Deliverable D9.2:

*Documentation of the new EUROCHAMP data portal:*

*new functionalities and tools for data provision*

*Author(s):* Cathy Boonne, Marjorie Salvetat, Bénédicte Picquet-Varrault

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D9.2. EUROCHAMP data portal: new functionalities and tools for data provision – EUROCHAMP-2020

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1. INTRODUCTION

EUROCHAMP-2020 project [A1] aims at further integrating the most advanced European atmospheric simulation chambers into a world-class infrastructure for research and innovation. The project is composed by a coordinated set of networking activities, which deliver improved chamber operability across the infrastructure, as well as standard protocols for data generation and analysis. All EUROCHAMP existing data and data generated during the project are archived and distributed through a new EUROCHAMP-2020 Data Centre (DC) which architecture is described in document A2.

The overall goal of the EUROCHAMP-2020 DC is to provide scientists and other user groups with free and open access to all EUROCHAMP-2020 infrastructure data, complemented with access to new data products, together with tools for quality assurance (QA), data analysis and research.

The new Data Centre (https://data.eurochamp.org) is structured in three topical databases indexing the measurement data and providing a single access point to all data:

- Database of Atmospheric Simulation Chamber Studies (DASCs): https://data.eurochamp.org/data-access/chamber-experiments,
- Library of Analytical resources (LAR) split into:
  - FTIR Reference Spectra database: https://data.eurochamp.org/data-access/spectra,

1.1. PURPOSE OF THE DOCUMENT

This document describes the new functionalities and tools developed and implemented within the new Data Centre in order to generate metadata contents and populate automatically the metadata repositories. For each EUROCHAMP-2020 topical database, dedicated web functionalities have been created and installed for data providers to feed databases with new data and metadata. This document outlines the different steps to handle these tools and considers also the way to check the format of data files uploaded. To conclude, tools for statistics of provision and usage will be featured.

1.2. INTENDED READERSHIP

This deliverable is intended for a public use. At the current stage of the project, the implementation of tools described will evolve and will be delivered all along the project.

1.3. DOCUMENT OUTLINE

The document consists of the following sections:

- **Section 2** gives an overview of the new EUROCHAMP-2020 Data Centre handling.
- **Section 3** describes the tools developed and implemented to generate automatically metadata contents and to check the format of the data files uploaded for:
  - Simulation chamber experiments,
  - FTIR Reference Spectra,
- **Section 4** presents tools for statistics data provision and usage.
1.4. APPLICATION AREA
The prime focus of this document will be on EUROCHAMP-2020 Virtual Access (WP9), as specified in the EUROCHAMP-2020 project document. [A1].

1.5. APPLICABLE DOCUMENTS AND REFERENCE DOCUMENTS

Applicable documents
[A1] EUROCHAMP-2020 project document

1.6. ABBREVIATIONS

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<tr>
<td>CNRS</td>
<td>Centre National de la Recherche Scientifique</td>
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<tr>
<td>DASCS</td>
<td>Database of Atmospheric Simulation Chamber Studies</td>
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<td>EDF</td>
<td>Eurochamp Data Format</td>
</tr>
<tr>
<td>FTIR</td>
<td>Fourier Transform Infrared</td>
</tr>
<tr>
<td>IPSL</td>
<td>Institut Pierre Simon Laplace</td>
</tr>
<tr>
<td>LADP</td>
<td>Library of Advanced Data Products</td>
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<tr>
<td>LAR</td>
<td>Library of Analytical Resources</td>
</tr>
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2. OVERVIEW OF THE NEW EUROCHAMP-2020 DATA CENTRE

2.1. PRESENTATION OF THE NEW SITE

The new EUROCHAMP-2020 Data Centre is available to the research community since September 2017 and reachable from this internet address: https://www.eurochamp.org/Data.aspx. Currently, two databases are operational (DASCS and LAR), the third one (LADP) being under development so far.

