PATHWAYS TO PRODUCE RENEWABLE CHEMICALS FROM AMBIENT CO2

THE CASE OF ETHYLENE

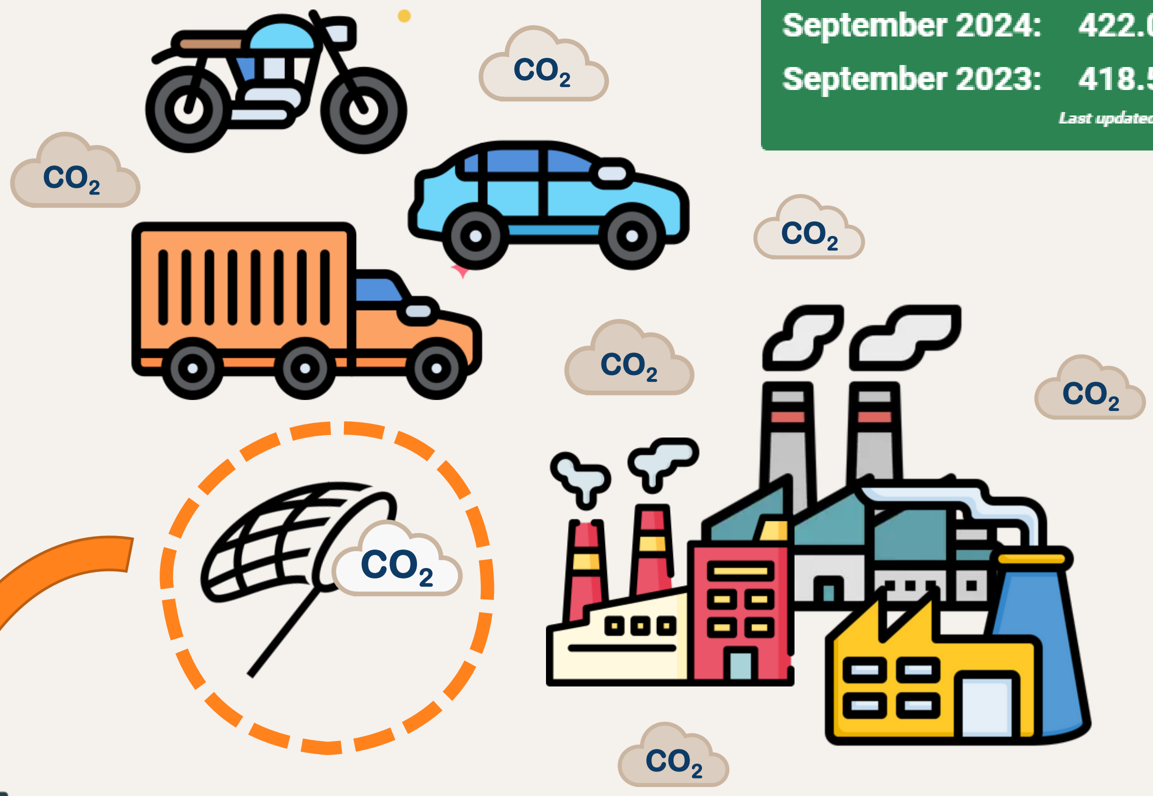
ISABELLA QUARANTA
PhD Researcher
i.c.cavalcante-quaranta@sms.ed.ac.uk
THE UNIVERSITY of EDINBURGH

RENEWABLE CHEMICAS FROM AMBIENT CO_2

September 2024: 422.03 ppm

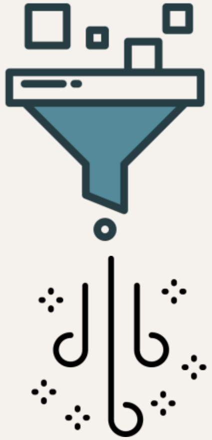
September 2023: 418.51 ppm

Last updated: Oct 05, 2024



Direct Air Capture

- ✓ Employed in different of locations
- ✓ Net-Zero Negative Emissions
- ✗ Large energy consumption
- ✗ High removal cost



CO_2

Formic acid   Propanol

Ethylene   Propane and C_{3+}

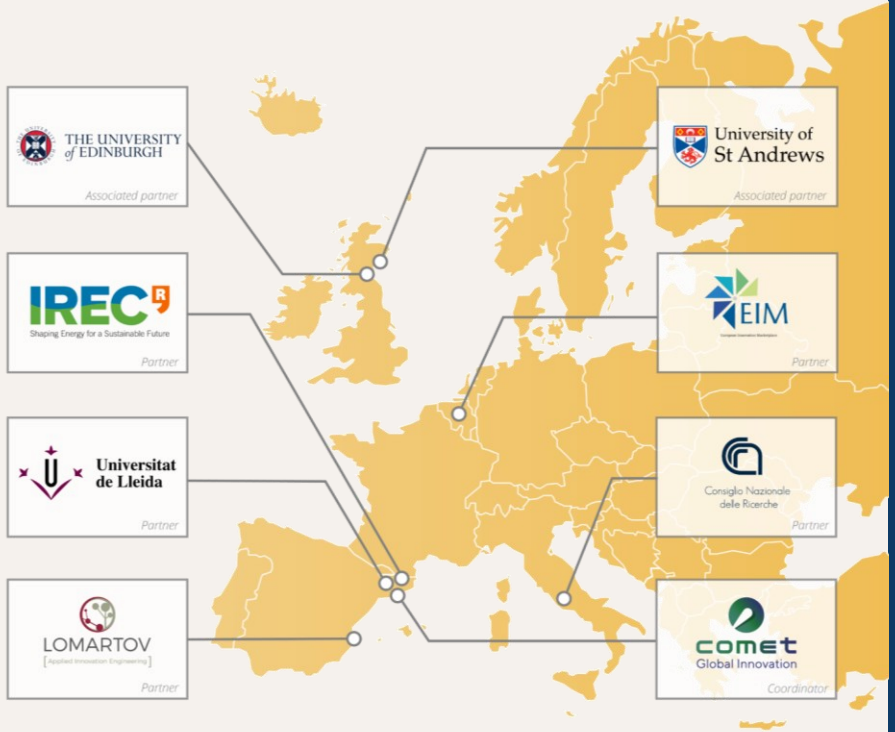
Ethanol H_2 Methane

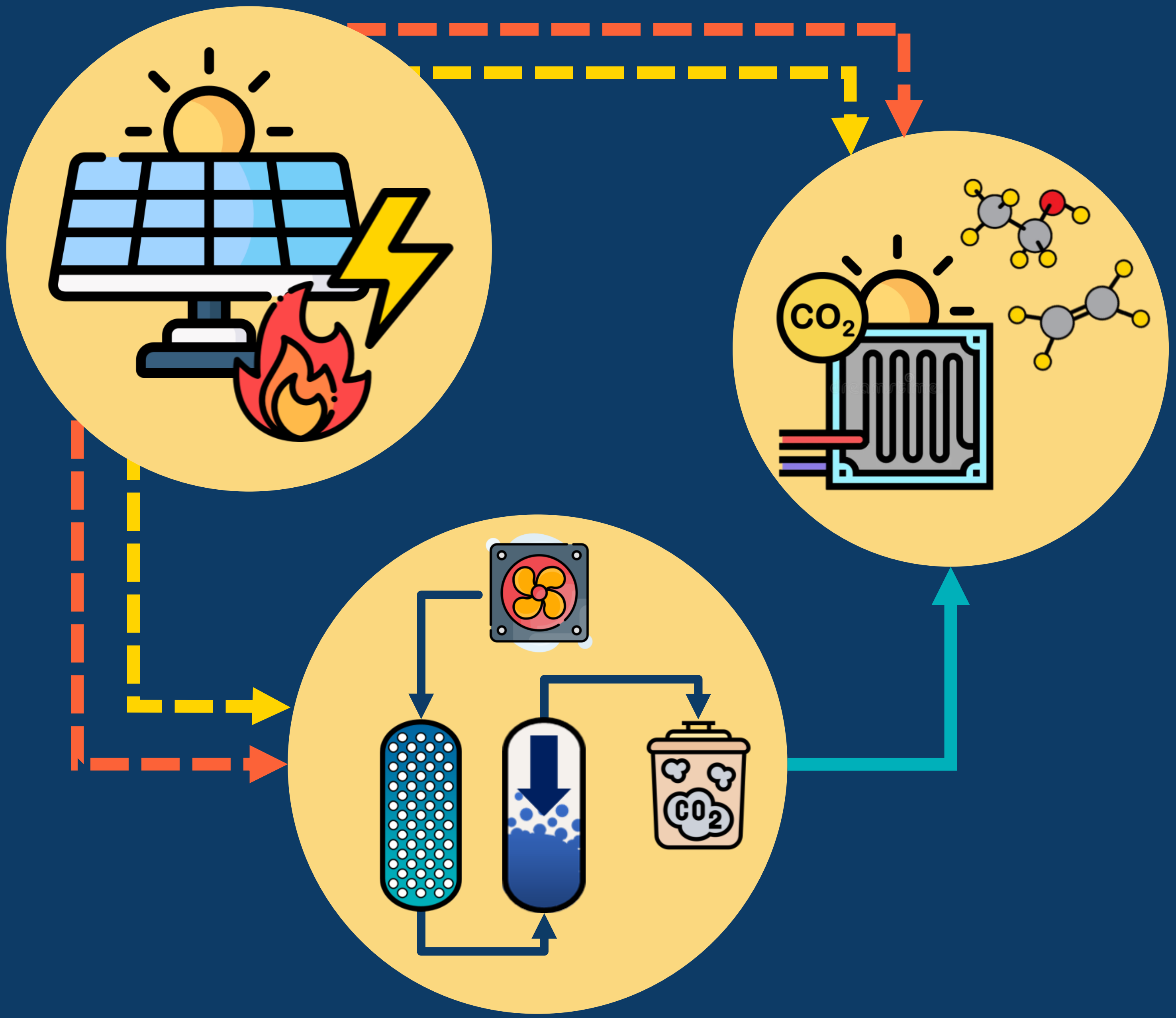
CO   Methanol

(i.c.cavalcante-quaranta@sms.ed.ac.uk)

