



D 4 R U N O F F

Data driven implementation of hybrid nature-based solutions for preventing and managing diffuse pollution from urban water runoff

D2.1 Online monitoring systems requirements and specifications

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R=Document, report; **DEM**=Demonstrator, pilot, prototype; **DEC**=website, patent fillings, videos, etc.; **OTHER**=other

PU=Public, **SEN**=Sensitive, limited under the conditions of the GA

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Executive Summary

WP2 is aimed on the development of a set of novel online sensors for the remote measurement of selected target microplastics, metals and CECs in urban runoff waters. Establishing the initial requirements and specifications for this online monitoring system is the first step for WP2. The main aim of this document is understanding the case studies' conditions and environment (WP5) as well as the limitations of the technologies that will be used for the system and how it will interact with the AI-assisted platform (WP4) to describe how the online monitoring system should be at the end of the WP2.

The deliverable reports the initial information collected from the different stakeholders (case studies' and AI-assisted platform responsible, mainly, involving in WP4 and WP5) and a preliminary description of the specifications of the measuring devices included in the monitoring system. A fully detailed specifications' datasheet and user manual will be produced at the end of the WP2 when the online monitoring system is completed and ready to use.

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1 Introduction

1.1 Purpose of the document

This deliverable describes the monitoring platform's initial specifications according to the project needs. At the end of the WP2 execution, further details on the sensors' final characteristics and performance should be provided.

Initially, a survey was conducted to collect information from the specific sites where the measurement device should operate in the last year (WP5). Continuous communication between WP2 and WP5 is needed to establish the optimal specification of the monitoring system according to the cases of study. Moreover, interaction between WP2, WP1 and WP4 is important. WP1 will analyse field samples, feeding WP2 with the occurrence and distribution of the target CECs, microplastics and metals. WP4 is in charge of the development of an AI-assisted platform to enable urban runoff management, and the data generated by WP2 sensors will be sent to this platform. Consequently, the selection of the proper communication protocols between the sensor and the AI platform is one of the key specifications that is addressed in this deliverable.

The initial sensors' specifications have been established, trying to fit as much as possible the site conditions, requirements, and needs to the measuring devices' limitations already identified in this early stage of the project development.

1.1.1 Scope of the document

The initial sensors' specifications have been established, trying to fit as much as possible the site conditions, requirements, and needs to the measuring devices' limitations already identified in this early stage of the project development.

2 Operation conditions based on the results of the surveys

A survey (Annex I) was prepared and distributed to the case studies involved in the WP5. Case studies are located in 1) Odense-Denmark, 2) Santander-Spain, and 3) Pontedera-Italy. In this stage of the project, the nature-based solutions where the monitoring system will be placed are not yet selected. Therefore, the operation conditions are based on the general requirements according to the geographical localization and the nature-based solutions

available in each case of study. Continuous communication between WP2 and WP5 via online meetings and emails is of vital importance to achieve the objective of WP2.

2.1 Environment

- Temperature: Measuring device should be able to operate in a range of ambient temperatures from 0°C to 40°C according to the seasonal variations established by the case studies.
- Vibrations: measuring device contains fiber optics and focusing that could lose alignment under heavy vibrations. Thus, although the system will contain dampeners, it should be used far from strong vibration forces such as heavy machinery, high speed roads, strong pumping stations, etc.
- Rain: the measuring device should be placed, when possible, in a shelter. Even so, open air operation should be possible by adding a protected enclosure.

The measuring device will be packaged in a box/suitcase to prevent temperature, vibration, and humidity interference. Temperature sensors will be included in the measuring devices to correct the data accordingly.

2.2 Reference water physico-chemical parameters

Reference physico-chemical parameters are being registered during the first sampling campaigns of the project taking place in the following months. Historical data, although of interest for comparison, cannot be fully used as the conditions of the surroundings can change (construction works, roads maintenance, etc). The analysis of those parameters will be performed in WP1 using reference analytical techniques and the information will be fed into WP2 to be considered in the measuring device specifications.

