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CO_2-WIN: Workshop zur Elektro- und Photokatalyse

ProMet: CO_2 to Propylene via eMethanol

01.02.2020 – 31.01.2023

12.07.2022

Dr. Katja Weichert (Covestro)

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Katja Weichert

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Martin Rothaemel

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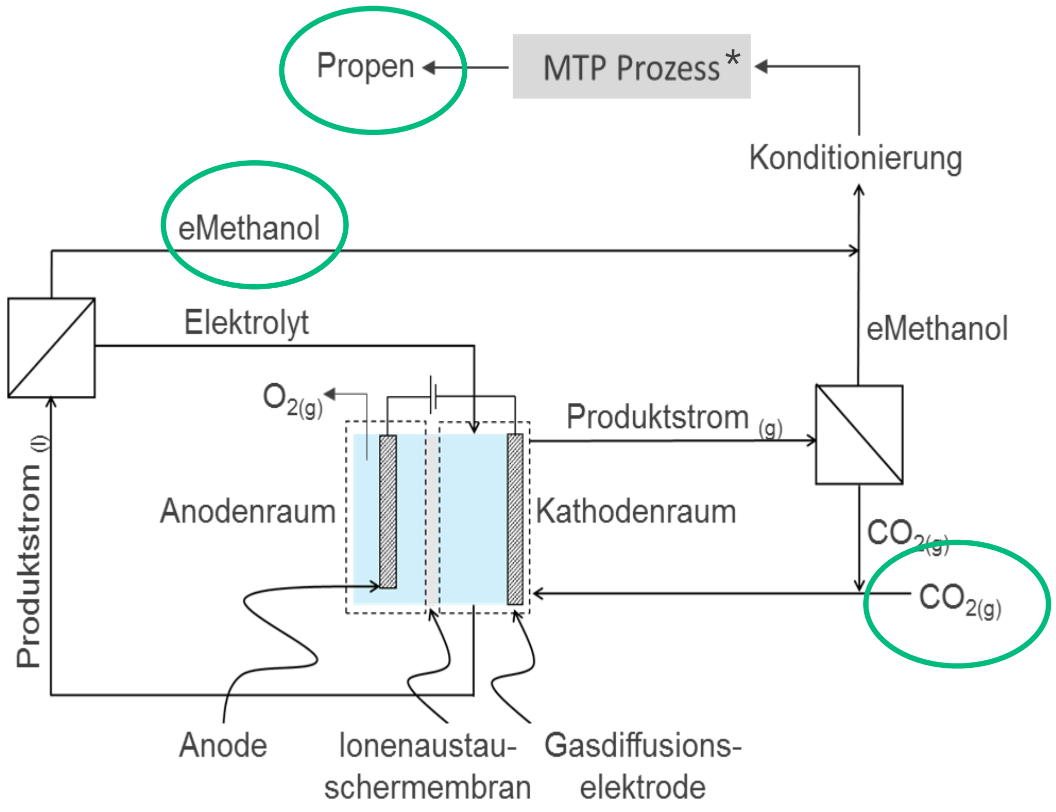
Goal

Combination of academic and industrial know-how for the development of the whole process.

Starting with fundamental work, the economic feasibility of the full industrial process will be evaluated.

The sustainable use of carbon will be assessed with an ecologic study (life cycle assessment).



* Methanol-to-Propylen process

Anticipated ProMet process

ProMet: CO_2 to Propylene via eMethanol

Material	FE* Methanol [%]			
Current Density (mA/cm²)	-5	-50	-100	-200
Ag_2S (2h)	0	0	0	0
Ag_2S (24h)	0	0	0	0
Ag_2S HCl	0	0	0	0
COV-C Cu (bottom)	0	0	0	0
COV-C Cu (top)	0	0	0	0
CuSe from Cu	0	0	**0.07**	0
CuSe from CuO	0	0	0	0
CuAl	0	0	0	0
Cu@Co, core@shell	0	0	0	0
Co@Cu, core@shell	0	0	0	0
Cu/SiO_2 (H_2)	0	0	0	0
Cu/SiO2 (N_2)	0	0	0	**0.03**
Zn/Cu @ N-doped C (800°C)	0	0	0	**0.08**
B-Cu/Zn (TU Clausthal)	0	0	0	0
B-Zn-In	0	0	0	0
Zn/Bi2S3	**2.77**	0	0	0
Zn-Bi-S*	0	0	0	0
Bi2S3	0	0	0	0
Cobalt Carbonate Hydroxide	0	0	0	**0.05**
Fe2P/C	0	0	0	0

After ~1 year intensive work on synthesis of a methanol electrocatalyst, the first milestone** was postponed by 6 month to 31.12.2021 and parallel activities for a new approach were started.

