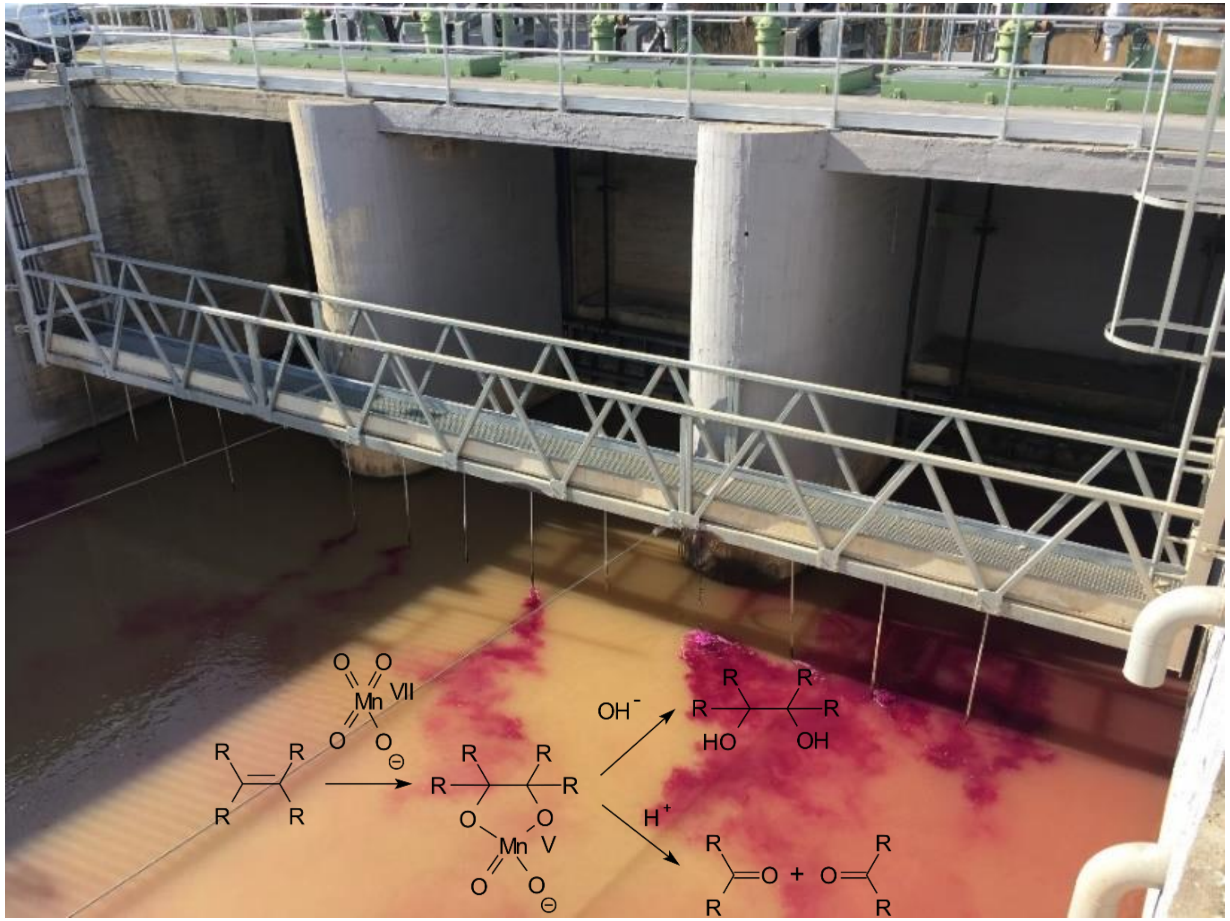
Predicting the oxidant demand in a surface water treatment plant: Model development and integration into an environmental decision support system.

Godo-Pla, L., Emiliano, P., Valero, F., Poch, M., Sin, G., Monclús, H., **2019**. Predicting the oxidant demand in full-scale drinking water treatment using an artificial neural network: Uncertainty and sensitivity analysis. Process Saf. Environ. Prot. 125, 317–327. https://doi.org/10.1016/j.psep.2019.03.017

Godo-Pla, L., Emiliano, P., González, S., Poch, M., Valero, F., Monclús, H**., 2020**. Implementation of an environmental decision support system for controlling the pre-oxidation step at a full-scale drinking water treatment plant. Water Sci. Technol. 81 (8), 1778-1785. https://doi.org/10.2166/wst.2020.142

Llobregat DWTP





Potassium permanganate ($KMnO_4$)

- Iron and manganese
- Odour and tase compounds
- Disinfection by-products (DBP) precursors

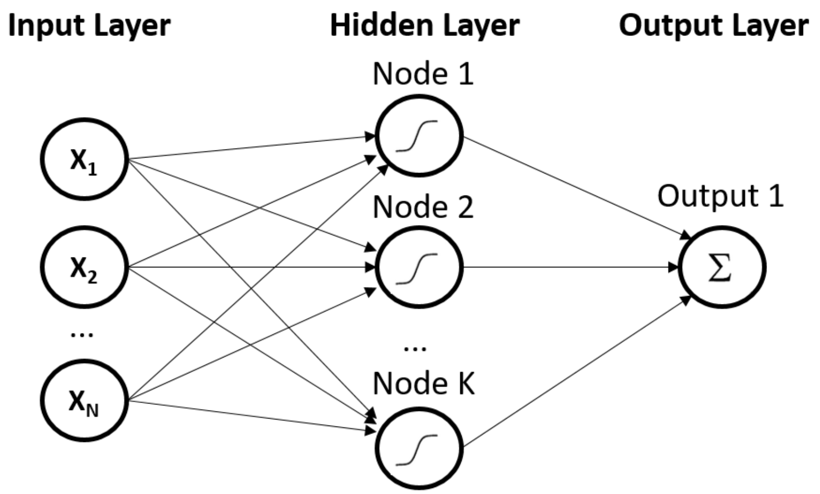
To develop a model for predicting the oxidant dose

Results I. Preoxidation

Data-driven model development

Model architecture selection

Multi-layer perceptrons (MLPs)



Multiple linear regression (MLR)

$$Y=\beta_0 + \beta_1 \cdot X_1 + \beta_2 \cdot X_2 + \ldots + \beta_n \cdot X_n$$

Results I. Preoxidation

Data-driven model development

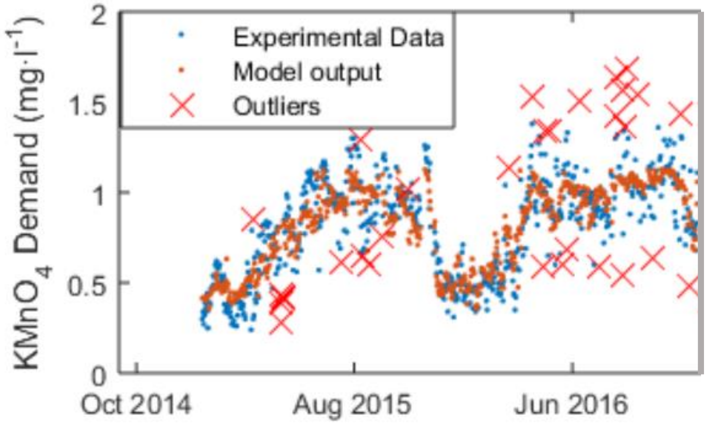
Model architecture selection

Data handling

Features selection
Best subset selection
James et al. (2013)

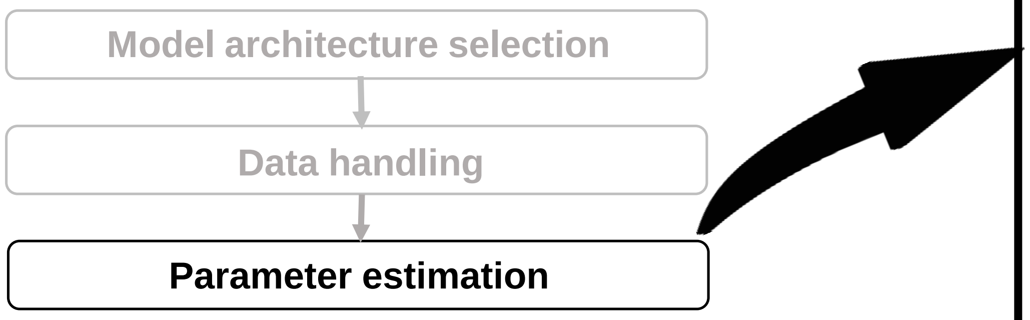
Input features:
- UV_{254}
- Turbidity
- Temperature
- HRT

Outliers detection
Empirical cumulative Distribution function (ECDF)
Frutiger et al. (2015)



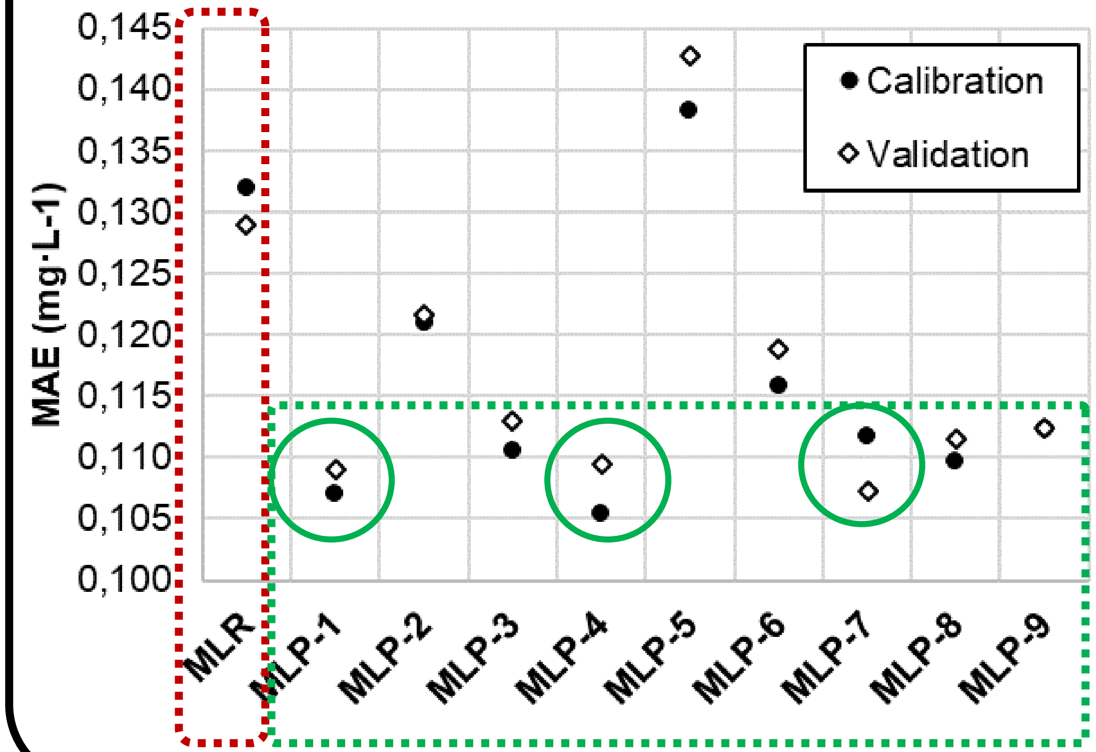
Data division
Self-organising map algorithm
May et al. (2010)

Data-driven model development



Bootstrap method (N=50) *Sin and Gernaey (2017)*

$$\hat{\theta} \sim D\left(\mu(\hat{\theta}), COV(\hat{\theta})\right)$$



Results I. Preoxidation

Data-driven model development

Model architecture selection

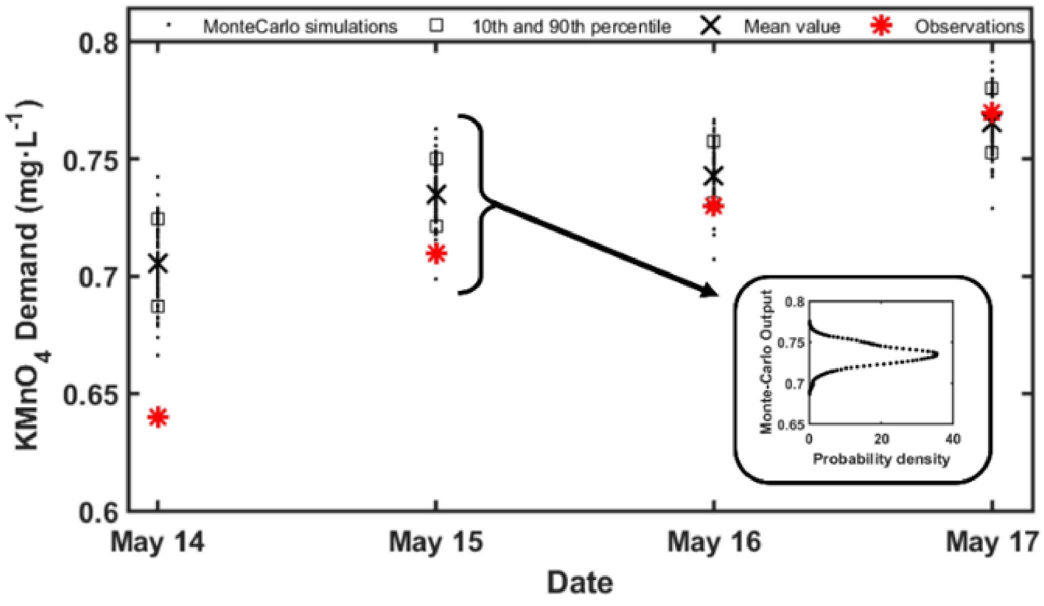
Data handling

Parameter estimation

Uncertainty analysis

MonteCarlo propagation (N=100) *Sin and Gernaey (2017)*

$$\hat{\theta} \sim D\left(\mu(\hat{\theta}), cov(\hat{\theta})\right)$$



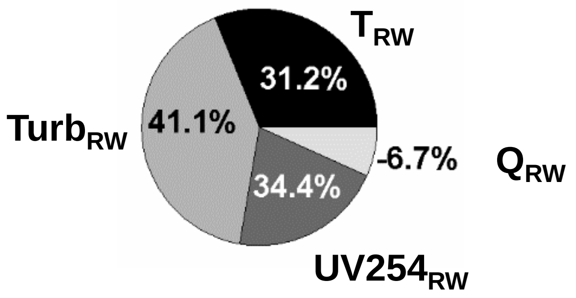
Data-driven model development

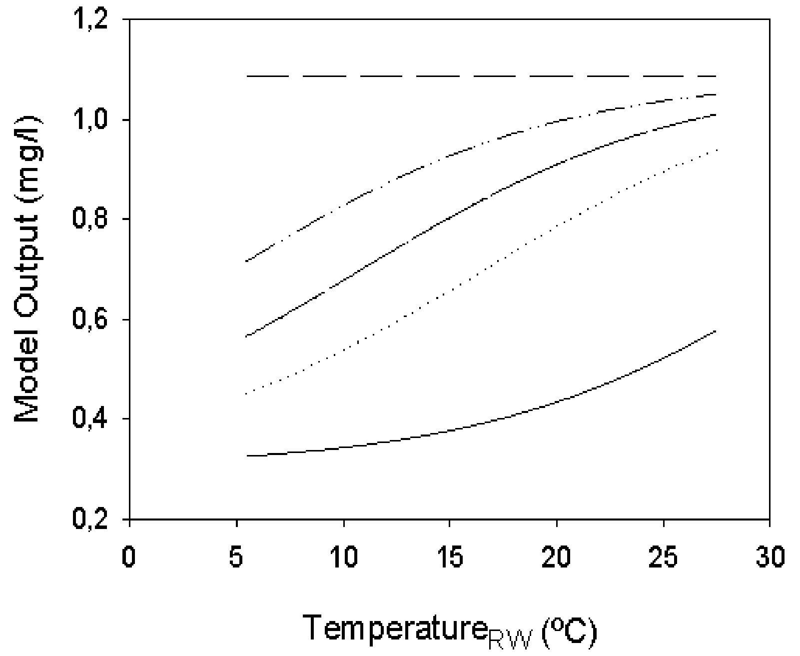
- Model architecture selection
- Data handling
- Parameter estimation
- Uncertainty analysis
- **Sensitivity analysis**