At least the following parameters will be taken into account for lab validation: pH, total organic carbon, turbidity, biological oxygen demand, chemical oxygen demand, nitrates/nitrites, total ammonia, and metals.

An analysis of interferences will be carried out later on the project (in WP2) considering the acquired information during the sampling campaigns.

2.3 Data acquisition rates, operation time, and maintenance requirements

The measuring device will perform measurements every 30 minutes during a heavy rain event, taking samples from nature-based solutions (NBS). The minimum data acquisition will be up to 4 measurements during the first 2 hours of the event. When possible, continuous data acquisition will be applied.

The cartridges in the measuring device will last at least 20 measurements. After that time, they will need to be replaced or regenerated. Consequently, operation time and maintenance periodicity will depend on the occurrence of rain events and the desired periodicity of measurements between those.

3 Automated monitoring system for remote detection and quantification of microplastics, metals and CECs: General Specifications

The monitoring platform developed in WP2 will be composed of:

- A measuring device involving a portable Raman system. This system will identify and quantify small microplastics ($\leq 50 \mu\text{m}$) by Raman spectroscopy and triazines (total) and 6PPD-Quinone by Surface-enhanced Raman Scattering. Details of this detection module will be reported on Deliverable 2.3 (confidential).
- A measuring device based on electrochemical sensors for zinc and nickel ions. Details of this detection module will be reported on Deliverable 2.3 (confidential).
- Sample processing modules specific for each type of contaminants and measuring systems. Details of this module will be reported on Deliverable 2.2.
- Control system(s), data analytics, and communication channels for the final user interface. Details of their integration will be reported on Deliverable 2.4.

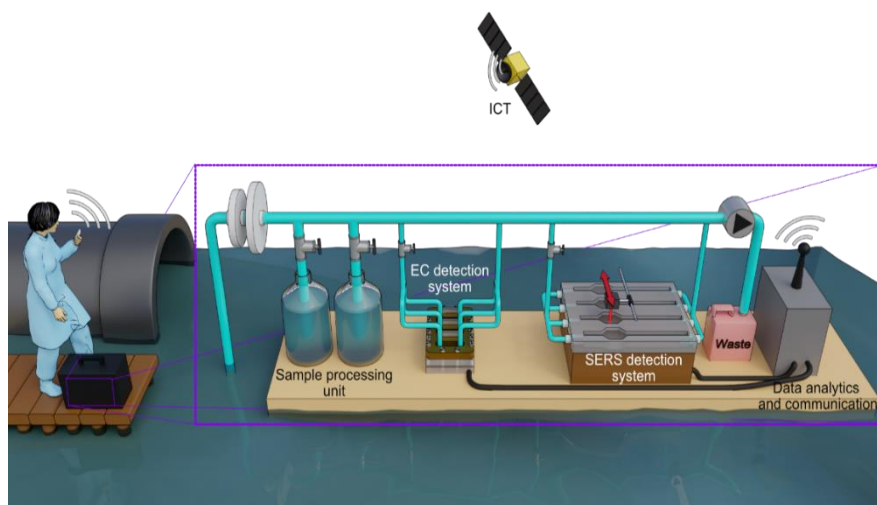


Figure 1 Online monitoring system for CECs scheme.

***Note: The monitoring device is at 4:1 scale compared to the operator to improve the visibility of the components**

The monitoring system will be assembled in a compact format that can be transported by one single operator making possible its relocation (Figure 1). However, the system will require some minimum installation at the place of operation, and calibration afterwards. Thus, despite its portability, it should be used as a monitoring station that can be relocated. This platform will contain the sample preparation and clean-up modules (sample processing unit) needed for each target compound/analyte. This unit will include the sample acquisition system: pumps and tubing that will collect the water sample from the pond or water reservoir and bring it to the measuring devices. According to the initial information provided by the case studies (WP5), measurements are expected in 2 points: inflow and outflow points of the nature-based solutions. Additionally, the distance between these 2 sampling points could be between 100 and 500 meters. The monitoring system should be placed where there is a minimum distance to the sampling points and at equal distance between the 2 collection points, however, the impact of the length of the tubing and the interactions between the tubing and the target analytes will be considered and studied from the beginning. Investigation on the most appropriate materials and tubing cross-sections will be performed to avoid problematics, such as biofilm formation.

