21st - 24th OCTOBER 2024

# Book of ABSTRACTS

# Empowering the FUTURE with HYDROGEN

MH2S

Munich Hydrogen Symposium 2024

# Imprint

**Book of Abstracts:**
Munich Hydrogen Symposium 2024 (MH2S 2024)
October 21st - 24th, 2024, Garching, Germany

**Organized by:**
Chair of Energy Systems

**Contact:**
Email: *h2symposium.les@ed.tum.de*

**PUBLISHER**:
Dr. Sebastian Fendt
Chair of Energy Systems
TUM School of Engineering and Design
Technical University of Munich
Boltzmannstrasse 15
85748 Garching

**Publication Date:** 19.12.2024
**DOI:** *10.14459/2024md1765595*

**Please cite this as:** *Author(s) of abstract. Title of abstract [abstract].* In: Munich Hydrogen Symposion 2024; October 21-24, Munich: S. Fendt; 2024. DOI: 10.14459/2024md1765595

# Organizing Committee

## Conference Chairman

Prof. Dr.-Ing. Hartmut Spliethoff
Dr.-Ing. Sebastian Fendt

## Conference Organization Team

Andreas Hanel (Lead)
Norina Auburger
Rebecca Singer
Lukas Martetschläger
Johannes Waßmuth
Theresa Hauth
Svenja Knösch
Vincent Dieterich

# Scientific Committee

| | |
|---|---|
| Prof. Dr. Peta Ashworth | *Curtin University* |
| Dr. Sebastian Fendt | *Technical University of Munich* |
| Dr. David Harris | *CSIRO* |
| Dr. Stephan Herrmann | *Reverion GmbH* |
| Prof. Dr. Svetlana Ikonnikova | *Technical University of Munich* |
| Prof. Dr. Gilberto Jannuzzi | *State University of Campinas* |
| Prof. Dr. Harald Klein | *Technical University of Munich* |
| Prof. Dr. Inês Cardoso Pereira | *Universidade NOVA de Lisboa* |
| Prof. Dr. Nicolas Plumere | *Technical University of Munich* |
| Prof. Dr. Volker Sieber | *Technical University of Munich* |
| Prof. Dr. Hartmut Spliethoff | *Technical University of Munich* |
| Prof. Dr. Kentaro Umeki | *Lulea University of Technology* |
| Prof. Dr. Johannes Völkl | *Rosenheim Technical University of Applied Sciences* |

## Main Sponsors

ChemDelta
Bavaria

H2 reallabor
burghausen

## Supporting Sponsors

Reverion

## Presented by

Technische
Universität
München

reallabor
burghausen

REDEFINE H2E
INTERNATIONAL FUTURE LAB

GEFÖRDERT VOM
Bundesministerium
für Bildung
und Forschung

# Opening Statement

**Dear Participants of MH2S 2024,**

**Dear readers,**

It is my pleasure to welcome you to the 2024 edition of the Munich Hydrogen Symposium (MH2S). This *Book of Abstracts* has been prepared to serve as an essential resource for all attendees of the symposium, as well as for researchers, industry professionals and stakeholders who share a deep interest in the advancements of hydrogen technologies but may not be able to join us this year.

As we gather in Garching (Munich) to exchange knowledge, insights, and innovative ideas, this symposium provides a unique platform to foster collaboration and explore new frontiers in hydrogen research and development. The symposium builds on the momentum of two exceptional initiatives: the International Future Lab "REDEFINE H2E" and the $H_2$ Reallabor Burghausen ($H_2$ Living Lab Burghausen). These projects underline our commitment to engage with the global research community and advance the hydrogen economy.

The contributions presented here span a broad spectrum of cutting-edge topics, from hydrogen production techniques and circular economy principles to comprehensive system studies and the future role of hydrogen across various sectors. Additionally, we delve into Power-to-X technologies, exploring their potential to elevate hydrogen's role in building sustainable energy systems. Each contribution highlights the critical role of hydrogen in driving the transition towards a resilient and circular economy, while also addressing the challenges that lie ahead.

I extend my sincere gratitude to all the contributors for their invaluable work, and to all participants for their active engagement in this pivotal dialogue. Together, we are laying the foundation for a cleaner, more sustainable future powered by hydrogen.

I hope this collection of abstracts inspires you as we collectively embark on this journey toward innovation and sustainability in the hydrogen sector. May MH2S 2024 be an exciting, informative, and visionary event, filled with inspiring discussions, fruitful networking, and new partnerships that will advance our shared vision of a hydrogen-powered, circular future.

Enjoy the Munich Hydrogen Symposium 2024, and happy reading!

Warm regards,

**Dr.-Ing. Sebastian Fendt**

# Content

# M.1a – System Studies

## Social acceptance of green hydrogen in Europe

Lydia Maketo

*Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: lydia.maketo@tum.de*

During the mid to late 2000s, there was a noticeable dearth of research attention dedicated to exploring the perceptions and acceptance of Hydrogen Energy Technologies (HETs) (Hugo Seymour et al. 2008). While there is evidence suggesting positive perceptions of and support for HETs (Häussermann, Maier et al. 2023), other research has found neither full support, nor complete opposition to HETs (Smith, Bucke and van der Horst 2023). It is apparent that the public has yet to reach a conclusive decision regarding HETs. This underscores the necessity for additional research to gain deeper insights into the determinants shaping public attitudes towards HETs. The aim of this study is to investigate social acceptance of green hydrogen in Germany and Europe.

Social acceptance is increasingly used in association with energy technologies associated with the energy transition and has been understood through diverse perspectives (Lundheim, Pellegrini-Masini et al. 2022). This study defines social acceptance as a favorable or positive reaction toward proposed or existing technology or social-technical systems by individuals within a specific social entity (such as a country, region, community, town, house hold, or organization)(Upham, Oltra and Boso 2015).

Twenty-five online semi-structured interviews were conducted using Microsoft Teams mostly in Germany. Semi-structured interviews allow the design of a catalog of questions, without appointing a strict procedure or unique set of questions (Crano, Brewer and Lac 2014). In-depth-qualitative data is particularly useful when looking to explore and understand social issues (Adams and Cox 2008). By employing a qualitative approach, this research seeks to unearth valuable insights into the factors shaping individuals' perceptions and acceptance of HETs, contributing to a more nuanced understanding of the societal dynamics influencing the adoption of HETs.

The majority of participants express a significant concern about climate change and demonstrate a strong willingness to adopt green hydrogen as a viable solution to mitigate the adverse effects of fossil fuels. It is evident that the definitions associated with green hydrogen significantly influence its social acceptance. There is a growing momentum to transition from categorizing hydrogen based on colours to defining clean hydrogen in terms of its carbon emissions. Lack of communication, regulation and policy are perceived to be barriers of acceptance of green hydrogen. The social acceptance of hydrogen can be examined through the lens of the challenges and opportunities presented by renewable hydrogen. The perceived benefits of green hydrogen extend potentially to a global scale, including the prospect of involving new energy stakeholders from the Global South. Discussions on global challenges have centered around the influence of politics and political unrest on the hydrogen value chain.

Through the lens of semi-structured interviews, this study endeavors to illuminate unexplored facets of green HETs acceptance, paving the way for informed policy decisions and future research directions in the field of renewable energy.

### References

Adams, A. and A. L. Cox (2008). Questionnaires, in-depth interviews and focus groups, Cambridge University Press.

Crano, W. D., M. B. Brewer and A. Lac (2014). Principles and methods of social research, Routledge.

Häussermann, J. J., et al. (2023). "Social acceptance of green hydrogen in Germany: building trust through responsible innovation." Energy Sustainability and Society 13(1).

Lundheim, S. H., et al. (2022). "Developing a Theoretical Framework to Explain the Social Acceptability of Wind Energy." Energies 15(14): 4934.

Smith, C., C. Bucke and D. van der Horst (2023). "Green hydrogen powering sustainable festivals: Public perceptions of generators, production and ownership." International Journal of Hydrogen Energy 48(23): 8370-8385.

Upham, P., C. Oltra and À. Boso (2015). "Towards a cross-paradigmatic framework of the social acceptance of energy systems." Energy Research & Social Science 8: 100-112.

# Emissions along the Green Hydrogen Value Chain and Their Regulatory Relevance in the EU

Regina Reck[1]*, Sophie Ströhler[1], Tapio Schmidt-Achert[1]

[1]*Forschungsstelle für Energiewirtschaft, Munich, Germany*
**Corresponding author: rreck@ffe.de*

---

## Motivation

Green hydrogen, defined for the purpose of this study as hydrogen produced via electrolysis powered by renewable electricity production, plays a central role for decarbonizing certain sectors and applications. The regulatory framework acknowledges the relevance of emission accounting of hydrogen. A threshold for the carbon footprint is defined to ensure reductions in greenhouse gas (GHG) emissions. In the EU regulation and current certification schemes of green hydrogen, different methodologies, system boundaries and thresholds exist for the calculation of the carbon footprint [1]. In literature, several studies compare the carbon footprint of different production pathways [2, 3]. For the production of hydrogen via electrolysis, the emission intensity of the electricity used is decisive [4]. Nevertheless, renewable hydrogen consumption always requires further steps following the hydrogen production. Therefore, the influence of transport and storage of hydrogen should also be considered in the carbon footprint. This is underlined by the EU definition for renewable hydrogen, where system boundary in the emission accounting methodology includes the emissions stemming from transport and production. As these emissions are rarely included in existing studies, the aim of the work is to give a comprehensive overview the scale of emissions occurring in the different stages of the hydrogen value chain. Hence, the carbon footprint of green hydrogen is determined using the methodology of life cycle assessment (LCA). Subsequently, the results are placed in the context of emissions accounting in EU legislation. analysis was developed within the framework of the interdisciplinary research project Trans4ReaL which scientifically accompanies the German hydrogen living labs.

## Method and Results

A LCA model is used for a holistic ecological assessment of a generic value chain of renewable hydrogen produced and consumed in Germany. Wherever possible, the model and necessary assumptions are based on real word projects (Reallabore der Energiewende / living labs). The life cycle inventory is based on a comprehensive literature review.

The aim is to provide an assessment for the contribution of each stage of the value chain to the carbon footprint of green hydrogen. Figure 1 shows the modelled steps in the value chain including the system boundaries and functional units. The overall functional unit is 1 kg of renewable hydrogen supplied. For each step in the value chain, different options are modelled. A modular approach is chosen, which enables the assessment of the carbon footprint of the connected combinations of the elements along the value chain. Hence, especially for the emissions attributed to the transport and storage of hydrogen, the separation of "variable" emissions from "fixed" emissions is required. "Variable" emissions are those that depend on the carbon footprint of the product, for example the leakage of hydrogen during transportation and storage. The "fixed" contributions refer to emissions independent of the product transported and stored, i.e. the electricity supply and chosen electrolysis technology.

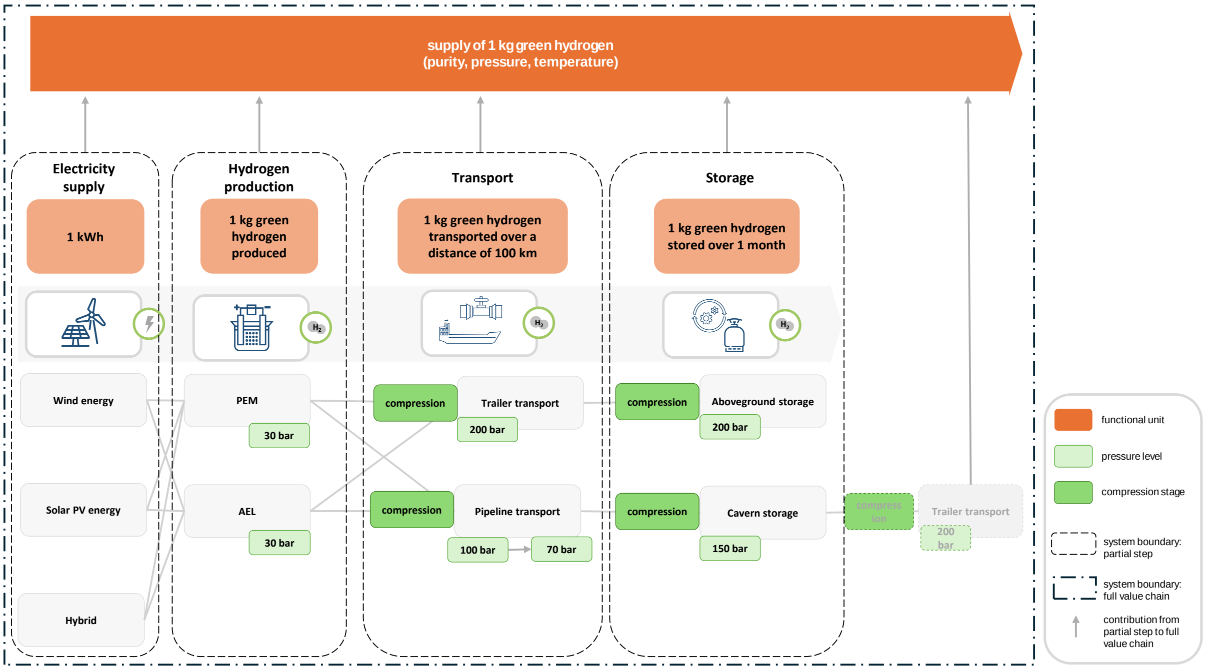


*Figure 1: Methodological assumptions for the LCA model of the renewable hydrogen value chain (own illustration)*

The assessment shows that despite the emission intensity of the electricity used for hydrogen production, transport and storage also significantly contribute to the carbon footprint of renewable hydrogen. Especially the energy consumption for compression at the different stages is relevant in Germany due to the emission intensity of the electricity mix. This is relevant in the context of hydrogen certification, where these steps are sometime excluded from the system boundary. When the energy required for the operation of hydrogen transport and storage infrastructure does not stem from renewable sources, larger transport distances for gaseous green hydrogen influence the carbon footprint. Especially for the compliance with the threshold for renewable hydrogen of 3.4 kg $CO_2e$ per kg hydrogen in the EU, long distance transport can increase the carbon footprint above this threshold.

## References

[1] G. G. Dias Ponzi, V. H. Jacks Mendes dos Santos, P. de Medeiros Engelmann und F. Dalla Vecchia, "The hydrogen life cycle assessment methodology: an overlooked puzzle piece in harmonizing hydrogen certification and trade", Clean Techn Environ Policy, 2024, doi: 10.1007/s10098-024-02752-y.
[2] G. H. Patel, J. Havukainen, M. Horttanainen, R. Soukka und M. Tuomaala, "Climate change performance of hydrogen production based on life cycle assessment", Green Chemistry, Jg. 26, Nr. 2, S. 992–1006, 2024, doi: 10.1039/D3GC02410E.
[3] IEA, "Towards hydrogen definitions based on their emissions intensity", France, Apr. 2023.
[4] R. Reck, S. Haas, T. Schmidt-Achert und A. Neitz-Regett, "Relevance of Emission Accounting Methods for the Classification of Green Hydrogen", 13. Internationale Energiewirtschaftstagung an der TU Wien, 2023.

# Open-source energy system model for evaluation of gigawatt-scale hydrogen production in Brazil

Simon Herzog[1]*

*[1]Chair of Renewable and Sustainable Energy Systems, Technical University Munich, Germany*
**Corresponding author: simon.herzog@tum.de*

---

Green hydrogen, produced from renewable energy sources, is a promising option for decarbonizing the global energy system. However, large-scale green hydrogen production requires huge amounts of low-cost electricity, mainly from wind and solar power, and sufficient land availability without major conflicts. To identify and quantify the potential of green hydrogen production in different regions of the world, energy system models are needed that can provide optimal system design and operation under various scenarios and constraints. In this work, we present an open-source energy system model for Brazil, a country with abundant solar and wind resources and diverse regional characteristics. [1] The model is based on the existing linear programming framework "urbs" and is implemented in Python and MATLAB. [2] It uses regional dependent data on solar and wind potential, electricity grid infrastructure, existing hydroelectricity, and hydropower reservoirs as a relevant flexibility option. Figure 1 shows a sketch of the model design for one of three Brazilian regions. The model optimizes the total system cost, subject to various constraints on supply, demand, and technology costs. We investigate several scenarios for the possible future development of the Brazilian energy system, including giga-watt scale production of green hydrogen. Outcome of the model were regional dependent capacities for generation, transmission, battery storage to balance the operation of electrolysis. The space need for wind and photovoltaic generation capacity by selected scenarios is depicted in figure 2. The resulting amount of green hydrogen produced in Brazil is in the same order as the total natural gas demand of Germany. [3] Therefore, these results can be used to discuss import of hydrogen-based energy carriers to Germany, such as ammonia or synthetic fuels, or bring energy intensive industry to Brazil, e.g. green steel production. The scientific community is invited to use the open-source model for further investigations, not only related to Brazil, but also for other countries with considerable potential for green hydrogen production, e.g., United States of America, North Africa, or Europe.

This work is based on a research project under the supervision of Gilberto De Martino Jannuzzi, Universidade Estadual de Campinas (UNICAMP), São Paulo, Brazil, and Thomas Hamacher, Technical University of Munich.

## References

[1] S. Herzog, Distributed and Centralized Integration of Fluctuating Renewable Power: The Case of Brazil, Munich, 2022, https://mediatum.ub.tum.de/1647418
[2] J. Dorfner, et al., urbs – a linear programming optimization model for capacity expansion planning and unit commitment for distributed energy systems, 2024, https://github.com/tum-ens/urbs
[3] S. Herzog, Brazil as a Global Leader for Green Hydrogen, 2024, Energy Review, vol. 5, no. 6, 2023, https://www.energyreview.in/post/adviser-s-note-june-2023

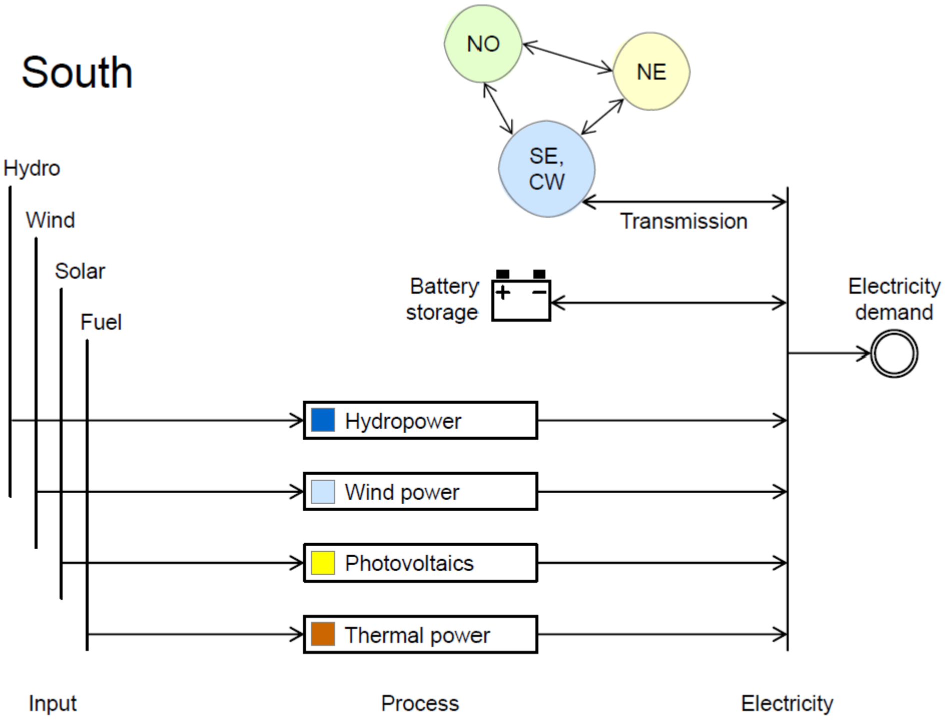


*Figure 1: Model representation of supply, processes, and demand in one Brazilian region*

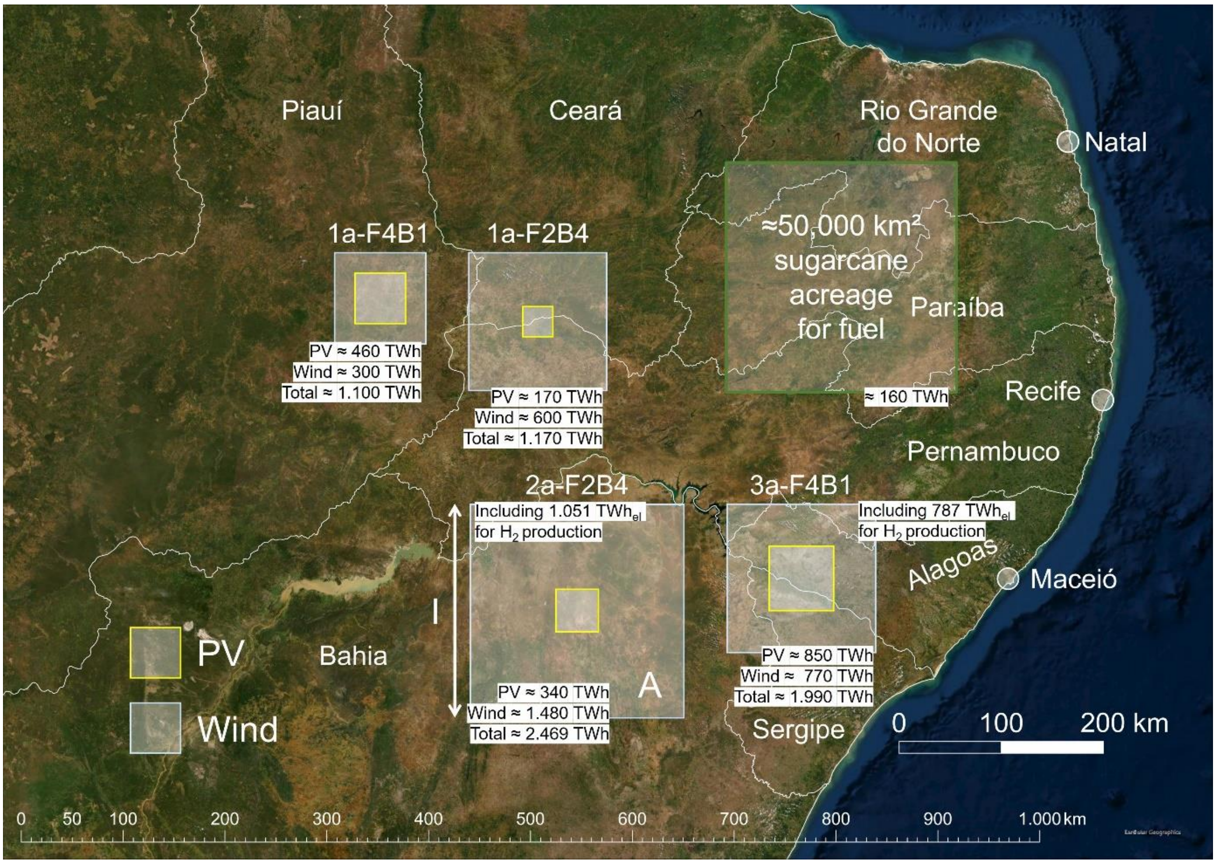


*Figure 2: Space need for wind farms and photovoltaic arrays by scenario.*

# Scotland can meet its 5 GW hydrogen target sooner than 2030!

Arash Badakhsh[1]*, Sivapriya Mothilal Bhagavathy[2]

*[1]Department of Chemical and Process Engineering, University of Strathclyde, Glasgow, United Kingdom*
*[2]PNDC, University of Strathclyde, Glasgow, United Kingdom*
**Corresponding Author: arash.badakhsh@strath.ac.uk*

---

## Introduction

Scotland was Europe's third country for renewable electricity (RE) generation in 2019, behind only Norway and Iceland [1]. Scotland is extremely rich in renewable energy resources including on- and offshore wind, hydropower, and marine energy such as tidal. Therefore, the opportunities for decarbonisation are ample in the birthplace of whisky. To this end, in January 2023, the Scottish Government released their strategy for the energy transition [2].

One of the main objectives is to reach 5 GW of “low-carbon hydrogen ($H_2$)” production to support 15% of Scotland’s energy demand by 2030 [2]. This strategy estimates that 5 GW of $H_2$ will equal 450,000,000 kg of $H_2$. This requires large investments in infrastructure and intersectoral collaborations nationwide. However, resources to sustainably produce suffiecint $H_2$ must be considered to evaluate the feasibility of such an ambitious goal. This prompted us to conduct an analysis to identify possible gaps and challenges in this journey to 2030. To that end, the required resources for meeting this target are quantified and reported here.

To date, different shades of $H_2$ have been identified; For example, other than water electrolysis (green $H_2$), there are other methods of producing low-carbon $H_2$, namely by steam methane reforming coupled with $CO_2$ capture (blue $H_2$) and methane pyrolysis (turquoise $H_2$). Resources needed for these methods are also quantified and compared with green $H_2$.

The principal research questions here are:

1. What is the required water feedstock for producing sufficient green $H_2$ to meet the 5 GW target?
2. How much oversizing is required for the installed RE capacity to meet water purification, plant cooling, and electrolysis demands?
3. What are the potential alternatives to fulfil Scotland’s hydrogen target?

## Methods

The following assumptions are made in the analysis carried out:

For water resourcing, the latest report by H. T. Madsen [3] states that 1.4, 1.5, and 3.3 $m^3$ of water feedstock are needed when using groundwater, treated wastewater or surface water, and seawater, respectively, to produce 1 $m^3$ of ultrapure water.

For green $H_2$, the electricity consumption is claculated according to the data provided by R. Niekerk [4]. The report highlights that 32 MW cooling capacity is installed per 100 MW of electrolysis capacity.

For blue $H_2$, the electricity consumption was reported in detail by M. Al-Breiki and Y. Bicer [5]. They report an electricity consumption of 22.31 $kWh_e/kgH_2$ for the reactor (including the steam methane reforming and water-gas shift reactions) with $CO_2$ capture. Water consumption of 1.8 $kg/kgH_2$ for the $CO_2$ capture process was retrieved from [6]. The balance of plant (BoP) for a blue $H_2$ plant consists of: a multi-stage flash seawater desalinator (0.05 $kWh_e/kgH_2$) and evaporator (1.12 $kWh_e/kgH_2$) [5].

For turquoise $H_2$, a recent report by L. Fulcheri *et al.* [7] highlights the actual breakdown of electricity consumption in an electrified (via plasma) turquoise $H_2$ plant. Their experimental data implies a 21.54 $kWh_e/kgH_2$ consumption for the plasma reactor. Balance of plant (BoP) for a turqoise $H_2$ plant consists of: carbon black retrieval (0.68 $kWh_e/kgH_2$), and additional minor power usage (0.86 $kWh_e/kgH_2$) [7].

In addition to the above, for blue and turquoise $H_2$ scenarios, an additional electricity requirement of 1.19 $kWh_e/kgH_2$ [5] and 1.92 $kWh_e/kgH_2$ [7] is considered to account for the $CO_2$ capture in the upstream raw natural gas processing and downstream $H_2$ purification.

## Findings

**Table 1** summarises overall RE and water requirements to meet Scotland's 2030 target of 5 GW of $H_2$. The installed RE capacity in Scotland in 2020 is 13.9 GW [8].

*Table 1. Summary of required resources via different hydrogen production scenarios.*

| **Scenario** | **RE requirement (including BoP and Capacity Factor of 33.8% [9]) [GW]** | **Water requirement [Mm$^3$/yr]** | | |
|---|---|---|---|---|
| | | **Groundwater** | **Surface water** | **Seawater** |
| Green $H_2$ | 18.2–28.2 | 35.1–42.9 | 35.5–43.3 | 41.6–49.4 |
| Blue $H_2$ | 4.0 | 5.1 | 5.5 | 10.9 |
| Turquoise $H_2$ | 4.0 | 1.1 | 1.2 | 2.4 |

These findings suggest that the RE needed to power green hydrogen production could be only realised if the current installation and commissioning rate (*ca*. 1.4 GW [8]) of renewable generators like wind turbines can be maintained. However, comparing the current installed RE capacity and the electricity requirement of a blue hydrogen plant or an electrified turquoise hydrogen plant, 5 GW of hydrogen would require 4 GW of RE. This is within the current capacity of Scotland, and hence, allows for a more seamless transition of assets to achieve net zero even before the target deadline.

As shown in **Figure 1**, the adoption of electrified turquoise hydrogen can expedite Scotland's journey to net zero by at least 3 years, whilst also eliminating the need for resourcing large quantities of water. Our high-level analysis suggests a major commercial case for adopting electrified turquoise hydrogen in Scotland, but further evaluation of logistics (*i.e.*, geospatial distribution of resources) is required on a case-by-case basis.

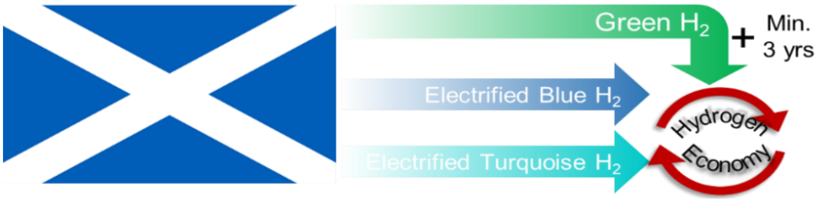


*Figure 1. Timeline to meet Scotland's hydrogen target via different production scenarios.*

## References

[1] G. Davidson, Scotland reaches the renewables top three, URL: https://www.thescottishfarmer.co.uk/news/19504045.scotland-reaches-renewables-top-three/, 11/08/2021 (Accessed on 18/01/2023).
[2] Draft Energy Strategy and Just Transition Plan, Scottish Government, Cabinet Secretary for Net Zero, Energy and Transport, URL: https://www.gov.scot/publications/draft-energy-strategy-transition-plan/, 10/01/2023 (Accessed on 17/01/2023).
[3] Madsen HT, Water treatment for green hydrogen: what you need to know, Hydrogen Tech World, 27/10/2022.
[4] Niekerk R, Thermal management in green hydrogen production: design considerations, Hydrogen Tech World, 10/11/2022.
[5] Al-Breiki M, Bicer Y. Liquified hydrogen vs. liquified renewable methane: Evaluating energy consumption and infrastructure for sustainable fuels. Fuel. 2023;350:128779.
[6] Mehmeti A, Angelis-Dimakis A, Arampatzis G, McPhail SJ, Ulgiati S. Life Cycle Assessment and Water Footprint of Hydrogen Production Methods: From Conventional to Emerging Technologies. Environments. 2018;5:24.
[7] Fulcheri L, Rohani V-J, Wyse E, Hardman N, Dames E. An energy-efficient plasma methane pyrolysis process for high yields of carbon black and hydrogen. International Journal of Hydrogen Energy. 2023;48:2920-8.
[8] Statistics: Energy Consumption by Sector, Scottish Renewables, URL: https://www.scottishrenewables.com/our-industry/statistics, (Accessed on 17/01/2023).
[9] Average load factor of renewable energies in Scotland in 2021, by source, Statista. September 2022. URL: https://www.statista.com/statistics/383335/renewable-energy-load-factor-in-scotland-uk/ (Accessed on 08/04/2023).

# Climate neutral chemistry inspired by Chemelot

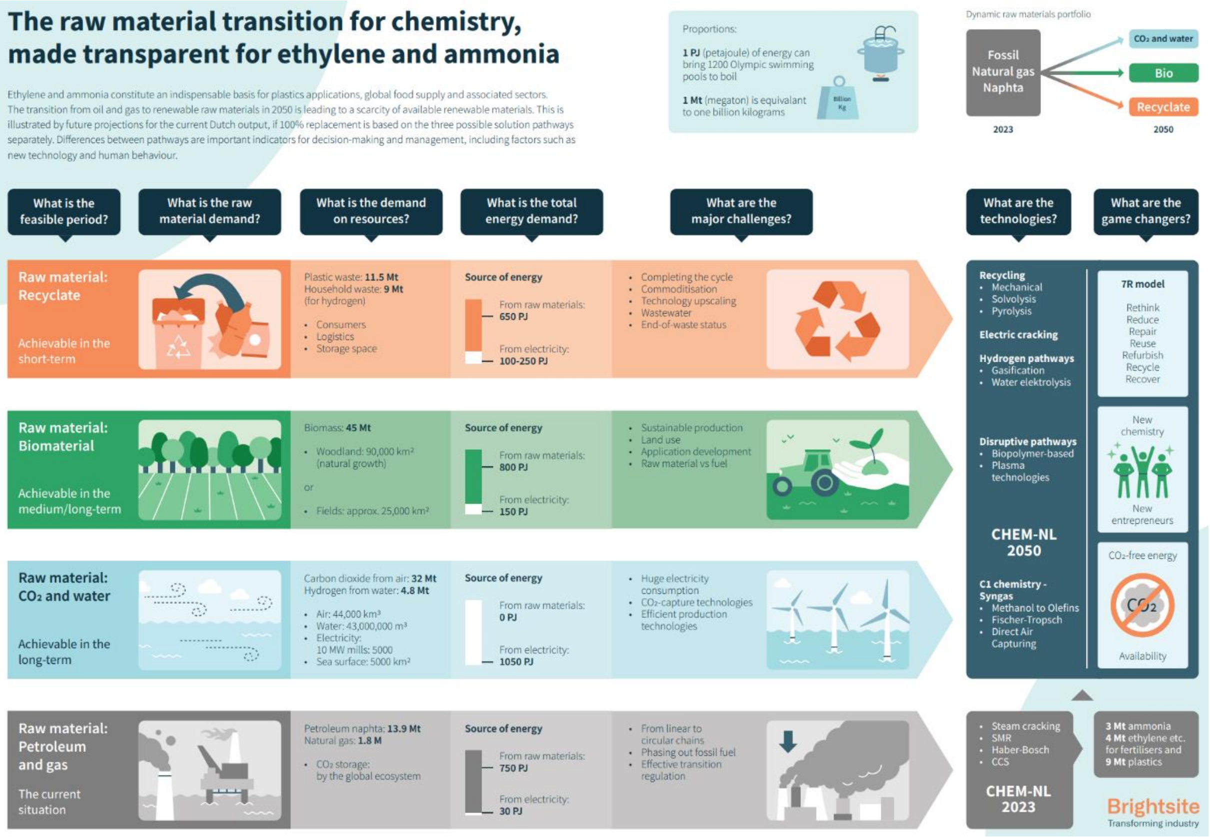
Céline Fellay*[1], Paul Brandts[1], Arnold Stocking[1], Rene Slaghek[1], Geert de Cremers[1], Zowi Maijer[1]

*[1]Brightsite Center, Brightlands Chemelot Campus, The Netherlands*
*Corresponding author: celine.fellay@sitech.nl*

---

The mission of Brightsite [1], founded by Brightlands Chemelot Campus, Maastricht University, TNO and Sitech Services, is 2-fold: demonstrate that climate goals can be reached at Chemelot Industrial Site and educate the next generation of scientists, researchers, engineers and coworkers. Chemelot is an integrated chemical site located in the south of the Netherlands where 60 highly integrated and interconnected plants produce >7,5 million tons of products per year. Among other topics, Brightsite is looking into transition scenarios and system integration to support the mission for Chemelot and the chemical industry in general. It releases a yearly BTO (Brightsite Transition Outlook) in which main dimensions of required feed and product streams are identified.