SolDAC

FULL SPECTRUM SOLAR DIRECT AIR CAPTURE & CONVERSION





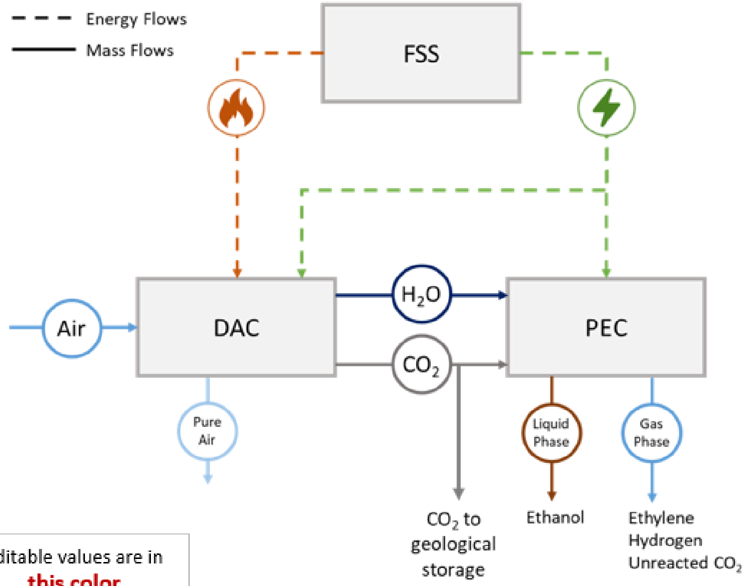
SolDAC

FULL SPECTRUM SOLAR DIRECT AIR CAPTURE & CONVERSION

THE UNIVERSITY of EDINBURGH

THERMO*Model*

Developed by:
Isabella Christina Cavalcante Quaranta (i.c.cavalcante-quaranta@sms.ed.ac.uk)
Giulio Santori (g.santori@ed.ac.uk)



Editable values are in **this color**

Quick Evaluation	
Environmental Analysis	✓
Economic Analysis	✓
Power from FSS : Required to PEC	✓
Thermal Power FSS : Required DAC	✓
Electrical Power FSS : Fan motion in DAC	✓

Run

Clear Results

RESULTS SUMMARY

PEC		
Electrochemical Reaction		
Ethylene production	3.65	kg/year
Ethanol production	0.75	kg/year
Hydrogen production	0.39	kg/year
Total Power Required		
To process 0.01 kg/day of Ethylene	13.13	W
Energy generation or excess in PEC		
Heat Power	9.23	W

PEC	value	units	Observations:
Ethylene Production (single unit)	0.01	kg/day	Total target: 1 kg/day
Electrode area	5	cm^2	
Cell current density	250	mA/cm^2	
Cell potential	3.5	V	
CO_2 Excess factor for PEC inlet	0.3		Excess factor of CO2 demand for the electroch no excess. 1 means a 100% of excess.
Ethanol Faradaic Effecency	10	%	
Ethylene Faradaic Efficiency	80	%	Target: 70%; Current state-of-the-art: 40-60%
Cell equilibrium potential (Ethylene)	1.3	V	Aproximation based on Nernst equation
Cell Arrangement	Parallel		Needs to be either Parallel or Series

DAC		units	Observations:
CO2 atmospheric mass concentration	410	ppm	
Relative humidity	1	%	
Process recovery to product stream	0.8		
Required purity of CO2 product	0.95		
Contactor pressure drop	0.01	kPa	Due to the size of the contactor, we expect no r
Fan efficiency	0.4		
Process efficiency	0.1		
Ambient Temperature	25	°C	
Hot water temperature	60	°C	Target: 60 °C; Current state-of-the-art: 80 °C
Primary thermal energy intensity (no fans)	3	kJ/g	Target: 3 kJ/g; Current state-of-the-art: 8.51 kJ/
DAC Outlet Excess factor (Pure CO2 for storage)	0.1		Excess production of DAC outlet used for geolo product flowrate. Enter zero for no excess. Ente

FSS	value	units	Observations:
Solar radiation	0.4	kW/m^2	Between 0.2 - 1kW/m², average value in Southe
Cold light fraction - electricity	0.7		Wave lenghts of 400-1100 nm
UV/IR fraction - heat	0.3		Wave lenghts of 1100-2500 nm and below 400
Field area	0.6	m^2	✓
Fresnel Optical Efficiency	0.55		
Thermal efficiency	0.53		Minimum: 0.35; Maximum: 0.7
Photovoltaic fraction	0.7		
Photovoltaic conversion efficiency	0.22		Light to electricity conversion efficiency (Theor
Radiation time	7.25	h	
Extra Operation time from renewable energy excess	1	h	

DAC and PED operation	value	units	Observations:
Working hours	8	h/day	If this value is higher than the radiation time,
Working days	365	day/year	

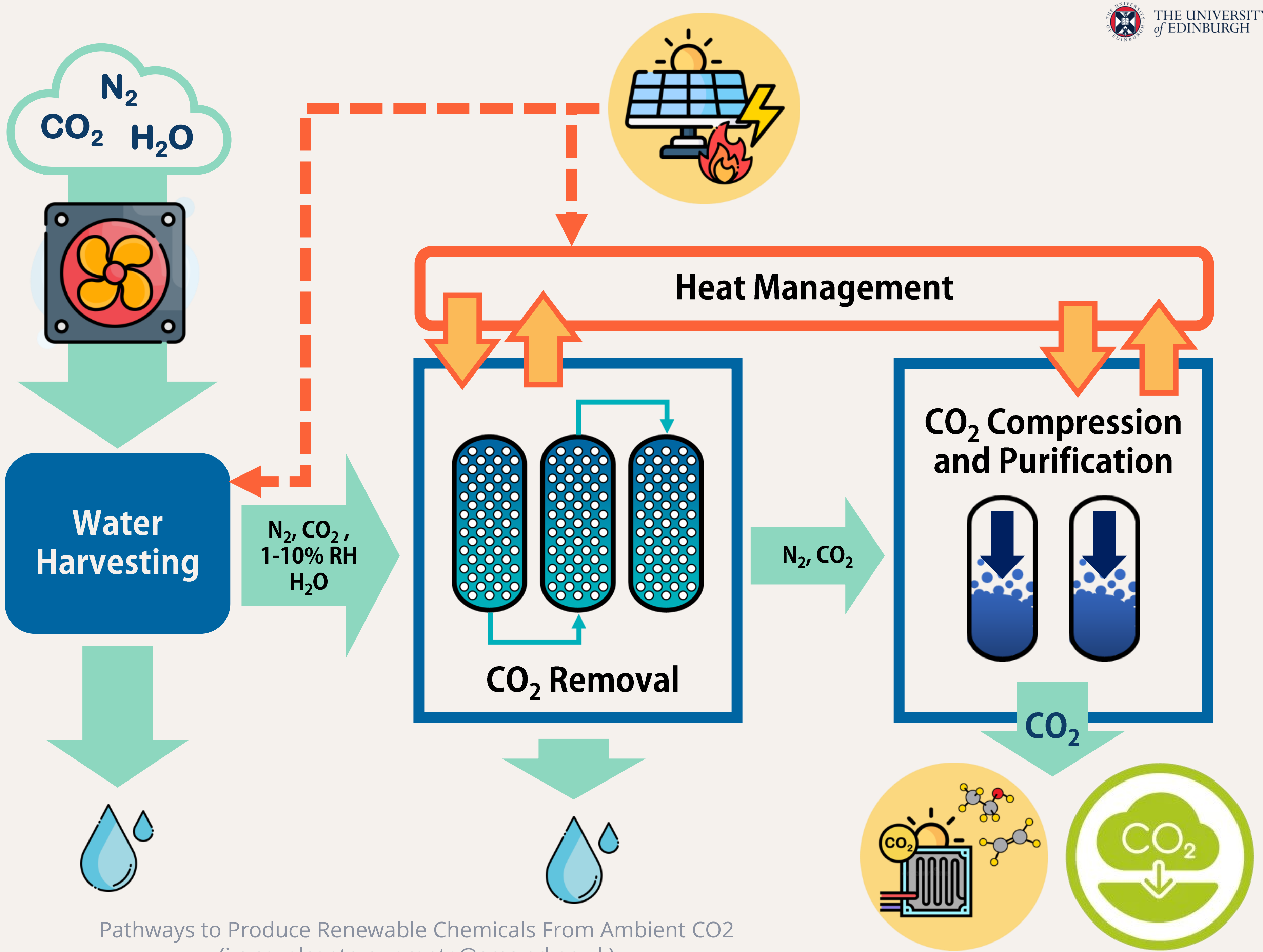
DETAILED RESULTS:

