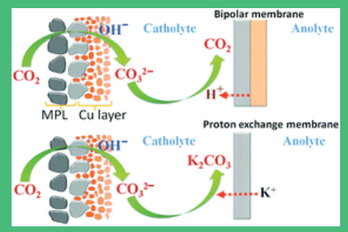
Technical consistency plan

The SELECTCO2 consortium has implement a technical consistency plan reporting a set of operating parameters that all partners use as a default value when testing for electrochemical CO_2 reduction. This document consists of parameters on both characterization and testing and relates to catalysts, gas diffusion electrodes and membranes.

These benchmarking conditions allows comparable results across the entire consortium and also gives those modelling mass transfer effects detailed parameters on which to base their models.

Publication

Role of ion-selective membranes in the carbon balance for CO_2 electroreduction via gas diffusion electrode reactor designs
M. Ma, S. Kim, I. Chorkendorff and B. Seger
Chem. Sci., 2020, 11, 8854
https://doi.org/10.1039/D0SC03047C



Consortium

- DE NORA — Industrie De Nora
- DTU — Coordinator Technical University of Denmark
- TU Berlin — Technical University Berlin
- TU Delft — Delft University of Technology
- EPFL — Swiss Federal Institute of Technology Lausanne
- RINA — RINA Consulting SpA
- University of Surrey — University of Surrey
- PRETEXO — Pretexo
- SLAC — SLAC National Accelerator Laboratory

Website: www.selectco2.eu

SELECT CO2

NEWSLETTER #1
FEBRUARY 2021

SELECTIVE ELECTROCHEMICAL REDUCTION OF CO_2 TO HIGH VALUE CHEMICALS

A very productive first year !

With the goal of selectively producing CO, ethanol and ethylene at industrially relevant current densities the SELECTCO2 project has had a very productive first year.

A **technical consistency plan** along with identical reactors distributed to all of the testing groups has allowed for uniform results and rapidly accelerated development. Both consortium produced gas diffusion layers, membranes and ionomers have been produced and now being tested.

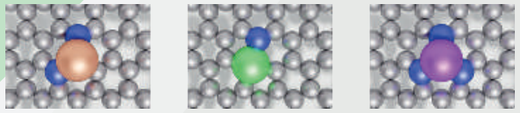
We have hit milestones with respect to **high selectivity for CO_2** to CO, integrating a **recycle loop**, and visualizing **gas diffusion layers**.

We have **new models** describing the ethylene/ethanol branching ratio and single site catalysts as well as more thorough models describing mass transfer within gas diffusion layers.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 851441.

CO Production

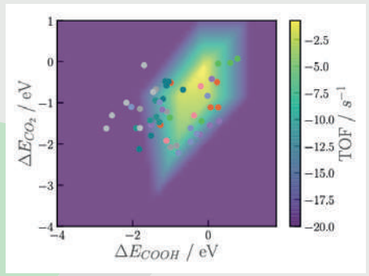
Single site catalysts embedded in 2D materials have recently emerged as potential earth-abundant catalysts for several electrochemical processes. In particular, metal- and nitrogen-doped graphene has shown promising activity and selectivity towards CO_2 reduction (CO2R) to CO. In WP2, Denmark Technical University-th (DTU-th) is working towards the computation-guided design of efficient single-site catalysts in nitrogen-doped graphene for the SELECTCO2 project, which has the objective of designing CO2R electrolyzers with high conversion efficiency and selectivity towards high value products. In particular, SELECTCO2 has the objective of achieving electrolyzers with with 90% selectivity for CO2R to CO.



Schematic of a few site motifs of M-N-C catalysts considered

In collaboration with Technical University of Berlin (TUB), DTU-th has conducted fundamental methanistic studies found new descriptors for the activity of CO2R to CO. Single-site catalysts are unique in that they deviate significantly from the scaling relations of transition metals and therefore have potential for higher intrinsic activity.

The contour plot with predicted catalysts in the high activity region, which will undergo experimental testing at TUB.

