ACT LAUNCH Project No 299662

The LAUNCH project is funded through the ACT programme (Accelerating CCS Technologies, Horizon2020 Project No 294766). Financial contributions are made from: Netherlands Ministry of Economic Affairs and Climate Policy, the Netherlands; Federal Ministry of Economic Affairs and Climate Action on the basis of a decision by the German Bundestag, Germany; Gassnova SF (GN), Norway; Department for Business, Energy & Industrial Strategy (BEIS) together with extra funding from NERC and EPSRC research councils, United Kingdom; US-Department of Energy (US-DOE), USA.
All funders are gratefully acknowledged.

Lowering **A**bsorption process **UN**certainty, risks and **C**osts by predicting and controlling amine degradation

Technical Memorandum, Solvent Degradation database

(related to the data base application)

Dissemination level	Public	
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Issue date	07.04.2023	

Executive summary

A public database for amine degradation data was established during the LAUNCH project. This is a unique platform for sharing and searching for data related to the stability and degradation of amine solvents for CO_2 capture and facilitates knowledge sharing and application of real data in models and simulations of the CO_2 capture process. Data from a range of lab and pilot scale degradation tests are made available and searchable in this database, which is currently administered by SINTEF Industry. The database currently contains 45 different datasets, which are all connected to published literature. In the database, a collection of data, metadata and additional information about setups and experiments can be found and shared. This memo introduces how the database works and how it can be used.

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1 Introduction

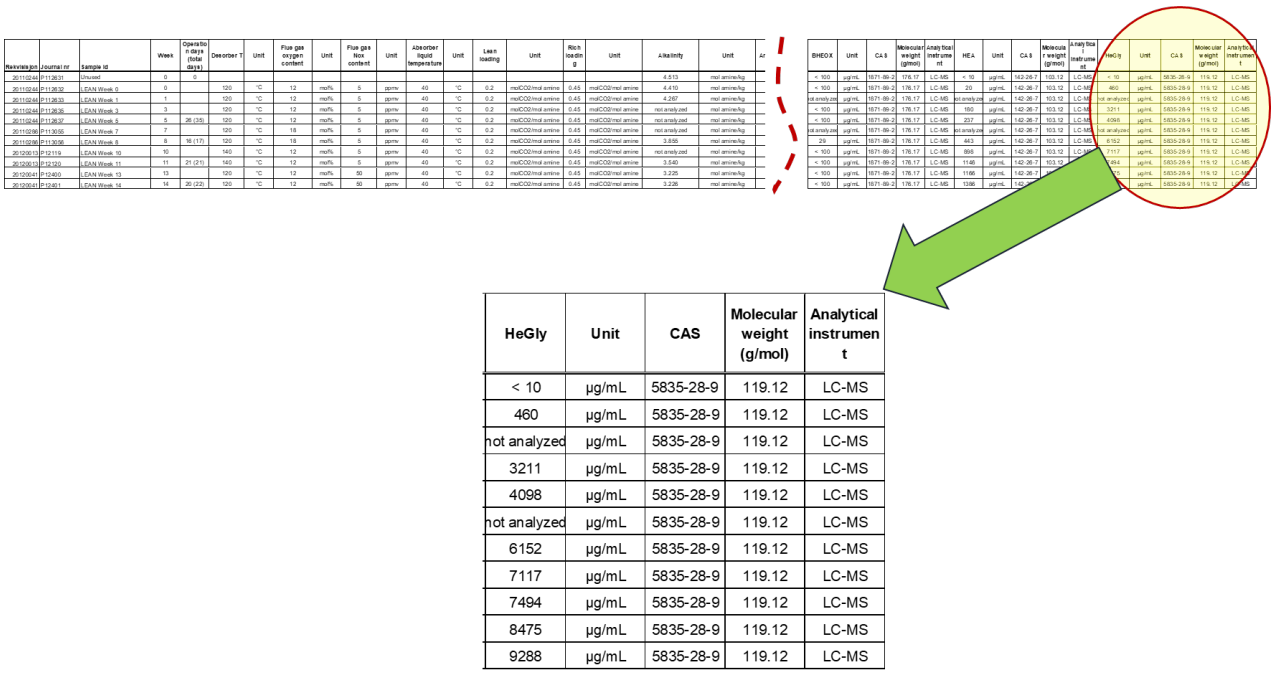
As part of the LAUNCH project a solvent degradation database is established. In this database the main focus is analytical results of degradation compounds in solvents during bench scale solvent degradation, pilot testing, etc. The first version of the database was based on available literature data, incorporating data from lab to pilot scale, and was later extended with data generated in the project. During the project the access to the database was limited to the project partners, but now as the project is ended the database is made publicly available. This MEMO gives a short description of the database, how to access it as well as how to add new data.

