Imperial College London

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# UKCCSRC Core Research Projects Capture Theme - Solid Sorbents

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A1b: Clemens Patzschke, Matt Boot-Handford, Paul Fennell

September 4th, 2019

BarrerCentre

CleanFaB

EPSRC Engineering and Physical Sciences Research Council

# Sorbent materials for advanced solid looping cycles

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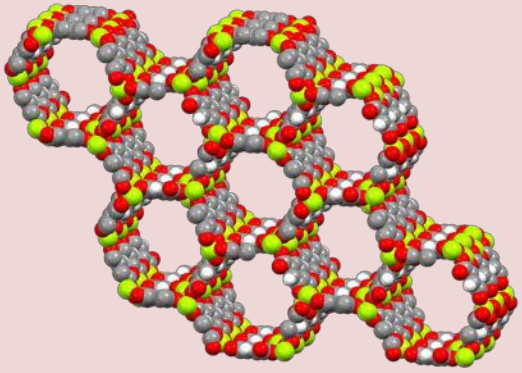
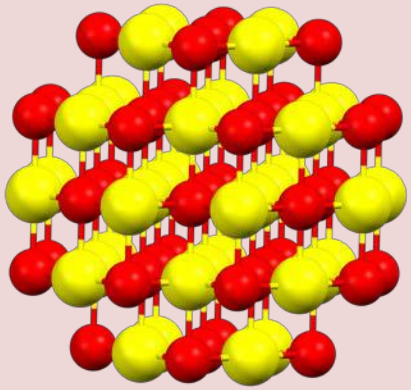
## Research theme scope

### Post-combustion capture



Porous low T sorbents
*e.g.* metal organic frameworks (MOFs), activated carbons, zeolites

### Chemical looping combustion



Porous high T sorbents
*e.g.* CaO, $Fe_2O_3$, CuO

- Measure materials sorption and physical properties
- Develop 'basic' process models

## Links with other themes

- Advanced process models
- Pilot plant demonstrations

# Post-combustion capture – WP A1a

**Research questions:**

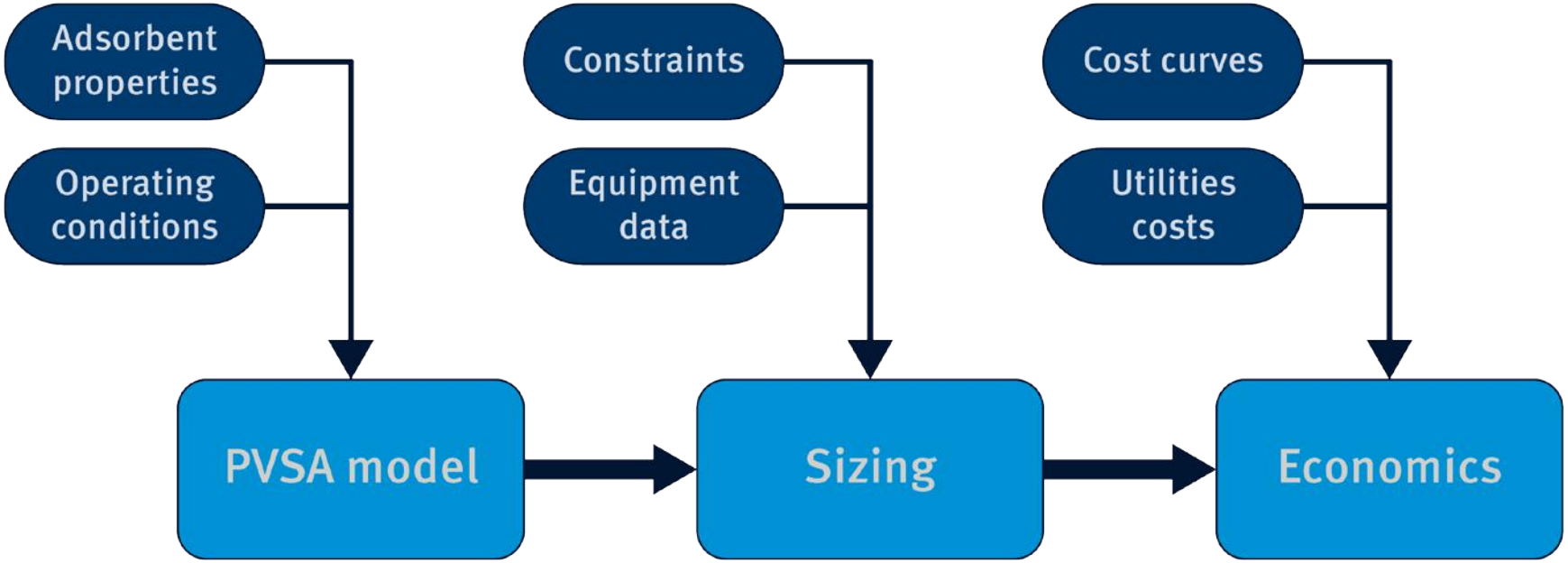
- Can adsorption be used for post-combustion $CO_2$ capture?
- What does a *good* adsorbent 'look like'?
- Which experimental data is missing/needed to assess an adsorbent?