Connection weight

Profile method

Humphrey et al. (2017)
Olden and Jackson (2002)

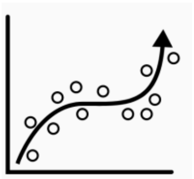


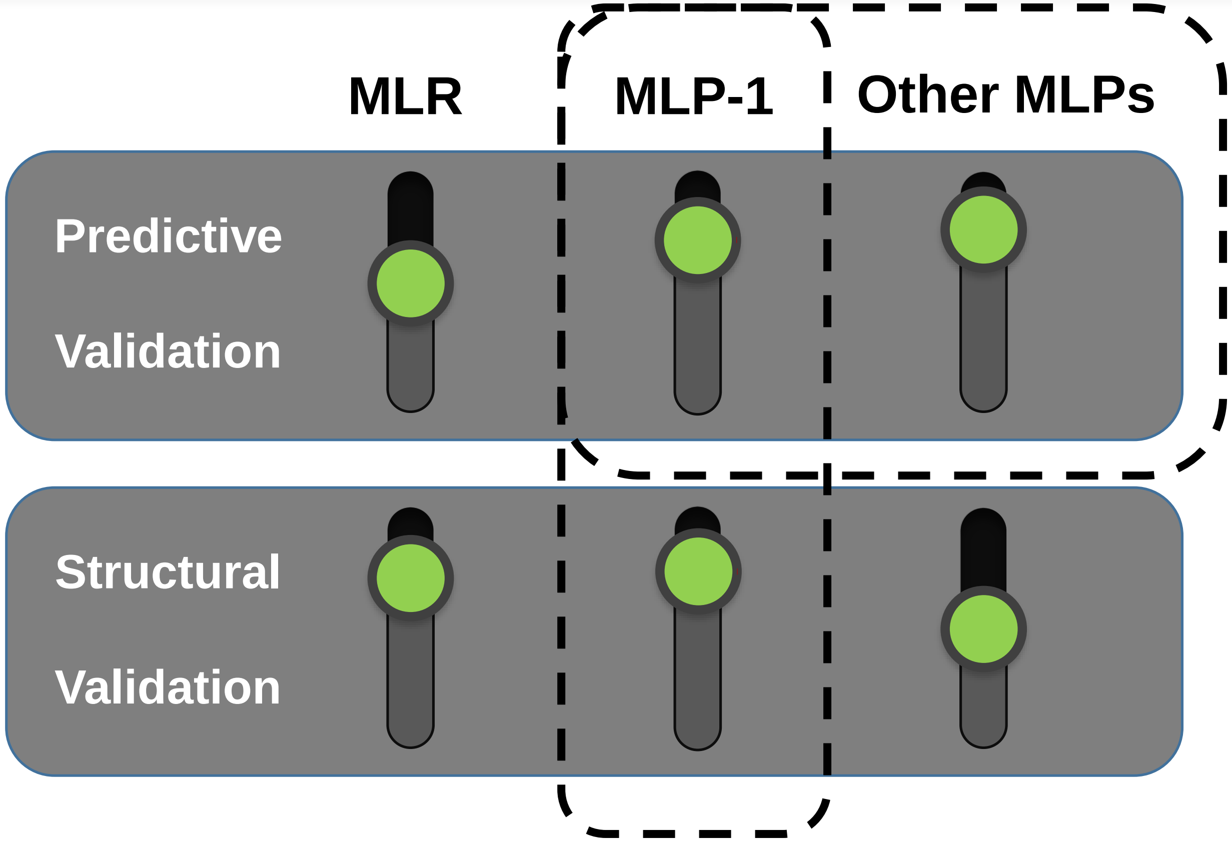


Data-driven model development

- Model architecture selection
- Data handling
- Parameter estimation
- Uncertainty analysis
- Sensitivity analysis

Predictive model

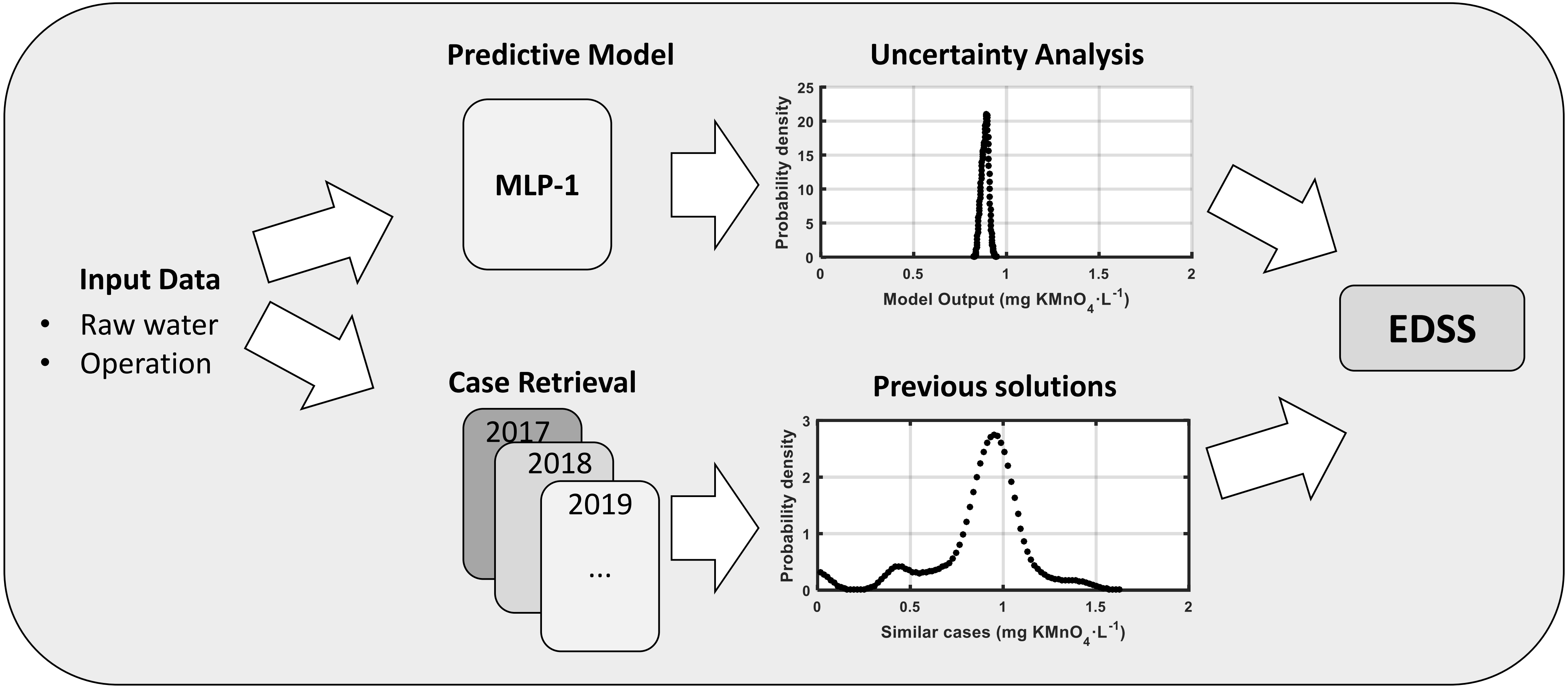




- **Best balance**
- **MAE ≈ 0.13 $mg \cdot L^{-1}$**
- **$\rho^2_{Spearman} = 0.80$**

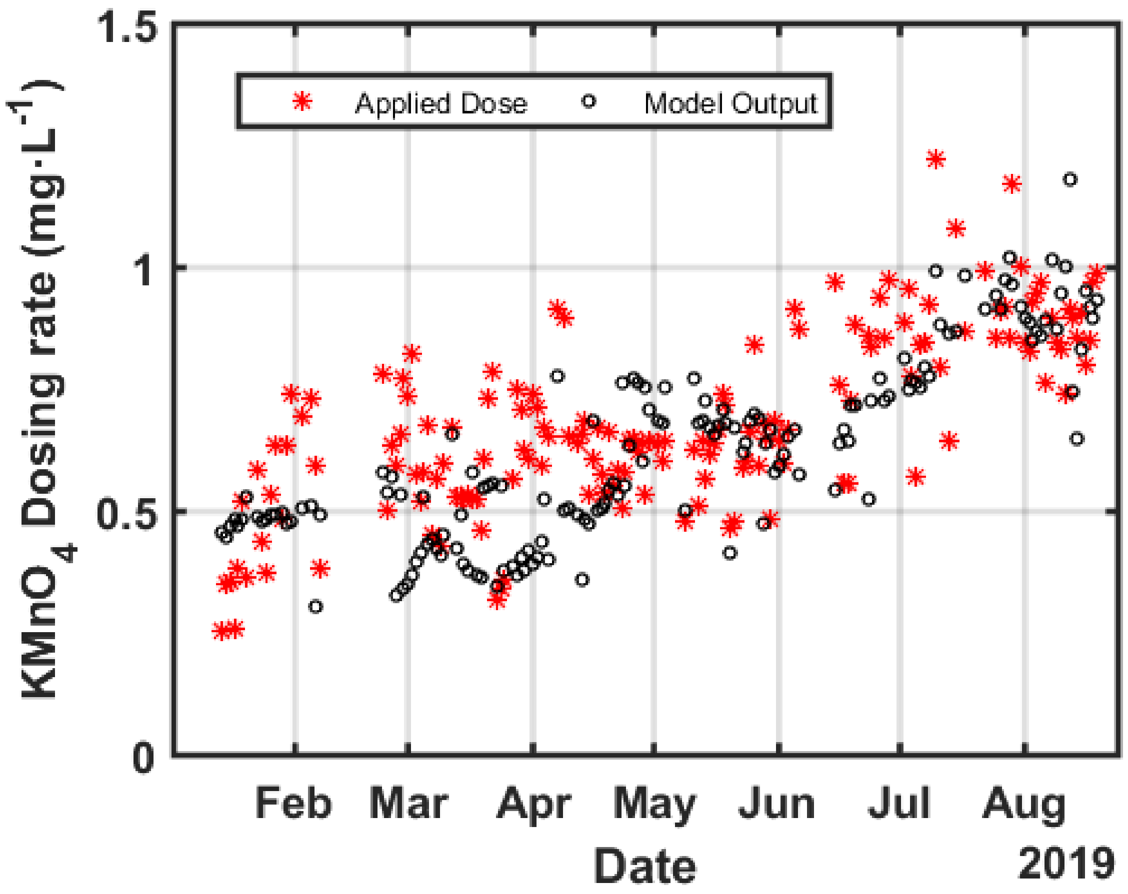
Results I. Preoxidation

Implementation for decision support



Results I. Preoxidation

Implementation for decision support



- Validation period (January-September 2019)
- Baseline values were modified based on experience, visual inspection and laboratory analyses.

Results I. Preoxidation

Keypoints

- New model for preoxidation process with MLP
- Predicted error <0.15 mg/L
- Uncertainty and sensitivity analysis
- Integration of MLP and CBR models in an EDSS

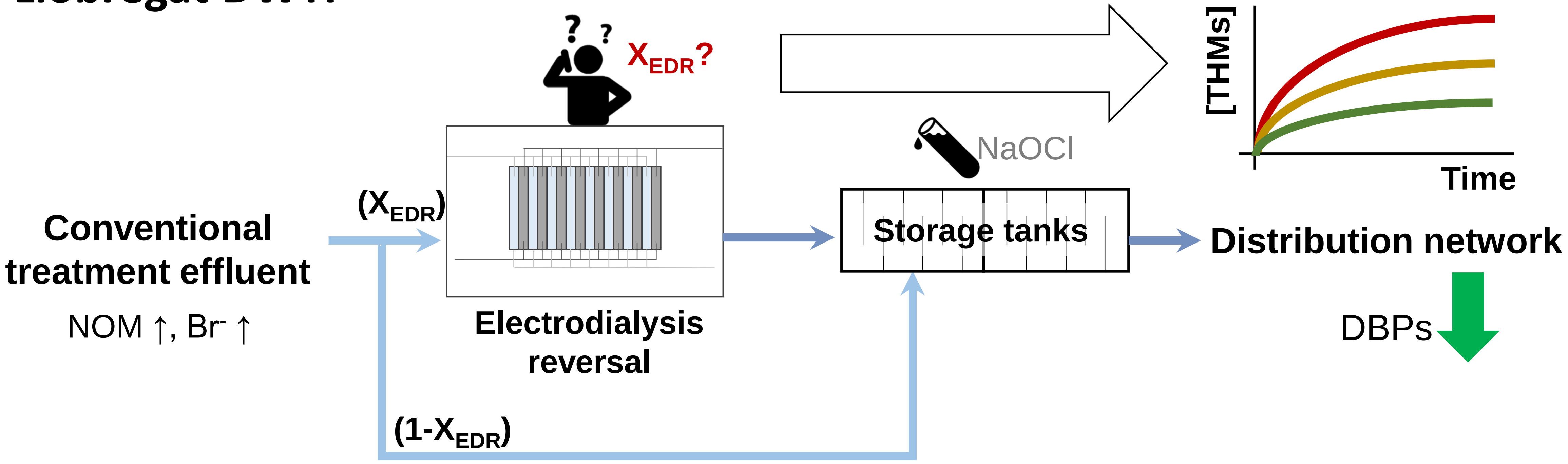
Results II

Benchmarking empirical models for THMs formation in drinking water systems and integration into an EDSS

Godo-Pla, L., Emiliano, P., Poch, M., Valero, F., Monclús, H., **2020**. Benchmarking empirical models for THM formation in drinking water systems: An application for decision support in Barcelona, Spain. (Under review in Science of the Total Environment).