Regarding the measuring device based on Raman spectroscopy, a modular Raman system with optical fiber configuration was selected to be integrated in the sensing module. The optical fiber configuration of the Raman probe will allow a better integration with the microfluidic chips fabricated for the detection of small microplastics and CECs (i.e. triazines and 6PPD-Quinone). The wavelength of the laser is 785 nm, which will reduce the auto-fluorescence of some matrix

components. Also, this laser is the optimal for SERS measurements since the optical enhancer selected (i.e. gold nanostars) is in resonance with the wavelength of the laser. The spot size, 100 μm , and the working distance, 7.5 mm, is given for the specification of the Raman probe. A dedicated and optimized pair of linear stages will be developed. One stage with fine Z-movement for the focusing of the Raman spectrometer and another one for the XY-displacement of the Raman probe above the observation microfluidic chambers. The range of displacement (Stroke) of these stages will be dependent on the design of the microfluidic chamber and the working distance of the Raman Probe. As such, all the mechanical design will depend on the features of the microfluidic system. The above-mentioned stages as well as the microfluidics chamber should be mounted on top of an anti-vibration board (for example, Thorlabs - PTT600600). In order to control the above developed linear stages, dedicated electronic control boards will also be developed. These control electronic boards will contain all the required motor control circuitry, power control and communication channels.

Regarding the measuring device based on electrochemical sensors, a pre-calibration system will be included in the sample processing modules to define the optimum analytical range for the measurement of the contaminants, due to the expected large differences between the different case studies. The system will process the collected sample and analyze it afterwards in static conditions.

A temperature sensor will also be included in the electronics module. A USB port will also be integrated to supply power to the stages and to establish the mentioned communication channels between the control electronics and the developed software (user interface).

A computer with the following requirements will be necessary:

- multiple USB3 ports (to dock spectrometer, fluidic components, electrochemical platform, and control boards);
- mobile internet connectivity (4G);
- battery autonomy for at least 2-3 h, supporting all the platform components (for permanent ability to perform measurements upon request a connection to the power grid is required).

A suitcase or enclosure will be purchased to protect all the platform's components (computer, stages, pumps, valves, measuring devices, and electronics) from external weather.

3.1 Detection limits for the different target analytes

The measuring devices should attain detection limits that are fit for purpose. Considering the available quality standards in water and up-to-date literature about the occurrence of our target

CECs, microplastics, and metals in runoff waters, the following detection limits have been established, and the minimum required for:

- Electrochemical (EC) detection of Zn and Ni ions. The first generation of this electrochemical sensor was developed under project NGQC IoRT—Next-Gen Quality Control IoRT System, supported by COMPETE 2020, FEDER. Thus, Table 1 summarizes the initial specifications of this sensor adapted for metal detection in runoff waters.
- SERS detection of triazines and 6PPD-quinone. This sensor's starting TRL is 2. Therefore, the initial requirements are based on the water quality standards and up-to-date literature and are summarized in Table 1. For instance, the maximum concentration to measurement was established taking into account the solubility in water (e.g., the solubility of 6PPD-Q is 67 $\mu\text{g/L}^1$) and the maximum concentration detected in run-off waters (e.g., the concentration of 6PPD-Q varies from 86 ng/L to 20 $\mu\text{g/L}^2$). For triazines, WP1 shared with us the concentration of triazines determined in previous studies in Odense: concentrations are usually between 5-60 ng/L in runoff. In some events, terbutryn reached concentrations above 1000 ng/L.

Response time and measurement frequency in both EC and SERS sensors must be optimized when the full system is operative, involving the sample preparation and detection modules.