**Approach:**

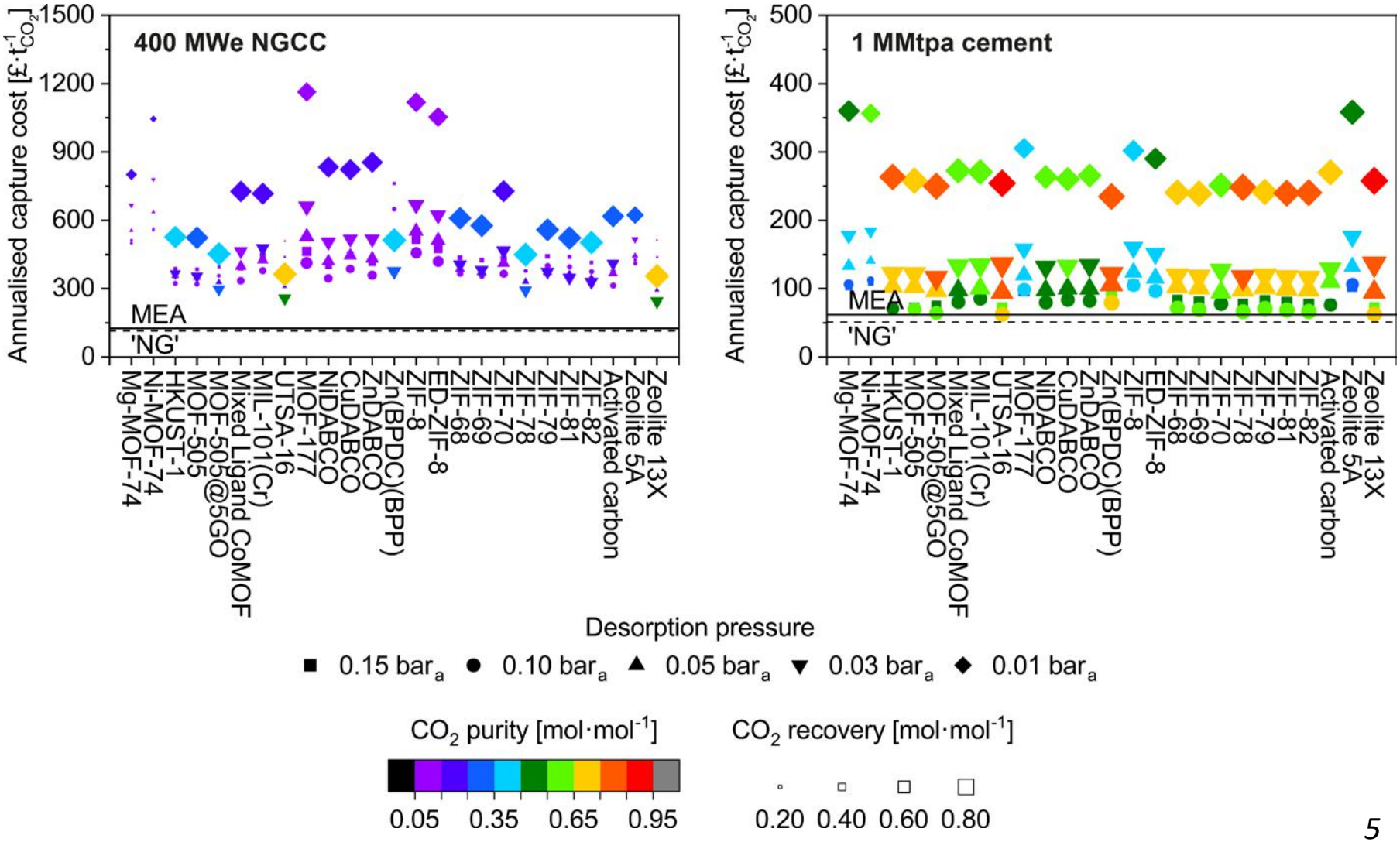
- Adsorbent screening tool for various $CO_2$-containing streams - *completed*
- Surrogate model for screening of new adsorbents - *completed*
- Identification of links between material properties and capture performance and cost - *completed*
- Evaluation of missing physical properties data of adsorbents - *on-going*

# Adsorbent screening tool

- PVSA model with integrated process economics



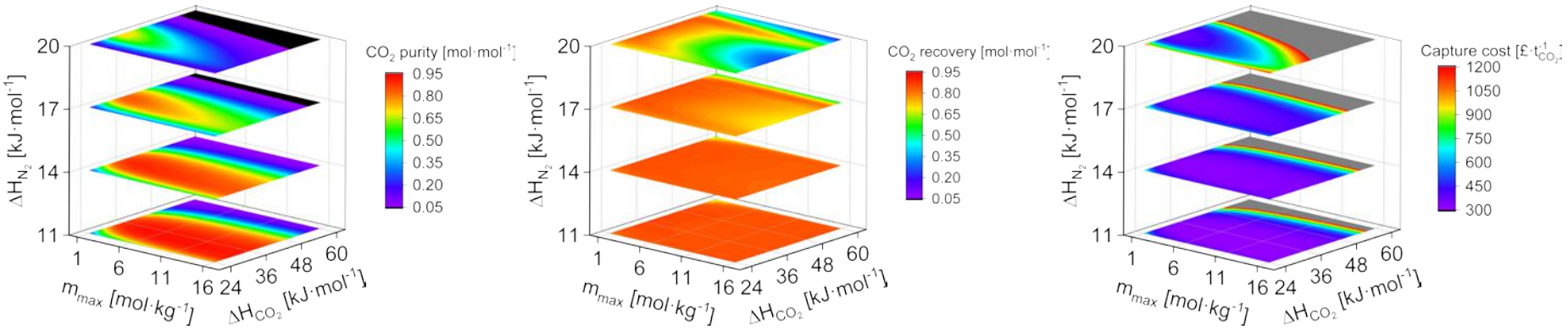
# MOF screening output



# Surrogate model (ROM)

- Data generated using screening tool
  - Surrogate model generated using ALAMO
  - Swift preliminary evaluation of new adsorbents
  - Will be publicly available

$$n_j = \frac{m_{\max} \cdot b_0 \cdot \exp\left(\frac{\Delta H_j}{RT}\right) \cdot P}{1 + b_0 \cdot \exp\left(\frac{\Delta H_j}{RT}\right) \cdot P}$$

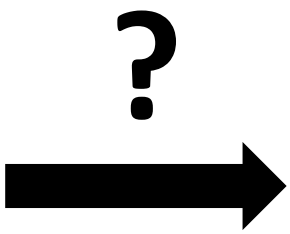


# Influence of adsorbent properties

- Vary input parameters which describe adsorption and observe changes
  - Physical interpretation of those parameters to adsorbent properties

