



Conceptual Design support  
tool for adaptable Drinking  
Water Treatment Plants

Deliverable 6.1

WP6 Design-support tool for  
flexible, small-scale drinking  
water treatment plants



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## Abbreviations

### *General*

EU	-	European Union
DWTP		Drinking Water Treatment Plant
DST	-	Design Support Tool
Lpppd	-	Litres per person per day
WP	-	Work Package

### *Water quality, treatment processes and technologies*

AIEX	-	Anion Ion Exchange
CIEX	-	Cation Ion Exchange
DBPs	-	Disinfection by-products
DAF		Dissolved Air Flotation
GAC	-	Granular activated carbon
IEX	-	Ion exchange (process)
LP-UV		Light Pressure Ultra Violet
NOM	-	Natural Organic Matter
NF	-	Nanofiltration
MF	-	Microfiltration
MP-UV		Medium Pressure Ultraviolet
OMP	-	Organic micropollutants
PAC	-	Powdered activated carbon
RO	-	Reverse Osmosis
UF	-	Ultrafiltration
WQ		Water Quality

### *Database and software architecture*

ERD	-	entity relationship diagram
FK	-	foreign key
PK	-	primary key
REST	-	<b>RE</b> presentational <b>S</b> tate <b>T</b> ransfer

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## Executive summary

The present document is the Deliverable 6.1 from Work Package 6 (WP6) of the ToDrinQ project. This Deliverable is an output of the work carried out in Tasks T6.1, T6.2 and T6.3, from the start of the project, until M24. Tasks 6.1 and 6.2 have been completed. Task 6.3 is ongoing.

The ToDrinQ project is an EU funded project with an overall objective to support the implementation of the revised Drinking Water Directive by enhancing the scientific and technical knowledge on drinking water quality protection and treatment. The aim of Work Package 6 is to develop a Design-Support Tool (DST) for flexible, small-scale water treatment plants by identifying the different required treatment technologies and corresponding trains, the key factors for designing a drinking water treatment plant and the key design goals.

The DST follows an automated procedure for the identification of the treatment technologies and trains related to the source of the water (groundwater, surface water, river-bank water). The user has the option to select from a range of technologies stored in the DST based on the source water type and the quality of the source water. Additional uncertainty parameters for each technology are quantified, these are the complexity, the robustness, the flexibility and the environmental impact and a final score is provided to the user. The DST also calculates four additional parameters, the efficiency, the footprint, the head losses and the total costs. Thus, the user gets a full information regarding the treatment train that has been selected and has also the option to change the train based on their parameters' importance. The current version of the tool is developed in Python and the upcoming version will be a Django web application. A presentation of the current, proof-of-concept, version of the DST could be found in the following link:

<https://youtu.be/PtWiVbBbQWo?si=ZP-2nUA9B5KN26Fw>

The next version of this Deliverable (D6.2) is due for M36.

## 1. Introduction

### 1.1. *The ToDrinQ project*

The ToDrinQ project is an EU funded project with an overall objective to support the implementation of the revised Drinking Water Directive and to significantly enhance the scientific and technical knowledge on drinking water quality protection, monitoring and treatment by developing and testing a compendium of modular complementary innovations (hereafter termed the 'ToDrinQ Toolkit'), including novel real time sensing and water quality parameters technologies, innovative treatment processes (especially suitable for modular, adaptable treatment plants) and interoperable, easy to deploy decision tools that support resilient, evidence-based treatment plant design and improved overall water system operational awareness and risk-based response. The ToDrinQ Toolkit aspires to increase the resilience of drinking water systems in terms of both increased robustness (against short term stresses) and adaptability (against longer term uncertainties) and ensure high-quality drinking water, minimising micro-pollutants, pathogenic micro-organisms and disinfection by-products (DBPs).

### 1.2. *Objectives for Design-support tool for flexible, small-scale drinking water treatment plants*

The present document is part of Work package 6 of the ToDrinQ project, named **Design Support Tool (DST) for flexible, small-scale drinking water treatment plants**. It reports on activities carried out in Task 6.1 (Finished), Task 6.2 (Finished) and Task 6.3 (ongoing).

The aim of WP6 is to provide a design-support tool for flexible/adaptable drinking water treatment plants (DWTPs). The tool will generate and evaluate (in terms of costs, environmental impact and resilience) alternative treatment trains for a variation of drinking water sources, including the effect of water quality variability, to meet high water quality standards.

The specific objectives are:

- To identify and characterize treatment technologies and treatment trains applicable for DWTPs;
- To define key uncertainties and goals to be considered when designing DWTPs;
- To develop a tool that can identify optimal design alternatives making DWTPs more flexible.

The Work package basically consist of four tasks:

1. Identification of key characteristics of drinking water treatment technologies and their corresponding treatment trains
2. Identification of key factors and their uncertainty for designing DWTPs
3. Identification of key design goals
4. Development of the design-support tool

In the present document, results of the first three tasks are addressed, as well as a first draft software architecture for the design support tool. The work is still ongoing and the next version of this deliverable will be submitted in M36 (Deliverable 6.2).

## 2. Identification of key characteristics of drinking water treatment technologies and their corresponding treatment trains

Drinking water treatment technologies are usually placed in a treatment train to transform source water into drinking water. The used sources are usually fresh (aerobic/anoxic/anaerobic) groundwater or surface water (from rivers and lakes), or a combination of both, being riverbank filtration or managed aquifer recharge, respectively.

In this report, we do not consider seawater or brackish groundwater as a source for drinking water, being beyond the scope of the ToDrinQ project. In addition, we mainly focus on state-of-the-art/proven technologies for drinking water treatment, not considering treatment of residues (such as backwash water).

For each treatment stage, different key treatment technologies were selected and their treatment efficiency for the removal of specific water quality contaminants were identified (by TUD) and saved in a database (developed by KWR). The conceptual design supporting tool follows an automated procedure to generate treatment trains based on the water source and the concentrations of key different drinking water parameters, such as heavy metals, turbidity, pathogens, natural organic matter (NOM),. The final version of the supporting tool will provide, for every selected treatment train, an overall evaluation based on all the aforementioned criteria and an evaluation for each unique criterium separately. Thus, the supporting tool will aid decision makers in their final decision regarding the selection of the most appropriate water treatment approach based on the water quality requirements, the available space for the plant and the cost estimations.

### 2.1. Groundwater characteristics and treatment trains

Groundwater can be characterised as aerobic, anoxic and anaerobic. The characteristics of well-protected groundwater are described below. A typical treatment train for a groundwater source is presented in Figure 1. When groundwater has not been well-protected additional (organic) contaminants, such as pesticides, herbicides and industrial persistent pollutants can be infiltrated. In this case, well-management and/or additional treatment steps have to be added to remove these contaminants. However, this is not in the scope of the ToDrinQ project.

Well protected **aerobic groundwater** will have (a low concentration of) oxygen and can have a relatively low pH. Sometimes the alkalinity of the water is also low. The rest of the parameters are usually within the drinking water standards. Therefore, this type of source water only (optionally) requires a **remineralisation/conditioning** step for addition of bicarbonate (through dosing or marble/limestone filtration) and/or an **aeration step** (by spraying, cascades, or a like) to add oxygen.

Well protected **anoxic groundwater** will not contain oxygen, but can contain iron, manganese, ammonium and/or hydrogen sulphide, due to reduction processes, frequently at a low pH. Sometimes, depending on the composition of the underground, hardness can be high, but the rest of the parameters are usually within the drinking water standards. Therefore, treatment will minimally consist of an **aeration** step, for addition of oxygen and stripping of carbon dioxide and hydrogen sulphide (by spraying, cascades, stripping towers, or alike) and a (sub-merged) **rapid filtration** step (single or dual media) to remove iron, manganese and ammonium (biologically). In specific cases where the hardness, the arsenic

concentration, natural organic matter content, nitrate concentration and/or the fluoride concentration are too high, specific measures must be taken (WHO,2017).

Well protected **anaerobic groundwater** will not contain oxygen, but can contain (high concentrations of) iron, manganese, ammonium, hydrogen sulphide and/or methane, due to reduction processes, frequently at a low pH. Sometimes, depending on the composition of the underground, hardness can be high, but the rest of the parameters are usually within the drinking water standards. Therefore, treatment will minimally consist of an **aeration step**, for addition of oxygen and stripping of carbon dioxide, hydrogen sulphide and methane (by spraying, cascades, stripping towers, or alike) and a **double filtration** step, being trickling filtration and (sub-merged) rapid filtration step (single or dual media) to remove iron, manganese and ammonium (biologically). In specific cases where the hardness, the arsenic concentration, natural organic matter content, nitrate concentration and/or the fluoride concentration are too high, specific measures must be taken.

In several countries in the Europe, the distribution system is such (due to leakages, pressure drops and excessive regrowth) that additional safety **chlorination** is needed after standard treatment.

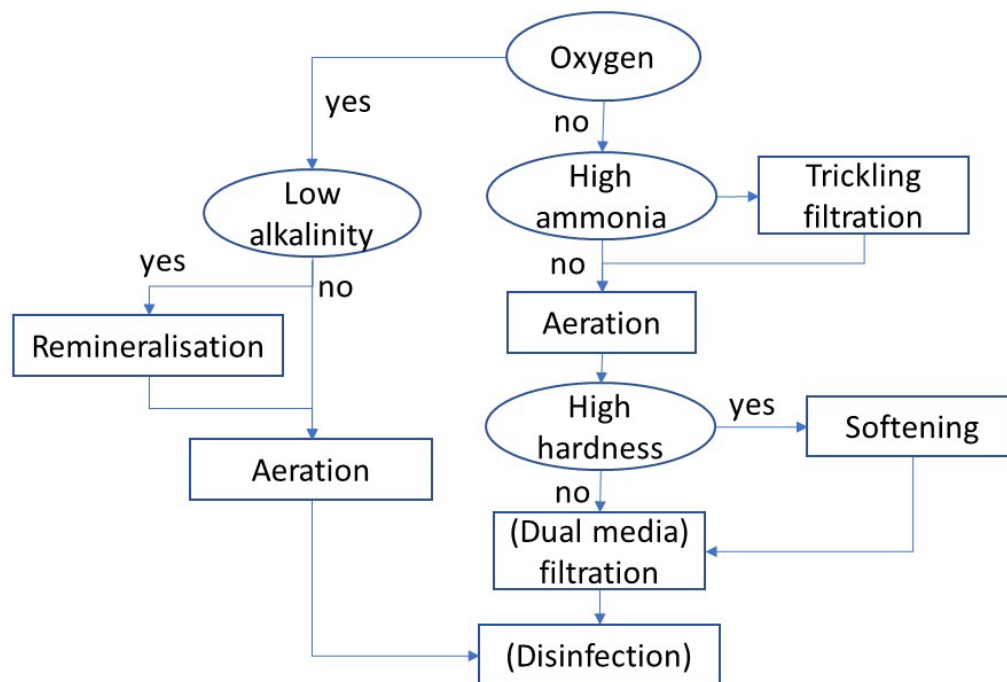


Figure 1: Conventional options for groundwater treatment

## 2.2. Surface water characteristics and treatment trains

Surface water is characterised by (high) turbidity, and the presence of pathogenic micro-organisms and (organic) micro-pollutants. In addition, in (eutrophic) lakes the algae concentration can be too high, also leading to taste and odour problems. It is further assumed that in (reasonably protected) surface waters oxygen levels are sufficiently high and ammonium is not present. Therefore, a surface water treatment plant should consist of a coagulation (static or dynamic mixing), flocculation (static or dynamic mixing), floc removal (flotation, sludge blanket, or (titled-plat) settling) and rapid sand filtration (single- or dual media) step, to remove suspended particles and inorganic micropollutants. Additionally, a main disinfection step (chlorination, Ozonation, UV disinfection, slow sand filtration) and one or more organic

micro pollutant (OMP) removal step(s) (activated carbon filtration, powdered activated carbon dosing, UV/peroxide, Ozonation) should be present. The flocculation-floc removal and rapid sand filtration step could occasionally be substituted by Ultrafiltration (UF)/ microfiltration (MF) membrane systems. In specific cases where the hardness, and/or natural organic matter content are too high, specific measures must be taken.

In several countries in the Europe, the distribution system is such (due to leakages, pressure drops and excessive regrowth) that additional safety **chlorination** is needed after standard treatment. Conventional options for treatment trains for surface water are presented in figure 2 and non-conventional options are presented in figure 3.

