Data Management Plan - initial

Deliverable D6.2, WP6

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History of Versions		
Version	**Publication Date**	**Change**
1	17.04.2023	Submitted to Commission
1.1	11.07.2024	Final review
2	12.07.2024	Submitted to Commission

History of Changes	
Date/section	**Nature of change and reason**
11.07.2024 page 2	To address the reviewers' comment: When updating the deliverable, please include in the history of changes where and what have been added comparing to the initial version of the deliverable. This will facilitate to review the deliverable: Previous "History of Changes" renamed to "History of Versions". "History of Changes" added.
11.07.2024 page 6	The list of abbreviations has been expanded.
11.07.2024, section 5, page 14-15	To address the comment "The name of the project Data Manager (announced in the GA), the reference in section 5 is not explicit enough": The following sentence has been added: "Anissa Grieb has been assigned as the project Data Manager." Also, a list with persons responsible for the implementation of the data management plan for each partner have been added.
11.07.2024, section 1.1 page 7	To address the comment "-the explanation of the main EU rules about data management, as open science is a legal obligation under Horizon Europe; the FAIR principles are explained, but not the aim and meaning of open science, of the "as open as possible, as closed as necessary" principle, or of the open access to research,": Paragraph 1.1 has been rewritten significantly.
11.07.2024, section 1.1 page 7	To address the comment "-the specific rules concerning the scientific publications, notably the associated costs eligibility (as these rules have change compared to H2020 projects), the following sentence has been added: Only publication fees in full open access venues for peer-reviewed scientific publications are eligible for reimbursement.
	To address the comment "The following information is missing: […] the chosen repositories to store and make data accessible (Zenodo, Argos, …) and the ad-hoc procedures to collect, name, store and deposit datasets (a metadata template is mentioned but not the procedure)" the changes below have been made
11.07.2024, Section 2.1, page 10	"Data, that will be re-used" replaced by "External and open-source data, that will be re-used"
11.07.2024, Section 2.3, page 11	In the first paragraph, several examples for the usage of historic data have been added. In the second paragraph, fifth line, "and climate projections (https://cds.climate.copernicus.eu/index.php/cdsapp#!/home)" has been added
09.07.2024, section 2.4, page 11	"The data are generated" replaces "The date is generated"; "The data are originated" replaces "The data originates" ; In the third line of the second paragraph: "resilience" replaces "adaptation"

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09.07.2024, section 3.1, page 11-12	Section 3.1 has been significantly rewritten
Section 3.2.1, page 13	The final paragraph has been rewritten.
Section 3.2.2, page 13	To clarify the meaning “Research data that are required to verify published results will be released on open-source repositories under FAIR guidelines. ”replaces “ Research data that are required to verify published results will be published on open source repositories under FAIR guidelines.”
Section 3.3, page 14	The following has been added to the first sentence “(See Section 3.1 for further details)”.
Section 3.4, page 14	The following has been added to the first sentence “(See Section 3.1 for further details)”. The order of the sentences has been changed. “journals” replaces “articles”
	To address the recommendation “In addition, to complement the sections 2.1 and 2.3, a preliminary list of datasets that will be reused/ collected/generated, per WP and per task, would be recommended” the change below has been made:
09.07.2024, section 2.1 page 10	“Table 1: Preliminary list of data sets in SafeCREW” has been introduced.

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Abstract

The data management plan ensures that SafeCREW's data follows the FAIR guidelines and adheres to the Guidelines on the Rules on the Open Access to Scientific Publications and Open Data Access to Research Data in Horizon Europe.