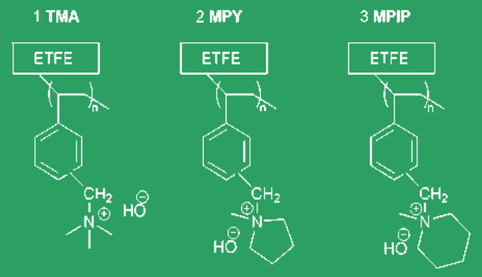


Results of activity screening using new descriptors, with candidates in the high activity region.

Optimization of Membranes & Ionomers

University of Surrey has now delivered batches of six different benchmark (generation 1) radiation-grafted anion-exchange membranes (RG-AEMs) to the DTU-EX team for initial evaluations in CO2RR cells.

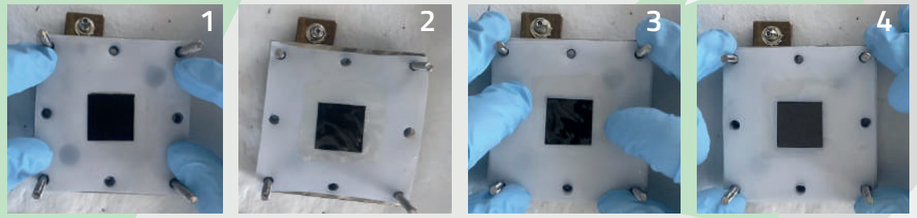
The RG-AEMs range from 50 to 100 micrometres in hydrated thicknesses and contain one of three different positively charge head-groups (TMA, MPY, and MPIP, see scheme). The different head-group chemistries are known to have high stabilities in alkali when hydrated, while they have similar ionic conductivities but very different water uptakes and transport properties.



These RG-AEMs will form the basis of the planned development of the next-generation of RG-AEM, which will be specifically tailored for low resistance in CO2ER cells and enhanced faradaic efficiencies for the electro-generation of the desired high-value C1 and C2 products (they will inhibit the parasitic hydrogen evolution in the CO2RR cells that can occur with suboptimal water transport properties).

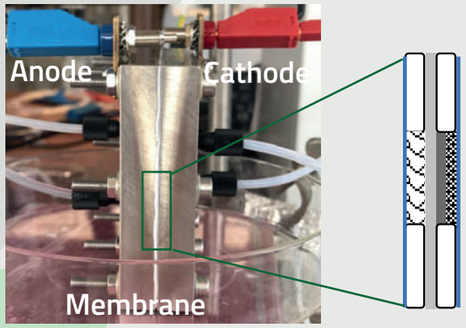
- Highlights -

MEA-type flow-cell "layer-by-layer" manufacturing



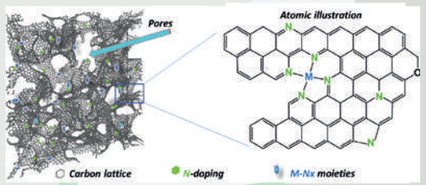
Mounting of the zero-gap MEA-type electrolyzer (TUB)

1) Gas diffusion electrode (GDE), with catalyst layer located on the cathode part. The back side of the GDE is attached on the flow field, and the catalyst layer contacts the membrane. This GDE is stabilized in a polytetrafluoroethylene gasket, to guarantee the cathode chamber (gas/liquid) leaktight.
2) The membrane is added on the catalyst layer of the GDE to allow ion transfer.
3) A second gasket material is put on the membrane, leaving the space for the anode.
4) Addition of the anode, leaving the anode material on the membrane for the counter oxygen evolution reaction catalyst. This allows the overall cell reaction.



Complete MEA Cell

Cell "cross section"



M-N-C catalyst

Optimization of Gas Diffusion Layers

De Nora's R&D team is working in a dedicated laboratory in Milan to develop a novel Gas Diffusion Electrode (GDE) specific for CO_2 electrochemical reduction. In Work Package 5 De Nora will develop a stable GDE, with hydrophobicity and pore size optimized to aid selectivity, activity and rates for a given CO_2 reduction product.

DE NORA
our research - your future

De Nora is a well-known manufacturer and supplier of GDE in many commercial applications.