Figure 1 gives a view of the home page of the EUROCHAMP-2020 Data Centre site. From this page, users can access:

- Data and metadata of the DASCS and LAR databases in the tab “data access”,
- Chambers description and management in the tab “Chambers”. The tool “Chamber Management” has been developed in order to allow partners to manage the rights for the provision of new data,
- Documentation (Data Management Plan, data description ...) in the tab “documents”,
- Tools for the generation and the handling of data by data providers and users in the tab “toolbox”,
- Video tutorials access presenting main features of the Data Centre in the tab “help”.

In a new future, it is also planned to add a tab “statistics” where statistic on data provision and usage will be given.

This page permits also to access functionalities and tools developed and implemented exclusively for data providers in order to generate and populate the EUROCHAMP-2020 metadata and data repositories and databases. For that purpose an ORCID account is necessary as described in the architecture document [A2].

Figure 1: Snapshot of the home page of the new EUROCHAMP-2020 Data Centre site.

2.2. ACCESS AND RIGHTS

Access to the entire website, in particular to the metadata catalogue as well as the summary sheet of the data is possible without any authentication. However, in order to being able to provide statistics on data usage, users are invited to connect with their ORCID for the download of data.

For data providers, authentication with the ORCID account is required to get the rights to provide new data.
- **Why an ORCID?**
  ORCID provides a persistent digital identifier that distinguishes a user from other researchers and supports the linkages between the researcher and his professional activity. This account is not dedicated to EUROCHAMP-2020 Data Centre and can be used on other websites sharing the same authentication method.

- **How to create an ORCID account**

**Step 1:** Data providers have to connect to the ORCID site:

This illustration on the left is a view of the home page of the ORCID site.

**Step 2:** Click on “sign in” (highlight in green) opens a new window (see fig. 2a). From this new window, choose the item “For researchers” (highlight in green).

**Step 3:** Register by filling the form (see fig. 2b).

Figure 2: Snapshots of the ORCID register windows, a) ORCID for researchers (on the left), b) ORCID register form (on the right).

After registration, the ORCID site sends automatically a message to the user delivering the ORCID number. The ORCID number looks like this template: XXXX-XXXX-XXXX-XXXX.

This number has to be sent to EUROCHAMP Data Centre administrator (currently: Marjorie Salvetat, ) in order to give rights to data providers to use the functionalities and tools developed.

- **How to access to the functionalities tools developed**

The data providers have just to sign in the EUROCHAMP-2020 Data Centre by clicking on the item “login” (see figure 1). This window below in the left will appear, click on the button “ID” in green to sign into ORCID (window in the right). The item “login” is refreshed and a “logout” item appears on the home page of the site.
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3. DESCRIPTION OF THE NEW FUNCTIONALITIES AND TOOLS DEVELOPED

A set of functionalities and tools have been developed to facilitate the automatic management of metadata and data in order to populate the EUROCHAMP-2020 Data Centre. These functionalities are reserved to data providers. Because of the specificities of the different metadata and data to ingest, specific functionalities and tools developments have been achieved and implemented for each topical database. They are described in the paragraphs below.

3.1. TOOLS DEVELOPED FOR THE DATABASE OF ATMOSPHERIC SIMULATION CHAMBER STUDIES

3.1.1. Description of the automatic management of metadata tools

Data providers can easily create, edit, modify or delete metadata using the tools developed. The figure 3 shows how to access to the tools for Simulation Chamber experiments (menu item highlighted in light grey). A click on this selection opens a new interface shown in figure 4.

![Figure 3: Snapshot of the home page of EUROCHAMP-2020 site with “Data Access” menu expanded.](image1)

![Figure 4: Snapshot of the metadata creation interface.](image2)
- **The metadata creation functionality**

A simple click on the button + (in orange in figure 4) permits to create a new metadata sheets. For Simulation Chamber experiments, five information boxes have to be filled:

- Reactants,
- Contacts,
- Experiments,
- EDF files upload,
- PDF file upload.

They are displayed in the figure 5 below. For each box a click on the button + (in orange in figure 5) permits to fill the information content of the related box. The information needed for each box is depicted in Appendix 1.

These three buttons shown in figure 5 permit the following functionalities:

- to open the window in full screen (the first one),
- to close the window (the second one),
- to save the new metadata sheet you have created (the third one).