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Abbreviations

CC0	Creative Commons Public Domain Dedication
CC BY	Creative Commons Attribution International Public Licence
CS#2, CS#3	Case study #2, case study #3
DBP	Disinfection by-product
DBPFP	Disinfection by-product formation potential
DMP	Data Management Plan
DOC	Dissolved organic carbon
DOI	Digital Object Identifier
DWDN	Drinking water distribution network
DWSS	Drinking water supply systems
DWTP	Drinking water treatment plant
EC	European Commission
FAIR	Findable, Accessible, Interoperable, Reusable
GA	Grant Agreement
GC	Gas chromatography
IPR	Intellectual Property Rights
LC-FT-ICR-MS	Liquid chromatography Fourier-transform ion cyclotron resonance mass spectrometry
LC-OCD	Liquid chromatography – organic carbon detection
NOM	Natural organic matter
PI	Persistent identifier
THM	Trihalomethane
TOC	Total organic carbon
URI	Uniform resource identifier
WP	Work package

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1 Introduction

This document is the initial version of the Data Management Plan (DMP) of the SafeCREW project. It is part of Task 6.2 of Work Package 6 "Management" and will be updated twice for Deliverable 6.4 (DMP midterm) and Deliverable 6.5 (DMP final).

The DMP ensures that SafeCREW's data follow the FAIR guidelines and adheres to Rules on the Open Access to Scientific Publications and Open Data Access to Research Data in Horizon Europe.

1.1 Open Access to Scientific Publications and Open Data Access to Research Data

Open science is a policy priority for the European Commission. Open science[1] is an approach to research based on open cooperative work that emphasizes the sharing of knowledge, results and tools as early and widely as possible. It is mandatory under Horizon Europe, and it operates on the principle of being 'as open as possible, as closed as necessary'. 'As open as possible, as closed as necessary' means that results and data may be kept closed if making them public in open access is against the researcher's legitimate interests. Examples include to commercially exploit their research results, or if it is against any obligations mentioned in the Grant Agreement (e.g., personal data protection).

The Specific Rules for Open Science and Open Research Data Management refer to Article 17 of the SafeCREW Grant Agreement and are set out in Annex 5 (p. 169-171 GA). Open science requires open access publications and to make research data as open as possible and as closed as necessary.

Open access means the provision of online access to scientific information free of charge. This shall result in more efficient science and innovation. Open access to scientific research refers to two categories:

- Peer-reviewed scientific publications (like research articles)
- Scientific research data (in particular data underlying these publications)

The Specific Rules in Annex 5 of the GA define the obligations for SafeCREW beneficiaries with respect to peer-reviewed scientific publications and scientific research data. In particular, beneficiaries must ensure that:

- a machine-readable electronic copy of the published version or the final peer-reviewed manuscript accepted for publication is deposited in a trusted repository latest at the time of publication and
- immediate open access is provided to the deposited publication via the repository, under the latest available version of the Creative Commons Attribution International Public Licence (CC BY) or a licence with equivalent rights.

The Specific Rules also define obligations regarding information about related research output and the specification of metadata (see the GA for details).

Only publication fees in full open access venues for peer-reviewed scientific publications are eligible for reimbursement.

[1]The text is based on the guidance of the European Research Executive Agency (REA) on Open Science in Horizon Europe (https://rea.ec.europa.eu/open-science_en) and on Annex 5 of the SafeCREW GA referring to Art 17 GA, p. 169-171).

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Regarding the research data management, the beneficiaries must manage the digital research data generated in the action ('data') responsibly, in line with the FAIR principles and by taking all of the actions listed in the Specific Rules referring to Article 17 GA. These actions comprise:

- the establishment of this Data Management Plan and its regular updates;
- depositing the data in a trusted repository as soon as they are validated as laid down in this DMP;
- ensuring open access to the deposited data via the repository as soon as possible after the validation, under the latest available version of the Creative Commons Attribution International Public License (CC BY) or Creative Commons Public Domain Dedication (CC 0) or a licence with equivalent rights, following the principle 'as open as possible as closed as necessary'.

'As open as possible as closed as necessary' may include exceptions from the principle of Open Research Data Access, if

- it is against the beneficiary's legitimate interests, including regarding commercial exploitation, or
- it is contrary to any other constraints, as they are justified in section 3.2.1 of this DMP.