PEC | DAC | FSS

Energy Requirements | Economic Check | Environmental Check

DEFINE PROJECT SCALE

DIRECT AIR CAPTURE UNIT

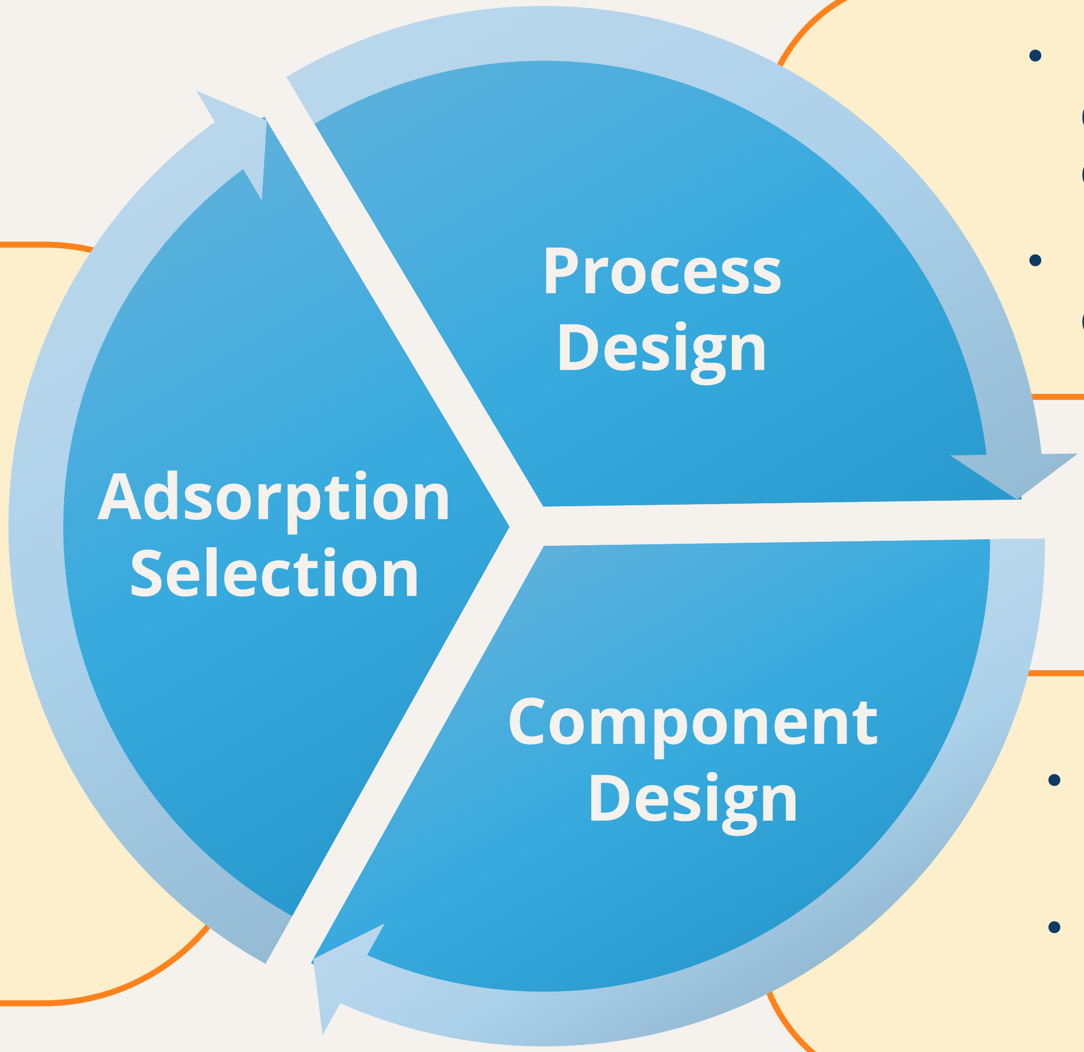


(i.c.cavalcante-quaranta@sms.ed.ac.uk)

CO_2 REMOVAL:

THE UNIVERSITY of EDINBURGH

- High CO_2 capacity and favourable kinetics in ultra-dilute conditions
- Selectively for CO_2 in different levels of humidity

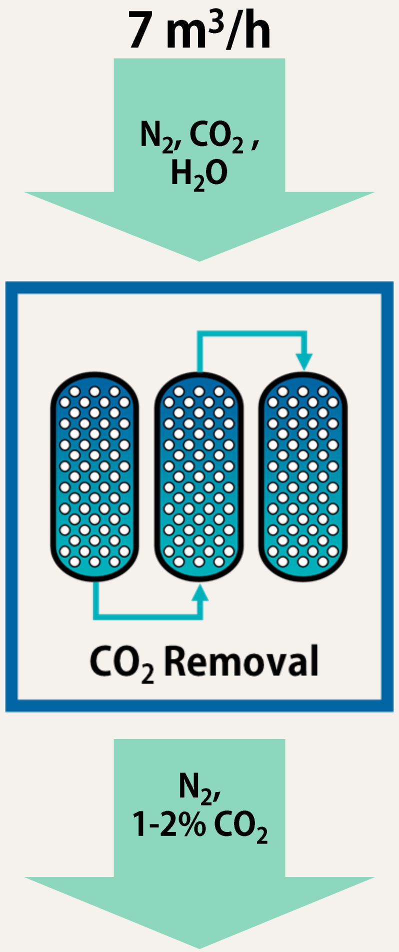


- Focus on ultra dilute components
- Low energy consumption

- Reduced pressure drop
- Favourable mass transfer

CO_2 REMOVAL:

PROCESS DESIGN



Use of low grade heat/waste heat (< 80° C)

Energy 238 (2022) 121967

Thermal Energy Source:

Solar Energy

No vacuum

Reduce processing costs

CO_2 concentration 80+%

Multiple beds to pre-concentrate CO_2

Energy 162 (2018) 1158 - 1168

Ultradilute CO_2

Temperature Swing Adsorption (TSA)

(i.c.cavalcante-quaranta@sms.ed.ac.uk)

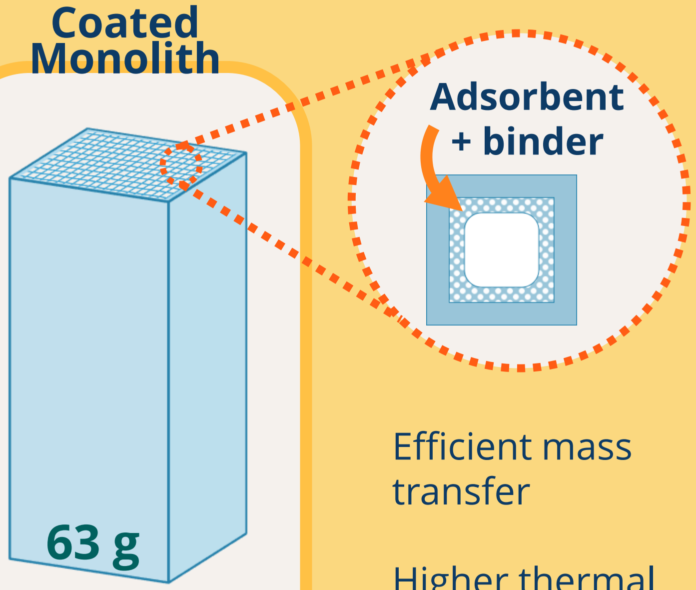
CO_2 REMOVAL:

COMPONENT DESIGN

- Contactor

Reduced pressure drop

Favourable mass transfer



L=15 cm, D = 6 cm

ΔP = 36.9 Pa

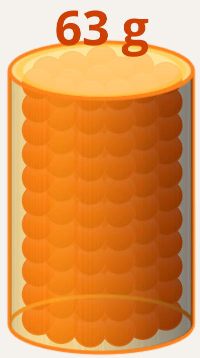
AIChE J. 2022;68:e17650

Efficient mass transfer

Higher thermal stability

Reduced pressure drop

Packed Bed



L=6.6 cm, D = 6 cm

ΔP = 100.8 Pa

Darcy Equation

High bed density

More control on the concentration front

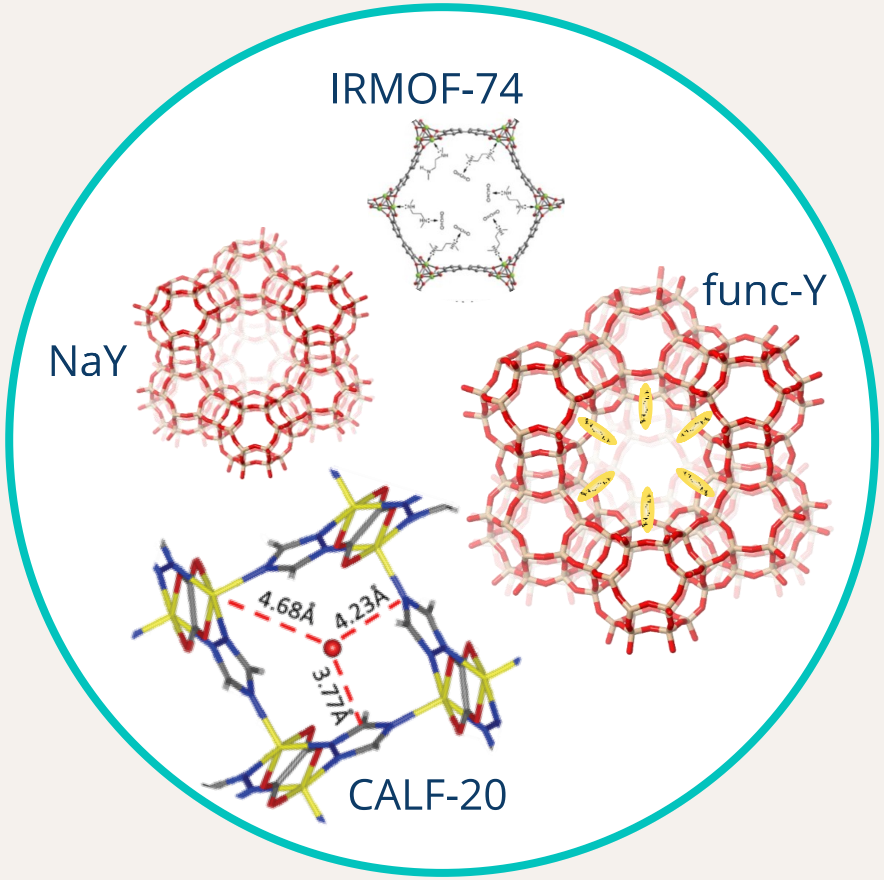
- Collector

High adsorption capacity

Favourable mass transfer

CO_2 REMOVAL:

ADSORBENT SELECTION



Equilibrium measurements

Gravimetric apparatus (DVS, ASAP 2020)

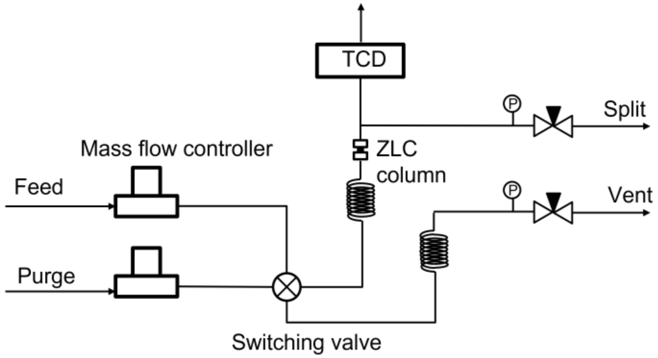
Volumetric apparatus (Autosorb)

Chromatograph apparatus (ZLC)

Kinetic measurements

Volumetric apparatus

Chromatograph apparatus (ZLC)

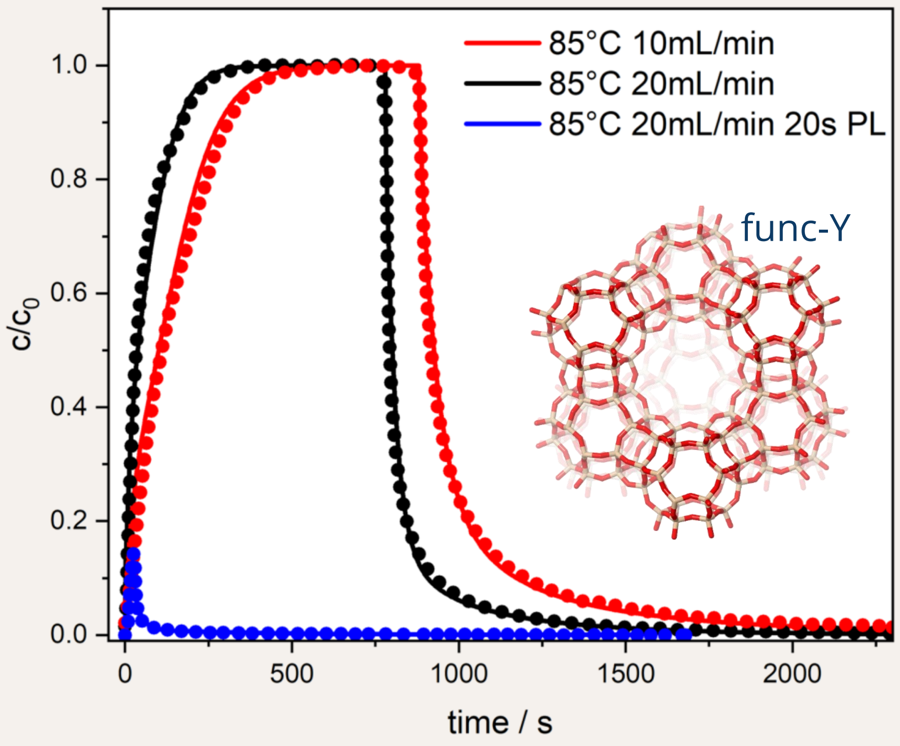


Materials were kindly provided by Prof. Paul Wright and Dr Harpreet Kaur from University of St Andrews

Pictures and results were kindly provided by Zhenye Xu

CO_2 REMOVAL:

ADSORBENT SELECTION



Materials	Capacity	Kinetics	Application
Na-Y	Small	Very fast	Compression
CALF-20	Small	Very fast	Concentration/ Compression
func-Y	Large	Fast	Removal area
IRMOF-74	Large	Slow	Compression

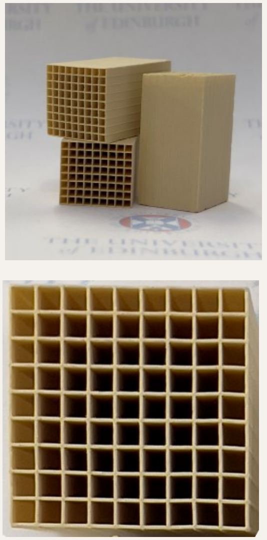
Can it be coated on the monolith?

Materials were kindly provided by Prof. Paul Wright and Dr Harpreet Kaur in University of St Andrews

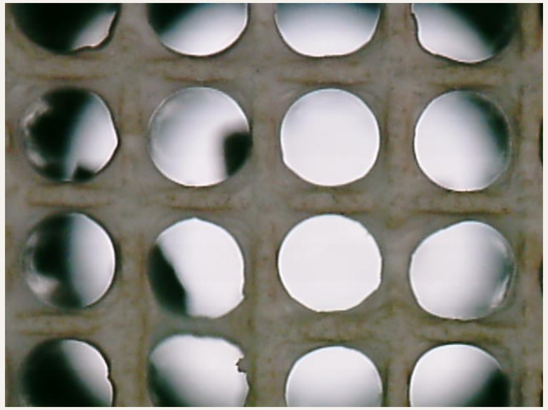
Pictures and results were kindly provided by Zhenye Xu

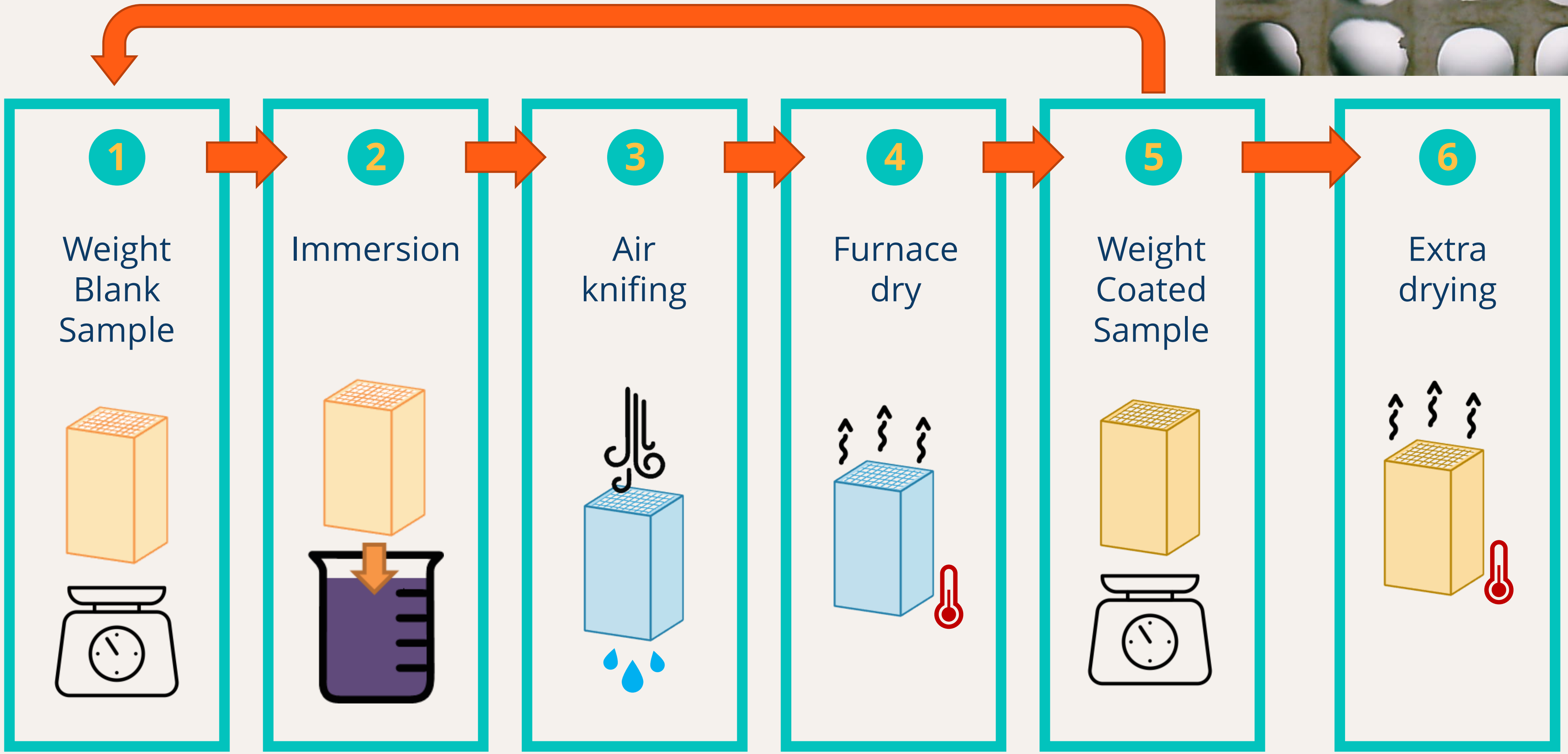
CO_2 REMOVAL:

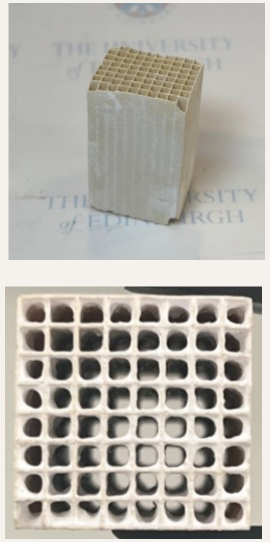
MONOLITH COATING



Bare monolith



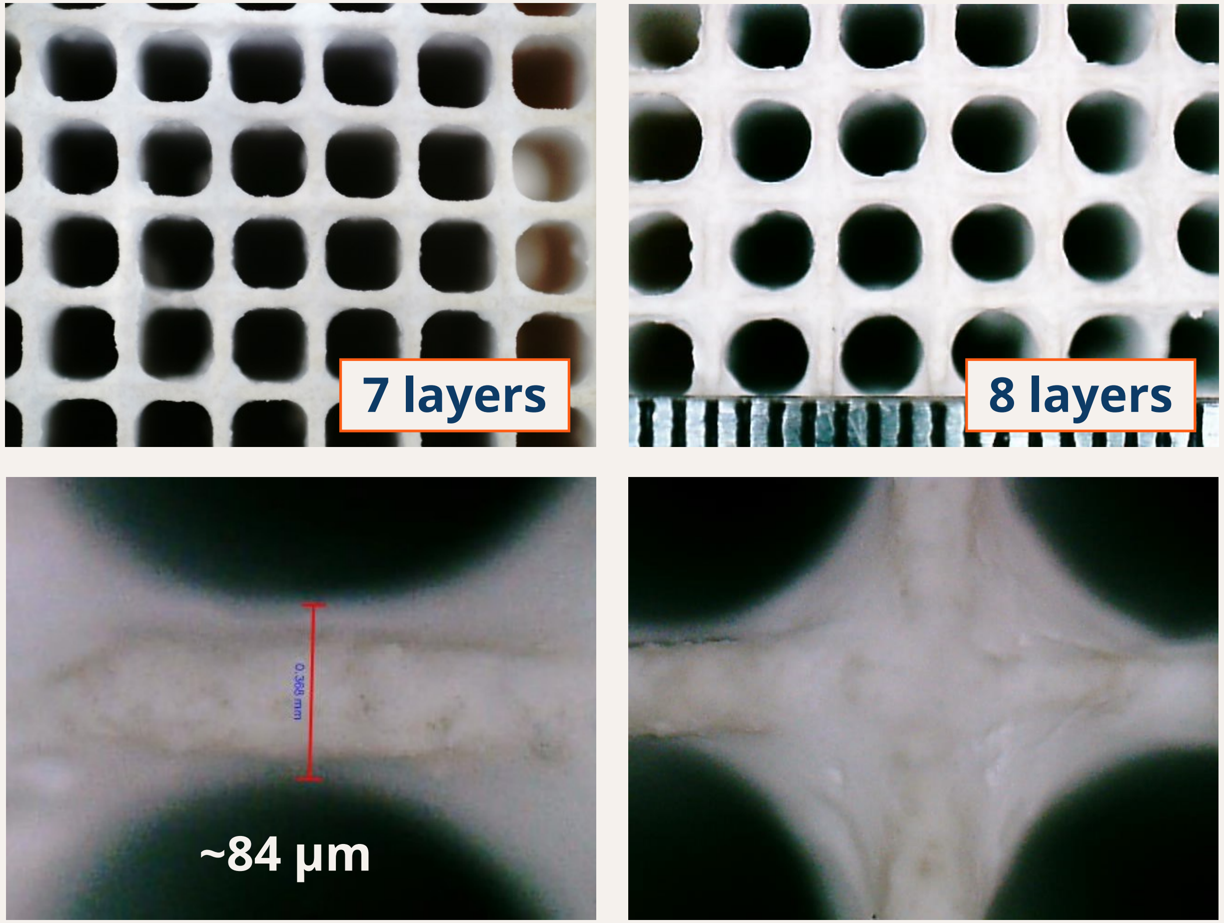


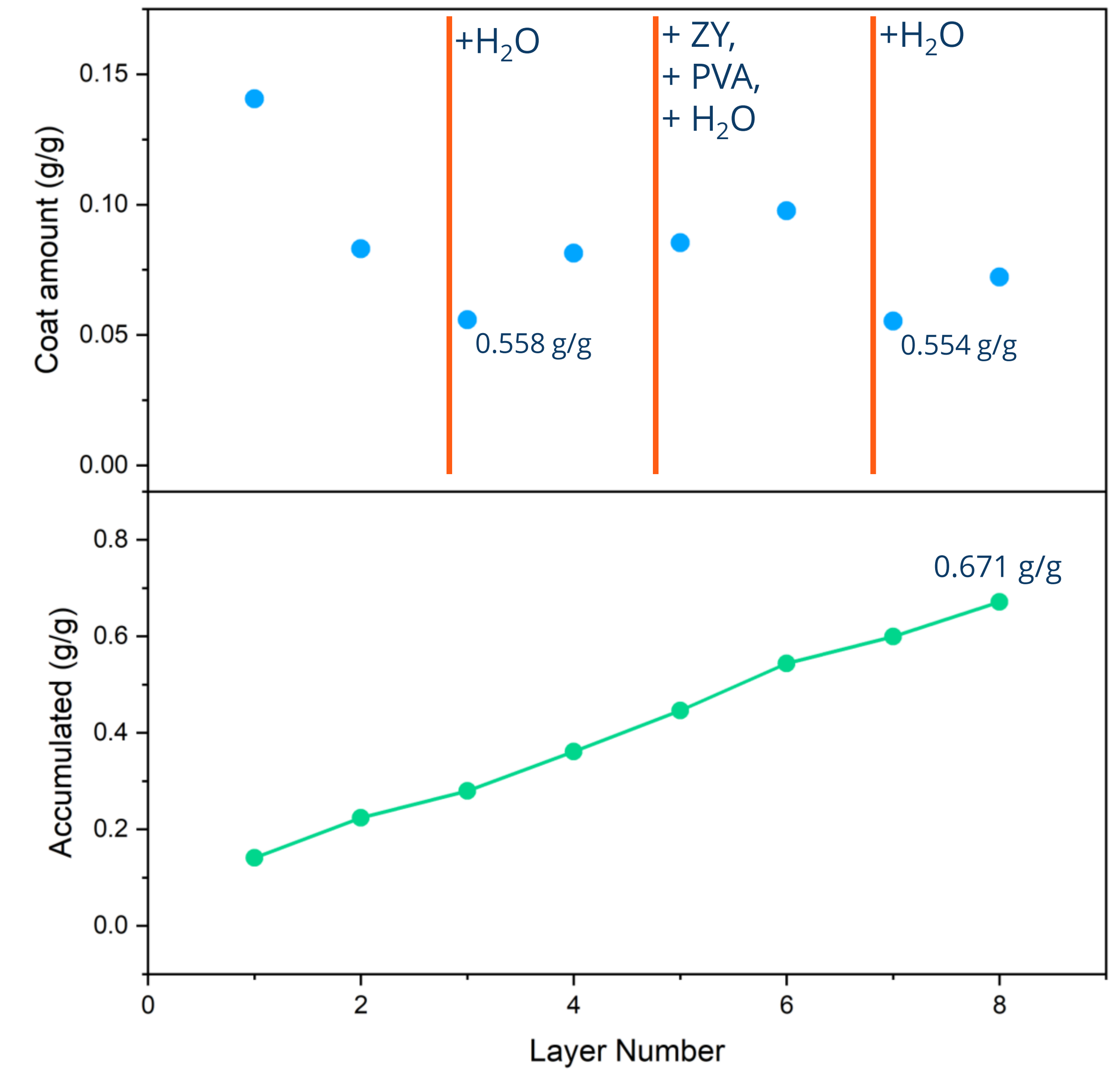


Coated Monolith

CO_2 REMOVAL:

MONOLITH COATING

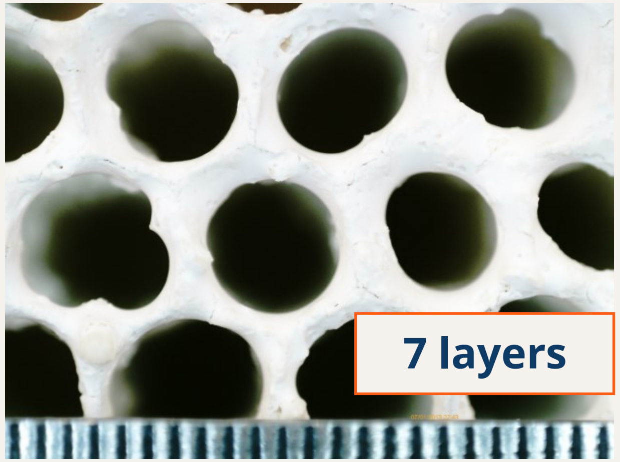


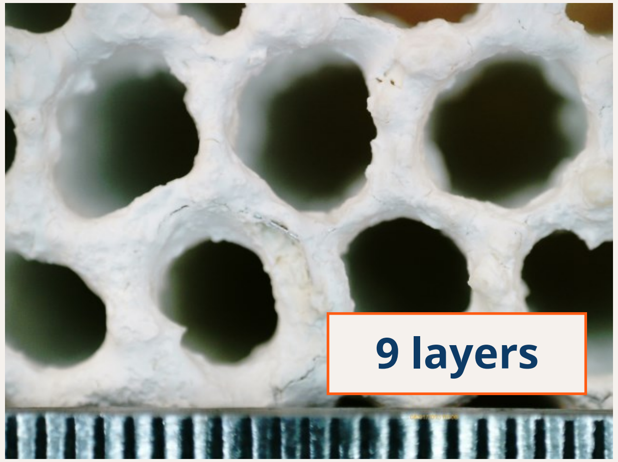


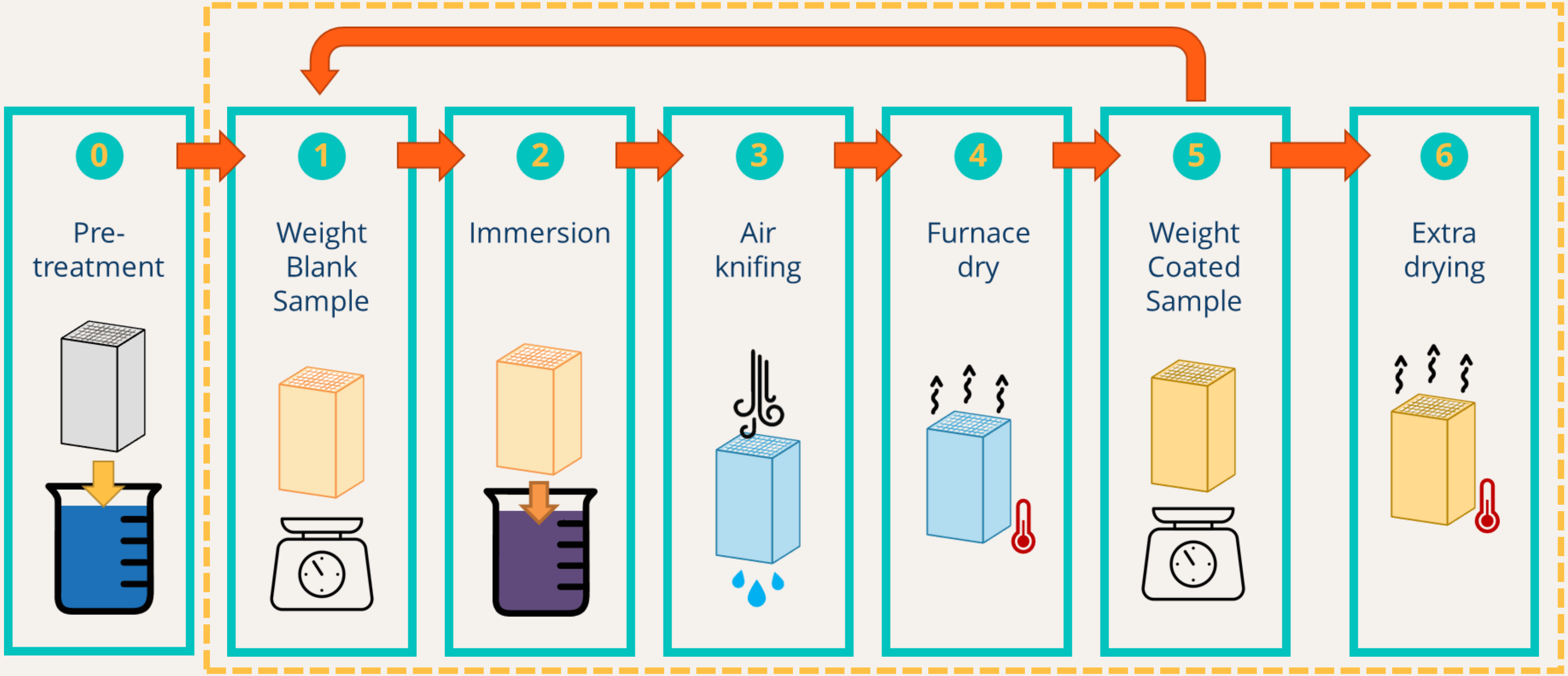
(i.c.cavalcante-quaranta@sms.ed.ac.uk)

CO_2 REMOVAL:

METAL SUPPORT COATING







Pictures kindly provided by Man Zhang

SHANGHAI JIAO TONG UNIVERSITY

CO_2 REMOVAL:

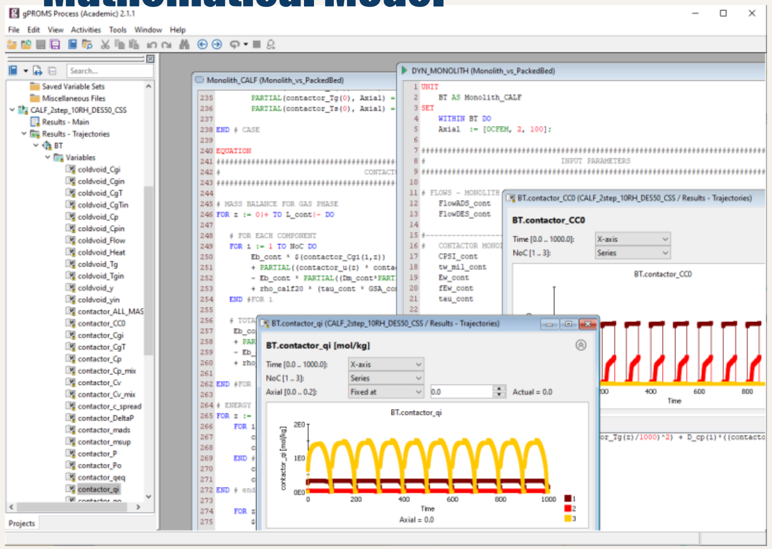
MODELLING

- **Feed limit composition**
- **Adsorbent amount**
- **Desorption temperature**
- **Cycle scheduling**
- Adsorption beds integration
- Prototype design

- **Desorption Temperature:**
  - 50 °C
  - 60 °C
  - 70 °C

- **Water in feed:**
  - 1% RH
  - 10% RH
  - 15% RH

Mathematical Model



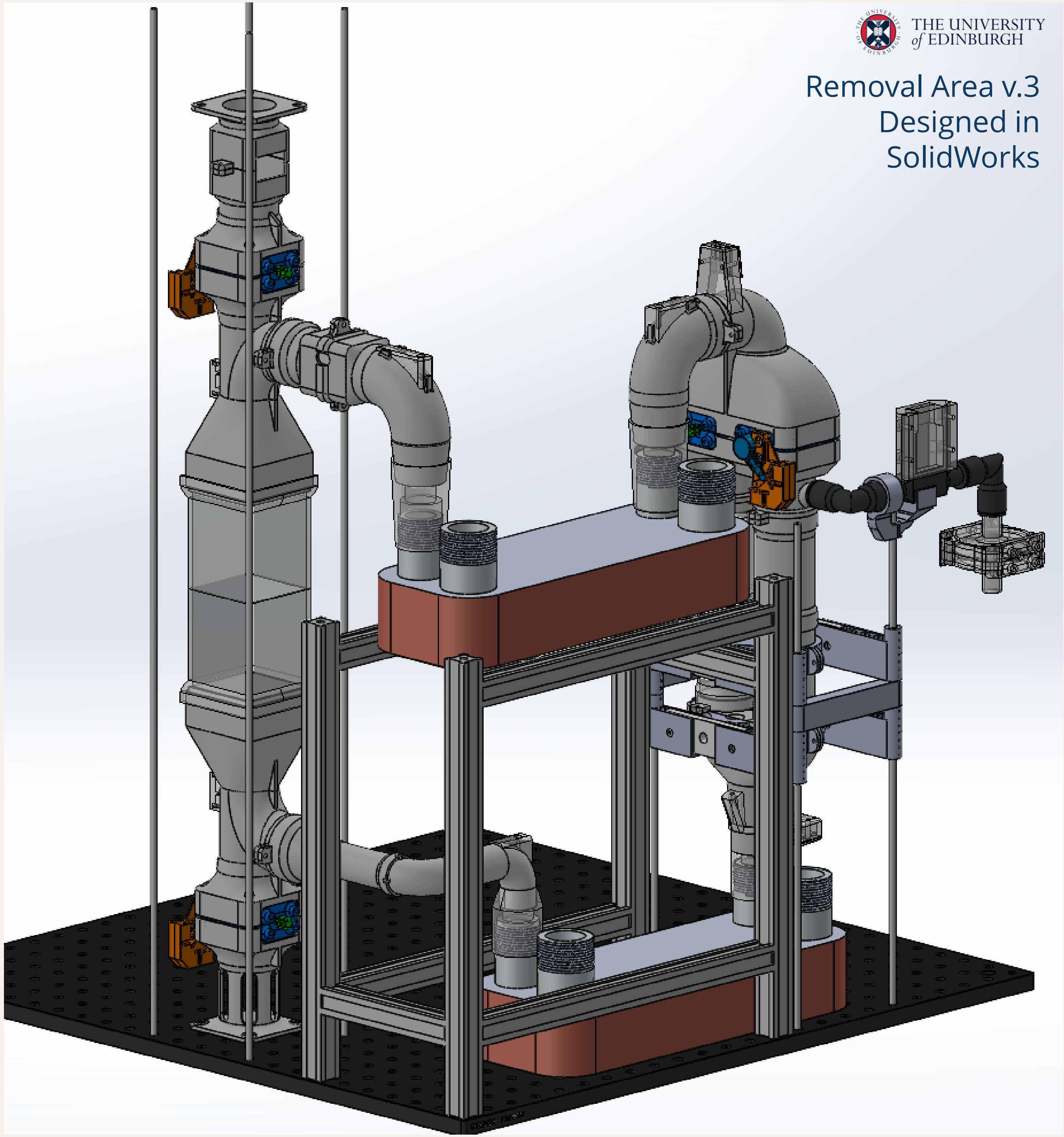
Pathways to Produce Renewable Chemicals From Ambient CO2