**Material properties**

- Adsorbed amount
- Gas-solid interactions
- Selectivity

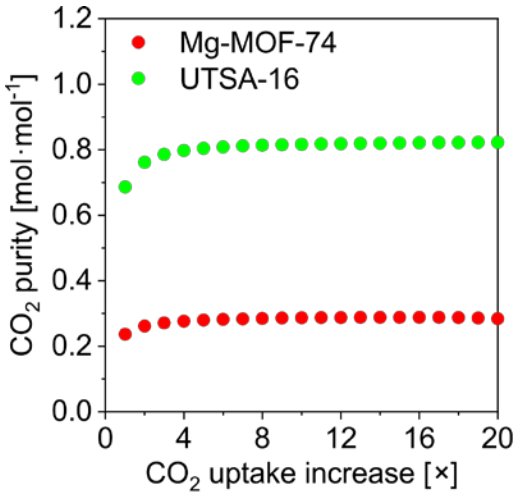


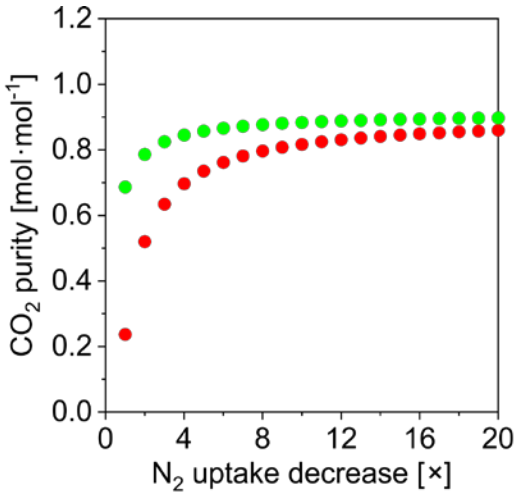

**Performance metrics**

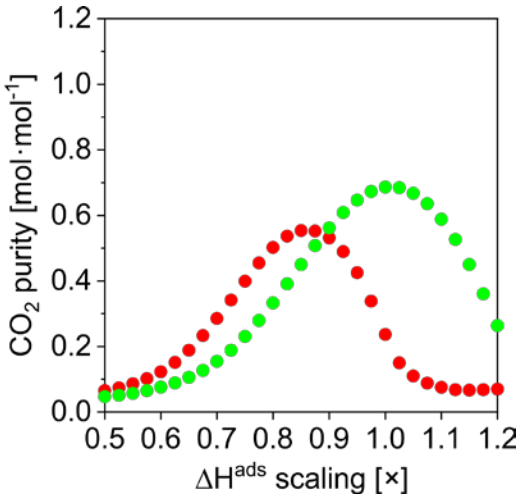
- $CO_2$ purity
- $CO_2$ recovery
- Capture cost

# Influence of adsorbent properties

- Vary input parameters which describe adsorption and observe changes
  - Physical interpretation of those parameters to adsorbent properties



# Come by our poster!

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## Adsorbent evaluation and design for post-combustion $CO_2$ capture (WP A1a)

Co-Investigator: Camille Petit, Niall Mac Dowell
Key researchers: David Danaci, Mai Bui
Funded by the UKCCSRC as part of its Core Research Programme
Dates: 01/2019 – current

CleanFaB

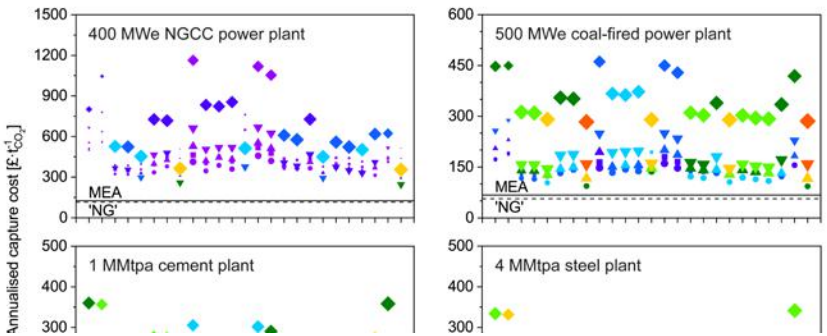
bit.ly/PetitGroup
bit.ly/CleanFaB
bit.ly/ddanaci

### Project overview

- Investigate the suitability of adsorption for post-combustion $CO_2$ capture
- Consider a range of flue gas sources for separation by pressure-swing (PSA) & temperature-swing adsorption (TSA)
- Identify the 'ideal adsorbent' characteristics which maximise performance
- Identify required input data to accurately assess an adsorbent, and populate missing data

Key objectives:

### Adsorbent screening results for post-combustion and industrial capture



# Chemical looping combustion – WP A1b

**Research questions:**

- What is the potential of mixed metal oxygen carriers in chemical looping?
- What are the reaction pathways involved?
- How can the thermodynamics and kinetics of the reaction be optimised?
- What is the potential of the materials for scale-up?

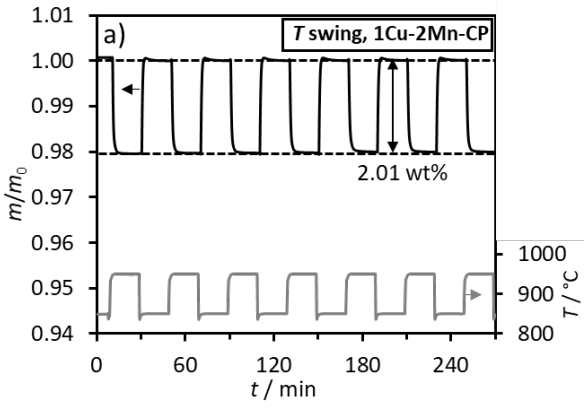
**Approach:**

- Study on copper manganese oxides for chemical looping - *completed*
- FBR tests and TG analyses for long-term cycling - *completed*
- Reaction kinetics from FBR experiments - *completed*
- Bench-scale co-precipitation batch reactor synthesis scale-up - *on-going (Cranfield U.)*