![Figure 5: Snapshot of the information boxes to be filled.](image)

It is important to note that a click on the “save” button generates the new metadata sheet and populate automatically the metadata repositories. A simple check of the extension of the uploaded file is done.

- **The metadata edition and modification functionalities**

Functionalities to edit or modify a metadata sheet have been also implemented. From a chosen metadata sheet (see figure 6), it is possible to edit, change or add information within the different content of the boxes described in Appendix 1.

To achieve this purpose just a click on this button is necessary, a new interface (figure 7) opens and the edition and modification functionalities are available.
Figure 6: Snapshot of a metadata sheets within the metadata repository.

Figure 7: Snapshot of a metadata sheet edition or modification functionalities.

- **The metadata deletion functionality**

Functionality to delete a metadata sheet has been also implemented. Just click on this button (see figure 6) to delete the selected metadata sheet. The following window (figure 8) appears.

Figure 8: Snapshot of a metadata sheet deletion functionality.
A confirmation of the user is expected.

3.1.2. Description of the “EDF” tools

A toolbox item within the home page of the EUROCHAMP-2020 Data Centre site (see figure 1) gives access to a lot of scripts to help users to convert, check or visualize their data. A list of these scripts is given in Appendix 2. Among these scripts, the tool called “E2020-EDF_IDL_checkerTools” permits to check the content of an “EDF” data format file before uploading it through the metadata creation interface. The program is written using the IDL language.

To use this tool, you have to follow these steps:
• Downloading the file “EDF_IDL_checkerTools.zip” by clicking on it,
• Unzip the file by using the following command:
  ▪ for linux environment, unzip EDF_IDL_checkerTools.zip
  ▪ for windows environment, the unzip is done when the file is opened.
• Execute the command:
  >idl –rt edf_checker.sav –args “name of the file with path if necessary”

A result file called “name of the file”.check.log is created giving the status of the file and the errors encountered when checking it. If the file follows the right description of the EDF data format, a message like this one is written. STATUS:= data successfully processed
!! successfully checked at 2018-03-29 18:48:45 160..... (check_edf.pro)
!!
!! edf_checker --- finished check at: 2018-03-29 18:48:45 160
!! edf_checker --- time used for check: 0.007 s

3.2. TOOLS DEVELOPED FOR THE LIBRARY OF ANALYTICAL RESOURCES

As the DASCS, data providers can easily create, edit, modify or delete metadata using the tools developed for FTIR or mass spectra. The figure 9 below shows how to access to these tools (menu item highlighted in light grey).

Figure 9: Snapshot of the home page of EUROCHAMP-2020 site with “Data Access” menu expanded.
3.2.1. Description of the automatic management of metadata tools for FTIR reference spectra

A click on IR spectra selection (see figure 9) opens a new interface shown in figure 10.

![Snapshot of the metadata creation interface for FTIR reference spectra.](image)

- **The metadata creation functionality**

  A simple click on the button + (in orange in figure 10) permits to create a new metadata sheets. For FTIR reference spectra, five information boxes have to be filled:

  - Contacts,
  - Molecule,
  - Instrument,
  - Experimental conditions,
  - JCAMP-DX files upload.

  For each box a click on the button + permits to fill the information content of the related box. The information needed for each box is depicted in Appendix 3.

  The same three buttons shown in figure 5 permit the following functionalities:

  - to open the window in full screen (the first one),
  - to close the window (the second one),
  - to save the new metadata sheet you have created (the third one).

  It is important also to note that a click on the “save” button generate the new metadata sheets and populate automatically the metadata repositories. A simple check of the extension of the uploaded file is done.

- **The metadata edition and modification functionalities**

  Functionalities to edit or modify a metadata sheet have been also implemented. From a selected metadata sheet (see figure 11), it is possible to edit, change or add information within the different content of the boxes described in Appendix 3.
A click on this button is necessary, a new interface (figure 11) opens and the edition and modification functionalities are available.

Figure 11: Snapshot of a metadata sheet edition or modification functionalities.

- **The metadata deletion functionality**

In the same way as Simulation Chamber experiments, a click on this button (see figure 6) to delete the selected metadata sheet.

### 3.2.2. Description of the automatic management of metadata tools for mass spectra

A click on mass spectra selection (see figure 9) opens a new interface shown in figure 12.