*FE = Faraday Efficiency: corresponds to the yield of the product in an electrochemical reaction.
FE = current used for product/overall current * 100 %

**Milestone 1 (after 18 month): catalyst and gas diffusion electrode available with FE(Methanol) ≥ 50% and current density > -50 mA/cm^2

<u>Testing parameters</u>
1 M KOH, ~21 ml/min CO_2 flow, ~16 ml/min N_2 flow, 2 mg catalyst powder + 1 mg PTFE drop-coated onto Freudenberg H23C2 carbon paper, *j* = -5 to -200 mA/cm². Prereduction ~30-60 min @ -5 mA/cm².

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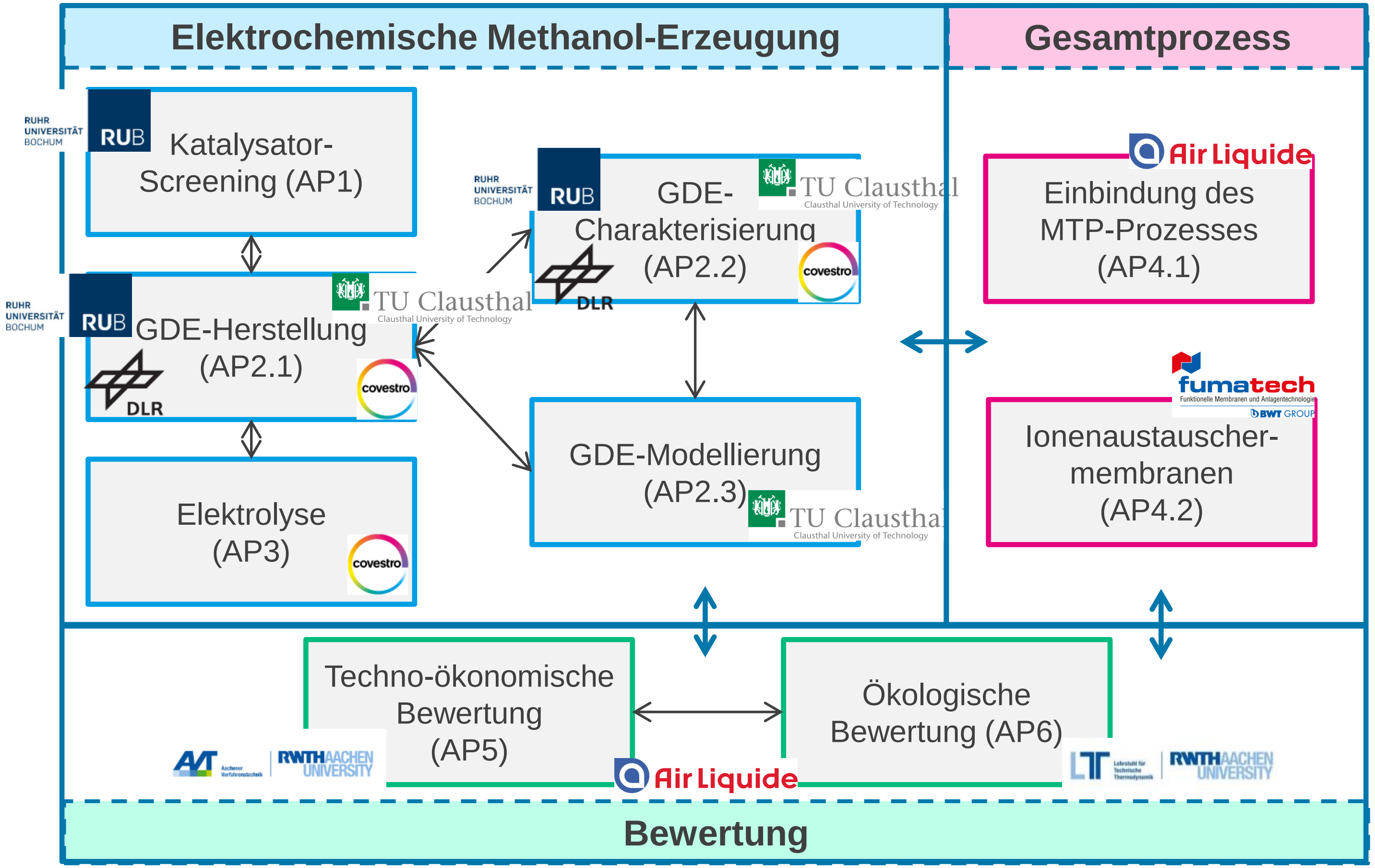
Focus on proven electrocatalyst for different products: ethylene, ethanol, n-propanol und acetate [1]