We are presenting here the approach and outcome of the BTO 2023, which focuses on the raw material transition for chemistry in the Netherlands, made transparent for ethylene and ammonia [2]. The alternative feedstock sources needed to replace the current fossil based annual Dutch production of 3 Mton of ammonia and 4 Mton of ethylene are explained and quantified in order to illustrate the size of the challenge and the intrinsic connection with the energy transition. The expected scarcity in sustainable resources requires a systemic and central-integrated approach on national and European level, to allocate the renewable resources where better alternatives are lacking, as well as encouraging an efficient use.



**The raw material transition for chemistry, made transparent for ethylene and ammonia**

Ethylene and ammonia constitute an indispensable basis for plastics applications, global food supply and associated sectors. The transition from oil and gas to renewable raw materials in 2050 is leading to a scarcity of available renewable materials. This is illustrated by future projections for the current Dutch output, if 100% replacement is based on the three possible solution pathways separately. Differences between pathways are important indicators for decision-making and management, including factors such as new technology and human behaviour.

Proportions:
**1 PJ** (petajoule) of energy can bring 1200 Olympic swimming pools to boil
**1 Mt** (megaton) is equivalant to one billion kilograms

Dynamic raw materials portfolio
2023: Fossil Natural gas Naphta
2050: CO₂ and water; Bio; Recyclate

| What is the feasible period? | What is the raw material demand? | What is the demand on resources? | What is the total energy demand? | What are the major challenges? |
|---|---|---|---|---|
| **Raw material: Recyclate**<br>Achievable in the short-term | | Plastic waste: **11.5 Mt**<br>Household waste: **9 Mt** (for hydrogen)<br>• Consumers<br>• Logistics<br>• Storage space | **Source of energy**<br>From raw materials: **650 PJ**<br>From electricity: **100-250 PJ** | • Completing the cycle<br>• Commoditisation<br>• Technology upscaling<br>• Wastewater<br>• End-of-waste status |
| **Raw material: Biomaterial**<br>Achievable in the medium/long-term | | Biomass: **45 Mt**<br>• Woodland: 90,000 km² (natural growth)<br>or<br>• Fields: approx. 25,000 km² | **Source of energy**<br>From raw materials: **800 PJ**<br>From electricity: **150 PJ** | • Sustainable production<br>• Land use<br>• Application development<br>• Raw material vs fuel |
| **Raw material: CO₂ and water**<br>Achievable in the long-term | | Carbon dioxide from air: **32 Mt**<br>Hydrogen from water: **4.8 Mt**<br>• Air: 44,000 km³<br>• Water: 43,000,000 m³<br>• Electricity: 10 MW mills: 5000<br>• Sea surface: 5000 km² | **Source of energy**<br>From raw materials: **0 PJ**<br>From electricity: **1050 PJ** | • Huge electricity consumption<br>• CO₂-capture technologies<br>• Efficient production technologies |
| **Raw material: Petroleum and gas**<br>The current situation | | Petroleum naphta: **13.9 Mt**<br>Natural gas: **1.8 M**<br>• CO₂ storage: by the global ecosystem | **Source of energy**<br>From raw materials: **750 PJ**<br>From electricity: **30 PJ** | • From linear to circular chains<br>• Phasing out fossil fuel<br>• Effective transition regulation |

| What are the technologies? | What are the game changers? |
|---|---|
| **Recycling**<br>• Mechanical<br>• Solvolysis<br>• Pyrolysis<br>**Electric cracking**<br>**Hydrogen pathways**<br>• Gasification<br>• Water elektrolysis | **7R model**<br>Rethink<br>Reduce<br>Repair<br>Reuse<br>Refurbish<br>Recycle<br>Recover |
| **Disruptive pathways**<br>• Biopolymer-based<br>• Plasma technologies<br>**CHEM-NL 2050** | New chemistry<br>New entrepreneurs |
| **C1 chemistry - Syngas**<br>• Methanol to Olefins<br>• Fischer-Tropsch<br>• Direct Air Capturing | CO₂-free energy<br>Availability |
| • Steam cracking<br>• SMR<br>• Haber-Bosch<br>• CCS<br>**CHEM-NL 2023** | **3 Mt** ammonia<br>**4 Mt** ethylene etc. for fertilisers and **9 Mt** plastics |

Brightsite
Transforming industry

*Figure 1: Infographic from Brightsite Transition Outlook 2023*

## References

[1] Home - Brightsite (brightsitecenter.com)
[2] M20230319_Brightsite_BTO_ENG_def_web_LR-1.pdf (brightsitecenter.com)

# T.1a – Hydrogen Production

## CO2 recovery and H2 generation by perovskite solar-assisted chemical looping

Massimo Santarelli[1]*, Francesco Orsini[1], Salvatore Cannone[1], Domenico Ferrero[1], Marta Boaro[2], Ahmed F. Ghoniem[3]

*[1]Department of Energy, Politecnico di Torino, Italy*
*[2]Department of Engineering and Architecture, University of Udine, Italy*
*[3]Department of Mechanical Engineering, Massachusetts Institute of Technology, US*
**Corresponding author: massimo.santarelli@polito.it*

The C-capture and utilization, together with the RES energy partner and the $H_2$ chemical/energy partner, represents a significant paradigm of sector coupling (climate change + energy + chemicals) developing a practice of molecular circularity (with a strong emphasis on C-circularity).

In this context, an interesting chemical looping process can be defined as a $CO_2$-waste-assisted production of solar fuels ($H_2$/CO at tunable percentages) by a thermochemical redox cycle. This process is based on perovskite oxygen carriers, primarily molybdates, that are continuously regenerated in redox cycles composed of the following two steps:

1. Reduction step: perovskite thermal reduction (solar-fed) assisted by a biological reducing agent (Carbon emissions from the agricultural sector, such as biogas/syngas), with a production of CO/$H_2$ syngas whose composition can be tuned by addition of $H_2O$.
2. Oxidation step: re-oxidation of perovskites with Carbon ($CO_2$) emissions from the energy/industrial sector, with further production of CO/$H_2$ syngas, again of tunable composition by addition of $H_2O$.

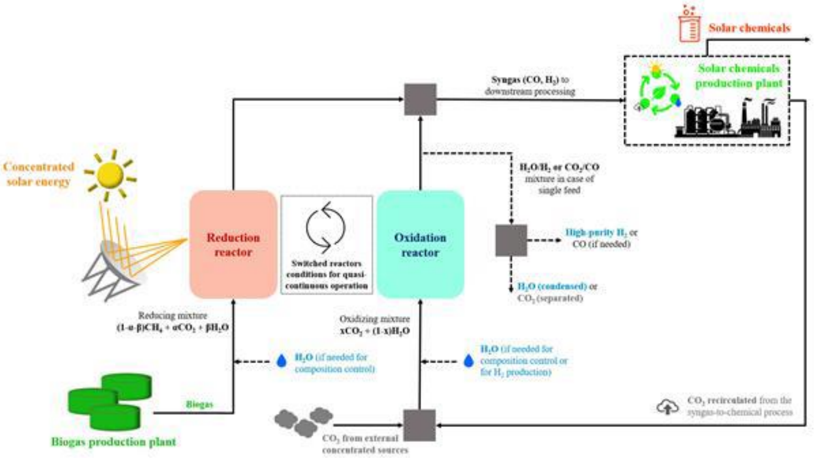


*Figure 1. Schematic concept of the symbiotic biological-synthetical processes defined biogas-solar-driven, $CO_2$ waste-assisted production of solar fuels by a thermochemical CL redox cycle*

In this general context, we have started to analyze the behavior of suitable materials in the case of a Chemical Looping Reverse Water Gas Shift reaction (RWGS-CL), in which the reduction is performed in presence of $H_2$, and the oxidation is performed in presence of $CO_2$. In particular, the RWGS-CL performance of the double perovskite $Sr_2FeMo_{0.6}Ni_{0.4}O_{6-\delta}$ (SFMN) during reduction/oxidation cycles in $H_2$/$CO_2$ are investigated, as well as the material's redox behavior and structural-morphological evolution during cycling.

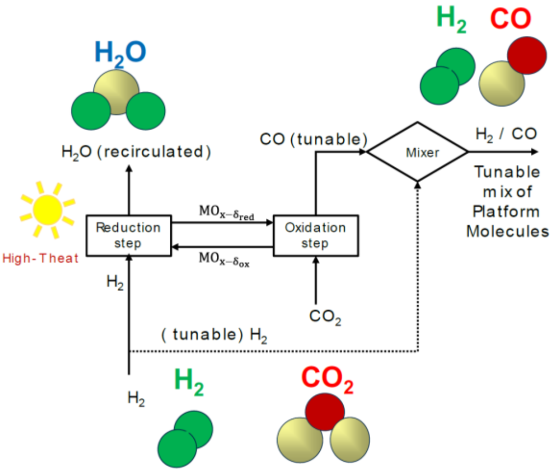


*Figure 2. Concept of RWGS-CL used to produce a tunable mix of platform molecules H2/CO precursor of solar chemicals*

As an example, Figure 3a shows the three complete redox cycles performed at $T_{red}$ = 850°C, $T_{oxy}$ = 750°C. Figure 3b shows the averaged oxidation curves at $T_{red}$ = 750 – 850°C.

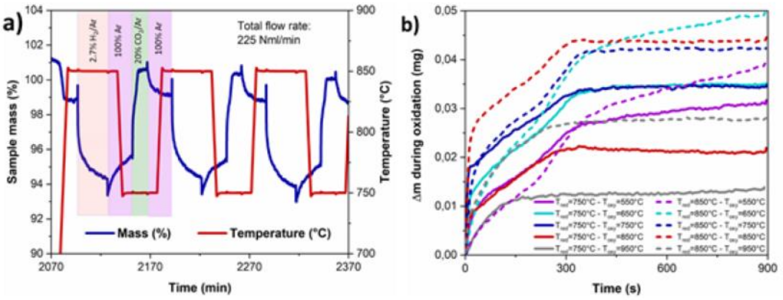


*Figure 3. (a) Representative thermograms from TGA at Tred = 850°C, Toxy = 750°C. Total flow rate of 225 Nml/min – Reduction in 2.7% H2/Ar – Oxidation in 20% CO2/Ar. (b) Cycleaveraged oxidation profiles from TGA for Tred = 750 and 850°C*

Then, we finally analyse the option of $CH_4$-assisted Chemical Looping Water Splitting (CLWS) using the same double perovskite structure, in which $CH_4$ is used to reduce the perovskite and H2O is used for its reoxidation. We also consider reference $H_2$/$H_2O$ cycles for comparison. This process is an option of interest in the symbiosis of biological-synthetical processes.

## References

[1] Farooqui, A.; Boaro, M.; Llorca, J.; Santarelli, M. Solar Fuels via Two-Step Thermochemical Redox Cycles. In Advances in Greener Energy Technologies; Bhoi, A. K., Sherpa, K. S., Kalam, A., Chae, G.-S., Eds.; Springer Singapore: Singapore, 2020; pp 31–84. https://doi.org/10.1007/978-981-15-4246-6_3. V.

[2] Orsini F., Ferrero D., Cannone S., Santarelli M., Felli A., Boaro M., de Leitenburg C., Trovarelli A., Llorca J., Dimitrakopoulos G., Ghoniem A.F., Exsolution-enhanced reverse water-gas shift chemical looping activity of Sr2FeMo0.6Ni0.4O6-δ double perovskite, Chemical Engineering Journal, p. 146083, set. 2023, doi: 10.1016/j.cej.2023.146083

# Thermal Complications in Direct Ammonia-Fed Solid Oxide Fuel Cells Elaborated by Numerical Modelling

Özgür Aydın[1,2]*

*[1]Department of Mechanical Engineering, Faculty of Engineering, Karadeniz Technical University, Trabzon, Türkiye*
*[2]Department of Energy and Process Engineering, Technical University of Munich, Garching, Germany*
**Corresponding author: ozguraydin@ktu.edu.tr*

The limited infrastructure of $H_2$ is still standing as the heaviest obstacle before the wide deployment of Solid Oxide Fuel Cells (SOFCs), like the other types of fuel cells. As an $H_2$ carrier, the potential of $NH_3$ is rather high owing to its comforting thermo-physical properties [1]. Besides, $NH_3$ can be decomposed to $H_2$ and $N_2$ within an SOFC, and the endothermic Ammonia Cracking Reaction (ACR) can proceed relying on the heat released in the SOFC, enhancing the system efficiency significantly. However, for producing 3 moles of $H_2$, 2 moles of $NH_3$ must be decomposed for which 91.9 kJ/mol thermal energy is required. Considering the rather high decomposition rate of ACR at the SOFC operating temperatures [2], the endothermic cooling due to $NH_3$ decomposition arises as a serious phenomenon to be concerned with [3].

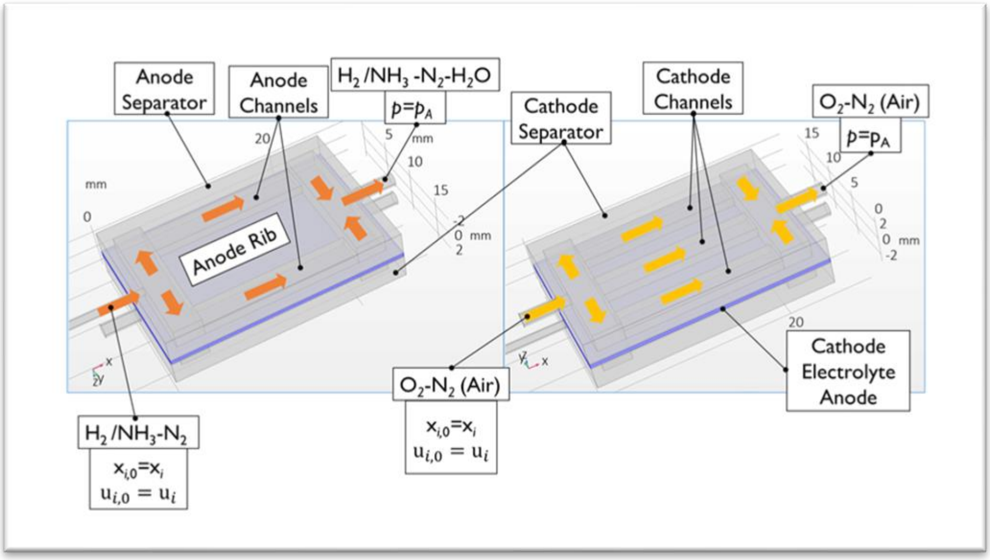


*Figure 1: The computational domain representing the laboratory-size SOFC [4].*

For investigating the thermal complications introduced by the ACR to ammonia-utilizing SOFCs (A-SOFC), the numerical modeling appears to be a great tool. Several numerical studies were published on the endothermic cooling in A-SOFCs [3]. However, the equations they relied on for describing the ACR rate were not obtained from real anodes of SOFCs, so the reported findings are not realistic, and they differ significantly from the experimental data reported [5]. In this study, we developed a 3D numerical model where we adopted a kinetics model of ACR that was derived from the well-established and nickel-based SOFC anode [6]. Besides, the mass, momentum, and charge balances in the numerical model were rigorously validated leaning upon the polarization data measured from a laboratory-size SOFC fed by $H_2$ [4]. Upon validating the model completely, the geometry was also extended to the commercial-scale (ca. 10x10 cm) and thermal complications were elaborated.

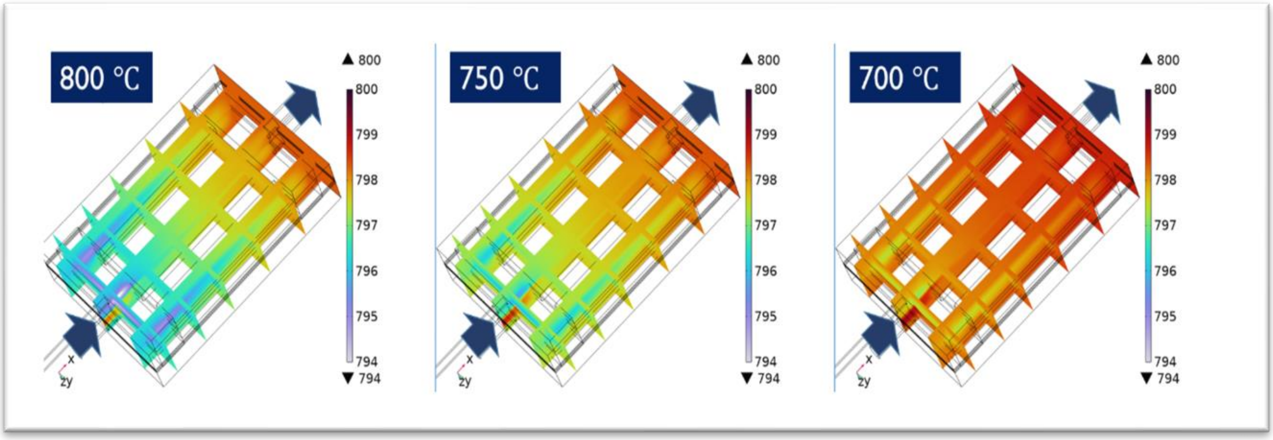


*Figure 2. The temperature (°C) fields in the one-cell stack of SOFC for the operating temperatures of 800 °C, 750 °C, and 700 °C where the cell potential is 0.7 V.*

It appears that the extent of the endothermic cooling depends highly on the size of the SOFC. The larger the active area, the greater the endothermic cooling. The calculations reveal that a higher operating temperature makes the temperature gradients along the flow field greater. The numerical data also show that the cell potential affects the temperature field remarkably. It seems that the temperature gradients along the flow field become smaller at a higher cell potential or a smaller current density.

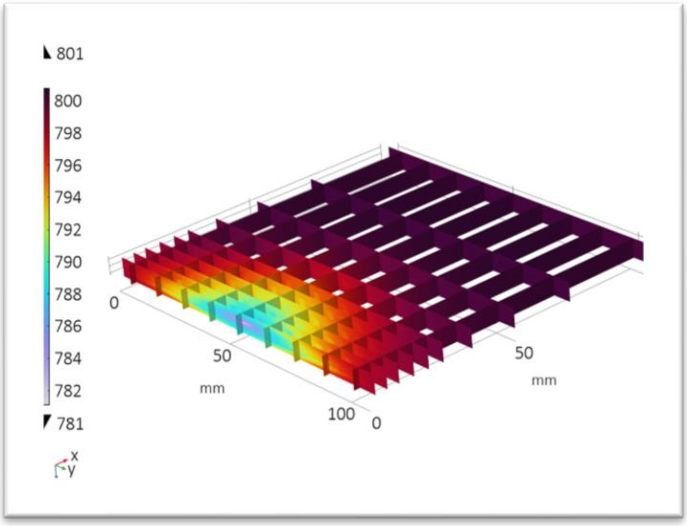


*Figure 3. The temperature (°C) field in the commercial-size (ca. 10 × 10 cm) A-SOFC at the operating temperature of 800 °C and cell potential of 0.7 V.*

## References

[1] R. Metkemeijer et al., “Ammonia as a Feedstock for a Hydrogen Fuel Cell; Reformer and Fuel Cell Behaviour”, J. Power Sources, vol. 49, 1994, pp. 271.
[2] K. Teramoto et al., “Direct Reforming of Methane–Ammonia Mixed Fuel on Ni–YSZ Anode of Solid Oxide Fuel Cells”, Int. J. Hydrogen Energy, vol. 45, 2020, pp. 8965.
[3] M. Ni, “Thermo-Electrochemical Modeling of Ammonia-Fueled Solid Oxide Fuel Cells Considering Ammonia Thermal Decomposition in the Anode”, Int. J. Hydrogen Energy, vol. 36, 2011, pp. 3153.
[4] T. Ochiai et al., “In-Situ Analysis of the In-Plane Current Distribution Difference between Electrolyte-Supported and Anode-Supported Planar Solid Oxide Fuel Cells by Segmented Electrodes”, ECS Trans., vol. 78, 2017, pp. 2203.
[5] B. Stoeckl et al. “Characterization and Performance Evaluation of Ammonia as Fuel for Solid Oxide Fuel Cells with Ni/YSZ Anodes”, Electrochimica Acta, vol. 298, 2019, pp. 874.
[6] M. Kishimoto et al., “Formulation of Ammonia Decomposition Rate in Ni-YSZ Anode of Solid Oxide Fuel Cells”, Int. J. Hydrogen Energy, vol. 42, 2017, pp. 2370.

# Electrochemical Investigation of Ni-GDC Electrodes on Fuel Electrode-Supported Solid Oxide Cells

Benjamin Steinrücken[1]*, Florian Kerscher[1], Sören Ohmstedt[1], Alexander Schwiers[2,3], Christian Lenser[2], Norbert H. Menzler[2,3], Hartmut Spliethoff[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University of Munich, Germany*
*[2]Inst. Of Energy and Climate Research, IEK-1. Materials Synthesis and Processing, Forschungszentrum Jülich GmbH, Germany*
*[3]RWTH Aachen University, Institute of Mineral Engineering, Aachen, Germany*
**Corresponding author: benjamin.steinruecken@tum.de*

---

Solid oxide cells are a highly promising technology for decarbonizing various sectors due to their reversible operation ability and high efficiency. However, the state-of-the-art fuel side electrode material Ni-YSZ (yttria-stabilized zirconia) of fuel electrode-supported cells (FESC) is limited by degradation effects and limitations in the maximum current density. To address this, a transition to mixed ionic conductors such as Ni-GDC (gadolinia-doped ceria) can improve the performance and robustness of the cells. This study experimentally investigated a Ni-GDC electrode on 5x5 cm² Ni-YSZ-supported full cell with a La-Sr-Co-Fe-oxide perovskite as air-electrode, developed by Forschungszentrum Jülich [1]. The characterization was performed in a metallic housing [2], and the experimental set-up is described elsewhere [3]. The reversible operation is investigated under relevant gas compositions for steam electrolysis, co-electrolysis, and syngas produced by biomass gasification. Electrochemical impedance spectroscopy and i-V curves are measured and compared to those of a Ni-YSZ electrode reference cell.

## Results

Exemplary, the results of the variation of the operational temperature in the fuel cell mode are shown in Figure 1. Both cells are operated under a $H_2/H_2O$ mixture with a molar ratio of 90/10 and a total flow of 0.2 Nl/min. The impedance of the cells is measured at a current density of 0.1 A/cm². The i-V curves in a.) show a lower performance of the Ni-GDC cell (dashed line) compared to the Ni-YSZ reference cell (solid line). The open circuit voltage (OCV) of the Ni-GDC cell is reduced by an average of 10.9 mV compared to the respective Ni-YSZ operational temperature. The reduced OCV indicates either a gas leakage of air into the fuel stream or a leakage of gas or electrons through the electrolyte of the cell. For the reference cell, the deviation from the theoretical OCV is associated with a gas leakage, resulting in an increased steam content of 26%. Due to the further decreased OCV of the Ni-GDC cell, an imperfect electrolyte with either gas or electronic leakage is assumed. Additionally, the i-V curves of the Ni-GDC cells are steeper, which indicates a generally lower cell performance. Here, also the leakage of the electrolyte can be the reason. The reference cell's measured impedance spectra (b.) show the expected dependence of the ohmic resistance and high-frequency arc from the operational temperature [4]. The DRT (c.) confirms this by matching the observed changes in the polarization resistances to the high-frequency processes. The Ni-GDC cells are showing completely different spectra (d.). One low-frequency process dominates the whole spectra. The DRT (e.) identifies the characteristic time constant for this process at 0.5-1 Hz. For Ni-GDC electrodes, the chemical capacity of the ceria overlaps with the gas diffusion resistance at this frequency range [5]. The temperature dependency of the observed DRT process identifies the Ni-GDC capacity as the main driving force. The operational temperature only has a minor influence on the gas diffusion resistance, but a major temperature influence on the process is observed. A similar dominating low-frequency process was observed for a Ni-GDC FESC operated at 600 °C under a 50/50 H2/H2O gas mixture [6]. In previous experiments, no dominating process has been observed for similar Ni-GDC FESCs at a temperature variation under internal reforming conditions [3]. The temperature dependency of the Ni-GDC cell’s ohmic resistance behaves similarly to the Ni-YSZ cell.

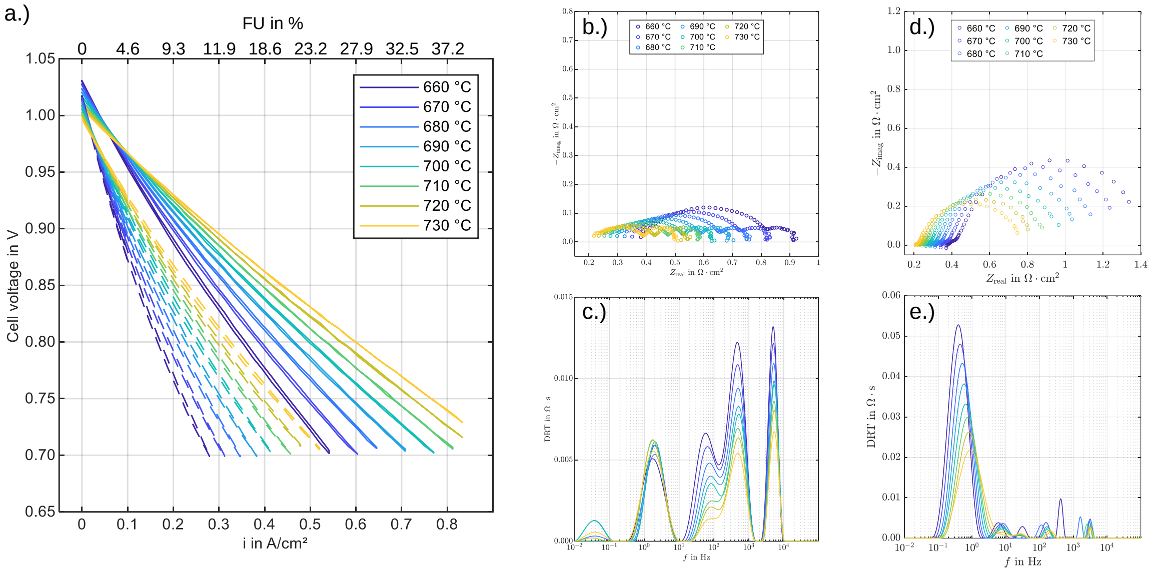


*Figure 1: Comparison of the Ni-YSZ FESC and the Ni-GDC FESC at different operational temperatures via: a.) i-V curves, b.) (Ni-YSZ) and d.) (Ni-GDC) electrochemical impedance spectra, c.) (Ni-YSZ) and e.) (Ni-GDC) distribution of relaxation times of these spectra.*

## Conclusion

Due to leakage within the electrolyte, the investigated Ni-GDC FESC cell did not offer the expected performance improvement compared to the Ni-YSZ FESC reference cell. Further research and development in the manufacturing process of the cells is required and currently ongoing. The sealing concept of the test rig at TUM showed room for improvement to further increase the OCVs and the cell's performance at high fuel utilization.

## References

[1] A. Schwiers, *Investigation and implementation of improved and degradation-tolerant fuel electrodes for solid oxide cells*, 2024.

[2] B. Steinrücken, S. Herrmann, M. Hauck et al., “Flexible and Modular Fully Metallic Housing Concept for Solid Oxide Fuel Cells,” *ECS Transactions*, vol. 103, no. 1, pp. 1817–1826, 2021.

[3] B. Steinrücken, S. Herrmann, F. Kerscher et al., “Experimental Investigation of Naphthalene Induced Degradation of Reversible Solid Oxide Cells Operated on Bio-Syngas,” *Journal of The Electrochemical Society*, vol. 171, no. 3, p. 34505, 2024.

[4] A. Leonide, “SOFC Modelling and Parameter Identification by means of Impedance Spectroscopy,” 2010.

[5] C. Grosselindemann, N. Russner, S. Dierickx et al., “Deconvolution of Gas Diffusion Polarization in Ni/Gadolinium-Doped Ceria Fuel Electrodes,” *Journal of The Electrochemical Society*, vol. 168, no. 12, p. 124506, 2021.

[6] Y. Liu, M. Juckel, N. H. Menzler et al., “Ni/GDC Fuel Electrode for Low-Temperature SOFC and its Aging Behavior Under Accelerated Stress,” *Journal of The Electrochemical Society*, vol. 171, no. 5, p. 54514, 2024.

# Macroeconomic Implications of Implementing 40t Fuel-Cell Trucks: Simulation Analyses of Roll-Out Scenarios for Austria

Katharina Rusch[1]*, Sebastian Goers[1], Andreas Zauner[1]

*[1] Energieinstitut an der JKU Linz, Linz, Austria*
**Corresponding author: rusch@energieinstitut-linz.at*

Aiming to reduce greenhouse gas emissions, carbon dioxide ($CO_2$)- and pollutant-free vehicle propulsion systems, such as fuel cell (FC) trucks, present a significant opportunity for the transportation sector. Particularly for medium and long-distance heavy-duty transport, the integration of fuel cell trucks into the road freight market paves the way for a sustainable and interoperable mobility system. Within the FC4HD (Heavy duty fuel-cell road demonstrator) project (https://www.wiva.at/project/fc4hd/), the world witnesses the development and demonstration of the first fully emission-free 40-ton fuel cell commercial vehicle. The transition from diesel trucks to FC trucks necessitates regional investments in both refueling infrastructure and the vehicles themselves. This shift, along with reduced diesel consumption, boosts the economy by enhancing positive economic stimulus and creating jobs. This study quantifies these benefits in terms of their impact on economic growth and employment opportunities.

The macroeconomic impacts of expanding the FC truck fleet in Austria are quantified using the multi-sectoral model MOVE2, a time series-based simulation model developed at the Energieinstitut at the Johannes Kepler University in Linz [1, 2]. The simulation model allows the estimation of various economic and structural changes within Austria, thereby focusing on energy-related effects based on different political and/or investment decisions. The simulations are used to analyze the economic effects triggered **(i)** by investments in FC trucks and hydrogen ($H_2$) fueling stations and **(ii)** the substitution of decreasing diesel imports due to the use of (partly domestically produced) $H_2$. The study explores two scenarios: a *moderate* and a *progressive* one, differing mainly in the intensity at which diesel trucks and trailers are replaced by $H_2$-powered alternatives and the development of refueling infrastructure These scenarios are projected over a timeframe from 2025 to 2050.

Based on the outcomes of the ex-ante simulation analyses, noticeable positive impacts on the Austrian economy are observed with the expansion of the FC truck fleet and the corresponding refueling infrastructure development. The simulated macroeconomic effects for Austria can be attributed to several factors: (1) Investment impulses stemming from the expansion of the FC truck fleet and the $H_2$ refueling station infrastructure serve as primary catalysts. (2) The reduction in diesel imports, facilitated by the adoption of $H_2$ (partly produced domestically), yields beneficial effects on the trade balance or net exports, offsetting potential negative impacts due to FC truck fleet expansion and the use of $H_2$. (3) These positive outcomes are further amplified by multiplier effects triggered by heightened production activities, which elevate Gross Domestic Product (GDP) and subsequently spur broader investment activities. This chain reaction culminates in enhanced employment rates, thereby increasing household spending capacity.

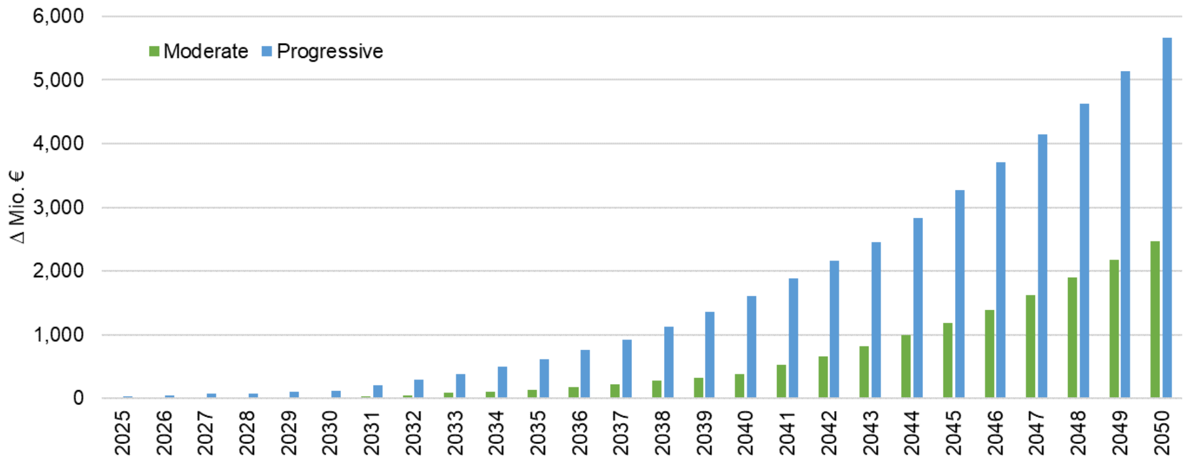


*Figure 1: Simulated change in GDP for moderate (green) and the progressive (blue) scenario in Austria for the expansion of the FC truck fleet and the implementation of the necessary $H_2$ refueling infrastructure. Notes: Nominal values. Results include direct and induced effects. Investments made in domestic $H_2$ plants and their macroeconomic effects were not considered. (Source: Own calculation based on MOVE2)*

Austria faces the challenge of taking effective and efficient measures to create jobs and increase economic growth in the short, medium and long term in light of the current macroeconomic and geopolitical changes. Simultaneously, expanding the production, storage and use of renewable energy (green electricity and $H_2$) will be essential for achieving Austria's climate and energy goals. Our research in the framework of the FC4HD project shows that a double dividend can be generated, with additional economic growth and an ecological dividend from reduced fossil energy use via the integration of fuel cell trucks into the road freight sector.

## References

[1] Baresch, M., Goers, S., Tichler, R., Schneider, F., 2014. MOVE2 - Modell zur Simulation der (ober-)österreichischen Volkswirtschaft mit einem speziellen Schwerpunkt auf Energie. Update des Modells MOVE (Linz: Energieinstitut an der Johannes Kepler Universität).

[2] Tichler, R., 2009. Optimale Energiepreise und Auswirkungen von Energiepreisveränderungen auf die oberösterreichische Volkswirtschaft: Analyse unter Verwendung des neu entwickelten Simulationsmodells MOVE, 1. Aufl. ed, Energiewissenschaftliche Studien. Pro Libris Verl.-Ges, Linz.

# T.2a – Synthetic Energy Carrier

## Hydrogen and syngas retrieval from methanol with electrically heated steam reforming reactors

Marcelo Dal Belo Takehara[1], Kentaro Umeki[1,2]*

[1]*Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden,*
[2]*Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author:* kentaro.umeki@ltu.se

Significantly increased demand of hydrogen in coming decades adds a potential risk in electricity grid stability especially the production becomes more and more intermittent renewable electricity.

Long-term storage and long-distance hydrogen transport would open a new opportunity to maximize the utilization of green hydrogen by decoupling the regional and temporal mismatching of renewable electricity availability and hydrogen demand. Among the different storage options, methanol has many interesting advantages because of its high hydrogen storage density, the lack of the demand for cryogenic or pressure vessels, existing global trade infrastructure, among others. In some industries that benefit from the mixture of hydrogen with carbon monoxide (e.g. steel and petrochemical industries), methanol conversion process can be operated in conditions where the gas output consists of both gases. The biggest challenge is, however, potential conversion loss and expensive retrieval equipment (steam reformers).

