
# Mechanistic study and kinetic modeling of isopropanol Guerbet coupling in a continuous plug-flow reactor over Ni/MoC catalysts

## Data Management Plan

23 March 2026

*Corresponds with Data Management Plan Template of the Horizon Europe Program v1.1 (1/4/2022)*
*Data Management Plan created in Data Stewardship Wizard*

| HISTORY OF CHANGES | | |
|---|---|---|
| **Version** | **Publication date** | **Changes** |
| *There are no named versions* | | |

## Contributors

The following contributors are related to the project of this DMP:


- **Kaluža Luděk - Czech Academy of Sciences, Institute of Chemical Process Fundamentals - *Catalysis and Reaction Engineering Research Group* - 0000-0002-0723-6679 kaluza@icpf.cas.cz**

  Czech Academy of Sciences, Institute of Chemical Process Fundamentals (ÚCHP AV ČR) **ORCID: 0000-0002-0723-6679 kaluza@icpf.cas.cz**
  Roles: Contact Person , Project Leader , Researcher

- **Soukup Karel - Czech Academy of Sciences, Institute of Chemical Process Fundamentals - *Catalysis and Reaction Engineering Research Group* - 0000-0001-8563-0340 soukup@icpf.cas.cz**

  Czech Academy of Sciences, Institute of Chemical Process Fundamentals (ÚCHP AV ČR) **ORCID: 0000-0001-8563-0340 soukup@icpf.cas.cz**
  Roles: Project Member , Researcher

# Projects

We will be working on the following project and for those are the data and work described in this DMP.

## Mechanistic study and kinetic modeling of isopropanol Guerbet coupling in a continuous plugflow reactor over Ni/MoC catalysts

Acronym:

*IPAinPFRoverCarb*

Project Number:

*27-25798S*

Start date:

*2027-01-01*

End date:

*2029-12-31*

Funding:

*Grantová Agentura České Republiky (Czechia): 27-25798S (planned)*

The project focusses the existing knowledge gap concerning low-chain bio-alcohol upgrading through heterogeneous catalyzed process of Guerbet reaction. The transition from batch to flow (B2F) is a critical step in adapting novel carbide Ni/MoC catalysts for large-scale processes. The research of reaction kinetic phenomena in plug-flow reactors (PFRs) will provide critical missing information that will enable the fusion of advanced catalyst synthesis, in situ/ex situ spectroscopy, mechanisms, and mathematical modeling of processes. The project places particular emphasis on the iso-propanol (IPA) C-C condensation reaction, which will elucidate the potential utilization of this least reactive bio-alcohol. The selectivity to the formation of highchain hydrocarbon derivatives (C6+) will be investigated. The project's findings promise to offer a comprehensive understanding of catalysis under real flow conditions. The result of this study will be the formulation of a knowledge-based strategy for designing robust catalysts and processes for next-generation biorefineries.

# 1. Data Summary

### Instrument datasets

The following instrument datasets will be acquired in the project:

- **TXT, JPEG, PDF, DOC, XY, TIFF, Microsoft Word, Excel**
  This dataset will be collected by experts in the project, with our own equipment.

  The equipment is less well described or not completely standard, so we will need to take extra care documenting the process.

  Researchers working in other fields of research could be interested in using this data.

### Re-used datasets

We identified the following datasets considered for potential re-use:

- NIST Chemistry WebBook
  It is available via: https://doi.org/10.18434/T4D303. It is used in the project.

  Owner of this dataset: NIST is an agency of the U.S. Department of Commerce. The U.S. Secretary of Commerce on behalf of the United States of America.

  The dataset can be used in the provided format without any conversion needed.

  We will use version "Last major update to the site: January, 2023. " of this dataset. If a new version becomes available during the project, all analyses will be redone with the new version.

  The provider keeps old versions around so the same reference data will be available to reproduce our results.