Table 1 Initial specifications for detection modules

Target contaminant	Detection type	Measurement Range ($\mu\text{g/L}$)	Accuracy $\mu\text{g/L}$	Resolution $\mu\text{g/L}$	Response time	T _{operation} range	Frequency	LoD $\mu\text{g/L}$
Zn	EC	50-1000 $\mu\text{g/L}$	$\pm 0.1 \mu\text{g/L}$	5 $\mu\text{g/L}$	1' + X' sample processing (TBO) (*)	0-40°C	every 30' (**)	< 10
Ni	EC	5-50 $\mu\text{g/L}$	$\pm 0.1 \mu\text{g/L}$	5 $\mu\text{g/L}$	2' + X' sample processing (TBO) (*)	0-40°C	every 30' (**)	< 10
Triazines (simetryn, terbutryn, metabolites)	SERS	0.1-50 $\mu\text{g/L}$	TBO	TBO	60' + X' sample processing (*)	0-40°C	every 60' (not optimized)	< 1
6PPD-quinone	SERS	0.04-20 $\mu\text{g/L}$	TBO	TBO	60' + X' sample processing (*)	0-40°C	every 60' (not optimized)	< 1

*Response time is the sum of the measurement time plus sample processing.** Measurement frequency indicates the minimum time between measurements.

Raman detection of small microplastics. We will use a microfluidic device developed in the framework of other projects (SbDToolBox NORTE-01-0145-FEDER-000047, supported by Norte Portugal Regional Operational Programme (NORTE 2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF) and H2020 LABPLAS project under grant agreement No. 101003954) with some modification to

adjust it for the detection, the size sorting and concentrating the microplastics (PS, PET, PE, PS and PVC) in the range of 50 – 1 μm found in runoff water.³ Additionally, the initial specifications of this device depend on the selected Raman system and the microplastic properties (i.e., plastic-type, size and shape):

- Measurement range. Depending on the type of plastic. We focus on PE, PP, PET, and PS. Due to the nature of the plastic, the range will be different due to Raman cross-section differences (higher sensitivity for PET and PS; lower for PE and PP). Additionally, size distribution will have an impact on it. The concentration estimation will also be relative to the number of positive spectra (identification of plastic) in the performed map. The measurement range will depend on size/shape. For spherical plastics: a. 50 μm : 1 particle - 200 particles; b. 25 μm : 2 particles - 400 particles; c. 10 μm : 5 - 1000 particles; d. 1 μm : 50 - 10000 particles.
- Accuracy. This will depend on the size/shape of the particle and the spatial step of the mapping (the initial conditions, 100 μm spatial step)
- Resolution. The spot size of the Raman probe is 100 μm . Therefore, the spatial resolution will be close to 100 μm , and consequently, depending on size and shape, the number of particles inside this 100 μm will be different. For instance, for spherical plastics, the resolution will be: 2 particles of 50 μm , 4 of 25 μm , 10 of 10 μm , 20 of 5 μm and 100 of 1 μm
- Measurement frequency. 3.5h [maximum 10 mL to pump at 100 $\mu\text{L}/\text{min}$, total 1 h + mapping (20-30 s per spectrum, minimum 50 spectra per array, step size 100 μm), total 30 min per array, 5 arrays=2.5 h]
- Limit of detection (LoD). Identify microplastics in each size range (50, 25, 10, 5, and 1 μm) and concentration-related into the device by correlating the number of positive spectra (identification of plastic) into the whole map.

These initial requirements for the three systems will be updated in Deliverable 2.3 (detection modules) and Deliverable 2.5 (lab validation).

3.2 Local AI algorithms and pre-processing function

The gathered spectra from the Raman spectrometer will be fed to a pre-processing data algorithm. This algorithm will comprise a set of functions able to filter data, and extract signal features, etc. AI algorithms will also be developed to perform data classification and extract meaningful information from the Raman spectra that will then be stored locally and communicated to the Cloud AI platform.

A Python-based algorithm will also be used for the automated analysis of the response of the electrochemical sensors and for the estimation of the concentration levels of the metals present in the samples. These algorithms will calculate the concentrations of the selected metals, based on the calibration curves obtained during sensor calibration. The raw data will be stored locally, and the final concentration value of the contaminants (metals) will be sent to the Cloud AI platform.