Figure 12: Snapshot of the metadata creation interface for mass spectra.

- **The metadata creation functionality**

A simple click on the button + (in orange in figure 12) permits to create a new metadata sheets. For mass spectra, four information boxes have to be filled:
- Contacts,
- Instrument,
- Experimental conditions,
  - Molecules,
  - Derivatives,
- JCAMP-DX files upload.

For each box a click on the button + permits to fill the information content of the related box. The information needed for each box is depicted in Appendix 4.

The same three buttons shown in figure 5 permit the following functionalities:

- to open the window in full screen (the first one),
- to close the window (the second one),
- to save the new metadata sheet you have created (the third one).

It is important also to note that a click on the “save” button generate the new metadata sheets and populate automatically the metadata repositories. A simple check of the extension of the uploaded file is done.

- The metadata edition and modification functionalities

Functionalities to edit or modify a metadata sheet have been also implemented. From a chosen metadata sheet (see figure 13), it is possible to edit, change or add information within the different content of the boxes described in Appendix 4.
A click on this button is necessary, a new interface (figure 13) opens and the edition and modification functionalities are available.

![Figure 13: Snapshot of a metadata sheet edition or modification functionalities.](image)

- The metadata deletion functionality

In the same way as the DASCS, a click on this button (see figure 13) deletes the metadata sheet chosen.
4. PRESENTATION OF STATISTICS DATA PROVISION AND USAGE TOOLS

Tools to provide statistics on data usage are under development so far. So they may evolve in the next months.

4.1. Data statistics

4.1.1. Statistics on data provision

The statistics on data provision are very useful to follow the amount of data provided by partners. As we can see on the snapshot (figure 14), the number of data provided will be monitored and will be accessible by partners in the tab “statistics”. A distinction will be made between i) data provided within Eurochamp-1 and -2 which have been recovered from the former data centre and ii) data provided within EUROCHAMP-2020.

Figure 14: Snapshot of statistics data provision page.

Furthermore, this information will also be sorted by institutes (see snapshot figure 15). Like so, each partner will be aware of the data provided by its institute. However, they won’t be able to have access to the statistics of the other institutes.

Figure 15: Snapshot of statistics data provision per institute page.

4.1.2. Data usage statistics

In order to help partners in the identification of the data that generate the most interest by the scientific community but also to better identify the type of users and the visibility of the DC around the world, statistics usage are also monitored. For that purpose, two types of information are collected: i) the
number of metadata sheet read and the number of files downloaded and ii) the country of the institute of the associated user.

In order to limit inconvenience for users, the collection of information is transparent for them. The only information which is requested to the user (for their first connection to the Data Centre) is the country of his institute. This method has been preferred to the IP collection as it appears more accurate: Indeed, what matters us is the country of its institute, not its current position. The snapshot (figure 16) illustrates this asking process.

![Update institute country](image)

Figure 16: Snapshot of the user distribution form window.

Finally, all these statistics will be displayed through charts and text on a dedicated page only available by the administrators.

4.2. General statistics

Up to now, we have only discussed about the statistics of the data. To handle more general statistics, we plan to use a tool off-the-shelf, like Piwik. It will allow us to know the number of visitors on the site, but also other information like the session duration or the number of pages per session.

As for the statistics about the data usage, this information will only be available by the administrators.
APPENDIX
APPENDIX 1: DESCRIPTION OF THE CONTENT OF THE DIFFERENT PARAMETERS CHOSEN TO DEFINE SIMULATION CHAMBER EXPERIMENTS METADATA

The snapshots below outline the content of these different parameters: reactants, contacts, experiment, EDF files upload, and PDF files upload.
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### APPENDIX 2: LIST OF EDF TOOLS