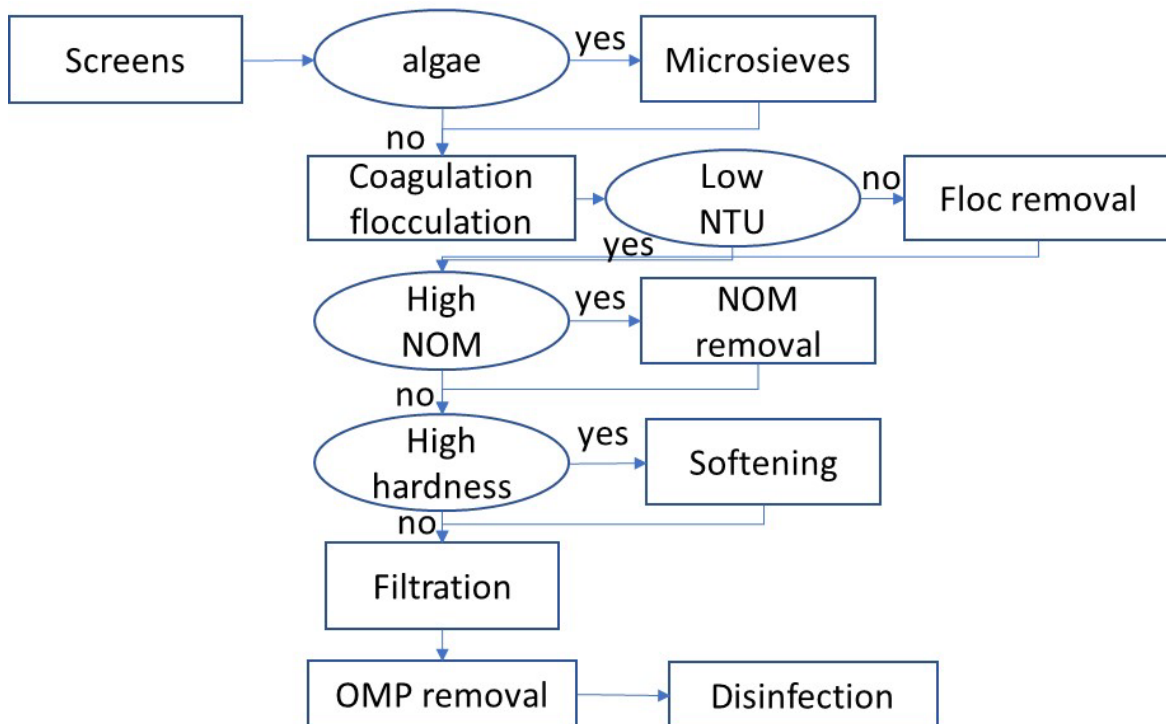


Figure 2: Conventional options for direct surface water treatment

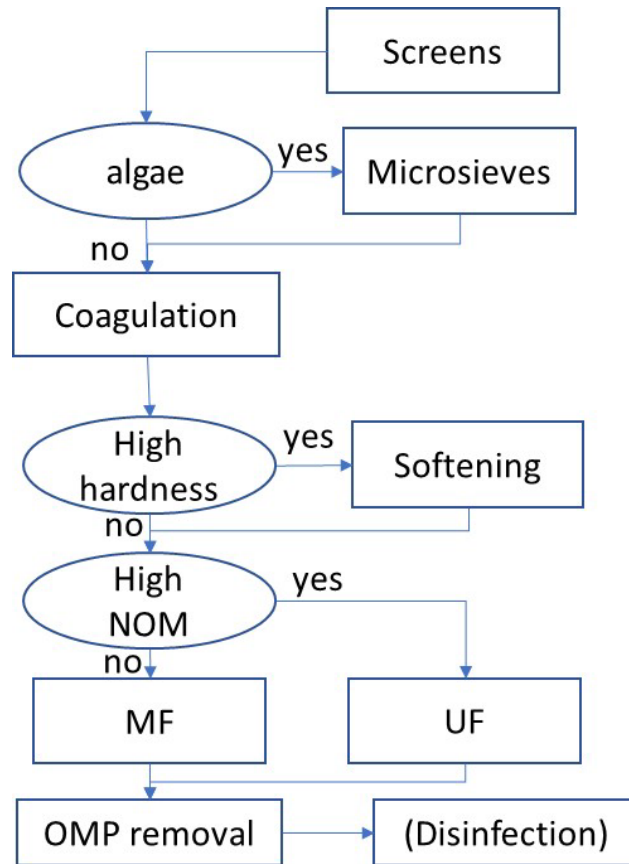


Figure 3: Low footprint, modern alternative for direct surface water treatment

### 2.3. (River)bank filtrate and infiltration water characteristics and treatment trains

River bank filtrate is characterised by the combination of anaerobic groundwater and surface water and will typically not contain oxygen, but can contain (high concentrations of) iron, manganese, ammonium, hydrogen sulphide and/or methane, due to reduction processes, frequently at a low pH. Sometimes, depending on the composition of the underground, hardness can be high. In addition, organic micro-pollutants will be present due to infiltration from the river (or lake), but the rest of the parameters are usually within the drinking water standards. Therefore, treatment will minimally consist of an **aeration step**, for addition of oxygen and stripping of carbon dioxide, hydrogen sulphide and methane (by spraying, cascades, stripping towers, or alike) and a **double filtration** step, being trickling filtration and (sub-merged) rapid filtration step (single or dual media) to remove iron, manganese and ammonium (biologically). Further, an **OMP removal step** must be added (activated carbon filtration, powdered activated carbon dosing, UV/peroxide, Ozonation). In specific cases where the hardness, the arsenic concentration, natural organic matter content, nitrate concentration and/or the fluoride concentration are too high, specific measures must be taken.

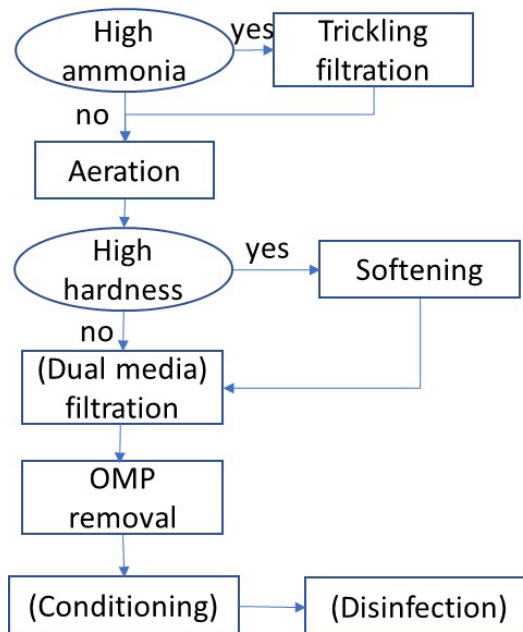


Figure 4: Conventional options for (river) bank filtrate treatment

Infiltrated water is characterised by the combination of surface water and anoxic groundwater and will not contain oxygen, but can contain (high concentrations of) iron, manganese, ammonium, and/or hydrogen sulphide, due to reduction processes, frequently at a low pH. Sometimes, depending on the composition of the (pre-treated) surface water and the underground, hardness can be high. In addition, organic micro-pollutants will be present due to infiltration from the pre-treated river (or lake) water, but the rest of the parameters are usually within the drinking water standards. Before infiltration, surface water has to be pre-treated, removing suspended particles and nutrients, to avoid clogging of infiltration ponds or wells. Furthermore, preferably, OMPs are being removed before infiltration, to avoid pollution of the subsoil in the infiltration area. The pre-treatment therefore consists of a conventional surface water treatment, consisting of coagulation, flocculation, floc removal and rapid sand filtration, preferably extended with an OMP removal step. Post-treatment, after infiltration, will minimally consist of an **aeration step**, for addition of oxygen and stripping of carbon dioxide, hydrogen sulphide and methane (by spraying, cascades, stripping towers, or alike) and a **double filtration** step, being trickling filtration and (sub-merged) rapid filtration step (single or dual media) to remove iron, manganese and ammonium (biologically). Further, an organic **micro-pollutant removal step** could be added (activated carbon filtration, powdered activated carbon dosing, UV/peroxide, Ozonation). In specific cases where the hardness, the arsenic concentration, natural organic matter content, nitrate concentration and/or the fluoride concentration are too high, specific measures must be taken.

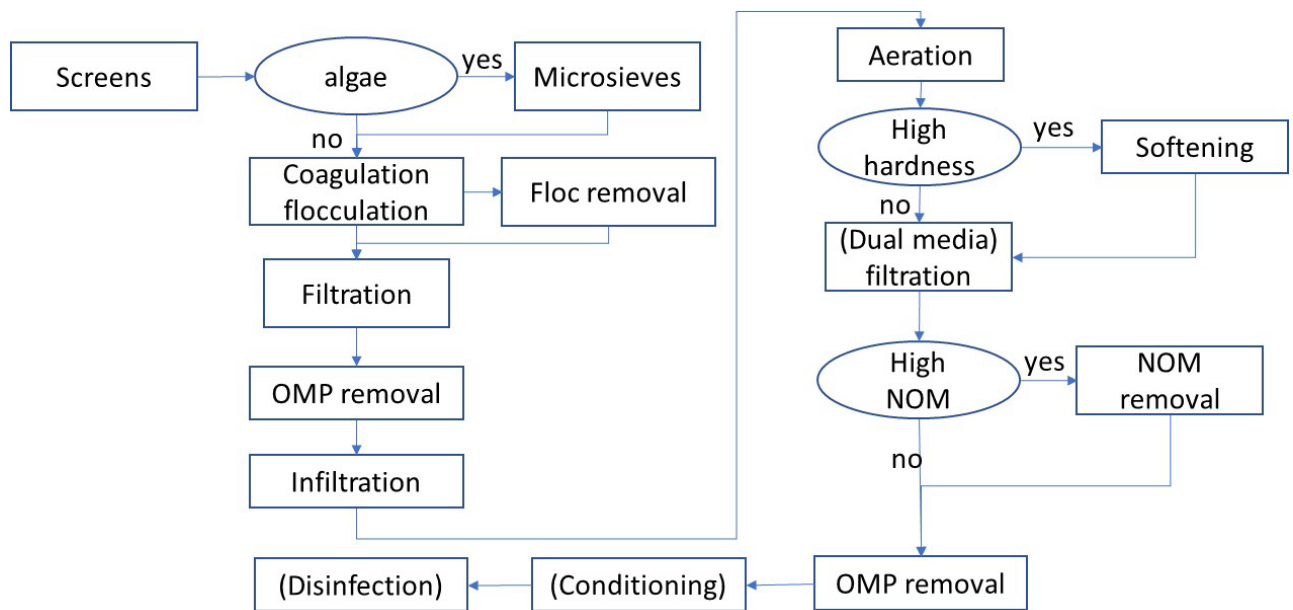


Figure 5: Conventional options for infiltration and infiltrated water treatment

## 2.4. Nominal capacity and security of drinking water treatment plants

The nominal capacity (in m<sup>3</sup>/day) of a (small) drinking water treatment plant is dependent on the average drinking water demand in the supply area (usually dominated by domestic use, as default 125 (Litres per person per day - lpppd), the number of (permanent) inhabitants, flow for other uses, such as commercial, industrial, agricultural or public, the leakage percentage of the total to be distributed flow (by default 20%), and a peak factor dealing with seasonal and weekly variations in the average day flow (by default 1.5 – Davis, 2011).

To increase the security of supply (and robustness) of the drinking water treatment plant the plant is usually divided into 4 lanes, each consisting of (all) processes of a treatment train in series. In this way, when one of the lanes is in maintenance, the plant will keep always a residual of 75% of the maximum capacity.

By applying the 4 lanes strategy the number of valves to direct the water to the subsequent process steps can be reduced to a minimum, increasing the robustness of the system. Finally, also for robustness reasons, it is required to minimize the pumping phases between the subsequent process steps. Therefore, the water should flow, after an initial pumping phase, as much as possible, under gravity through the treatment plant. Major elements in the hydraulics of the plant are: height of the individual treatment steps (in relation to ground level) and the head loss over the individual treatment processes. Head losses in between the process steps should be, as much as possible, avoided.

The supporting tool calculates the nominal capacity using information, provided by the user, regarding perspective population and estimated consumption per person per day (in lpppd). Moreover, the supporting tool includes any additional flow that are used for other purposes and requires from the user to provide a rough estimation of the % of leakage expected in the distribution network. The supportive tool is flexible and additional population numbers could be introduced by the user in any case of an expected population expansion in the area. Moreover, the supporting tool asks the user for

a potential drinking consumption pattern difference in the area during the year that it should be considered in the capacity calculations. Finally, the supportive tool asks the user to provide the number of different lanes and the number of the different units per lane to calculate the nominal flow per lane.

## *2.5. State of the art in treatment technologies and key comparison criteria in relationship to ToDrinQ goal*

### *2.5.1. Key treatment technologies included in the design support tool (DST)*

The different treatment stages (steps) of a treatment train are required for different treatment purposes. For example, coagulation – flocculation steps are required for NOM removal while OMP removal step is required for to tackle the presence of micropollutants. Therefore, the supporting tool should not compare potential technologies that are used in different treatment steps. Thus, the alternative technologies of the supporting tool database are grouped per treatment step and only a comparison between those belonging in the same treatment stage is possible. The database of the different technologies per treatment step is presented in the following table including a short description per technology and its main advantages and disadvantages.