To improve the round-trip efficiency of hydrogen delivery and at the same time, to reduce the capital cost of hydrogen retrieval system, this study suggests the electrification of steam reforming system using resistance or induction heating. The feasibility of the electrified hydrogen retrieval system was investigated from reactor and system perspectives in this study.

First, the variation in overall round-trip efficiency was evaluated between conventional and electrified systems. Simplified mass and energy balance models were developed to evaluate the whole value chain. Fig. 1 shows Sankey diagrams of hydrogen delivery system via methanol using conventional and electrified steam reforming processes. The operation condition of steam reformers was set to produce as pure hydrogen as possible. The values in the figures were normalized by the total electricity input to be 100. The electrified system shows much higher overall hydrogen utilization rate (43.0%) than the conventional system (36.8%). In the electrified system, electrolyser was responsible for only 87.7% of total electricity input, which in turn, decreased the generation of low grade heat (in case of low temperature electrolyser) that are difficult to recover.

Then, the advantage of electrification of steam reformers was further demonstrated with respect to the reactor scaling and the conversion efficiency using the reactor CFD simulation. As the reactor capacity gets larger, the electrified option started showing the advantage due to its ability to keep the uniform temperature through the reactor and to omit the heat exchanger section. The results are going to be validated by the experiments in future.

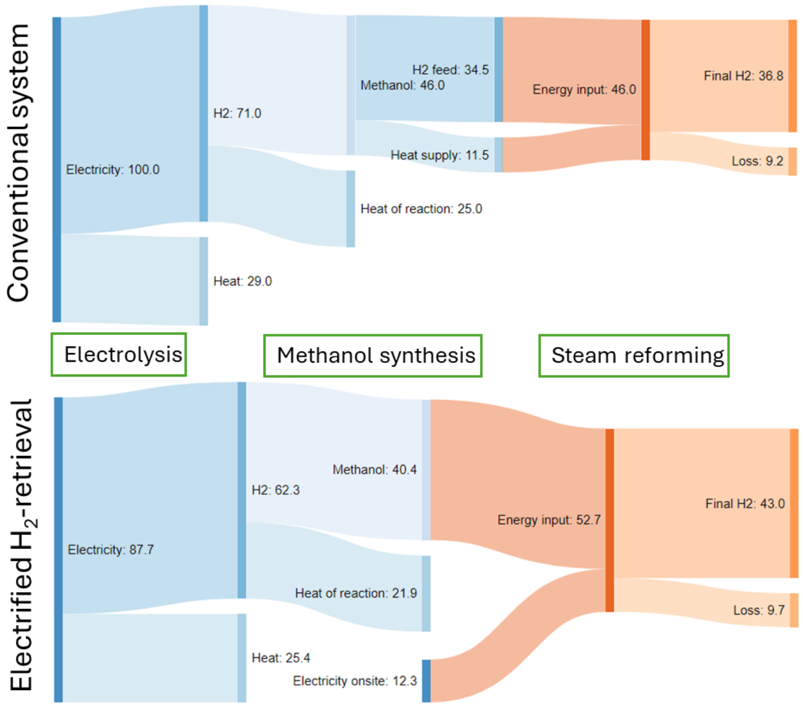


*Figure 1: The comparison of round-trip hydrogen delivery system via methanol steam reforming (top) conventional combustion based retrieval system; (bottom) electrified retrieval system.*

# Particle Circulation between Interconnected Slurry Bubble Columns for Sorption-Enhanced Fischer-Tropsch Synthesis

Wiebke Asbahr[1]*, Reinhard Rauch[1]

*[1]Karlsruhe Institute of Technology (KIT), Engler-Bunte-Institute, Department Fuel Technology (EBI-ceb), Engler-Bunte-Ring 1a, 76131 Karlsruhe, Germany*
**Corresponding author: wiebke.asbahr@kit.edu*

Sorption-enhanced Fischer-Tropsch (SEFT) synthesis has gained recent attention for producing liquid hydrocarbons with higher conversions compared to conventional FT synthesis [1]. The FT reaction is an exothermic polymerization reaction where synthesis gas (CO and $H_2$) is converted on iron- or cobalt-based catalysts to a range of hydrocarbons and water. Using water-gas-shift active iron-based catalysts, $CO_2$ can be directly used as carbon source. Removing the produced water shifts the equilibrium towards the production of CO, which is then converted to long-chain hydrocarbons in the FT reaction [2]. Furthermore, several authors [2,3,4] reported oxide formation and structural changes at high water partial pressures during FT synthesis on cobalt catalysts. Besides the deactivation of the catalyst and the associated reduced catalyst lifetime, kinetic inhibition is a significant issue to consider about. Jacobs et al. [4] postulated that a temporary decline in conversion is due to the kinetic inhibition of water molecules, blocking the active sides of the catalyst. Thus, SE operation enhances the process with faster reaction rates, conversion enhancement and extended catalyst lifetime.

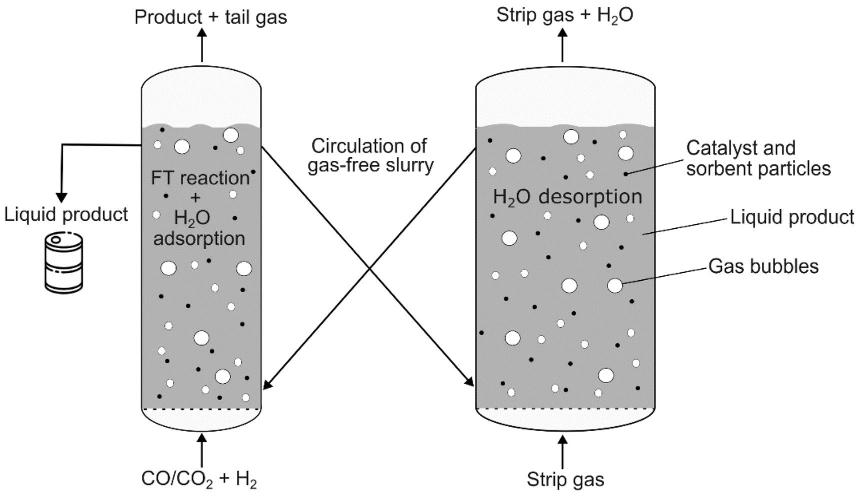


*Figure 1: Interconnected slurry bubble columns for SEFT synthesis [5].*

Asbahr et al. [5] proposed a new reactor concept (Figure 1) combining FT reaction and in-situ water adsorption in one slurry bubble column (SBC) and water desorption in a second SBC. The liquid circulation was successfully demonstrated in a cold flow model by Jafarian et al. [6], with main influencing parameters, i.e. gas holdup and reactor geometry, shown by Asbahr et al. [5]. In the same cold flow model, the volume and mass flow of the slurry between the two SBCs (circulation rate) were measured at ambient conditions using a Coriolis device (Optimass 7400C, Krohne). Initially, the volume circulation rate of water was compared between the Coriolis device and an ultrasonic flow sensor. Figure 2 shows that the measurements from the ultrasonic flow sensor (in blue) are consistently lower than those from the Coriolis device (in red), with a mean percentage error <4%. For the first time, a slurry circulation with 10 wt.% SiC (particle diameter: 53 - 75 µm) was achieved and measured only with the Coriolis device. Since gas holdup drives the circulation [5] and decreases with increasing mass fraction [7], the circulation rate of the slurry (10 wt.% SiC) is lower than the liquid circulation (0 wt.% SiC) for all superficial gas velocities. At $u_G$ = 0,2 m $s^{-1}$ a particle circulation of 393 g $min^{-1}$ was reached, corresponding to nearly 10 wt.% in the loop. This shows the suitability of the new reactor concept for slurry circulation and demonstrates the potential for SEFT synthesis. Further studies need to investigate the effect of higher mass fractions, up to 35 wt.%, to assess the feasibility of operating commercially relevant SEFT synthesis in the new reactor concept.

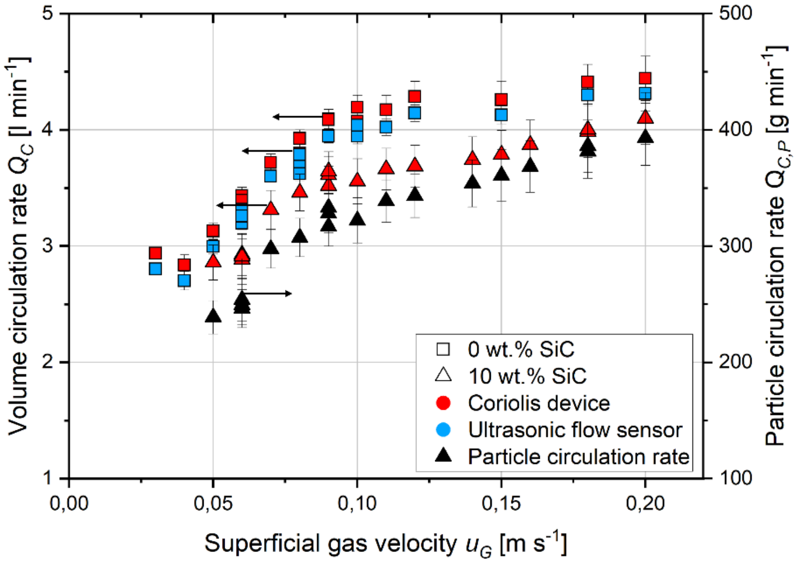


*Figure 2: Volume (Particle) circulation rate QC(,P) for different superficial gas velocities uG and mass fractions of SiC (0 and 10 wt.%).*

## References

[1] Lj. Gavrilović, S. S. Kazi, A. Oliveira, O. L. I. Encinas, and E. A. Blekkan, 'Sorption-enhanced Fischer-Tropsch synthesis – Effect of water removal', *Catal. Today*, vol. 432, Apr. 2024, doi: 10.1016/j.cattod.2024.114614.

[2] M. P. Rohde, G. Schaub, S. Khajavi, J. C. Jansen, and F. Kapteijn, 'Fischer–Tropsch synthesis with in situ H2O removal – Directions of membrane development', *Microporous Mesoporous Mater.*, vol. 115, no. 1–2, pp. 123–136, Oct. 2008, doi: 10.1016/j.micromeso.2007.10.052.

[3] C. H. Bartholomew and R. J. Farrauto, *Fundamentals of Industrial Catalytic Processes*, 1st ed. Wiley, 2005. doi: 10.1002/9780471730071.

[4] G. Jacobs, T. K. Das, P. M. Patterson, J. Li, L. Sanchez, and B. H. Davis, 'Fischer–Tropsch synthesis XAFS', *Appl. Catal. Gen.*, vol. 247, no. 2, pp. 335–343, Jul. 2003, doi: 10.1016/S0926-860X(03)00107-8.

[5] W. Asbahr, R. Lamparter, and R. Rauch, 'A Cold Flow Model of Interconnected Slurry Bubble Columns for Sorption-Enhanced Fischer–Tropsch Synthesis', *ChemEngineering*, vol. 8, no. 3, p. 52, May 2024, doi: 10.3390/chemengineering8030052.

[6] M. Jafarian, Y. Chisti, and G. J. Nathan, 'Gas-lift circulation of a liquid between two inter-connected bubble columns', *Chem. Eng. Sci.*, vol. 218, Jun. 2020, doi: 10.1016/j.ces.2020.115574.

[7] S. Orvalho *et al.*, 'Flow regimes in slurry bubble column: Effect of column height and particle concentration', *Chem. Eng. J.*, vol. 351, pp. 799–815, Nov. 2018, doi: 10.1016/j.cej.2018.06.115.

## T.3a – Power-to-X

# Design Parameter Optimization of a Membrane Reactor for Methanol Synthesis Using a Sophisticated CFD Model

Theresa Hauth[1]*, Konstantin Pielmeier[1], Vincent Dieterich[1], Nicolas Wein[1], Hartmut Spielthoff[1], Sebastian Fendt[1]

[1]*Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: theresa.hauth@tum.de*

Methanol is used as a versatile feedstock in the chemical industry, with a global production rate of 98 million tons per year, which is supposed to rise drastically over the next decades [1, 2]. Furthermore, Methanol is regarded as a key energy carrier for the transition to a sustainable future [3]. Methanol is mainly produced in large-scale plants by converting synthesis gas from steam reforming of fossil fuels. However, renewable methanol can be synthesized using captured $CO_2$ from unavoidable emission sites [2]. The reaction is limited by the chemical equilibrium, resulting in an achievable once-through conversion between 30 % to 40 %. Hence, large energy-intensive recycles need to be implemented. A membrane reactor removing the product water from the reaction site can circumvent the chemical equilibrium and could reduce the required compression energy [4].

This study presents a sophisticated CFD model that combines the kinetic model of the reactions with the permeation kinetic to optimize the construction of a membrane reactor with a $NaA^+$ zeolite membrane. Several kinetic models are investigated, and based on the experimental data of Gallucci et al. [5], the most appropriate is implemented. Temperature-dependent Langmuir isotherms are used to depict the permeation process, and the model is validated by data from Li et al. [6]. After validation, both kinetics are applied to the construction of a membrane reactor, and key parameters are elaborated that are crucial for $CO_2$ conversion and methanol yield. Based on these findings, an optimal membrane reactor is constructed, and the best operational modes are examined.

### References

[1] A. Nemmour, A. Inayat, I. Janajreh, C. Ghenai, Green hydrogen-based E-fuels (E-methane, E-methanol, E-ammonia) to support clean energy transition: A literature review, International Journal of Hydrogen Energy, vol. 48, no. 75, 2023
[2] S. S. Tabibian, M. Sharifzadeh, Statistical and analytical investigation of methanol applications, production technologies, value-chain and economy with a special focus on renewable methanol, Renewable and Sustainable Energy Reviews, vol.179, 2023
[3] G. Leonzio, “Methanol Synthesis: Optimal Solution for a Better Efficiency of the Process,” Processes, vol. 6, no. 20, 2018.
[4] V. Dieterich, N. Wein, H. Spliethoff et al., “Performance Requirements of Membrane Reactors for the Application in Renewable Methanol Synthesis: A Techno-Economic Assessment,” Advanced Sustainable Systems, vol. 6, no. 12, 2022.
[5] F. Gallucci, E. Fernandez, P. Corengia, M. van Sint Annaland, “Recent advances on membranes and membrane reactors for hydrogen production”, Chemical Engineering Science, vol. 92, 2013.
[6] H. Li et al., “Na+-gated water-conducting nanochannels for boosting CO2 conversion to liquid fuels,” Science, vol. 367, 2020.

# Power-to-X Technologies for a sustainable future

Christian Schuhbauer[1], Gunnar Ganzer[1], Sebastian Pichler[1]*

[1]*MAN Energy Solutions Deggendorf, Germany*
**Corresponding author: sebastian.pichler@man-es.com*

Power-to-X (PtX) is a collective term for processes that convert renewable electrical energy into hydrogen via electrolysis and subsequently into various forms of chemicals or synthetic fuels via synthesis technologies. The products can be utilized in manifold applications like marine propulsion, jet fuel, or as feedstock for chemical industries, enabling so-called "hard-to-abate" industry sectors to be defossilized.

This approach plays an indispensable role in achieving net-zero goals, as forecasted by various market research studies. Despite the anticipated enormous growth in synthetic fuels, the high associated costs are consistently highlighted. While utilization technology experiences heightened activity (especially in the marine sector), investments in production facilities are trailing behind, posing a challenge to the widespread adoption of synthetic fuels.

MAN Energy Solutions Deggendorf is a global leader in the design and manufacturing of multitubular reactors operating mainly with molten salt but also with boiling water, thermal oil, or exhaust gas from combustion as heat transfer media. As part of the MAN Energy Solutions corporation, which delivers renewable fuel utilization solutions within the marine industry like methanol or ammonia engines, the development of PtX technologies is an important element of the Group's future strategy.

In this presentation, the theoretical studies and market research activities of the various Power-to-X routes, which were carried out in the context of business development, are first presented. The goal was to estimate their future market potential by comparing their levelized production costs and exploit the possibility to place suitable products on the market.

A deep dive into current research and development activities focuses on the methanation of $CO_2$ and the $CO_2$-based methanol synthesis pathways.

In the former pathway MAN Energy Solutions is in the role of process owner and technology provider. Having operated a pilot-scale reactor since 2009, the company successfully developed an advanced reactant feeding system to optimize the flow arrangement within the reactor tube, which resulted in optimal hot spot control. This system has already been successfully deployed in two commercial plants. Additionally, a recent study found that the methanation process' load flexibility can meet renewable energy grid demands when optimizing the ratio control system of $H_2/CO_2$ properly. Lastly, a product quality optimization study to satisfy the requirements of Liquefied Natural Gas production processes is presented.

In the recent past, considerable efforts have also been made to advance the development of $CO_2$-based methanol synthesis. A single-pass reactor has been in operation in Deggendorf since 2022, which was upgraded to recycle operation at the end of last year and has already been successfully commissioned. The main aim of the process development, which is conducted in a long-lasting cooperation with BSE Methanol, is to achieve far-reaching process flexibility by maximizing permissible load change rates and minimizing the permissible turndown ratio.

The presentation concludes with an insightful outlook into MAN Energy Solutions' future projects, providing a roadmap for ongoing and upcoming development.

# Power to X: From cement flue gas to value added products

Dr. Alexander Beck[1]*, Dr. Ralph Freund[1], Raphael Gratzl[1], Thomas Mairegger[1], Dr. Philipp Stadler[1]

*[1]Net Zero Emission Labs GmbH, Sinning 1, 83101 Rohrdorf, Germany*
**Corresponding author: alexander.beck@rohrdorfer.eu*

---

Cement producers are significant contributors to global $CO_2$ emissions, accounting for 7-8% of the total and playing a crucial role in the ongoing climate transition. While Carbon Capture and Storage (CCS) serves as a short-term solution, Carbon Capture and Utilization (CCU) assumes greater importance for the long-term sustainability paradigm, aligning with principles of a circular economy. In light of this, Rohrdorfer is committed to spearheading advancements and scalability in $CO_2$ electrolysis and capture technologies. With this objective in mind, two pilot plants have been established, operational since October 2022: one dedicated to $CO_2$ capture (processing 2 tons per day) and the other to $CO_2$ electrolysis (producing 1 kg per hour).

The aim of these efforts is to research the comprehensive process from $CO_2$ removal from flue gas to the synthesis of value-added products. To achieve this goal, construction of a third pilot plant for $CO_2$ conversion has begun in 2024, focusing on the conversion to ethylene. This project paves the way for a highly relevant platform chemical, incorporating insights from the cell concept, peripheral adaptations and the scale-up of $CO_2$ electrolyzers.

Due to the development of specific configurations for both $CO_2$ electrolyzer systems (formic acid and ethylene), higher conversion efficiencies and current densities can be achieved while the downstream processing costs and energy consumption are reduced. This presentation highlights current developments in the field of ethylene synthesis on a pilot plant scale. Emphasis is placed on process optimization by means of design of experiment as well as on the specially designed system operation. Through the targeted use of geogenic $CO_2$ from cement flue gases and long-term carbon sequestration as formic acid and ethylene, we not only contribute to climate protection, but also create new opportunities for industrial development and resource utilization.

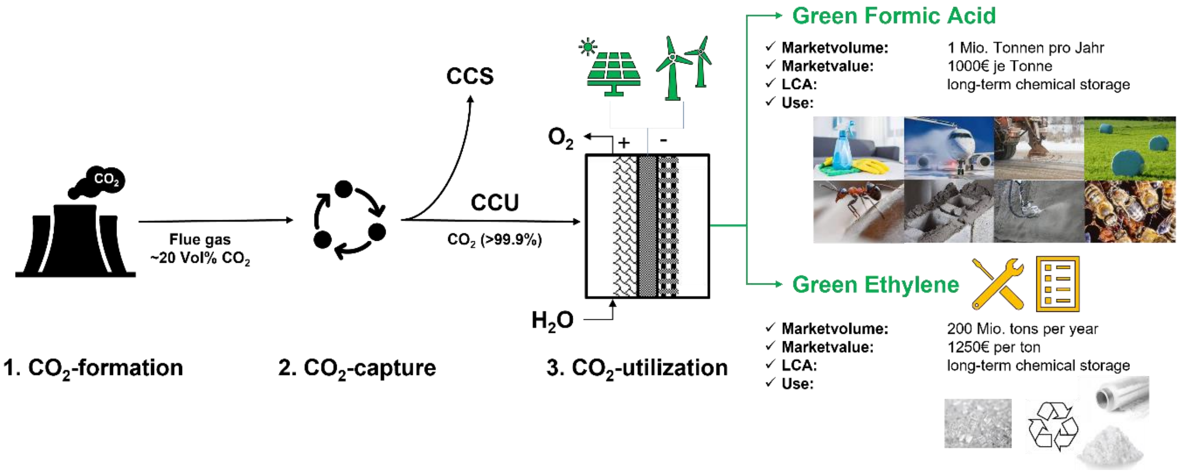


*Figure 1: Rohrdorfer path to CaCU – from flue gas to value-added products.*

# Electrification of Biomass- and Waste-to-X Processes

Marcel Dossow[1], Sebastian Fendt[1]*

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: sebastian.fendt@tum.de*

---

Climate change and its consequences pose one of the greatest threads and challenges humanity faces today. To mitigate climate change, it is essential to reduce anthropogenic greenhouse gas emissions significantly. Biomass-based chemicals and fuels can effectively replace fossil feedstock, while using existing infrastructure and regulatory frameworks. In addition, recycling of carbon from (difficult to avoid or unavoidable) waste streams will play a significant role in a circular economy especially as a growing carbon demand is projected for the chemical industry [1].

Gasification processes that convert biomass and waste into chemicals and fuels (Biomass-to-X, BtX and Waste-to-X, WtX) will play a key role in this transition due to their scalability and availability at relatively high Technology Readiness Levels (TRL). Entrained flow gasification is of special interest in this regard due to inherent advantages like a high-quality syngas, pressurized operation, scalability and technology maturity [2].

However, both biomass and waste feedstock is usually complex, inhomogeneous and not easy to handle. Due to a limited availability, maximizing product yield and carbon efficiency is crucial in future utilization. Electrification of BtX processes is a very promising and innovative way to improve biomass- and waste-derived chemical and fuel production by increasing product yield and carbon efficiency. Electrification could furthermore offer advantages over both, traditional BtX and electricity-based Power-to-X (PtX) stand-alone processes. Electrification options can be distinguished into "indirect electrification", which typically means adding hydrogen from water electrolysis (Power-and-Biomass-to-X, PBtX), and "direct electrification", which means power integration into specific processing steps using electricity for heat, electrochemical energy, or plasma (eBtX). Figure 1 shows the general outline of both the PBtX and the eBtX options.

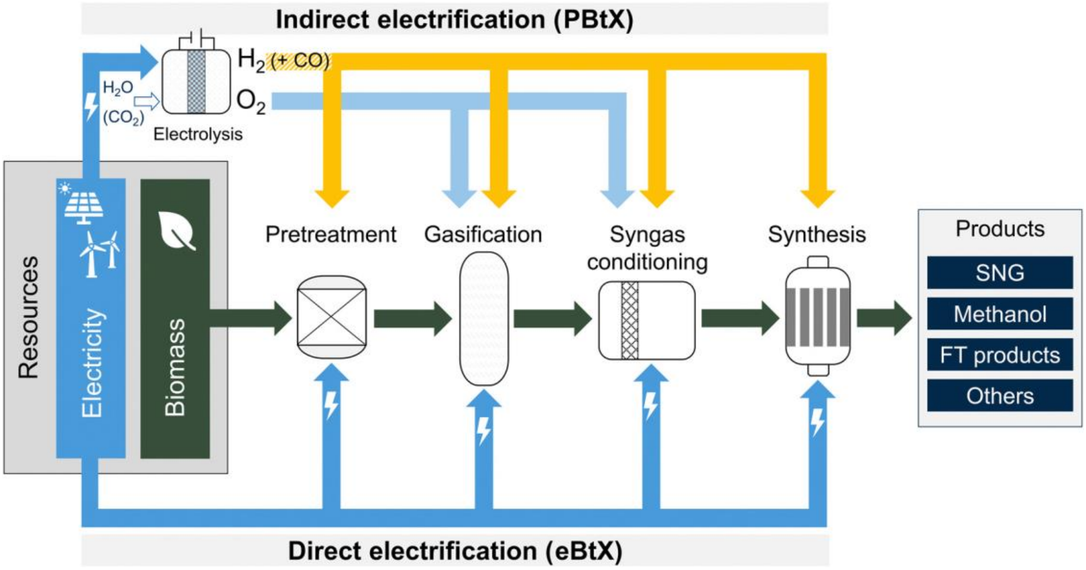


*Figure 1: Electrification options for Biomass-to-X processes based on gasification [3].*

For large-scale deployment and the definition of research and development demands, the technologies are assessed and evaluated based on performance, maturity, feasibility, land requirements, and operational dynamics. While hydrogen addition in PBtX has been extensively studied, research on direct electrification (eBtX) is limited due to its lower technological maturity. Further research is needed on both equipment and system-level technologies to assess performance, economics, environmental impact, and future regulations.

A detailed case study shows the potential for an optimized PBtX process producing renewable syncrude and Sustainable Aviation Fuel (SAF) at highest carbon efficiencies of up to 97% and significantly increased product yields (+140%) compared to the state of the art technology [4].

## References

[1] F. Kähler, O. Porc, M. Carus, RCI Carbon Flows Report: Compilation of supply and demand of fossil and renewable carbon on a global and European level, October 2023, available at: www.renewable-carbon-initiative.com

[2] A. Hanel, V. Dieterich, S. Bastek, H. Spliethoff, S. Fendt: Entrained flow gasification-based biomass-to-X processes: An energetic and technical evaluation, Energy Conversion and Management, 274, 116424, 2022

[3] M. Dossow, D. Klüh, K. Umeki, M. Gaderer, H. Spliethoff, S. Fendt: Electrification of gasification-based biomass-to-X processes - a critical review and in-depth assessment, Energy and Environmental Science, 2023, 17(3), pp. 925–973

[4] M. Dossow, V. Dieterich, A. Hanel, H. Spliethoff, S. Fendt: Improving carbon efficiency for an advanced Biomass-to-Liquid process using hydrogen and oxygen from electrolysis, Renewable and Sustainable Energy Reviews, Volume 152, 2021, 111670

## W.1a – Plasma Utilization

# A 50 kW Arc-Heated Plasma Torch for Hydrogen and Carbon Production via Methane Pyrolysis and for the Electrification of High Temperature processes

Hamid Reza Yousefi [1]*, Steffen Pauly[1], Bernd Glocker[1]

*[1]PlasmaAir AG, Weil der Stadt, Germany*
**Corresponding author: yousefi@plasmaair.de*

The Munich Hydrogen Symposium 2024 is a crucial forum for advancing of hydrogen-based technologies, and this abstract highlights a thorough study centered on a thermal arc-heated plasma torch. Operating with hydrogen and methane as plasma gas, this torch serves dual purposes: methane pyrolysis for turquoise hydrogen and black carbon production in an oxygen-free atmosphere, and as a hybrid high-temperature heater for electrifying high-temperature processes through a blend of electrical and chemical energies.

Key to these processes is a plasma torch engineered for prolonged operation without erosion or carbon buildup. Accompanying the torch itself, auxiliary equipment, including the power supply, has been developed. Initially configured for 50 kW, the system can be scaled up to higher power levels. The torch is designed with a liner configuration, featuring a hot cathode and cylindrical anode. This study focuses on fine-tuning operational parameters and thermal efficiency, particularly in determining the optimal hydrogen-to-methane ratio to maximize operational duration. Through careful adjustment of fuel mixture ratios, the objective is to achieve an optimal balance that enhances combustion stability, heat release patterns, and the efficient generation of hydrogen and carbon. This comprehensive strategy highlights a firm dedication to sustainable energy solutions.

The research outcomes hold promise for industries seeking to incorporate hydrogen and carbon production into their processes. Practical insights are offered for researchers, engineers, and industry professionals looking to achieve improved combustion efficiency, prolonged electrode lifespan, reduced erosion, and concurrent hydrogen and carbon generation. These advancements contribute to global efforts in establishing sustainable and versatile energy solutions.

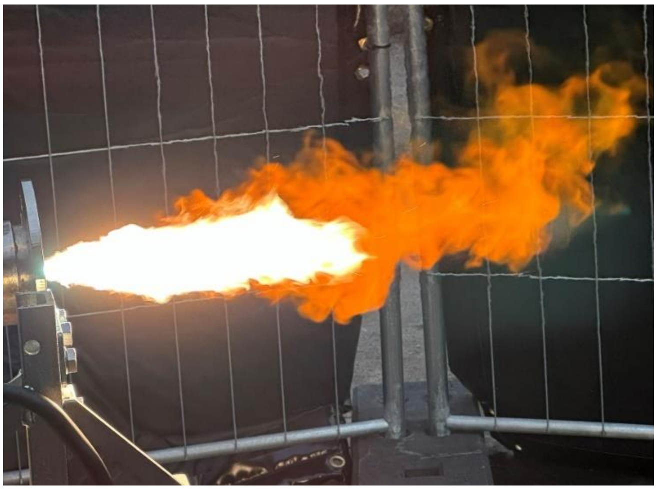


*Figure 1: An arc-heated plasma torch configuration operating at 27 kW with a gas mixture of 60 SLM methane and 24 SLM hydrogen.*

**References:**

[1] Mateusz Wnukowski, Methane Pyrolysis with the Use of Plasma: Review of Plasma Reactors and Process Products. Energies 2023, 16(18), 6441.
[2] Matheus Oliveira, Ana Ramos, Tamer M. Ismail at al., A Review on Plasma Gasification of Solid Residues: Recent Advances and Developments. Energies 2022, 15(4), 1475.
[3] Duy Khoe Dinh et al., Arc plasma reactor modification for enhancing performance of dry reforming of methane. Journal of CO2 Utilization, Volume 42, December 2020, 101352.

# Plasma Reforming Technologies for Low Carbon Hydrogen Production

*Bader Ali Alrasheed[1]*, Hao Zhang[2], and Massimiliano Materazzi[2]*

*[1]MSc Chemical Engineering, University College London, Torrington Place, London WC1E 7JE*
*[2]Department of Chemical Engineering, University College London, Torrington Place, London, WC1E 7JE, UK*
**Corresponding author: ucecbal@ucl.ac.uk*

## Introduction

Hydrogen is set to be one of the key energy sources in future industrial systems. However, the current approaches to hydrogen production still heavily rely on fossil fuels, presenting significant challenges either in the form of high carbon pollution or sustainability trade-offs. This has led to the development of bridge technologies based on fossil fuels with a low environmental impact, which has been the focus of countless studies in the last years. Natural gas is presently the leading source of hydrogen production among fossil fuels, accounting for 48%, with oil contributing 30% and coal 18%. In contrast, only 4% of the world's hydrogen production is derived from renewable resources[1].

While steam reforming (SMR) and gasification of fossil fuels are the mainstay of hydrogen production due to their industrial scalability, they come with a significant drawback-the production of large amounts of GHGs[2]. Retrofitting these plants with carbon capture facilities is a potential solution, but it's costly and faces its own set of challenges, including high energy consumption for solvent regeneration and the lack of carbon transportation and storage infrastructure.

Unlike SMR and autothermal technologies, which need to rely on CCS to deliver low-carbon hydrogen, the pyrolysis of methane (and hydrocarbons in general) appears as a potential process for the transition to a sustainable hydrogen economy. This is because carbon is generated from the process in solid, easy to store, and highly valuable form, providing an additional revenue stream and not an environmental burden anymore. The applications for this carbon by-product are numerous, e.g., steel additive, filler for car tires, graphite, dye, and soil improver. Hydrocarbon pyrolysis is the process in which thermal energy is applied to a molecule, e.g., methane, to break the chemical bond between carbon and hydrogen, generating hydrogen gas and a solid carbon product with no $CO_2$ emissions. The process is much more energetically favorable than water electrolysis and as efficient as SMR and gasification, too, when these are integrated with CCS[1]. In the absence of catalysts, the energy is typically provided by an electric source due to the inherent advantages related to fast ramp-up and high conversion efficiencies, but also the high costs associated.

## Methodology

It is crucial to thoroughly understand and characterize the process of producing clean hydrogen via methane plasma pyrolysis. This involves examining the interactions and synergies between the chemical feedstock (such as methane), heat, and the active species generated by plasma, all in the absence of catalysts. By doing so, we can evaluate the system's performance based on energy consumption, hydrogen yield, and the purity of the hydrogen produced.

Investigating the behavior of methane under plasma conditions allows us to optimize the process for maximum efficiency. Understanding how the heat and plasma-generated species interact with methane molecules can reveal ways to enhance hydrogen production while minimizing energy input. Additionally, assessing these interactions helps in identifying the optimal conditions for achieving high hydrogen purity, which is essential for various applications.

Focusing on these aspects can help us develop a more efficient and cleaner method for hydrogen production, reducing reliance on traditional methods that often involve significant $CO_2$ emissions. This approach promises a cleaner hydrogen production process and contributes to the broader goal of sustainable energy solutions.

The target is to develop a kinetic model in simulation software using Ansys Chemkin based on methane pyrolysis and reforming kinetic reactions, expand the kinetic model to include and implement kinetic reactions where plasma plays an active role, and then validate the model using the experimental apparatus at the UCL laboratory.

## Results

The results of this project will be finalized by early September and shared during the conference. They will be useful in identifying future research opportunities in clean hydrogen production and the role of novel plasma technologies in future production pathways.

## Conclusion

In conclusion, this research highlights the promising potential of methane plasma pyrolysis for sustainable hydrogen production, which contributes to the field of methane reforming by offering an alternative to high-temperature, energy-intensive conventional processes. It creates possibilities for environmentally friendly and potentially more economical methane conversion, particularly for distributed processes based on renewable energy sources. Furthermore, it aligns with the goals of reducing greenhouse gas emissions, as it can avoid $CO_2$ production associated with the combustion of fossil fuels during conventional heating processes[3].

## Reference

(1) Sánchez-Bastardo, N.; Schlögl, R.; Ruland, H. Methane Pyrolysis for Zero-Emission Hydrogen Production: A Potential Bridge Technology from Fossil Fuels to a Renewable and Sustainable Hydrogen Economy. *Ind Eng Chem Res* **2021**, *60* (32), 11855–11881. https://doi.org/10.1021/ACS.IECR.1C01679/ASSET/IMAGES/LARGE/IE1C01679_0008.JPEG.

(2) Holladay, J. D.; Hu, J.; King, D. L.; Wang, Y. An Overview of Hydrogen Production Technologies. *Catal Today* **2009**, *139* (4), 244–260. https://doi.org/10.1016/j.cattod.2008.08.039.

(3) Tu, X.; Whitehead, J. C. Plasma-Catalytic Dry Reforming of Methane in an Atmospheric Dielectric Barrier Discharge: Understanding the Synergistic Effect at Low Temperature. *Appl Catal B* **2012**, *125*, 439–448. https://doi.org/10.1016/J.APCATB.2012.06.006.