The existing rules on the metadata of SafeCREW's deposited data are specifically described in section 2 of this DMP.

1.2 FAIR guidelines

For the management of research data, the FAIR guidelines were described to ensure open access for research data. FAIR stands for:

- Findable
- Accessible
- Interoperable
- Re-usable

A more detailed description of the FAIR principles can be found in Figure 1 or on www.go-fair.org.

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Box 2 | The FAIR Guiding Principles

To be Findable:
F1. (meta)data are assigned a globally unique and persistent identifier
F2. data are described with rich metadata (defined by R1 below)
F3. metadata clearly and explicitly include the identifier of the data it describes
F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:
A1. (meta)data are retrievable by their identifier using a standardized communications protocol
A1.1 the protocol is open, free, and universally implementable
A1.2 the protocol allows for an authentication and authorization procedure, where necessary
A2. metadata are accessible, even when the data are no longer available

To be Interoperable:
I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
I2. (meta)data use vocabularies that follow FAIR principles
I3. (meta)data include qualified references to other (meta)data

To be Reusable:
R1. meta(data) are richly described with a plurality of accurate and relevant attributes
R1.1. (meta)data are released with a clear and accessible data usage license
R1.2. (meta)data are associated with detailed provenance
R1.3. (meta)data meet domain-relevant community standards

Figure 1: Wilkinson et al., 2016; DOI: 10.1038/sdata.2016.18

This document follows the template provided by the European Commission on DMP structure and dmponline.dcc.ac.uk. It will describe the type of data generated in the SafeCREW project, where it will be deposited and how FAIR guiding principles are kept.

2 Data Summary

2.1 Data created within SafeCREW project

The following research data will be collected and created in the project:

- Water quality parameters from three case study sites (chemical, microbiological, physical data, geo-location)
- Research data from lab experiments (chemical, microbiological, physical data)
- Correlations between parameters feeding into models and software

In detail the research data are:

- Toxicity data on DBP compounds
- Toxicity data on water (mixtures)
- NOM composition of water (mixtures)
    - At different locations
    - With different treatments
- Fluorescence values of water (mixtures)
- Cell counts in DWDN and wells
    - At different locations
    - With different treatments
- DBP composition of water
- THM composition of water

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  - At different locations
  - With different treatments
- Microbial indicators, e.g. *E.Coli*
  - At different locations
  - Time series

External and open-source data that will be re-used:

- Satellite data
- Historical water quality parameters from participating water works

From existing and generated data, correlations between various parameters will be analysed and fed to models and software that will be created.

The following table displays a preliminary list of data sets that is envisaged to be collected and/or generated in the course of the project. This list will be monitored, complemented and refined if the availability and suitability of existing data for the purposes of the project is evaluated.

Table 1: Preliminary list of data sets in SafeCREW

No	FAIR data set	WP, task, case study
1	Data sets for advanced analysis of NOM by coupling LC to FT-ICR-MS with LC-OCD/fluorescence data to evaluate treatment impact on NOM and associate generation of regulated and non-regulated (sulfonated) DBPs.	WP2, task 2.5, CS#1-3
2	Data set of NOM and DBPFP characterization through DWTP associated to different treatment steps	WP2, task 2.3, task 2.5, CS#2, CS#3,
3	Data set of microbiological characterization through DWTP associated to different treatment steps	WP2, task 2.5, CS#3
4	Data set of microbiological and chemical characterization and in vitro toxicity profiling, at the outlet of different DWTPs supplied by groundwater	WP2, task 2.6, CS#2
5	Data set enabling characterization of DBPs along the DWDN and the interactions with relining resins	WP3, task 3.1, CS#2
6	Data set of in vitro toxicity profiling in different kinds of water (treated, untreated) along the DWDN	WP3, task 3.2, CS#3
7	Data set of microbiological characterization in DWDN	WP3, task 3.2, CS#3
8	Data set of hydraulic online DWDN parameters for CS#3 model calibration	WP3, task 3.2, CS#3
9	Data set of water quality online DWDN parameters for CS#3 for early DBP prediction model	WP3, task 3.2, CS#3
10	Collected data from full scale DWDN lab monitoring of CS#3 for early DBP prediction model	WP3, task 3.2, task 3.3, CS#3
11	Simulated data set of DBPs predictions for optimal set-points for chlorination boosters in the network	WP3, task 3.4, CS#3
12	Dataset for DBPs-prediction models and decision support on DWDN management	WP3, task 3.4
13	Data sets defining climate change scenarios for relevant parameters for DWSS accompanying existing climate projections	WP4, task 4.1
14	Data set accompanying the development of soft sensors for three case studies in the drinking water sector to model target parameters by measuring easy-to-measure parameters	WP4, task 4.2, CS#2, CS#3
15	Data set for guidelines for climate change adaptation currently non-disinfected DWSS with high DOC	WP4, task 4.4, CS#1 (B)