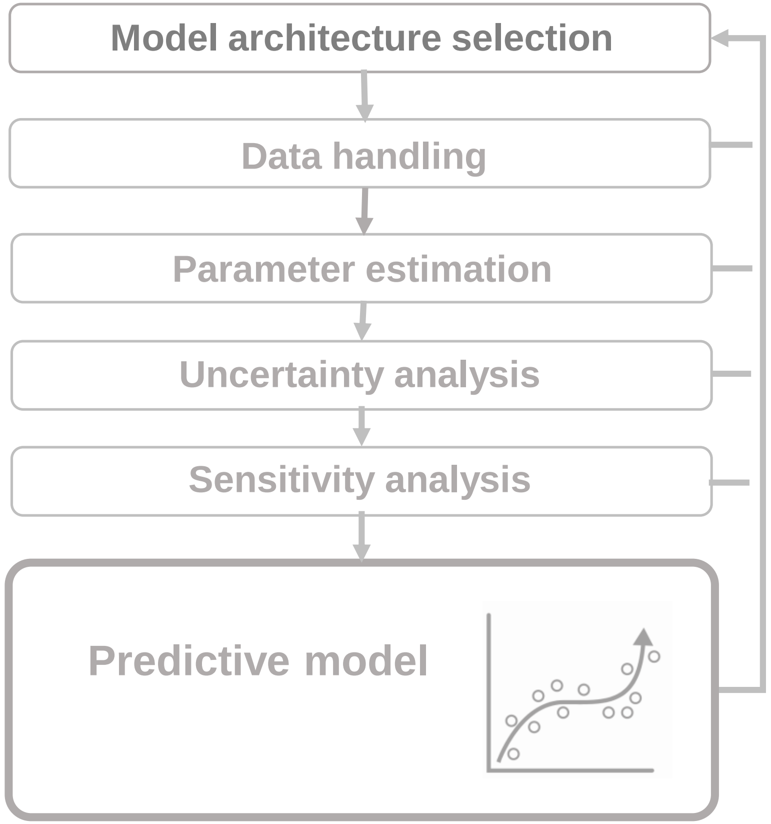
Results II. Electrodialysis reversal

Llobregat DWTP



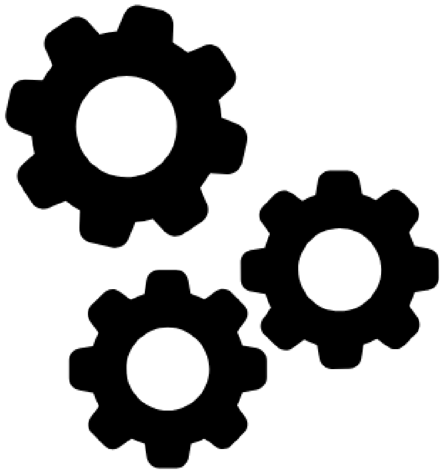
1. To develop a predictive model for THMs formation
2. To link EDR performance with THMs formation
3. Integration of models for real-time support in managing the DWTP

Predictive model for THMs formation



Data-driven model development

Historical Data 2019-2020 (N=573)



Predictive model for THMs formation

Model architecture selection

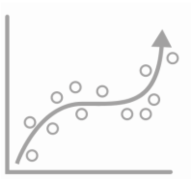
Data handling

Parameter estimation

Uncertainty analysis

Sensitivity analysis

Predictive model



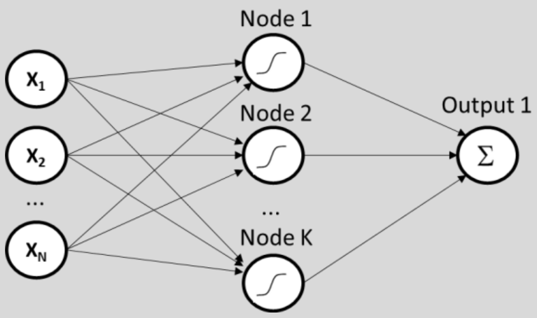
- Log-scaled multiple linear regressions **(MLR)**

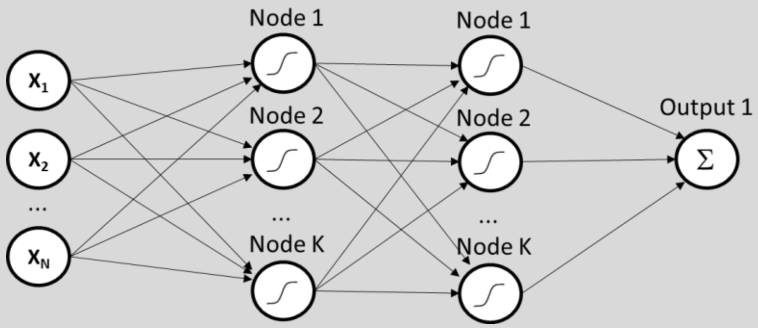
  Chowdhurry et al. (2009)

$$[THM] = a \cdot ([UV254]+1)^{b} \cdot [TOC]^{c} \cdot [D_{Cl}]^{d} \cdot ([Br]+1)^{e} \cdot T^{f} \cdot pH^{g} \cdot HRT^{h}$$

- Multi-layer perceptrons **(MLPs)** with different architectures

  Kulkarni et al. (2010)





Results II. Electrodialysis reversal

Predictive model for THMs formation

Model architecture selection

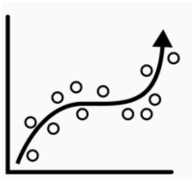
Dat ling

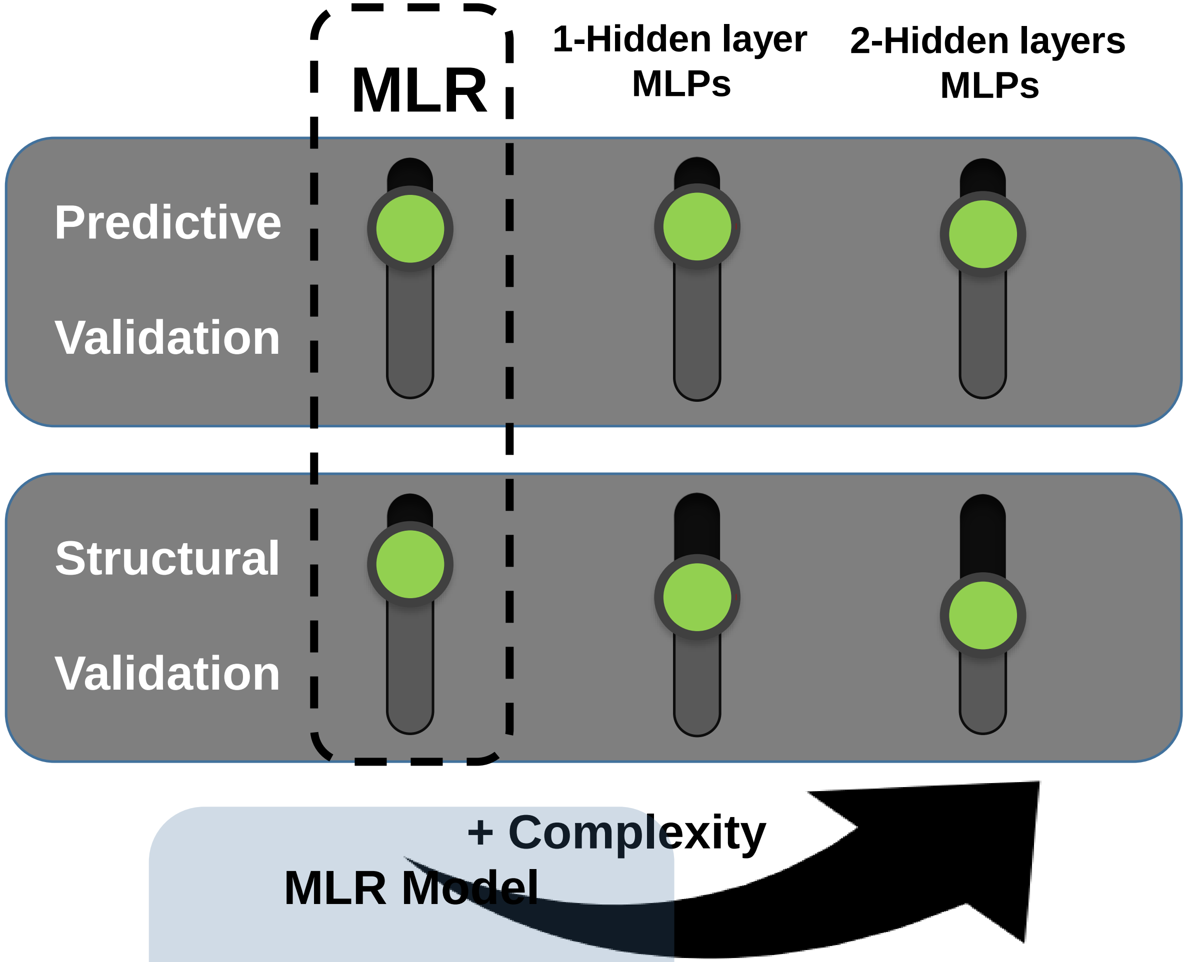
Parame imation

Uncert nalysis

Sens alysis

Predictive model



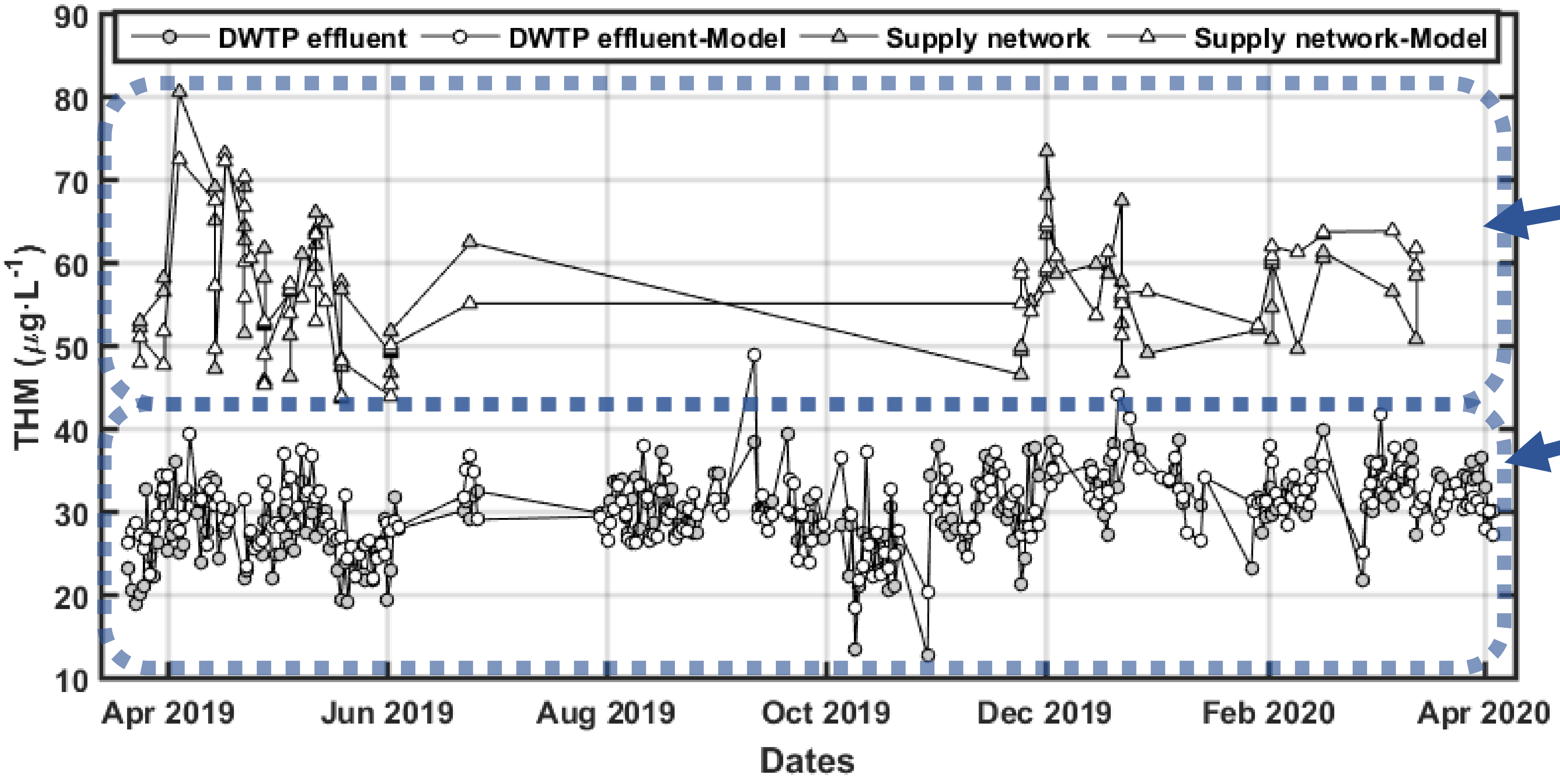


MLR Model

R^2= 0.88

MAE= 4 µg·L^{-1}

Predictive model for THMs formation



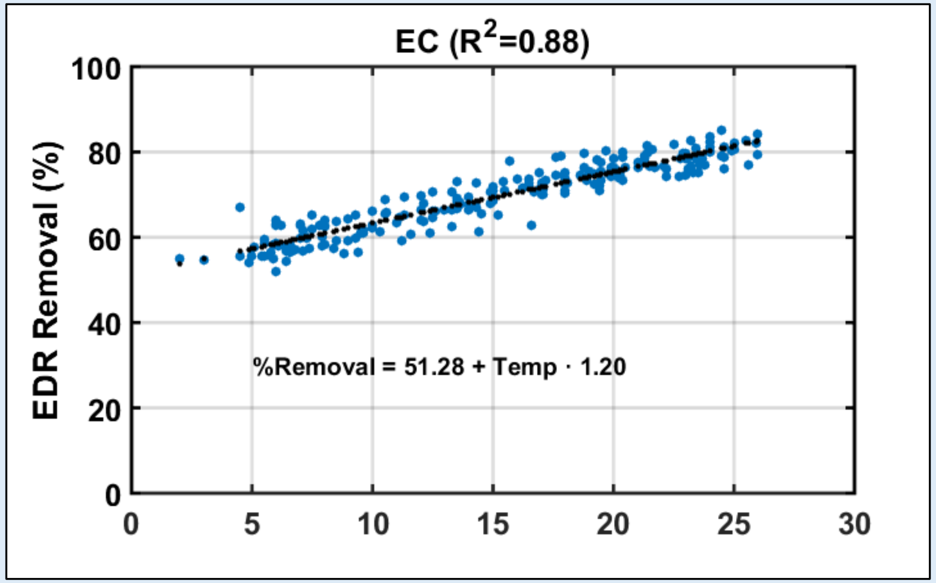
Supply network data

DWTP efluent data

Results II. Electrodialysis reversal

Linking EDR operation and THMs formation

Historical data 2015-2020

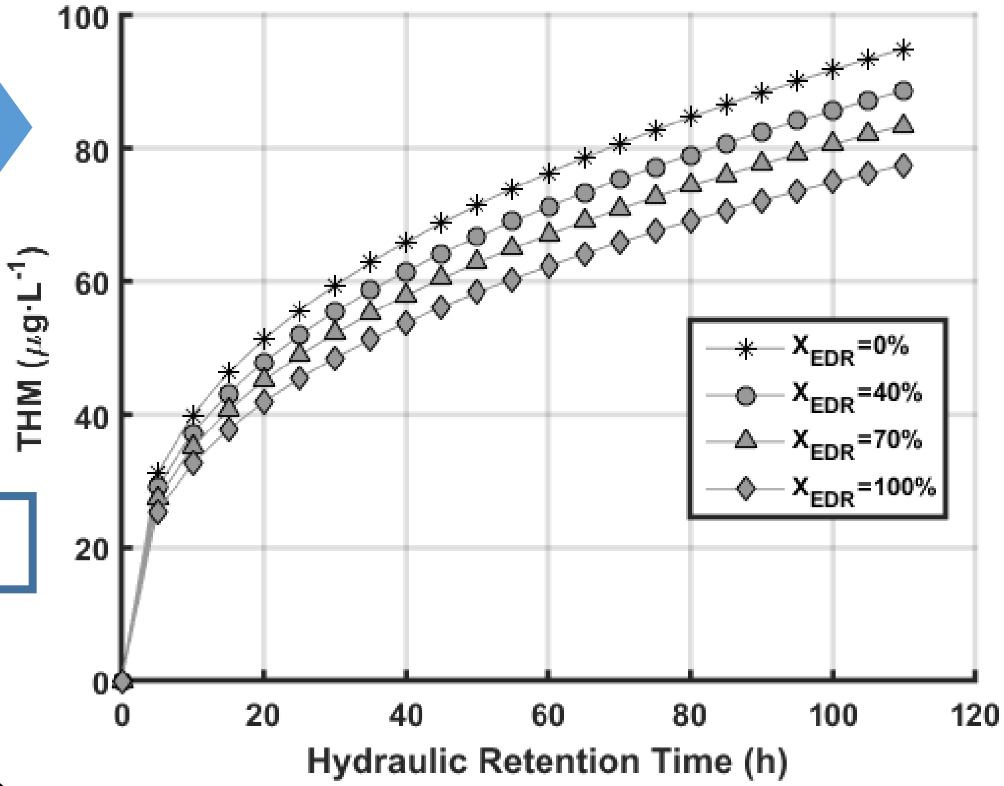


Removal characterization:

- EC, Bromide, TOC, UV_{254}
- Temperature dependent

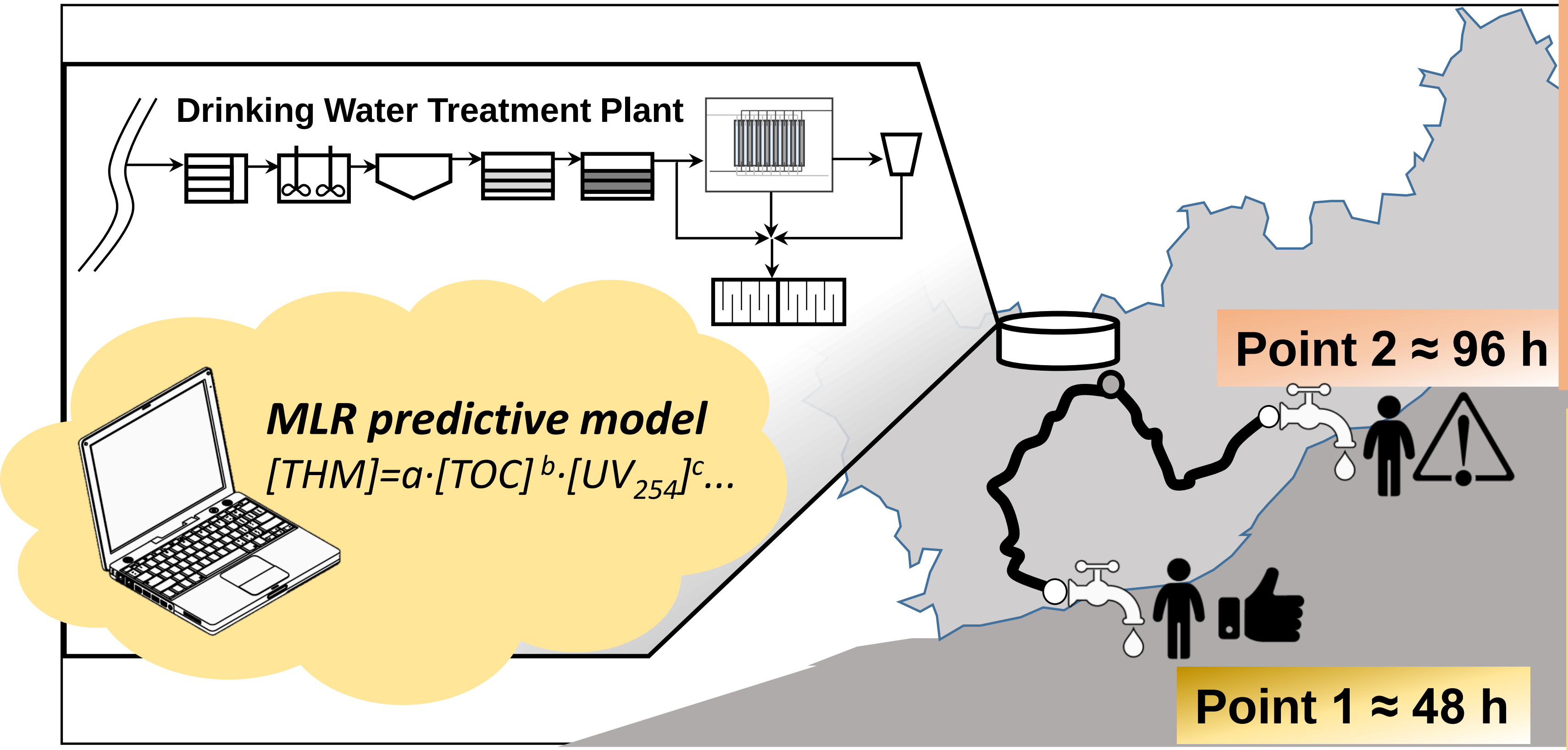
Predictive model MLR

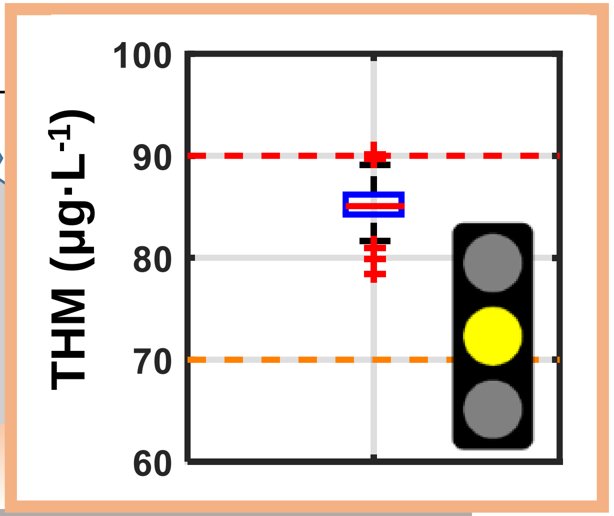
$[THM] = a \cdot ([UV254]+1)^{b} \cdot [TOC]^{c} \cdot [D_{Cl}]^{d} \cdot ([Br]+1)^{e} \cdot T^{f} \cdot pH^{g} \cdot HRT^{h}$

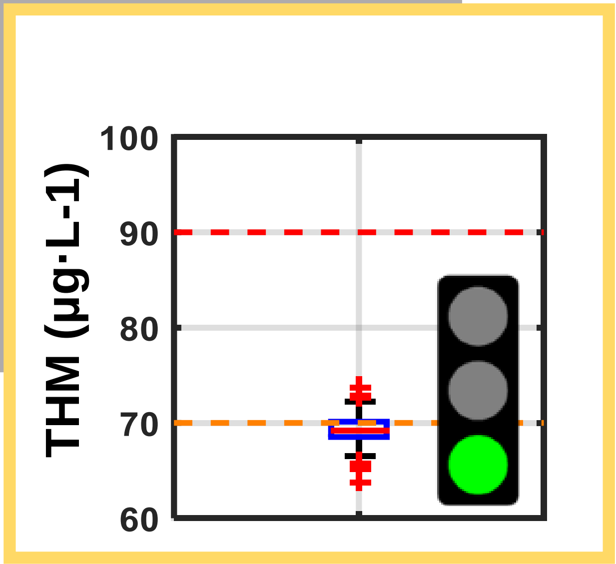


Results II. Electrodialysis reversal

Integration for real-time decision support







Keypoints

- Benchmark of empirical models to predict THMs with full-scale data
- Operation of EDR was linked with THMs formation at distribution network
- Integration in an EDSS for a real-time management of EDR.
- Feasibility of empirical models for operational purposes was demonstrated.

Results III

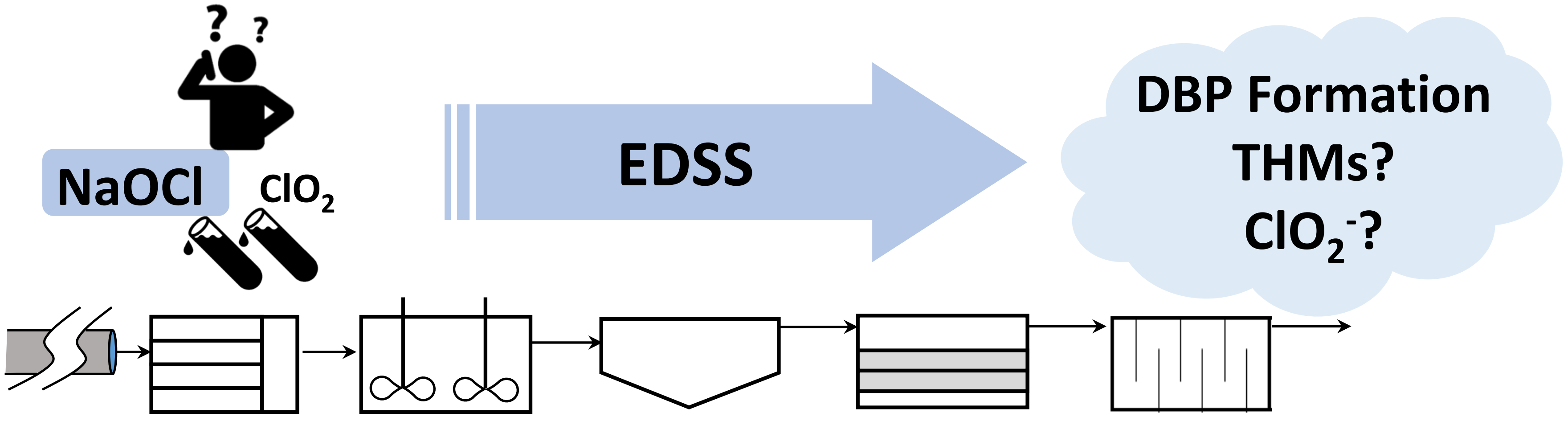
Control of primary disinfection in a drinking water treatment plant based on a fuzzy inference system

Godo-Pla, L., Rodríguez, J.J., Suquet, J., Emiliano, P., Valero, F., Poch, M., Monclús, H., **2020**. Control of primary disinfection in a drinking water treatment plant based on a fuzzy inference system. Process Saf. Environ. Prot. 145, 63–70. https://doi.org/10.1016/j.psep.2020.07.037

Ter DWTP

Primary disinfection

- Disinfection along the treatment process
- Oxidation of odour-causing compounds



✓ Accumulated experience
✓ Few availability of data
✓ Highly correlated

→ **Knowledge-based models**

Results III. Primary disinfection

Fuzzy Inference System (FIS)

- Consolidate process knowldge
- Data is difficult to obtain
- Imprecision related to human classification using fuzzy sets

1) Fuzzification
2) Inference System
3) Defuzzification

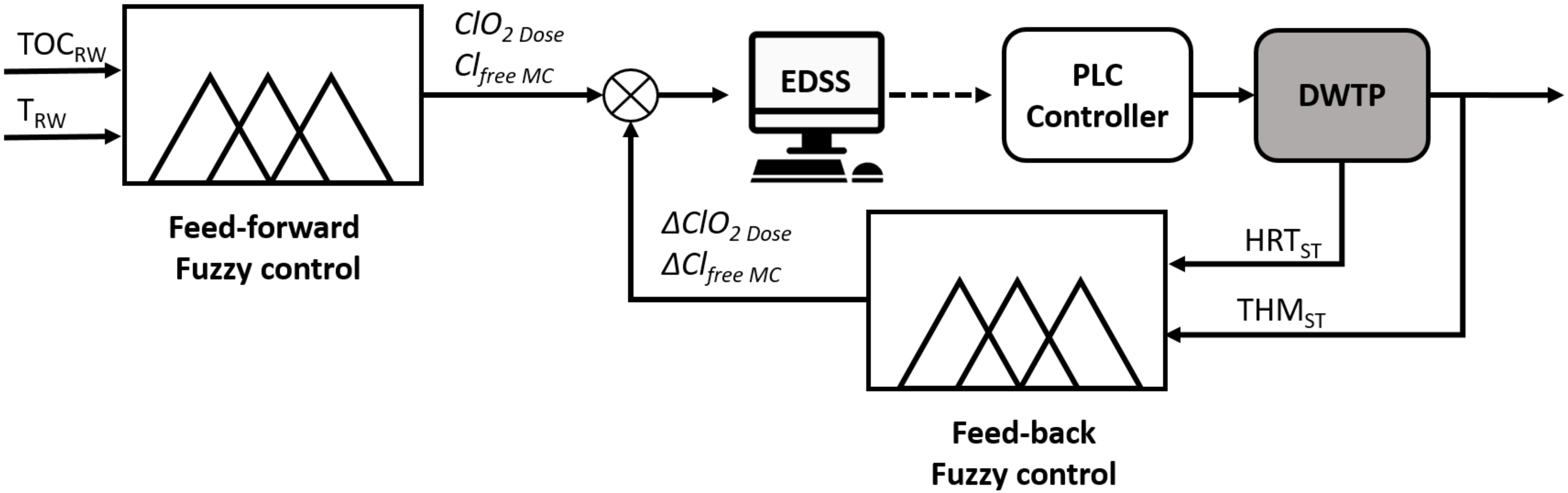
x_1, x_2

IF x_1 is ... **AND** x_2 is..., **THEN** y_1 is ...

y_1

Experience, process knowledge
Scientific basis

Design of the control system



Design of the control system

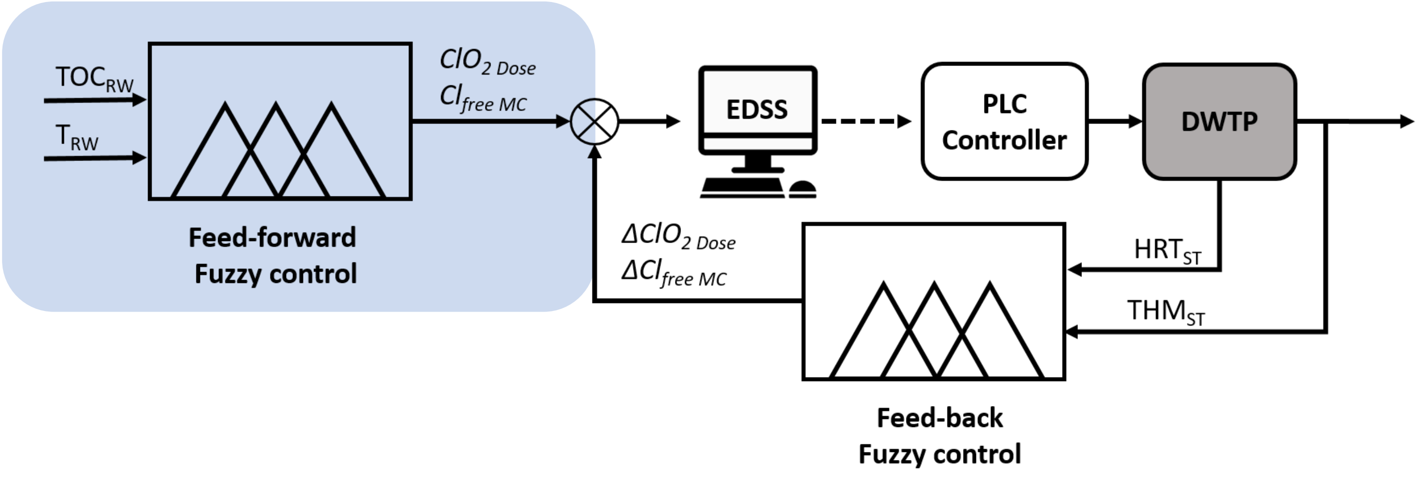
FIS_1

Objective:
Assess the THMs formation risk (THMFR) accordig to raw water quality and environmental conditions

Input variables:
TOC_{RW}, T_{RW}

Inference System:
(TOC_{RW}, T_{RW} → $ClO_{2\ Dose}$, Cl_{Free})

Controlled variables:
$ClO_{2\ Dose}$, Cl_{Free}



Design of the control system

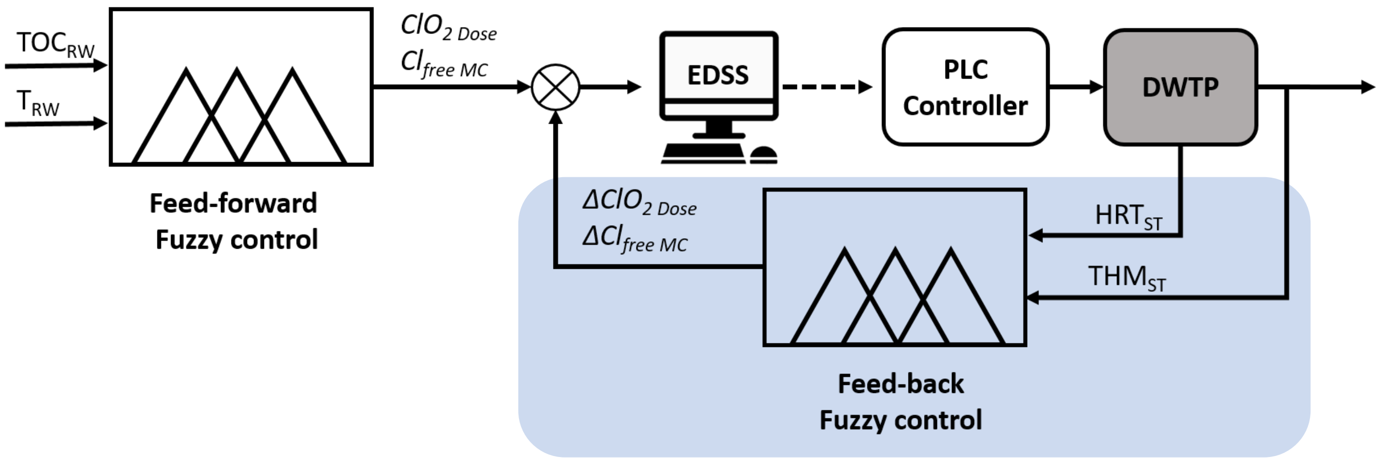
FIS_2

Objective:
Adjust the operational set-points accordig to THMs concentration and operational conditions.