2 The database

2.1 Database development

The database was developed by using Dataverse – Open-source research data repository software framework (https://dataverse.org/). A custom LAUNCH Dataverse repository was established. The database with web portal and REST-API deployed on Azure Cloud (with SINTEF access control during the project, but now made public)

2.2 Template for the analytical data



HeGly	Unit	CAS	Molecular weight (g/mol)	Analytical instrument
< 10	µg/mL	5835-28-9	119.12	LC-MS
460	µg/mL	5835-28-9	119.12	LC-MS
not analyzed	µg/mL	5835-28-9	119.12	LC-MS
3211	µg/mL	5835-28-9	119.12	LC-MS
4098	µg/mL	5835-28-9	119.12	LC-MS
not analyzed	µg/mL	5835-28-9	119.12	LC-MS
6152	µg/mL	5835-28-9	119.12	LC-MS
7117	µg/mL	5835-28-9	119.12	LC-MS
7494	µg/mL	5835-28-9	119.12	LC-MS
8475	µg/mL	5835-28-9	119.12	LC-MS
9288	µg/mL	5835-28-9	119.12	LC-MS

Figure 2.1: Structure of analytical data to be uploaded to the database

3 Accessing the database

Go to the Database which is located here: **https://launchdb.sintef.no**

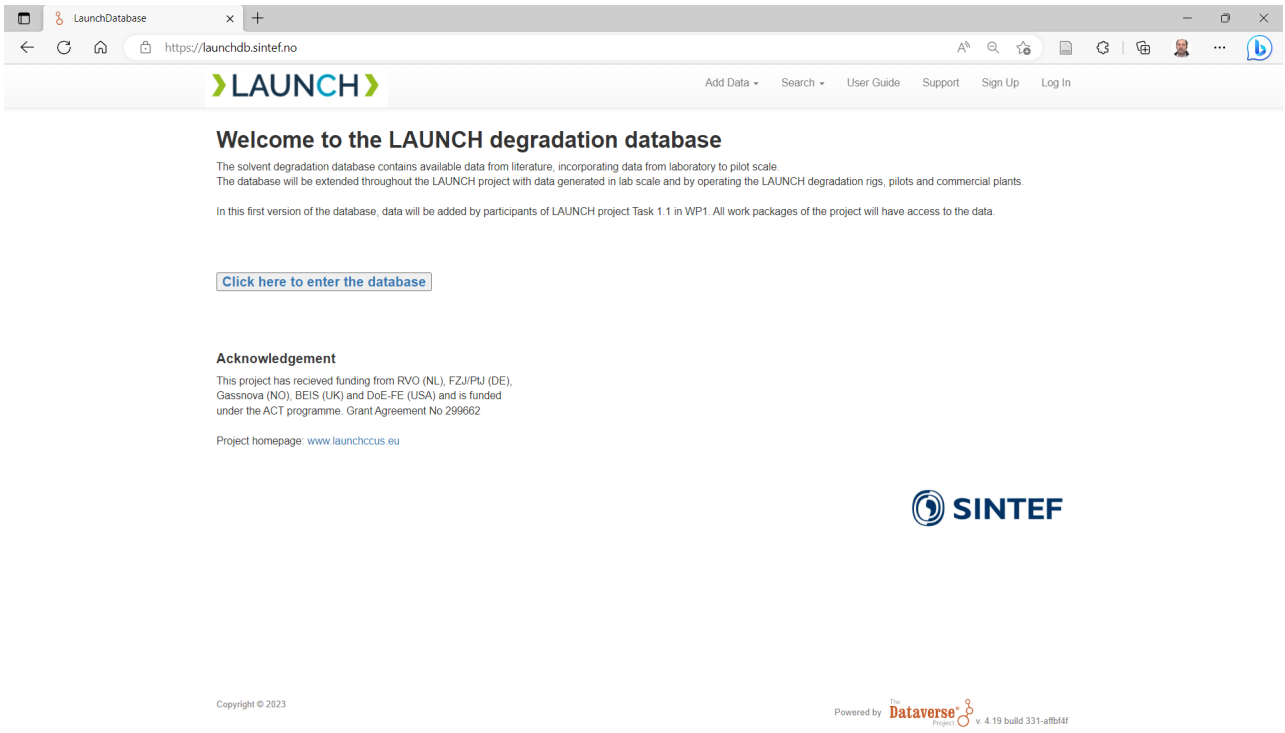


Figure 3.1 LAUNCH database, welcome page.

From the welcome page you click on the button marked *Click here to enter the database* to enter the database.

In the database there is a search field, which can be seen marked with yellow in *Figure 3.2*. Here it is possible to search for instance on chemical name (or abbreviation) or CAS number. It is also possible to click on the Subject and Author Affiliation and list with matching entries will appear in a new window. In the bottom you can scroll through all entries in the database. On the top there is also a User Guide if help or more info on the Dataverse is needed.