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2.2 Data formats

Most chemical and physical parameter data will be generated in table format (.xlsx, .csv, .txt, .asc, .fcs) or database format (.int, .float), whereas reports and papers are in text or table documents (.docx, .pdf, .xlsx) and mathematical models and software are in text code files (.txt, .r). To ensure compatibility with long-term archives and usability, we will preferentially store the data additionally as pdf/a, txt, asc or xml for documents, wav for audio and tiff/tif for images.

Large datasets will be generated in particular during high frequency on-line measurements. In total, we expect up to 10 GB of data, varying between the experiments.

2.3 Usage of existing data

We will use historic large data sets from case study sites (e.g., water quality and quantity parameters), open-source weather (like, temperature, precipitation, etc.) and satellite imagery data for model calibration and tools development, and climate projections (e.g., precipitation, water and air temperatures, water availability, etc.) to define future scenarios. These data has been previously validated by the owner. Existing data from previous projects will also be used, that are so far unpublished on internal servers.

These existing data is used to increase the knowledge on correlation between parameters and deducing consequences. The weather and satellite data will be exported from on-line and open-source databases (such as XEMA (meteocat, https://www.meteo.cat/observacions/xema) for meterological data and Copernicus for satellite data (https://cds.climate.copernicus.eu/#!/home) and climate projections (https://cds.climate.copernicus.eu/index.php/cdsapp#!/home) as well as images from Sentinel2 (https://scihub.copernicus.eu/dhus/#/home) and Landsat (https://earthexplorer.usgs.gov/)).

2.4 Purpose of data generation

The data are generated to increase knowledge on DWSS adaptation to face climate change impacts. The data are originated from sensors (e.g. pH, UV, chlorine, turbidity, conductivity, water level, water flow), and lab equipment (e.g. flow cytometer, GC, TOC, LC-OCD) as well as lab experiments (e.g. microbial cultivation).

The generated data and knowledge within the project might be useful to drinking water related organisations (utilities, industry, private companies, etc.) that are exploiting DWSS for a better resilience of their systems face to climate change impacts. Data might also be useful for other researchers in this research topic. The results generated from the raw data are useful for policy makers, government, other projects, regulators and the general public.

3 FAIR Data

3.1 Making data findable

SafeCREW's peer-reviewed scientific publications will be published in full open access journals to comply with the Horizon Europe obligations. Only in this case, publication costs can be reimbursed by the project. The open access journals will provide DOIs for the articles that are published and articles will be accessible immediately after the publication. Metadata for scientific publications must at least provide the following information:

- publication (author(s), title, date of publication, publication venue);
- Horizon Europe funding;
- grant project name, acronym and number;

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- licensing terms;
- persistent identifiers for the publication,
- the authors involved in the action and, if possible, for their organizations and the grant.

Where applicable, the metadata must include persistent identifiers for any research output or any other tools and instruments needed to validate the conclusions of the publication.