  We will use the dataset as follows: The identification of chemical compounds and their physical-chemical properties.

- Gas Chromatography/Mass Spectrometry (GC/MS)
  It is available via: https://www.agilent.com/. It is used in the project.

  Owner of this dataset: Agilent; Headquarters; 5301 Stevens Creek Blvd.; Santa Clara, CA 95051; United States.

  The dataset can be used in the provided format without any conversion needed.

  We already have a copy of this dataset.

  It is a fixed dataset, changes will not influence reproducibility of our results.

  We will make sure the selected subset will be available together with our results.

We will use the dataset as follows: The identification of chemical compounds.

There is no need to harmonize different sources of existing data in our case.

**Data formats and types**

We will be using the following data formats and types:

- TXT, PDF, Microsoft Word and Excel
  It is a standardized format. This is a suitable format for long-term archiving. We will have only a small amount of data stored in this format.

# 2. FAIR Data

## 2.1. Making data findable, including provisions for metadata

- **ASEP – Repository of the Czech Academy of Sciences** (will be published)
  The dataset has the following identifiers:
  - Handle: **https://hdl.handle.net/**

  We will distribute the dataset using:
  - *Our institutional repository*.
    A persistent identifier will be assigned by the repository. The repository will make sure that the persistent identifier can be resolved to a digital object.

  There won't be different versions of this data over time.
  We will be adding a reference to the published data to at least one data catalogue.

## 2.2. Making data accessible

We will be working with the philosophy *as open as possible* for our data.

All of our data can become completely open over time.

Data that is not legally restrained will be released after a fixed time period (Unless full open access, after the specified restriction conditions of a given journal Jimp.), unconditionally.

Metadata will be openly available including instructions how to get access to the data. Metadata will be available in a form that can be harvested and indexed.

Our data is legally not copyrightable, there is no legal owner.

For the reference and non-reference data sets that we reuse, conditions are as follows:

- NIST Chemistry WebBook

It is freely available for any use (public domain or CC0).
- Gas Chromatography/Mass Spectrometry (GC/MS)
  It is available under specific restrictions, which we will follow in our project: Software license.

For our produced data, conditions are as follows:

- **ASEP – Repository of the Czech Academy of Sciences** (will be published)
  The distributions will be accessible through:
  - *Our institutional repository*. The distribution will be available under the following license:
    - Starting 2027-01-01: Freely available for any use (public domain or CC0).

A user of this data can use it without any specific software.

The dataset will published after an embargo.

## 2.3. Making data interoperable

We will be using the following data formats and types:

- TXT, PDF, Microsoft Word and Excel
  It is a standardized format.

## 2.4. Increase data re-use

The metadata for our produced data will be kept as follows:

- **ASEP – Repository of the Czech Academy of Sciences** (will be published) – This data set will be kept available as long as technically possible.

As stated already in Section 2.2, all of our data can become completely open over time.

We will be archiving data in *cold storage* systems for long-term preservation already during the project. The data are expected to remain interpretable and reusable over time.

To validate the integrity of the results, the following will be done:

- We will run a subset of our jobs several times across the different compute infrastructures.
- We will run part of the data set repeatedly to catch unexpected changes in results.

# 3. Other research outputs

We use Data Stewardship Wizard for planning our data management and creating this DMP. The management and planning of other research outputs is done separately and is included in this Section. Still, we benefit from data stewardship guidance (e.g. FAIR principles, openness, or security) and it is reflected in our plans with respect to other research outputs.

We decide which additional research outputs should be retained as follows: Outputs necessary for reproducibility, reuse by others, legal compliance, or future reference are stored according to good laboratory practices.

We plan to produce the following additional research outputs:

- *The following is a list of relevant outputs for scale-up: - Conversions - Yields - Kinetic and thermodynamic constants - Procedures for operation*:
  It is valuable because they has received scant attention in the open scientific literature. It is expected to be reused by *researchers in the scientific and technical disciplines*. It will be made available at *reasonable request, these outputs can be provided by authors*.