Table 2: Treatment Technologies in the supporting tool database

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
Screening	coarse strainer	Easily separate and remove large matter carried along by the raw water, which might negatively affect the efficiency of later treatment procedures or make their implementation more difficult. Mesh opening larger than 4 cm.	Low maintenance required. Accommodate with high flow rate. Reduced risk of clogging	Limited removal of small particles. Not suitable for fine screening. Large footprint
	medium strainer	Strainers with mesh opening between 0.5 and 3 cm to remove large matter, e.g. leaves or duckweed. Usually applied for surface water intake.	Moderate maintenance required. Could be used for different treatment applications. Low risk of equipment damage.	Limited removal of fine particles. Limitations in accommodating high flow rates. Large footprint
	micro strainer/microsieve	Strainer with mesh opening between 10 to 40 micrometer to remove small particles and algae	Fine filtration. Enhanced water quality. Flexible installation. Low risk of damage.	High maintenance required. Limitations in accommodating high flow rates. Large footprint. High capital and maintenance costs.
Ammonia removal	trickling filtration unit	Trickling filtration is a wastewater treatment process that involves the biological degradation of organic matter and the removal of suspended solids and nutrients through microbial activity on the surface of a fixed-bed media	Biological treatment. Low energy costs. Compact design	Limited removal efficiency for micropollutants. Nutrient removal limitations. Media clogging.
Coagulation / Flocculation	cascade mixing	Cascade mixing works by passing water through a series of mixing stages or compartments, where chemicals or additives are introduced at each stage	Effective removal of suspended particles, turbidity. Flexibility in terms of adjusting coagulant dosages and mixing parameters based on water	Cascade mixing typically requires energy-intensive mixing equipment to ensure thorough dispersion of coagulants. The equipment requires

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
			quality variations. Proper mixing reduces the amount of coagulant needed. Enhances settling rates, facilitating easier separation of flocs.	regular maintenance to ensure proper functioning.
	inline mixing	Inline mixing, also known as in-line mixing, is a method of mixing chemicals or additives with water directly within a pipeline	Immediate and thorough dispersion of coagulants. Compact design that minimizes the footprint. Reduction of the chemical contact time. Lower Energy consumption.	May not provide sufficient mixing time or uneven mixing for the chemicals. Regular maintenance to prevent clogging and fouling. Flow changes may affect mixing efficiency.
	dynamic mixing	Dynamic mixing coagulation is a water treatment process that combines coagulation and flocculation with dynamic mixing to enhance the removal of suspended particles	Provides vigorous agitation, ensuring thorough dispersion of coagulants. Increases the contact between coagulants and suspended particles. Maintains consistent mixing intensity and distribution. Accelerates settling rates.	Energy Consumption. Proper design and operation of dynamic mixing systems are crucial to avoid issues such as uneven mixing, dead zones, or excessive turbulence. Intense mixing action in dynamic mixing systems can potentially cause shear damage to delicate flocs, leading to floc breakage.
Flocculation	static mixing	Static mixing devices to promote flocculation and particle aggregation in water	Static mixing elements provide consistent and uniform mixing throughout the water stream, ensuring thorough dispersion of coagulants and promoting the formation of well-developed flocs. Static mixing requires minimal energy input compared to dynamic mixing methods. Minimal space requirements. Require minimal maintenance	Static mixing may not provide as intense or vigorous mixing compared to dynamic mixing methods. Affected by flow rates variations. Limited scalability for larger treatment capacities

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
Floc Removal	sludge blanket clarifier	Uses a suspended blanket of flocculated particles to enhance the clarification process	Facilitates efficient separation of suspended solids from water by allowing particles to settle under gravity, forming a distinct sludge blanket at the bottom of the clarifier. Less space compared to other clarification techniques. Continuous operation without shutdowns for maintenance. Flexibility in treating different types of water sources	Managing and removing the sludge generated in the clarifier can be challenging and labour-intensive. Sensitive in hydraulic variations. Limitations in removing fine particles, not suitable for waters with low turbidity.
	horizontal settling	This process involves the flow of water in horizontal direction through a settling basin or tank, allowing suspended solids and flocs to settle out by gravity	Horizontal settling allows for longer settling distances compared to vertical settling, which can enhance the settling efficiency of flocs. Longer retention time for flocs to settle. Smaller footprint compared to vertical settling tanks. Simple to operate and require less maintenance.	Proper sludge removal mechanisms are required to prevent buildup and maintain clarifier efficiency. Not easily scalable for larger treatment capacities. Variations in hydraulic conditions can affect the settling efficiency.
	tilted-plate settling	This method increases the effective settling area by using multiple inclined plates or tubes, allowing for more efficient sedimentation in a smaller footprint compared to traditional horizontal settling basins.	Tilted plates provide a larger settling surface area allowing for more efficient particle capture. Compact design with less footprint required. Enhanced removal of TSS and turbidity.	Tilted plates are susceptible to clogging or fouling by suspended solids and organic matter that could reduce efficiency. Can be affected by variations in flow rates. Require regular control, inspection and maintenance.
	dissolved air flotation (DAF)	A floatation tank pumped with pressurized dissolved air bubbles that help suspend flocculated particles to	Efficient Solid-Liquid Separation. Very small footprint. Very flexible and	Requires careful monitoring and control of various parameters, including air flow, pressure, and

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
		the surface forming what's called a 'floc-foam bed' which is then scrapped or skimmed off.	customized design. High removal efficiency of NOM, algae, heavy metals	chemical dosing. It requires additional chemical dosing. Increased operational costs and higher energy consumption. Sludge handling of and disposal that may require additional treatment processes to dewater.
Rapid Sand Filtration	single media filtration unit	Filtration with a singular type of granular media	Simple to operate. Lower capital costs. Suitable when total suspended solids (TSS) are moderate.	Limited filtration efficiency for fine particles. Require more frequent backwashing or media replacement. Reduced flexibility in achieving filtration goals.
	dual media (sand) filtration unit	Filtration with two types of granular media	Double media filtration systems use two layers of different media with varying particle sizes, which can enhance filtration efficiency by capturing a wider range of particle sizes. More effective removal of TSS. Greater filtration flexibility. Less backwashing required.	High capital costs. Higher design, maintenance and operational complexity. The use of two media layers increases the potential for media clogging or fouling.
	moving bed filtration	Moving bed filtration is an advanced water treatment process that employs a bed of granular media, which is constantly in motion, to filter out suspended solids from water.	Moving bed filtration offers high filtration efficiency due to continuous agitation of the media, which helps prevent clogging and promotes effective removal of suspended solids. Has smaller footprint. The movement of filtration media prevents biofilm formation and reduces maintenance requirements.	High initial costs. Higher energy consumption to maintain the necessary flow velocity. Risk of media loss during backwashing. Operational and maintenance complexity.

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
	pressurized filtration vessel	Vessel(s) where pressure is used to force the water passing through the media.	High filtration quality. Small footprint. Fast processing. High Flexibility.	High energy consumption. High operational and maintenance complexity. High capital cost.
OMP removal	granular activated carbon (GAC)	Submerged packed bed filtration with activated carbon granules	High removal efficiencies (up to 99.9%) for many VOCs, including trichloroethylene (TCE) and tetrachloroethylene (PCE). In most cases, GAC can remove target contaminants to concentrations below 1 µg/l.	Media to be removed when GAC capacity is exhausted.
	powdered activated carbon (PAC)	Powdered activated carbon (PAC) in concentrations between 1 to 100 mg/l are added in the early stages of the treatment process to absorb the microorganisms and organic chemicals.	High adsorption capacity for pesticides, and organic material. Effective removal of taste and odour. PAC can be regenerated and reused to minimize operational costs	Expensive comparing to other options such as GAC. Proper mixing and dispersion equipment are required to ensure effective contact between PAC particles. Potential generation of airborne dust. Sludge generation that requires treatment and disposal.
	Medium pressure ultraviolet (mp-UV)/H <sub>2</sub> O <sub>2</sub>	The UV/H <sub>2</sub> O <sub>2</sub> system is an advanced oxidation process (AOP) in which hydrogen peroxide (H <sub>2</sub> O <sub>2</sub> ) is added in the presence of ultraviolet (UV) light to generate hydroxyl radicals (·OH).	The combination of UV and H <sub>2</sub> O <sub>2</sub> produces hydroxyl radicals which are powerful oxidants capable of breaking down and removing various organic and inorganic contaminants in water, including pesticides, pharmaceuticals, and industrial chemicals. Does not produce any harmful byproducts. Does not change the chemistry of the water.	Requires significant energy input and has high operational costs. Insufficient penetration in turbid or colour water. Dependency on H <sub>2</sub> O <sub>2</sub> that requires additional safety precautions and logistical arrangements.

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
	ozonation	Use of ozone (O <sub>3</sub> ) for removing OMPs through the oxidation process of those compounds.	Effective disinfection against a wide range of microorganisms, including bacteria, viruses, and protozoa. Oxidizes a variety of contaminants in water, including organic compounds, taste and odour compounds. No odour or taste residual unlike other disinfection processes and no chlorinated disinfection by-products (DBPs). Shorter Contact time for either OMP removal or disinfection, therefore, requires smaller footprint.	Expensive to implement and operate due to the high cost of ozone generation equipment, energy requirements, and maintenance costs. Does not provide a long-lasting residual effect unlike other disinfection solutions. Proper safety precautions for operators are required as ozone is hazardous to handle. High concentration of ozone oxidize bromide ions to bromate, a DBP with potential health risks.
OMP removal	Nanofiltration/ reverse osmosis (NF/RO)	Use of nanofiltration membranes where pressure forces water to pass through	Good for selective removal of dissolved ions, organic compounds, and other contaminants. Reduce the use of chemicals. Compact design with small footprint.	High energy consumption. Higher maintenance costs and high risk of membrane fouling. Limited removal of small solutes. Sensitive in pH variations in the feed water.
NOM removal	anionic IEX	Packed bed filtration with anion exchange resin beads as filter media	High removal efficiencies (greater than 99 percent) for negatively charged contaminants. When the capacity of the resin is exhausted, it can be regenerated to restore it to its initial condition.	The spent regenerant brine is a concentrated solution of the removed contaminants and will be high in dissolved solids and excess regenerant ions. Anion exchange treatment also can lower the pH of the treated water and, therefore, may require post-treatment corrosion control. Disposal of the resin may require a special hazardous waste handling permit.

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
	enhanced coagulation	Use of additional coagulants for reducing the NOM concentration in the water	Effective NOM removal.	High energy consumption. High maintenance required. Storage unit required to store the chemicals. Safety precautions required.
Softening	cationic IEX	Packed bed filtration with cation exchange resin beads as filter media	Cation exchange is a proven technology for water softening and removal of positively charged contaminants. It can achieve high removal efficiencies (greater than 99 percent) for positively charged contaminants. When the capacity of the resin is exhausted, it can be regenerated to restore it to its initial condition.	The spent regenerant brine is a concentrated solution of the removed contaminants and also will be high in dissolved solids and excess regenerant ions (e.g., sodium, chloride). This waste stream will require disposal or discharge.
	pellet softening	Pellet softening (lime and soda) is a water treatment process designed to remove hardness ions, primarily calcium ( $\text{Ca}^{2+}$ ) and magnesium ( $\text{Mg}^{2+}$ ), from water by converting them into insoluble calcium carbonate ( $\text{CaCO}_3$ ) and magnesium hydroxide ( $\text{Mg}(\text{OH})_2$ ) precipitates	Highly effective hardness reduction. Minimal chemical usage. Low maintenance required. High flexibility in treatment operations	Significant amount of sludge. Safety precautions required to minimize the chemicals risk. Additional pH adjustment may be required. Operational control required to minimize the precipitation of pellet chemicals in the following treatment stages or the distribution system.
	Nanofiltration/ reverse osmosis (NF/RO)	Use of nanofiltration membranes where pressure forces water to pass through	Can remove hardness ions while retaining essential minerals. High removal of calcium and magnesium ions	High energy consumption. Higher maintenance costs and high risk of membrane fouling. Risk of brine disposal.

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
Aeration	cascade unit	Mechanical introduction of air or oxygen into water to improve its quality for various purposes, such as enhancing biological processes, removing volatile organic compounds, or oxidizing contaminants	Simple and cost-effective solution. Provides efficient oxygen to water. Easily scalable to accommodate various flow rates	Potential water loss. Risk of aerosol formation. Sensitive to colder conditions. Limiting mixing capability.
	spray nozzles	Spray nozzles used for aeration are specifically designed to introduce air or oxygen into water bodies to enhance dissolved oxygen levels	Efficient oxygen transfer. Flexible for use in different water flow rates. Customization of the aeration patterns. Energy efficient. Low maintenance complexity.	Vulnerable to clogging. May produce noise. High operational costs.
	stripping tower	Aeration in stripping towers involves introducing air into water and allowing volatile compounds to evaporate and escape into the atmosphere.	Effective removal of VOCs. Simple and robust design. Adaptability – Flexibility. Minimal residuals.	Not suitable for non VOCs. High energy consumption. Potential release of stripped gasses. Affected by low temperatures.
	plate aeration unit	Plate aeration units, also known as plate aerators or diffused plate aerators, are devices used in water treatment processes to introduce air into water for the purpose of oxygenation and mixing	High oxygen transfer efficiency. Uniform oxygen distribution. Low energy consumption. Minimal maintenance.	Sensitive to clogging. Potential air entrapment. Potential release of VOCs or stripped gasses.
Conditioning	remineralization filtration unit	Filtration with limestone or calcium/magnesium carbonate containing granules to increase the water hardness		
	dosing of chemicals	Extensive use of chemicals to improve water condition and stabilize the quality of the water.		

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
	pH correction	Use of acids alkali to correct the pH and optimize the treatment		
Disinfection	baffled ozone contact reactor	Baffle containing vessel for ozone induced oxidation	Effective disinfection over against a wide range of microorganisms, including bacteria, viruses, and protozoa. Oxidizes a variety of contaminants in water, including organic compounds, taste and odour compounds. No odour or taste residual unlike other disinfection processes and no chlorinated disinfection by-products (DBPs). Shorter Contact time for either OMP removal or disinfection, therefore, requires smaller footprint.	Expensive to implement and operate due to the high cost of ozone generation equipment, energy requirements, and maintenance costs. Does not provide a long-lasting residual effect unlike other disinfection solutions. Proper safety precautions for operators are required as ozone is hazardous to handle. High concentration of ozone oxidizes bromide ions to bromate, a DBP with potential health risks.
	Light pressure ultraviolet (LP-UV) reactor	Use of low-pressure mercury lamps to emit ultraviolet (UV) light at a specific wavelength (typically around 254 nanometers) to inactivate microorganisms and pathogens present in water	LP UV technology effectively inactivates a wide range of microorganisms, including bacteria, viruses, and protozoa. LP UV is chemical free. Provides fast treatment. Requires minimal maintenance.	Limited penetration depth if microorganisms are shielded by particles, turbidity, or biofilms in the water. if microorganisms are shielded by particles, turbidity, or biofilms in the water. High energy consumption. Safety precautions are required to minimize exposure in the UV light.
	chlorine dosing	Use of chlorine containing compounds for disinfection	Chlorination is a highly effective method for killing a wide range of microorganisms, including bacteria, viruses, and protozoa. Provides a residual for protection over a potential	Can lead to the formation of disinfection byproducts (DBPs). Can impact taste and odour of the treated water. Safety precautions or hazardous gases are required. Chlorine

Treatment Step	Treatment Technology	Description	Advantages	Disadvantages
			regrowth. Provides rapid action in killing microorganisms.	can react with materials and metals in the distribution system, leading to corrosion of infrastructure.
	chloramine dosing	Use of chlorine in combination with ammonia to produce chloramines for disinfection	Chloramination produces a more stable residual compared to chlorine. Chloramination typically results in lower levels of disinfection byproducts (DBPs). Creates fewer taste and odour compounds.	Requires longer contact time than chlorination. Requires additional ammonia handling increasing operational and maintenance processes. Chloramines can promote the growth of nitrifying bacteria in distribution systems, leading to nitrification. Chloramines may be less effective against certain pathogens, such as Cryptosporidium.
Ultrafiltration and microfiltration	polymeric UF	UF employs semi-permeable ultra membranes made of synthetic polymers to separate suspended solids, colloids, bacteria, and macromolecules from water.	Effective removal of small particles. No chemical use required.	High maintenance and high operational costs to prevent fouling. High energy consumption. Complex maintenance of the membranes.
	polymeric MF	MF employs semi-permeable micro membranes made of synthetic polymers to separate suspended solids, colloids, bacteria, and macromolecules from water.	Effective removal of medium particles. No chemical use required. Minimal Fouling. Robust performance	Low filtration efficiency to small particles. High footprint.