Open data coming from the scientific results and outcomes will be published in Zenodo, OpenAire's trusted repository. A Zenodo Community (https://zenodo.org/communities/safecrew/) has been created. Research data that is deposited in a trusted repository, such as Zenodo, receives a persistent identifier. A universal repository like Zenodo allows the deposition of very different research data like the ones created in SafeCREW.

The SafeCREW consortium will develop a metadata template to ensure that all basic information is included in the metadata that is provided together with the research data to properly document them. The metadata template to be developed and implemented will include:

- Guidelines for the nomenclature and tags to be used as metadata
- Examples of good practices on how to store collected data (i.e., field samples, lab analysis, and on-line sensors)

The template will be presented among the partners and approved by the project consortium. Additionally, the template will be updated continuously if necessary. Metadata of deposited data will be preferably open under a CC0 -licence, in line with the FAIR principles. Based on these principles, the partners will be notified about the procedure to follow and the needed information. Thus, the information to be provided will include at least about the following:

- datasets (description, date of deposit, author(s), venue and embargo);
- Horizon Europe funding;
- grant project name, acronym and number;
- licensing terms;
- persistent identifiers for the dataset, the authors involved in the action, and, if possible, for their organisations and the grant.

In addition, they will include an adjunct text file to document the datasets containing relevant metadata, for example: sampling date and time, unit, source, location, and other relevant key words. Preferentially, standardized vocabulary from Wikidata with URI will be used, otherwise free text. For metadata standards the template will consider the usage of domain specific ontologies.

Zenodo's metadata is compliant with DataCite's Metadata Schema minimum with a few additional extensions. Fields that will be used, if applicable, are:

- Files
- Upload
- Basic information (DOI, publication date, authors & affiliation, title, description)
- Licence
- Related identifiers (if applicable)
- Subjects
- Contributors
- References
- Funding

The next updates of this section will enhance the level of information on how data will be made discoverable. The metadata template will be available on the SafeCREW Sharepoint.

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3.2 Making data accessible

3.2.1 Repositories

Research data will be deposited in trusted repositories, preferentially Zenodo. Software will be made open on GitHub and linked to on Zenodo. On Zenodo, data is stored safely and for a long term and the different datasets can be linked to the SafeCREW project. It is a trusted repository and operated by OpenAire. Every upload receives a DOI/PI that makes them citeable and trackable. Zenodo enriches all uploads with metadata like Publication date, DOI and versions.

Additional repositories that may be taken into account over the course of the project are IPChem, openfluor.lablicate.com and UFZ Archive system. These would be more specified repositories. All are running under CC license.

When publishing data on Zenodo, it is automatically indexed in OpenAire. Zenodo supports harvesting of all content via the OAI-PMH protocol, which is a widely used protocol for harvesting metadata. The metadata output is possible in the formats datacite (only original DataCite metadata), oai_dc (only minimal metadata) or marc21 (support may be discontinued by Zenodo).

Additionally, the Zenodo REST application programming interface currently supports Deposits (upload and publishing of research outputs), Records (search published records) and Files (download/upload of files).

The data deposited on the chosen repositories will be accessible using a standard browser via the http-protocol.

Zenodo is a long-term repository on which the data and metadata (to properly document collected and generated data) remain accessible and findable. The SafeCREW members agree to keep any additional data for additional two years after the project ends.

3.2.2 Open access of data

Research data that are required to verify published results, will be released on open-source repositories under FAIR guidelines. The repository is selected to guarantee long-term storage. A PID (permanent identifier) will be given and the availability of metadata will be under CCO license. Data will be published latest when related results are published.

3.2.2.1 Exceptions: Sensitive data

All data generated from water utility samples need approval from the respective water utility prior to publication. If the water utility does not consent, this data cannot be made open. Possibilities to provide data “on demand”/under restricted access or in anonymised form will be favoured in that case. For anonymization, the water work name is for example changed to a non-descriptive number in the readme file and file name. The description of samples will also be modified accordingly.