3.3 Software

A dedicated software to control the Raman spectrometer will be developed. This software will also control XZ stage where the spectrometer is mounted. Another interface will be created to control the components of the electrochemical measurement system, which will control the electrochemical readout system. A final interface will control all the fluidic components of the system.

Dedicated pre-processing, AI algorithms and data analytics (described in the previous section) will be developed and integrated into the software as virtual peripherals. Local file storage will also be provided.

Communication sockets will be created in both software interfaces to attend requests from the AI-assisted platform (WP4) located on the cloud. The communication between these nodes will be accomplished using an API exchanging a JSON format.

3.4 Communication protocols with the AI platform (WP4)

The sensing platform will also include the development of communication modules that allow communication within the proposed architectures, enabling process automation and digitalization and remote management of the entire monitoring system.

Due to the large transmission range, a permanent connection (socket) to the cloud (AI-assisted platform; WP4) will be used for communications, using a mobile (4G) connection. The IoT platform (based on FlyThings) developed by the Galicia Institute of Technology in the D4RUNOFF project is fully described in the WP4 documentation.

Flythings allows the processing of different types of information such as numerical, textual, boolean, geographical, spectral and even images. For the injection of data in the platform,

Flythings offers different types of messages where we can highlight a proprietary Rest-JSON API, the most used communication protocol on the Internet of Things (MQTT), industry standards such as ModBus or OPC-UA, different connectors for ETL (Extract, Transform, Load) and a API REST.

Table 2 Formats accepted by the platform.

Type	Data format
Industry	<ul style="list-style-type: none"> • OPC-UA, Modbus, Bac-net, Mbus
Energy	<ul style="list-style-type: none"> • OpenDomo, Sennet, XeoEnergy
BI y Machine Learning	<ul style="list-style-type: none"> • Birt, TensorFlow, R,
Standards	<ul style="list-style-type: none"> • SOS,
Message Formats	<ul style="list-style-type: none"> • json, csv, xml
Protocols	<ul style="list-style-type: none"> • http, mqtt, ftp, tcp
Calculation Engines	<ul style="list-style-type: none"> • Octave, Matlab, R
Programming Languages	<ul style="list-style-type: none"> • Python, Arduino, Java, JavaScript

Flythings also allows remote actuation or support over remote devices, including on-off standby, trigger setting, or even firmware update. Based on weather data, the possibility of actuating the sensing platforms to trigger the measurements when a rain event starts is being explored.

The modules allow bi-directional communication and distribute messages between devices and the cloud.

4 Conclusions

Herein, we describe the initial specifications of the monitoring platform being developed in WP2. These specifications were established considering the conditions of the case study sites involved in WP5, where the monitoring platform will operate, the measurement requirements and needs, and the sensor's characteristics and analytical performance. Herein, the communication protocols requested by the AI-assisted platform being developed in WP4 were also specified. After the integration and testing of the sub-systems and lab validations are completed (M30), this deliverable will be revised, and the requirements will be updated. It is important to remark that at the time of the collection of the information from the case studies the location of the online monitoring system has not been completely decided and is still in discussion.

5 References

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6 Acronyms

CEC – Contaminant of emerging concern

SERS – Surface-enhanced Raman Scattering

6PPD-Q – 6PPD-quinone

PP – Polypropylene

PE – Polyethylene

PET – Polyethylene terephthalate

PS – Polystyrene

PVC – Polyvinyl chloride

7 Annex A: SURVEY

SPECIFICATIONS OF MEASURING DEVICES

1. The measurement devices can be designed to be portable, in which case the operator will move them from one spot to another and will be responsible for triggering the measurement. Or to be installed in one single location and operate automatically. Which kind of system would you prefer?
2. Taking into account that the measuring device is expected to require intervention every 20 measurements, how often would consider necessary to get measurements:
 - a. During a heavy rainfall/storm event:
 - Every 30 min
 - Every 1h
 - Other:
 - b. Without heavy rainfall/storm event:
 - 1 day (accumulated water)
 - 1 week (accumulated water)
 - 2 weeks (accumulated water)
 - 1 month (accumulated water)
3. Add any other consideration that you deem necessary