Project structure could be maintained



[1] Y. Song, J. R. C. Junqueira, N. Sikdar, D. Öhl, S. Dieckhöfer, T. Quast, S. Seisel, J. Masa, C. Andronescu, W. Schuhmann, *Angew. Chem. Int. Ed.* **2021**, *60*, 9135

Upscaling Katalysatorherstellung

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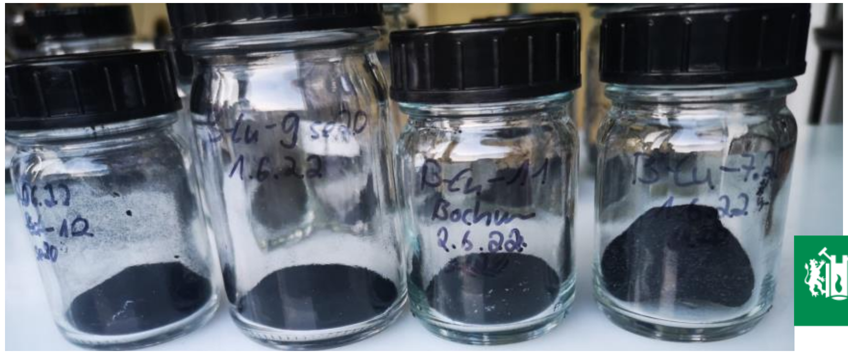
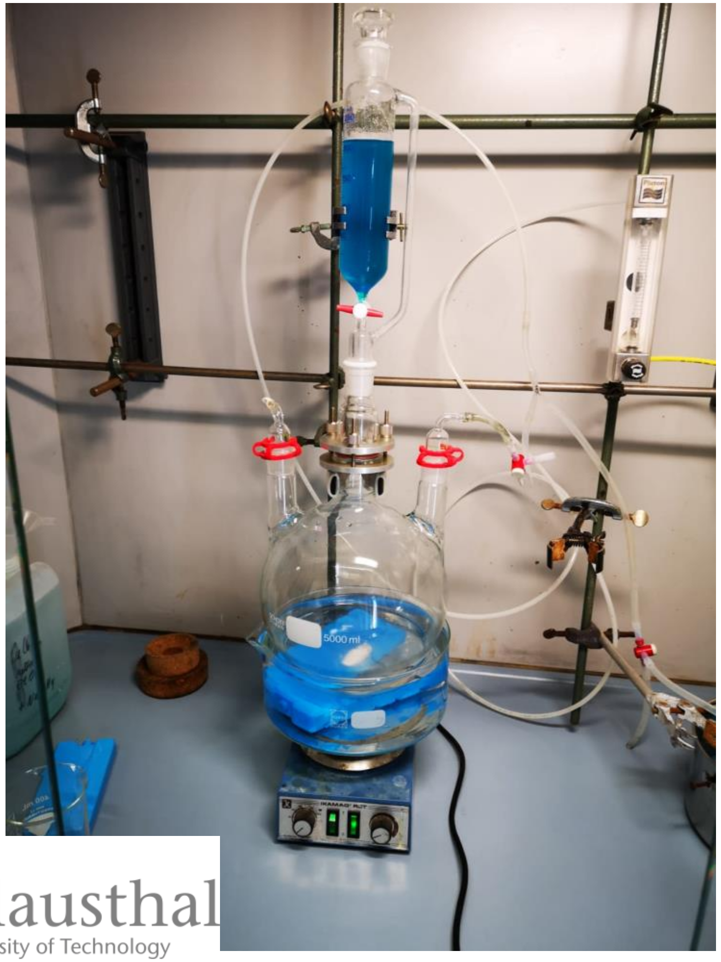
- Modification of the synthesis procedure [2] for preparation of higher quantities of catalyst
  - Temperature variations
  - Variation of reaction times
  - Variation of reactant concentration
- Successful production of >12 g per batch
- Catalyst production for all partners by TUC





