Cracking of Green Ammonia to Hydrogen by Synergistic Combination of Thermocatalysis and Plasma Technology

A Data Management Plan created using DMPonline.be

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Project abstract:

Ammonia is a promising hydrogen carrier due to its high hydrogen density, but a missing link is an energy-efficient technology for ammonia cracking to produce hydrogen gas. The most explored option is thermocatalytic cracking, but this solution requires high temperatures to achieve near complete conversion, especially when using noble metal-free catalysts. Plasma cracking of ammonia is not limited by the same thermodynamic equilibrium as the applied electrical energy selectively heats electrons, due to their small mass, creating a thermal non-equilibrium. The highly energetic electrons can break up ammonia molecules and achieve higher conversions at lower bulk temperatures. The main downside of plasma cracking is the relatively high energy cost. During this PhD, a process, which combines the benefits of thermocatalytic and plasma cracking, will be explored. A packed bed reactor partly converts ammonia to H2 and N2 (>50 %). The outlet of the catalytic reactor is sent to the plasma reactor, where the remaining ammonia is converted as much as possible (aiming at > 99%). The first objective of this PhD is to develop a noble metal-free catalysts with high activity for ammonia cracking, without aiming at complete conversion (WP1). The second objective is to join the catalytic and plasma reactor and find the optimal combination of process parameters (temperatures, flow rates, conversion efficiencies, energy requirements) to minimize total energy cost and maximize synergy production rate (WP2).

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FWO DMP (Flemish Standard DMP)

1. 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.

				Only for digital data	Only for digital data	Only for digital data	Only for physical data
Dataset Name	Description	New or reused	Digital or Physical	Digital Data Type	Digital Data format	Digital data volume (MB/GB/TB)	Physical volume
		Please choose from the following options: • Generate new data • Reuse existing data	*Please choose from the following options:* • Digital • Physical	*Please choose from the following options:* • Observational • Experimental • Compiled/aggregated data • Simulation data • Software • Other • NA	*Please choose from the following options:* • .por, .xml, .tab, .cvs,.pdf, .txt, .rtf, .dwg, .gml, … • NA	*Please choose from the following options:* • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • >50TB • NA	
1. Experimental data of catalytic reactor (WP1)	Numeric data on gas concentration of products formed in the catalytic reactor, generated by Mass Spectrometry.	Generate new data	Digital	Experimental data	.xls	< 100 GB	
2. Processed data & matlab codes (WP1)	Processing of the experimental data by Matlab	Generate new data	Digital	Simulation data/aggregated data	.mat .xls image data	< 100 GB	
3. numeric data on simulation results & matlab and Aspen Plus codes (WP2)	Results of simulations carried out in Matlab and Aspen Plus V12/V11.	Generate new data	Digital	Simulation data	.xls .mat .apw	< 1 GB	
4. Characterization data of catalyst samples (WP1)	Data generated by characterization of the catalyst samples, obtained by in-house instruments (including SEM and nitrogen physisorption).	Generate new data	Digital	Experimental data	image data .xls	< 1 GB	
5. Catalyst samples (WP1)	Powder catalyst samples in-house synthesized	Generate new data	Physical				< 1 g of each sample

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:

/

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? Describe these issues in the comment section. Please refer to specific datasets or data types when appropriate.

- No

Will you process personal data? If so, briefly describe the kind of personal data you will use in the comment section. Please refer to specific datasets or data types when appropriate.

- 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.

- Yes

Before publication of relevant data, there will be checked whether the data is patentable to protect the data with view on potential commercial exploitation.

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material/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

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

2. 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).

1. Experimental data of catalytic react or (WP1): numeric data on gas concentration of products formed in the catalytic reactor, generated by Mass Spectrometry. The exact test conditions (flowrate, feedgas composition, test duration, temperature and protocol) will be stored together with the concentration data.
2. Processed data (WP1): Processing of the experimental data (obtained in 1) by Matlab. The results carried out in Matlab will be stored in .xls format and in image data. The Matlab protocol will be stored in .mat format.
3. Numeric data on simulation results (WP2): results of simulations carried out in Matlab and Aspen Plus V12/V11. The results carried out in Matlab will be stored separately in .xls format. The simulation protocol of matlab will be stored in .mat format. For simulations in Aspen Plus, both results and protocol will be stored in .apw format.
4. Characterization data of catalyst samples (WP1): Data generated by characterization of the catalyst samples, obtained by in-house instruments (including SEM and nitrogen physisorption). The results of SEM characterization will be stored in images. The results of nitrogen physisorption and other instruments will be stored in .xls format.
5. Catalyst samples (WP1): Powder catalyst samples, which are synthesized in-house, will be phyisically stored in our lab.

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify (where appropriate per dataset or data type) which metadata standard will be used. If not, please specify (where appropriate per dataset or data type) which metadata will be created to make the data easier to find and reuse.

- Yes

Relevant data will be deposited and shared in KU Leuven Research Data Repository (RDR), which uses DataCite as metadata standard.

3. Data storage & back-up during the research project

Where will the data be stored?

Data will be stored on the pc's of the researchers (on the I network drive) and automatically also on the OneDrive cloud server.

How will the data be backed up?

Back-up of the files on the pc's of the researchers to the OneDrive cloud server will automatically happen. Also, every time adjustments to the data or added data will automatically be saved and back-uped in the OneDrive Cloud. In case data are lost due malfunctioning, lost or stolen pc's, they can be retrieved from the OneDrive cloud server.

Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely.
If no or insufficient storage or backup capacities are available, then explain how this will be taken care of.

- Yes

The required storage is relatively small. The standard storage space provided by the university is sufficient.

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

Access to the OneDrive cloud server is protected by the KU Leuven authenticator service. The pc's of the researchers working on the project are password protected.

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

No additional costs are expected.

4. Data preservation after the end of the research project

Which data will be retained for at least five 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 relevant data generated will be preserved for a period of 10 years, according to KU Leuven RDM policy.

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

The relevant data will be stored on the university's central servers (with automatic back-up procedures) for at least 10 years, conform the KU Leuven RDM policy. Physical data will be physically stored in the labs of KU Leuven.

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

No additional costs for data preservation are expected.

5. Data sharing and reuse

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

- Yes, in an Open Access repository

Relevant data accompanying any publications related to the research carried out will be uploaded as supplementary information (all data types in .xls format). Relevant data will be deposited and shared in KU Leuven RDR. Any other additional data will be available upon reasonable request via e-mail or via Belnet FileSender service for large files (all digital data types).

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

Everyone will be able to access the data uploaded as supplementary information to publications in scientific journals. Any additional data can be requested by anyone via e-mail.

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 in the comment section per dataset or data type where appropriate.

- No

Where will the data be made available? If already known, please provide a repository per dataset or data type.

The relevant data will be made publicaly available in the Research Data Repository (RDR) of KU Leuven.

When will the data be made available?

Upon publication of the research results.

Which data usage licenses are you going to provide? If none, please explain why.

not applicable

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.

- Yes

The relevant data will be made available in the Research Data Repository (RDR) of KU Leuven, which uses a DOI number to identify the data.

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

No additional costs for data sharing are expected.

6. Responsibilities

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

Johan Martens

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

Johan Martens

Who will manage data preservation and sharing?

Johan Martens

Who will update and implement this DMP?

Johan Martens