# Green Hydrogen as an Alternative for Sustainable Glass Production

Nerijus Striūgas[1]*, Andrius Tamošiūnas[2], Raminta Skvorčinskienė[1]

*[1]Lithuanian Energy Institute, Laboratory of Combustion Processes, Kaunas, Lithuania*
*[2]Lithuanian Energy Institute, Plasma Processing Laboratory, Kaunas, Lithuania*
**Corresponding author: nerijus.striugas@lei.lt*

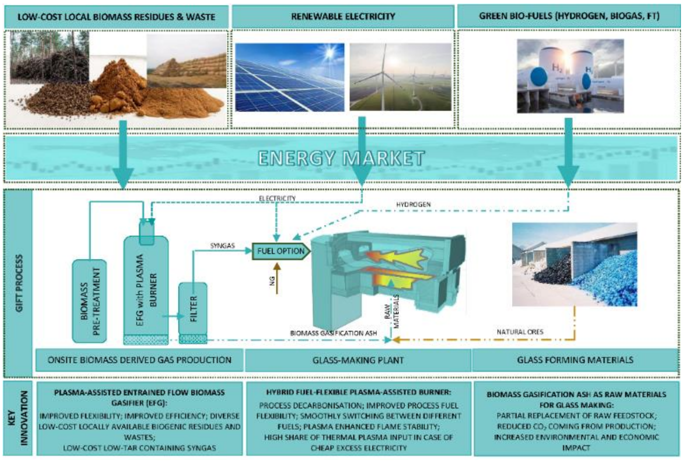


*Figure 1: GIFFT's conceptual idea of a sustainable glass industry with fuel-flexible technology*

The "Flexible Hybrid Furnace of the Future" is the European glass industry's vision to meet the European Green Deal's objective of reducing Europe's carbon emissions and contributing to EU climate neutrality. Effective decarbonisation of the entire glass sector as soon as possible requires the development of new methods and technologies and the search for environmentally friendly alternatives to natural gas as a carbon-neutral alternative fuel. This paper presents the vision and latest results of the Horizon Europe project GIFFT (Sustainable Glass Industry with Fuel-Flexible Technology), whose overall objective is to develop a sustainable, hybrid and biofuel-flexible heat generation technology and process that can be integrated into industrial glass production through the efficient use of plasma combustion and gasification systems.

The GIFFT concept is to develop and validate a flexible hybrid furnace that optimises using freely available low-cost green electricity and biofuels to facilitate the transition from natural gas to a new low-to-zero-carbon and more dynamic heat generation. By combining plasma gasification of biomass and flexible combustion of hybrid fuels, the GIFFT process offers high fuel flexibility operation in response to changes in energy and fuel markets. The process is designed to allow continuous operation of the glassmaking plant throughout the year, with many operating hours. The flexibility of the hybrid operation and fuels is analysed using standard flow diagrams to calculate the energy and mass balances when changing the four main regimes: the Bace case, the Biomass case, the Green electricity case and the Green hydrogen case. Preliminary results of combustion tests will also be made available during the conference to demonstrate the validity of the theoretical assessment.

**Acknowledgements**

This project has received funding from the European Union’s Horizon Europe research and innovation programme under grant agreement No 101122257. Views and opinions expressed are, however, those of the authors only and do not necessarily reflect those of the European Union or the European Climate, Infrastructure and Environmental Executive Agency (CINEA). Neither the European Union nor the granting authority can be held responsible for them.

# Integration of electrically assisted processes coupled with the use of Hydrogen in the Glass-Making Industry

Andrius Tamosiunas[1,2]*, Nerijus Striugas[3]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
*[2] Plasma Processing Laboratory, Lithuanian Energy Institute, Lithuania*
*[3]Laboratory of Combustion Processes, Lithuanian Energy Institute, Lithuania*
**Corresponding author: andrius.tamosiunas@tum.de*

## Introduction

Solutions in hard-to-decarbonize sectors, such as glass-making, steel-making, and/or chemical industries, to use resources and processes that are more sustainable are of the highest importance. Thus, the interest in sectors' electrification coupled with the use of hydrogen to reduce the dependence on fossil fuels and carbon footprint has been increasing. In this regard, the potential to integrate plasma-assisted processes and green or blue hydrogen use in the Glass-making industry is an object of this experimental research.

## Methodology

Direct current (DC) arc discharge plasma torch of up to 45 kW electric input was tested to be used as an electrical energy source, providing a high-temperature plasma stream into the glass melting furnace and thus reducing the amount of chemical energy needed. For plasma generation, oxygen was used as a main plasma-forming gas. Simultaneously, hydrogen or methane was injected at the exit nozzle of the plasma torch to be mixed with a high-temperature oxygen plasma stream at a stoichiometric ratio needed for complete combustion. Separate mixtures of hydrogen-oxygen and methane-oxygen were tested as an additional chemical energy required for the glass melting furnace. A smooth switch from one gas mixture to another was also tested.

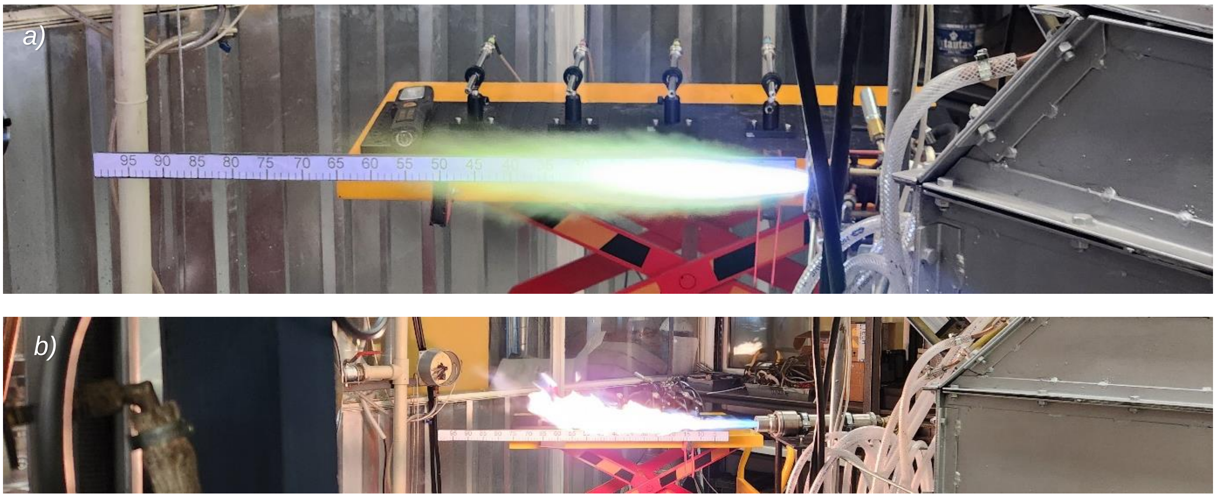


*Figure 1: a) Plasma torch in operation ($O_2$-$H_2$ mixture, up to 45 $kW_{el}$, up to 97 $kW_{chem}$); b) natural gas burner in operation used for the glass melting (100 kW burner capacity). For both cases, the oxygen-to-fuel equivalence ratio was 1*

## Results

The designed plasma burner could provide up to 70 kW of electrical and chemical energy required for the glass melting at the tested experimental conditions. It could flexibly operate, switching between gas mixtures, $O_2$-$H_2$ and $O_2$-$CH_4$, and their ratios and electrical and chemical power. The visible mean flame length in the plasma case was up to 0.55-0.65 m (total input electrical and chemical power 75–130 kW), while in the conventional gas burner case (input chemical power around 100 kW), it was up to 1.0 m.

## Conclusions

As a general conclusion, the first results showed that the DC arc plasma torch operated on an $O_2$-$H_2$ mixture could be successfully applied to replace conventional gas burners used in the glass melting industry. However, a more detailed research-based examination and comparison, especially flame radiation properties, is needed to investigate industrial-scale plasma technology applications for the sector's electrification.

## Acknowledgements

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101122257. Views and opinions expressed are, however, those of the authors only and do not necessarily reflect those of the European Union or the European Climate, Infrastructure and Environmental Executive Agency (CINEA). Neither the European Union nor the granting authority can be held responsible for them.

# W.1b – Biotechnology

## Intermittency in Biohybrid Hydrogen Production

Nicolas Plumeré[1]*

*[1] Professorship for Electrobiotechnology, Technical University Munich, Germany*
**Corresponding author: Nicolas.plumere@tum.de*

Biocatalysts have unmatched performance in terms of activity, selectivity and energy efficiency for the conversion of small molecules such as $H_2$, $CO_2$, $O_2$ or $N_2$. However, implementation of biocatalysts in devices for energy conversion cannot proceed without solutions that mitigate their intrinsic fragility. Protection strategies using a redox-active polymeric matrices can effectively stabilize biocatalysts such as the hydrogenase and significantly increase their operational lifetime for electrocatalytic $H_2$ oxidation or production [1, 2]. Mass transport and electron transfer limitations emerge as trade-offs when increasing matrix dimensions for protection considerations [3]. Quantitative analysis supported by kinetic modeling enable to pin-point such bottlenecks and guide the rational design of the immobilization matrix [4, 5] to enable high catalyst utilization that can theoretically provide robustness for non-limiting periods of time even when using highly fragile hydrogenases [6, 7]. Engineering catalytic reversibility [8] into the redox-active films embedding the hydrogenase enables $H_2$ oxidation and $H_2$ evolution at minimal overpotential, making the protected hydrogenase energy efficient in fuel cell and electrolyzers [9]. The same redox-active films were also successfully applied to construct energy efficient biohybrid systems based on $CO_2$ fixating enzyme [10]. We show that fine tuning of the reduction potential of the polymer is a prerequisite for both bidirectionality and protection under intermittent use.

### References

[1] Plumeré, Rüdiger, Oughli, Williams, Vivekananthan, Pöller, Schuhmann, Lubitz, *Nature Chemistry*, **2014**, *6*, 822–827.
[2] Oughli, Conzuelo, Winkler, Happe, Lubitz, Schuhmann, Rüdiger, Plumeré, *Angew. Chem. Int. Ed.*, **2015**, *54*, 12329 –12333.
[3] Fourmond, Stapf, Li, Buesen, Birrell, Rüdiger, Lubitz, Schuhmann, Plumeré, Léger, *JACS*, **2015**, *137*, 5494-5505.
[4] Li, Buesen, Williams, Henig, Stapf, Mukherjee, Freier, Lubitz, Winkler, Happe, Plumeré, *Chemical Science*, **2018**, *9*, 7596-7605.
[5] Buesen, Li, Plumeré *Chemical Science*, **2020**, *11*, 937 – 946.
[6] Li, Buesen, Démentin, Léger, Fourmond, Plumeré *JACS*, **2019**, *141*, 16734.
[7] Li, Münchberg, Alsheikh Oughli, Buesen, Lubitz, Freier, Plumeré *Nature Communications*, **2020**, *11*, 920.
[8] Fourmond, Plumeré, Léger, *Nature Reviews Chemistry*, **2021**, *5*, 348-360.
[9] Hardt, Stapf, Filmon, Birrell, Rüdiger, Fourmond, Léger, Plumeré, *Nature Catalysis*, **2021**, *4*, 251.
[10] Castañeda, Adam, Paczia, Buesen, Steffler, Sieber, Erb, Richter, Plumeré, *Angew. Chem. Int. Ed.*, **2021**, *60*, 21056.

# Hydrogen-driven synthesis of chemicals in whole cells

Dominik L. Siebert[1], Ammar Al-Shameri[1], Volker Sieber[1,2,3,4]*

[1] *Chair of Chemistry of Biogenic Resources, TUM Campus Straubing for Biotechnology and Sustainability, Technical University of Munich, Schulgasse 16, 94315, Straubing, Germany.*
[2] *Catalytic Research Center, Technical University of Munich, Ernst-Otto-Fischer-Straße 1, 85748, Garching, Germany.*
[3] *SynBiofoundry@TUM, Technical University of Munich, Schulgasse 16, 94315, Straubing, Germany.*
[4] *School of Chemistry and Molecular Biosciences, The University of Queensland, St. Lucia, QLD, 4072, Australia.*
**Corresponding author: sieber@tum.de*

Biocatalysis-based reactions have the potential to be a clean and renewable platform to produce fine chemicals. Previously we described an oxygen-free oxidative biocatalytic system for the conversion of sugars into fine chemicals based on hydrogen evolution. This study introduces a sustainable approach to chemical synthesis using green hydrogen within whole-cell systems. By harnessing the enzymatic properties of the soluble hydrogenase (SH), we propose a method where we couple SH with an ene reductase (OYE) for the chemical reduction of terpenoids. This method will minimize the reliance on traditional reducing reagents and reduces environmental impact. Moreover, by employing the substrate itself as a solvent, we further enhance the sustainability of the process by reducing the need for conventional aqueous/organic solvents. Through enzymatic catalysis, whole-cell biotransformation, and solvent optimization, we present a promising strategy for a green chemical synthesis applicable to pharmaceuticals, agrochemicals, and specialty chemicals. We discuss recent progress, challenges, and future directions in this field, underscoring the potential of green hydrogen-driven whole-cell catalysis for sustainable chemical synthesis.

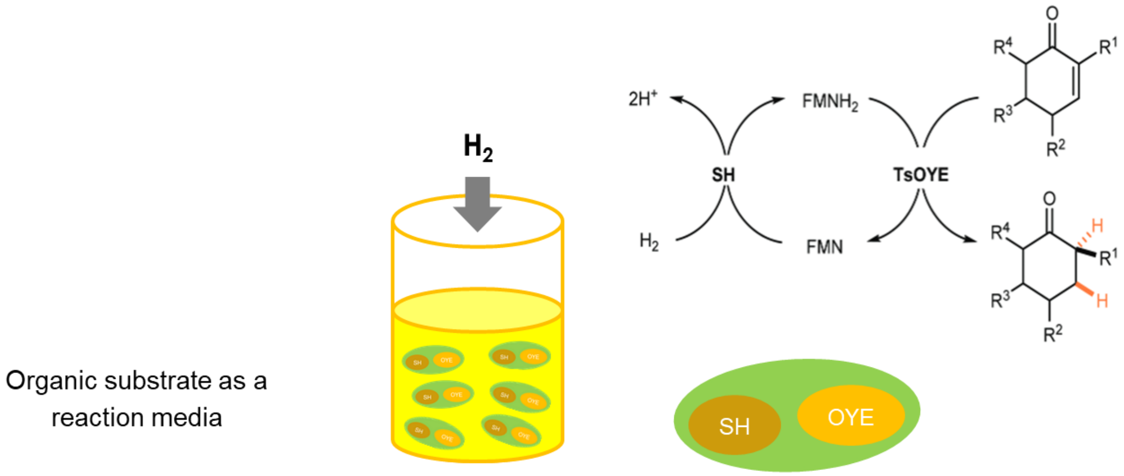


*Figure 1: Schematic illustration of concept of hydrogen-driven synthesis of chemicals in whole cells*

## References

[1] Al-Shameri A, Siebert DL, Sutiono S, Lauterbach L, Sieber V. “Hydrogenase-based oxidative biocatalysis without oxygen”. Nat Commun. 2023.
[2] Al-Shameri A, Willot SJP, Paul CE, Hollmann F, Lauterbach L. “ $H_2$ as a fuel for flavin- and $H_2O_2$-dependent biocatalytic reactions”. Chem. Comm. 2020.

# Hydrogen Driven Isobutanol Production

Tenuun Bayaraa[1, 2], Vivian Willers[1], Gary Schenk[2], Volker Sieber[1, 2]*

*[1]Chair of Chemistry of Biogenic Resources, TUM Campus Straubing, Technical University Munich, Germany*
*[2]School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Australia*
**Corresponding author: sieber@tum.de*

---

Given the increasing global energy demands, the task of obtaining sustainable alternatives to fossil fuels has become vital. The use and manufacture of biofuels is crucial for maintaining a sustainable bioeconomy. Isobutanol, a promising next-generation biofuel, offers a viable solution and can be efficiently obtained through biocatalysis. Our research focuses on establishing and optimising the production of isobutanol through various multi-enzyme cascades utilising different feedstocks. We have established a highly efficient one pot biocatalytic cascade consisting of 15 enzymes and two cofactors (NADP and ATP) that can produce isobutanol from xylose (biomass) and green methanol (produced via green hydrogen). The enzymes have been purified, characterised and succesfully integrated into the cascade. Through numerous optimisation efforts, current results show ~40 mM isobutanol can be obtained from 50 mM xylose and methanol corresponding to a theoretical yield of ~80% with a final titre of ~3 g/L isobutanol in 24 hours (Figure 1). Further optimisation of the biocatalysts and reaction conditions is crucial to reach a higher yield and titre and to become industrially attractive.

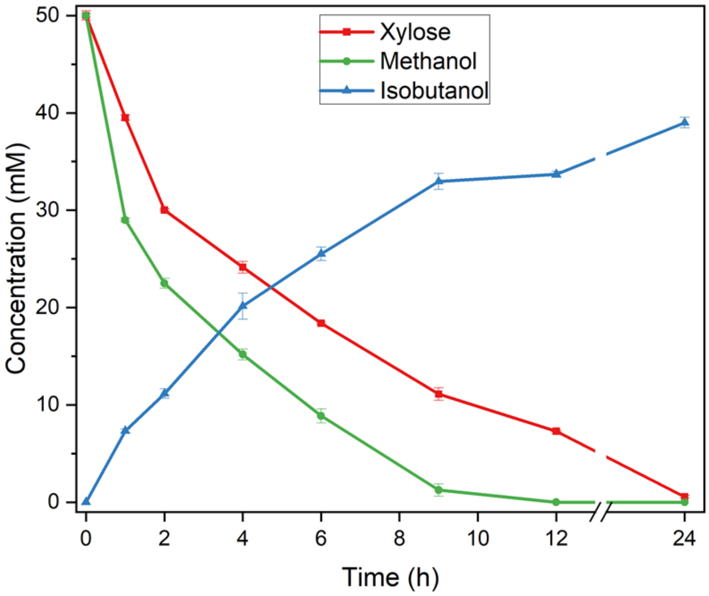


*Figure 1: Time course of isobutanol production by the multi-enzymatic cascade. The cascade efficiently produces ~40 mM of isobutanol from 50 mM xylose and methanol after 24 hours, corresponding to a theoretical yield of 80%.*

# Power-to-X-to-Y: Expanding Power-to-X and CCU by industrial biotechnology integration

Jonathan Thomas Fabarius[1]*, Carina Sagstetter[2], Melanie Speck[1], Luciana Vieira, Dhananjai Pangotra, Ferdinand Vogelgsang, Arne Roth[1]

*[1]Division Sustainable Catalytic Processes, Fraunhofer IGB, Germany*
**Corresponding author: jonathan.fabarius@igb.fraunhofer.de*

Harnessing $CO_2$ as a resource has the potential to access truly sustainable chemical production while driving the economy. New process cascades are required for this purpose: Our approach in this context is based on the initial conversion of $CO_2$ and hydrogen or water into energy-rich and water-soluble intermediates like formic acid or methanol. In particular, chemical and electrochemical processes are under investigation to produce methanol or formic acid, respectively. As additional advantage, the use of renewable energy makes the supply of these intermediates almost carbon-neutral. Both of the $C_1$ compounds methanol and formic acid can be utilized as substrates by specifically engineered methylotrophic and formatotrophic microbes to produce various targeted chemicals and energy carriers of interest [1]. In comparison to plant-based sugars used for fermentation, these $CO_2$-derived substrates enable highly scalable production routes while saving arable land for food and feed supply. Together with the vast potential of industrial biotechnology, i.e. combined application of synthetic biology, metabolic engineering and fermentation process development, the accessible product spectrum of CCU and Power-to-X is broadly enhanced.

The successful genetic engineering of methylotrophic and formatotrophic microorganisms requires interdisciplinary collaboration and a systematic approach, including detailed metabolic modeling. Particularly, the prediction of heterologous production pathways and obtainable yields serves as important guideline for the rational metabolic engineering of microorganisms. Furthermore, the *in silico* analysis of the central carbon metabolism sheds light on native key reactions limiting achievable product yields. When embedding these methods in an iterative circular engineering approach following the Design-Build-Test-Learn cycle (DBTL cycle), fast and knowledge-driven development is achieved [3].

Under this regard, we present two successful proof-of-concept studies for new CCU process cascades through integration of Power-to-X and industrial biotechnology. Specifically, we demonstrate methanol-based production of the feed/food-relevant amino acid L-lysine [2] as well as of the valuable polymer building blocks glycolic acid and lactic acid, in both cases by means of systems metabolic engineering and fermentation. These examples demonstrate that integrating synthetic biology (i.e., enzyme engineering) and metabolic modeling in modern industrial biotechnology is highly valuable.

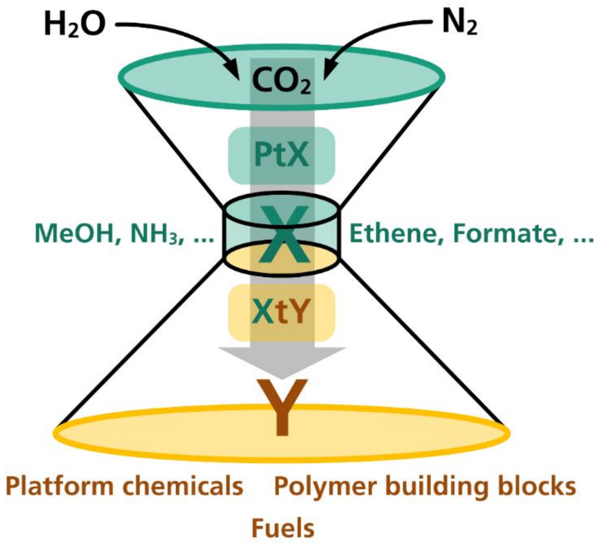


*Figure 1: The concept of Power-to-X-to-Y process cascades. Interdisciplinary connection of chemical, electrochemical and biotechnological processes enhances the accessible product spectrum of Power-to-X and CCU.*

## References

[1] Cotton, C. A. R., et al. (2020). "Renewable methanol and formate as microbial feedstocks." Current Opinion in Biotechnology 62: 168-180.

[2] Fabarius, J. T., et al. (2024). "Process Cascade for the Production of Green Polymers from CO2 and Electric Energy." Chemie Ingenieur Technik 96(5): 698-712.

[3] Carbonell, P., et al. (2018). “An automated Design-Build-Test-Learn pipeline for enhanced microbial production of fine chemicals.” Communications Biology 1(66).

# W2.a – Research Projects

## $H_2$-Reallabor Burghausen: Transformation of the Chemical Industry Towards a Hydrogen-Based Circular Economy

Christian Hackl[1]*

*[1]Reallabor Burghausen - ChemDelta Bavaria gGmbH, Germany*
**Corresponding author: christian.hackl@reallabor-burghausen.de*

The H2-Reallabor Burghausen is a pioneering project that is investigating the transformation of the chemical industry in the Bavarian ChemDelta towards a climate-neutral future. The aim is to reduce dependence on fossil fuels through the use of green hydrogen. A network of 35 partners from industry, science and politics is researching how hydrogen can be used in industrial production processes. The Federal Ministry of Education and Research (BMBF) is funding the project with 39 million euros over four years.

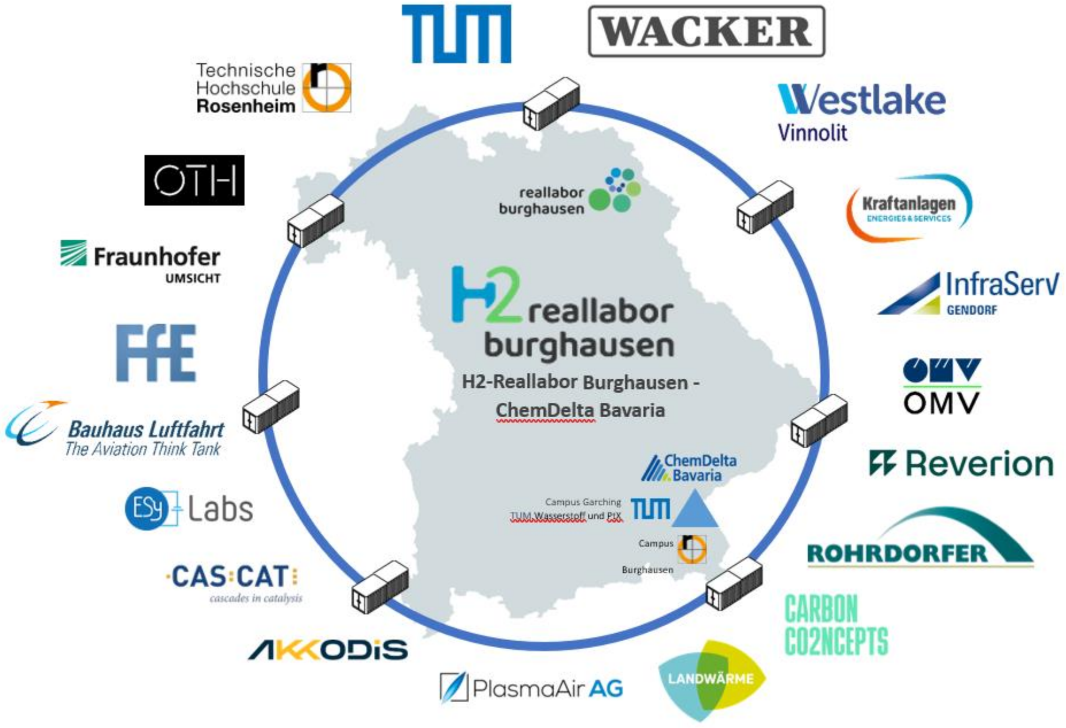


*Figure 1: Project consortium of the "$H_2$ Reallabor Burghausen - ChemDelta Bavaria"[1].*

The project is divided into various work packages that deal with the production and utilization of hydrogen, among other things. These packages include, for example, $CO_2$ capture and utilization (CCU), research into the circular economy and the integration of power-to-methanol technologies. Research is being conducted into how green hydrogen can be used to replace fossil fuels and drastically reduce $CO_2$ emissions.

One of the aims of the H2-Reallabor is to develop model solutions for the future industrial use of hydrogen in Germany. This is to be achieved through innovative technical solutions that are being trialed in the Burghausen region. The knowledge gained there will serve as a guide for the chemical industry to drive forward a sustainable transformation towards climate-friendly processes.

A key component of the project is the energy system analysis, which examines how the energy flows between the various sectors and plants can be efficiently organized. The aim is to optimize the interaction between renewable energies, hydrogen production and industrial processes. This is complemented by future planning, which analyses future development paths for the industrial use of hydrogen. A roadmap will be drawn up that defines clear steps and milestones on the path to a climate-neutral chemical industry. This roadmap serves as a guideline for the long-term planning and implementation of measures to establish a sustainable hydrogen economy.

In addition to the technical challenges, the cooperation of stakeholders from industry and science plays an important role in ensuring the acceptance and feasibility of the large-scale use of green hydrogen. The living lab is thus intended to make a significant contribution to the German energy transition and to achieving the national climate targets by developing and implementing practical solutions for the decarbonization of industry.

The H2 real-world laboratory can therefore be seen as an important building block on the way to a climate-neutral industry.

## References

[1] C. Hackl, “Project Website: $H_2$ Reallabor Burghausen”, https://www.reallabor-burghausen.de/h2-reallabor/, 2023

# SynergyFuels: where the bioeconomy meets the hydrogen economy

Júnior Staudt[1]*, Jakob Burger[1]

*[1]Laboratory of Chemical Process Engineering, Campus Straubing for Biotechnology and sustainability, Technical University Munich, Germany*
**Corresponding author: junior.staudt@tum.de*

---

Boosting the production and development of renewable fuels is essential to ensure the immediate reduction in the emissions of greenhouse gases (GHG) and thus limit the global warming. Advanced biofuels and electricity-based fuels (e-fuels) can provide pronounced reductions in the well-to-wheel emissions compared to fossil fuels, and there are ready-to-deploy technologies available for their production. However, significant parts of the carbon from the biogenic resources is emitted in the biofuel production as $CO_2$, whereas some source of carbon (e.g., $CO_2$) is needed for the e-fuel production.

This contribution gives an overview of the collaborative research project SynergyFuels (funded by the German BMDV ministry), which aims at the integration of existing concepts for the use of biogenic residues and $H_2$ provision from renewable energy. Thereby, the bioeconomy and the hydrogen economy are linked in a Power-Bio-to-X (PB2X) concept (see Figure 1). The resulting synergies from combining the individual concepts lead to high efficiency of energy and materials and novel integrated processes for the production of renewable fuels.

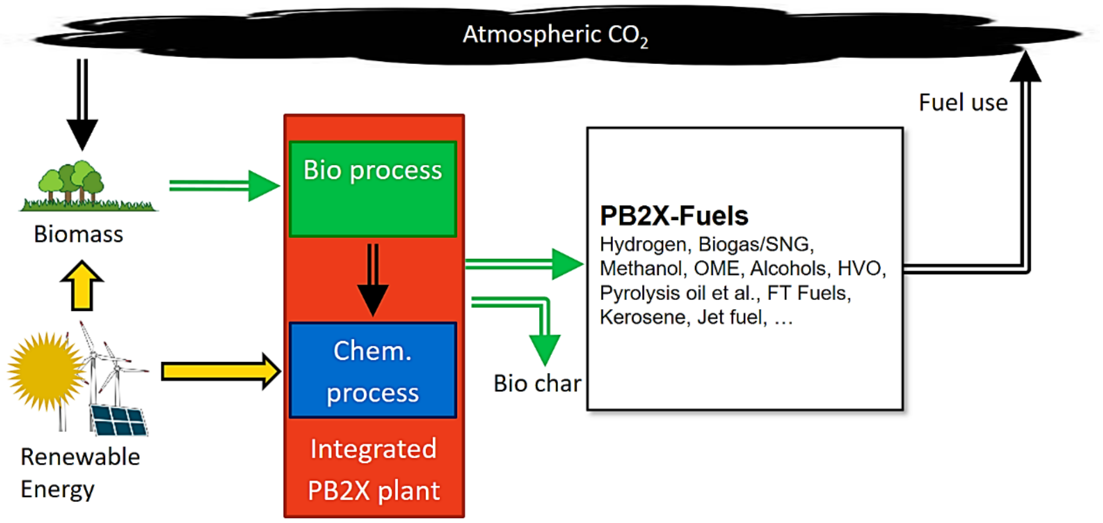


*Figure 1: Power-Bio-to-X concept integrating bioeconomy and hydrogen economy.*

The project is led by the Technical University of Munich (TUM) and counts on several partners from academia and industry: Technologie- und Förderzentrum Straubing (TFZ), Fraunhofer IGB, Fraunhofer UMSICHT, Volkswagen and CLARIANT. The goal is to develop and demonstrate an integrated refinery concept on a pilot plant scale, which combines thermochemical, electrochemical and biotechnological processes (see Figure 2). Biogenic residual and waste materials are used as carbon source. Hydrogen is produced from electrolysis. Central platform chemicals of the refinery are the methanol, ethanol, butanol, and pyrolysis oil.

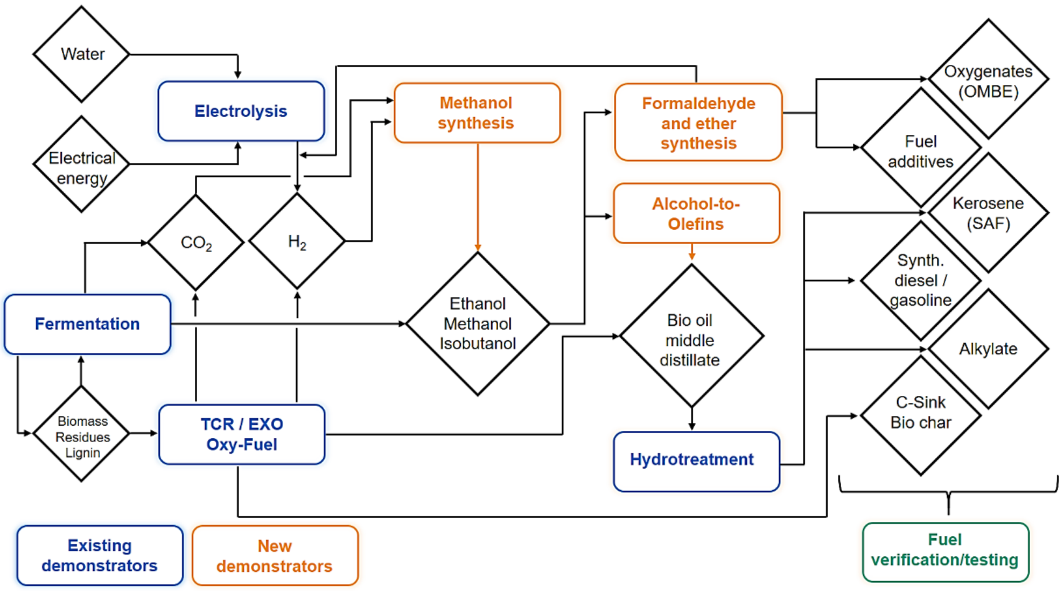


*Figure 2: Illustration of the integrated refinery concept within SynergyFuels.*

On the one hand, the platform chemicals are catalytically converted into liquid oligomers using alcohol-to-olefins processes and hydro treatment. Target products are hydrocarbons, e.g., kerosene as sustainable aviation fuel (SAF), diesel fuel or gasoline. On the other hand, oxygenated ether fuels are produced from methanol and butanol. These oxygenated fuels are intended as pilot fuel or blend components, e.g., in ship fuels. In summary, the SynergyFuels will be able to integrate the bioeconomy and the hydrogen economy to produce renewable drop-in fuels and contribute to the decarbonization of the transport sector.

## W.2b – Alternative Solid Feedstocks

# Waste-to-Methanol: Techno-economic Comparison ofPromising Methanol-Production Processes from Municipal Solid Waste

Sebastian Bastek[1]*, Christian Heiß[1], Johannes Waßmuth[1], Hartmut Spliethoff[1], Sebastian Fendt[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: sebastian.bastek@tum.de*

The chemical industry requires around 450 million tons of carbon as feedstock for a wide range of end products. Today the carbon demand is mainly covered by fossil sources which account for 84% of current carbon intake. By 2050 the carbon demand of the world's growing population is expected to surpass one billion tons. To achieve sustainable production of chemical products, the carbon will have to be provided by sustainable sources such as biomass, recycled carbon-containing waste and captured $CO_2$ – with recycled carbon expected to contribute the majority of total carbon demand.

Current mechanical recycling technologies are not able to supply enough sustainable carbon by just utilizing homogenous plastic waste streams. That is why, advanced chemical and thermochemical recycling technologies are needed which can process also difficult, inhomogeneous waste streams such as municipal solid waste (MSW).