Input variables:
THM_{ST}, HRT_{ST}

Inference System:
(THM_{ST}, HRT_{ST}) → ($\Delta ClO_{2\ Dose}$, ΔCl_{Free})

Controlled variables:
$\Delta ClO_{2\ Dose}$, ΔCl_{Free}



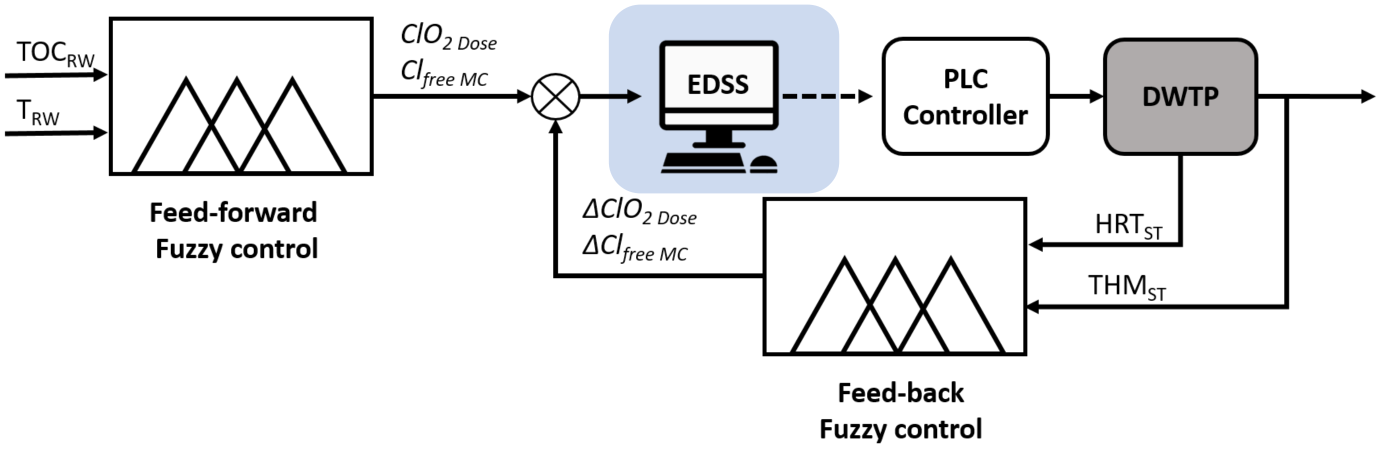
Design of the control system

Supervisor rule

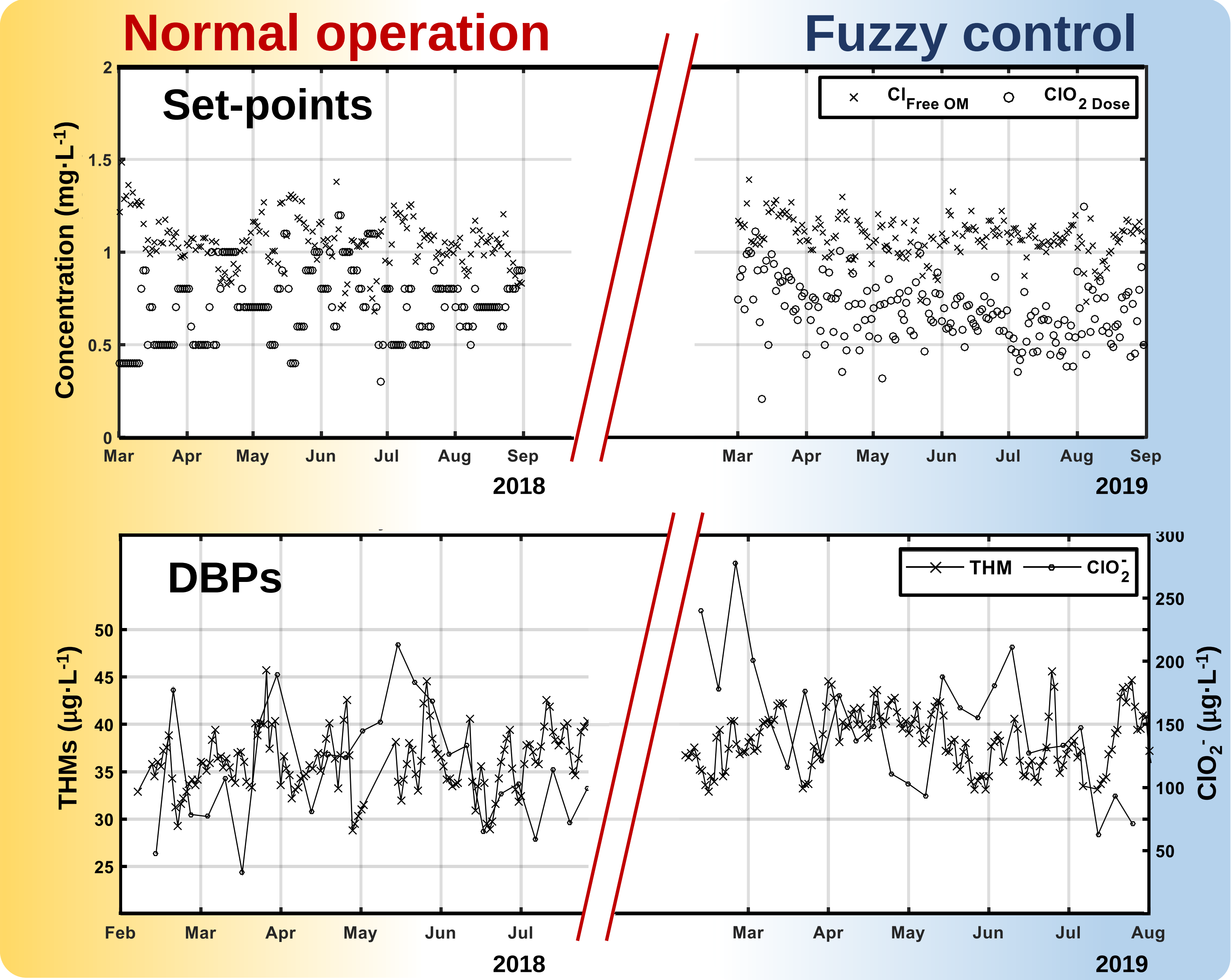
Objective:
To limit the total amount of chemicals to avoid high levels of ClO_2^- and ClO_3^-.

Input variables:
$ClO_{2\ Dose}$, Cl_{Free}

Controlled variables:
$ClO_{2\ Dose}$, Cl_{Free}



Results III. Primary disinfection



Full-scale implementation of fuzzy control system.

Positively Validated 85% of the time.

More systematic dosing of chemicals with the control system.

DBPs without exceeding threshold levels

Keypoints

A feedback and feedforward control system to control primary disinfection.

Process knowledge was modelled with a fuzzy inference system.

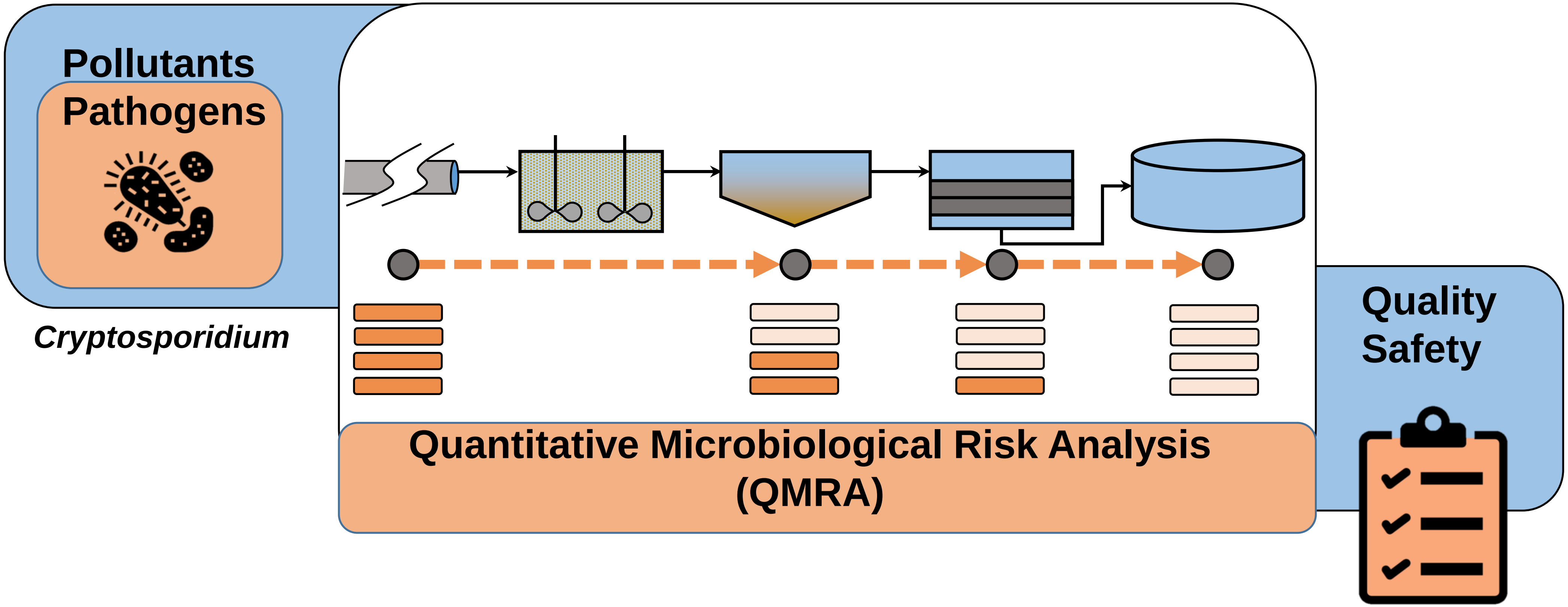
Implementation at full-scale was positively validated 85.5% of the time during 6 months.

DBPs concentration at the effluent at a safe range.

Results IV

Development of a key performance indicator based on quantitative microbial risk assessment

Results IV. QMRA Indicator



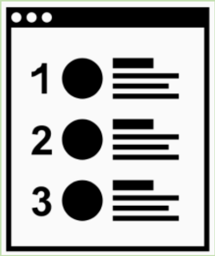
Results IV. QMRA Indicator

QMRA Quantitative Microbiological Risk Assessment

+

Quantification of risk

Used in the design phase



-

Site-specific data

Variabilities and uncertainties

Not applicable for real-time monitoring

QMRA methodology *(Medema et al., 2006; WHO 2009)*

1) **Pathogen load**
2) **Treatment units performance**
3) **Dose-response**
4) **Risk characterisation**

Real-time QMRA indicator

Results IV. QMRA Indicator

Real-time QMRA indicator

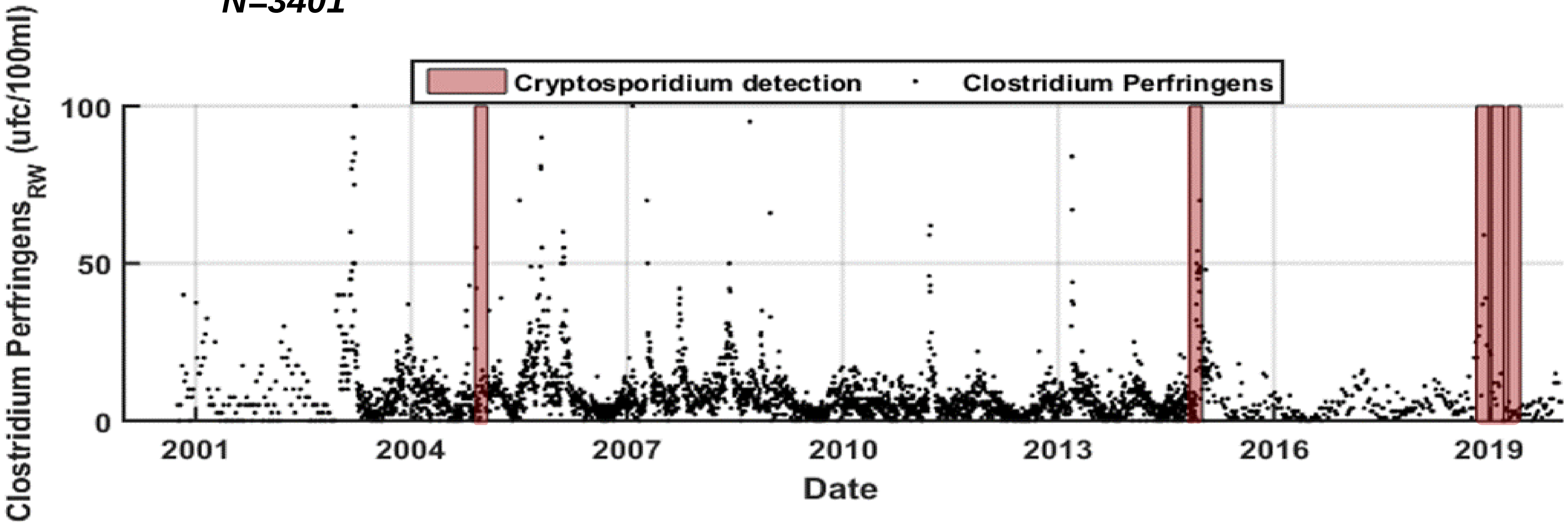
1) Pathogen load | **2) Treatment units performance** | **3) Dose-response** | **4) Risk characterisation**

Can we relate the pathogen load at DWTPs with online-available measures?