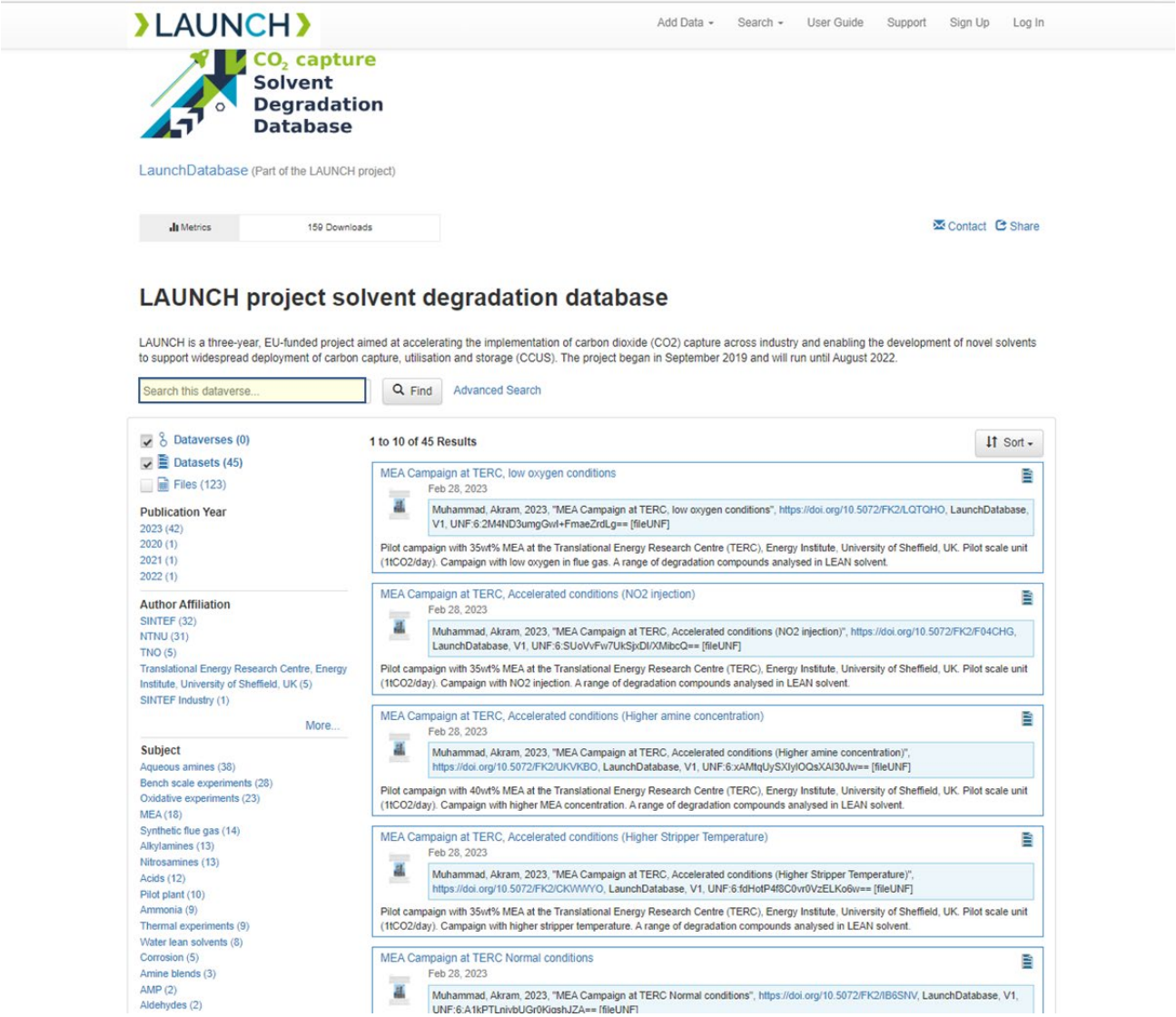


Figure 3.2 LAUNCH degradation database, Overview Window

To see the contents of an entry, just click on the name/title and that entries opens in a new window, as illustrated below (*Figure 3.3*). Here the entered metadata appears as well as all files that are available for this entry. In this case there were 7 files, which is also available to download. For this example, the XY data with the analytical results is in the file *RAW data SDR MEA 2016.tab*. There is also a supporting file with compounds name and more details of the analytical methods used (*Overview compounds and liquid analysis.xlxs*), file with a picture of the apparatus, file with procedure, as well as files with P&ID and Flow Diagram.