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[2] Y. Zhou, F. Che, M. Liu, C. Zou, Z. Liang, P. De Luna, H. Yuan, J. Li, Z. Wang, H. Xie, H. Li, P. Chen, E. Bladt, R. Quintero-Bermudez, T. K. Sham, S. Bals, J. Hofkens, D. Sinton, G. Chen, E. H. Sargent, *Nat. Chem.* **2018**, *10*, 974-980

Gas Diffusion Electrode (GDE)
Preparation and Characteriztion

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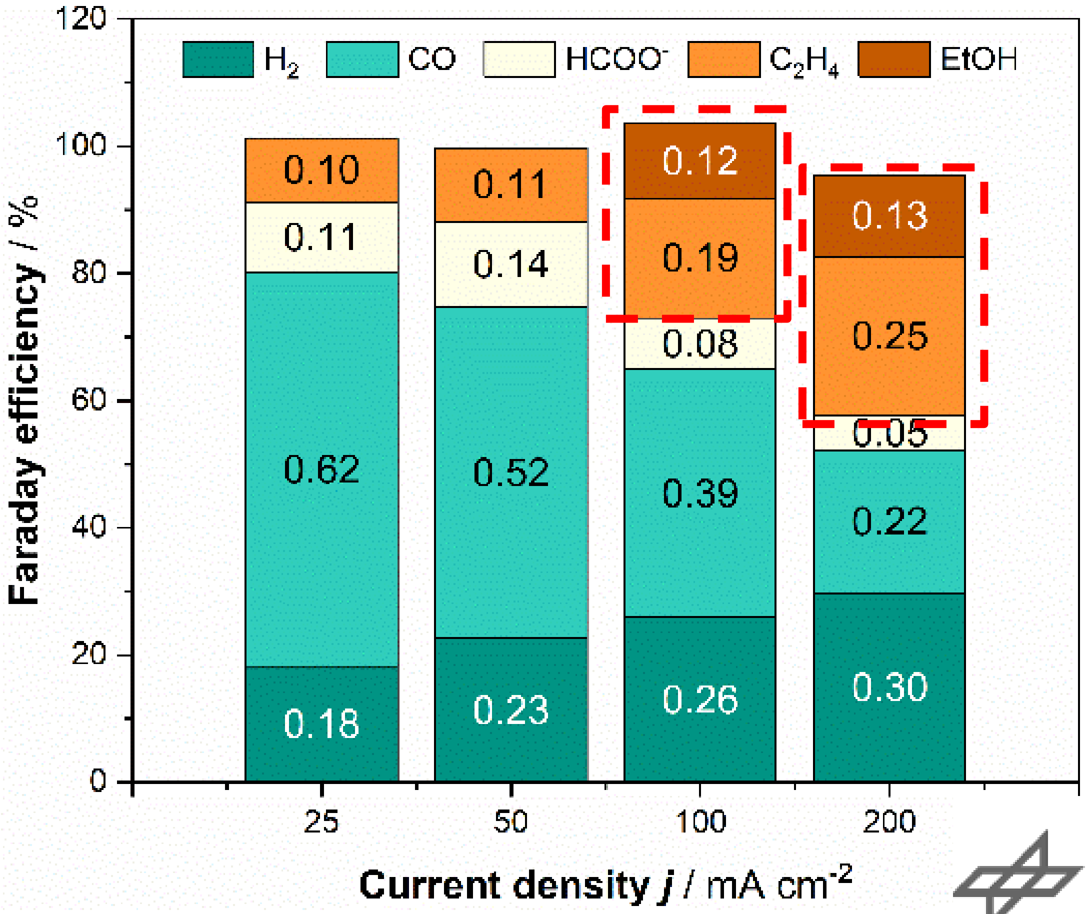
- Results from RUB with new catalyst could be reproduced qualitatively at DLR and TUC, but with different product distribution → probably due to different methods for GDE preparation and/or different cell designs