### 2.5.2. Criteria and constraints for the characterisation of technologies in relation to the project goals

Based on the project goals the following criteria are distinguished for the comparison of individual, alternative treatment technologies to be incorporated in the previously described treatment trains:

- Complexity (operational and maintenance)
- Flexibility (changes in demand/quality (seasonality), scalability, operational flexibility)
- Robustness/reliability
- Environmental impact (CO<sub>2</sub> emission – energy consumption, water losses, sludge/concentrate production, chemical use)

A score between 0 to 1 will be assigned to each different technology for each one of the different criteria where a score close to 0 indicates a low score and a score close to 1 indicates a high score. The score will be assigned based on the available literature, the EPA and the EEA guidance and KWR and TUD experience in the field (EPA, n.d., EEA, 2000). Thus, once the final treatment train is selected, the supportive tool will sum the total score for each different criterium and the overall score of all the criteria of treatment train. In the table below an example of the total score in these four criteria for GAC Filtration for OMP removal is presented.

Table 1: Indicative criteria scoring of the GAC filtration

Criteria/ Technologies	Complexity	Flexibility	Robustness	Environmental impact	Total Score
GAC filtration	0.5	0.8	0.8	0.3	2.4

### 2.5.3. Total costs of ownership calculations

The cost of the final treatment train will be calculated in terms of total costs of ownership per m<sup>3</sup> of treated water. The final cost will be dependent to the selected technologies and the calculations will be made using the Kostenstandaard tool (<https://kostenstandaard.nl/>) developed by RHDHV (Kostenstandaard Tool, n.d.) .

### 2.5.4. Drinking water treatment plant removal efficiency

The percentage or log removal rate for different water quality parameters per treatment technology is included in the supporting tool database. The removal rates are taken from the bibliography and from EPANET’s Drinking Water Treatability Database (*Drinking Water Treatability Database*, n.d.). In the following table, an indicative water quality removal rate per parameter for some of the treatment technologies are presented. The supportive tool calculates the final removal rate per parameter once the final treatment train is finalized.

Table 2: Removal efficiency per water quality parameter for some of the treatment technologies of the DST. Adapted from the Drinking Water Treatability Database (EPA, n.d.)

WQ Parameter	Coagulation - Flocculation - Clarification - Rapid Sand Filtration	Granular Activated Carbon (GAC)	Powdered Activated Carbon Dosing (PAC)	Ozonation	MP-UV/H <sub>2</sub> O <sub>2</sub>	NF/RO
NOM	30-70%	50-70%	50-80%	10-50%	20-60%	80-95%
Turbidity	90-99%	20%	20%			90-99%
DOC	30-70%	70-80%	40-80%	20-50%	30-50%	60-99%
TOC	40-80%	40-70%	50-80%	15-40%	20-60%	70-90%
<i>E. Coli</i>	1-3log			4-6log	3-5 log	4-6log
Coliform bacteria	2-3log			4-6log	3-5log	4-6log
Arsenic	50-90%	30-60%	20-40%	10-40%	10-30%	70-90%
Cryptosporidium	1-2log			0.5-2	2-4log	>3log
Micropollutants		1-3 log	1-3 log	2-3log	2-4 log	1-3log

### 2.5.5. Drinking water treatment plant footprint, energy consumption and head losses calculations

To determine the footprint of the DWTP it is needed to first determine the superficial velocity of the individual treatment processes, e.g. by using rule of thumb values for process based characteristic variables (retention time, chemical dosage etc.) from practice and the literature. The DST calculates key operational metrics for each treatment technology used in the plant. These metrics include:

#### 1. Footprint Calculation:

- The tool estimates the footprint area (m<sup>2</sup>) required for each treatment technology based on the number of lanes, nominal flow (Q), and required retention time.
- It also includes additional space estimates for secondary areas like offices, roads, and other essential facilities.

#### 2. Head Loss Estimation:

- The tool assesses head loss (pressure loss) associated with each technology.
- It then aggregates these values to provide the total head loss across all treatment processes.

#### 3. Total Footprint Area:

- The total footprint area is calculated as the combined area of all treatment processes and secondary facilities, giving a comprehensive view of the spatial requirements.

#### 4. Power and Energy Cost Estimation:

- For each treatment technology, the tool estimates power requirements and calculates the overall energy cost for the plant.

#### 5. Data Presentation:

- The tool includes a sample table showing information for each treatment technology, allowing users to compare footprint, head loss, and energy needs across options.

In the following table, a short database for the area and the head loss calculations is presented. In the area column of this table, the formula that calculates the footprint of each technology is presented. The footprint calculations are adopted from the “Water and wastewater engineering: design principles and practice” book (Davis, 2011).

Table 3: Head loss and footprint database per treatment technology

Key characteristics/ Technologies	Superficial velocity (m/h)	Retention time (T -min)	Height (H - m)	Area (m <sup>2</sup> )	Head loss (m)	Key characteristics/ Technologies
Coagulation: Cascade mixing			0.5-1.0		0.5-1.0	Coagulation: Cascade mixing
Coagulation: Inline mixing			0	0		Coagulation: Inline mixing
Coagulation: Dynamic mixing			2.5-3.5		0.1	Coagulation: Dynamic mixing
Flocculation: Static mixing	-	30	2.5-3.5	=Q*T/(60*H)		Flocculation: Static mixing
Flocculation: Dynamic mixing		30	2.5-3.5	=Q*T/(60*H)	0.1	Flocculation: Dynamic mixing
Horizontal settling				=Q/V	0.1	Horizontal settling
Dissolved air flotation				=Q/V		Dissolved air flotation
Single media filtration	5-10		2.5-3.0	=Q/V	0.5-1.0	Single media filtration
Dual media filtration	8-12		2.5-3.0	=Q/V	0.5-1.0	Dual media filtration
GAC filtration		10-20	3.0-5.0	=Q*T/(60*H)	0.5	GAC filtration
PAC dosing			0	0	0	PAC dosing
Ozonation				=Q*T/(60*H)	0.1	Ozonation
Anion IEX				=Q/v	0.3-0.5	Anion IEX
Pellet softening	60-100			=Q/v	5.0-10.0	Pellet softening

### 2.5.6. Constraints used in the DST

The following constraints have been distinguished:

- Incoming water quality
- Regulations/legislation (e.g. for drinking water quality)
- Material scarcity
- Footprint (dimensions)

If the final selected treatment train cannot follow one or more of the above constraints, the DST will receive a "non-available treatment" warning text and will be asked to modify their treatment technology selection or lose one of the constraints to get feasible solution.

#### *2.5.7. Introduction of weights for the different criteria*

The DST by default gives equal weight to each one of the aforementioned criteria including the head losses and the footprint. However, for some decision makers some criteria are more important than others. For example, minimal footprint or total cost could be more important parameters than environment impact. Thus, the DST introduce weights for each different criterium between 0 to 1 with 1 being an important criterium and 0 being a criterium that is ignored.

#### *2.5.8. Adjusting the drinking water treatment stage order*

In a typical treatment train, the treatment stage order is usually screens, coagulation, flocculation, floc removal, rapid sand filtration, OMP removal, disinfection (if required). However, there are treatment technologies in each different treatment stage that for their successful implementation should be added earlier or later in the treatment order. For example, Powdered Activated Carbon (PAC) should be placed before the sedimentation – floc removal and not after the rapid sand filtration. The supportive tool considers these constraints in the decision process and places the treatment stages based on the selection of the treatment technology made the user.

### 3. Web application framework for the design support tool

For the purpose of supporting the end-user to obtain a preliminary design of a water treatment chain, so-called user stories have been defined in order to obtain functional requirements.

#### 3.1. User stories and requirements

##### 3.1.1. Definition

User stories are a widely used concept for formulating software requirements in agile development projects by capturing the essential elements of a requirement: *who* it is for, *what* it expects and *why* it is important. A well-known format is: “As a <type of user>, I want to <goal> so that <some reason>” (Cohn, 2004).

A scientific, rigorous framework for defining a user story following quality guidelines, which will be followed and adapted also in ToDrinQ, is given in (Lucassen et al., 2015). Quality criteria for a user story are showed in Table 5 for reference.

Table 4: Quality criteria for a user story. Adopted from (Lucassen et al., 2015).

Criteria	Description
<i>Syntactic</i> Atomic Minimal Well-formed	A user story expresses a requirement for exactly one feature A user story contains nothing more than role, means and ends A user story includes at least a role and a means
<i>Semantic</i> Conflict-free Conceptually sound  Problem-oriented Unambiguous	A user story should not be inconsistent with any other user story The means expresses a feature and the ends expresses a rationale, not something else  A user story only specifies the problem, not the solution to it A user story avoids terms or abstractions that may lead to multiple interpretations
<i>Pragmatic</i> Complete  Explicit dependencies Full sentence Independent  Scalable  Uniform Unique	Implementing a set of user stories creates a feature-complete application, no steps are missing Link all unavoidable, non-obvious dependencies on user stories A user story is a well-formed full sentence The user story is self-contained, avoiding inherent dependencies on other user stories User stories do not denote too coarse-grained requirements that are difficult to plan and prioritize All user stories follow roughly the same template Every user story is unique, duplicates are avoided

### 3.1.2. User stories for the DST

For the development of the DST, a set of user stories have been defined along with three roles a user can have:

- An administrator role for user and data management purposes. An administrator can add or remove users and user groups, and add, modify or remove data entries.
- An end-user role, in this case a process engineer or water manager who is interested in a preliminary design of a water treatment.
- A developer role.

A list of user stories is given in

Table 6 Note that in some user stories, the ‘means’ (why) is omitted because of its obviousness.

*Table 5: List of user stories for the design support tool.*

<b>UDM1</b>	As an <i>administrator</i> , I want to <i>log in</i> so that I can add, remove or modify existing tables or records of the DST database related to the design of a water treatment.
<b>UDM2</b>	As an <i>administrator</i> , I want to <i>log in</i> so that I can add, change or remove users.
<b>UT1</b>	As an <i>end-user</i> , I want to <i>log in and obtain a preliminary design of a treatment</i> based on my input regarding the characteristics of the source water, process and scale.
<b>UT2</b>	As an <i>end-user</i> , I want to <i>store a (calculated) treatment configuration</i> so that I can load the configuration at a later moment.
<b>UT3</b>	As an <i>end-user</i> , I want to <i>log in and analyse the performance scores of different criteria of a preliminary design configuration of a treatment</i> based on my preferences regarding different criteria.
<b>UT4</b>	As an <i>end-user</i> , I want to <i>log in and load a pre-defined treatment configuration</i> so that I can proceed with a further analysis.
<b>UT5</b>	As an <i>end-user</i> , I want to <i>log in and remove a pre-defined treatment configuration</i> .
<b>UT6</b>	As an <i>end-user</i> , I want to <i>log out</i> so that other users cannot view preliminary design configurations, make changes or remove configuration settings.
<b>UD1</b>	As a <i>developer</i> , I want to <i>calculate criteria or obtain a preliminary design configuration without using a user interface</i> so that testing is simplified and the user interface can be modified without affecting the core functionalities of the tool.

For this document, the scope will be limited to describing the information flow regarding user stories UT1, UT2 and UT3 (Paragraph 3.3) because these user stories have the most direct relationship with the main objective of a DST.

### 3.2. Architecture and requirements

A minimal set of system requirements can be derived from the list of user stories, i.e.:

- The tool can be run standalone (locally), or can be run on a web server.
- A user authentication framework is needed so that multiple users will be able to use the tool.
- APIs (application programming interfaces) will provide the means to key functionalities of the DST, e.g. calculate performance criteria or calculate the ordering of stages in a treatment chain independent of front-end (the user interface) or back-end specific modules (database and related components).
- Information (settings, configurations and other data) are stored and managed in a database.

Based on the above considerations, a web application is developed using Django (*Django Documentation*, n.d.), a Python module for web frameworks. Django is a framework that contains an object-relational mapper (ORM). With the ORM technique, data of a relational database is converted to a virtual object database, i.e. all database tables and a session with the database are represented as objects. Furthermore, Django provides templates for developing web pages, e.g. forms or polls, so that Python can be used to design the user interface of the application. In software engineering terms, Django provides a framework for developing the front-end, i.e. the presentation layer or user interface, and the back-end which is the data access layer.