(i.c.cavalcante-quaranta@sms.ed.ac.uk)

CO_2 REMOVAL:

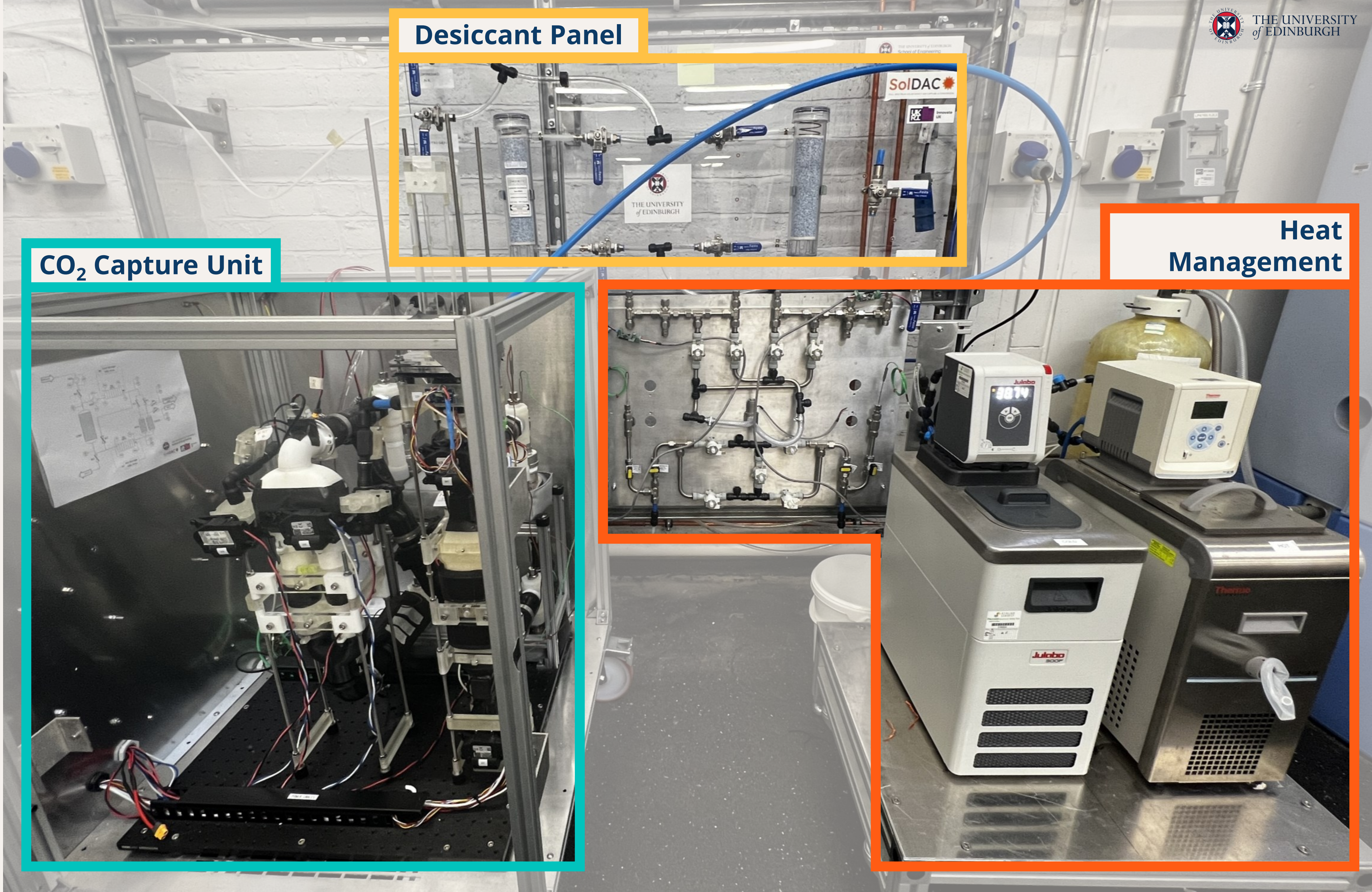
MODELLING

- Feed limit composition
- Adsorbent amount
- Desorption temperature
- Cycle scheduling
- **Adsorption beds integration**
- **Prototype design**



Removal Area v.3 Designed in SolidWorks

CO_2 REMOVAL: PROTOTY ASSEMBLY



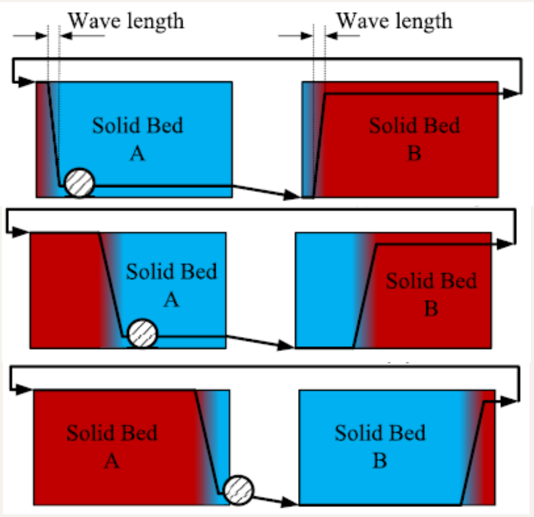
THE UNIVERSITY of EDINBURGH

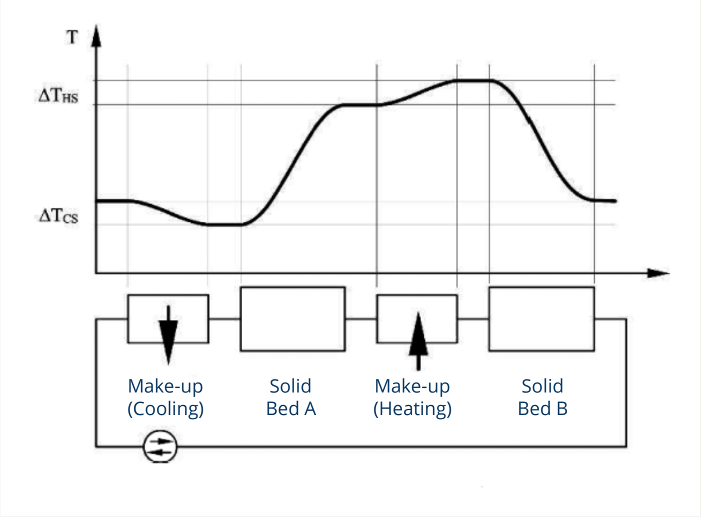
CO_2 REMOVAL:

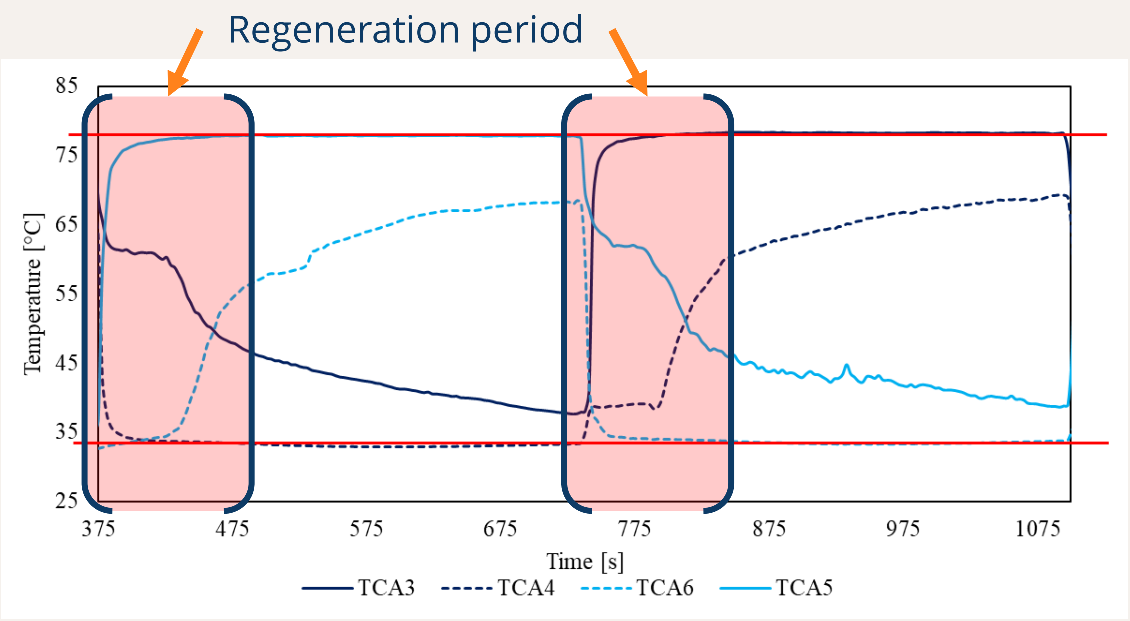
HEAT MANAGEMENT

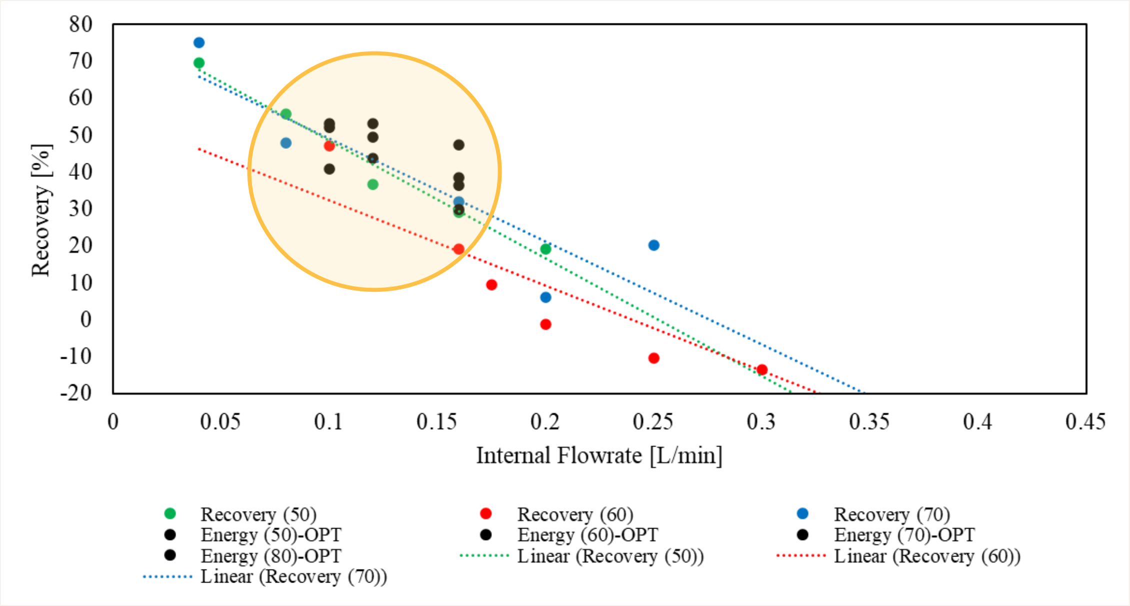
Thermal Wave Method

Reduce energy input by recovering sensible heat







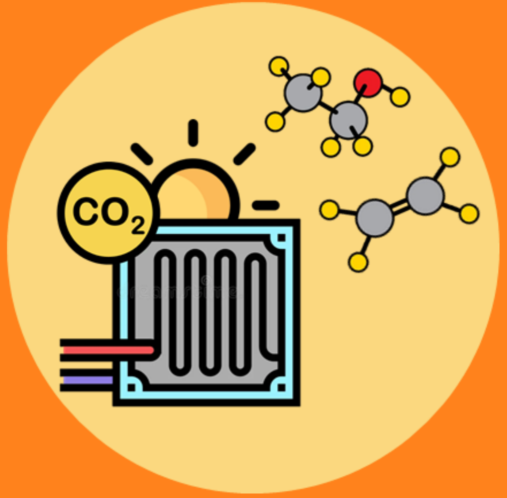


Experimental results were kindly provided by Marwan Mohammed

THE UNIVERSITY of EDINBURGH

Ethylene Conversion

Electrodeposition of Cu catalysts



Results kindly provided by Mayra Tovar

THE UNIVERSITY of EDINBURGH

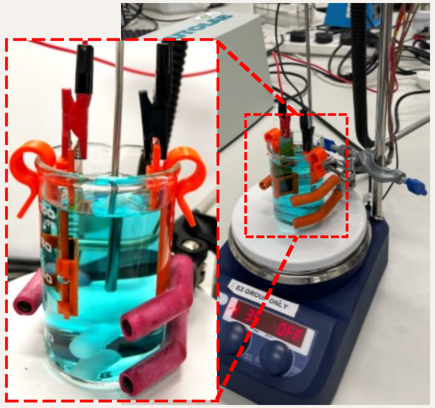
Catalyst

Electrolyte preparation → Cu catalyst

Optimisation

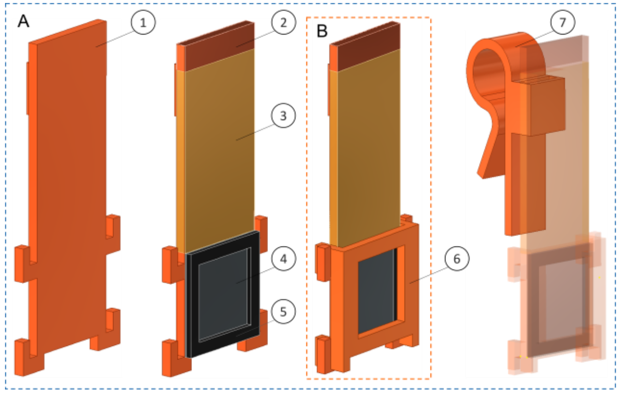
Preparation of GDLs → HNO_3 treatment → Assembly of electrodeposition jigs

Set-up



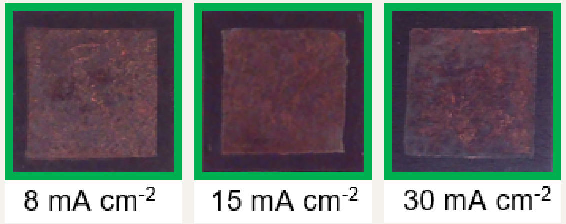
Optimising parameters

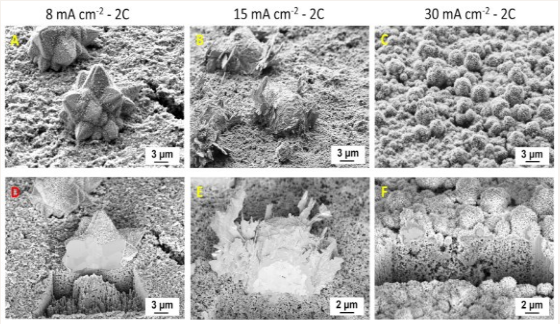
pH | Temperature | Charge | Current



Before

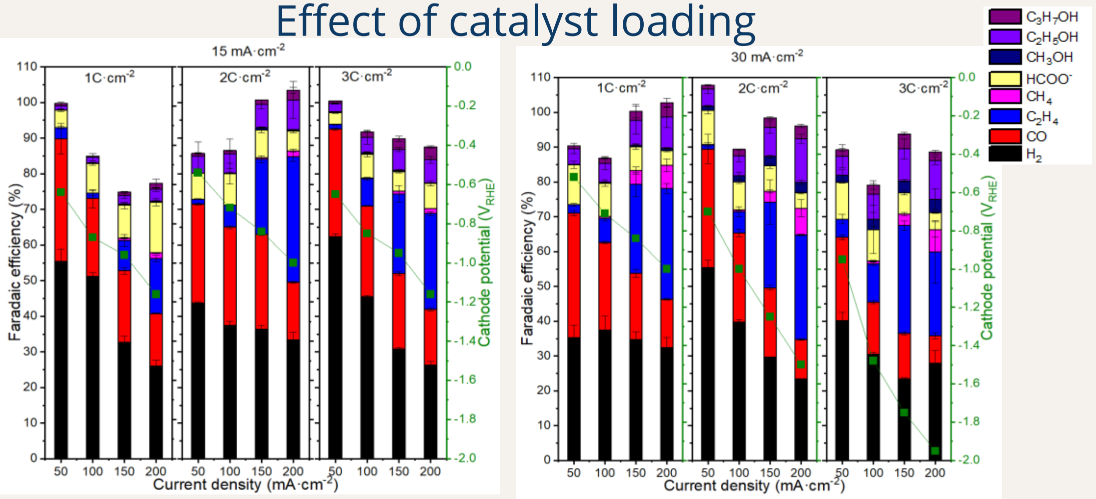
After





Faradaic Efficiency

Effect of catalyst loading



Pathways to Produce Renewable Chemicals From Ambient CO2

(i.c.cavalcante-quaranta@sms.ed.ac.uk)

ISABELLA QUARANTA

PhD Researcher
The University of Edinburgh
i.c.cavalcante-quaranta@sms.ed.ac.uk

THANK YOU!

SCCS PhD Consortium 2024

This project has received funding from UK Research and Innovation - Innovate UK under Innovation Funding Service (ISF) 10039331 – Full spectrum solar direct air capture and conversion: https://soldac-project.eu/