SURVEY CASE STUDIES CONDITIONS RELEVANT FOR MEASURING DEVICES

1. Does your case study, in the localization where the measuring devices will be operating, have:
 - Internet connectivity
 - Electrical power
 - Isolation from the external environmental conditions (booth or cabin)
 - Stability of the ground (vibrations?)
2. Which are the ranges of environmental conditions in your case study?
 - Ambient temperature (differentiating between seasons)
 - Rainfall
 - Solar radiation
 - Distance between inflow and outflow
3. Which are the known water quality parameters expected?
 - pH
 - TOC
 - Turbidity
 - BOD
 - COD



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- Nitrates/nitrites
 - Total ammonia
 - Metals
 - Etc
4. Which is the availability of dedicated staff for device operation or maintenance?
- Frequency: daily, weekly, bi-weekly, monthly
 - Maximum time available

8 Annex B: Replies to the survey collected

SURVEY 1

AQUALIA. PARQUE DE LAS LLAMAS: URBAN WETLAND + POND IN SANTANDER.

SPECIFICATIONS OF MEASURING DEVICES

1. The measurement devices can be designed to be portable, in which case the operator will move them from one spot to another and will be responsible for triggering the measurement. Or to be installed in one single location and operate automatically. Which kind of system would you prefer?

As the surface of the site is large, it would be interesting a portable device that we can install in different locations during different periods of time. Ideally, the triggering of the measurement will be automatic, using level indicator, data from meteorological stations (rain), conductivity sensors, or something similar.

2. Taking into account that the measuring device is expected to require intervention every 20 measurements, how often would consider necessary to get measurements:
 - a. During a heavy rainfall/storm event:
 - Every 30 min X
 - Every 1h
 - Other:
 - b. Without heavy rainfall/storm event:
 - 1 day (accumulated water) X
 - 1 week (accumulated water) X
 - 2 weeks (accumulated water)
 - 1 month (accumulated water)Daily or weekly. Not completely decided.
3. Add any other consideration that you deem necessary

SURVEY CASE STUDIES CONDITIONS RELEVANT FOR MEASURING DEVICES

1. Does your case study, in the localization where the measuring devices will be operating, have:
 - Internet connectivity. Yes, using 3G SIM card.

- Electrical power. Depending on the location. In the pumping station and probably in the parking is possible to have electrical power. In the inflow or outflow of wetland probably no electrical power.
- Isolation from the external environmental conditions (booth or cabin). NO
- Stability of the ground (vibrations?). Depending on the location. Vibrations in the parking and in the pumping station.

2. Which are the ranges of environmental conditions in your case study?

Data from Santander Airport. Data collected from <https://es.weatherspark.com/>.

- Ambient temperature (differentiating between seasons).

Average daily temperature in Santander per month (2017-2022).

Average daily temperature	Jan	Feb	Mar	Apr	May	Jun	Jul	Ago	Sep	Oct	Nov	Dec
Maximum	13	13	14	16	18	21	22	23	22	20	17	14
Mean	10	10	11	12	15	17	19	20	18	16	13	11
Minimum	6	6	7	8	11	13	15	16	14	12	9	7

- Rainfall

	Jan	Feb	Mar	Apr	May	Jun	Jul	Ago	Sep	Oct	Nov	Dec
Number of days with rain	10,5	8,5	8,4	9,0	7,0	4,6	3,2	3,7	5,9	8,9	10,7	10,3
mm of rain	73,8	70,1	58,8	64,2	44,7	32,9	17,7	21,6	41,2	68,1	89,7	75,4

- Solar radiation. Average daily incident shortwave solar energy.

Solar energy	Jan	Feb	Mar	Apr	May	Jun	Jul	Ago	Sep	Oct	Nov	Dec
kWh	1.7	2.6	3.9	5.1	6.2	7.0	7.2	6.2	4.7	3.1	1.9	1.5

- Distance between inflow and outflow. More than 300 m

3. Which are the known water quality parameters expected?

- pH
- TOC
- Turbidity
- BOD
- COD
- Nitrates/nitrites
- Total ammonia
- Metals
- Etc

All these parameters can be measured in lab. Probably pH, Turbidity and Ammonia will be measured with online sensors.