More specifically, the architecture consists of the following components:

- **Front end:** the user interface is designed as a web site, composed of HTML and CSS (cascading style sheets which are used to define the layout), and JavaScript. The styling of the web pages and components (buttons, check boxes, etc.) is taken care of by using Bootstrap, a popular HTML/CSS and JavaScript package. Django provides the building blocks for the front end, by providing HTML templates and Python code which relate the HTML (page) requests to the ORM.
- **Back end:** the back end consists of four parts:
  - A communication layer with an ORM, including (Python) methods which allow to query from and store data into the database. In addition, the communication layer handles forms and other HTML requests, and forwards these requests to calculation modules if extra processing is needed. Finally, the communication layer comprises of application programming interfaces (APIs). By using APIs, the communication is further generalized and abstracted, enabling easier scaling up, or enabling the use of another front end than the one included in Django. APIs are developed using the Django REST framework. REST is an architectural style and acronym for **RE**presentational **S**tate **T**ransfer (Fielding, 2000). A Web API, or Web Service, conforming to the REST architectural style is called a REST API or RESTful API. By the use of web services, the DST is more future-proof.
  - The main DST ('ToDrinQ') database, an SQLite database containing data related to process technologies, treatment stages, chemical compound names, removal efficiencies, scenario settings, etc. User management data is also included. This database is extended with a separate database for storing literature references.
  - Calculations modules which serve different functionalities of the DST, like the ordering logic involved in determining the treatment chain of stages, or a multi-criteria analysis (MCA) when scoring the different performance criteria of the treatment design.

Figure 6 shows a schematic overview of how the architecture of the DST is set up.

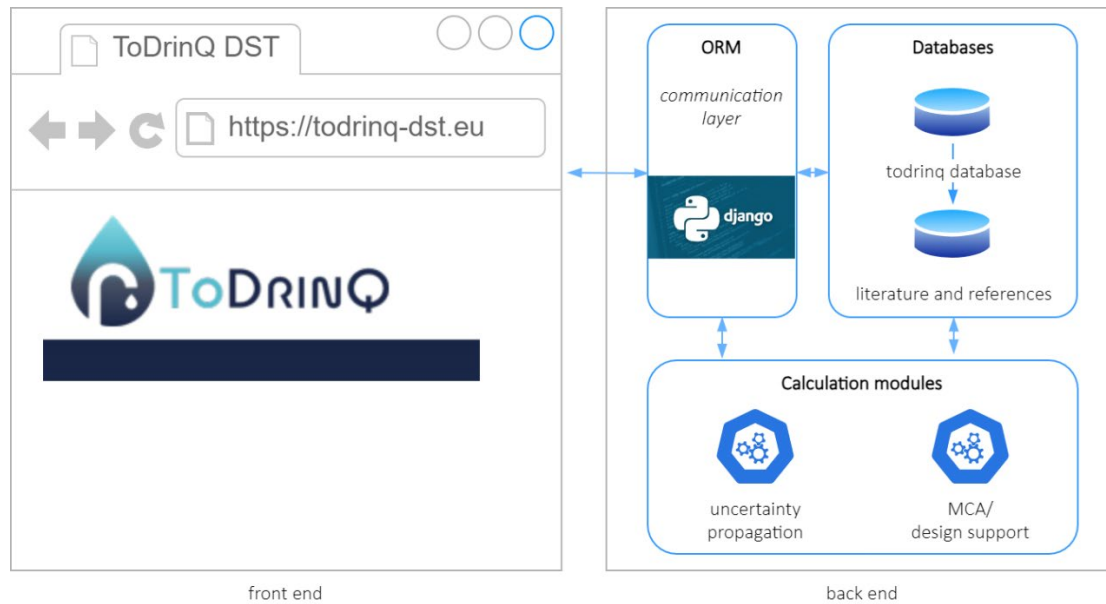


Figure 6: Software architecture scheme of the design support tool, consisting of a front-end part (the user interface, i.e. a website) and the back-end with databases, calculation modules and a communication layer (ORM). APIs (not shown here) are part of the communication layer

Finally, functional requirements are deduced from the user stories:

- guide the user to define (scenario) input settings (e.g. changing characteristics of the source water quality, an estimation of an increasing trend in water consumption, etc.);
- guide the user to select technologies based on water quality and technology characteristics;
- provide a means to tune the resulting treatment design, based on criteria preferences (e.g. weigh environmental impact as more important than costs).
- provide an overview of criteria scores (KPIs) regarding the chosen design and the chosen treatment configuration;
- enable the user to modify settings, like storing and restoring treatment configurations.

### 3.3. Information flows

#### 3.3.1. User authentication and obtain a preliminary water treatment design

In user story UT1, the user logs in and subsequently starts a new preliminary design of a water treatment by answering questions and/or selecting the desired characteristics of the treatment. U1 consists of the following 3 steps:

1. User authentication
2. Decision guidance: by the aid of statements or questions about (predominantly) the water quality of the source, the user is guided in the selection of treatment stages. To this aim, a web form will be used where the user can select relevant characteristics of the drinking water source and

process. The selected options are used to query the database and get the relevant stages and technologies.

3. Show treatment configuration and characteristics.

User story UT2 (storage of a treatment configuration) depends on a calculated preliminary design as obtained by UT1. A schematic representation of the information flow in UT1 and UT2 is shown in Figure 7.

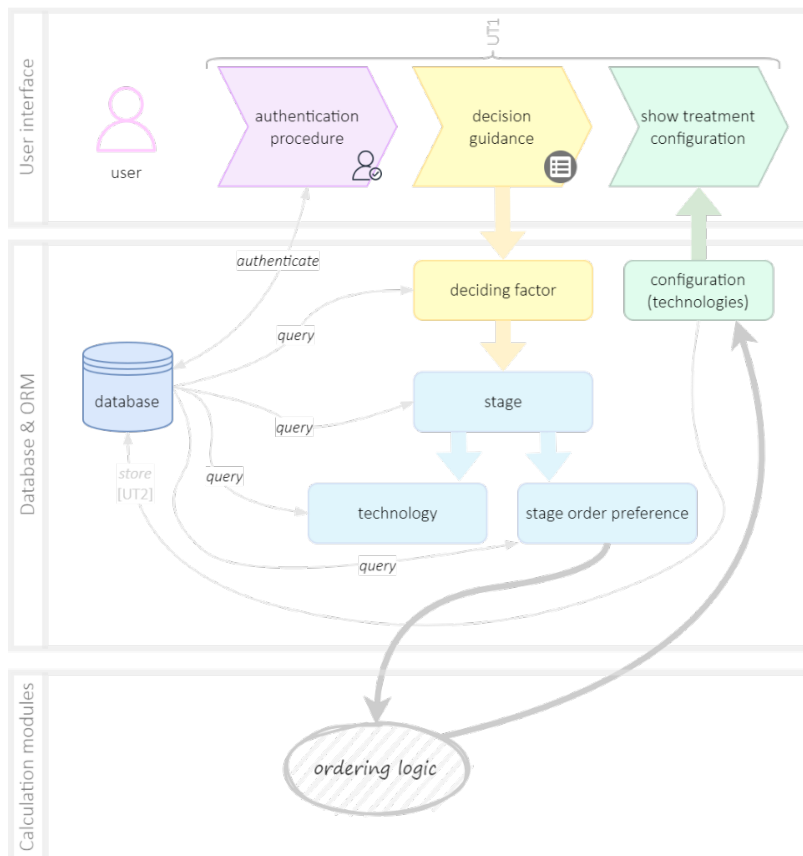


Figure 7: Schematic overview of the steps involved in user story UT1 and UT2. The information flow (top frame) within the user interface translates to querying the database (middle frame) and calculations (frame below) to obtain a treatment configuration. Note that, to simplify the scheme and improve its readability, not all the queried tables are depicted

### 3.3.2. Show the performance of a preliminary water treatment design

UT3 goes one step further by calculating the performance scores of different criteria and presenting these to the end-user based on additional end-user preferences so that performance scores can be analysed and evaluated. Hence, UT3 adds two additional steps to UT1:

1. Specify weight factors for different criteria, uncertainties regarding specific process or input characteristics, and specify inputs for different scenarios (e.g. changing water consumption, changing drinking water quality requirements, etc.). Again, a web form is used to send the weight factor values and other settings which will be used by the KPI and uncertainty propagation module. Moreover, these settings can be stored in the current configuration.
2. Show the key performance indicators as a result of step (1 to) 4.

Figure 8 shows the full information trajectory from user authentication to guidance in designing a treatment configuration (UT1) to showing its performance (UT3).

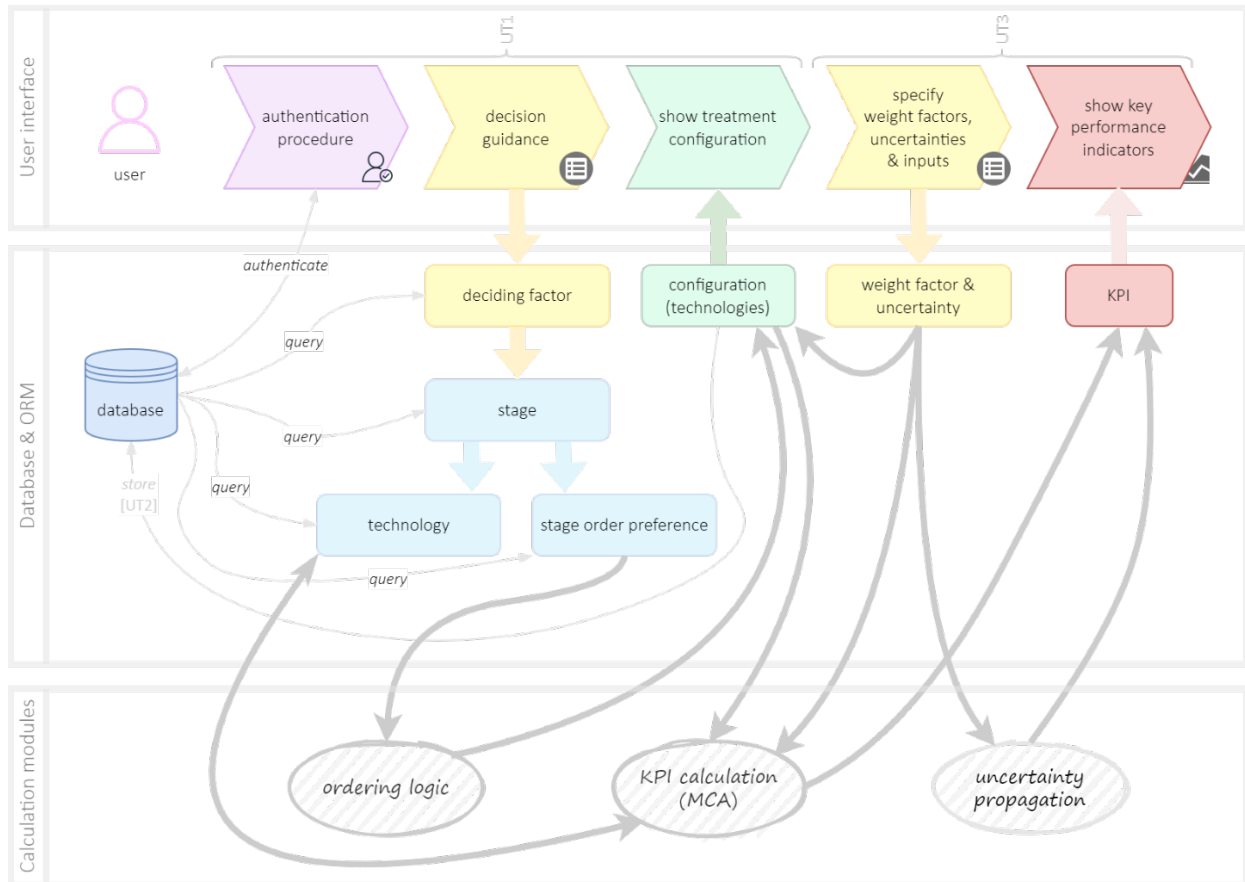


Figure 8: Schematic overview of the steps involved in user story UT1, UT2 and UT3. The information flow (top frame) within the user interface translates to querying the database (middle frame) and calculations (frame below) to obtain a treatment configuration, and finally, after specifying weight factors and other settings, scores for key performance criteria indicators. Note that, to simplify the scheme and improve its readability, not all the queried tables are depicted

Note that UT4 (loading a selected configuration) and UT5 (removing a selected configuration) depart from having a stored configuration (UT2).

### 3.3.3. Key elements in obtaining a preliminary treatment configuration

As explained in Chapter 2, much of the design logic stems from the characteristics of the drinking water source. These characteristics are directly related to the decision tree involved in designing a treatment plant. In the sequel, process technology determining characteristics will be referred to as *deciding factors*. For example, for surface water treatment a deciding factor is whether the surface water contains a high level of algae, consequently determining the need of an extra treatment step (stage) using micro-sieves as a technology.

Elaborating on the example use case, the design support decision tree (see also Paragraph 2.2) consists of decision nodes (here called ‘decision factors’) which led to the selection of stages to be included in the treatment train. Each stage contains a set of technologies suitable for the removal criterion at hand. By adding more decision factors (e.g. based on footprint, costs or other technology properties), a set with

more than one technology can be further reduced until the set contains only one technology. As an illustration, a decision tree where water quality related decision factors lead to a treatment configuration with several stages and their corresponding technologies is depicted in Figure 9.