Cryptosporidium
N=112

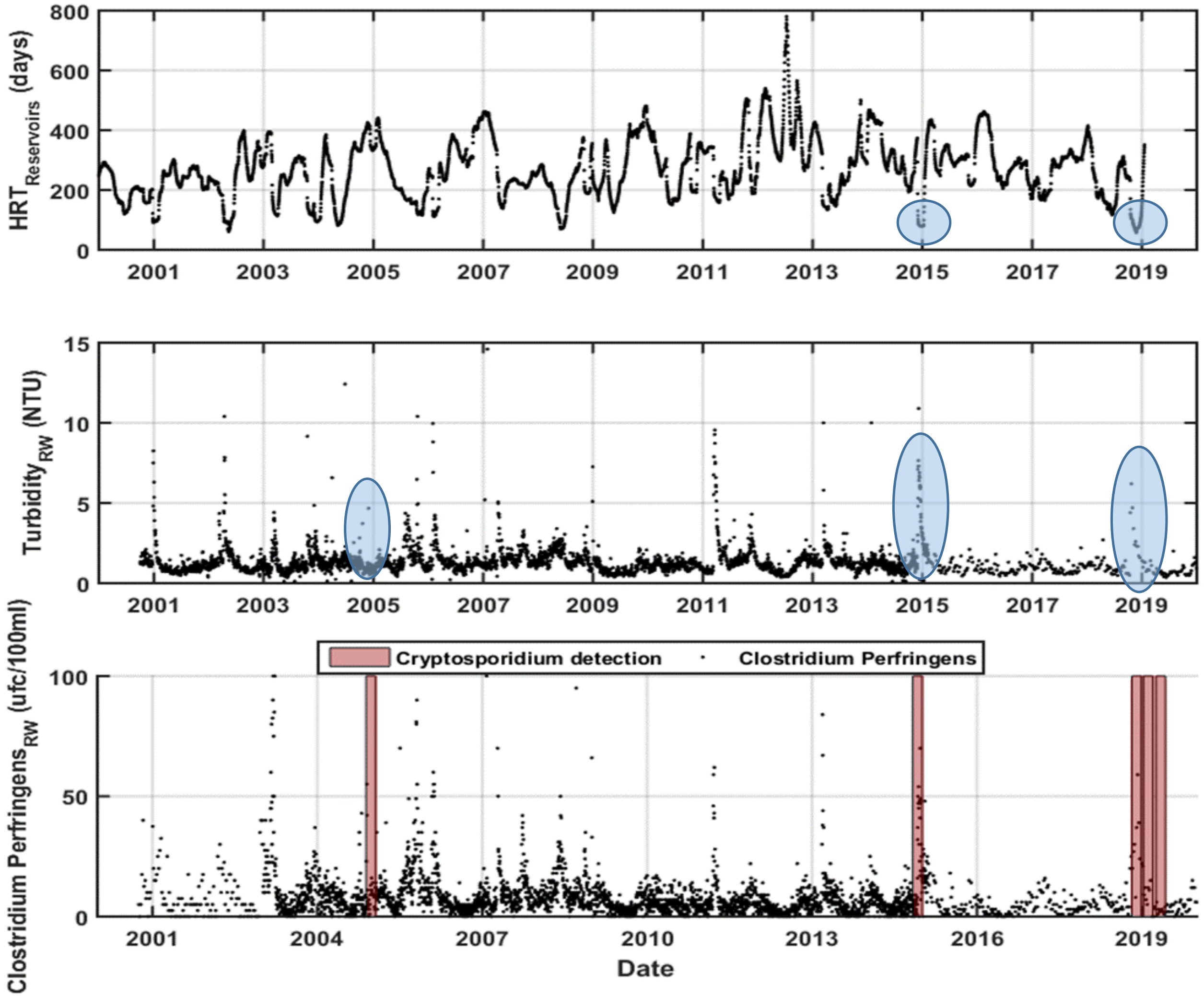
Clostridium perfringens
N=3401

Surrogate measure (Medema et al., 2006)



Real-time QMRA indicator

1) Pathogen load | **2) Treatment units performance** | **3) Dose-response** | **4) Risk characterisation**



Correlation between:

Clostridium perfringens

and
- $Turb_{RW}$ (P value<<0.05)
- HRT_{Res} (P value<<0.05)

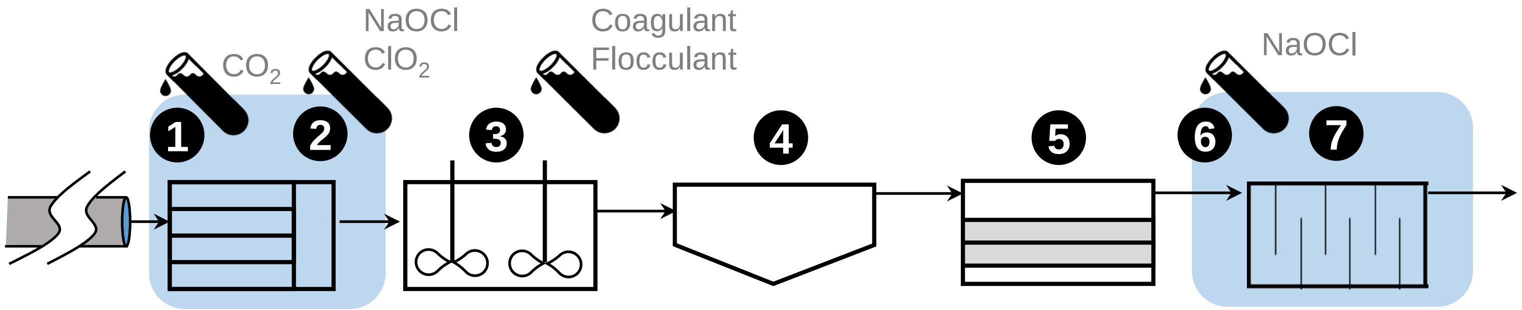
Relationship between online-availbale parameters and pathogen load

Real-time QMRA indicator

1) Pathogen load | **2) Treatment units performance** | 3) Dose-response | 4) Risk characterisation

Can we estimate the treatment units performance with online measures?

Ter DWTP



Chemical inactivation

1. Primary disinfection
2. Secondary disinfection

CSTR model

$$LRV_{Disinfection} = -\log\left(\frac{1}{1 + k_e \cdot c \cdot t_h}\right)$$

Results IV. QMRA Indicator

Real-time QMRA indicator

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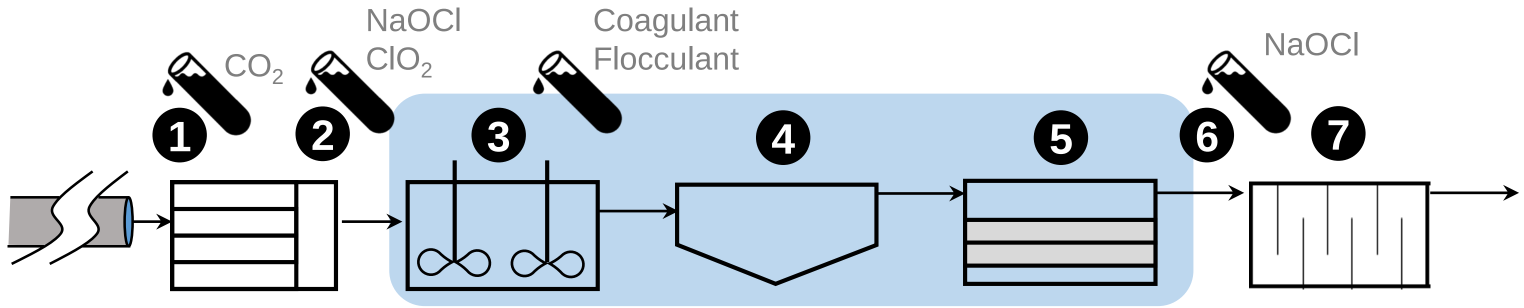


Physical removal

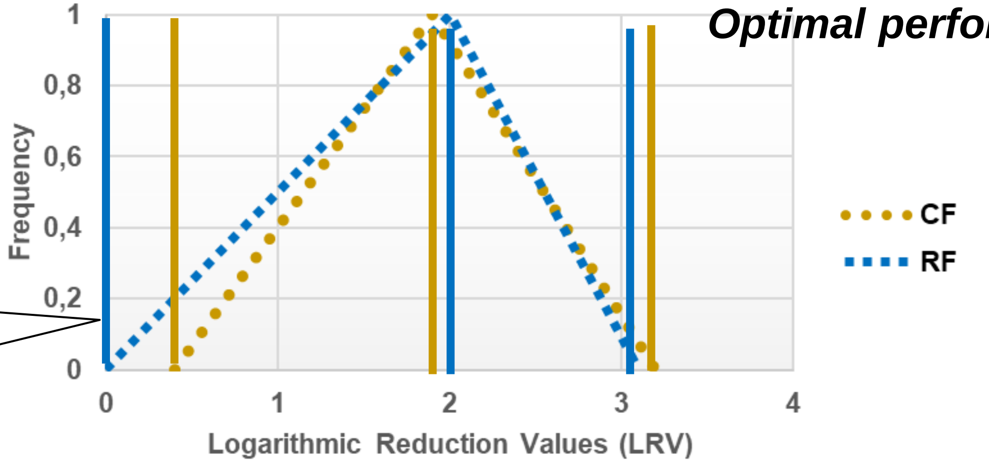
1. Coagulation/focculation (CF)
2. Rapid filtration (RF)

Triangular Distribution fu

(Medema et

Need of online performance indicators I_{CF} and I_{RF}

Min. values: PooMECfomues:Intermediate:performance
Max. values: Optimal performance



Real-time QMRA indicator

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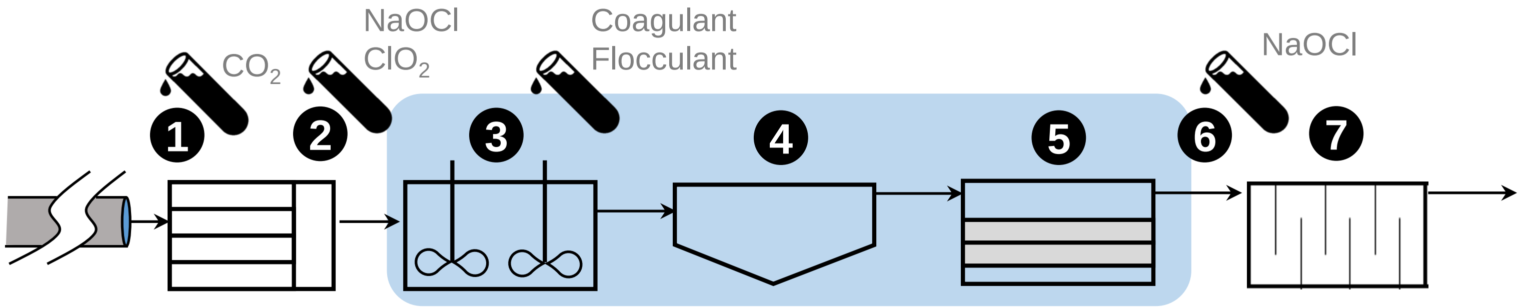


Physical removal

1. **Coagulation/focculation (CF)**
2. **Rapid filtration (RF)**

Triangular Distribution functions

(Medema et al., 2006)

Online performance indicators

I_{CF} (0-1)

Quality parameters

~ Average turbidity ($Turb_{AVG}$)

Operational parameters

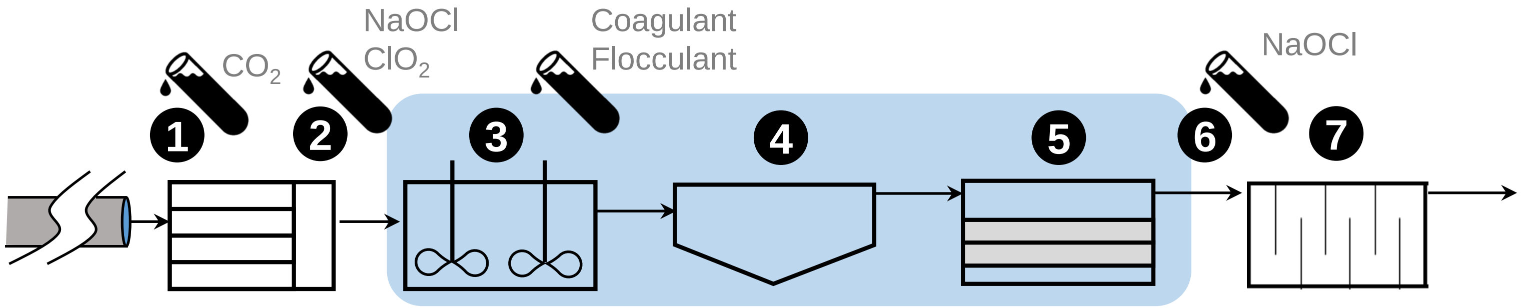
~ Mean sludge age (MSA)

Real-time QMRA indicator

1) Pathogen load | **2) Treatment units performance** | 3) Dose-response | 4) Risk characterisation

Can we estimate the treatment units performance with online measures?

Ter DWTP



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1. Coagulation/focculation (CF)
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Triangular Distribution functions

(Medema et al., 2006)

Online performance indicators

I_{RF} (0-1)

Quality parameters

~ **Average turbidity ($Turb_{AVG}$)**

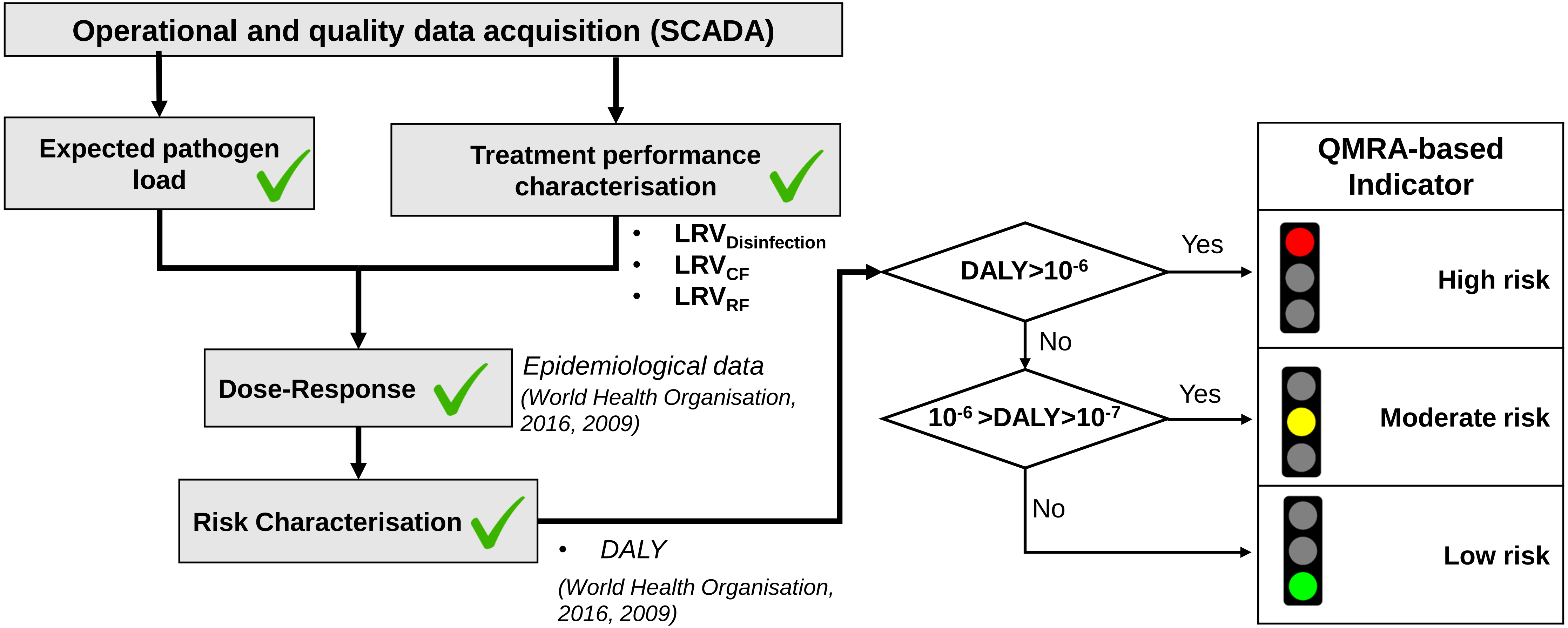
Operational parameters

~ **Mean flow rate (MFR)**

Results IV. QMRA Indicator

Real-time QMRA indicator

1) Pathogen load 2) Treatment units performance 3) Dose-response 4) Risk characterisation



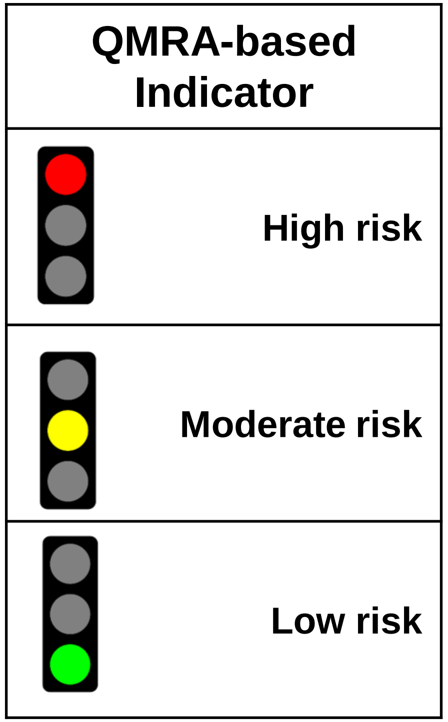
Real-time QMRA indicator

1) Pathogen load 2) Treatment units performance **3) Dose-response 4) Risk characterisation**

