SAlBAGE

Sulfur-Aluminium Battery with Advanced Polymeric Gel Electrolytes

H2020-FETOPEN-2016-2017

FET-Open – Novel ideas for radically new technologies

GA 766581

Type of action: RIA (Research and Innovation action)

Start date of the project: 01/11/2017

Duration: 36 months

Deliverable D 1.3

Data Management Plan

Project partners

LOGO	Partner full name	Acronym
albufera Energy Storage	Albufera Energy Storage S.L.	AES
UNIVERSITY OF LEICESTER	University of Leicester	UoL
Scionix	Scionix Ltd.	Scionix
ICTP CSIC	Agencia Estatal Consejo Superior de Investigaciones Científicas	CSIC
TU Graz Graz University of Technology	Technische Universität Graz	TUG
UNIVERSITY OF Southampton	University of Southampton	UoS
DTU Danmarks Tekniske Universitet	Danmarks Tekniske Universitet	DTU

Deliverable Name: Data Management Plan
Led by: Albufera Energy Storage
Partners: All

Date	Version	Author	Institution	Comments*
23/01/2018	V01	Ana L. Cudero	AES	creation
20/04/2018	V01	Ana L. Cudero	AES	Final version

* Creation, modification, final version for evaluation, revised version following evaluation, final

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List of Acronyms

Acronym	Description
DMP	Data Management Plan
EU	European Union
OA	Open Access
WP	Work Package
IL	Ionic Liquid
DES	Deep Eutectic Solvents
FAIR	Findable, accessible, interoperable and reusable.
DFT	Density Functional Theory
SEM	Scanning Electron Microscope

Content

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1. Introduction

According to the EU regulations, projects participating in the core areas of Horizon 2020 starting from 2017 must participate in the Open Research Data Pilot (ORD Pilot). This includes Future and Emerging Technologies (FET) projects. Thus, the SALBAGE Project as a H2020-FET funded project is bounded to participate in the ORD pilot action on open access to research data.

Open access implies unrestricted online access to research outputs such as journal articles, without access fees. The goal of the EU with this program is fostering access to and re-use of data generated by EU funded projects in order to improve and maximize public financial European resources and avoid duplication of efforts. According to the EU guidelines[1], ORD pilot applies primarily to the data needed to validate the results presented in scientific publications. More specifically, projects participating in the Pilot are required to deposit and make public, as soon as possible, the research data described below:

- The data, including associated metadata, needed to validate the results presented in scientific publications
- Other data, including associated metadata, as specified and within the deadlines laid down in a data management plan (DMP).

2. Plan Description

The Data Management Plan (DMP) of the SALBAGE project describes the data management life cycle including specific standards of the databases in terms of formats, metadata, sharing, archiving and preservation.

The DMP will be developed during the project life and periodically updated. This document represents the initial version of the data management life cycle for all datasets to be collected, processed or generated by the project partners.

The present document has been prepared with aid of the DMP Online tool.

1 http://ec.europa.eu/research/participants/data/ref/h2020/grants_manual/hi/oa_pilot/h2020-hi-oa-data-mgt_en.pdf

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3. Data summary

SALBAGE project intends to explore the feasibility of using Aluminium-Sulfur batteries with polymerized electrolytes based on ionic liquids and deep eutectic solvents.

The project is structured in 6 work packages. Three main WPs will be devoted to the study of materials properties and electrochemical reactions of the main components of a battery, namely Anode, Cathode and Electrolyte. Thus, WP2 is focused in the study of the electrolyte; WP3 in the study of the Aluminium anode and WP4 for the case of the Sulphur cathode. On top of that, data resulting from the combination of these elements will be generated. Most of these data will come from a combination of computational simulations (DFT) in WP5 and confirmed by experimental results from different electrochemical and testing techniques in WP6.

Therefore, in SALBAGE project, data coming from the above mentioned WP and its corresponding tasks will be generated and collected. In this first approach, three data types can be distinguished and foreseen:

3.1. Experimental data

WP2, WP3 and WP4 are devoted to the study of the chemical, electrochemical and material properties of the materials composing the basic cell of the battery. For the correct development of the tasks included in these WP, a variety of electrochemical and surface science techniques will be used. The data will be use to recognize performance of the proposed materials in the proposed battery. In deeper detail:

- WP2 will gather data regarding the capability of a set of proposed ILs and DES to be incorporated into polymer gels or blends. Their further application as electrolytes will be studied also for which conductivity measurements will be performed. Data obtained in the characterization of the electrolyte will be shared with the other partners, especially those involved in WP3, 4 and 5.
- WP3 will study the stripping and electrodeposition of Al from the proposed electrolytes on different aluminium anodes and alloys, including the formation of dendrites on the surface. Different techniques will be used such as cyclic voltammetry, impedance spectroscopy and SEM imaging. Results will provide insights on the performance of the proposed electrolytes to be coupled with an aluminium anode, allowing determining which might be employed and which might not. Outputs will be internally provided to the other partners, namely those involved in WP2 and WP5 and WP6. The most successful results will be retained for their use in the battery and promising and results beyond the state of art will be published.