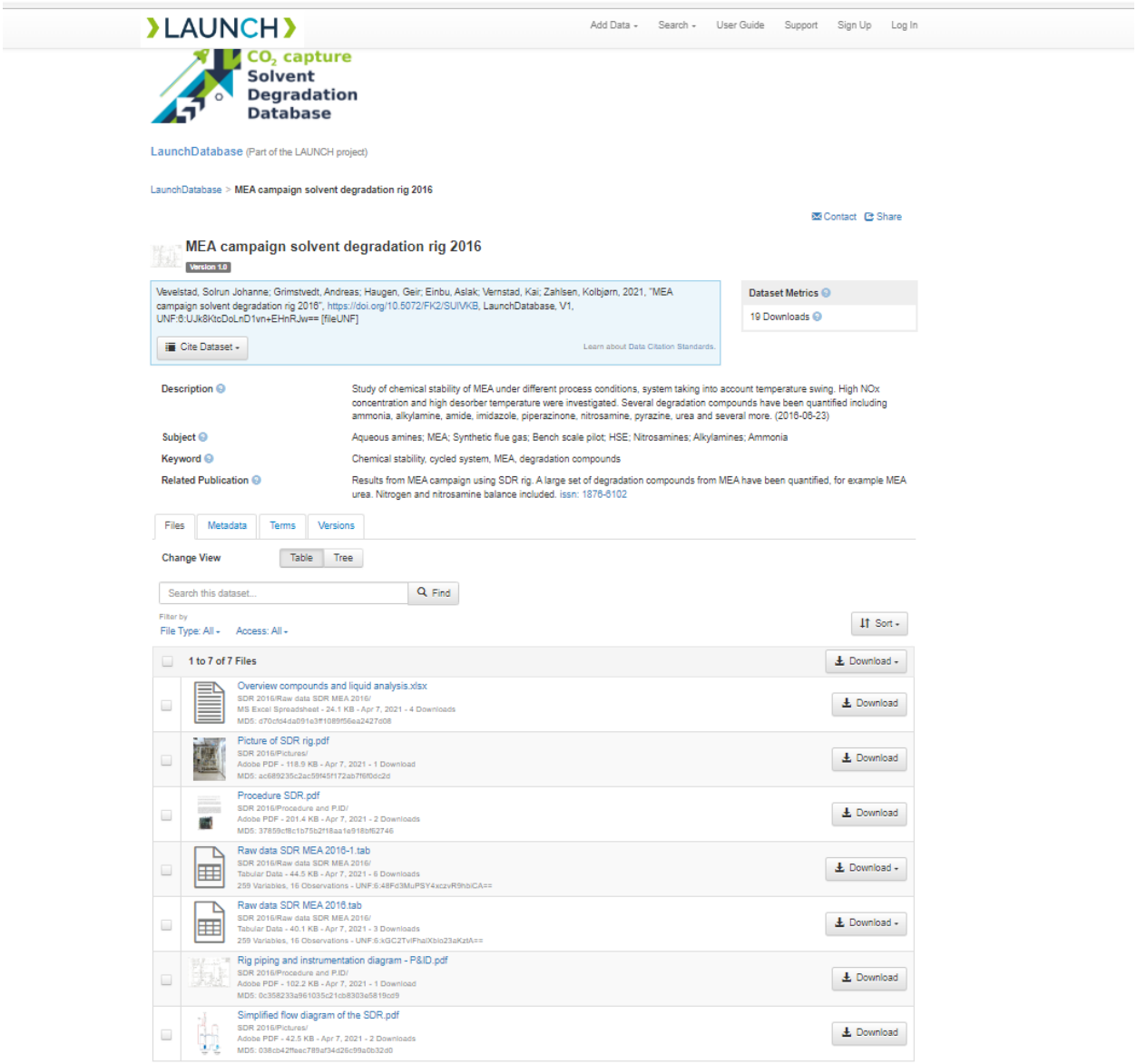


Figure 3.3 Example of a dataset in the database, with Metadata and files available for download.

4 Adding new data to the database

To add new data to the database, you must first create an account which is done by clicking Sign Up (*see Figure 4.1)*

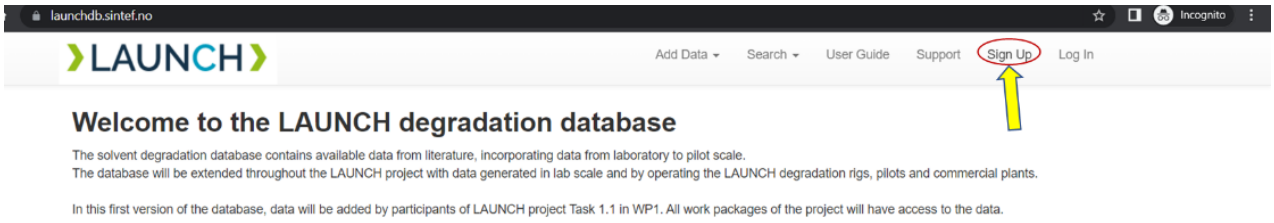


Figure 4.1 Sign up

When you sign up, you will be given access to add new data. Please note that this you take some days before the account is ready.

When you have the account, you then need to Log in (Log In is on the upper right side of the page). Then you choose Add Data and New Dataset (as illustrated in *Figure 4.2*)

Figure 4.2 Adding New Dataset

You then get a form where you fill in the metadata, and upload the relevant files (see *Figure 4.3*)