Operational and quality data acquisition (SCADA)

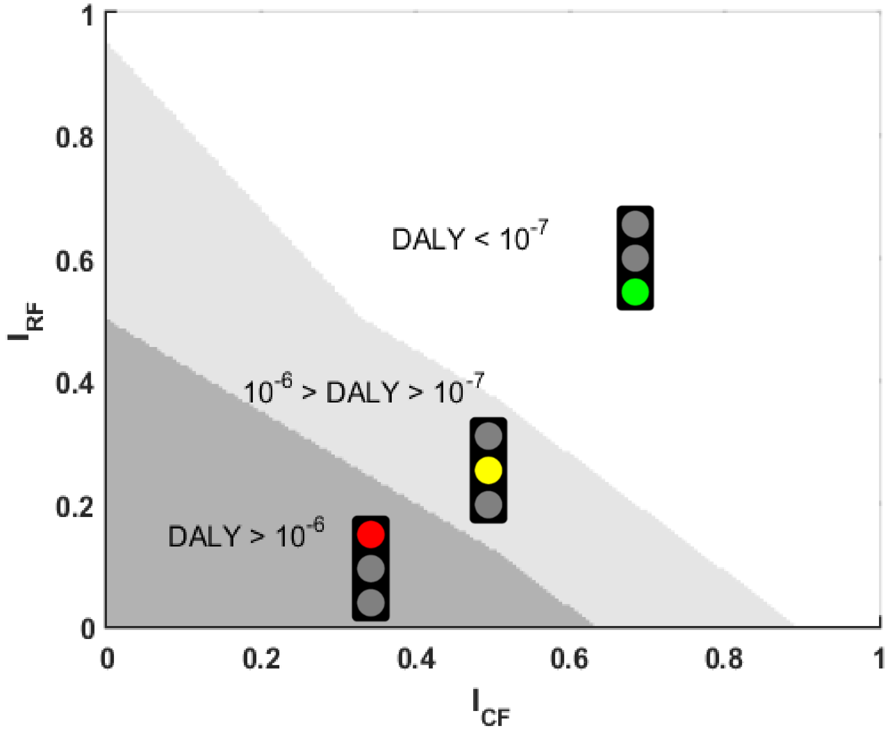
Online surrogates of microorganisms

Development of online treatment performance indicators

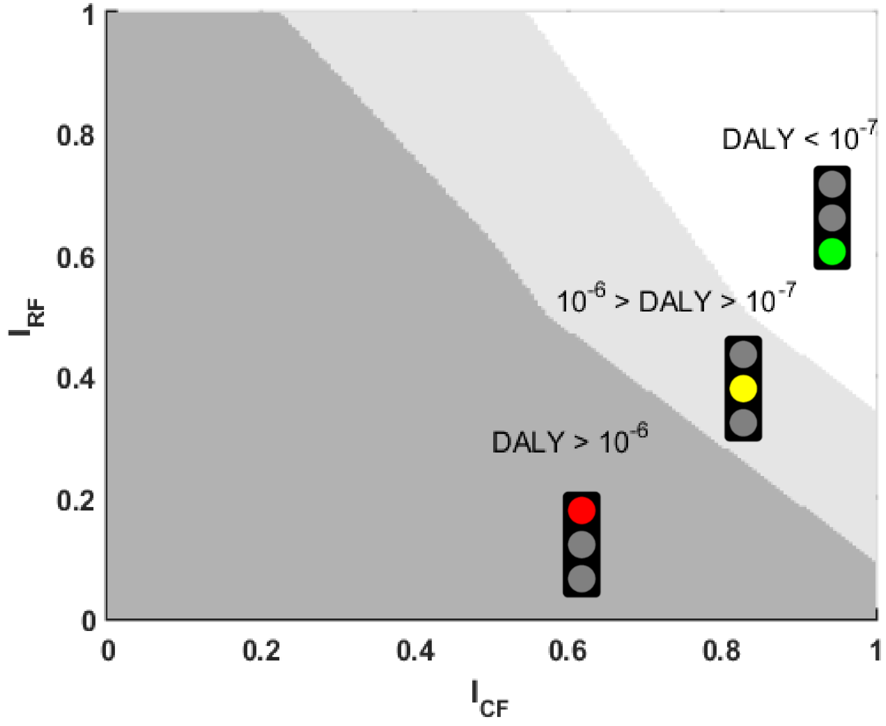


Scenario analysis for Ter DWTP

Crypto $_{RW}$**= 0.2 oocysts·L^{-1}**
(Peak event) ✓



Crypto $_{RW}$**= 0.6 oocysts·L^{-1}**
(WWTP tertiary effluent) ✗



⚠ Additional barrier needed!

⚠ Other pollutants (DBPs, etc.)

Keypoints

- Online QMRA indicators were developed
- Treatment performance characterisation upon process knowledge
- Alert DWTP managers about poor or suboptimal performance
- Scenarios leading to increase the risk can be detected

OUTLINE

1. Introduction
2. Objectives
3. Materials and methods
4. Results
    1. Results I
    2. Results II
    3. Results III
    4. Results IV

5. General discussions

6. General conclusions

General Discussion

Objectives

- **Preoxidation**
- **DBP formation**
- **Microbiological safety**

Case studies

- **Llobregat DWTP**
- **Ter DWTP**

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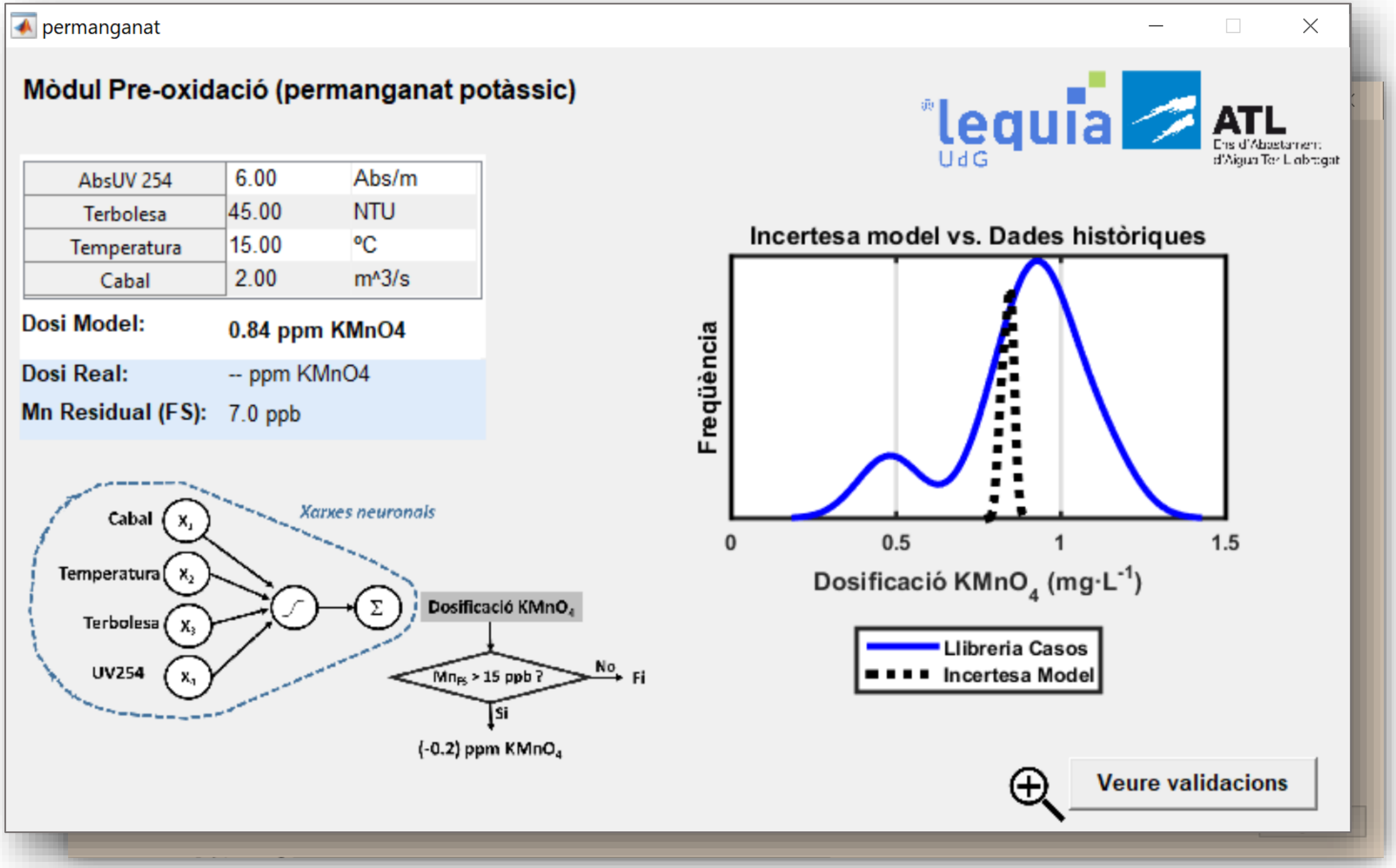

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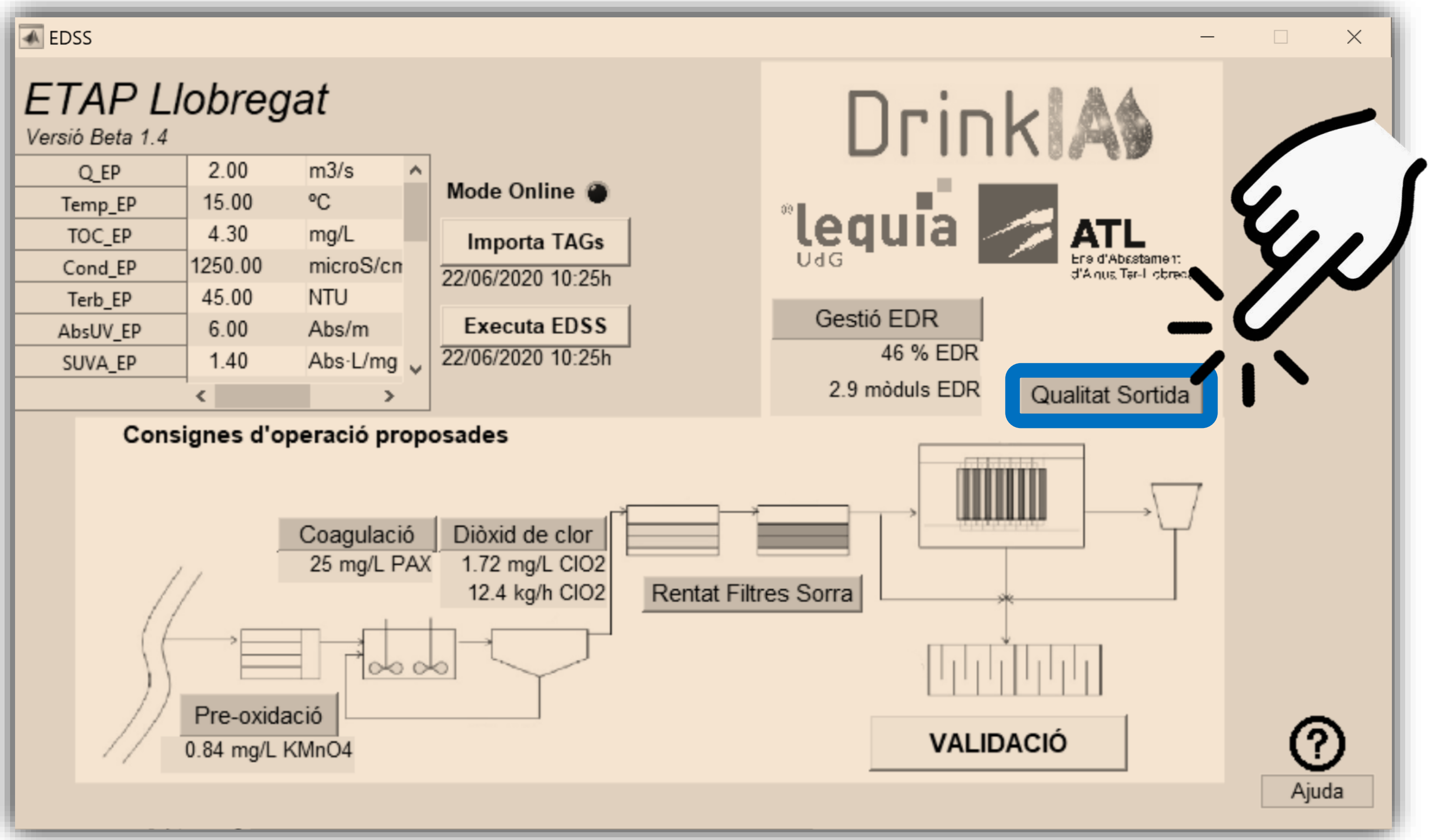

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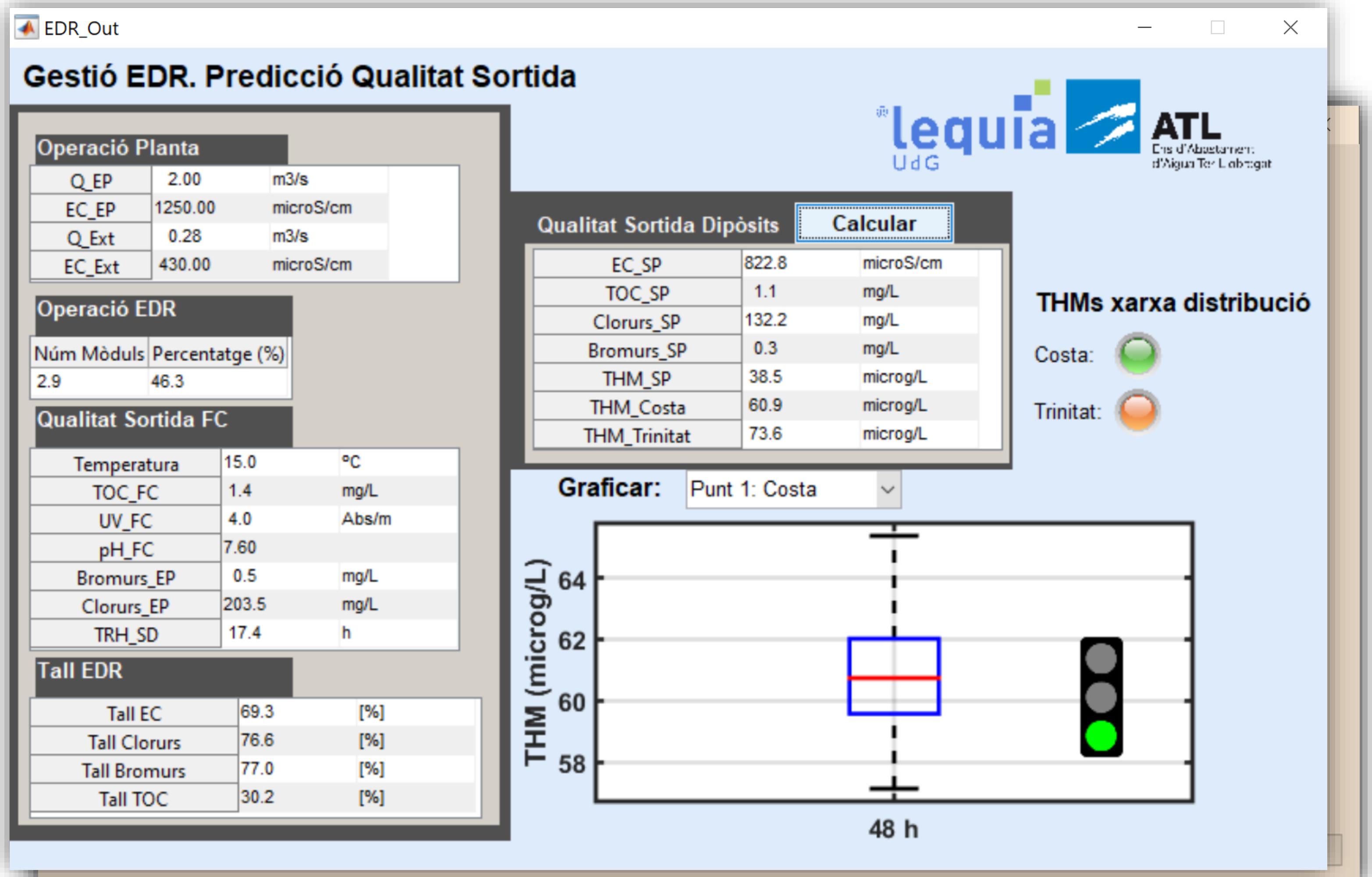