3.2.3 Metadata

Readme files under CC0 license will be provided with each dataset that is uploaded to a repository. It will provide information on the samples (metadata like location, timestamp, unit) that describe the scientific data, provides contact to the creator of the dataset as well as provide keywords to help finding relevant datasets. If necessary, the readme file will explain how to process the data that it is linked to.

The metadata will document the obtained data during monitoring activities and sampling campaigns. It will include the parameters measured as well as their units, the location of the measurements, the

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equipment used. The equipment will be described. It will be differed between time series and lab measurements. Keywords will be provided in order to make data findable.

3.3 Making data interoperable

Within the SafeCREW consortium, we will decide on a naming convention for samples and files. This includes a list of abbreviations (for case studies, water works, treatments, etc.) that will be provided within the readme files for all samples that are deposited in a repository. A suggestion has been made that can look like:

Field samples: **<Case-study>_<Point of sampling>_<Date&timestamp>**

Lab samples (modified water from case studies): **<Case study>_<Point of sampling>_<Type of experiment>_<Operating parameters nr>_<Running nr>**

Lab samples (artificial water)**: <Partner>_<Synthetic water recipe>_<Type of experiment>_<Operating parameters nr>_<Running_Nr>**

On-line sensors: **<Case study>_<Point of sampling>_<start date&time stamp>_<End date&time stamp>_<Running Nr>**

A codebook will be created that deciphers abbreviations used (See Section 3.1 for further details). This is accessible for all SafeCREW members and may be adapted over the course of the project. Relevant parts are pasted in the readme files for metadata provision of deposited datasets. For description of data and devices, we will consider the preferential use of terms from commonly used ontologies.

Within the SafeCREW consortium the naming convention ensures a facilitated sharing and usability of datasets.

3.4 Increase data re-use

The readme file will include information on methodology, abbreviations and sample collection details (see section 3.1 for further details). The description of data will include the sampling location (perhaps anonymised), if useful with geo-coordinates.

The data will be published under creative commons license with the exceptions stated above. With the readme files provided with the samples, all data is usable by third parties.

Research articles will be published in peer-reviewed journals. Deliverables that are finished within the SafeCREW project are written and checked by different persons to assure quality and correctness. For data, the processing parameters are given, so calculations can be re-done to check quality and correctness.

4 Other research outputs

Digital outputs such as software or models will be treated as research data like stated above. Protocols and workflows are publications and will be published open access as well.

5 Allocation of resources

The approximate costs are 1 person month per beneficiary and already covered by the project budget.

The data management is organized by the project Coordinator and each partner named one responsible person for the implementation. Anissa Grieb has been assigned as the project Data Manager.

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The partners have assigned the following persons per partner as responsible for the implementation of the Data Management Plan:

Partner	**Responsible person**
DVGW-TUHH (project data manager, coordinator)	Anissa Grieb, Deputy: Jon Wullenweber
POLIMI	Manuela Antonelli
KWB	Christoph Sprenger
BDS	Peter Behnisch
EUT	Queralt Plana Puig
UBA	Aki Sebastian Ruhl
UFZ	Thorsten Reemtsma
CAT	Andreu Fargas Marques
TUTECH	Margarete Remmert-Rieper
MM	Fabio Marelli, Angela Manenti
MSS	Andrew McInnes

6 Data security

Servers are located in the EU and aligned with the EU legislation on data security and privacy.

Each institution responsible for their own backup. Recommendations are to store data at least 3 times on 2 different media, of which 1 is located at another place (physical distance).

Once deposited on the repository, Zenodo (or other used repositories) has its own backup strategies.

6.1 Website privacy and policy

SafeCREW's Website Privacy and Cookie Policy is published on https://safecrew.org/privacy-policy/.

7 Ethics

There are no ethical issues for this project.

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