The goal of thermochemical recycling is to turn the MSW into a feedstock such as methanol which can be directly used by the chemical industry. Given a wide range of potential process options, the purpose of this research is to perform a process route comparison based on process simulations for the conversion of MSW into methanol (MeOH). The following routes have been simulated in Aspen Plus:

- Waste incineration and CCU: Conventional incineration of waste followed by carbon capture and hydrogen addition via electrolysis with subsequent MeOH synthesis
- Oxy-fuel combustion: Oxy-fuel incineration of waste followed by exhaust gas upgrading and hydrogen addition via electrolysis with subsequent MeOH synthesis
- Pyrolysis and entrained flow gasification (Noell process): Pretreatment of MSW via rotary kiln pyrolysis, oxygen-blown entrained flow gasification, gas cleaning, syngas upgrading with $H_2$ from electrolysis and subsequent MeOH synthesis
- Pyrolysis and steam plasma gasification: Rotary kiln pyrolysis followed by steam plasma-assisted entrained flow gasification and gas cleaning, syngas upgrading with $H_2$ from electrolysis and subsequent MeOH synthesis

Each sub-system of the different processes has been modelled independently with respective sub-models. The process comparison has been performed with a focus on the respective energy and mass balances as well as key performance indicators such as recycling rate, energy yields, and carbon conversion efficiencies. In addition, a techno-economic assessment has been performed.

## References

[1] D. Stapf, "Trends and Drivers in Alternative Thermal Conversion of Waste: Task 36 - Material and Energy Valorisation of Waste in a Circular Economy," Sep. 16 2020.

[2] Hanel A., Dieterich V., Bastek S., Spliethoff H., Fendt S. (2022): Entrained flow gasification-based biomass-to-X processes: An energetic and technical evaluation. *Energy Convers. Manag.* 274, 116424.

[3] Dossow, M.; Dieterich, V.; Hanel, A.; Spliethoff, H.; Fendt, S. (2021): Improving carbon efficiency for an advanced Biomass-to-Liquid process using hydrogen and oxygen from electrolysis. Renewable and Sustainable Energy Reviews, Volume 152, 111670

[4] Dieterich, Buttler, Hanel, Spliethoff, Fendt (2020): Power-to-liquid via synthesis of methanol, DME or Fischer-Tropsch-fuels: a review. Energy Environ. Sci., 13, pp. 3207-3252

# High-Purity Hydrogen Production from Bark via Dual Fluidized Bed Steam Gasification

Veronica Gubin[1]*, David Kadlez[1], Alexander Bartik[1], Hermann Hofbauer[1], Stefan Müller[1]

[1]*Institute of Chemical, Environmental and Bioscience Engineering, TU Wien, Austria*
**Corresponding author: veronica.gubin@tuwien.ac.at*

## Introduction

In this work, hydrogen production from a real product gas obtained by thermochemical conversion of bark mulch pellets by advanced dual fluidized bed (DFB) steam gasification was experimentally investigated. Based on previous works of Fail et al. [1] and Loipersböck et al. [2], who conducted long-term experiments with real product gas from DFB gasification of wood chips, a similar pilot-scale process chain was set up. The aim was to prove the technical feasibility of high-purity hydrogen production from a biogenic residue.

## Methodology

A 100 $kW_{th}$ DFB gasifier was operated with bark mulch pellets as fuel, steam as gasification agent, and carbon dioxide ($CO_2$) as a purging medium for measurement equipment. Due to the use of $CO_2$ as a purging medium, only a small amount of nitrogen ($N_2$), originating from the fuel-nitrogen, is expected to be found in the product gas. A partial product gas stream was extracted downstream of the DFB gasifier and fed into process chain for product gas cleaning, conditioning, and hydrogen purification using the following process units: a hot gas filter, a two-staged water-gas shift (WGS) unit, a rapeseed methyl ester (RME) scrubber, activated carbon adsorbers, a Zn adsorber, a silica gel adsorber, and a pressure swing adsorption (PSA) unit. Figure 1 shows photos of the DFB gasifier and the pilot-scale process units.

Downstream of the hot gas filter, steam is added to the product gas and then passed through two fixed-bed reactors of the WGS unit to convert carbon monoxide (CO) with steam to $CO_2$ and hydrogen ($H_2$) in the presence of a commercial Fe/Cr-based catalyst (ShiftMax 120). The RME scrubber and the adsorbers remove water and impurities such as tar compounds, ammonia, and hydrogen sulfide. A compressor feeds the shifted product gas into the PSA unit to separate the hydrogen (raffinate) from all other gas components (tail gas). Activated carbon and 5Å Zeolite are used in the PSA to retain $CO_2$, methane ($CH_4$), ethylene ($C_2H_4$), and ethane ($C_2H_6$) as well as CO and $N_2$, respectively.

Three NGA 2000 analyzers, a Perkin Elmer ARNEL Clarus 500 gas chromatograph, and an X-Stream Enhanced XEGP analyzer were used to measure the gas compositions during the experiment. Furthermore, tar, ammonia, and hydrogen sulfide sampling were carried out. The experimental data is validated with their measurement uncertainties by using the IPSEpro tool PSValidate.

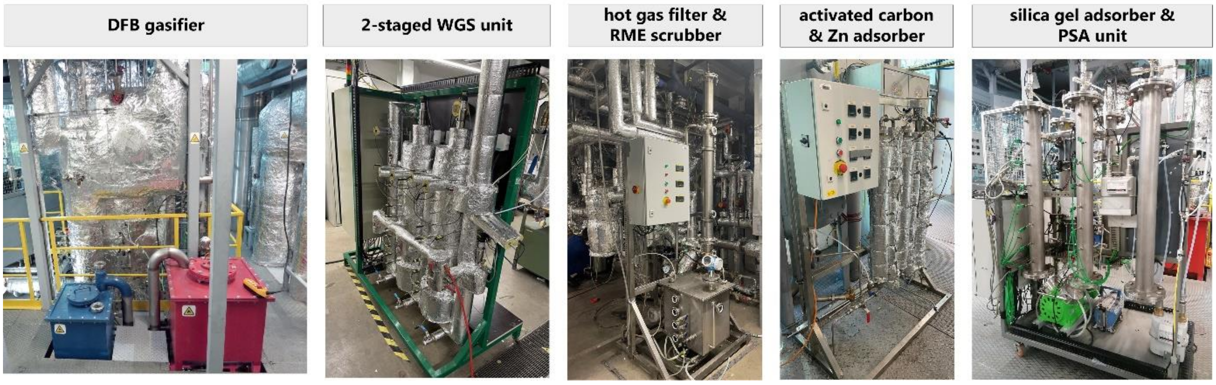


*Figure 1: DFB gasifier and pilot-scale process units for hydrogen production from bark mulch pellets*

## Preliminary Results

The WGS unit was operated with a wet gas hourly space velocity (GHSV) of 1100 $h^{-1}$ per reactor and inlet temperatures of 348 °C and 321 °C for the first and second reactor, respectively. A steam-to-carbon ratio (STCR) of approximately 2.4 was applied. Table 1 shows the measured gas composition of the product gas downstream of the DFB gasifier and the shifted product gas downstream of the WGS unit. The residual CO content was found to be 0.98 vol.-$\%_{db}$, corresponding to an overall conversion rate of 93.2%, which agrees well with the results of Binder [3].

*Table 1: Measured product gas and shifted product gas composition with standard deviation*

| Gas composition | Value | | Unit |
|---|---|---|---|
| | Product gas | Shifted product gas | |
| $H_2$ | 42.37 ± 0.25 | 50.30 ± 0.15 | vol.-$\%_{db}$ |
| CO | 17.32 ± 0.33 | 0.98 ± 0.03 | vol.-$\%_{db}$ |
| $CO_2$ | 26.82 ± 0.57 | 37.59 ± 0.10 | vol.-$\%_{db}$ |
| $CH_4$ | 8.65 ± 0.16 | 7.40 ± 0.06 | vol.-$\%_{db}$ |
| $C_2H_4$ | 2.13 ± 0.07 | - | vol.-$\%_{db}$ |
| $C_2H_6$ | 0.22 ± 0.01 | - | vol.-$\%_{db}$ |
| $N_2$ | 0.44 ± 0.08 | - | vol.-$\%_{db}$ |

In the PSA raffinate, no $CH_4$ (LOD[1]=10 $ppm_v$), $C_2H_4$ (LOD=100 $ppm_v$), $C_2H_6$ (LOD=100 $ppm_v$), and CO (LOD=0.5 $ppm_v$) were detected. As adsorption strength typically increases with molecular weight [4], it can be assumed that $C_2H_4$ and $C_2H_6$ were not present in the raffinate if $CH_4$ was not detected. $N_2$ was found to be lower than 200 $ppm_v$. The $CO_2$ content showed a decreasing trend, indicating that a $CO_2$ content lower than 30 $ppm_v$ can be expected with further experiment duration. The hydrogen recovery amounts to 75.3% at an adsorption pressure, equalization pressure and adsorption time of 6.4 $bar_a$, 5 $bar_a$ and 500 s, respectively.

## Conclusion

Hydrogen could be successfully produced from bark mulch pellets via advanced DFB gasification with a purity of ≥99.97 vol.-%. Preliminary results have shown that the $CH_4$ and $N_2$ content in the raffinate did not exceed the thresholds according to the standard ISO 14687:2019 [5]. The LOD of the CO analyzer (0.5 $ppm_v$) is slightly above the maximum allowable CO content (0.2 $ppm_v$). Future research should address, on the one hand, the optimization potential regarding the hydrogen recovery, and, on the other hand, prove in longer-term experiments whether the $CO_2$ threshold of 2 $ppm_v$ can be undercut.

## References

[1] S. Fail *et al.* "Wood Gas Processing To Generate Pure Hydrogen Suitable for PEM Fuel Cells". In: *ACS Sustainable Chem. Eng.* 2 (2014), pp. 2690-2698. DOI: 10.1021/sc500436m.
[2] J. Loipersböck, M. Luisser, S. Müller, H. Hofbauer, and R. Rauch. "Experimental Demonstration and Validation of Hydrogen Production Based on Gasification of Lignocellulosic Feedstock". In: *ChemEngineering* 2 (2018), p. 61. DOI: 10.3390/chemengineering2040061.
[3] M. Binder. "Long Term Performance of an Fe/Cr Based Water Gas Shift Catalyst Processing Tar-Rich Wood Gas". Master Thesis. Vienna: TU Wien, 2015.
[4] J. Benson and A. Celin. "Recovering hydrogen - and profits - from hydrogen-rich offgas". In: *Chemical Engineering Progress* 114 (2018).
[5] International Organization for Standardization. "International Standard ISO 14687". Ed. by ISO Copyright Office. 2019. URL: https://www.iso.org/standard/69539.html

---

[1] LOD – Limit of detection

## W.3a – Gasification

# Entrained flow gasification of circular raw materials in the Swedish chemical industry

Fredrik Weiland[1]*, Johannes Fernberg[1], Marcus Gullberg[1], Jonas Wennebro[1]

[1]*RISE Research Institutes of Sweden AB, Sweden*
**Corresponding author: fredrik.weiland@ri.se*

---

Sweden has an overall climate goal of net zero emissions of greenhouse gases by 2045 [1]. One way towards reduced industrial $CO_2$ emissions is to replace virgin fossil raw materials with recycled materials and biomass. In order to facilitate this transition, the Swedish Energy Agency funded a research project in which RISE, Perstorp AB, Stena Recycling, Scandinavian Enviro Systems, Rejlers, Josefsson Sustainable Chemistry and Stenungsund municipality, jointly investigated the possibilities for replacing natural gas with circular oil raw materials in the chemical industry [2]. In practice, the project involved pilot-scale entrained flow gasification experiments under different operating conditions to investigate the influence on yields, syngas impurity levels, and process efficiency when gasifying two circular oils. The two oils were a waste lubricant oil (WLO) supplied by Stena Recycling and a pyrolysis oil from end-of-life tires (tire pyrolysis oil, TPO) produced by Scandinavian Enviro Systems. The results from oil gasification experiments were compared against the results from gasification of natural gas (NG) in the same pilot reactor.

The gasification pilot plant was previously described by Simonsson et al.[3], whose experiments involved gasification of pulverized feedstocks. In this work, for natural reasons, two different burners were used, one for the oils and another one for the natural gas, respectively. Both burners had a central fuel injection. A full cone spraying nozzle with an outlet diameter of 0.51 mm (Spraying Systems Co.®) was used for spray atomization of the oils, whereas the NG was supplied through a 6 mm hole in the centerline of the burner. In both burners, oxygen was supplied through four holes (2.0 mm and 3.5 mm in diameter for the NG and oil burners, respectively), evenly spaced concentrically outside the central fuel injection. All inlet gas flows were controlled by mass flow controllers, whereas the oil injection was monitored by a Coriolis mass flow meter.

Experiments with all feedstocks were separately executed at different operating conditions of the gasifier. The fuel feeding was controlled to correspond to a thermal input of 150 $kW_{th}$. And the oxygen supply was adjusted to different oxygen stoichiometric ratios ($\lambda$) in the range $0.30<\lambda<0.65$. Analytical instruments included micro-GC and FTIR for analysis of the gas components, while a low-pressure impactor (LPI) was used to sample particulate matter in the syngas after the gasifier.

The main results are presented in Figure 1, where the top row (panes a and b) show the yields of $H_2$ and CO, respectively. NG, mostly composed of $CH_4$, resulted in the highest yield of $H_2$. The $H_2$ yield from both oils were lower due to a lower overall H/C ratio of the feedstocks compared to NG. The yields of CO were more similar, approx. 40-50 mol/kg of fuel, independent of feedstock type. The $CH_4$ concentration in the produced syngas is an important parameter to minimize if $H_2$ and CO are the major species of interest for downstream synthesis. The results indicated large differences in $CH_4$ concentrations for the different feedstocks as functions of $\lambda$ (Figure 1c). If instead compared to the measured gas temperature in the gasification reactor, the results were much more similar (Figure 1d). The yield of $CH_4$ decreased with increasing process temperature (increased $\lambda$). So did the yields of other unwanted gas species such as $NH_3$ and HCN. However, sulfur compounds such as $H_2S$ and COS did not follow a similar relationship.

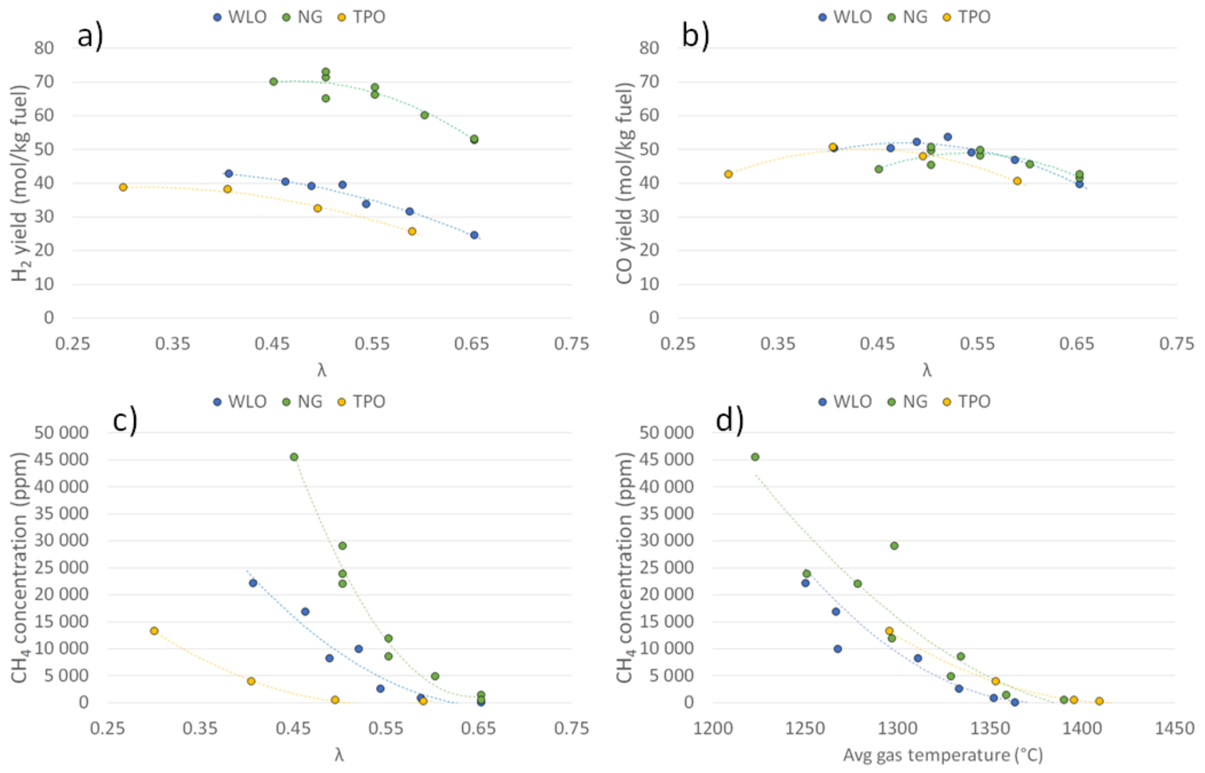


*Figure 1. Top row present the yield (mol/kg of fuel) of the most important syngas species, $H_2$ and CO in panes a) and b), respectively, as functions of λ. Bottom row visualizes the syngas concentration of $CH_4$ as function of λ and average gas temperature of the gasifier in panes c) and d), respectively.*

The major conclusion from this work was that it was possible to produce a syngas with sufficiently low $CH_4$ content and handleable amounts of trace impurities for further downstream processing in the chemical industry. However, gas cleaning adaptations will most likely be necessary to accommodate for the higher yields of sulfur species and soot resulting from circular raw materials in comparison with natural gas.

## References

[1] Naturvårdsverket, ”Sveriges klimatmål och klimatpolitiska ramverk,” 2020. [Online]. Available: http://www.naturvardsverket.se/Miljoarbete-i-samhallet/Miljoarbete-i-Sverige/Uppdelat-efter-omrade/Klimat/Sveriges-klimatlag-och-klimatpolitiska-ramverk/. [Använd 25 05 2021].

[2] Energimyndigheten, "Projektinformation - Cirkulära och förnybara råvaror till svensk kemiindustri," Energimyndigheten, [Online]. Available: https://www.energimyndigheten.se/forskning-och-innovation/projektdatabas/sokresultat/?registrationnumber=2021-037434. [Accessed 12 03 2024].

[3] J. Simonsson, H. Bladh, M. Gullberg, E. Pettersson, A. Sepman, Y. Ögren, H. Wiinikka and P.-E. Bengtsson, "Soot concentration in an atmospheric entrained flow gasifier with variations in fuel and burner configuration studied using diode-laser extinction measurements," Energy and Fuels, pp. 2174-2186, 2016.

# Kinetics of Biomass Devolatilization with Thermal Plasma

Kentaro Umeki[1,2]*, Johannes Waßmuth[1], Robert Lewtak[1], Sebastian Bastek[1], Andrius Tamošiūnas[1,3], Hartmut Spliethoff[1], Sebastian Fendt[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
*[2]Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden,*
*[3]Lithuanian Energy Institute, Kaunas, Lithuania*
**Corresponding author: kentaro.umeki@ltu.se*

Electricity-biomass hybrid system, also known as power and biomass to X (PBtX) system, is a promising route to produce sustainable biofuels and chemicals with high carbon conversion efficiency. A plasma-assisted entrained-flow gasification (PEFG) technology can play a key role in PBtX. By substituting a part of heat input to the gasifier, the PEFG requires much lower oxygen input than conventional gasification processes. As a consequence, it reduces the $CO_2$ content of product gases while keeping the benefit of entrained flow gasification technologies, such as low tar content. However, there is a lack of knowledge on how biomass converts under the influence of plasma in order to design the PEFG reactors based on CFD (computational fluid dynamic) simulation.

In this work, we aim to elucidate the conversion of pulverized biomass driven by thermal plasma generated by DC arc. Particular focus is on the initial stage of fuel conversion (devolatilization) because biomass passes through the high-temperature zone generated by plasma during the devolatilization step. The time required for devolatilization (conversion time) was evaluated to highlight the conditions that ensure complete devolatilization in the plasma zone. Conversion modes (uniform or non-uniform temperature and reaction profiles) were investigated to estimate the likelihood of particle fragmentation because of their strong influence on the kinetics of the consecutive reaction step (char gasification).

One-dimensional particle simulation was carried out, including heat and mass transfer as well as devolatilization kinetics, to examine the effect of particle size and gas temperature on the conversion time and conversion mode. The main governing equations are the continuity equation, Darcy's law (velocity-pressure correlation), species balance equations, heat balance equation, ideal gas law, solid phase conservation, and chemical reaction sub-models. The particle was discretized into smaller cells, and the above-mentioned conservation equations were solved numerically.

The results showed that having small particles is much more critical than the conventional gasification process because of the extremely short residence time at high-temperature zones.

The first and most important result from the particle simulation is the time required to heat and devolatilize particles. Fig. 1a shows the time for a single particle to reach 95% of the devolatilization reaction from the initial state of 300 K. The required time for the conversion decreases significantly as the plasma temperature increases and the particle size reduces. The effect is especially significant for relatively large particles (200 µm). The decrease in the required time for devolatilization is much more significant at the lower temperature ranges (2000 to 5000 K) than at the higher temperature ranges (5000 to 8000 K). Moreover, it shows the importance of decreasing the particle size rather than pursuing a higher plasma temperature. For example, the devolatilization time becomes below 20 ms for 50 µm particles even at the plasma temperature of 5000 K, while 200 µm particles cannot reach the same devolatilization time even with the plasma temperature of 8000 K.

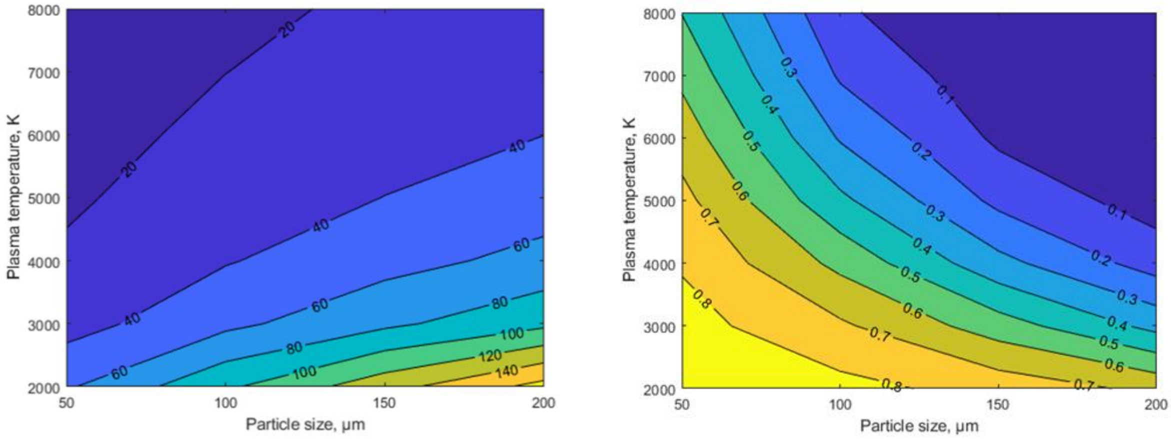


*Figure 1 (a) The time required for the completion of devolatilization in ms; (b) The indication for the uniformity of the particle conversion by plotting the local conversion at the particle centre at the moment when the local conversion of particle surface reaches 0.9*

The next question is how uniformly particles are converted during devolatilization. Fig. 1b shows the local conversion (the fraction of biomass converted to char) at the particle centre at the moment when the particle surface reaches the local conversion of 0.9. It shows that particles convert more uniformly if the particle size is small and the plasma temperature is low. Typical conventional entrained flow gasification conditions (ca. <200 µm particle and gas temperature of 2000 K) show relatively uniform conversion of particles. Meanwhile, the 200 µm particles undergo devolatilization highly non-uniformly with a 5000 K plasma gas stream, such that the conversion at the particle centre barely starts before the particle surface completes the conversion. If the reference condition for uniform particle conversion is taken from conventional gasification conditions (200 µm and 2000 K), the particle should be below ca 50-70 µm at the plasma gas temperature of 5000 K.

The results would be important for elucidating the potential physical transformation of biomass particles during devolatilization, such as fragmentation. If the particles release large amounts of gas in a very short time while reacting uniformly, there is a high possibility of causing fragmentation via micro explosion due to the simultaneous plasticization of solid and pressure buildup. On the other hand, highly non-uniform reactions may result in the ablation-like fragmentation of char particles. When the biomass near the particle surface is completely converted to char, it can be exposed to strong shear stress from high-speed gas surrounding the particles. Since inner particles remain physically intact biomass particles, this would most likely cause the surface to scale off and produce small char particles, leaving unreacted biomass particles.

# Numerical simulations of plasma-assisted biomass gasification in a vertical entrained flow gasifier

Robert Lewtak[1]*, Sebastian Bastek[1], Kentaro Umeki[1], Andrius Tamosiunas[1],
Sebastian Fendt[1], Hartmut Spliethoff[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: robert.lewtak@tum.de*

---

**Topic: Hydrogen Production, Sub-topic: Thermochemical** (e.g.: pyrolysis and gasification of biomass and waste for hydrogen and syngas production)

## Introduction

Plasma-assisted gasification is an attractive option for closing the carbon cycle in a circular economy and is the most popular and cheapest method of hydrogen production, compared to, for example, water electrolysis, where the amount of hydrogen obtained per unit of energy consumed is much greater.

## Mathematical model of gasification

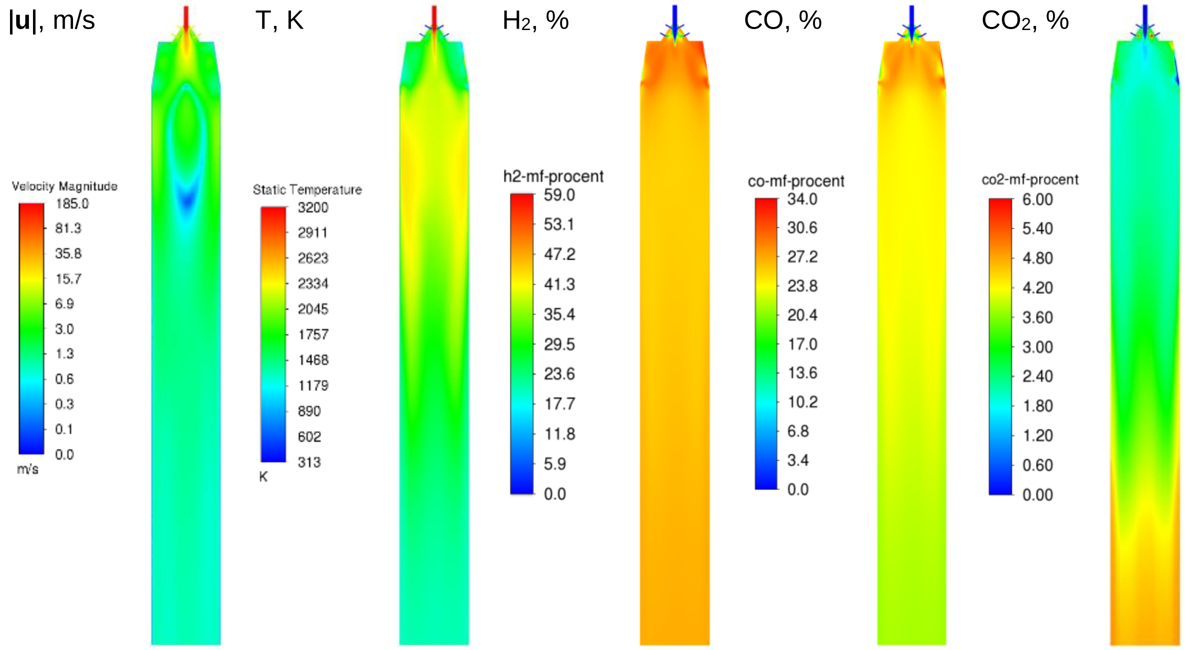
In this work, the numerical simulations were performed to model the plasma-assisted biomass gasification in a vertical entrained-flow gasifier equipped with a 30kW thermal plasma torch. The simulations were carried out using CFD software ANSYS Fluent 2023R1. The numerical setup solved the governing equations for the gas mixture and species mass, momentum, and energy conservation laws, and additionally the equations describing the turbulence model and the radiation transfer equation. In the current simulations, the following reactions were considered for the gas phase:

- oxidation of volatiles released during devolatilization of biomass fuel:
$$C_mH_nO_lN_k + (m+n/2-l)/2\ O_2 \rightarrow m\ CO + n/2\ H_2O + k/2\ N_2\ ,$$
- water steam reforming (WSR) of volatiles released during devolatilization of biomass:
$$C_mH_nO_lN_k + (m-l)\ H_2O \rightarrow m\ CO + (m-l+n/2)\ H_2 + k/2\ N_2\ ,$$
- oxidation of carbon monoxide:
$$CO + 0.5\ O_2 \rightarrow CO_2\ ,$$
- oxidation of hydrogen:
$$H_2 + 0.5\ O_2 \rightarrow H_2O\ ,$$
- water gas shift reaction (WGSR):
$$CO + H_2O = CO_2 + H_2\ ,$$
that is assumed to be in equilibrium.

For the biomass fuel the following reactions were applied: oxidation and gasification of char carbon described by the following reactions:

$$C + 0.5\ O_2 \rightarrow CO,$$
$$C + O_2 \rightarrow CO_2,$$
$$C + H_2O \rightarrow CO + H_2\ ,$$
$$C + CO_2 \rightarrow 2\ CO.$$

The biomass gasification model was implemented into Ansys Fluent using the UDFs Other equations, describing the processes in the gas phase, were solved using the coupled algorithm available in Fluent with second order discretization method. The SST k-ω model was used to describe the turbulent flow of the gas medium. The discrete-ordinates method was used to solve the radiation transfer equation (RTE) describing the radiation heat transfer and the weighted-sum-of-gray-gases model (WSGG) was applied for the emissivity of the gas phase.



a) velocity b) temperature c) $H_2$ mole frac. d) CO mole frac e) $CO_2$ mole frac.

*Figure 1: Selected numerical results*

## Numerical results

Figure 1 shows selected numerical results, i.e. contours of velocity, temperature, mole fractions of $H_2$, CO and $CO_2$. The contours are shown in two vertical cross sections mutually perpendicular to each other. Biomass particles flow directly adjacent to or through the plasma jet, and subsequently undergo significant heating at a rate of $10^4$-$10^5$ K/s depending on the particle diameter. The biomass inlets are aligned in such a way as to guide the particles through the intensely hot plasma jet, which results in evaporation of moisture and the release of volatile components as the biomass temperature rises. Due to the presence of water vapour and the immediate surroundings of the hot plasma jet, the released volatiles, which may include tars and hydrocarbons, rapidly undergo water steam reforming to produce CO and $H_2$. Apart from the area around the plasma torch and the reactor outlet, the concentrations of $H_2$ and CO as gasification products are uniform. In the area of the plasma torch, intense evaporation of moisture and devolatilization of the fuel take place. Due to the high heating rate of the fuel, a high volatile yield is achieved. Then, in the steam reforming reaction, the volatiles are converted into CO and $H_2$.

## Conclusion

The gasification reactor acts as a reactor for the steam reforming of the volatiles and the gasification of the char carbon remaining as fixed coal. The amount of $CO_2$ obtained in the process depends on the steady-state equilibrium of the WGS reaction, i.e. on the temperature reached in the reactor. The syngas produced is of high quality (high concentrations of $H_2$ = 47%v db. and CO = 21%v db) and high purity due to the absence of problematic tars and hydrocarbons, which is a characteristic feature of plasma-assisted gasification.

## Acknowledgments

This study was carried out in the framework of the International Future Lab on Green Hydrogen Technologies “REDEFINE Hydrogen Economy (H2E)” (project no.: 01DD21005) sponsored by the Federal Ministry for Education and Research (Germany). The financial support is gratefully acknowledged.

# Characterizing Solid Fuel Particle Behavior in Thermal Plasma Flows: Insights from CFD Simulations

Aleksandra Kiedrzynska [1,2]*

[1]*Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
[2]*Institute of Power Engineering - National Research Institute, Warsaw, Poland*
**Corresponding author: aleksandra.kiedrzynska@tum.de*

This study investigates the behavior of solid fuel particles in thermal plasma flows through computational fluid dynamics (CFD) simulations. Thermal plasma flows play a crucial role in various industrial processes, including gasification, where solid fuel particles interact with high-temperature plasma. Understanding the dynamics of these interactions is essential for optimizing process efficiency and product yield. Utilizing CFD simulations, this research explores the complex phenomena governing solid fuel particle behavior in thermal plasma flows. Insights gained from this study provide valuable knowledge for the design and optimization of plasma-assisted processes, contributing to advancements in energy production and environmental sustainability.

## W.3b – Energy Vectors and Supply Chains

# Dimethyl Ether as a Potential Vector for Large-Scale Hydrogen Import: Leveraging LNG Terminals for Hydrogen Import

Patrick Preuster[1,2]*

*[1]Fraunhofer IEG, Fraunhofer Research Institution for Energy Infrastructure and Geothermal Systems IEG, Bochum, Germany*
*[2]Campus Burghausen, Rosenheim Technical University of Applied Sciences, Rosenheim, Germany*
**Corresponding author: patrick.preuster@th-hosenheim.de*

In recent years, the transition towards a hydrogen-based economy has gained significant momentum, driven by the imperative to mitigate climate change and achieve energy security. As the demand for renewable energies and thus hydrogen continues to rise, innovative solutions for its efficient production, storage, and distribution are paramount. In this context, dimethyl ether (DME) emerges as a promising candidate for facilitating the import of large quantities of hydrogen, utilizing existing infrastructure. [1]

The political conditions that have prevailed since the Russian invasion of Ukraine have made it necessary for Germany in particular to create large LNG import capacities in order to reduce its dependence on Russian gas. The TransHyDE LNG2Hydrogen project aims to evaluate how these capacities can be used to import green hydrogen in the future.

DME is characterized by a high hydrogen density, as half of the hydrogen from the steam reforming of DME results from the water vapor used and therefore effectively does not need to be transported but still contributes to the storage density. [1]

$$CH_3OCH_3 + 3\,H_2O \rightleftharpoons 2\,CO_2 + 6\,H_2 \tag{1}$$

This presentation explores the feasibility of utilizing DME as a vector for hydrogen importation, leveraging the well-established infrastructure of LNG terminals for its handling and distribution. Unlike gaseous hydrogen, DME offers the advantage of being a liquid at ambient conditions, simplifying storage and transportation logistics. The conversion of DME to hydrogen can be efficiently achieved through established catalytic processes, ensuring a seamless integration into existing hydrogen supply chains.

A key consideration in this paradigm is the management of carbon dioxide generated during the production of hydrogen from DME by steam reforming. The carbon dioxide ideally has to be captured by technical measures and has to be transported back to regions with abundant renewable energies. By strategically locating DME production facilities near regions abundant in renewable energy sources, such as wind or solar the captured and transported carbon dioxide emissions can be utilized in the DME synthesis processes, effectively closing the carbon loop [2]. Moreover, the potential for carbon dioxide transport back to renewable energy hubs for utilization or sequestration enhances the environmental sustainability of the proposed system.

This presentation will outline a conceptual framework for a DME terminal dedicated to the importation of large volumes of hydrogen and its integration into the planned hydrogen backbone of Germany. Through comprehensive techno-economic analysis and strategic planning, the proposed terminal aims to serve as a pivotal node in the european hydrogen supply chain, facilitating the transition towards a carbon-neutral future.