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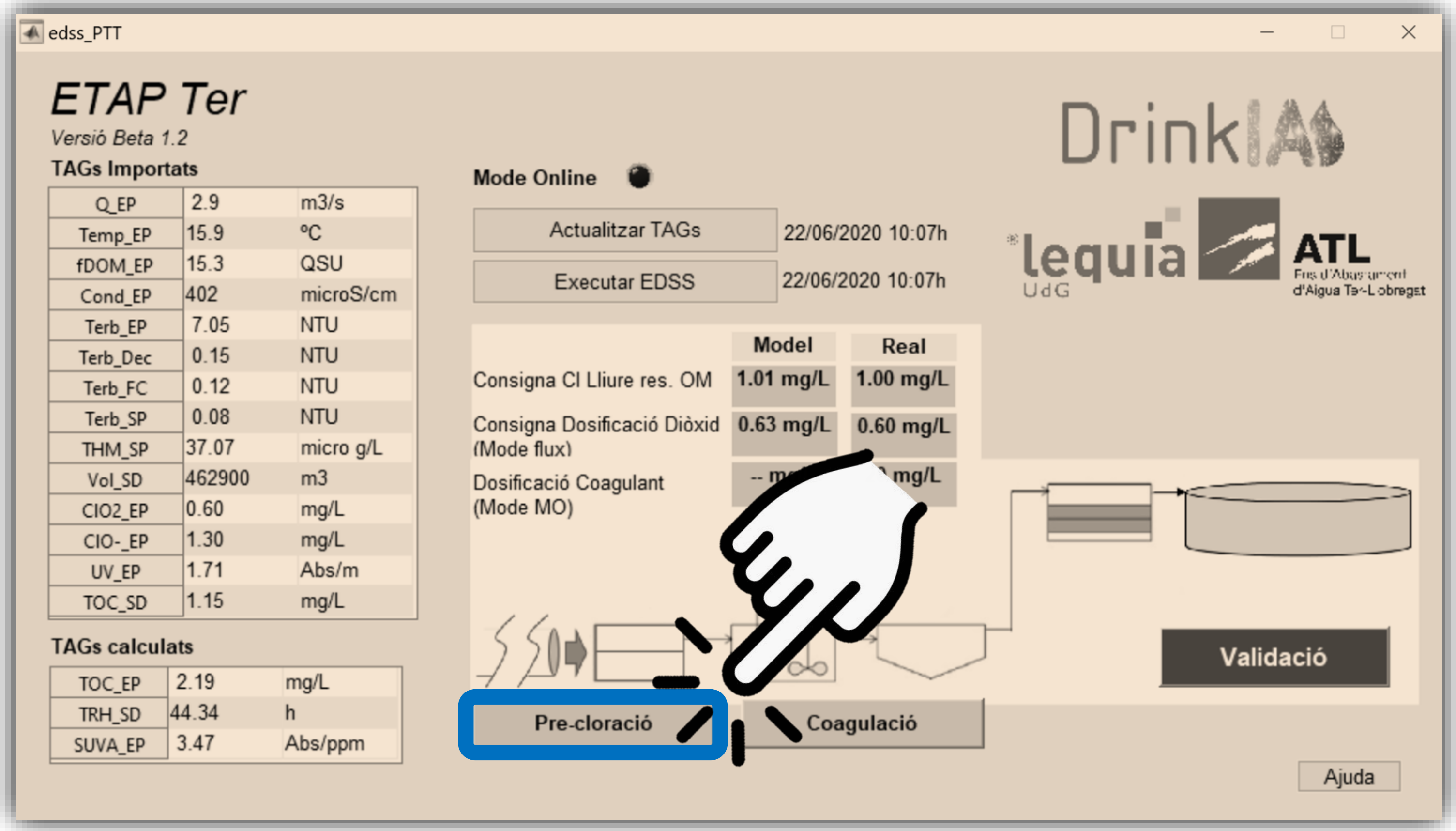

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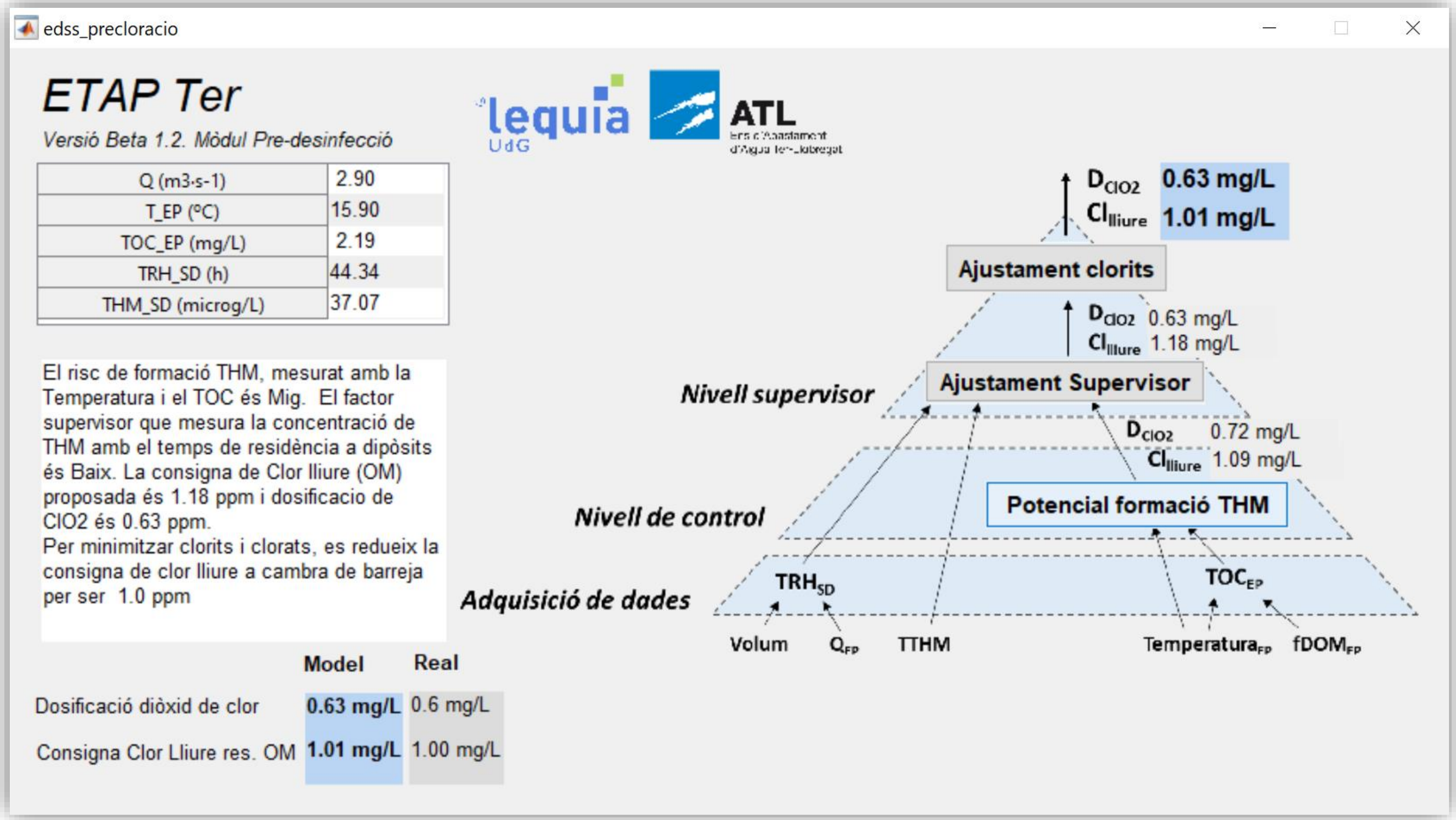

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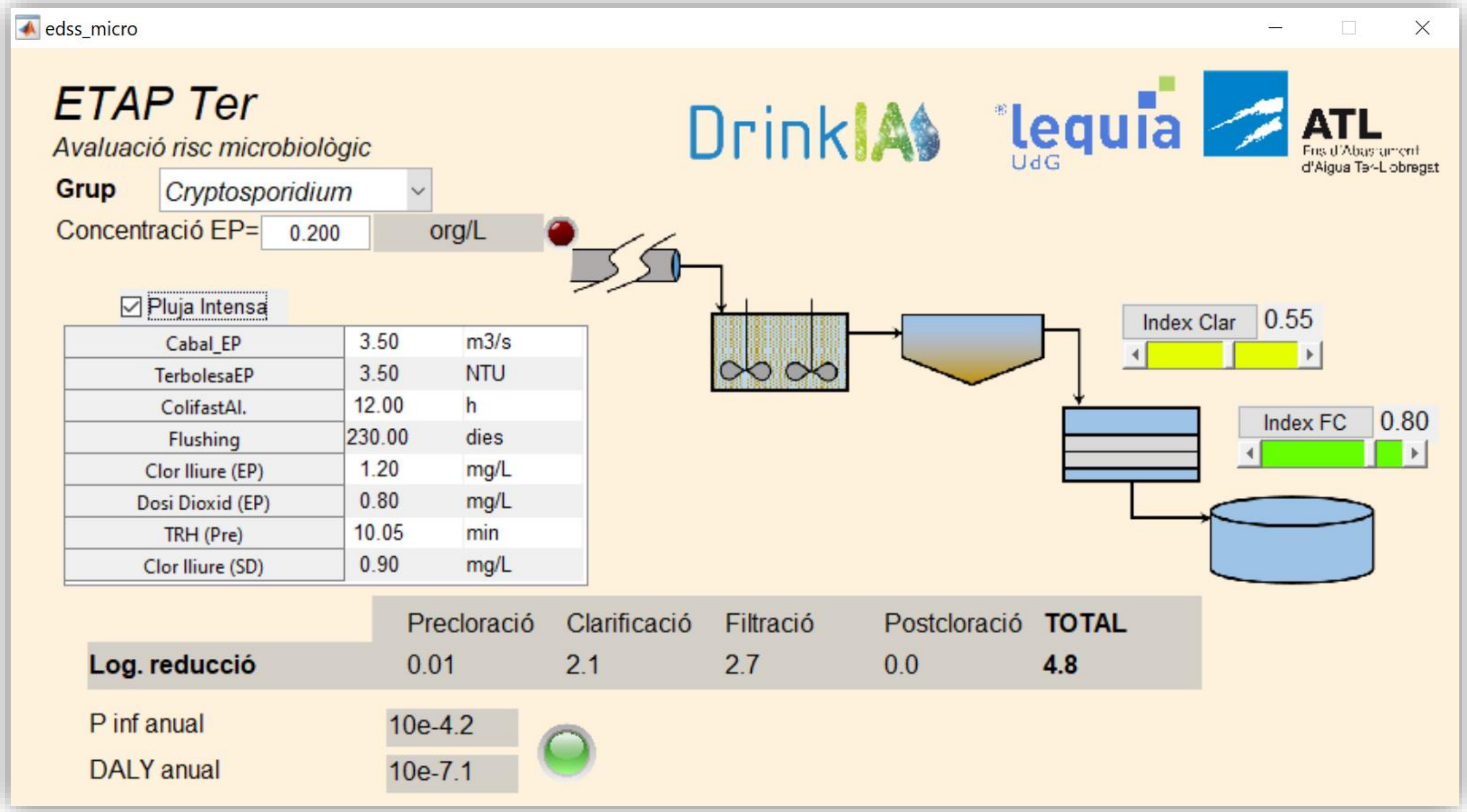

General Discussion

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General conclusions

- New data-driven and knowledge-based mathematical models were developed
- Expert knowledge was codified to systematise decision-making
- Real-time response to raw water variations
- EDSS implemented at full-scale DWTPs
- Application at the control center

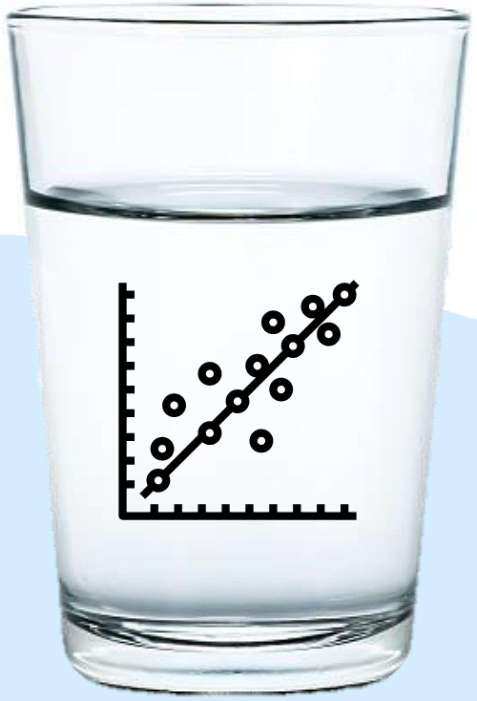
Main limitations

- **Diversity of DWTPs**
- **Limitations inherent to data-driven models**
- **Non-regulated DBPs**

Future work

- **Consolidation of developed tools for managing treatment units**
- **Integrated management of the Distribution network**

General Conclusions



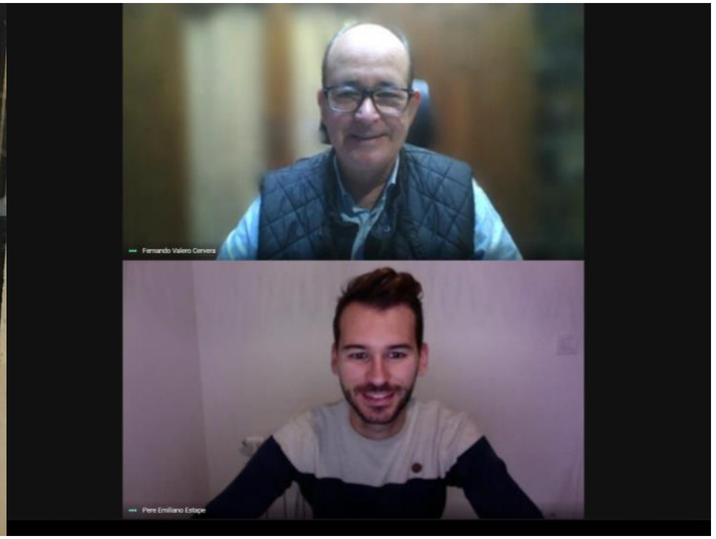
"All models are wrong but some are useful"

George E. P. Box

Acknowledgements

Thanks for your attention!!!

Acknowledgements



Design and implementation of an

Environmental Decision Support System

for the control and management of

Drinking Water Treatment Plants

Doctoral Thesis | 5th November 2020

Lluís Godo Pla

Advisors: Dr. Hèctor Monclús, Dr. Fernando Valero