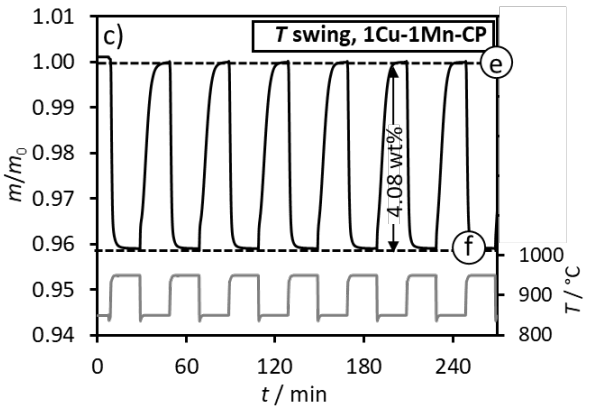
# $Cu_xMn_yO_z$ – kinetics optimisation

- Fast kinetics, good capacity, reversible for CLAS

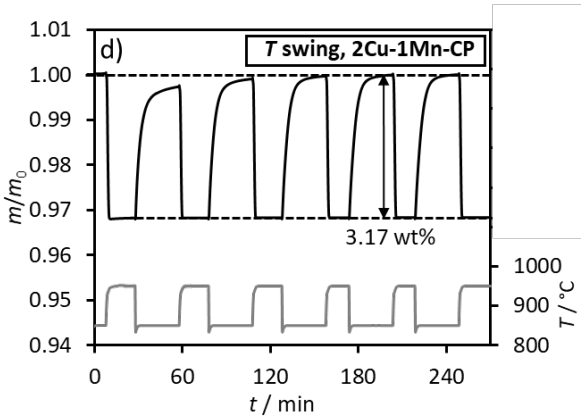
Cu:Mn = 1:2




Cu:Mn = 1:1




Cu:Mn = 2:1

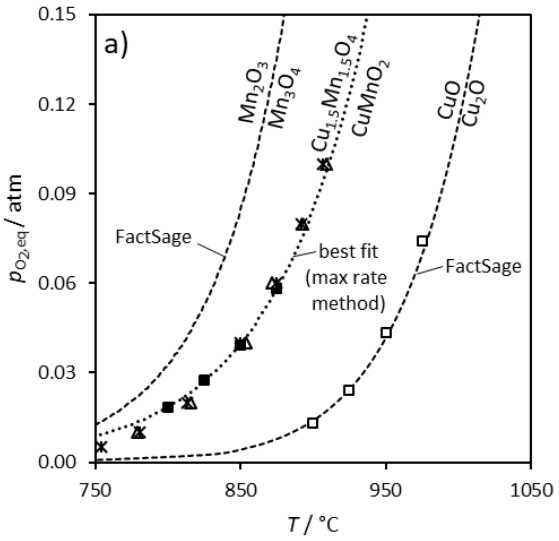



- Oxidation – 10 % $O_2$ in $N_2$ @ 850 °C
- Reduction – 10 % $O_2$ in $CO_2$ @ 950 °C
- Flow rate constant @ 170 $mL_{STP} \cdot min^{-1}$

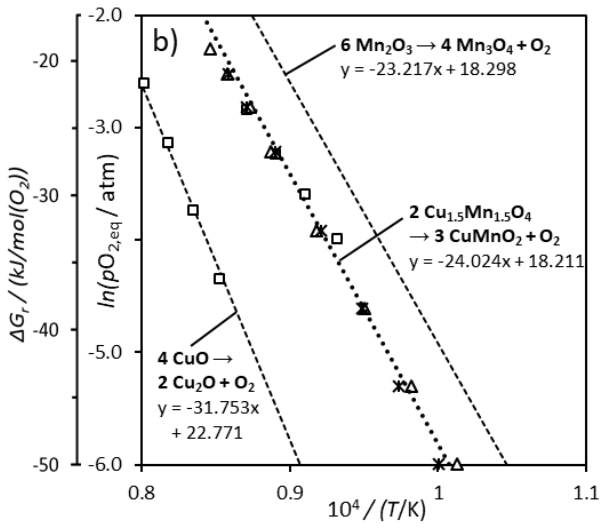
# $Cu_xMn_yO_z$ – equilibria optimisation

- Novel experimental method developed for $O_2$ equilibria, $\Delta H_r$
  - $P_{O2,eq}$ calculated from observed reaction kinetics data
  - Allows calculation of $P_{O2,eq}$ for complex MMOs

$P_{O2,eq}$ *vs* T




$\ln(P_{O2,eq})$ *vs* 1/T



# $Cu_xMn_yO_z$ – further findings

**Reaction kinetics**

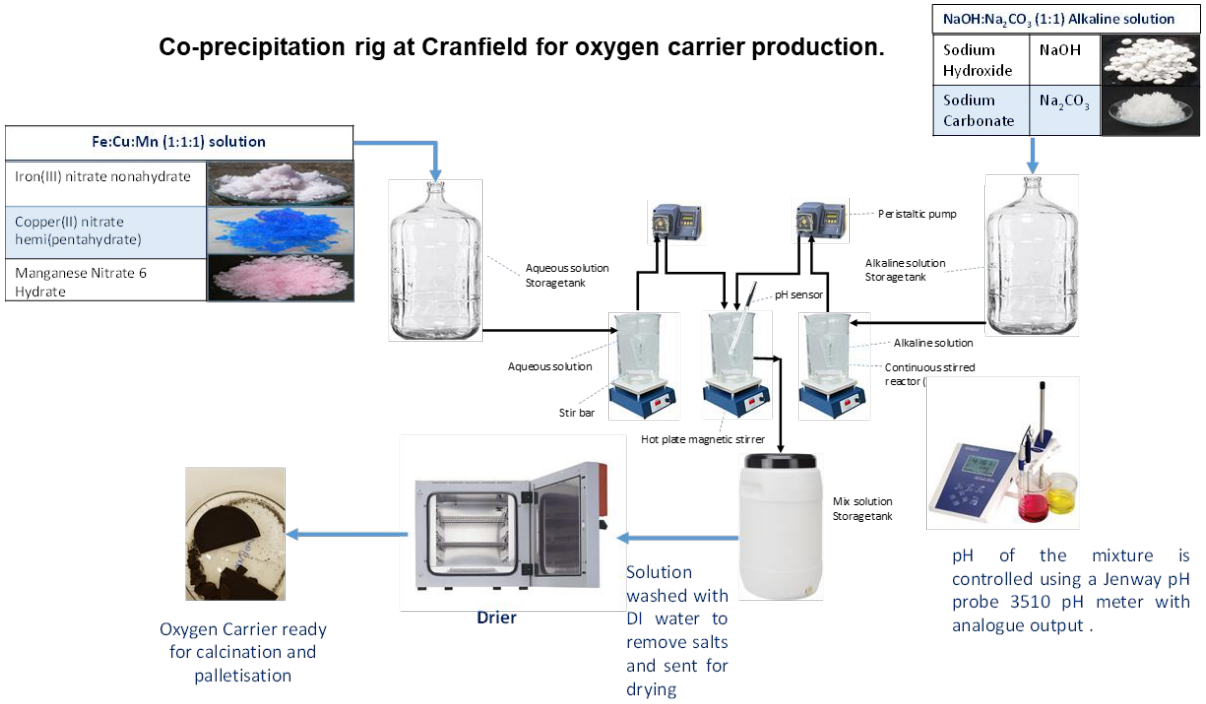
- Fundamental reaction mechanisms established
- Reaction model for $O_2$ release and oxidation developed