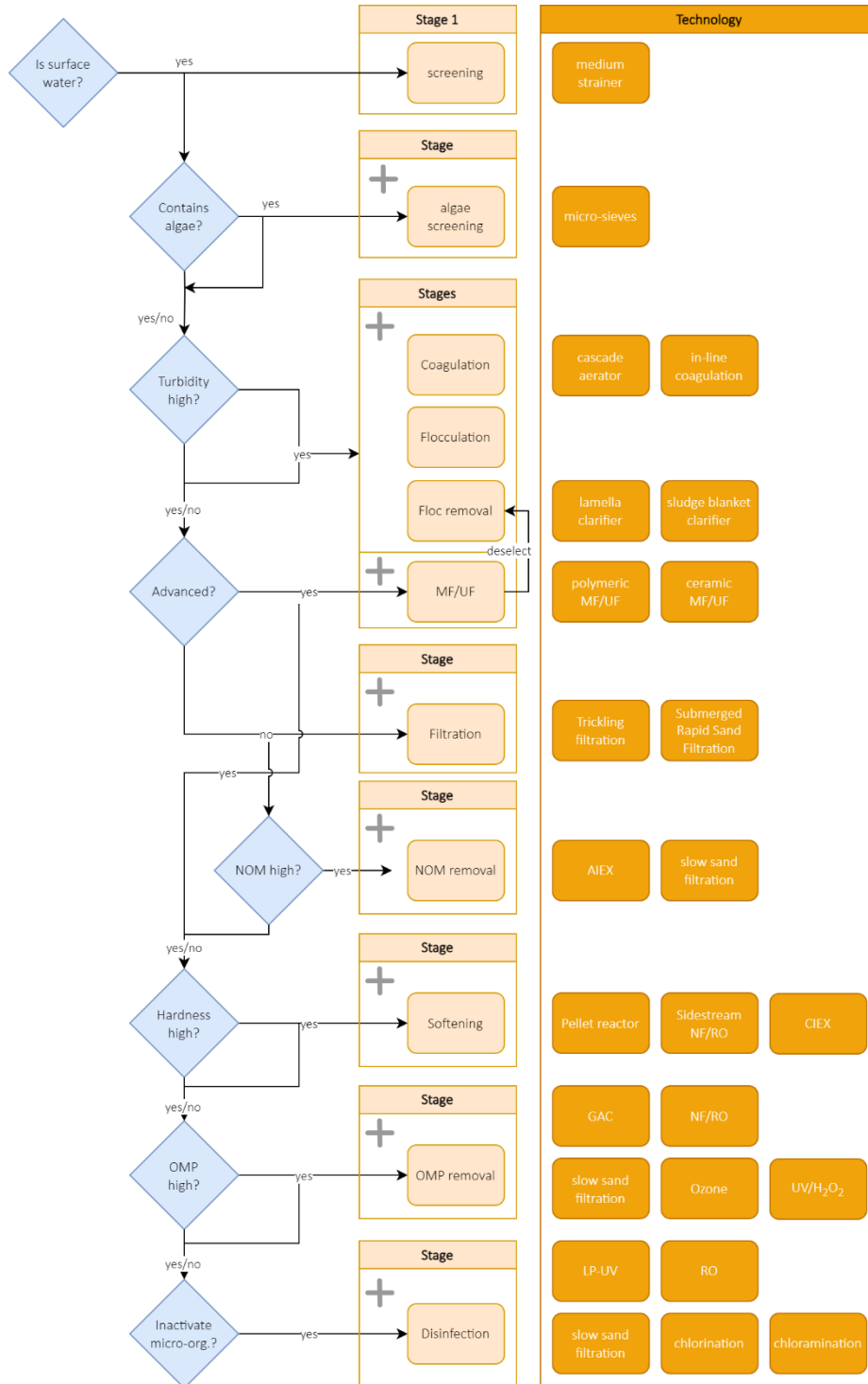


Figure 9: Decision tree where decision factors lead to the selection of stages and corresponding treatment technologies. Note that the stages are still unordered. Decision factors, stages and technologies are stored in database tables, as well their inter-relationships

After the selection of stages, the ordering of stages is determined by the aid of a look-up in a pairing table (also called junction, associative or cross-over table) referred to as the ‘stage\_stage’ table of the DST database. More information about the relationship between stages, technologies and deciding factors are contained in Paragraph 3.4.

Next to the decision guidance in UT1, other tables will be queried when the user is asked for setting the importance of performance criteria and setting scenario settings and/or other inputs. A simplified scheme of how the guidance process (UT1) relates to a proposal of a water treatment design and how the calculation of performance criteria scores relates to technology properties (UT3) is given in Figure 10. In the next section, the focus is set on how the guidance part of UT1 is embedded in the database structure.

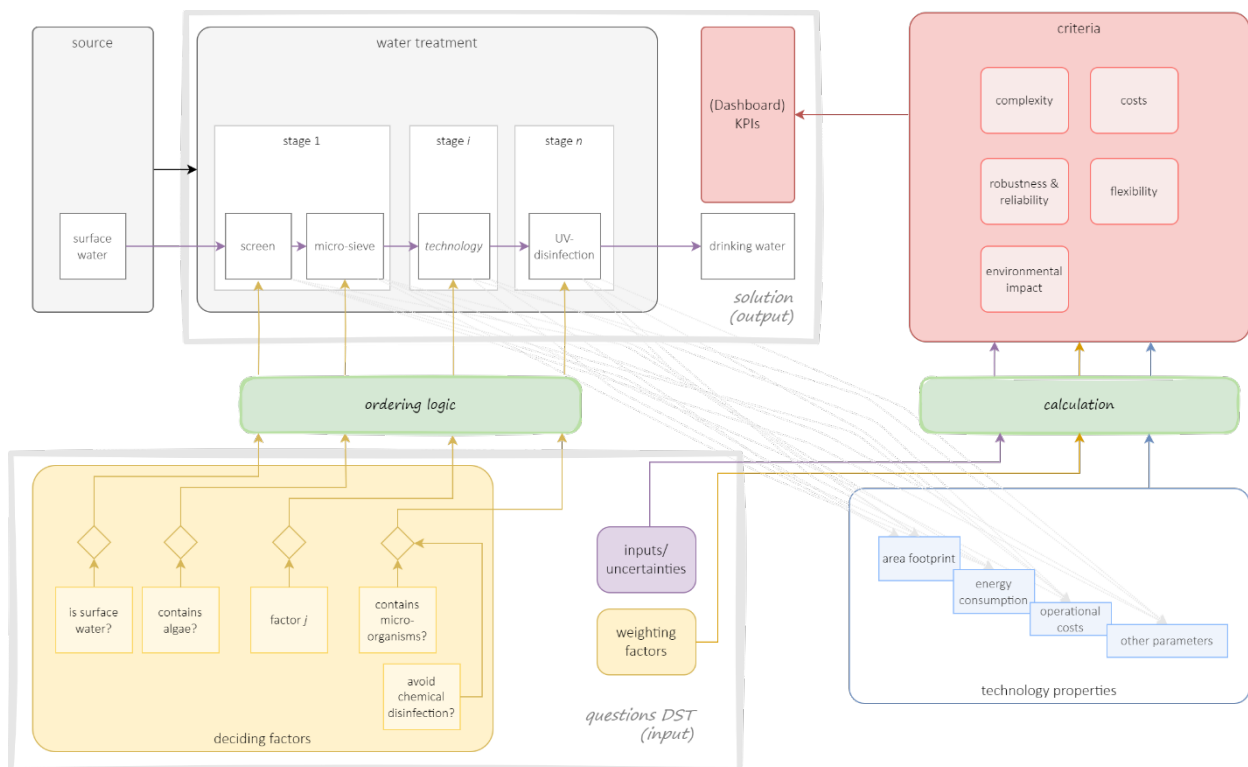


Figure 10: Example of how the decision guidance in UT1 leads to a water treatment configuration via the use of so-called deciding factors, and how each technology is related to its properties and criteria for further evaluation in UT3

### 3.4. Decision guidance part in database structure

The relationships with the different entities (stages, technologies, decision factors) in the decision guidance part of UT1 are fixed within the structure of the database. Each entity is stored as a table, and each entity has its own characteristics. The interrelationship of an entity (the ‘child’ table) is set by a foreign key to another entity (the ‘parent’ table). A foreign key (FK) is a set of attributes in a table that references another key, i.e. the primary key (PK) of another table. Hence, an FK links these two tables. If a table contains a one-to-many or a many-to-many relationship, the name of the table follows the convention to use an underscore to separate the table names which are given by the FKs (e.g. the table ‘stage\_technologies’ which links a stage with technologies).

For the DST, integer numbers are used for the PKs and in most cases, the PK is named as **id**.

### 3.4.1. Stages

For stages, we have the following tables link to a stage:

- **process:** contains characteristics of a treatment process (e.g. submerged rapid sand filtration). The database table ‘process’ is needed to link removal efficiencies to treatment processes. A treatment process can be carried out by different technologies, e.g. removal by activated carbon is possible via granular activated carbon (GAC) or powdered activated carbon (PAC).
  - **id** [PK]
  - **description:** description of the process
  - **name:** (short) name of the process
  - **slug:** the URL slug, i.e. the last part of the URL address that serves as a unique identifier of the page. Can be used to quickly have a web page with information about the entity, in this case a treatment process.
- **stage\_technologies:** a one-to-many relationship table where each stage relates to (possibly many) technologies.
  - **id** [PK]
  - **stage:** FK to stage
  - **technology:** FK to technology
- **stage\_stage:** a many-to-many relationship table, or junction table. A junction table maps two or more tables together by referencing the primary keys of each data table using FKs. See Table 7 for an example.
  - **id** [PK]
  - **stage\_current:** the stage which is placed before the next stage (stage\_next)
  - **stage\_next:** the stage which is placed after stage\_current.

Table 6: Example showing the records of the junction table ‘stage\_stage’. Primary keys and foreign keys are written in bold-face

<b>id</b>	<b>stage_current</b>		<b>stage_next</b>	
<b>1</b>	<b>1</b>	[name: Water intake]	<b>2</b>	[name: Screening]
<b>2</b>	<b>2</b>	[name: Screening]	<b>3</b>	[name: Algae screening]
<b>3</b>	<b>13</b>	[name: Aeration]	<b>4</b>	[name: Trickling filtration]
<b>4</b>	<b>6</b>	[name: Coagulation]	<b>7</b>	[name: Flocculation]
..	..	..	..	..

### 3.4.2. Technologies

Treatment technologies form the backbone of the designed treatment configuration. Each stage consists of one or more technologies. The following tables are linked to technology characteristics:

- **technology:** a table with the names, descriptions, advantages and disadvantages of different treatment technologies, i.e.:
  - **id** [PK]
  - **name:** name of the treatment process
  - **description:** description of the treatment process.
  - **advantage:** each technology has one or more advantages. These are listed for the user during the technology selection.
  - **disadvantage:** each technology has one or more disadvantages. These are listed for the user during the technology selection.
- **stage\_technologies:** the same table as described in paragraph 0.
- **goal\_per\_technology:** a table where the goal of each technology is listed.
  - **id** [PK]
  - **goal:** FK to goal
  - **technology:** FK to technology
- **configured\_technologies:** once a treatment chain of technologies has been selected, the configuration is stored in the parent table 'configuration'. The current (many-to-many) table relates to a configuration in which a technology is present, and in what order.
  - **id** [PK]
  - **configuration:** FK to configuration
  - **technology:** FK to technology
  - **order:** the ordering integer number of the technology (starting with 1 at the drinking water source).
- **technology\_decidingfactors:** for each deciding factor which is considered to be valid (true), one or more technologies are effective.
  - **id** [PK]
  - **deciding\_factor:** FK to table 'decidingfactor'.
  - **threshold\_value:** a numeric value, or null. For dichotomous deciding factors, the threshold value is null.
- **configuration:** this table stores a user-defined name of a treatment configuration, along with the user id and creation date.
  - **id** [PK]
  - **name:** user-defined name of the treatment configuration.
  - **creation\_date:** date and timestamp of creation of the configuration.
- **configured\_techproperties:** each configured technology has properties which are specific to the design configuration, for instance a nominal filtration rate of a rapid sand filter. Furthermore, each technology has its own position in the treatment chain specified by an ordinal number.
  - **id** [PK]
  - **configured\_technology:** FK to table 'configured\_technology'
  - **technology\_property:** FK to table technology\_property
  - **property\_value:** numeric value of the technology property.
  - **technology\_ordinal:** position (integer) number in the treatment chain

### 3.4.3. Deciding factors

A deciding factor is in most cases a dichotomous variable, meaning the answer to the question at hand is either True or False. However, in some cases it is more practical to work with a categorical variable which has more than 2 levels, e.g. in case of removal efficiencies which are binned into discrete categories (3: 'very good removal', 2: 'moderate removal' or 1: 'no removal'). This way, a filtering threshold can be defined by the user to have at least e.g. a 'good removal'. The following tables are part of, or linked to deciding factors:

- **decidingfactor**
  - **id** [PK]
  - **name**: name of the deciding factor
  - **description**: description of the deciding factor
  - **form\_label**: label or short description of the deciding factor which will show up in the HTML web page.
  - **categorical\_variable**: FK to a categorical variable.
- **categoricalvariable**: table with categorical variables
  - **id** [PK]
  - **name**: name of the categorical variable
  - **n\_levels**: integer number of levels. For example, a dichotomous variable (e.g. the variable 'water\_contains\_algae') only has 2 levels: it can be either True or False. When 'n\_levels' > 2, the threshold value in the table **technology\_decidingfactors** has to be specified as a floating or integer number (not NULL).
- **technology\_decidingfactors**: see paragraph 0.
- **technologyform\_decidingfactors**: the sequence of decision factors which is presented in the user interface as a HTML form, is queried from this table. Although graph databases are far more efficient than relational databases for storing, updating and querying decision tree data, there are ways to store the decision tree structure. A possible, suitable candidate which is used for hierarchical data storing in relational databases, is the use of *closure tables* (Karwin, 2010). A closure table is a many-to-many table, where each path from each (decision) node to each of its descendants are stored. Furthermore, a node is even connected to itself. For easier querying, the path length (**path\_length**) is stored as an extra column. Finally, we define whether a path to a child is independent of the answer with the **child\_if\_parent\_true** attribute (e.g. the technology for 'the turbidity is high' question is independent of the previous question) and gets a NULL value; or whether is dependent of a Yes or No answer to the deciding factor (e.g. 'NOM is high' leading to the use of AIEX is dependent of whether UF/MF is used).
  - **id** [PK]
  - **parent\_deciding\_factor**: FK to the table 'decidingfactor'.
  - **child\_deciding\_factor**: FK to the table 'decidingfactor'.
  - **child\_if\_parent\_true**: integer number (0: false, 1: true) for *yes* or *no* answers on the parent node, or NULL value if it is independent of the parent deciding factor.
  - **path\_length**: integer number. If the child node is directly connected to the parent node, then the path length is 1.
  - **form\_tree**: there can be multiple questionnaires, for each drinking water source there is at least one decision tree.