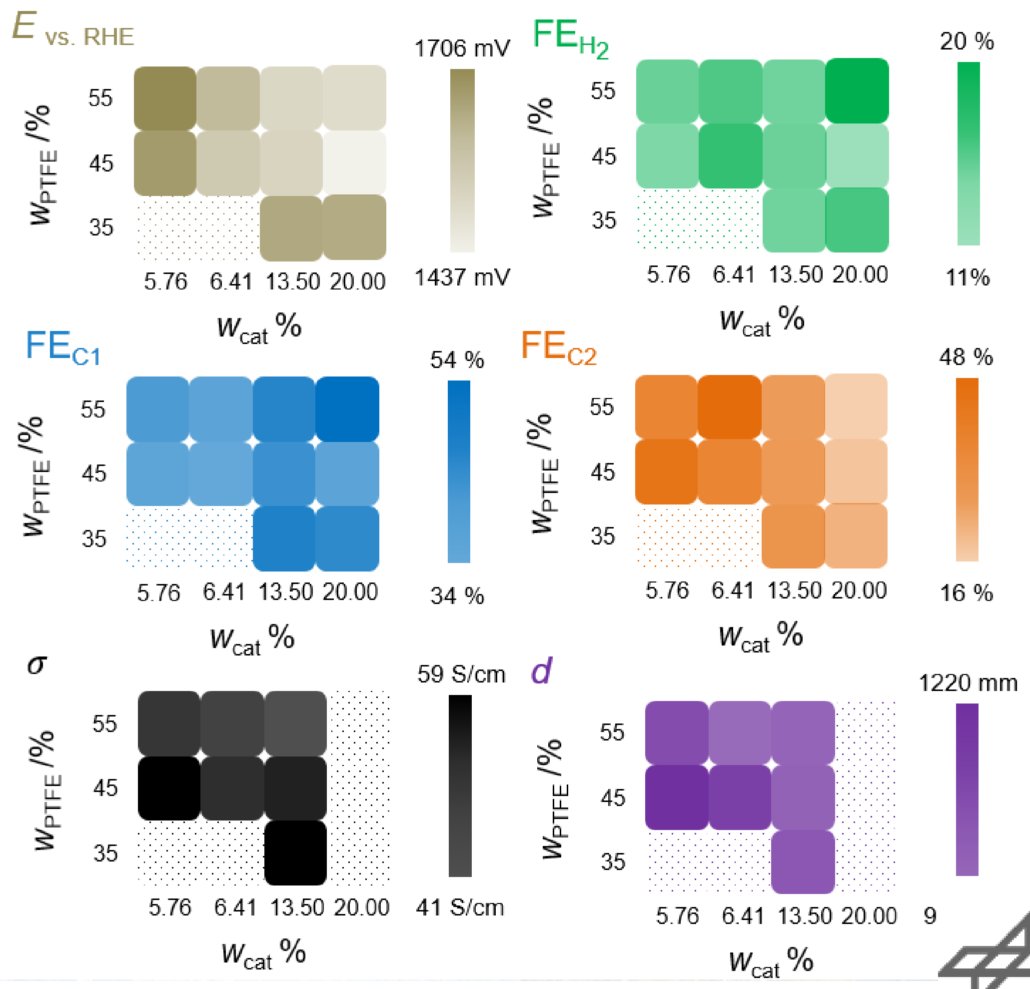


For 100 & 200 mA cm^{-2}:
+ Acetate
+ n(!)-PrOH

Deutsches Zentrum für Luft- und Raumfahrt DLR

Gas Diffusion Electrode (GDE) Preparation and Characteriztion

- GDE engineering: several aproaches to modifiy GDE structure: pore size, thickness, load of catalyst, multi-layers with different functions
- Goal: identify structure-performance relationships of GDEs for electrochemical CO_2 reduction