**Particle evolution**

- Long term cycling and particle evolution over different cycling modes
- Studied the effect of various support materials on the change of the pore morphology and porosity over extended cycling periods

# Material scale-up

- Spent time at Cranfield University to assist with co-precipitation reactor commissioning
- Trials are ongoing at CrU to improve particle strength



# Acknowledgements


- Mr. Wouter Arts for MOF isotherm data survey
- Funding to undertake this work is provided by the EPSRC

# Appendices

- Petit Group appendix

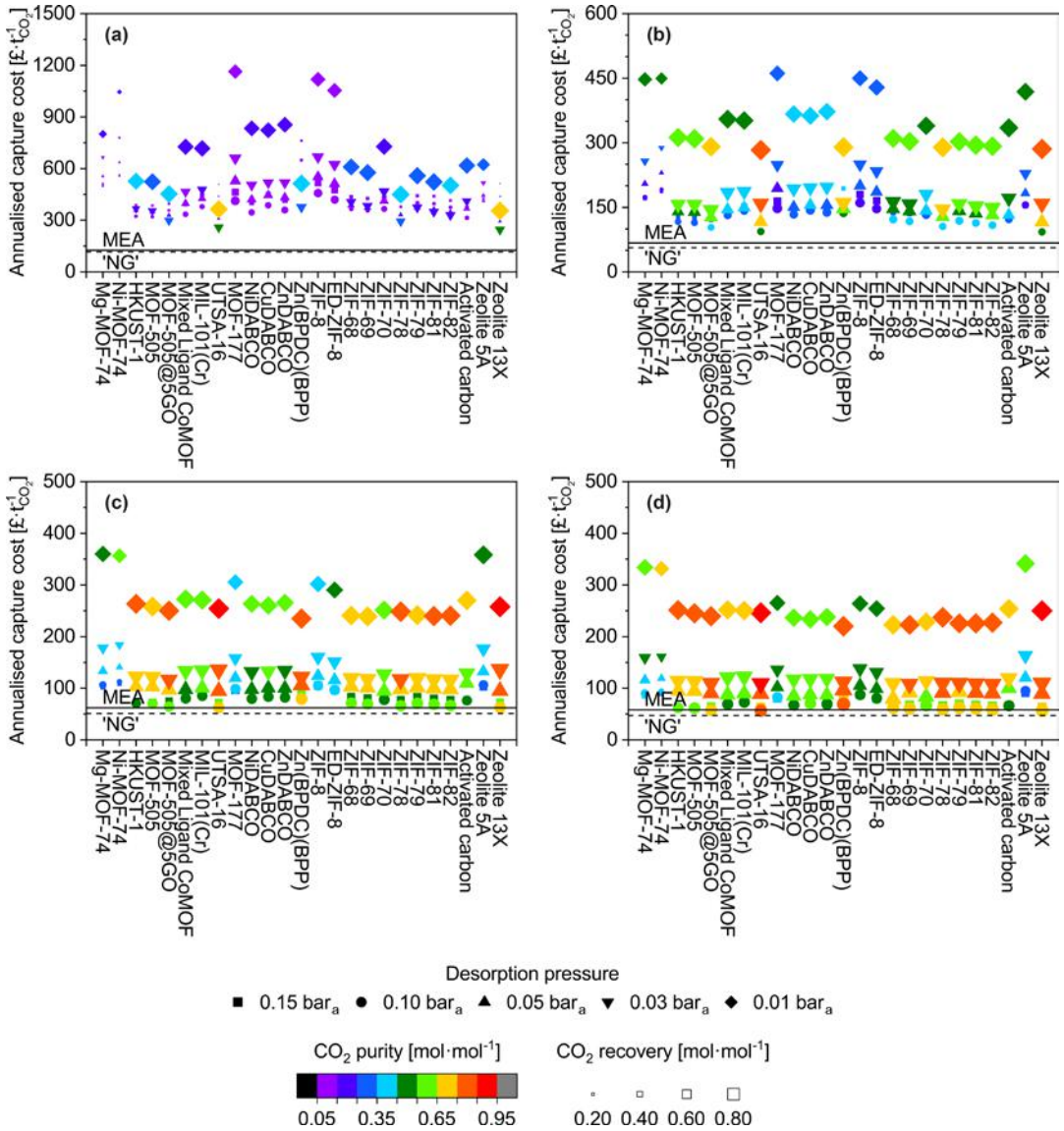
- Adsorbent evaluation results for all scenarios investigated