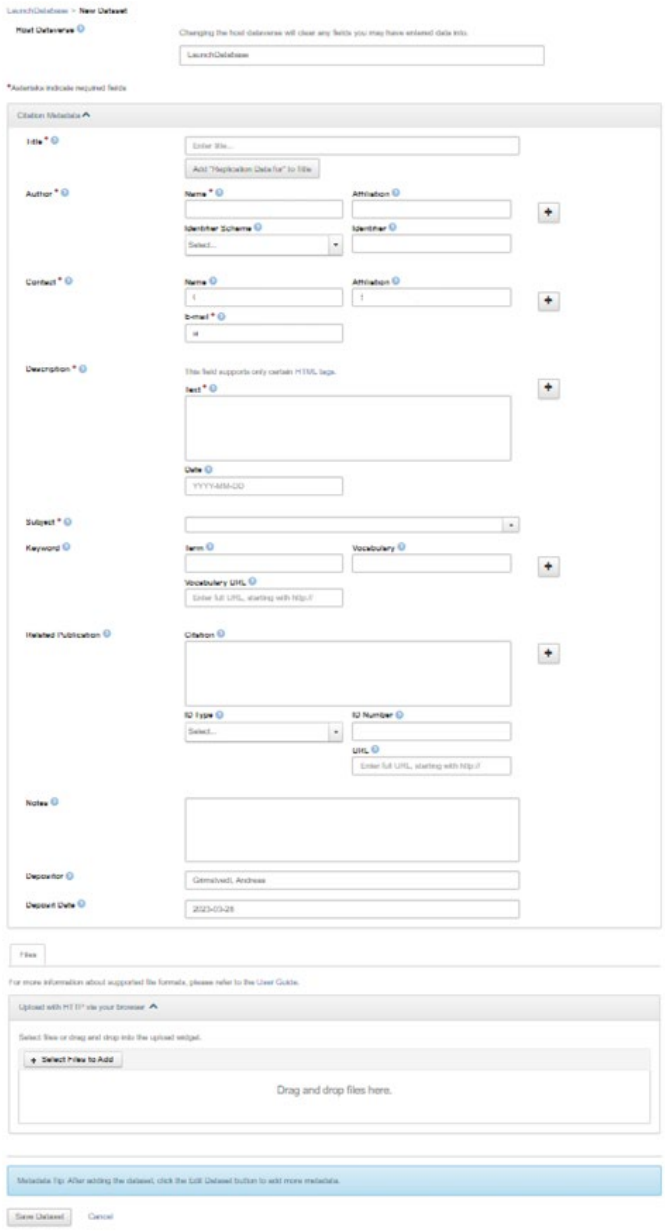


Figure 4.3 Form to enter metadata and upload files.

The analytical data (i.e., chemical analysis) of samples from experiment/pilot campaign must be added as an XY table and it is most convenient to upload an MS-Excel or Tab separated file. All analyzed results and compounds should be uniquely described, i.e., heading should include unit, analysis method and CAS number. It is worth noting that the search bar of the LAUNCH database searches only through the header row of the data tables, which is why descriptive headings facilitate finding the data you need when searching. The first columns should be used for sample id, time or sequence number, values for conditions that were varied. If you have many literature references for your set, this could be listed in a separate file which then also should be uploaded. Further details may be described in separate files which can also be uploaded. It is recommended to look at already published data sets in the database as examples.