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- WP4 is devoted to the study of Sulfur electrode. The use of Sulfur as cathode in a battery is not straightforward due to the variety of species that Sulfur can form. In order to improve and boost its performance, the use of redox mediators is foreseen in the project. Thus, electrochemical studies will be carried out regarding the performance of Sulfur modified with different species (redox mediators) as cathode and results will be provided to the partners involved n WP2, WP5 and WP3.

3.2. Simulation data

WP5 involves all the simulation activities that will allow reducing the number of species to be tested experimentally in WP3 and WP4. The stability of different molecules in the given conditions will be examined by means of DFT simulations in order tell which would be the most stable and probable. Outputs of this WP will allow WP4 and WP3 to reduce the number of experimental tests to carry out to the most stable species, reducing efforts and optimizing resources. Likewise, a continuous feedback between WP4, WP3 and WP5 will be stablished in order to refine results.

Reports and deliverables of WP5 will be made public. Additionally, the results obtained beyond the state-of-art will be published.

3.3. Testing data

The information gathered with the outputs of WP2, WP3 and WP4 as performance of the individual elements of the battery will be actually combined in a battery cell and tested as a whole. Results on the performance of this cell will give information about the real performance and capabilities of an Aluminium/Sulfur battery. Tests will be carried out in relevant conditions and results will provide the basis to determine the viability and possibilities of this sort of battery beyond the state-of-art. Results from this WP will be provided to the partners involved in WP2, WP3 and WP4 in order to improve the materials combination. In addition, a potential market analysis depending on the battery performance will be prepared and made public.

In all cases, details of the equipment used, such as the make and model of the instrument, the settings used and information on how it was calibrated will be provided along with each set of data.

The techniques used for the characterization of materials may include specific software but the data created by the acquisition devices will be transformed into figures and tables in

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order to better share with the other partners and beyond. Thus data will be presented as text including images and/or figures.

Other formats that might be used in the case of other documents different form texts are the following: Mendeley database (.ris); ASCII or MS Excel spreadsheet (.xlsx and comma-delimited .csv); and/or MS Word for text documents (.docx); Microsoft Word 2007 for text-based documents. MP3 or WAV for audio files. Images will be saved and stored in JPG with the maximum quality available. Windows Media Video for video files. Quantitative data analysis will be stored in SAV file format (used by SPSS) from which data can be extracted using the open-source spss read Perl script.

These file formats have been chosen because they are accepted standards and in widespread use.

These results will be useful to material scientist and battery development industry.

It is not envisaged that there will be any privacy issues with respect to the data as there aren't personal data involved.

4. FAIR data

In accordance with the EU Guidelines, data produced in the present project should be FAIR, that is: Findable, Accessible, Interoperable and Reusable.

4.1. Making data findable, including provisions for metadata:

In order to make the documents **findable** within the repositories metadata will be inserted along with the document. For that, relevant and sufficient keywords will be used, some examples could be the words Battery, Aluminium, Sulfur /Sulphur, Ionic Liquids, Polymerization, Deep Eutectic Solvents, and any other more specific keyword relevant to the content of the publication as well as appropriate and relevant titles.

All data and metadata will be stored using English as language in order to make them more easily findable for the scientific community. Besides, IUPAC standards will be used for units and chemical names.

For identification purposes, the repositories offer the assignation of persistent and unique identifiers such as Digital Object Identifiers **(DOI)** identification numbers to clearly and univocally identify documents. In the case of Zenodo, it also supports DOI versioning of the document for further editions.

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In the case of the project deliverables (some of which will be public), they will be identified with number and version, date and type of document. Following the rules below:

Type: DEC/R/ DEM according to the description presented in the deliverable table 3.1 of the proposal.

Dissemination Level: Choose one PU/ CO (public/ confidential) according to the deliverable list table on the proposal

Name: same as in table 3.1

Document ID: should be D.X.x- TYPE- deliverable number-year.

The deliverable number is the order on the list and it also appears in the Grant agreement data.