## References

[1] P. Schühle, R. Stöber, M. Semmel, A. Schaadt, R. Szolak, S. Thill, M. Alders, C. Hebling, P. Wasserscheid, O. Salem *d, “Dimethyl ether/CO2 – a hitherto underestimated H2 storage cycle,” Energy Environ. Sci., 16, 3002-3013, 2023

[2] E. Catizzone, G. Bonura, M. Migliori, F. Frusteri, G. Giordano, “$CO_2$ Recycling to Dimethyl Ether: State-of-the-Art and Perspectives”, Molecules, 23, 31, 2018

# Hydrogen and PtX fuel logistics for optimized Sustainable Aviation Fuel production for Bavaria

Leonard Moser*[1], Benjamin W. Portner[1], Lennart Rieger[1], Christina Penke[1], Valentin Batteiger[1]

[1]*Bauhaus Luftfahrt e.V., Munich, Germany*
**Corresponding author: leonard.moser@bauhaus-luftfahrt.net*

Germany is aiming for climate neutrality by 2045 in order to comply with the Paris Agreement [1]; this target requires action in all major sectors of the economy including air transport. Within the European Union, fuel suppliers are mandated to meet the ReFuelEU Aviation quotas for sustainable aviation fuels (SAFs) starting from 2026, with a target of reaching 70% by 2050. This necessitates a radical transformation of the fuel production landscape, with new infrastructure emerging and repurposing of existing infrastructure to expand SAF production capacity significantly.

In this work, the focus will be on different technological and logistical options for supplying the Bavarian Aviation industry with Power-to-X fuels, induced by the sub-quota requirements in the ReFuelEU Aviation initiative and the huge theoretical production potential. PtX technologies convert renewable electricity into hydrogen and further into various synthetic fuels, such as methanol and kerosene. While the latter two energy carriers are liquid and can be easily transported over long distances, hydrogen is a gas under typical conditions and therefore requires either liquefaction or transport via pipeline. The SouthH2Corridor (SH2C) pipeline project, scheduled to commence operation by 2030, represents a pivotal development in this context. [2] The SH2C pipeline, which will be part of the European Hydrogen Backbone, will extend from Tunisia to Europe and offers a strategic opportunity to channel hydrogen into the European market. [3] Tunisia, as the entry point of the SH2C pipeline, was selected as the focus area of production of this work.

So far, all SAF production pathways incur higher production cost than conventional jet fuel. Consequently, the economic optimization of conversion paths and logistics is of high importance. Individual cost items for each investigated import and fuel production option will be detailed. Notably, a possible integration of the Bavarian “Chemical Delta” (Burghausen-Trostberg-Aschau) into the production path is analyzed, as it is directly connected to the SH2C / EHB. Access and repurposing existing infrastructure can be a pivotal factor in terms of fuel production cost, especially for conversion pathways that require large amounts of hydrogen.

## References

[1] Paris Agreement to the United Nations Framework Convention on Climate Change, Dec. 12, 2015, T.I.A.S. No. 16-1104
[2] SoutH2 Corridor (SH2C). (2024, July 24). https://www.south2corridor.net/
[3] The European Hydrogen Backbone (EHB) initiative | EHB European Hydrogen Backbone. (2024, February 09). https://ehb.eu/

# A Concept for Data-Driven Decision Support in Renewable Hydrogen Supply Chains

Julian Stang[1]*, Alexander Klimenko[2], Niklas Lindholm[1], Yuanshen Lu[2], Marc Wegmann[1], Ruediger Daub[1,3]

[1]*Institute for Machine Tools and Industrial Management, TUM School of Engineering and Design, Technical University of Munich, Germany*
[2]*Centre for Multiscale Energy Systems, School of Mechanical and Mining Engineering, The University of Queensland, Australia*
[3]*Fraunhofer Institute for Casting, Composite and Processing Technology (IGCV), Augsburg, Germany*
**Corresponding author: julian.stang@iwb.tum.de*

## Problem Statement

The pressure for governments and industry to shift towards renewable energy resources is increasing [1]. Renewable hydrogen (RH2) can potentially replace fossil fuels in various applications [2]. However, one of the main challenges is that the supply chain of RH2 is in the early stages of its development. Consequently, there is a lack of data to support decision-making and to understand the effects of the selection of different RH2 methods for production, transport, storage, and utilization (PTS&U) on key performance indicators (KPIs) in economic, ecologic, and social sustainability [3]. An RH2 method in this context can be, for example, hydrogen electrolysis for production, a ship for transportation, a high-pressure tank for storage, and a steel manufacturer for consumption. Therefore, this article proposes a concept to artificially generate RH2 supply chain data for various methods of PTS&U using a simulation approach and assessing their impacts on the relevant sustainability KPIs. The assessment allows decision-makers to choose suitable RH2 supply chain configurations according to company-specific objectives.

## Methodology and Results

The concept follows the Design Research Methodology proposed by Blessing and Chakrabarti [4]. First, an initial literature review confirmed the outlined problem statement and the importance of resolving these issues. Therefore, resolving these issues is crucial for RH2 adoption and development. Afterward, a systematic literature review combined with empirical research methods (e.g., surveys) identifies the relevant sustainability KPIs. Furthermore, the parameters for the simulation building blocks that model the various RH2 methods of PTS&U are identified. With the help of a Design of Experiment approach, various RH2 supply chain configurations consisting of different combinations of RH2 methods for PTS&U are simulated according to the VDI 3633. The generated data is analyzed in the subsequent step by developing a suitable artificial intelligence (AI)-based methodology. The AI methodology will be employed in a manner analogous to data-driven supply chain management methodologies for risk assessment in the RH2 supply chain [5]. The simulation data will be utilized as training data for the AI methodology, which will then be employed with real data once it becomes available [6]. The AI methodology enables forecasting and optimizing RH2 supply chain operations under various configurations, thereby aiding decision-makers in selecting suitable RH2 supply chain configurations according to company-specific KPIs. The concept will be validated with the help of industry experts. Figure 1 summarizes the proposed concept.

The result is a data-driven decision support system (DSS) consisting of the simulation approach and an AI-based decision support. The DSS allows critical decision-makers to generate artificial RH2 supply chain data for different methods for PTS&U of RH2 and identify optimally suited RH2 supply chain configurations based on company-specific objectives.

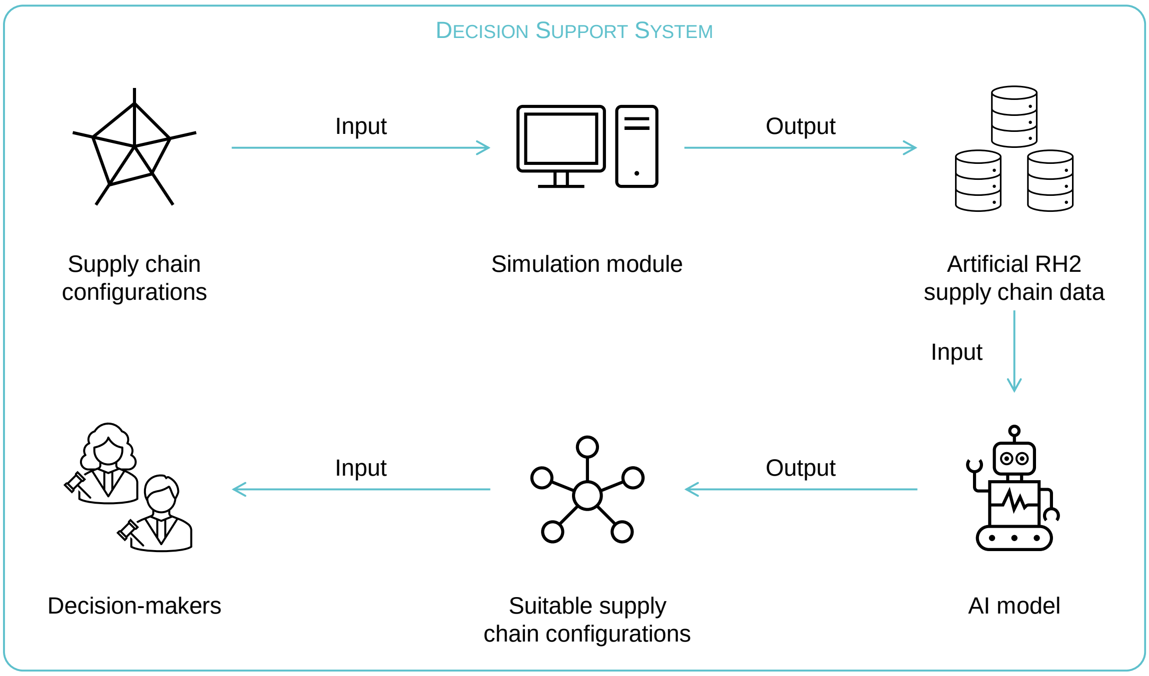


*Figure 1: Concept for a data-driven DSS*

## Conclusion

The authors of this article propose a data-driven, simulation-based DSS for the RH2 supply chain. The proposed concept will generate and analyze artificial data of methods for PTS&U for RH2, utilizing simulation models and AI technologies. This approach will allow for multiple simulations of supply chain configurations and for assessing their impact on KPIs within the three pillars of sustainability: economic, ecological, and social.

## References

[1] UNFCCC, “The Paris Agreement - Publication,” in *Paris Climate Change Conference,* UNFCCC, Ed., pp. 1–54, 2018.
[2] U.S. Department of Energy, “Hydrogen Strategy: Enabling A Low-Carbon Economy,” 2020.
[3] B. Purvis, Y. Mao, and D. Robinson, “Three pillars of sustainability: in search of conceptual origins,” *Sustainability Science*, vol. 14, no. 3, pp. 681–695, 2019.
[4] L. T. Blessing and A. Chakrabarti, *DRM, a Design Research Methodology*, Springer London, London, 2009.
[5] F. Schlüter, “Procedure Model for Supply Chain Digitalization Scenarios for a Data-Driven Supply Chain Risk Management,” in *Revisiting Supply Chain Risk,* G. A. Zsidisin and M. Henke, Eds., vol. 7, pp. 137–154, Springer International Publishing, Cham, 2019.
[6] T. Zhang, M. Lauras, G. Zacharewicz et al., “Coupling simulation and machine learning for predictive analytics in supply chain management,” *International Journal of Production Research*, pp. 1–18, 2024.

# Circular economy strategies for green electrolyzer supply chains

Sarah Haßlacher[1], Magnus Fröhling[1*]

[1]*Professorship Circular Economy, Technical University of Munich (TUM), Campus Straubing, Am Essigberg 3, 94315 Straubing, Germany*
*Corresponding *author: sarah.hasslacher@tum.de*

---

To face the devastating consequences of climate change, the international community has reached the Paris Agreement in 2015, which aims to limit the overall global warming to 1.5 °C compared to pre-industrial levels in 1990. As a national implementation, Germany has to reduce its greenhouse gas emissions by 65% by 2030 compared to the 1990, according to the German Climate Change Act [1]. With the goal of becoming climate neutral by 2045, Germany is going to transform its complete energy system towards nearly 100% renewable energy sources [1, 2]. As a significant key player of the energy transition, hydrogen offers myriad application possibilities. The demand for this resource is continuously increasing. The hydrogen demand is predicted to be 90 - 110 TWh in Germany by 2030. Until 2050, the hydrogen demand is estimated at 1000 TWh including hydrogen based synthetic products [3, 4]. As a matter of fact, legislators and policy advisors focus starkly on the important gas, with a prominent example being Germany's National Hydrogen Strategy. This coherent framework deals with the holistic hydrogen supply chain of scaling-up production, promoting industrial use and uptake, developing associated infrastructure and creating coherent regulatory conditions for the market [3, 5]. The green hydrogen production excels perfectly as a suitable protagonist in promoting a green energy transformation. This environmentally friendly production method is characterized by water electrolysis using renewable energy sources and highly purified water [2]. However, along the green hydrogen value chain, several barriers impede the progress in green hydrogen deployment. The faster the production scale expands, the higher the material and manufacturing inputs for electrolyzer production increase. Especially, the demand for highly important and critical raw materials such as aluminum, titanium and rare earth elements have to be considered. In order to align material demand and sustainability standards, the circular economy concept encloses a regenerative industrial economy including closed-loop material flows, circularity by design and the value retention of raw materials and compounds over multiple life stages as well as social and techno-economic improvements. This transformative shift decouples the classical economic growth from resource consumption, thereby fostering sustainability and resilience in the long term. As long as possible, products, materials and resources are retained within this loop by so-called R imperatives. Figure 1 represents the R imperatives embedded in the green electrolyzer supply chain. These core elements for the transformation towards a circular economy offer concrete ways to reduce the consumption of primary resources and promote the use of secondary raw materials throughout the complete life cycle, from manufacturing to end-of-life treatments [6, 7].

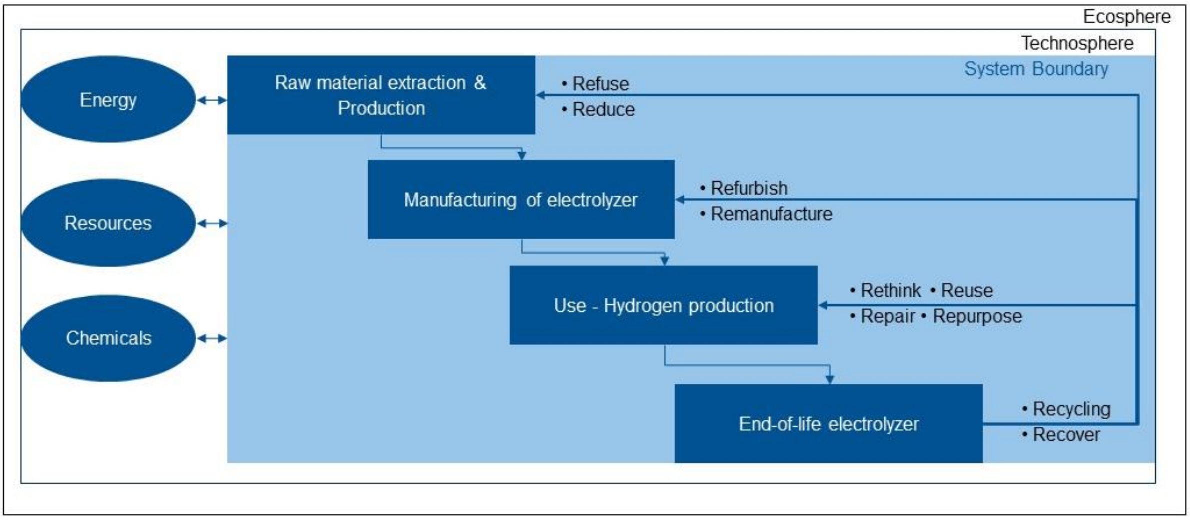


*Figure 1: R imperatives for a green electrolyzer supply chain*

To assess the circular economy strategies for the electrolyzer system, the literature lacks a comprehensive framework that applies circular economy strategies on a green and sustainable electrolyzer supply chain. The contribution of this research is the implementation of various R imperatives on the different life cycle steps of a holistic green electrolyzer supply chain. First, we conduct a structured literature research focused on circular economy strategies for electrolyzer supply chains including European and German based legislative frameworks. To identify the status quo, a material flow analysis highlights the materials and resources within the technical system in order to identify hotspot pathways especially with a closer look on critical and valuable raw materials. Based on this as-is analysis, we derive a complete holistic circular economy framework for green electrolyzer supply chains. This circular economy framework for electrolyzer supply chains promotes the pathway towards a comprehensive decarbonization strategy for Germany.

## References

[1] Bundestag, "Federal Climate Change Act of 12 December 2019 (Federal Law Gazette I, p. 2513), as last amended by Article 1 of the Act of 18 August 2021 (Federal Law Gazette I, p. 3905)," [Online]. Available: https://www.gesetze-im-internet.de/englisch_ksg/englisch_ksg.html

[2] F. Dawood, M. Anda, and G. M. Shafiullah, "Hydrogen production for energy: An overview," *International Journal of Hydrogen Energy*, vol. 45, no. 7, pp. 3847–3869, 2020, doi: 10.1016/j.ijhydene.2019.12.059.

[3] Bundesministerium für Wirtschaft und Energie, Ed., "Nationales Reformprogramm 2020 - Die Nationale Wasserstoffstrategie," Berlin, 2020.

[4] R. Neugebauer, Ed., *Wasserstofftechnologien*. Berlin, Heidelberg: Springer Vieweg, 2022.

[5] Bundesministerium für Wirtschaft und Klimaschutz, Ed., "Fortschreibung der Nationalen Wasserstoffstrategie," Berlin, 2023.

[6] J. Potting, M. P. Hekkert, E. Worrell, and A. Hanemaaijer, "Circular Economy: Measuring Innovation in the Product Chain," *Planbureau voor de Leefomgeving*, no. 2544, 2017. [Online]. Available: https://dspace.library.uu.nl/handle/1874/358310

[7] J. Kirchherr, D. Reike, and M. Hekkert, "Conceptualizing the circular economy: An analysis of 114 definitions," *Resources, Conservation and Recycling*, vol. 127, pp. 221–232, 2017, doi: 10.1016/j.resconrec.2017.09.005.

# W.4a – Innovative Technologies and Applications

## Reflecting the potential role of REDEFINE technologies in a future low-emission energy system

Doronina Iryna [1]

[1]*Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: iryna.doronina@tum.de*

The vast majority of countries around the world have committed to sharply reducing greenhouse gas emissions and becoming climate-neutral by 2050. The REDEFINE Hydrogen Economy (H2E) project, which includes representatives of countries from around the world, reflects the processes of transition and the application of new technologies, as well as their impact on shaping a future low-emission energy system. At the core of reducing greenhouse gas emissions is the shift to renewable energy sources for energy production and the use of renewable energy carriers, such as hydrogen, for hard-to-abate, energy intensive applications such as long-range transportation, high-grade heat production, and as a feedstock in industrial processes. With the adoption of the Paris Agreement and the establishment of the Global Development Goals in 2015, countries have accelerated the transition to renewable energy sources, gradually reducing the use of fossil fuels. Using the example of the countries involved in the REDEFINE H2E project, the changes in energy share are illustrated in Figure 1.

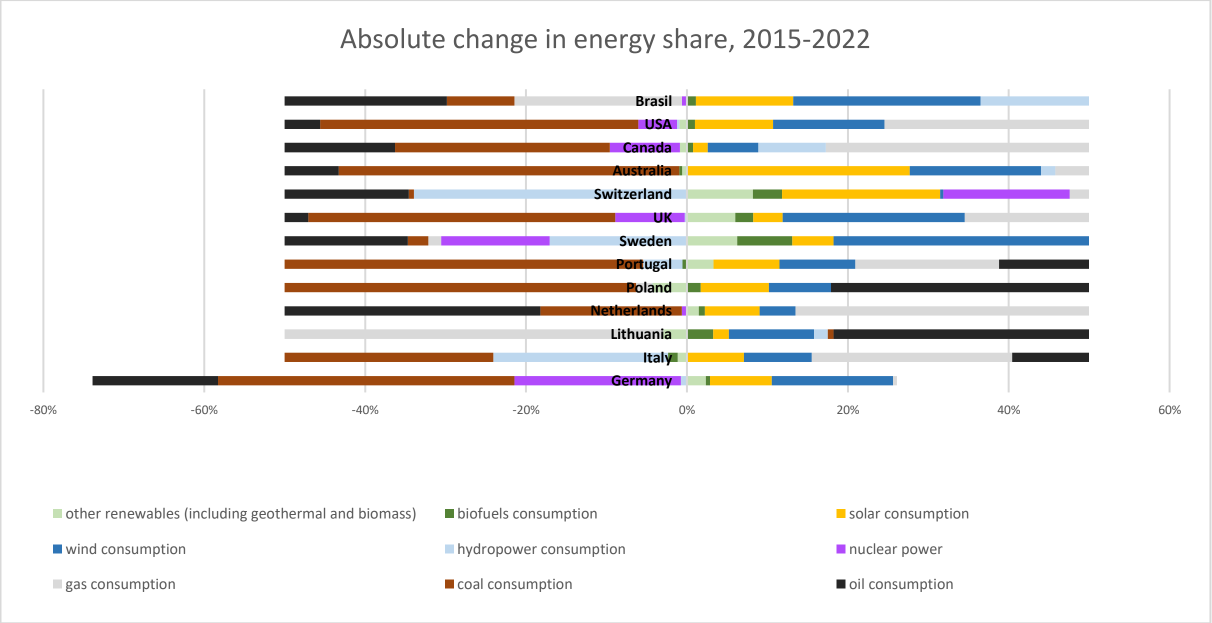


*Figure 1: Changes in energy share of the partner countries of the REDEFINE H2 project*

Although the goal for all countries is the same, the paths to decarbonization vary. Germany has completely abandoned nuclear generation since 2024 and reduced the use of coal and oil. Countries like the Netherlands, Sweden, the UK, Canada, and the USA have also reduced their use of nuclear generation, whereas Switzerland has increased its consumption of nuclear energy. Some countries are substituting one fossil resource for another. For instance, Lithuania has reduced its gas consumption but increased its oil consumption. In the Netherlands, the situation is the opposite. Poland and Portugal, while reducing coal consumption, have increased their oil consumption. The general trend among the countries under study is a move towards decreasing coal consumption. However, all of these countries are still looking for optimal hydrogen technology solutions based on local characteristics and potential, and so far, the energy systems of these countries still have a significant share of fossil fuels in their energy mix.

Most of the hydrogen produced today comes from fossil resources. Pure hydrogen production is still a small share of total production, as is its overall use and demand (Figure 2).

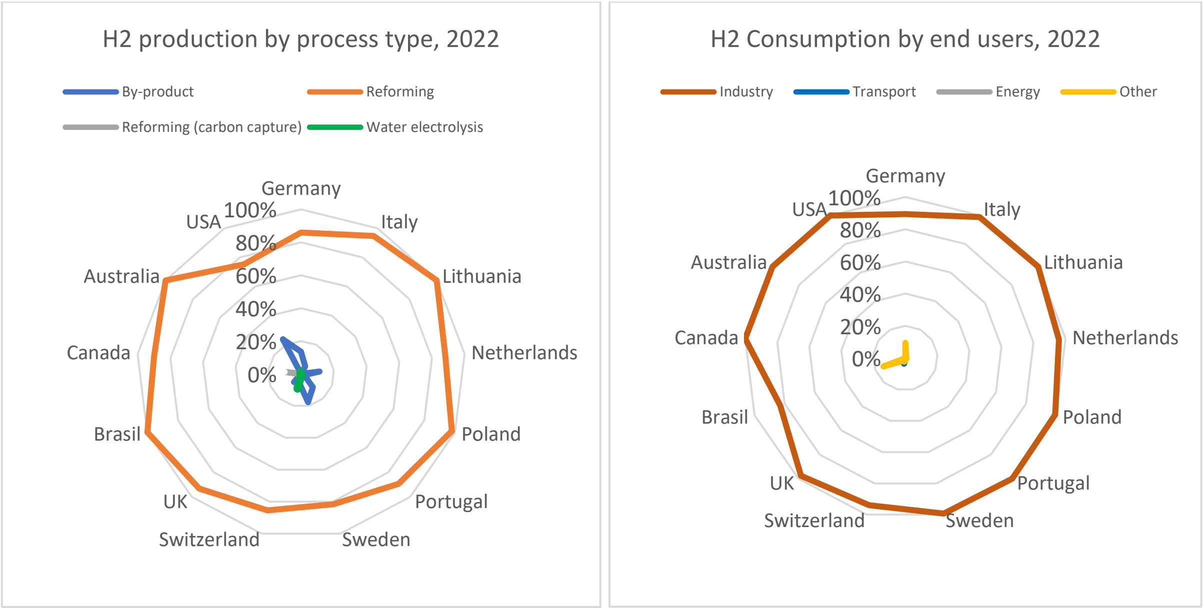


*Figure 2: Current production and use of hydrogen in the countries under study*

Nonetheless, the demand for hydrogen is expected to explode over the next 10-30 years in all these countries: The analysis of future demand for H2 scenarios and the calculation of the amount of hydrogen production according to the planned projects in the IEA database indicate a progressive increase.

For now, 43 governments around the world have a hydrogen strategy in place. Analysis of NHS in countries under study provides the direction of movement in these countries toward forming the hydrogen economy. The hydrogen strategies all focus on a similar target picture by defining the future usage of hydrogen in the following sectors: transport, energy, and industry. The production of hydrogen fundamentally reshapes power, gas, chemical, and fuel markets because hydrogen can be produced from electricity and used as - or converted into -fuels, chemicals, and power. Potential end-uses for hydrogen demand are: Injection in gas grids for space heating and heating for industry (oil and gas, steel, cement), and for export; Feedstock for industry (synthetic fuels, ammonia, methanol, oil refining, metals and steel); Transport (long distance, heavy duty, rail, sea, material transport); Electricity storage (stationary plants, remote areas, back-up power).

Sectors that are difficult to decarbonize require not only the end product, such as hydrogen, but also technologies that can produce this product on-site. Transporting hydrogen over long distances is still expensive and also has an environmental impact. Global interest in hydrogen is leading to efforts and investments in new technologies. As demand for hydrogen increases, production volumes are growing, and production methods are evolving.

Strategies indicate the planned capacity of electrolysers for hydrogen production, but fossil-free hydrogen can be produced by combining different hydrogen production routes, as proposed by the REDEFINE H2E concept.

# Optimal Res-Electrolyser Coupling- A Flexible Technoeconomic Assessment Tool

Nikolaos Skordoulias[1]*, Sotirios Karellas[1], Dimitrios V. Lyridis[2], Emmanuel Stamatakis[3], Emmanuel Zoulias[4]

*1National Technical University of Athens, Laboratory of Thermal Processes, 9 Heroon Polytechniou, Zografos, 15780, Athens, Greece*
*2National Technical University of Athens, Laboratory of Maritime Transport, 9 Heroon Polytechniou, Zografos, 15780, Athens, Greece*
*3Institute of Geoenergy/FORTH, M1 Building, Technical University of Crete Campus, 73100 Chania*
*4New Energy & Environmental Solutions &Technologies (NEEST), Agia Paraskevi, 15341 Athens, Greece*
**Corresponding author: nikosskordoulias@mail.ntua.gr*

---

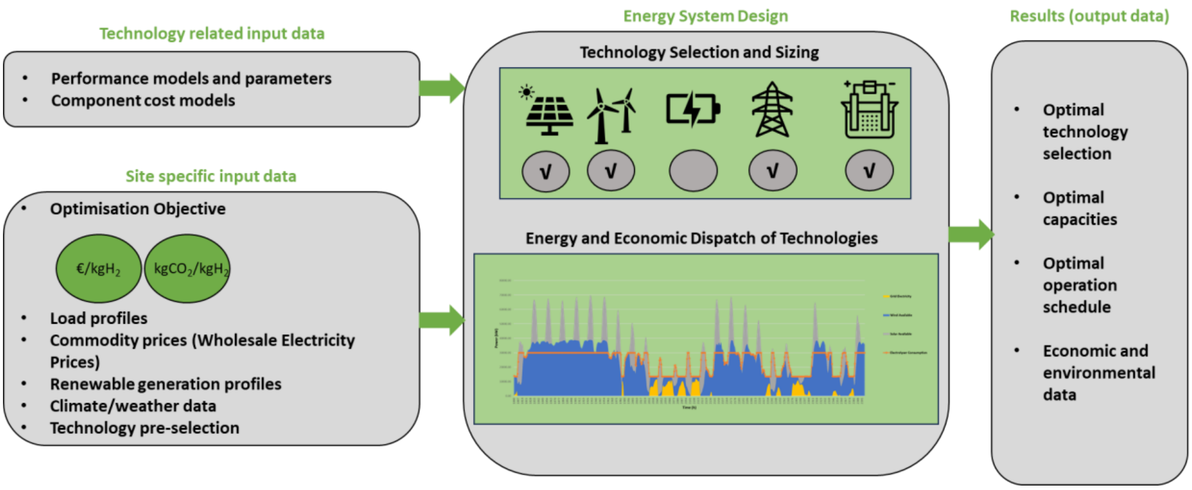


*Figure 1: Research Methodology.*

The escalating urgency to address climate change has sparked unprecedented interest in green hydrogen as a clean energy carrier. The intermittent nature of Renewable Energy Sources (RES) like wind and solar can introduce unpredictability into the energy supply, potentially causing mismatches in the power grid. To this end, green hydrogen production can provide a solution by enhancing system flexibility, thereby accommodating the fluctuations and stochastic characteristics of RES. Furthermore, green hydrogen could play a pivotal role in decarbonizing hard-to-abate sectors and promoting sector coupling.

This research article endeavors to delve into this subject by developing a dynamic techno-economic analysis tool, capable of flexibly assessing the optimal setup of Alkaline (AEL) electrolysis coupled with Renewable Energy Sources (RES) in a specific region or hub. The focus lies on achieving cost-effectiveness, efficiency, and sustainable production of green hydrogen. The tool leverages a comprehensive dataset covering a full year of hourly data on both renewable electricity production from intermittent RES and wholesale electricity market prices, alongside customizable inputs from users. It can be applied across various scenarios, including direct coupling with dedicated RES plants and hybrid configurations utilizing the electricity grid as a backup source. Moreover, the tool can integrate multiple electricity sources to minimize electricity costs. Extensive analyses are conducted within the context of the Peloponnese region, where TRIERES, the Greek Hydrogen Valley, is taking shape. The model optimizes RES and electrolyzer capacities to minimize the Levelized Cost of Hydrogen (LCOH) and surplus renewable electricity. By incorporating real operating maps of electrolysis systems from industrial manufacturers, the model accounts for factors such as maximum and minimum PEM electrolyzer operating loads, degradation phenomena, and makes hourly decisions regarding the electrolyzer operation load, partial-load efficiency, water consumption, and green hydrogen production. Additionally, the tool calculates the equivalent $CO_2$ emissions associated with hydrogen production, considering the carbon intensity of the electricity utilized. This enables the assessment of the environmental impact of various hydrogen production scenarios. Overall, the dynamic techno-economic tool scrutinizes operational strategies of the AEL electrolysis system when interfacing with stochastic RES, aiming to optimize economic, technical, and environmental parameters.

## ACKNOWLEDGEMENT

The authors would like to acknowledge funding received within the framework of the **TRIERES** research project, funded by the Clean Hydrogen Partnership and its members Hydrogen Europe and Hydrogen Europe Research under Grant Agreement No. 101112056 (TRIERES).

# Utilization of Oxygen from water electrolysis for applications in the chemical industry

Kajetan Mühlbock[1], Johannes Völkl[1*]

*[1]Campus Burghausen, Rosenheim Technical University of Applied Sciences, Germany*
**Corresponding author: johannes.voelkl@th-rosenheim.de*

---

Hydrogen is generally considered to be a corner stone for achieving “Zero Emission” targets. This has led to the development of several numbers of Hydrogen strategies of different governments. Based on current studies a European demand of 1,800 TWh Hydrogen in 2050 seems to be possible [1]. For the Chemical industry Hydrogen is not only part of the transition towards sustainable energy supply but also plays a major part in the transition towards sustainable chemical synthesis based on green feedstock. The most important source of Hydrogen is splitting of water, e.g. via water electrolysis (see eq. (1)):

$$2\,H_2O \leftrightharpoons 2H_2 + O_2 \qquad (1)$$

Based on stoichiometry 8 tons of Oxygen are produced for each ton of Hydrogen as by-product. Utilization of this $O_2$ from water electrolysis seems to be an interesting option. In different studies this utilization in medical use, waste water treatment or as gasification agent has been investigated [2,3]. In this work the focus is on the utilization of $O_2$ for applications in the Chemical industry. The technological and economical feasibility of the usage of $O_2$ from different water electrolysis technologies is compared with $O_2$ from cryogenic air separation as the current reference technology. As application routes the production of Ethylene Oxide EO, vinyl acetate monomer VAM and vinyl chloride monomer VCM are selected. These components are important intermediates and are produced on a large scale. It can be shown that based on a scenario of local water electrolysis $O_2$ fits very well with the subsequent processing as it is produced already at a suitable pressure at the required purity. As a synergistic effect selling $O_2$ could also improve production costs of $H_2$ from electrolysis (see Fig. 1).

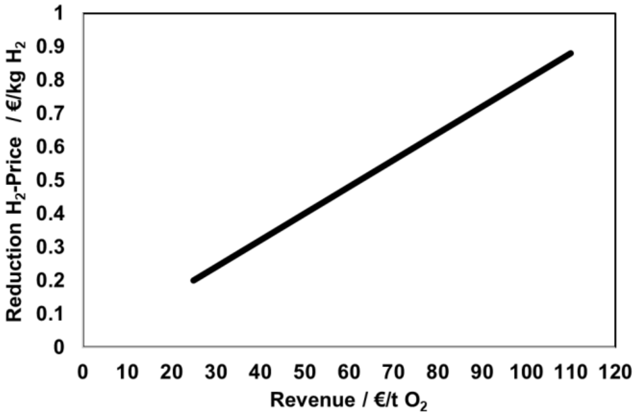


*Figure 1: Influence of $O_2$ revenue on $H_2$ production price from water electrolysis*

## References

[1] T. Fleiter et al., METIS 3, study S5 – The impact of industry transition on a CO2-neutral European energy system, Publications Office of the European Union, 2023.
[2] M. Dossow, D. Klüh, K. Umeki et al., “Electrification of gasification-based biomass-to-X processes – a critical review and in-depth assessment,” *Energy & Environmental Science*, vol. 17, no. 3, 2024.
[3] T. Kato, M. Kubota, N. Kobayashi et al., “Effective utilization of by-product oxygen from electrolysis hydrogen production,” *Energy*, vol. 30, no. 14, 2005.

# Techno-economic and profitability assessment of stand-alone photoelectrochemical hydrogen generation technology

C-T. Yang [1,2]*, D. Adner [2,3], M. Turek [2], C. Hagendorf [2,4], C-N. Chen[1]

*[1] National Taiwan University of Science and Technology, Taipei, Taiwan*
*[2] Fraunhofer Center for Silicon Photovoltaics CSP, Halle, Germany*
*[3] The Martin Luther University of Halle-Wittenberg, Halle, Germany*
*[4] Freiberg Instruments GmbH, Freiberg, Germany*
**Corresponding author: d10618002@mail.ntust.edu.tw*

Hydrogen production from renewable energy sources without $CO_2$ emissions is a major part of emerging hydrogen-based economies. Many countries and regional governments list hydrogen and related technologies as essential national strategies and long-term roadmaps [1]. Worldwide interest in hydrogen technologies lies in their great potential for energy storage and the chemical and materials industry [2]. In addition to a combination of photovoltaics and electrolysis, direct conversion of solar power to hydrogen can be technologically realized through photoelectrochemical water splitting [3,4], which is not currently commercialized.