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Techno-economic Assessment

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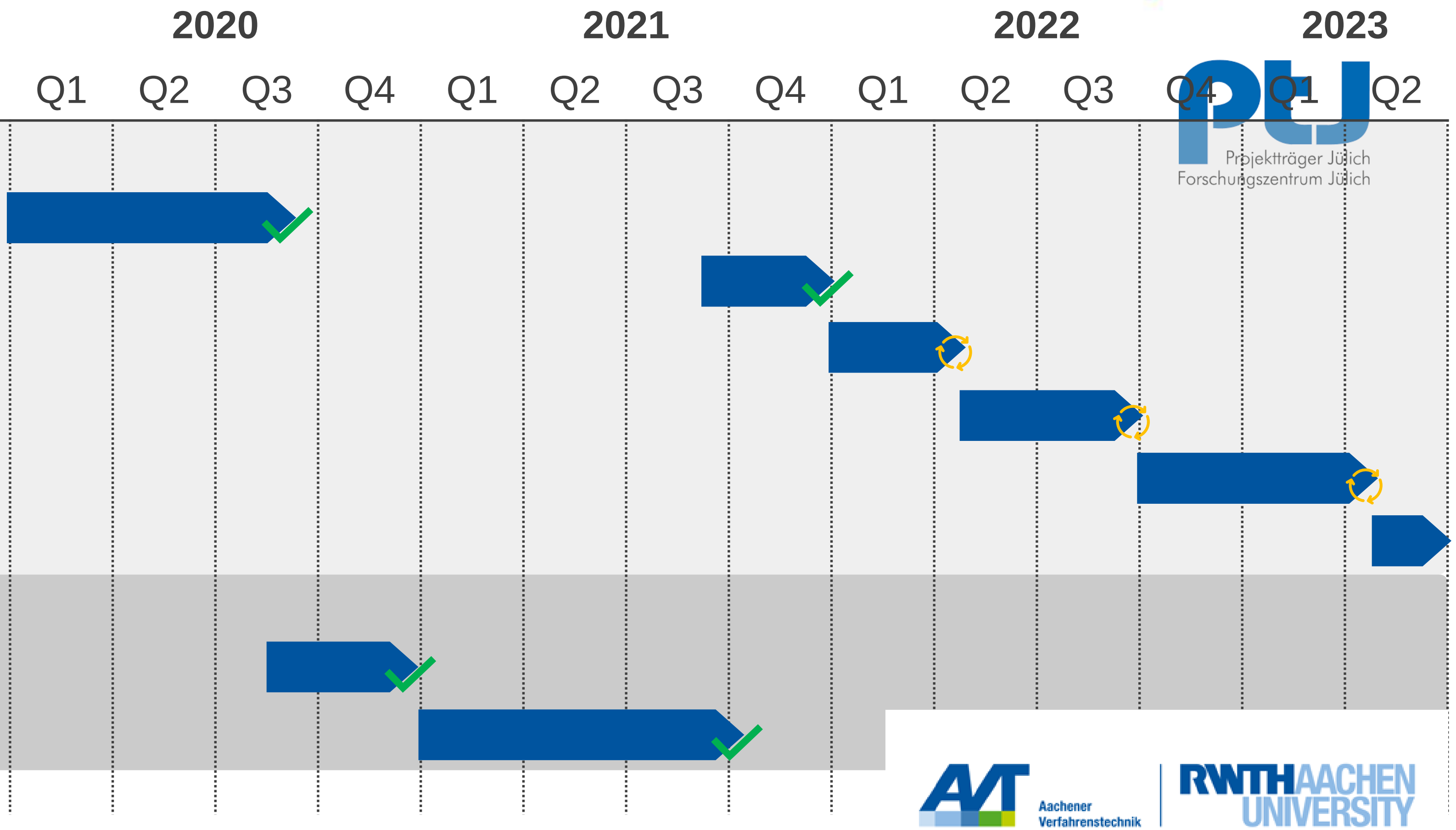
- Transfer of the model from methanol to n-propanol

AP5.1	**Benchmarking**
AP5.1.1	Modelling benchmark processes
AP5.1.2	Modelling CO_2 reduction to MeOH
AP5.1.3	Modification of CO_2 reduction model
AP5.1.4	Modelling benchmark n-propanol separation
AP5.1.5	Modelling overall process
AP5.1.6	Techno-economic evaluation
AP5.2	**Validation**
AP5.2.1	Modification exp. setups
AP5.2.2	Membrane screening



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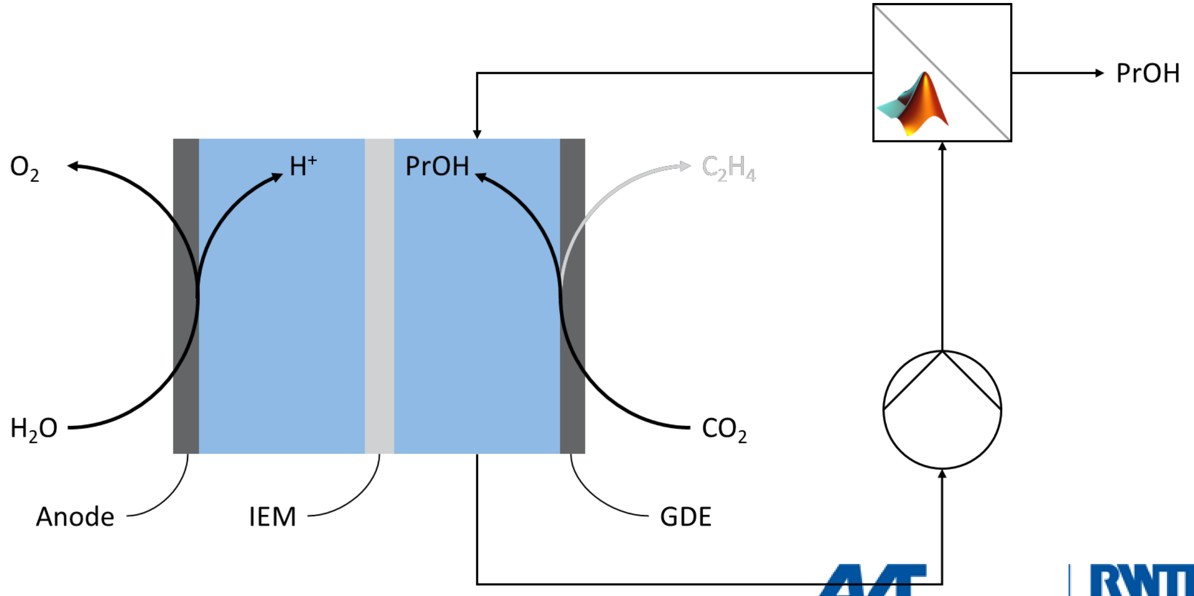
Techno-economic Assessment