4. Which is the availability of dedicated staff for device operation or maintenance?
 - Frequency: daily, weekly, bi-weekly, monthly
 - Maximum time available

Ideally, 1 h per month. 1 h each 15 days possible.

Parque de las Llamas: Urban Wetland + Pond

Phase 1 (11 Ha): 30 M €

Future phase 2: 50 M€



Parking
Draining Pavement



WW pumping station
Below Wetland
(Design up to 300 L/s)



San Roman
WWTP
430,000 IE

SURVEY 2

PONTEDERA (ITALY)

SPECIFICATIONS OF MEASURING DEVICES

4. The measurement devices can be designed to be portable, in which case the operator will move them from one spot to another and will be responsible for triggering the measurement. Or to be installed in one single location and operate automatically. Which kind of system would you prefer?
It would be preferable installed in one location

5. Taking into account that the measuring device is expected to require intervention every 20 measurements, how often would consider necessary to get measurements:
 - c. During a heavy rainfall/storm event:
 - Every 30 min
 - Every 1h
 - Other: **15 min**

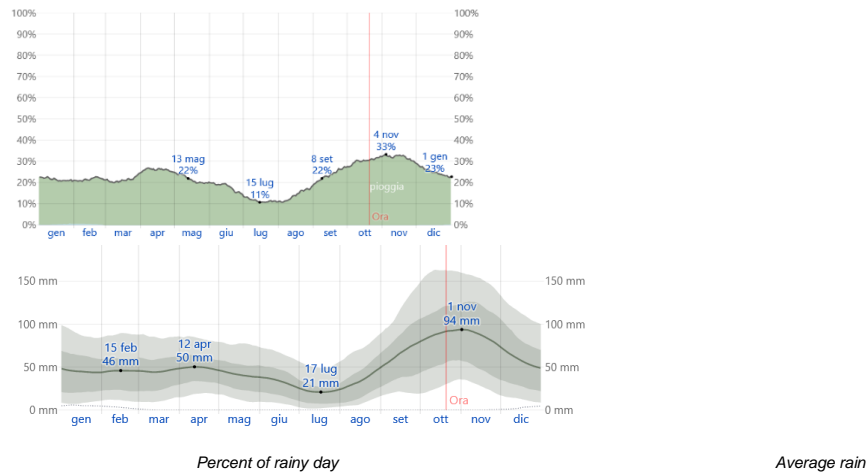
 - d. Without heavy rainfall/storm event:
 - 1 day (accumulated water)
 - 1 week (accumulated water)
 - 2 weeks (accumulated water)
 - 1 month (accumulated water)
 - **Other every 6-8 hours, this because the outflow during a day is not always the same**

6. Add any other consideration that you deem necessary

SURVEY CASE STUDIES CONDITIONS RELEVANT FOR MEASURING DEVICES

5. Does your case study, in the localization where the measuring devices will be operating, have:
 - Internet connectivity **Yes**
 - Electrical power **Yes**
 - Isolation from the external environmental conditions (booth or cabin) **Yes**
 - Stability of the ground (vibrations?) – **vibration for what? Like traffic?**

6. Which are the ranges of environmental conditions in your case study?
 - Ambient temperature (differentiating between seasons) **Winter min=2°C,Max=10°C, Summer min=18°C,Max=31°C**
 - Rainfall **October is the most rainy month with average h=90mm, July is the less rainy with an average of 21 mm**



- Solar radiation
- Distance between inflow and outflow -

7. Which are the known water quality parameters expected?

- **pH X**
- **TOC X**
- Turbidity
- BOD
- COD
- Nitrates/nitrites
- **Total ammonia X**
- Metals
- **Etc (conduibility) X**

8. Which is the availability of dedicated staff for device operation or maintenance?

- Frequency: daily, **weekly**, bi-weekly, monthly
- Maximum time available