400 MWe NGCC

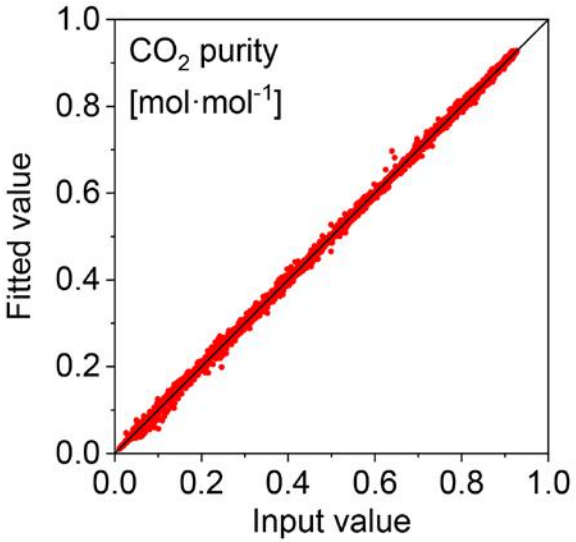
500 MWe coal

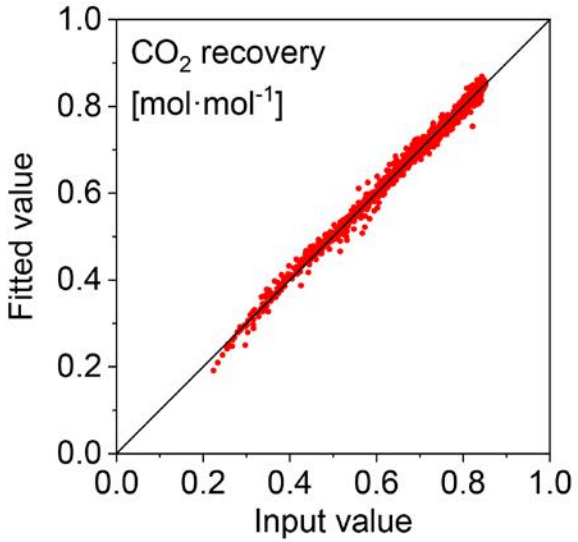
1 MMtpa cement

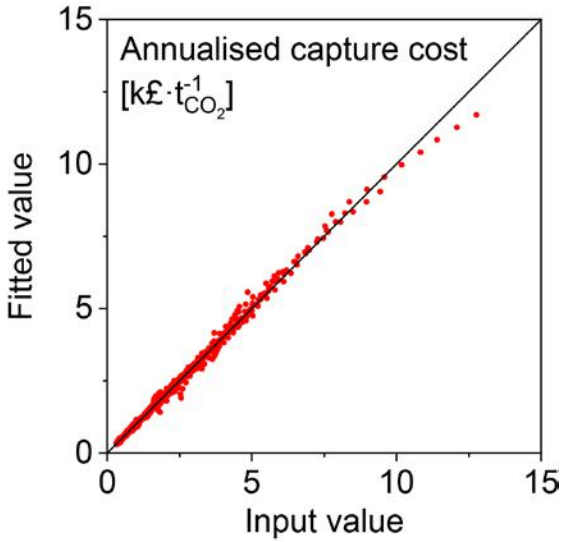
4 MMtpa steel



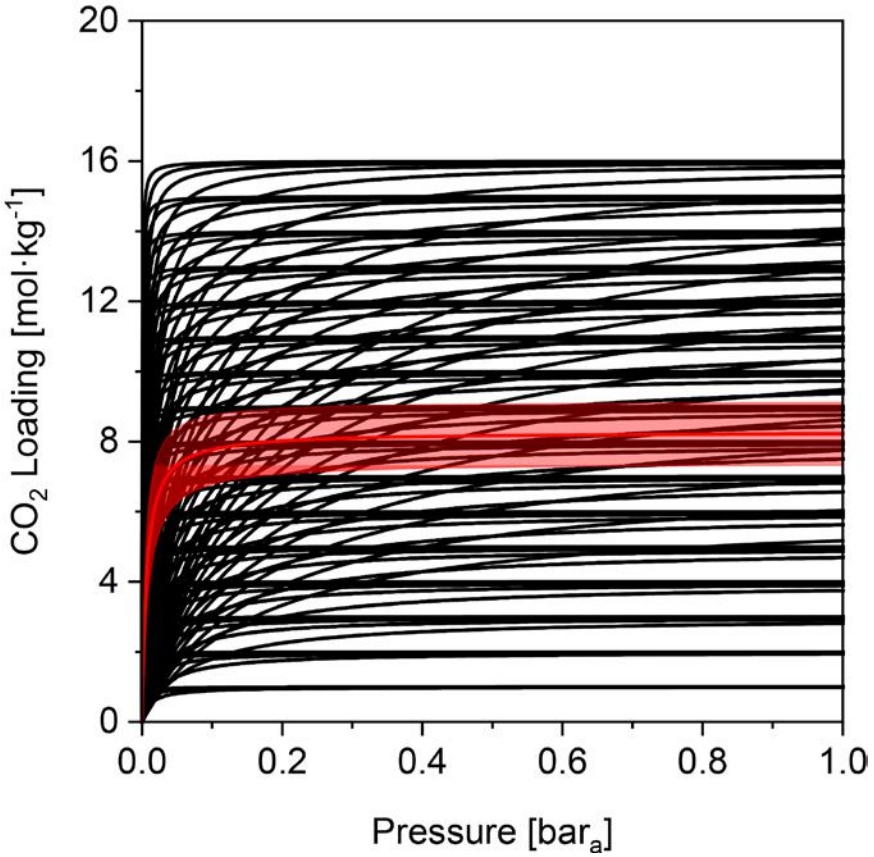
- ROM goodness of fits for NGCC scenario