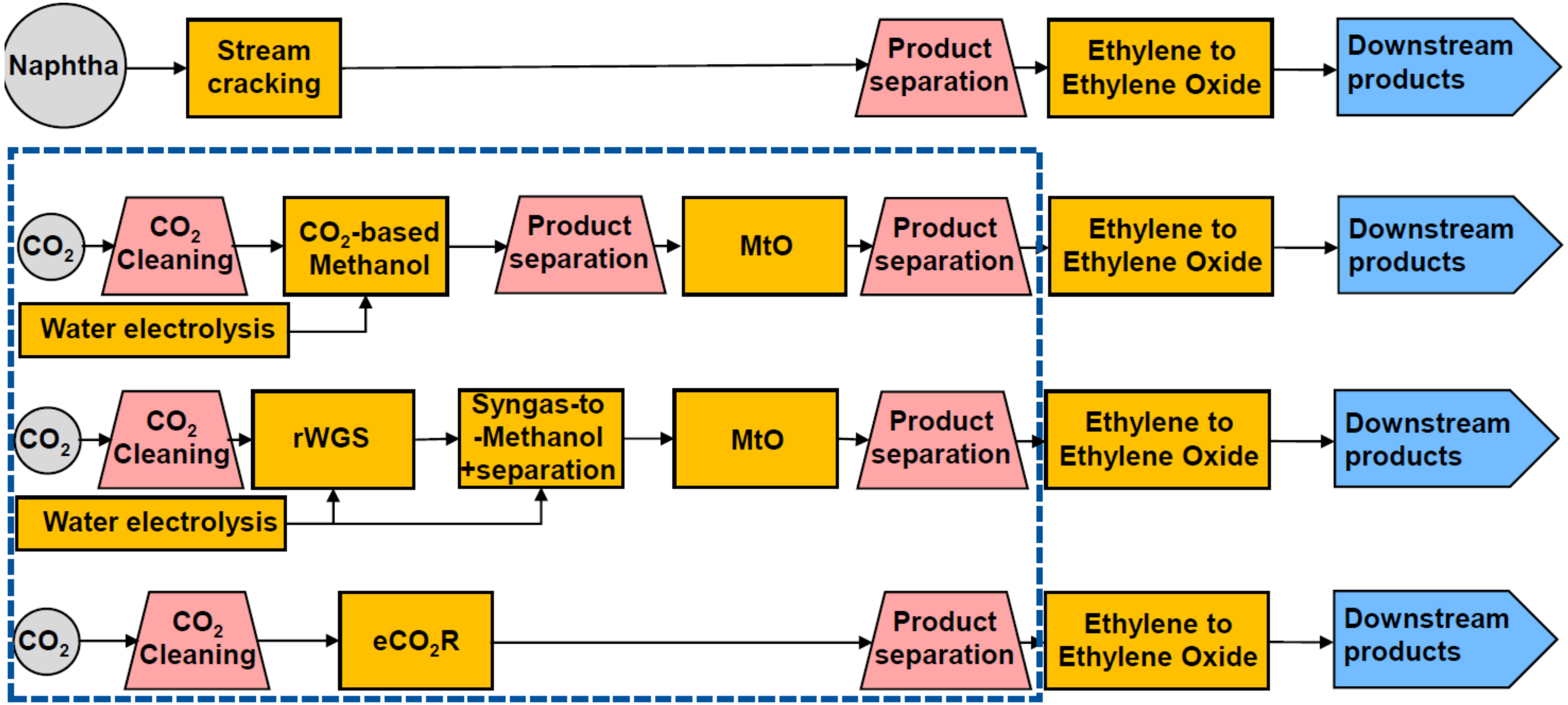
- Modelling with Aspen+
- Focus on membrane separation of n-propanol from electrolysis cell and modelling of different parameters:
  - Pressure loss
  - Real gas behaviour
  - Concentration polarization
  - Permeability temperature dependence