In order to bridge the gap and provide practical insights to stakeholders and policymakers, this study presents a financial feasibility analysis of stand-alone photoelectrochemical reactors in Germany. A detailed cost structure of the photoelectrochemical reactor is carried out. The total cost of photoelectrochemical reactor with 500 $cm^2$ active area is around 94.2 € based on real-world data. The levelized cost of hydrogen for the off-grid photoelectrochemical in Munich is calculated to be 83.71 €/kg, with a solar-to-hydrogen efficiency of 5%. Policymakers and investors are interested in the financial feasibility of PEC systems under different financial and technological conditions. The sensitivity analysis shows that the two most sensitive factors are hydrogen production, which is affected by solar-to-hydrogen efficiency and solar irradiance, and lifetime. We propose potentially feasible scenarios to reach the 2 €/kg target cost in upscaling production. Increasing lifetime to 20 years, improving solar-to-hydrogen efficiency to 20%, reducing initial capital expenditure by approximately 80%, and financing favorably, either 10% or 5% of weighted average cost of capital, can result in achieving target levelized cost of hydrogen.

## References

[1] IEA Global Hydrogen Review 2023; IEA, 2023
[2] Fuel Cells; Hydrogen Joint Undertaking “Hydrogen Roadmap Europe: A Sustainable Pathway for the European Energy Transition.” 2019.
[3] S. Kirner, P. Bogdanoff, B. Stannowski et al., “Architectures for Scalable Integrated Photo Driven Catalytic Devices-A Concept Study.” Int. J. Hydrogen Energy, 41, 20823–20831, 2016.
[4] T.J. Jacobsson, V. Fjällström, M. Edoff et al., “CIGS Based Devices for Solar Hydrogen Production Spanning from PEC-Cells to PV-Electrolyzers: A Comparison of Efficiency, Stability and Device Topology.” Sol. Energy Mater. Sol. Cells, 134, 185–193, 2015.

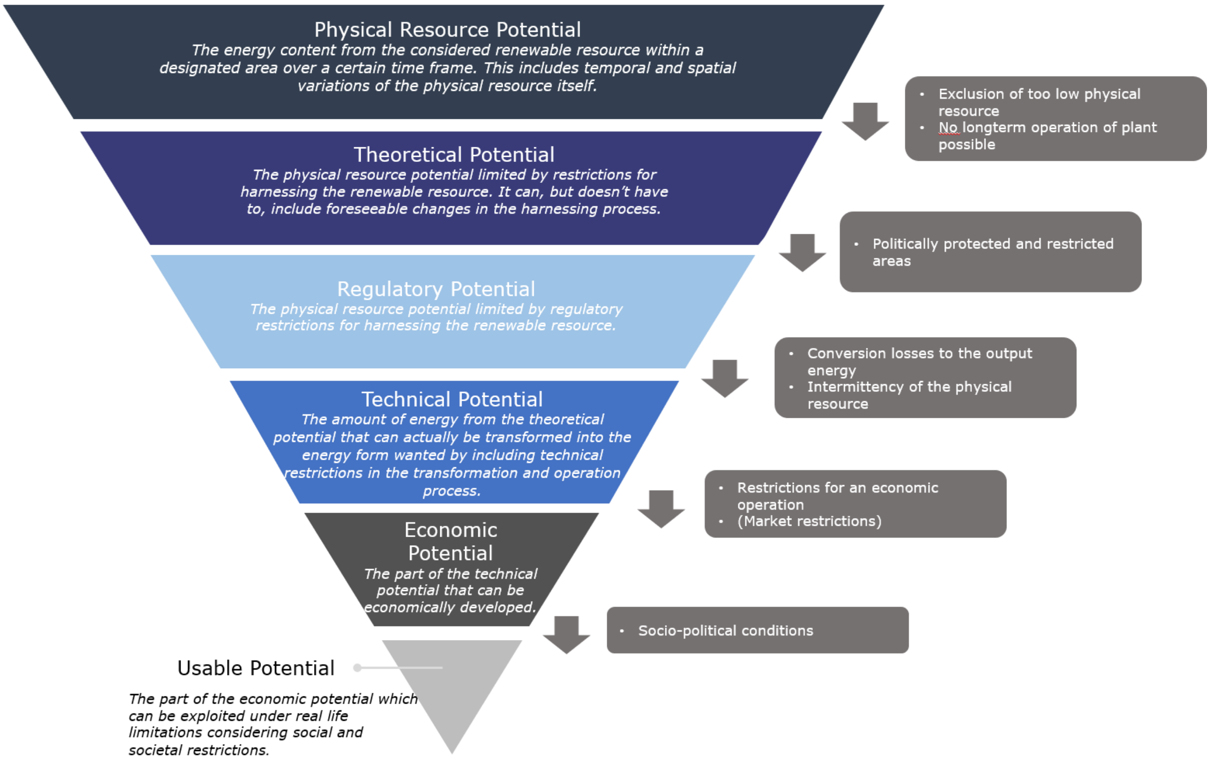
# Novel Definition of Renewable Energy and Sustainable Hydrogen Potential

Alina Kerschbaum[1]*, Lennart Trentmann[1], Andreas Hanel[1], Sebastian Fendt[1], Benedikt Schweiger[1], Hartmut Spliethoff[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University of Munich, Germany*
**Corresponding author: alina.kerschbaum@tum.de*

Energy system analysis is an important tool to evaluate the influence of increasing shares of renewable energy and sustainable hydrogen for an energy system. One vital input parameter in this context is the potential of each technology. The process of potential determination is called potential analysis and can be conducted through a variety of methods.

However, before a comparison of different potential methods is possible, there should be agreement on the definition of different types of potential (theoretical, technical, economic, usable,…). It was found that across technologies but also within a certain one, oftentimes there is either no definition of the potential given at all or it is poorly defined. On top of that, it was found that one term can have different meanings which can lead to confusion.



Physical Resource Potential
*The energy content from the considered renewable resource within a designated area over a certain time frame. This includes temporal and spatial variations of the physical resource itself.*

- Exclusion of too low physical resource
- No longterm operation of plant possible

Theoretical Potential
*The physical resource potential limited by restrictions for harnessing the renewable resource. It can, but doesn't have to, include foreseeable changes in the harnessing process.*

- Politically protected and restricted areas

Regulatory Potential
*The physical resource potential limited by regulatory restrictions for harnessing the renewable resource.*

- Conversion losses to the output energy
- Intermittency of the physical resource

Technical Potential
*The amount of energy from the theoretical potential that can actually be transformed into the energy form wanted by including technical restrictions in the transformation and operation process.*

- Restrictions for an economic operation
- (Market restrictions)

Economic Potential
*The part of the technical potential that can be economically developed.*

- Socio-political conditions

Usable Potential
*The part of the economic potential which can be exploited under real life limitations considering social and societal restrictions.*

*Figure 1: Overview of different potentials based on [1,2] and completed with novel regulatory potential*

In order to address this problem, a new technology-wide definition of different types of potentials is proposed. It is differentiated between a physical resource, a theoretical, a regulatory, a technical, an economic, and a usable one as seen in Figure 1. The introduction of a regulatory potential is novel and is based on the goal in mind of identifying key reasons for restrictions in the potential. This definition also leads to a better understanding of impediments to growing the share of renewables and sustainable hydrogen production while helping to inform policymakers about the implications of their decisions.

In conclusion, the proposed definitions facilitate the understanding of both scientists and other stakeholders, such as policymakers, in the definition of renewable energy and sustainable hydrogen potentials. It also enables better comparison of the potentials and thereby decreases the uncertainty in the potential estimation process.

### References

[1] M. Kaltschmitt, Energy from Organic Materials (Biomass), New York, Springer New York, 2019

[2] L. Rybach, Classification of geothermal resources by potential, Geothermal Energy Science, 3(1), 13-17, 2015

# Chemelot Integrated Model System “CIMS”

Céline Fellay[1]*, Zowi Maijer[1], Geert Cremers[1], Paul Schouten[2], Puck Wammes[2]

*[1] Brightsite Center, Brightlands Chemelot Campus, The Netherlands*
*[2] TNO (Netherlands Organisation for applied scientific research), The Netherlands*
**Corresponding author: celine.fellay@sitech.nl*

---

The mission of Brightsite [1], founded by Brightlands Chemelot Campus, Maastricht University, TNO and Sitech Services, is 2-fold: demonstrate that climate goals can be reached at Chemelot Industrial Site and educate the next generation of scientists, researchers, engineers and coworkers. Chemelot is an integrated chemical site located in the south of the Netherlands where 60 highly integrated and interconnected plants produce >7,5 million tons of products per year. Among other topics, Brightsite is looking into transition scenarios and system integration to support the mission for Chemelot and the chemical industry in general. New methods, models and analyses are being developed to evaluate transition pathways towards a climate neutral system, based on starting points and assumptions. These tools allow for a transparent, fact- and science based integral assessment of the complex transition which the chemical industry is facing. Insights from the model results can support decision and policy making for companies and governments.

The Chemelot Integrated Model System (CIMS) is one of the modelling tool developed within Brightsite (Figure 1). Consider a set of chemical processes, whether it is a chemical production site, a chemical cluster or a region. If one takes a step back as an observer the collection of processes can be seen as an integrated system. Following this approach the different aspects that influence and affect the systems can be collected and studied. CIMS is based on such a holistic view to parameterize the factors relevant for chemical industry and uses a mathematical model to study this system. This allows one to objectively study the private, political and generic (public) societal aspects which are inherent to the transition the chemical industry is facing.

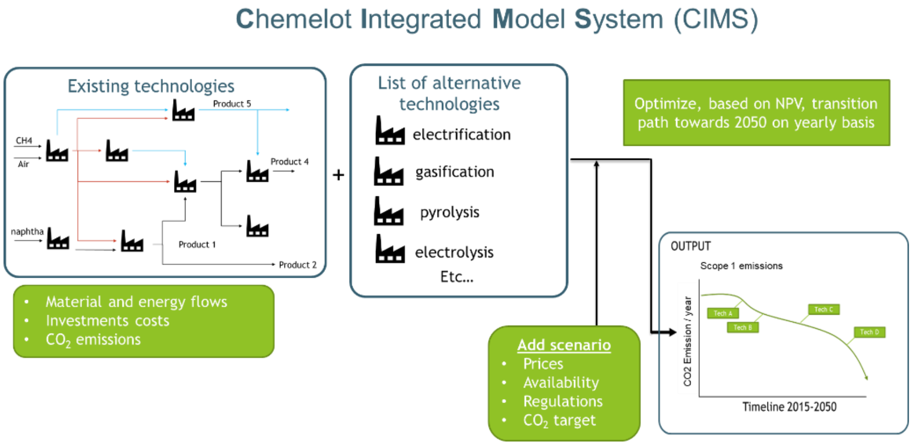


*Figure 1: Schematic view of the Chemelot Integrated Model System CIMS*

The CIMS model identifies the optimal investment trajectory (called transition path) in producing assets as a function of imposed changing external circumstances. The model utilizes a so-called Mixed-Integer-Linear-Programming algorithm to find the optimum. It has been built and developed based on the Chemelot configuration but is applicable generically to other chemical sites.

CIMS is designed to answer the following questions:
'Given an assumed, parameterized set of available alternative energy, raw materials and technologies in time: how, between now and 2050, can a defined product package best be manufactured that must gradually become greener and whose fossil emissions must gradually decrease to net-zero in 2050? Which technologies should be used for this purpose, when, and with what quantities of energy and raw materials? What are the consequences when energy, raw materials or technologies are not available?‘
Examples of results obtained with CIMS will be presented.

## References

[1] Home - Brightsite (brightsitecenter.com)

# Few layer $MoS_2$ as a catalyst for the hydrodeoxygenation of fatty acids to alkanes

Fuli Deng[1], Ruixue Zhao[1,*], Johannes A. Lercher[1,2,*]

[1] *Department of Chemistry and Catalysis Research Center, School of Natural Sciences, Technical University of Munich, 85747 Garching, Germany*
[2] *Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA 99352, United States*
**Corresponding author: ruixue.zhao@tum.de, johannes.lercher@ch.tum.de*

---

## Introduction

The production of long-chain alkanes from renewable biomass instead of fossil resources is very attractive and important for sustainable energy and chemical supply. Long-chain alkanes are vital in transportation fuels, making their sustainable production of utmost significance. In this context, bio-derived fatty acids emerge as promising alternatives. To facilitate this transformation, transition metal sulfide (TMS) materials stand out as the catalyst of choice for the defunctionalization process[1]. However, these TMS catalysts are susceptible to instability, primarily due to sulfur loss in the face of harsh operational conditions. Without sulfur compensation from an external source, the catalyst's contamination and eventual deactivation become inevitable[2,3.] This work reports the development of an efficient unsupported $MoS_2$ catalyst designed for the hydrodeoxygenation of stearic acid into long-chain alkanes. This $MoS_2$ catalyst is facilely synthesized, offering high activity and stability.

## Materials and Methods

Two-dimensional molybdenum disulfide (2D-$MoS_2$) materials were synthesized using hydrothermal techniques. The catalytic hydrodeoxygenation of stearic acid was conducted within a high-pressure stainless-steel autoclave (300 mL) equipped with a mechanical stirrer and a heating jacket. During the reaction, in situ sampling was carried out by extracting 1 mL of reaction liquid through a sampling tube fitted with a filter. The resulting products were analyzed using gas chromatography-mass spectrometry (GC-MS). Furthermore, the physical and chemical properties of the catalysts were comprehensively characterized through $N_2$ adsorption, TEM, XRD, and XAS.

## Results and Discussion

The depicted reaction network on Few-layer $MoS_2$ in **Fig. 1a** reveals that the deoxygenation of stearic acid on $MoS_2$ mainly follows an HDO pathway, exhibiting a 97% selectivity for octadecane. Additionally, carbon loss reaction pathways produce a minor amount of heptadecane (3%).

Stearic acid undergoes an identical reaction pathway on both Rod-$MoS_2$ and Bulk-$MoS_2$. However, in comparison to the high initial rate of stearic acid consumption observed on Few layer-$MoS_2$ (182 $mmol_{SA}$ $g_{Cat.}^{-1}h^{-1}$), the conversion rates on Rod-$MoS_2$ and Bulk-$MoS_2$ are significantly lower (19 and 13 $mmol_{SA}$ $g_{Cat.}^{-1}h^{-1}$, respectively) (**Fig. 1b**). This superior catalytic performance is attributed to the richer vacancies on $MoS_2$ with lower stacking degree[4,5]. Furthermore, it exhibits remarkable stability with no apparent deactivation after 10 cycles of reactions (**Fig. 1c)**. The stearic acid consumption rates and octadecane selectivity remain stable. Characterization results confirmed no noticeable structure change or sulfur loss from the $MoS_2$.

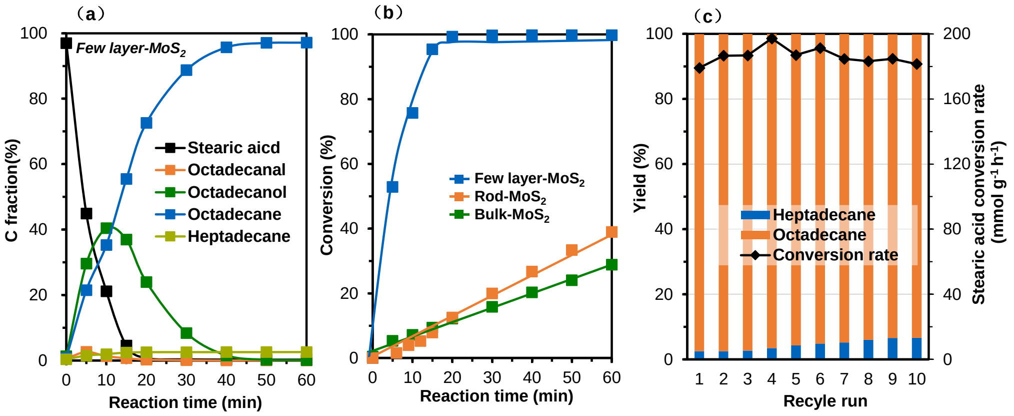


*Figure 1: (a) Conversion of stearic acid vs. reaction time on three types $MoS_2$ catalysts, (b) Carbon fraction of stearic acid and products vs. reaction time on few-layer $MoS_2$, (c) Stability test of few-layer $MoS_2$ (Reaction condition: 50 mg catalyst, 5 MPa $H_2$ at 300 °C, 20 mM stearic acid, decalin as the solvent.)*

## Conclusion

The Few-layer $MoS_2$ catalyst described exhibits exceptional catalytic performance since it is active, selective, and stable for the conversion of fatty acid to alkanes in hydrogen, revealing the promising prospects of unsupported transition metal sulfide materials in catalysis and could inspire the development of innovative catalysts for the highly efficient upgrading of bio-derived chemicals.

## References

[1] Douglas C. Elliott," Historical developments in hydroprocessing bio-oils," Energy and Fuels, vol. 21, 1792–1815, 2007.

[2] Majid. Saidi, Bruce. C. Gates, and Mohammad Reza Rahimpour et al., " Upgrading of lignin-derived bio-oils by catalytic hydrodeoxygenation," ' Energy and Environmental Science, vol 7, 103–129, 2014.

[3] Daniel A. Ruddy, Jesse E. Hensley et al., " Recent advances in heterogeneous catalysts for bio-oil upgrading via "ex-situ catalytic fast pyrolysis": Catalyst development through the study of model compounds" Green Chemistry, vol 16, 454–490, 2014.

[4] Hemamala I. Karunadasa, Christopher J. Chang et al., Science, vol 335, 698–702, 2012.

[5] Guoliang Liu, Shik Chi Edman, Tsang et al., "$MoS_2$ monolayer catalyst doped with isolated Co atoms for the hydrodeoxygenation reaction," Nature Chemistry, Vol 9(8), 810-816, 2017.

# Investigations on Ce-doping of NiAlO$_x$ Catalysts for CO$_2$ Methanation

Heike Plendl[1,2]*, Tim Kratky[1,2], Sebastian Günther[1,2] and Olaf Hinrichsen[1,2]

*[1]Technical University of Munich, School of Natural Sciences, Lichtenbergstraße 4, D-85748 Garching near Munich, Germany*
*[2]Technical University of Munich, Catalysis Research Center, Ernst-Otto-Fischer-Straße 1, D-85748 Garching near Munich, Germany*
**Corresponding author: heike.plendl@tum.de*

---

Concerning global warming and increasing energy demand, the topic of renewable energies is becoming more important than ever before. [1] Since these sources cannot provide the energy continuously, ways must be found to store the energy effectively. The so-called power-to-gas (PtG) concept offers a much-discussed possibility for this. Here, the energy that comes from renewable sources is converted into hydrogen using water electrolysis. The hydrogen is then converted into methane together with carbon dioxide as part of the methanation reaction (see Fig. 1). [2]

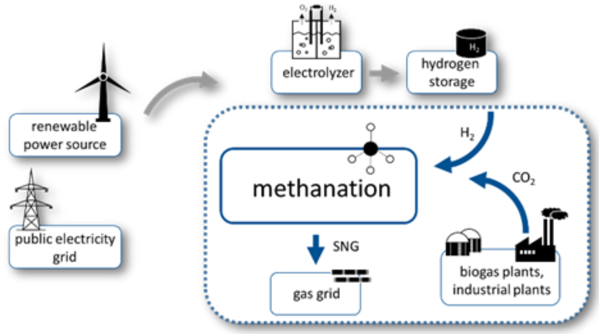


*Figure 1: Methanation in the context of the power-to-gas concept. Adapted from [2].*

NiAlO$_x$ catalysts, which are characterized by high activity and selectivity, have been established to ensure highly efficient methanation. These materials can be further improved by adding CeO$_{2-x}$ which is a popular support material in catalysis, particularly through the formation of highly reactive oxygen vacancies. [3] For this purpose, a series of Ni-Al-Ce catalysts with Ce/Ni ratios between 0.05 - 0.4 were produced by means of coprecipitation, impregnation and mortaring.

Coprecipitation was carried out with 1M Ni$^{2+}$, Al$^{3+}$ and/or Ce$^{3+}$ nitrate solutions at a constant pH of 9, the precipitation reagent was a mixture of 0.5 M NaOH and 0.5 M Na$_2$CO$_3$. The materials were calcined at 450 °C in synthetic air for 5 h and activated in 5% H$_2$ in Ar at 485 °C for 8 h. Impregnation was carried out *via* incipient wetness and wet impregnation of a coprecipitated NiAlO$_x$ sample with the molar ratio Ni/Al = 1/1. Ce$^{3+}$ nitrate solutions in the appropriate concentration were used, calcination was carried out at 450 °C for 5 h in synthetic air. Additionally, a coprecipitated NiAlO$_x$ sample with the molar ratio Ni/Al = 1/1 was ground with appropriate amounts of CeO$_2$. The samples were analyzed using inductively coupled plasma – optical emission spectrometry, X-ray powder diffraction, X-ray photoelectron spectroscopy, N$_2$ physisorption analysis, H$_2$ chemisorption analysis, temperature programmed reduction and transmission electron microscopy. To measure the activity of the samples, 25 mg of each sample with 225 mg of SiC were placed in a 4 mm diameter tubular reactor. Before the actual methanation, the samples were first activated *in situ* at 485 °C for 8 h in 5% H$_2$ in Ar. The CO$_2$ conversion was then measured between 175 °C and 400 °C at 8 bar and 10% CO$_2$ and 40% H$_2$ diluted in Ar at a total flow of 58 sccm. In addition, the samples were measured under differential conditions ($X_{CO2}$ < 15%) at 240 °C and 8 bar to determine the turnover frequencies.

By comparing the co-precipitated and the ground samples, two phases could be determined after co-precipitation using X-Ray diffractometry: A Ni-Al takovite-like phase and a $CeCO_3OH$ phase. After calcination, a NiAl mixed oxide forms alongside a $CeO_2$ phase for all three synthesis methods. After activation in $H_2$, the active species $Ni^0$ is formed alongside residues of unreduced Ni-Al mixed oxide and $Ce^{3+}/Ce^{4+}$ redox couples. Smaller Ce/Ni ratios appear to have a positive effect on the size and dispersion of the nickel particles, as seen by transmission electron microscopy in comparison with pure $NiAlO_x$. Using $H_2$ chemisorption, it was also shown that small Ce proportions lead to larger nickel surfaces and better metal dispersions. Compared to the other two synthesis methods, the co-precipitated samples featured the highest dispersions. Additionally, temperature programmed reduction showed that the addition of Ce leads to a decrease of the reduction temperature. *In-situ* X-ray photoelectron spectroscopy revealed that upon activation in $H_2$, metallic Ni and $Ce^{3+}/Ce^{4+}$ redox couples are formed. Methanation of $CO_2$ showed no visible differences to the freshly activated state. Oxidation and further reduction showed that the process is completely reversible (see Fig. 2). Test reactions under methanation conditions revealed that small Ce/Ni ratios can promote methanation and lead to higher activities.

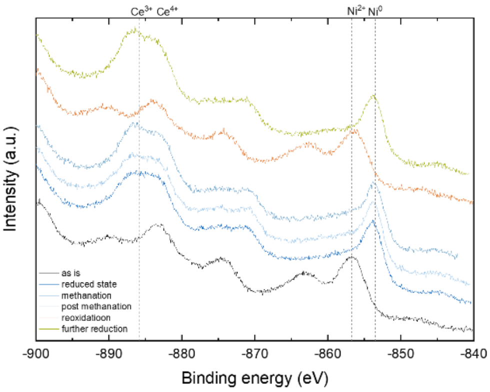


*Figure 2: Quasi in-situ XPS of a coprecipitated sample with a molar Ce/Ni ratio of 0.4.*

The results show that the addition of Ce to $NiAlO_x$ catalysts leads to an improvement in catalytic properties and methanation activity when an optimal Ce/Ni ratio is used. Oxygen vacancies in the cerium oxide most likely play a crucial role here. Further studies should investigate the exact role of the oxygen vacancies and determine to what extent Ce intervenes in the methanation mechanism. Long-term stability tests are also planned.

## References

[1] C. A. Huff, M. S. Sanford, Journal of the American Chemical Society 2011, 133, 18122–18125.
[2] G. Gahleitner, international Journal of Hydrogen Energy 2013, 38, 2039–2061.
[3] C. Yang, Y. Lu, L. Zhang, Z. Kong, T. Yang, L. Tao, Y. Zou, S. Wang, Small Struct. 2021, 2, 2100058.

# Investigating the Influence of Thermal Plasma on Biomass Particles

Johannes Waßmuth[1]*, Jonas Brandstetter[1], Ranjeet Kafle[1], Kentaro Umeki[2], Sebastian Bastek[1], Omar Dacres[1], Andrius Tamošiūnas[3], Sebastian Fendt[1], Hartmut Spliethoff[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
*[2]Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden,*
*[3]Lithuanian Energy Institute, Kaunas, Lithuania*
**Corresponding author: johannes.wassmuth@tum.de*

The utilization of thermal plasma for entrained flow gasification processes is said to produce high-quality syngas with low tars and a high content of hydrogen [1-2]. This is ideal for use in further processes such as Methanol or Fischer-Tropsch synthesis. Since the influence of thermal plasma on biomass particles has not yet been observed, it is of great importance to investigate fundamental phenomena to increase the probability of success for upscaling.

This study examines the influence of thermal plasma on biomass particles, focusing on pyrolysis and gasification processes. Optical as well as solid analysis methods were used to delve into the field of plasma treatment of biomass. For optical analysis, a high-speed camera was employed to capture the rapid particle dynamics and interactions in the environment of thermal plasma (see Figure 1). The plasma treated particles, e.g. plasma char, were collected and analyzed by proximate and ultimate analysis. Furthermore, EDX analysis was performed to determine the composition of the plasma char surface. In addition, the influence on the gasification kinetics was analyzed using thermogravimetric analysis (TGA) combined with surface area determination.

Both pyrolysis and gasification processes can be studied as the plasma system can be operated with either nitrogen or air. The plasma reactor setup is designed to provide direct quenching and inertization after the reaction zone to focus only on the influence of the thermal plasma on the biomass particles. The information obtained will be used to validate and improve plasma entrained flow gasification CFD models and can be used as a guide value for the design of plasma burners for entrained flow gasification processes.

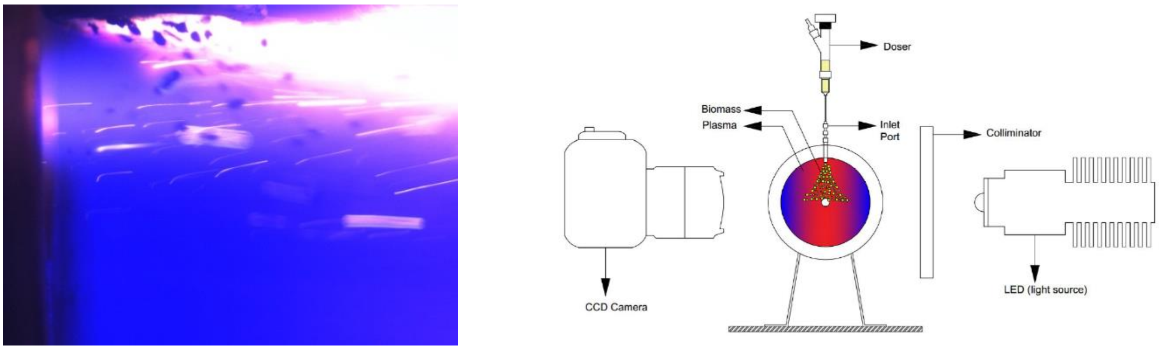


*Figure 1: Biomass particles in contact with thermal nitrogen plasma (left); Schematic of the setup for the optical analysis (right)*

## References

[1] Materazzi, M. et al., Reforming of tars and organic sulphur compounds in a plasma-assisted process for waste gasification, Fuel Processing Technologies, 2015, 137, 259–268.
[2] Mountouris et al., Plasma gasification of sewage sludge: Process development and energy optimization, Energy Conversion and Management, 2008, 49, 2264–2271.

# Experimental Comparison of Plasma-Assisted Entrained Flow Gasification and Conventional Entrained Flow Gasification in a Pilot-Scale Gasifier

Jonas Brandstetter1*, Johannes Waßmuth1, Philipp Leuter1, Sebastian Bastek1, Sebastian Fendt1, Hartmut Spliethoff1

[1]*Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: jonas.brandstetter@tum.de*

---

Entrained flow gasification has gained prominence as an advanced technology for converting carbonaceous feedstocks such as coal and biomass into valuable syngas, which can be used energetically or for the synthesis of chemicals. In recent years, there has been a shift in the feedstock for gasification – from coal through biomass to residues. This has resulted in a deterioration of fuel properties. Simultaneously, there is an increasing demand for syngas quality as the focus moves away from energetic use towards utilization for syntheses. Introducing plasma into the gasification process is one way to align with these contradictory trends. It provides an external heat source, enhancing the independence of the reactor temperature from the feedstock characteristics. However, the advantage comes at the cost of higher energy demands [1].

This paper presents a comparative analysis of conventional and plasma-assisted entrained flow gasification. The study aims to evaluate the performance and efficiency of these two processes to further investigate the advantages and disadvantages of plasma integration. Critical operational parameters such as carbon conversion, wall temperatures, main and trace components, and tar formation are studied for that.

The experiments were conducted using an industrial-like pilot-scale SIEMENS-type gasifier with a fuel power of around 100 kW [2]. Torrefied non-debarked mixed wood is used for the experiments. It is fed into the gasifier with a pneumatic conveying system. Oxygen was used as the gasification agent for conventional gasification, with steam added as a moderator. The gasifier is retrofitted with a 50 kW plasma torch by changing the burner of the reactor. Steam is used as a plasma gas flowing coaxially with the feedstock. Furthermore, oxygen is added as a gasification agent around the burner mouth to ensure a specific lambda.

This research contributes valuable insights into the potential benefits and challenges of adopting plasma-assisted entrained flow gasification, offering a foundation for future developments in sustainable and efficient gasification technologies. The findings aim to inform decision-makers and researchers in pursuing cleaner and more effective routes for producing syngas from carbonaceous feedstocks.

## References

[1] V. Subramanyam, A. Gorodetsky, “Municipal wastes and other potential fuels for use in IGCC Systems”, ”Integrated Gasification Combined Cycle Technologies”, 2017.
[2] L. Briesemeister, M. Kremling, et al., “Air-Blown Entrained-Flow Gasification of Biomass: Influence of Operating Conditions on Tar Generation” Power Generation from Solid Fuels”, Energy Fuels, vol. 31, 2017.

# Dynamic Operation and Optimization of a Containerized Pilot Plant for $CO_2$-Based Methanol Production

Lukas Anthofer*, Theresa Hauth[1], Vincent Dieterich[1], Sebastian Fendt[1], Hartmut Spliethoff[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: lukas.anthofer@tum.de*

---

$CO_2$-derived methanol serves as a promising energy carrier and chemical precursor, offering opportunities for both $CO_2$ utilization and energy storage. Achieving dynamic operation in methanol production is crucial for rapid response to fluctuating renewable energy inputs and varying $CO_2$ capture rates. This research aims to enhance process dynamics through the development of a containerized pilot plant, enabling in-depth investigations into startup/shutdown sequences and load transitions. [1]

In the container plant, a proton exchange membrane (PEM) electrolyzer is employed to supply hydrogen, chosen for its rapid response capabilities to load variation. [2] $CO_2$ is supplied by an amine wash that captures the carbon dioxide of the flue gas of an incineration plant. Due to limited conversion a recycle is essential for the process. [3] Control strategies are devised to modulate critical process parameters, including the recycle-to-feed ratio, gas hourly space velocity, and stoichiometric ratios.

Optimization efforts focus on identifying economically viable operational strategies based on electricity prices. Scenarios include full-load operation under optimal conditions, partial load operation, exclusive hydrogen production for commercial sale, or temporary shutdown of the methanol production unit with $CO_2$ sales from the carbon capture system.

Initial optimization will target the existing pilot plant, followed by process simulations to determine threshold electricity prices for optimal operation. Finally, optimization strategies will be applied to scale up the process for the complete conversion of $CO_2$ emissions from a chemical plant's residual combustion into methanol.

This study contributes to advancing sustainable methanol production technologies, providing insights into dynamic operation and optimization strategies essential for commercial viability.

## References

[1] F. Schorn, J. L. Breuer, R. C. Samsun et al., “Methanol as a renewable energy carrier: An assessment of production and transportation costs for selected global locations,” *Advances in Applied Energy*, vol. 3, p. 100050, 2021.

[2] H. Lange, A. Klose, W. Lippmann et al., “Technical evaluation of the flexibility of water electrolysis systems to increase energy flexibility: A review,” *International Journal of Hydrogen Energy*, vol. 48, no. 42, pp. 15771–15783, 2023.

[3] V. Dieterich, N. Wein, H. Spliethoff et al., “Performance Requirements of Membrane Reactors for the Application in Renewable Methanol Synthesis: A Techno-Economic Assessment,” *Advanced Sustainable Systems*, vol. 6, no. 12, 2022.

# Facilitation of Machine Learning Methods for Waste Plastic Pyrolysis

Lukas Martetschläger[1]*, Simon Meilinger[1], Darius Junginger[1], Sebastian Fendt[1], Hartmut Spliethoff[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: lukas.martetschlaeger@tum.de*

---

The pressing environmental challenges posed by increasing mixed plastic waste necessitate the development of efficient recycling technologies. Pyrolysis presents a viable solution for advancing the circular economy, particularly by closing the carbon cycle through the conversion of plastic waste into valuable oils that can be reused as feedstock for the chemical industry. However, despite several experiments with varying parameters, accurately predicting liquid yields remains challenging, underscoring the need for improved models.

In this study, we apply machine learning techniques to predict liquid yield in plastic pyrolysis processes. Utilizing a combined dataset from two published pyrolysis databases [1,2], we evaluate four machine learning models: Decision Trees (Random Forest and eXtreme Gradient Boosting), Support Vector Machines, Gaussian Processes, and Artificial Neural Networks. After data processing, the database contains entries with information about process parameters (e.g., temperature, heating rate) and feedstock properties (e.g., plastic blend composition, particle size).

Trained and optimized models were compared with each other and benchmarked against base models for assessment. The mean absolute error of the Decision Tree algorithm on the test-split is lower compared to the baseline K-Nearest Neighbors model yielding and the other machine learning models. Figure 1 illustrates the parity plots and SHapley Additive exPlanations (SHAP) summary plots generated by the best-performing algorithm, Decision Tree with eXtreme Gradient Boosting.

The comprehensive evaluation reveals that despite reports of high performance, these models often fail to generalize to unseen data, thus limiting their practical applicability. Future research focuses on evaluating model applicability within narrowly defined domains and revisiting model suitability with more extensive and accurate pyrolysis data, including solid and non-condensable components to close the mass balance. Enhanced predictability can lead to a better understanding of economic feasibility, facilitating advancements in chemical recycling technologies.