Some examples:

-D1. Deliverable D.1.1 launch of website. ID would be D1.1-PU-01-2017

-D16. Deliverable D3.3. Effect of inorganic additives on the anode performance ID would be D3.3-CO-16-2018

Date: Day/Month/Year

4.2. Making data openly accessible:

The most effective way to spread the data generated by the SALBAGE project is by means of scientific publications. In accordance with the OPEN Pilot plan, research data results must be granted Open Access. This means that scientific publications of the research findings directly coming from the project must be made openly and publically available by the partners involved and its institutions, at least in its almost-final version. In any case the principal investigators on the project and their institutions will hold the **intellectual property rights** for the research data they generate but they will grant redistribution rights to repository for purposes of data sharing.

In order to make data publically available, paper will be uploaded to repositories as PDF file to public internet sites. Each partner will be responsible of making its data resulting from the SALBAGE project open according to the H2020 FAIR guidelines. In order to do that, data will be stored in either the institution's repositories or in ZENODO (www.zenodo.org). ZENODO is an open repository from OpenAIRE H2020 project and CERN. Data uploaded to ZENODO is linked to OpenAIRE and the EC portal what guarantees its **accessibility** to all public.

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In addition to those repositories, copies can be uploaded to social networks either scientific platforms, such as ResearchGate.net, or professional, such as LikedInd, as well as to the project website hosted at **www.salbageproject.eu.**

In the case of SALBAGE project, a combination of the above mentioned forms will be used.

The procedure will be as follows:

- As soon as results from the project are published, PDF copies along with any complementary data will be uploaded to the selected repository and to ResearchGate.
- In parallel, they will be announced in the website including links to the publication location.
- In addition, project results will also be disseminated by other means such as newsletters, conferences etc., as well as by the corresponding LinkedIn and twitter profiles in order to make the data reach the widest possible audience.

On top of that, some of the project deliverables are public, such as those coming from the simulation activities. In these reports the most stable species for the given conditions will be presented for all the public to know. The report will include the list of possible species that might form as a result of the redox processes when the battery is charged and discharged and which of them are the most probable according to the simulation data. Complementary experimental data supporting the results will also be provided.

For preservation, we will supply periodic copies of the data and public deliverables to Zenodo repository. That repository will be the ultimate home for the data generated along the project life and beyond.

4.3. Making data interoperable:

In order to make the data **interoperable**, data stored in public repositories will include description of the equipment, conditions and settings used to acquired data as well as a comprehensive explanation and description on of the experimental procedures followed to obtain data, whenever it applies. In the case of DFT data, all the boundary conditions and assumptions will be provided with the data.

In order to be able to reproduce experiments, publications might include additional supporting information with complementary data that help verifying the results presented for the sake of interoperability in order to make the data presented fully reproducible in other laboratories

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IUPAC nomenclature will be used as well as International Standards and metric units in order to facilitate interoperability.

Public press releases and Social Media news in LinkedIn and Twitter will use common language for the general public to understand.

4.4. Increase data re-use (through clarifying licenses):

Data presented in the public repositories might be used by third parties for research purposes as state-of art, in order to avoid duplication of efforts and as the basis for future investigations and research on the topic.

The generated data can be re-used in similar configurations, whenever the aluminium anode the sulphur cathode or the polymeric electrolyte would be used as part of an electrochemical setting (battery, super-capacitor), in combination with each other or not. For instance, data regarding the stability and species formed in the cathode can be extrapolated for its use in Li-S batteries.

Nevertheless, the **commercial** use of the data generated by the project might be restricted if any patent or exploitation agreement has been filled or signed by the consortium members. In which case, information about the patent will also be provided by the project foreseen ways.

With regard to **quality assurance,** research groups and institutions participating in this project are top-level and with great reputation and trajectory within their respective fields what assures the reliability and quality of their findings and results. In addition, the strict procedures that researchers must follow in order to be able to publish results in a peer-review journal guarantees their quality.

5. Allocation of resources

The responsible of the data preservation corresponds to the partner(s) generating the data. For the compilation of the documents, the coordinator is responsible of gathering and reporting to the EU. In addition, dissemination of the results generated will be made by the means foreseen in the Dissemination Plan (deliverable 2.2 of the project).

Each partner is responsible of making its data and results open and of uploading the results to their repositories, being the cost of this eligible for reimbursement during the duration of the project.

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The coordinator is responsible of creating and updating the DMP. The cost of documentation preparation and uploading is included in the WP1 management tasks, eligible for reimbursement in accordance with EU rules.