PrOH – n-propanol
IEM – Ion Exchange Membrane
GDE – gas diffusion electrode

Ecologic Assessment (Life Cycle Assessment)

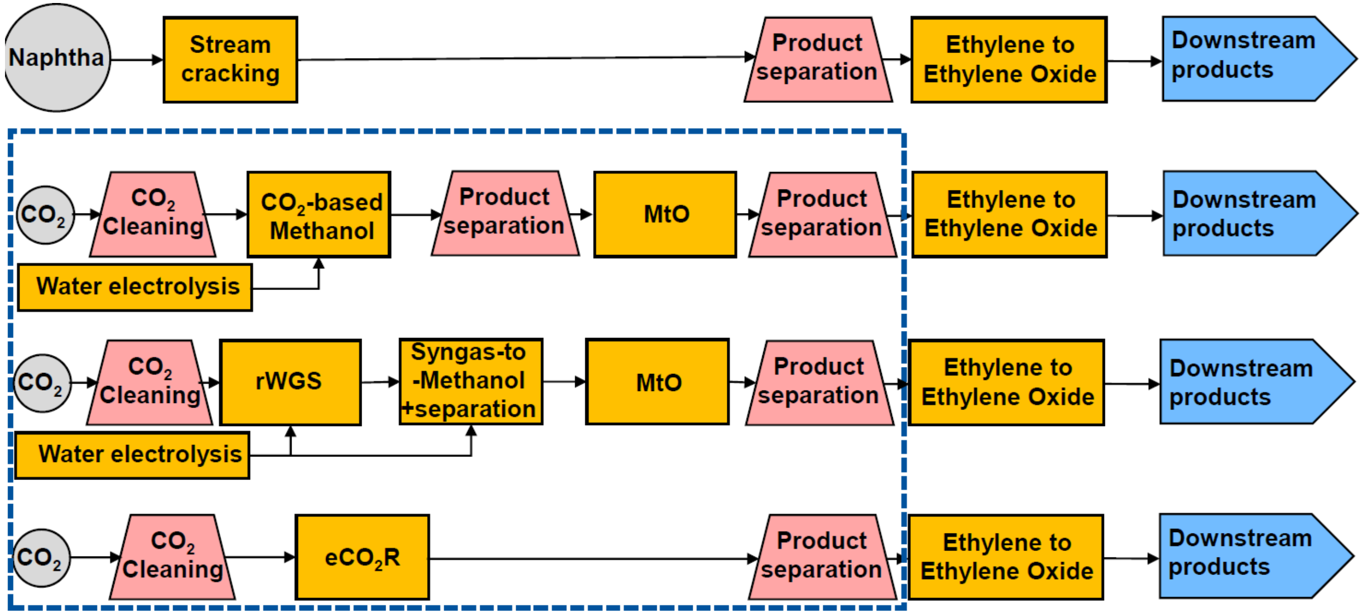
- Comparison of different routes for ethylene production: fossil route (state of the art) and sustainable alternative routes



MtO: Methanol to Olefine
rWGS: reverse water gas shift
eCO_2R: electrochemical CO_2 reduction

Ecologic Assessment (Life Cycle Assessment)

- All alternative routes have a significantly reduced Global Warming Potential (emissons of CO_2-eq per kg ethylene) compared to fossil route
- Direkt CO_2 electrolysis to ethylene could be best-in-class, if Faradaic Efficiency > 58 %, cell voltage < 2.5 V



MtO: Methanol to Olefine
rWGS: reverse water gas shift
eCO_2R: electrochemical CO_2 reduction

Summary

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- New target molecules, but still aiming for sustainable production of basic chemicals by electrochemical CO_2 reduction
- Successful upscaling of electrocatalyst synthesis
- Preparation of gas diffusion electrodes (GDE) by different methods and characterization in electrochemical flow cells
- Modelling of Cu-GDEs for CO_2 reduction
- Membrane characterization
- Life cycle assessment with focus on ethylene
- Techno-economic study with focus on n-propanol for futher use in Methylen-to-Propylen process
- Evaluation of the use of n-propanol for Methanol-to-Propylene process

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Thank you for your kind attention!