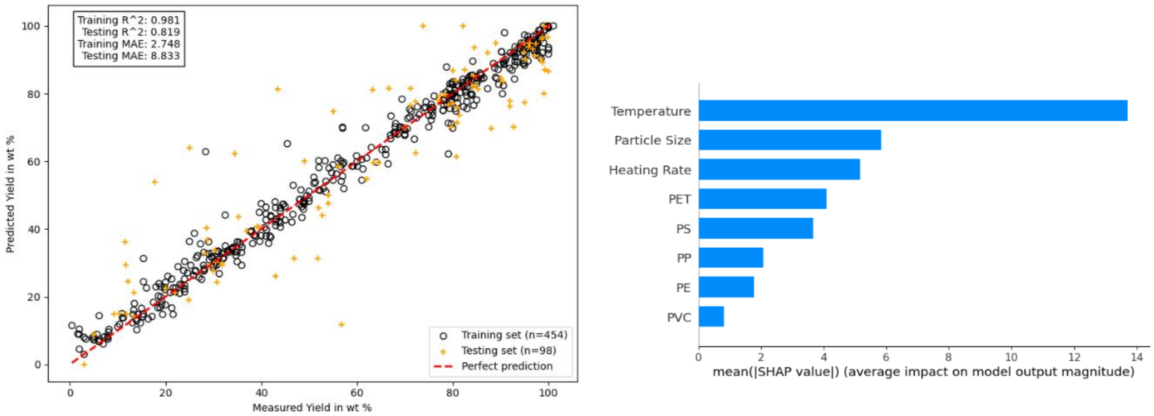


*Figure 1: Result of the Decision Tree with eXtreme Gradient Boosting algorithm, (l) parity plot and (r) SHapley Additive exPlanations (SHAP) summary plot*

**References**:

[1] Y. Cheng, et al. “Applied machine learning for prediction of waste plastic pyrolysis towards valuable fuel and chemicals production”, Journal of Analytical and Applied Pyrolysis, doi: 10.1016/j.jaap.2023.105857.
[2] E. Belden, et al. ”Machine learning predictions of oil yields obtained by plastic pyrolysis and application to thermodynamic analysis.” ACS Engineering Au, doi: 10.1021/acsengineeringau.2c00038

# Biomass-to-Liquid Opportunities: Sustainable Aviation Fuel from Australia's Sugar Industry

Marcel Dossow[1]*, Weiss Naim[2], Vahid Shadravan[2], Hartmut Spliethoff1, Sebastian Fendt[1]

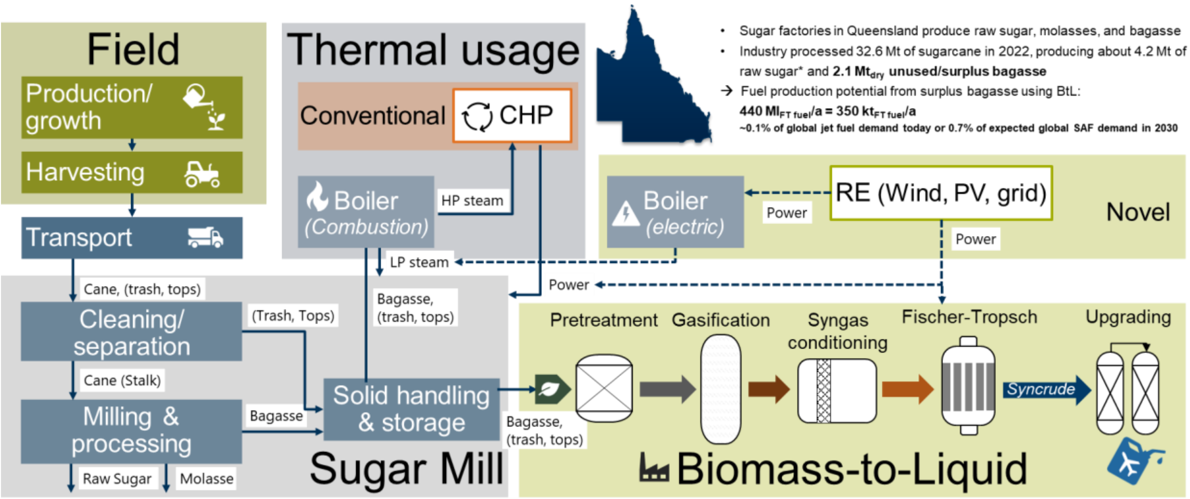
*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
*[2]Commonwealth Scientific and Industrial Research Organisation (CSIRO) Energy, 1 Technology Court, Pullenvale QLD 4069, Brisbane, Australia*
**Corresponding author: marcel.dossow@tum.de*

---

Sustainable Aviation Fuel (SAF) is ready to play a key role in decarbonizing the global aviation industry by reducing emissions while maintaining todays aircrafts and infrastructure. Australia has the opportunity to establish a domestic SAF industry, building on its existing industries and infrastructure to utilize a variety of biomass resources, such as sugarcane bagasse, and other renewable waste streams. Producing SAF from bagasse offers a way to integrate current sugar industry operations with the growing demand for drop-in fuels, providing a stable market and supporting the diversification of the sugar industry. A local SAF industry would also help reduce Australia's reliance on fossil fuel imports while contributing to its renewable energy and emissions reduction goals.

Among the various SAF production pathways, gasification-based thermochemical Biomass-to-Liquids (BtL) processes are particularly promising for the efficient use of surplus bagasse in Australia, thanks to their technological readiness and scalability. Leveraging existing infrastructure and refining technologies could facilitate the large-scale adoption of BtL processes within the sugar industry, enabling a transition of current supply chains and fostering economic diversification and a renewable fuels sector.

Since bagasse recovery and transport costs significantly affect the viability of BtL plants, special attention is required for optimizing the supply chain in the sugar industry. As Figure 1 shows how today's sugar mill operation is based on the thermal use of bagasse and other residues, and how an alternative process, based on BtL and renewable electricity could be integrated. To allow efficient logistics, BtL facilities must be strategically located near the biomass sources. While biomass residues are often concentrated in rural and regional areas, the sugar industry offers a localized and plentiful source of lignocellulosic biomass for BtL applications.



- Sugar factories in Queensland produce raw sugar, molasses, and bagasse
- Industry processed 32.6 Mt of sugarcane in 2022, producing about 4.2 Mt of raw sugar* and **2.1 $Mt_{dry}$ unused/surplus bagasse**

→ Fuel production potential from surplus bagasse using BtL:
**440 $Ml_{FT\ fuel}$/a = 350 $kt_{FT\ fuel}$/a**
**~0.1% of global jet fuel demand today or 0.7% of expected global SAF demand in 2030**

*Figure 1: Simplified sugar processing flow diagram from field to raw sugar including the conventional and proposed use of bagasse, trash, and tops in a novel Biomass-to-Liquid (BtL) process*

Not all Australian sugar mills produce sufficient bagasse to reach the economies of scale required for commercially viable BtL application. However, an initial analysis shows that larger mills in Queensland could independently support a gasification plant with a capacity of 60-130 $MW_{th}$, using only the surplus bagasse currently available. For smaller mills, a more centralized approach would be necessary, with up to five mills supplying a single gasifier, resulting in transport distances for feedstock in the range of

100-200 km. Estimates suggest that converting all available 2.1 Mt/a of surplus bagasse in Australia into Fischer-Tropsch (FT) syncrude could yield approximately 440 million liters of syncrude annually. Changes in mill operations or harvesting practices could further unlock additional quantities of bagasse, while incorporating sugarcane trash and tops could boost that capacity to about 1 billion liters per year. Economically, the estimates suggest that transportation distances below 200 km would be viable, with gasifier sizes ranging from 100-255 $MW_{th}$ potentially offering a 10-15% cost advantage over previous projections.

In summary, the Australian sugar industry has significant potential to produce SAF on an industrial scale via the proposed BtL process, supporting national goals for fuel security, industry diversification, and renewable energy. The key engineering challenges remaining in the BtL pathways primarily relate to the Biomass-to-Syngas conversion stages. Managing impurities in the syngas and adapting technologies to the unique characteristics of the sugar industry's residues are critical, though syngas cleaning and processing technologies are well-developed in other industries and could be adapted for this purpose.

# Structural Optimization of an ideal Chemical Park towards $CO_2$ Neutrality

Maximilian Kerschbaum[1]*, Sebastian Fendt[1], Hartmut Spliethoff[1]

[1]*Chair of Energy Systems, TUM School of Engineering and Design, Technical University of Munich, Germany*
**Corresponding author: maximilian.kerschbaum@tum.de*

Many processes in the chemical industry are fossil-based and require a reliable heat and power supply. Thus, the transformation towards $CO_2$ neutrality is a great challenge. Synthetic energy carriers, direct electrification, and various storage technologies could pave the way to a climate-neutral chemical industry [1]. Energy system optimization plays a crucial role in identifying economic transformation pathways towards $CO_2$ neutrality. Here, the linear programming (LP) open-source software PyPSA (Python for Power System Analysis) [2] is used to implement a model of an ideal chemical park. The initial build-up and demand profiles of the ideal chemical park were adapted from previous publications [3]. Various technologies, such as direct electrification, synthetic fuels, biomass, and fossil-based energy carriers, are considered. In addition, storage systems and direct investment in renewables are also integrated. The ideal chemical park is structurally optimized following a greenfield approach for two key years, 2019 as a reference and 2045, with an hourly resolution. Both years' technical and economic data was taken from the DEA technology database [4]. Except for electricity prices, carrier prices are assumed constant each year.

Our results show that power-to-heat technologies such as electrode boilers can already be integrated in 2019 to benefit from temporal low electricity costs. High-temperature heat pumps are not considered for 2019 since the required sink temperature is assumed to remain infeasible until 2030 [5]. The reference model also consists of a fossil-based CHP and two gas boilers, which fit the general build-up of today's chemical parks [3]. On the other hand, we find that our initially assumed $CO_2$ price of 150 €/$t_{CO_2}$ in 2045 does not lead to a $CO_2$-neutral system. However, wind and PV and short- and long-term energy storage systems are expanded until their maximum allowed potential. Fossil-based CHP and electricity storage are integrated into the system to make it more independent of high temporal electricity prices. The main contributors to a forced $CO_2$-neutral energy system are high-temperature heat pumps for low-pressure demand and electrode and hydrogen boilers for high-pressure demand. With this, hydrogen boilers are mainly used for peak shaving in the summer and contribute to the base load in the winter season. In addition, lithium-ion batteries and PEM electrolyzers combined with hydrogen storage tanks are expanded until their maximum allowed potential to benefit from frequently low electricity prices. The total energy demand of the $CO_2$-neutral accounts for 80.6 % of the 2019 reference energy system. This underlines the higher total efficiency of electrified heat generation.

## References

[1] Kochenburger, Thomas, et al. "Fine chemicals production in a carbon-neutral economy: the role of electrification." Chemical Engineering 40 (2023): 100904.
[2] T. Brown, J. Hörsch, D. Schlachtberger, "PyPSA: Python for Power System Analysis", Journal of Open Research Software (2018), DOI:10.5334/jors.188.
[3] Bauer, Thomas, et al. "Ideal-Typical Utility Infrastructure at Chemical Sites – Definition, Operation and Defossilization." Chemie Ingenieur Technik 94.6 (2022): 840-851.
[4] Danish Energy Agency. Energinet. Technology data: Technology Data for Industrial Process Heat. https://ens.dk/en/our-services/technology-catalogues/technology-data-industrial-process-heat. [Accessed August 2024].
[5] Neusel, Lisa, Simon Hirzel, and Matthias Rehfeldt. "Still alive, but different in the future? Decarbonisation of industrial steam boilers from a multi-dimensional perspective." (2022).

# CFD Modeling of Plasma-Assisted Entrained Flow Gasification

Sebastian Wilhelm[1]*, Sebastian Bastek[1], Dr. Sebastian Fendt[1], Prof. Hartmut Spliethoff[1]

[1] *Chair of Energy Systems, TUM School of Engineering and Design, Technical University of Munich, Germany*
**Corresponding author: sebastian.g.wilhelm@tum.de*

---

CFD modeling is an essential tool in designing entrained flow gasification reactors for solid fuels. At the Chair of Energy Systems, a detailed entrained flow gasification model is developed based on the CFD-software ANSYS Fluent. The two-phase gas-solid flow is described with a coupled Eulerian-Lagrangian approach. This work investigates the integration of a plasma torch in the simulation model.

In the conventional gasification process, the necessary process energy is supplied by partial oxidation of the feedstock with oxygen or air. Adding an electric plasma torch in the rector as an energy supply is seen as an attractive alternative, especially at times when there is excess electricity production by renewable energy sources. With this allothermal plasma gasification, syngas yield and composition, as well as fuel conversion, can be improved. Within this work, the integration of plasma gasification in the existing gasification model is investigated. To keep the modeling complexity manageable, the effect of the ionization of the plasma gas on reaction kinetics is neglected.

Within the first approach, a hot gas stream represents the plasma gas coming out of the torch. The outlet of the plasma torch is depicted by an inlet boundary condition in the model. With this relatively simple approach, a first estimation of the effect of plasma gasification on the conversion behavior and the overall gasification process is provided.

First simulations are carried out on a model of the pilot-scale reactor BOOSTER located at the Chair of Energy Systems, which is currently under construction, to add a plasma torch to this reactor for an experimental investigation of the plasma gasification process. Results from these experiments will act as validation data in the future.

The simulation results for both pilot-scale and industrial-scale reactor models reveal similar trends. In the case of steam plasma gasification, there is a significant improvement in the hydrogen content of the syngas compared to conventional gasification processes. However, a major challenge identified in both plasma cases is the reduced char burnout, as conversion rates decrease significantly. The primary reasons for this include shorter particle residence times, mainly due to the high gas velocities in plasma torches, and the lower availability of gasifying agents needed for heterogeneous char reactions in many regions of the reactor.

Based on these findings, design optimizations of the industrial-scale reactor are being carried out to enhance the overall process performance, focusing on improving char conversion rates under plasma conditions. Sensitivity studies support that the modeling approach is practical in providing insights into the conversion behavior of biogenic feedstocks under plasma gasification conditions.

# Waste-to-X: Two-Step Process for Thermochemical Recycling of Municipal Solid Waste and its Characterization

Simon Meilinger[1*], Lukas Martetschläger[1], Matias Fierro Rivas[1], Sebastian Bastek[1], Matthias Gaderer[2]
Hartmut Spliethoff[1], Sebastian Fendt[1]

*[1]Chair of Energy Systems, Technical University of Munich, Germany,*
*[2]Regenerative Energy Systems, Technical University of Munich, Germany*
**Corresponding author: simon.meilinger@tum.de*

In 2018, roughly 11 million tons of municipal solid waste (MSW) was produced in German households (residual waste only), leading to one of the highest specific waste production rates of 128 kg/capita in Europe. In theory however, only 33 wt-% of this waste stream needs to be incinerated (e.g., sanitary products), while the great majority (67 wt-%) consists of recyclable components (e.g., organics (39 wt-%) and plastics (12 wt-%)).

Especially for central European countries with high resource exploitation, material recycling is essential on the way to a complete circular economy. While current recycling technologies mostly focus on mechanical recycling of homogeneous streams such as plastic or paper waste, heterogeneous municipal solid waste (MSW) is typically incinerated without recycling carbon-based compounds to substitute fossil carbon sources.

To address this task, alternative (thermo)chemical recycling technologies are necessary, converting MSW and other difficult carbon-containing feedstocks into valuable input materials for the chemical industry. Our proposed technology embraces a high-temperature rotary kiln pyrolysis reactor followed by a plasma-assisted gasification. The produced high-calorific syngas with low tar content and increased H2/CO ratio can ultimately be refined into methanol or Fischer-Tropsch syncrude. This two-stage approach enables high carbon conversion and cold gas efficiencies together with low CO2 emissions.

The detail engineering of the plant is still ongoing and requires a profound feedstock screening. Consequently, the purpose of this research is to perform a comprehensive characterization of the MSW (residual waste only) in Munich (> 1.5 million residents) considering it as a potent input stream yet impaired by limited data available. It was carried out to shed light on the complex composition and differences in three social strata (suburban areas, dense residential areas, and residential - commercial area). The analysis includes the differentiation in main and sub categories and an extensive fuel analysis (e.g., heating value, elemental composition, ash content) to assess its chemical recycling potential and process behavior in our future Waste-to-X pilot plant.

Our contribution will focus on the presentation of the plant concept (highlighting recycling potentials and Aspen Plus® process simulation results) and the characterization of Munich’s residual waste according to our progress.

### References

[1] German Environment Agency, “Abfälle privater Haushalte”, https://www.umweltbundesamt.de/daten/private-haushalte-konsum/wohnen/abfaelle-privater-haushalte#nur-geringer-ruckgang-beim-hausmull, accessed May 01 2024
[2] German Environment Agency, “Vergleichende Analyse von Siedlungsrestabfällen aus repräsentativen Regionen in Deutschland zur Bestimmung des Anteils an Problemstoffen und verwertbaren Materialien“ https://www.umweltbundesamt.de/sites/default/files/medien/479/publikationen/texte_113-2020_analyse_von_siedlungsrestabfaellen_abschlussbericht.pdf, accessed May 01 2024
[3] D. Stapf, “Trends and Drivers in Alternative Thermal Conversion of Waste: Task 36 - Material and Energy Valorisation of Waste in a Circular Economy,” Sep. 16 2020.
[4] Hanel A., Dieterich V., Bastek S., Spliethoff H., Fendt S. (2022): Entrained flow gasification-based biomass-to-X processes: An energetic and technical evaluation. Energy Convers. Manag. 274, 116424.
[5] Bavarian State Office for Statistics, “Genesis Online-Database”, https://www.statistikdaten.bayern.de/genesis/online?operation=ergebnistabelleQualitaetSeparatAUS&levelindex=1&levelid=1715075861092&downloadname=12411-003r#abreadcrumb, accessed May 01 2024.

# Development and Design of a Pressurized Test Rig for Reversible Solid-Oxide Short Stacks

Sören Ohmstedt[1]*, Benjamin Steinrücken[1], Florian Kerscher[1], Hartmut Spliethoff[1]

[1]*Chair of Energy Systems, TUM School of Engineering and Design, Technical University of Munich, Germany*
**Corresponding author: soeren.ohmstedt@tum.de*

Reversible Solid-Oxide Cells (rSOC) represent a promising technology pivotal for the decarbonization of diverse energy applications. With the ability to function as both a fuel cell and an electrolyzer within the same system at high efficiencies, rSOCs offer considerable potential to enhance flexibility through the provision of both negative and positive regulating power and thereby enabling a more efficient integration of renewable energies in the energy system. The required installed power of renewables can therefore be reduced in comparison to an energy system without this conversion technology ultimately lowering the cost of the energy transition. Additionally hard-to-decarbonize sectors can be supported in their transition through the supply of green base chemicals facilitated by the option to use renewable carbon feedstocks for $CO_2$- or co-electrolysis in rSOCs.

This paper introduces a test rig to investigate the advantageous effects of pressurized operation on both stack and individual stack cell levels. At the cell level, elevated operating pressures enable better kinetics due to the equilibrium shift while minimizing diffusion effects which lead to more reactions per time. These effects indicate improved fuel cell efficiency in fuel cell mode and certain improvements in electrolysis mode. Furthermore, an increased pressure level of the reactants reduces the compression work required for storing and utilizing product gases post-electrolysis. This not only leads to an improved base technology for the design of flexibilization power plants but shows potential for lower investment and operating costs.

Despite the significance of pressurized operation, current literature lacks comprehensive experimental research on stack level at reversible operation under such conditions. Thus, this study introduces a purpose-designed test rig for short stacks, along with a systematic approach for their characterization of performance and degradation as well as temperature distribution and electrochemical reaction behavior. Conversion of multiple gas-feedstocks can be investigated.

The test rig made up of a pressurized reactor area and its supporting peripherals accommodates short stacks containing up to 15 cells, with horizontal plane outer dimensions of 230 by 210 mm, and allows for operation pressures ranging from 1 bara to 11 bara in the pressurized vessel. The periphery regulates the media supply of the educt gases and the media disposal to minimize pressure alternations inside the stack cells. Measurement devices record pressure, temperature, gas composition, and electrochemical impedance spectroscopy readings (single cell voltage and stack current), facilitating comprehensive characterization of internal processes and discerning differences between cell loadings.

This research constitutes a crucial step toward implementing rSOCs in commercially available systems for grid integration, underscoring the importance of advancing our understanding of short stack performance and behavior.

# Electrolysis vs. Battery: Flexibility dynamics in Europe's energy system amid varying renewable expansion rates

Stephan Mohr[1]*, Stephan Kigle[1,2], Tapio Schmidt-Achert[1]

*[1]FfE Munich, Germany*
*[2]TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: smohr@ffe.de*

---

The transition to an energy system based on renewable energies leads to profound changes in the price-setting dynamics of the energy-only market. Electricity storage and flexibility technologies are expected to be of vital importance for balancing variable renewable energy supply with electricity demand. From an economic perspective, this is possible because of the increasing magnitude of electricity price fluctuations: Flexibility and storage technologies can take advantage of price differences by reducing electricity demand or storing energy in times of low prices, and by increasing demand or discharging energy during times of high prices. On a functional market, the price is an indicator of the scarcity of the good in question. Hence, this mechanism leads to shifts in energy from times of low residual load to times of high residual load.

However, by balancing supply and demand, flexibility and storage technologies reduce the need for further balancing and, therefore, are in competition with each other. The lower the fluctuations in residual load and hence in the electricity price, the more severe the competition. This raises the question which levels of flexibility are sustained by a market with a given amount of variable renewable energy and whether there are complementary effects allowing for two different technologies to be present simultaneously.

As investments in new technologies take long lead times and have to pay off over a period of 20 years or more, there is a growing need to take investment decisions now. The outcome of these decisions will be affected by the state of the energy system in 2045 or later, when renewable energies are expected to dominate supply. However, despite national and EU-wide targets, the levels of installed renewable power in the future market is unknown. Lower shares of renewable power might reduce the available market for flexibility and storage technologies. Therefore, there is a need to identify figures for the market capacity for flexibility and storage technologies that are robust against deviations of renewable energy expansion from the targets.

In this study, we employ the multi-energy system model ISAaR to simulate the transformation of the European energy system in the years until 2050 under seven different scenarios of renewable energy expansion. ISAaR captures the interactions between seven different energy carriers in hourly resolution and identifies a cost-optimal pathway for the expansion and dispatch of the encompassed energy technologies that satisfies the total energy demand and constraints regarding the total greenhouse gas emissions. Covering the geographical scope of the EU27+3 (Norway, Switzerland, UK), the model also considers the import of natural gas, crude oil, hydrogen and synthetic energy carriers. The expansion is modelled starting in 2019 and continuing from 2025 in five-year steps, reaching up until 2050.

To investigate the effect of varying levels of renewable expansion, seven different scenarios with exogenous renewable build up were explored. In the base case, renewable energy sources are expanded according to the national and EU-wide plans and targets. In the other scenarios, renewable power expansion is changed in 10% steps from –30% to +30% with respect to the base scenario. The effects of the different renewable expansion levels on different demand flexibilization and storage technologies (flexibilization of industrial processes, industrial heating rods, heat pumps, electrolysis and PtX, batteries and smart and bidirectionally charged electric vehicles) is investigated. In particular, we focus on the installed capacities of these technologies and on typical running patterns to draw distinctions between the technologies' uses.

The results show that the installed capacities of the flexibility technologies in 2045 depend on the levels of installed renewable energy. In general, the higher the amount of renewable energy in the system, the larger the installed capacities of the flexibility technologies. However, trends differ between the technologies: While the installed capacity of electrolysis increases monotonically with the installed renewable electricity, batteries have their highest installed power in the scenario with -10% renewable energy expansion compared to the base case, while no batteries are installed in the -30% and +30% scenarios.

An analysis of the sorted shadow electricity price curve shows two plateaus of electricity prices (one in summer, one in winter), each making up around 20 to 30 % of the total hours of the year. Certain flexibility technologies (batteries, smart charging and flexible industrial consumers) run mainly in the hours where the shadow price is lower than that of the plateaus, making use of low-residual-load-situations. Electrolysis, on the other hand, also has significant running hours during the price plateaus, with no running hours at prices higher than the plateaus. This leads to the conclusion that electrolysis and other flexibility technologies can benefit from distinct market situations.

We underpin this result by two observations on the differences in running patterns between batteries and electrolysis. First, particularly in summer, there is a significant amount of battery discharging while electrolysis is running at more than 50 % of its full capacity. Second, particularly in winter, there is a significant number of battery charging events during hours electricity prices above the plateau level during which electrolysis is running. Both observations are independent of the expansion of renewable energy.

We conclude that batteries and electrolysis serve mutually different functions on the electricity market. While the levels of installed battery power vary with renewable energy expansion, the optimal installed powers of electrolysis is more robust. Outside of the extreme scenarios of high and low renewable energy expansion, there is significant potential for battery and electrolysis expansion compared to current levels.

# Development of a Dynamic Carbon Capture and Utilization Pilot Plant

Svenja Knösch[1]*, Vincent Dieterich[1], Dr.-Ing. Sebastian Fendt[1], Prof. Dr.-Ing Hartmut Spliethoff[1]

*1Chair of Energy Systems, TUM School of Engineering and Design, Technical University Munich, Germany*
**Corresponding author: svenja.knoesch@tum.de*

---

Carbon capture technology has emerged as an efficient way of reducing $CO_2$ emissions, while enabling the direct utilization of the captured greenhouse gas in power-to-X processes. For carbon capture and utilization (CCU) plants, absorption of $CO_2$ employing amine solutions is a state-of-the-art technology.

The main focus of this work is the development of a dynamic CCU pilot plant as part of the H2 living lab Burghausen, aiming to establish an emission-free power to methanol process. To validate the described process chain, the $CO_2$ isolated from the flue gas of a waste incineration plant by means of a post-combustion CCU process, is supplied to a methanol synthesis plant. As shown in Figure 1, the CCU process in general consists of an absorber, the main heat exchanger for the heat integration of the amine solution, and a desorber.

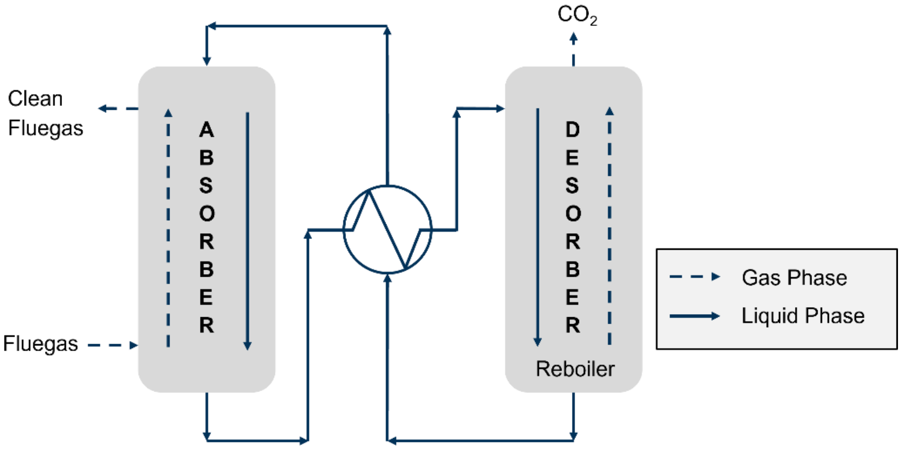


*Figure 1: Generic process scheme of the carbon capture pilot plant.*

The research focus of this work lies on designing a non-stationary CCU pilot plant within a 20-foot container, that enables dynamic operation and serves as a model for future scalability of the process. Dynamic operation is required to ensure a constant $CO_2$ absorption rate of 80% despite fluctuations in volume flow and $CO_2$ concentration within the flue gas. Due to the geometric constraints of the container, the absorption columns are split into 5 compartments, necessitating a decreased absorption rate of 80%, compared to 90% in conventional CCU units, however, enabling the aforementioned dynamic operation [1].

For a reliable process validation, the well-established solvent monoethanolamine (MEA, 30 wt% in water) is employed as the absorbing agent due to its extensive investigation in literature, providing a trustworthy database of physicochemical characteristics, as well as the possibility of a reasonable comparison to other CCU plants.

Using the Aspen Plus software, simulations extending over a broad parameter space have been performed as a first step towards specifying the process limitations. Based on a working CCU process within the pilot plant-specific restrictions, process parameters, including reboiler duty, desorption pressure, column height, and detergent flow rate, were optimized. In addition, the influence of varying flue gas volume flow and $CO_2$ concentration was simulated to gain preliminary insights into the system's behavior under dynamic operation.

## References

[1] J. N. Knudsen, J. N. Jensen, P. Vilhelmsen, O. Biede, "Experience with CO2 capture from coal flue gas in pilot-scale: Testing of different amine solvents", Energy Procedia,vol 1, no. 1, 2009.

# Power-to-X: Process Modeling and Assessment of Pathways to Produce Sustainable Aviation Fuel

Vincent Eyberg[1]*, Vincent Dieterich[1], Sebastian Bastek[1], Marcel Dossow[1], Hartmut Spliethoff[1], Sebastian Fendt[1]

*[1]Chair of Energy Systems, TUM School of Engineering and Design, Technical University of Munich, Germany*
**Corresponding author: vincent.eyberg@tum.de*

---

The aviation sector accounts for about 3 % of global $CO_2$ emissions [1] and aviation $CO_2$ emissions will further increase as air travel is predicted to grow in the future [2]. Planes are difficult to electrify, therefore sustainable aviation fuel (SAF) will be an option to defossilize aviation [3]. Power-to-Liquid processes can be applied to produce SAF, whereby carbon dioxide and hydrogen from electrolysis are raw materials. If $CO_2$ is extracted from the air via Direct Air Capture (DAC) technologies the potential scale of PtL processes is significantly larger compared to Biomass-to-Liquid (BtL) processes based on biogenic waste materials [4]. The two currently most considered pathways for PtL based SAF production are the Fischer–Tropsch (FT) and Methanol-to-Jet (MtJ) routes [4].

This study is related to a recently published research article of the authors [5]. FT and MtJ pathways, with $CO_2$ from DAC and $H_2$ from Solid Oxide Electrolysis (SOEL) as educts, are considered. An electrified reverse Water-Gas-Shift (rWGS) reactor is applied to generate CO from $CO_2$. The whole process chains are displayed in Aspen Plus V12 based on experimentally validated sub-models. In the evaluation, the technical performance is assessed based on the carbon efficiency to liquid hydrocarbons ("syncrude"), the energy efficiency and the obtained product composition. For the economic assessment, the TUM CESTEA method [6] is used to calculate the capital investment and production costs. The economic performance is evaluated by comparing the Levelized Cost of Production (LCOP) of syncrude. The LCOP consist of variable costs (VCOP), fixed costs (FCOP) and the annual depreciation ($a_{year}$) depending on the interest rate $i$ and the amortization period $n_A$ [6]:

$$\mathrm{LCOP} = \mathrm{VCOP} + \mathrm{FCOP} + a_{year} \text{ with } a_{year} = \mathrm{FCI}\,\frac{i(1+i)^{n_A}}{(1+i)^{n_A}-1} \qquad (1)$$

Nine different process configurations, regarding the usage of by-products and unconverted educts, are investigated. The three major approaches are the burning of light gases from FT/MtJ to fuel the DAC process ($CO_2$ is recycled), the reforming of light gases in the rWGS to produce fresh syngas and the upgrading of unconverted syngas to methane (synthetic natural gas). For more details on process modeling and the economic assessment it is referred to the related research article [5].

The FT and MtJ process configurations with reforming of light gases to syngas show the best performance. Figure 1 displays the carbon and energy efficiencies as well as the resulting LCOP of the optimal configurations. FT and MtJ show minor differences in their technical and economical results. However, MtJ products show better fuel properties, resulting from branched molecules and no wax range products. The resulting LCOP is 0.81 €/kWh$_{Syn}$ for both pathways. Applying SOEL cost projection for 2050 and electricity costs of 40 €/MWh$_{el}$ as an optimistic scenario, the LCOP reaches about 0.23 €/kWh$_{Syn}$. Compared to fossil jet fuel, the LCOP are about three times higher as fossil fuel costs [7].

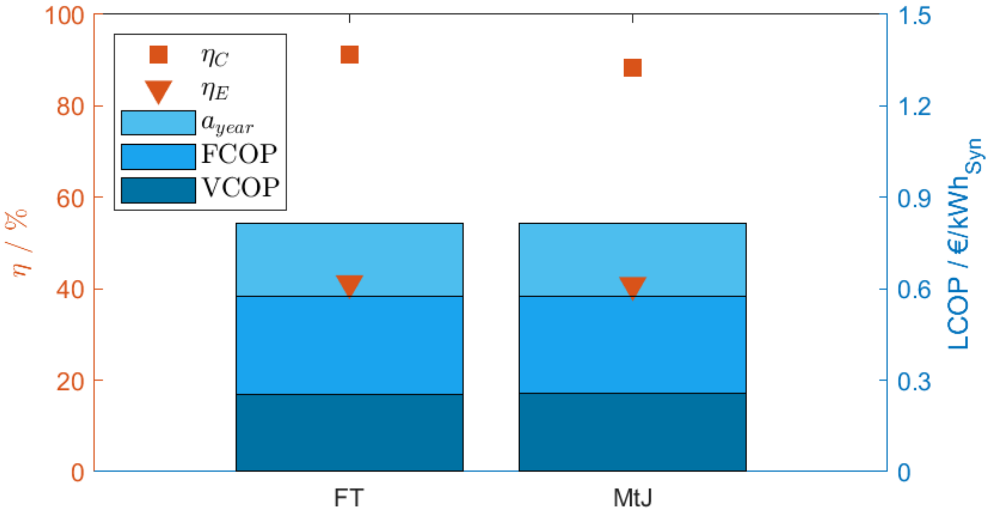


*Figure 1: Carbon efficiency to liquid products (based on the captured amount of $CO_2$), energy efficiency and LCOP (divided in variable costs, fixed costs and depreciation) for the optimal FT and MtJ configurations.*

## References

[1] A. Gonzalez-Garay, C. Heuberger-Austin, X. Fu, M. Klokkenburg, D. Zhang, A. van der Made, N. Shah, Unravelling the potential of sustainable aviation fuels to decarbonise the aviation sector, Energy Environ. Sci. 15 (2022) 3291–3309. doi:10.1039/D1EE03437E.

[2] K. S. Ng, D. Farooq, A. Yang, Global biorenewable development strategies for sustainable aviation fuel production, Renewable and Sustainable Energy Reviews 150 (2021) 111502. doi:10.1016/j.rser.2021.111502.

[3] J. Ruokonen, H. Nieminen, A. R. Dahiru, A. Laari, T. Koiranen, P. Laaksonen, A. Vuokila, M. Huuhtanen, Modelling and cost estimation for conversion of green methanol to renewable liquid transport fuels via olefin oligomerisation, Processes 9 (2021). doi:10.3390/pr9061046.

[4] Schmidt P, Batteiger V, Roth A, Weindorf W, Raksha T. Power-to-liquids as renewable fuel option for aviation: A review. Chem Ing Tech 2018;90(1–2):127–40. doi:10.1002/cite.201700129.

[5] V. Eyberg, V. Dieterich, S. Bastek, M. Dossow, H. Spliethoff, S. Fendt, Techno-economic assessment and comparison of Fischer–Tropsch and Methanol-to-Jet processes to produce sustainable aviation fuel via Power-to-Liquid. Energy Convers Manage 315 (2024) 118728. doi:10.1016/j.enconman.2024.118728.

[6] M. Dossow, V. Eyberg, V. Dieterich, H. Spliethoff, S. Fendt, CESTEA: The TUM chair of energy systems techno-economic analysis method. TUM-CES White Paper Series ‘‘Energy System in Transition’’ (2024). doi:10.14459/2024md1743206.

[7] US EIA. U.S. Gulf Coast Kerosene-Type Jet Fuel Spot Price FOB. 2023.