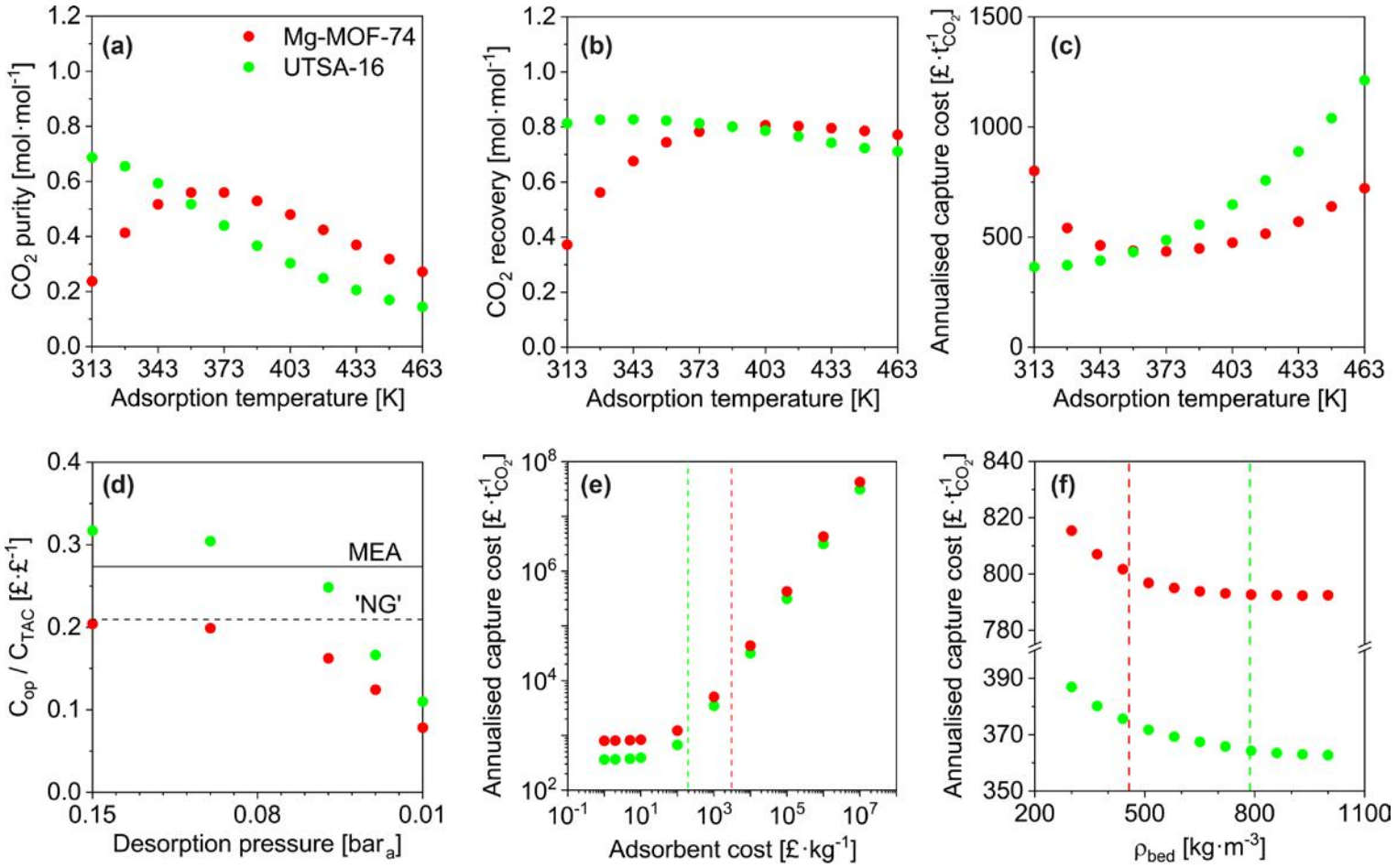



- All isotherms that meet performance criteria for NGCC case



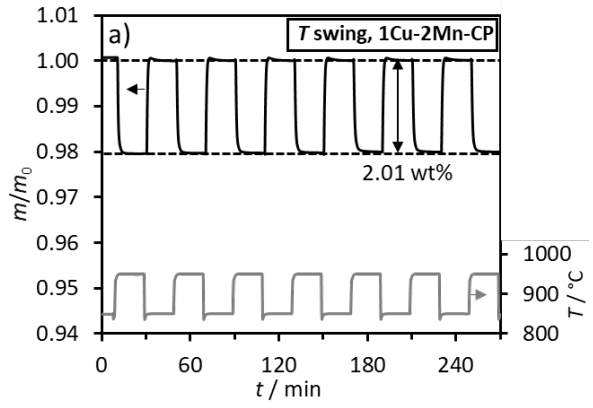
- Effect of process parameters – NGCC case