### 3.4.4. Entity Relationships

The relationships between the tables as mentioned in paragraphs 0, 0 and 0 are schematically depicted by Entity-Relationship-Diagrams (ERDs) in Figure 11.

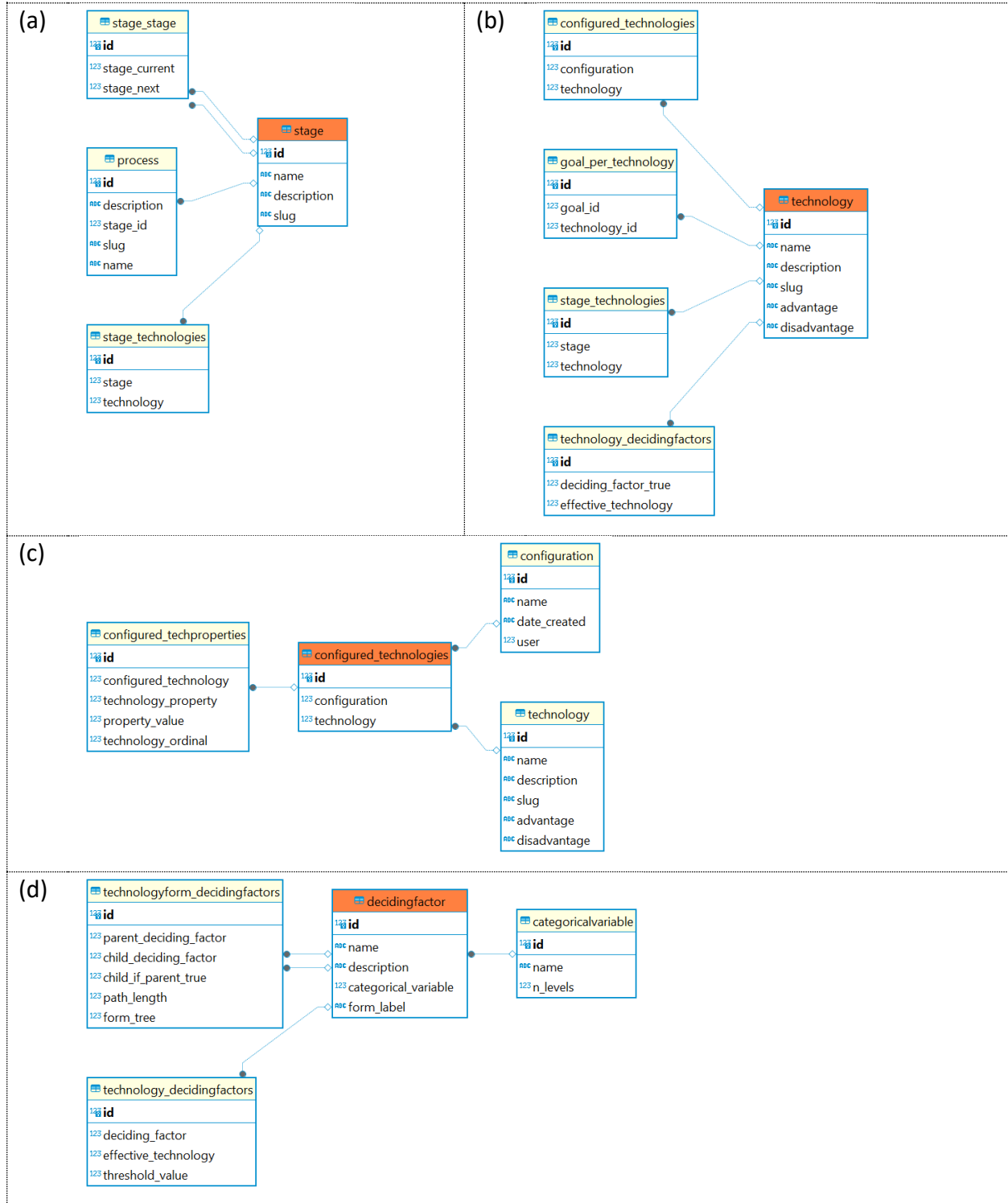


Figure 11: ERD of the 'stage' (a), 'technology' (b), 'configured\_techproperties' (c) and 'decidingfactor' (d) table

For reference purposes, the ERD of the complete database is given in Figure 12 Note that some tables and relationships are subject to change, because not all tables are translated to code, and tested.

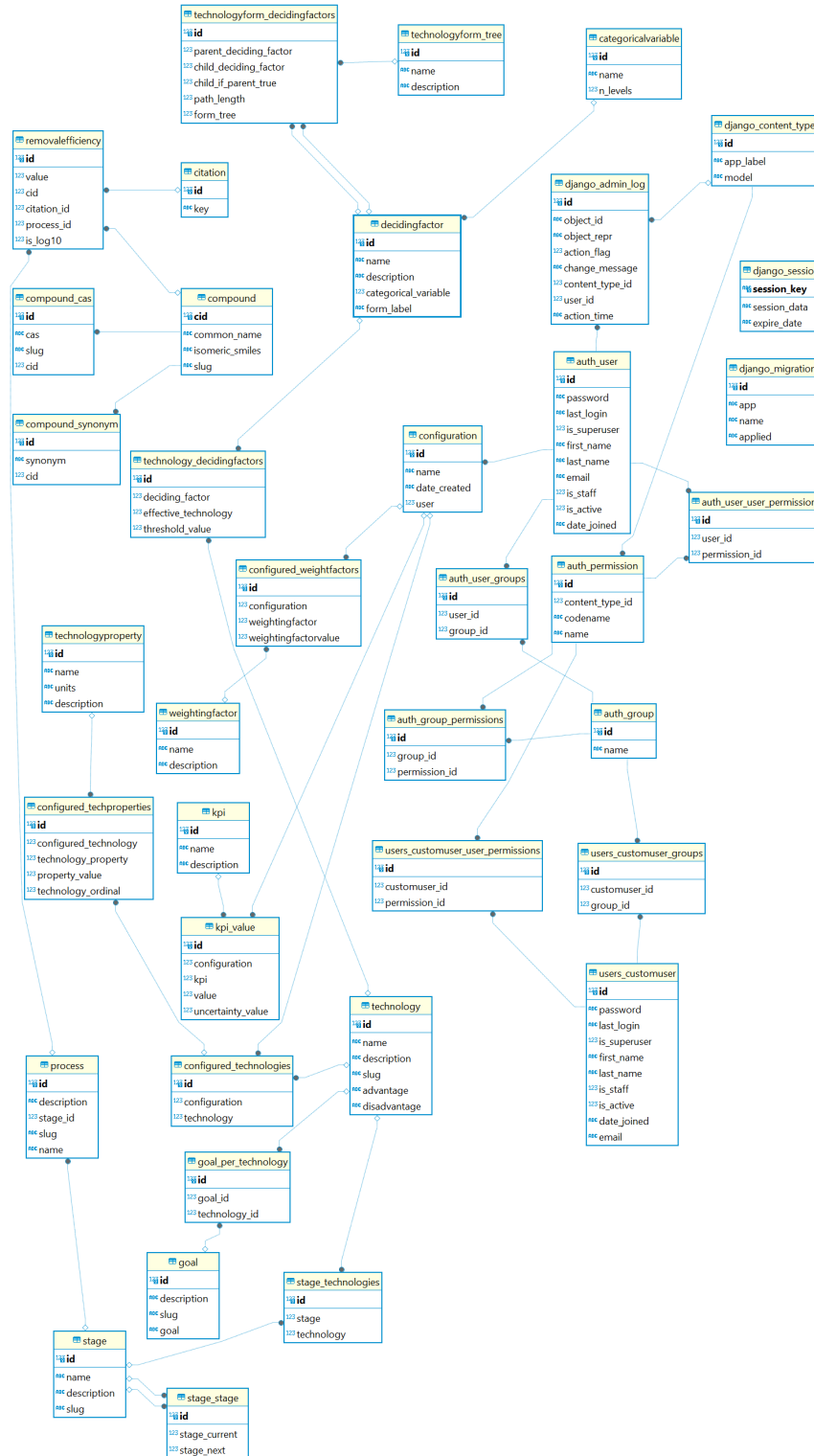


Figure 12: ERD of the complete ToDrinQ database, version v1.

## 4. Identification of key factors and their uncertainty for designing DWTPs

Four key factors for water treatment plant design will be identified and translated to code:

1. change in the future demand (e.g., the number of users)
2. change in the supply capacity (e.g., addition of treatment equipment)
3. change in the operating rules (e.g., a new design of treatment trains, more stringent water quality standards)
4. change in the technology (e.g., a new treatment technology which boosts treatment efficiency or lowers operating costs).

Factors (i) and (ii) bring (deep) uncertainty in the design process. With this supporting tool we aim to tackle these issues by introducing flexibility and adaptability into factors (iii) and (iv). Therefore, both operational flexibility (i.e., flexible decisions made by system operators) and capacity flexibility (e.g., shifting between raw water sources, buffer capacities only used in emergent cases or new technology boosting the capacity) will be considered. Besides these factors, 'hedging measures' to mitigate the consequence of (un)expected events (e.g., reserved spare capacities to deal with severe droughts or equipment malfunction) will be considered.

The full development of these features is part of Task 6.3 and will be reported in Deliverable 6.2 (M36).

## 5. Current DST development status

The first (alpha) version ( as a proof of concept) of the DST is developed as a Python notebook. Upcoming versions will be a Django web application. This refactoring is deemed necessary in order to

- (i) improve the interface such that it is more user friendly,
- (ii) improve the flexibility of the tool by enabling the user to modify settings, store and restore treatment configurations with the aid of a database,
- (iii) provide an overview of criteria scores (KPIs) regarding the chosen design,
- (iv) provide a web (graphical) interface such that process technologists and water managers have global access to the tool without knowledge of Python. Additionally, all settings and data are stored in a database and selected data can be added, modified or removed.

A blueprint of the web application architecture and database structure is given in .

In the following subsections, screenshots the present condition of the first (alpha) version of the DST is showcased. The current version does not have a graphical user interface (GUI).

The preliminary design procedure is based on the following workflow:

1. *Identification of nominal flow.* Determine the nominal flow of the DWTP based on population numbers, consumption, irrigation needs, industrial needs and number of units per lane.
2. *Selection of water source.* The user has to select which drinking water source is available.
3. *Identify and select treatment stages.* The user has to define and identify the required treatment processes given a list of feasible options.
4. *Select treatment technology and determine technology order.* An example of this step is presented in line 4 of the 5-1 table.
5. *Show DWT preliminary design of selected technologies.* An example output of a treatment step based on certain user selections is presented in line 5 of the 5-1 table.
6. *Output performance indicators.* The footprint calculation is presented in line 6 of the 5-1 table.

A video presentation of the present form of the tool can be found in the following link: <https://www.youtube.com/watch?v=PtWiVbBbQWo&t=8s>.

In Table 8, the design steps of the workflow are shown using screenshots of the proof-of-concept DST.

Table 7: A brief presentation of the current version of the DST

1. Identification of nominal flow	Population numbers (comma-separated):5000 Water consumption per person per day (l/p/day): 125 Leakage estimation (0-1): 0.2 Are there any irrigation needs? (Yes/No): No Are there any industrial needs? (Yes/No): No Set the number of different consumption periods: 2 Maximum water consumption per person per day (l/p/day): 250 Set the number of independent lanes: 2 Number of units per lane:2
2. Selection of water source	Select one option: 1. Groundwater 2. Surface 3. River bank water Enter the number corresponding to your choice: <input style="width: 100px;" type="text"/>