# 4. Allocation of resources

FAIR is a central part of our data management; it is considered at every decision in our data management plan. We use the FAIR data process ourselves to make our use of the data as efficient as possible.

- **Mechanistic study and kinetic modeling of isopropanol Guerbet coupling in a continuous plugflow reactor over Ni/MoC catalysts**

  **- 27-25798S**
  Following resources will be dedicated to data management and ensuring that data will be FAIR:

  - **Eligible costs of the consortium - Open Access** - Planned grant project eligible costs from all funding sources .
    The amount is 50000 Czech Republic Koruna, CZK.

    This resource is allocated for ensuring findability, ensuring accessibility, ensuring interoperability, ensuring reusability, and supporting management of data.

    This cost will be covered by funding grant (grant number: 27-25798S)

We will be archiving data in cold storage systems for long-term preservation after the project but also already during the project. The costs for archiving data will be paid out of departmental budgets from one or more of the project participants. The minimum lifetime of the archive is 15 years. The archival period can be extended – library or archive staff will decide. The decision whether or not to extend the renewal

be based on the predicted use of the archived data. Data formats in cold storage will be upgraded if they become obsolete. Archived data will be migrated regularly to more modern storage media (e.g. newer tapes).

None of the used repositories charge for their services.

We have a reserved budget for the time and effort it will take to prepare the data for publication. For making data or other research outputs FAIR, we budgeted: 50000 CZK.

To execute the DMP, additional specialist expertise is required and we have such trained support staff available.

We do not require any hardware or software in addition to what is usually available in the institute.

# 5. Data security

Project members will not store data or software on computers in the lab or external hard drives connected to those computers. They will not carry data with them (e.g. on laptops, USB sticks, or other external media). All data centers where project data is stored hold appropriate certifications. All project web services are accessible via secure HTTP (https://...). Project members have been instructed about both generic and specific risks to the project.

The possible impact of information loss is small. The risk of information leak, and vandalism is acceptably low.

We are not using any personal information.

The archive will be stored in a remote location to protect the data against disasters. The archive needs to be protected against loss or theft. It is clear who has physical access to the archives.

We are running the project in a collaboration between different groups and institutes. However, there is no collaboration agreement in the project that describes who can have access to what data.

# 6. Ethics

**Data we produce**

For the data we produce, the ethical aspects are as follows:

- **ASEP – Repository of the Czech Academy of Sciences**
  - It does not contain personal data.
  - It does not contain sensitive data.

**Data we collect**

We will not collect any data related to individuals, i.e. "personal data".

The data collection is not subject to ethical legislation.

# 7. Other issues

We use the Data Stewardship Wizard with its *CAS Common DSW Knowledge Model* (ID: 053avzc18:CAScommon:3.1.0) knowledge model to make our DMP. More specifically, we use the https://avcr.fair-wizard.com/wizard DSW instance where the project has direct URL: https://avcr.fair-wizard.com/wizard/projects/e4c2e276-b7d0-42d8-95e2-66af7c759641.

We will be using the following policies and procedures for data management:

- **Code of Ethics for Scientific Research of the Czech Academy of Sciences**
  https://www.avcr.cz/en/about-us/legal-regulations/code-of-ethics-for-researchers-of-the-czech-academy-of-sciences/
  The policy finds application in all contexts involving the principles of scientific work, the dissemination of scientific knowledge and results, the assessment, evaluation, peer review, and expert activities, or procedures for dealing with breaches of the principles of proper conduct in scientific research.
- **Open Science Principles of the Czech Academy of Sciences**
  https://www.avcr.cz/en/about-us/legal-regulations/open-science-principles-of-the-czech-academy-of-sciences/
  The policy finds application in all contexts involving support for open science by the CAS, publication - open access, research data - FAIR principles, and research software - open source.