When the metadata and files has been entered, remember to save the dataset (button on the left bottom of the page). You can later edit the entry, this you do by choosing the dataset in the database and then select the Edit button (*see Figure 4.4*), where you can edit the metadata. or upload more files etc.

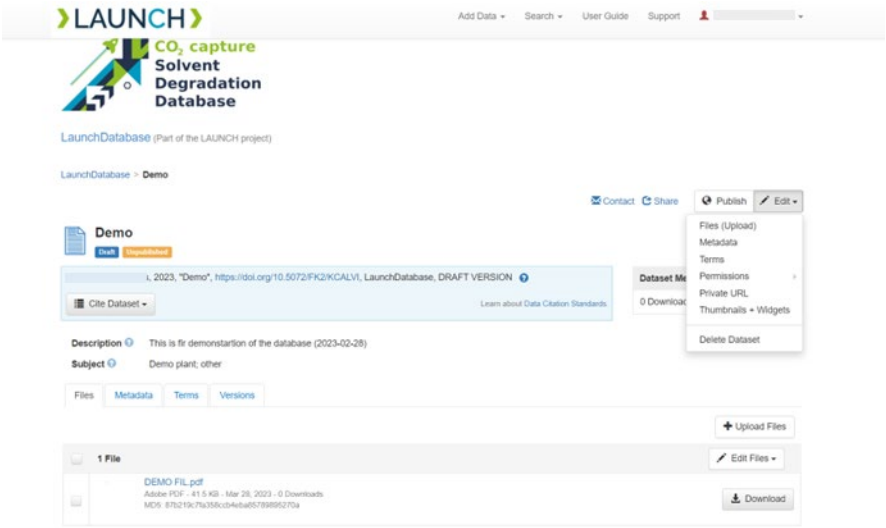


Figure 4.4 Edit of dataset.

At this stage the data is not yet published in the database (it is only you who see the dataset), but will at this point be reviewed (currently by SINTEF) before it is published to the database. After you have submitted your dataset for review, you may no longer edit it, until the review process is done. Once the review has been completed and the dataset is approved, it will become searchable, and you may also edit the submission. If you make changes and resubmit the dataset, another review of the data will take place before the changes become publicly available.