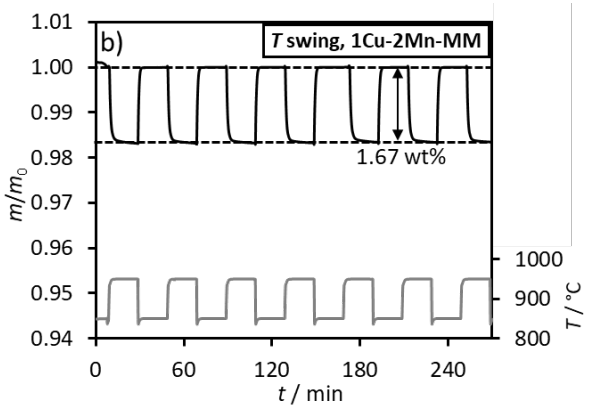


- Fennell Group appendix

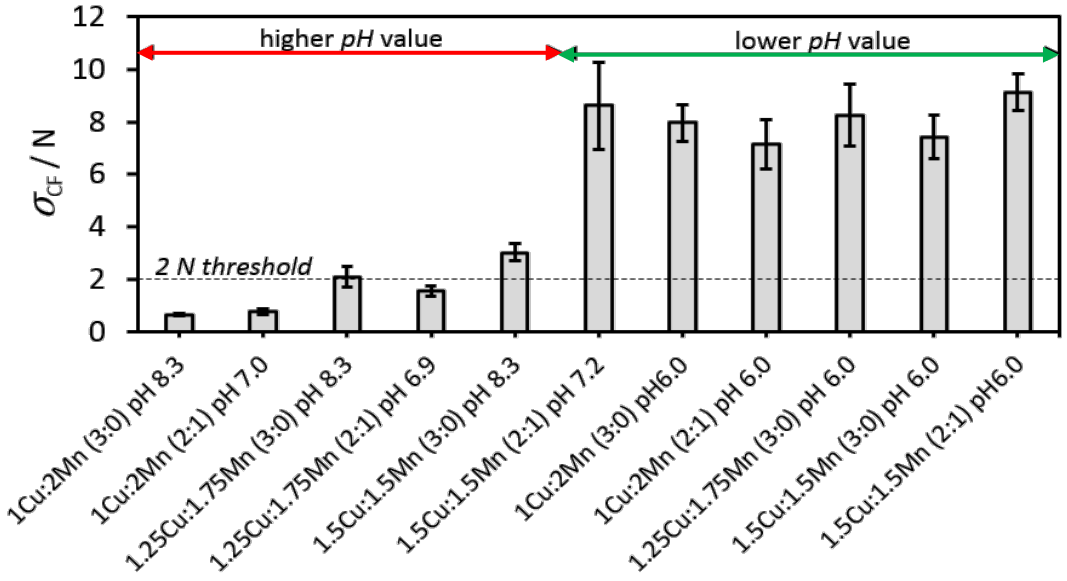
# Fennell Group appendices

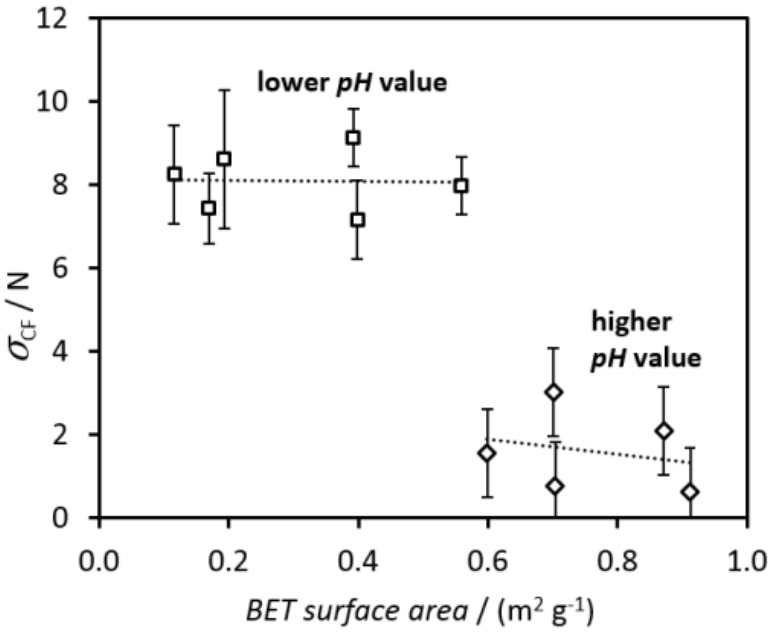
- Co-precipitation (CP) *vs.* mechanical mixing (MM)



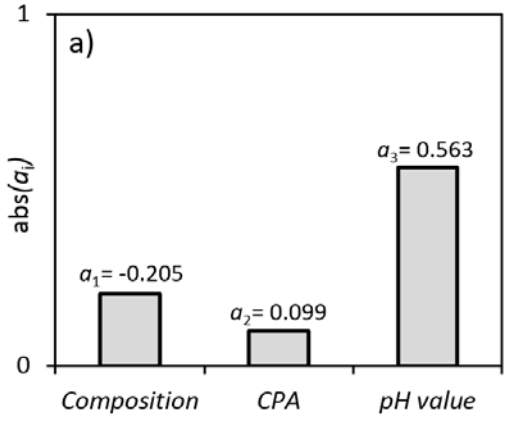
- Crushing strength and BET surface area of oxygen carriers (co-precipitated)



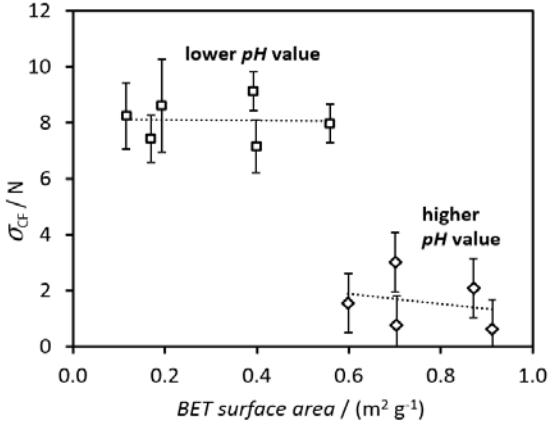



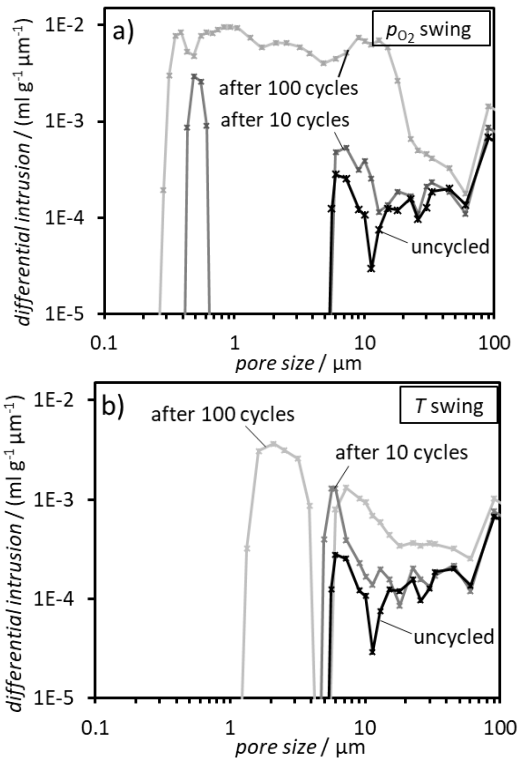
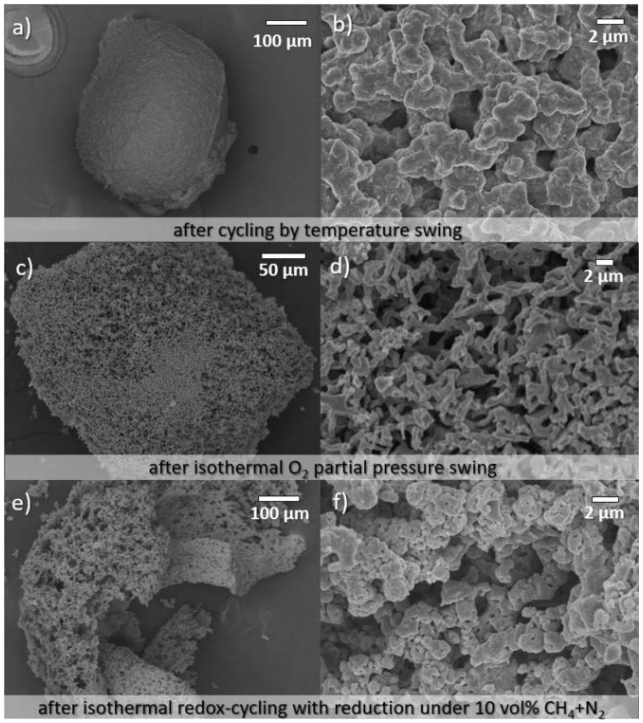
- Optimal synthesis procedures for co-precipitated and mechanically mixed CMO oxygen carriers have been developed.

- The relationship between oxygen carrier properties and synthesis conditions has been determined.




*The results of the linear regression analysis of the BET surface area values.*




*A plot of the crushing strength against the BET surface area of the co-precipitated oxygen carriers co-precipitated, □, at a lower pH value and, ◇, at a higher pH value.*

- Particle evolution based on different cycling methods (isoT, non-isoT, with $CH_4$)
  - ➢ Novel TGA + FBR experimental method