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<td>The description of IDL procedure is contained in the zip file.</td>
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<tr>
<td>E2020 – EDF_IDL_Routines_V1.0</td>
<td>EDF_IDL_Routines_V1.0.zip</td>
<td>Read and write EDF file.</td>
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</table>
| E2020 – IGOR_EDF_Exporter | IGOR_EDF_Exporter.zip         | Create a panel to select waves for export intoDDF file:  
- export the selected waves,  
- Input : information for EDF file via userinterface  
- Output in Igor : folder withEDF variables  
- Side effects : if T or RH in chamber DMPS is exported the stdev will be added if waves exist. |
| E2020 – Excel_to_EDF-builder 1.0.R | Excel_to_EDF_v1.0.zip        | From a txt file easily produced from excel, it aims:  
- at formatting all the parameter given in excel in column into the EDF format,  
- at plotting the data in a series of graphs one above the other in a pdf file.  
The data must be given as in indicated in the model file "exemple.txt".  
Disclaimer, authors and instruction for use are contained in the header. |
| E2020 – EDF_read_all-5-per-page_portrait v1.0.R | EDFReadAll.zip               | It aims at producing reports of data contained in a EDF file. It produces a PDF file located in the original data directory. Each category of data will be displayed on a separate plot. All the plots are displayed 5 plots per page oriented in “portrait”.  
Up to twelve parameters can be plotted (more is feasible but issues on the readability of the plot may occurs).  
Disclaimer, authors and instruction for use are contained in the header. |
| E2020 – EDF_read_all-in-one-page_portrait v1.0.R | EDFReadAll.zip               | It aims at producing reports of data contained in a EDF file. It produces a PDF file located in the original data directory. Each category of data will be displayed on a separate plot. All the plots are on a single page oriented in "portrait".  
Up to twelve parameters can be plotted (more is feasible but issues
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<th>EDFMergerSynchronizer_v1.2.zip</th>
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<td><strong>Description</strong>: It aims at merging data contained in a series EDF files related to the same experiment by synchronizing them to the same time base. It produces an EDF file of the synchronized data together with an ASCII datafile (.DAT) that can be easily read by other data analysis software. As a report, it produces a PDF file located in the original data directory. Each category of data will be displayed on a separate plot (5 plots per pages). Three files are provided as example but there is virtually not limit to the number of files that can be synchronized.</td>
<td><strong>Disclaimer</strong>: authors and instruction for use are contained in the header.</td>
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<td><strong>Description</strong>: It aims at producing a continuous long EDF file from a serie of EDF files of the same type (eg. 7 seven identical files recorded along a week can be “glued” together to make a single one covering 7 days”.</td>
<td><strong>Disclaimer</strong>: authors and instruction for use are contained in the header.</td>
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<th>Compare2edf_v1.0.zip</th>
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<tr>
<td><strong>Description</strong>: It aims at producing a report that allows to compare the data of two EDF files of exact similar structure (same variables, same order). The data are synchronized with respect to a similar event (e.g. the time of light on in two different experiments). It produces a PDF file located in the original directory of the first dataset. Each category of data will be displayed on a separate sheet (landscape orientation). The routine allows to compare a huge number of variable group two by two on separated pages.</td>
<td><strong>Disclaimer</strong>: authors and instruction for use are contained in the header.</td>
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APPENDIX 3: DESCRIPTION OF THE CONTENT OF THE DIFFERENT PARAMETERS CHOSEN TO DEFINE FTIR REFERENCE SPECTRA METADATA

The snapshots below outline the content of these different parameters: contacts, molecule, instrument, experimental conditions and JCAMP-DX files upload.
APPENDIX 4: DESCRIPTION OF THE CONTENT OF THE DIFFERENT PARAMETERS CHOSEN TO DEFINE MASS SPECTRA METADATA

The snapshots below outline the content of these different parameters: contacts, instrument, experimental conditions and JCAMP-DX files upload.

Contacts

Name
  e.g., John Doe

Email
  e.g., john.doe@email.org

Institute
  e.g., CNRS-LISA

ORCID
  e.g., 0000-0000-0000-0000

Instrument

Type

Make
  e.g., Thermo Scientific

Brand
  e.g., Orbitrap

Specie detector
  e.g., QqQ

Resolution
  e.g., 50,000

Observations
  Insert any further information about the instrument.

Experimental conditions

Ion source
  Elctrospray

Information
  Insert any further information about the experimental conditions.

Molecule

Name

CAS number
  e.g., 1402-30-1

SMILES
  e.g., "C8H8N2O2"
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