In a first approach, only free repositories such as those provided by the institutions and Zenodo will be used. On the new versions of the DMP a revision of costs will be made.

6. Data security

The research data from this project will be deposited with the institutional repository on the partner's official pages. The research data from this project will be deposited in those repositories to ensure that the research community have long-term access to the data.

The data files from this study will be managed, processed, and stored in a secure environment (e.g., lockable computer systems with passwords, firewall system in place, power surge protection, virus/malicious intruder protection) and by controlling access to digital files with password protection. Universities involved have self-stored mechanisms that are intend to preserve data. SME's have also backup systems that preserve their information.

In a deeper detail:

- **Albufera:** Computers are password protected and equipped with all the due virus and firewall protections. Computers for collection of data in measurement equipment such as potentiostats or battery cyclers are connected to UPS in order to avoid the loss of data due to an unpredicted electrical failure. User's data are backed up locally in hard copy once a week. A remote copy is also kept in a cloud based storage system and regularly backed up and stored in a different place.
- **DTU:** Computers and clusters are protected by password, antivirus and firewall. The data are produced using the Niflheim cluster hosted at DTU. Niflheim is currently assuring for the standards required by the Danish research council and DTU in terms of preservation of data (from daily backups to long-term storage of the data). All the post-processing scripting will be run and saved in the project folder of the same cluster. Periodic local updates (on removal disks) will also be performed. When the person responsible for the project will move, the data will be transferred to the PI of the project (Tejs Vegge, DTU Energy, Section for Atomic Scale Modelling and Materials). The final data, protected by a DOI, will also be stored in the computational materials repository (CMR - https://cmr.fysik.dtu.dk/) which is hosted at DTU Physics and has been active for more than 8 years. The properties collected in a database will be accompanied by ReadMe files to understand how the

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data was obtained and what exactly is included. Code will be commented in the python script, as well as additional ReadMe instructions will be attached describing how to use and run the script.

- **TU Graz:** All computers are protected by password, antivirus and firewall. These are regularly updated. User data is stored on several computers and backed up regularly. A remote copy in a cloud and object based TU Graz internal storage system is used for data exchange between project members within the TU Graz. The storage nodes and the server that monitor and balance the system are located at three sites within the TU Graz. The system is capable of autocorrection in case of failure of single disks or whole storage nodes. For a disaster recovery, data are synchronized in a separate data storage unit on a daily basis.
- **Univ. of Southampton:** Computers are password protected and equipped with virus and firewall protections. Computers for collection of data in measurement equipment such as potentiostats or battery cyclers are connected to UPS to avoid the loss of data due to an unpredicted electrical failure. User's data are stored in several computers. Remote copies of the files are also kept in the University storage system and regularly backed up.
- **Scionix:** All client computers and servers are protected by a strong-password methodology. All computers have a virus and firewall installed and set up. These are cloud controlled and updates threats and suspected activities are managed centrally all updates and changes are automatically pushed to the clients. All data is maintained and collected on servers at the central site and data is managed, protected and backed up locally and remotely. All data is stored and managed in compliance with current regulation and policies
- **Univ. of Leicester:** Computers are protected by a strong-password methodology for which there is a compulsory 90-day replacement cycle. All computers (managed desktop and stand-alone) are equipped with virus and firewall protections, these are regularly and automatically updated. Computers used for collection of data attached to measurement equipment such as potentiostats, microscopes or battery cyclers are adminstered through central desktop management consistent with the Universty Data Management policies (https://www2.le.ac.uk/services/research-data). This means that all data are backed up centrally and thereofre protected against unscheduled local or regional power failures. Additionally, user data are stored on several redundant hardware encrypted remote backup devices. All data are stored and managed in compliance with new regulation and policies governing the secure storage of research and personal data (General Data Protection Regulations).
- **ICTP-CSIC:** At CSIC all computers are password protected and equipped with virus and firewall protections according to CSIC protocols. Computers for collection of

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data in measurement equipment are connected to UPS in order to avoid data loss caused by unpredicted electrical failure. User's data are stored in several computers and backed up regularly. Researchers from CSIC have access to the data management services provided by DIGITAL.CSIC which includes data storage and open access data publication, repositories and DOI assignation (https://www.re3data.org/search?query=DIGITAL.CSIC). DIGITAL.CSIC meets the quality criteria of the global directory of repositories and has the Data Seal of Approval Certificate.

7. Ethical aspects

This project does not involve ethical issues to be managed.

8. Other

Each institution has implemented procedures to guarantee the preservation and curation of data which are in good alignment with the EU guidelines.

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