# Thermochemical engineering for enhanced control and recovery of valuable inorganic compounds in high-temperature reactors for unrecyclable wasted materials in the Circular Economy

*A Data Management Plan created using DMPonline.be*

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**Project abstract:**

As consumer goods come to an end-of-life, they cannot always be recycled without potential threats to the environment and/or public health. One of the reasons for non-recyclability is the presence of dispersed inorganic additives in materials. Such additives are often essential to provide materials with desired functional properties or to extend the lifetime of consumer goods. Hence, they cannot be entirely avoided in newly manufactured materials. As a consequence of the Waste Hierarchy principle in EU waste policy, thermochemical processes, such as incineration and gasification, are to be applied for a safe and irreversible treatment of non-recyclable wasted materials. This creates also chances for the advanced recovery of inorganic compounds of high interest in the Circular Economy. As waste enters a thermochemical process, metallic elements in the waste exhibit a behaviour of partitioning and speciation. This behaviour is not well understood yet and complicates the operation of existing industrial incineration processes, as well as the further development of emerging processes for gasification of waste. The project aims at establishing the missing knowledge, to predict and control the fate of metallic elements from waste in typical solid-gas environments of thermochemical reactors, through adapting conditions of flow, and heat and mass transfer. The research combines a reactor engineering approach with computational chemical modelling, advanced analytical chemistry and unique validation experiments on a dedicated pilot-reactor for in-depth study of the thermal decomposition of solid wasted materials.

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## Research Data Summary

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

| Dataset name / ID | Description | New or reuse | Digital or Physical data | Data Type | File format | Data volume | Physical volume |
|---|---|---|---|---|---|---|---|
| | | *Indicate:*<br>***N****(ew data) or* ***E****(xisting data)* | Indicate: **D**(igital) or **P**(hysical) | Indicate:<br>**A**udiovisual<br>**I**mages<br>**S**ound<br>**N**umerical **T**extual<br>**M**odel<br>**SO**ftware<br>Other (specify) | | Indicate:<br><1GB<br><100GB<br><1TB<br><5TB<br>>5TB<br>NA | |
| Analytical data | chemical analyses of samples | N | D | N | .csv; .xls | <1GB | |
| Process data | process data extracted from PLC | N | D | N | .csv; .xls | <1GB | |
| Experimental results | interpreted data | N | D | N | .xls(x) | <1GB | |
| CFD data | numerical simulation data | N | D | M | ANSYS Fluent | <1GB | |
| Python code | Jupyter notebook code | N | D | M/N | binary | <1GB | |
| Reports | presentation and discussion of results | N | D | T/N | .doc; .pdf | <1GB | |

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

N/A

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.

- No

Will you process personal data? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).

- No

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, …)? If so, please comment per dataset or data type where appropriate.

- No

N/A

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or Data transfer agreements, Research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

- No

N/A

Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.

- No

N/A

## Documentation and Metadata

Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, codebook.tsv etc. where this information is recorded).

An overview of Analytical and Process data will be maintained in the (Excel) files containing the Experimental results (e.g., tab sheet with list of source files interpreted).

A dedicated .xls file will list
- all different source files established during CFD modelling (ANSYS Fluent)
- all different binary files established with Python
A short description will be added for each (group of) files listed.
Reports are kept together with the above (in a shared storage place / folder).

**Will a metadata standard be used to make it easier to find and reuse the data ?**
**If so, please specify which metadata standard will be used.**

**If not, please specify which metadata will be created to make the data easier to find and reuse.**

- Yes

RDR KU Leuven

## Data Storage & Back-up during the Research Project

**Where will the data be stored?**

- OneDrive (KU Leuven)
- Shared network drive (J-drive)

Low-volume data (such as, analytical and process data, experimental data, reports etc.) are kept in OneDrive.
High-volume data (such as data from CFD simulations) are stored on Shared network drive J.

**How will the data be backed up?**

- Standard back-up provided by KU Leuven ICTS for my storage solution

**Is there currently sufficient storage & backup capacity during the project?**

**If no or insufficient storage or backup capacities are available, explain how this will be taken care of.**

- Yes

**How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?**

OneDrive: sharing folders with only relevant persons
J-drive: password on folder

**What are the expected costs for data storage and backup during the research project? How will these costs be covered?**

N/A

## Data Preservation after the end of the Research Project

**Which data will be retained for 10 years (or longer, in agreement with other retention policies that are applicable) after the end of the project?**

**In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).**

- All data will be preserved for 10 years according to KU Leuven RDM policy

**Where will these data be archived (stored and curated for the long-term)?**

- Shared network drive (J-drive)
- KU Leuven RDR

**What are the expected costs for data preservation during the expected retention period? How will these costs be covered?**

N/A

## Data Sharing and Reuse

**Will the data (or part of the data) be made available for reuse after/during the project?**
**Please explain per dataset or data type which data will be made available.**

- Yes, as restricted data (upon approval, or institutional access only)

Since waste samples are studied in experiments on a thermal pilot plant, data sharing/access will depend upon approval of the provider of the waste samples.

**If access is restricted, please specify who will be able to access the data and under what conditions.**

Only members of our own research group.

**Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?**

**Please explain per dataset or data type where appropriate.**

- Yes, other

Since specific waste types are studied (in experiments on a thermal pilot plant), data sharing/access depends upon approval of the provider(s) of the waste samples in order to avoid (indirect or unintended) disclosure of commercially sensitive data.

**Where will the data be made available?**

**If already known, please provide a repository per dataset or data type.**

- KU Leuven RDR (Research Data Repository)

**When will the data be made available?**

- Upon publication of research results

**Which data usage licenses are you going to provide?**

**If none, please explain why.**

To be specified later

**Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here.**

- No

**What are the expected costs for data sharing? How will these costs be covered?**

N/A

## Responsibilities

**Who will manage data documentation and metadata during the research project?**

PhD researchers (Raf Vandevelde, Zouhir Bouchaar)
PIs (Johan De Greef and Jo Van Caneghem)

**Who will manage data storage and backup during the research project?**

N/A (I.e., internal storage is used --> via ICTS KU Leuven)

**Who will manage data preservation and sharing?**

Johan De Greef

**Who will update and implement this DMP?**

Johan De Greef

Jo Van Caneghem

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