<p>3. Identification of treatment stages</p>	<p>Is the algae concentration high?:            1. Yes            2. No            Enter your choice (1/2): 1            Use of an advanced technology (UF or MF)?:            1. Yes            2. No            Enter your choice (1/2): 2            The average maximum measured turbidity is 14.937999999999999            Is turbidity above 1 NTU?:            1. Yes            2. No            Enter your choice (1/2): 1            The average maximum measured DOC is 3.3732999999999995            NOM concentration in the water in (mg/l): 4            The average maximum measured hardness is 237.0            Is hardness in the water high?            1. Yes            2. No            Enter your choice (1/2): 1            Is disinfection required?            1. Yes            2. No            Enter your choice (1/2): 1            Treatment process: ['Screens', 'Microsieves', 'Coagulation', 'F'</p>																				
<p>4. Select treatment technology and determine technology order</p>	<p>Coagulation:            1. Cascade Mixing            2. Inline Mixing            3. Dynamic Mixing            Enter your choice (1/3): 1            Flocculation:            1. Static mixing            2. Dynamic Mixing            Enter your choice (1/2): 1            Floc Removal:            1. Sludge Blanket Clarification            2. Horizontal Settling            3. Titled-plate Settling            4. Dissolved Air Flotation            Enter your choice (1/4): 4            Softening:            1. Cationic IEX            2. Pellet Softening            3. NF/RO</p>																				
<p>5. Show DWT preliminary design of selected technologies</p>	<table border="1" data-bbox="566 1400 1428 1635"> <thead> <tr> <th>Treatment Steps</th> <th>Treatment Technologies</th> </tr> </thead> <tbody> <tr> <td>0 Screens</td> <td>Screens</td> </tr> <tr> <td>1 Microsieves</td> <td>Microsieves</td> </tr> <tr> <td>2 Coagulation</td> <td>Cascade Mixing</td> </tr> <tr> <td>3 Flocculation</td> <td>Static mixing</td> </tr> <tr> <td>4 Floc Removal</td> <td>Dissolved Air Flotation</td> </tr> <tr> <td>5 Softening</td> <td>Cationic IEX</td> </tr> <tr> <td>6 Sand Filtration</td> <td>Dual Media Filtration</td> </tr> <tr> <td>7 OMP Removal</td> <td>Granular Activated Carbon Filtration (GAC)</td> </tr> <tr> <td>8 Disinfection</td> <td>Chlorination</td> </tr> </tbody> </table> <p>The proposed treatment train based on preceding user choices.</p>	Treatment Steps	Treatment Technologies	0 Screens	Screens	1 Microsieves	Microsieves	2 Coagulation	Cascade Mixing	3 Flocculation	Static mixing	4 Floc Removal	Dissolved Air Flotation	5 Softening	Cationic IEX	6 Sand Filtration	Dual Media Filtration	7 OMP Removal	Granular Activated Carbon Filtration (GAC)	8 Disinfection	Chlorination
Treatment Steps	Treatment Technologies																				
0 Screens	Screens																				
1 Microsieves	Microsieves																				
2 Coagulation	Cascade Mixing																				
3 Flocculation	Static mixing																				
4 Floc Removal	Dissolved Air Flotation																				
5 Softening	Cationic IEX																				
6 Sand Filtration	Dual Media Filtration																				
7 OMP Removal	Granular Activated Carbon Filtration (GAC)																				
8 Disinfection	Chlorination																				
<p>6. Output performance indicators, e.g. area footprint</p>	<p>Footprint per unit (m2) 25.0            Footprint of Sand Filtration(m2) 50.0            Total number of units 4            Total number of lanes 2            Sand filtration Length 4.0            Sand filtration width 25.0</p> <hr/> <p>An example of the footprint calculations for dual media rapid sand filtration</p>																				

## 6. Conclusions and future work

This deliverable includes the technical background and the alpha version of the DST tool for the Adaptable design of small drinking water plants. There are several pending and future activities for further development. Future work will focus on several activities. Some can be considered refinements and implementation related to T6.1 (key characteristics) and T6.2 (key factors and uncertainties) to be included in the next versions of the DST. In addition, development and implementation is scheduled for T6.3 (design goals) and T6.4 (development of the DST-final version):

- Refinements and implementation related to T6.1
  - Refactoring and finalising footprint calculations for the treatment technologies which are included in the database.
  - Collect removal efficiencies per treatment technology for water quality parameters and include these in the database.
  - Define the methodology to calculate scores per criterium for each treatment technology.
- Refinements and implementation related to T6.2
  - Introduce uncertainty factors and develop methods to calculate the propagation of these uncertainties.
  - Identify pathways to mitigate deep uncertainties associated with decisions in the design of DWT, like institutional or regime changes, severe flooding, etc.
  - Define the methodology to calculate and visualise the effect of a change in a key factor (e.g. water consumption).
- Ongoing and future work related to T6.3 and T6.4
  - Import values of different technology properties (e.g. head losses), including removal efficiencies, into the database.
  - Functionality to add new treatment processes;
  - Identify and implement the key design goals in the DST;
  - Translate the structure of the database to the ORM and finalise and test the decision tree storage into/querying from the database;
  - Develop and test APIs for the calculation modules and querying or sending data to the database.
  - Develop and test the ordering logic, MCA (KPI) and uncertainty propagation.
  - Develop and test the visualisation of KPIs/performance criteria, also when there is a change in key factors.
  - Give feedback to the user when either no technology (or treatment chain) satisfies the user-specified constraints, or, alternatively, yield the best possible treatment configuration even if one or more water quality, or other constraints are not satisfied.
  - Test a beta version of the tool by end users

A further explanation of two key aspects in this work is given in paragraph 6.1 and 6.2.

### *6.1. Further refinements regarding uncertainty*

Due to the fact that many factors influence the decision workflow and their associated uncertainties (climate change and its impact on water quality, future water demand, technological advancements, institutional preferences for environmental impact, flexibility and/or economical costs, etc.), it is not feasible to determine and quantify the uncertainty for every key design parameter. Instead, key design

parameters are identified and selected where uncertainty heavily impacts design choices. These parameters are referred to as uncertainty factors, e.g. the uncertainty amount of water consumption per inhabitant.

Next to the identification and selection of uncertainty factors, a methodology framework will be selected to prioritize (deep) uncertainty pathways and a means to qualitatively or quantitatively determine uncertainties and their mitigation measures. The uncertainty pathways can be obtained by for instance using methods from Decision Making Under Deep Uncertainty (DMDU) and methods from Transition Management (Malekpour et al., 2020). For some pathways, the tool will include quantified uncertainty propagation, as will be the case for e.g. area footprint calculations and nominal flow calculations. For other pathways, a qualitative approach will measure the amount of uncertainty associated with a preliminary design.

## 6.2. Next steps regarding key design goals

Key design goals referring to (i) the use of produced water for different end-users and their water quality requirements, (ii) the annual turnover of a treatment plant and other, relevant associated costs will be further explored and defined and (iii) the resilience and flexibility of the DWT system, and its environmental impact will be investigated. Methods will be selected that quantify these design goals.

## 6.3. Next steps regarding development of the DST

The development of the Django web version of the DST will consist of a couple of phases, i.e.:

1. Development of a *prototype Django web tool* where a preliminary design is selected based on a limited set of criteria, e.g. water demand and water source. The ordering logic is implemented in this version, translated into ORM and stored in the database, along with calculation methods of the needed capacity (e.g. area footprint, nominal daily flow). The prototype version and subsequent versions will act as a means to gather feedback from end-users about user requirements, (missing) features and expected outcome.
2. Development of a *beta Django web tool* where the MCA procedure acts as a means to weigh key performance indicators for resilience, costs, environmental impact and end-usage as defined in Task 6.3. Technological properties which relate to these indicators and which will be used for the MCA will be defined and stored in the database. Also, quantified uncertainty and qualitative measures of uncertainty will be stored in the database and used to calculate an uncertainty metric for different end-points, like expected water demand.
3. Inclusion of plausible future scenarios in the release candidate of the DST as identified in Task 6.2, will be included. The methodology following from Task 6.2 acts as a basis for further development of the tool and (workshop) sessions with end-users will feed the refinement of the user interface as well as the workflow when using the tool. Finally, the tool will include a flexible selection of designs that enhance adaptability.

#### 6.4. Innovation, impact and impact pathways

Several design and engineering software tools exist to support engineers in the design planning and engineering phase when new drinking water plants are to be constructed. A non-extensive overview of software packages which actively market their solution on (except for the proposed solution in this work) the website *XPRT environmental* is listed in Table 6-1, and their main features are listed in Table 6-2. Software packages focused on only membrane and ion exchange treatment processes, like the WAVE DuPont Software® are excluded from the overview, while iNode is focusing only on conventional processes. To the best of our knowledge, no similar software package to this one exists as an alternative.

What makes the DST innovative is: (i) the ability to compare different designs based on different criteria related to environmental impact, costs, flexibility and robustness and (ii) that methods are included that deal with uncertainty in various aspects of the design process. In contrast, EVS water designer is a tool aimed at process technologists and engineers to support in getting a (refined) design needed for construction and engineering phase of a DWTP. It can generate a process flow diagram, equipment lists, etc. but lacks the (planned) features of the DST. The features of iNode WTP are comparable to Water designer, but the application only covers conventional treatment processes. An overview of these functionalities is given in Table 6-3.

The foreseen impact of the DST lies in the ability to support, in Open Access, a design team to better deal with an uncertain future where extreme weather due to climate change, socio-economic or (geo)political changes and/or major demographic changes can impact water availability, water quality, costs and resources for treatment (e.g. chemical dosing or energy). Additionally, the tool could also be used by investment banks like the European Investment Bank (EIB) to have a quick-scan, preliminary assessment or audit when new, climate-resilient water systems are tendered, leading to a cheaper and more transparent design process with a higher quality end product. The impact pathway will be paved by having workshops with stakeholders and end-users in order to shape its features regarding environmental and resilience criteria, get acquainted with the tool and dissemination within national and international water network groups.

Table 8: design supporting software packages or services

Name/Abbreviation	Tool [company]	Commercial (C) or Public (P)	Stand-alone, Web-based service (SaaS <sup>1</sup> )	Country/Region
Water designer	<a href="#">EVS Water designer</a> [envirosuite]	C	Web-based	Australia
iNode WTP	<a href="#">iNode WTP</a> [inode design]	C	SaaS	India
DST*	Design support tool	P	Web-based	European Union

<sup>1</sup> SaaS: Software-as-a-Service

Table 9: Main features and included technologies of software water treatment design tools. \*DST: current work.

Tool	Commercial (C) or Public (P)	Technologies	Main features
Water designer	C	(A.o.) Flocculation, Granular media filtration (sand/activated carbon), Ion exchange, Pressure (media) filters, RO, NF, ozone, pellet softening, clarifiers, aeration tanks, cartridge filter, dissolved air flotation, settling pond, UV disinfection, UF, storage tank, screening and rotating equipment (pumps)	Multiuser application with drag and drop flow sheeting, with operating or design calculation modes. Can generate among others process diagram, mass and heat balance and equipment lists.
<a href="#">iNode WTP</a>	C	Only conventional processes, i.e. cascade aeration, rapid sand filtration, flocculation (e.g. radial flocculators, mechanical flocculators)	Web-based forms, generates hydraulic design reports and drawings
Design support tool*	P	Filtration processes, Coagulation softening, RO/NF, UF/MF, GAC, PAC, Advanced oxidation (ozone, UV + H <sub>2</sub> O <sub>2</sub> ), slow sand filtration	Web-based forms

Table 10: Main functionalities of water treatment design software applications.

Tool	Treated water (ind: industrial, dw: drinking water sources)	Environmental impact	Speciation	Material balance	Hydraulic sizing	Reporting	Operational costs	Investment costs	TCO or whole-life costs	Flexibility criterion	Resilience criterion
Water designer	DW, Ind	-	✓	✓	✓	✓	✓	?	✓	-	-
iNode WTP	DW	-	-	-	✓	✓	-	-	-	-	-
DST	DW	✓	-	-		-	✓	✓	✓	✓*	✓*

## References

- Cohn, M. (2004). *User Stories Applied: For Agile Software Development*. Addison-Wesley. <https://dl.acm.org/doi/abs/10.5555/984017>
- Davis, M. L. (2011). *Water and wastewater engineering : design principles and practice*. McGraw-Hill.
- Django documentation*. (n.d.). Retrieved May 23, 2024, from <https://docs.djangoproject.com/en/5.0/>
- Drinking Water Treatability Database*. (n.d.). (2024) Database available from KWR
- European Parliament and Council of the European Union. (2000). *Directive 2000/60/EC of the European Parliament and of the Council establishing a framework for Community action in the field of water policy*. Official Journal of the European Communities, L 327, 1–73. Retrieved from <https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32000L0060>
- Fielding, R. T. (2000). *Architectural Styles and the Design of Network-Based Software Architectures* [Doctoral thesis, University of California]. <https://cir.nii.ac.jp/crid/1571135651036132480>
- Karwin, B. (2010). *SQL Antipatterns. Avoiding the Pitfalls of Database Programming* (J. Carter, Ed.). The Pragmatic Bookshelf.
- Kostenstandaard Tool*. (n.d.). <https://kostenstandaard.nl>.
- Lucassen, G., Dalpiaz, F., Martijn, J., Van Der Werf, E. M., & Brinkkemper, S. (2015). Forging high-quality user stories: towards a discipline for agile requirements. *IEEE 23rd International Requirements Engineering Conference (RE)*. <https://doi.org/10.1109/RE.2015.7320415>
- Malekpour, S., Walker, W. E., de Haan, F. J., Frantzeskaki, N., & Marchau, V. A. W. J. (2020). Bridging Decision Making under Deep Uncertainty (DMDU) and Transition Management (TM) to improve strategic planning for sustainable development. *Environmental Science and Policy*, 107. <https://doi.org/10.1016/j.envsci.2020.03.002>
- U.S. Environmental Protection Agency. (n.d.). *Drinking Water Treatability Database (TDB)*. Retrieved 18-11-2024, from <https://tdb.epa.gov>
- World Health Organisation. (2017). *Guidelines for drinking-water quality: Fourth edition incorporating the first addendum*. Geneva: World Health Organization. Retrieved from <https://www.who.int/publications/i/item/9789241549950>

The revised EU Drinking Water Directive promotes a risk assessment and risk management approach for securing drinking water supply in the context of climate change and increased pollution. However, this approach is challenged by insufficient information that is available to operators, especially in real time, on compounds and organisms of emerging concern, such as pesticides, pharmaceuticals, disinfection by-products, heavy metals and pathogenic microorganisms. We argue that if drinking water treatment could leverage novel technologies and design philosophies, and more agile operational actions could be supported, drinking water supply systems could become more adaptable and robust without expensive infrastructural investments. In this context, ToDriNq develops and tests a compendium of modular, complementary, innovative solutions (the 'ToDriNq Toolkit') that provide new information and better support tools to operators and designers to adapt to (short- and long-term) changes in water quality, while obtaining high drinking water quality at the tap. ToDriNq develops novel real time sensing and water quality monitoring technologies, innovative treatment systems (especially suitable for small-scale/modular, adaptable treatment plants) and interoperable decision tools that support resilient, evidence-based treatment plant design and improved overall water system operational awareness and response.



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