The potential of advanced sorbents to reduce CO_2 capture cost capture via temperature swing adsorption

Joint project DCC3

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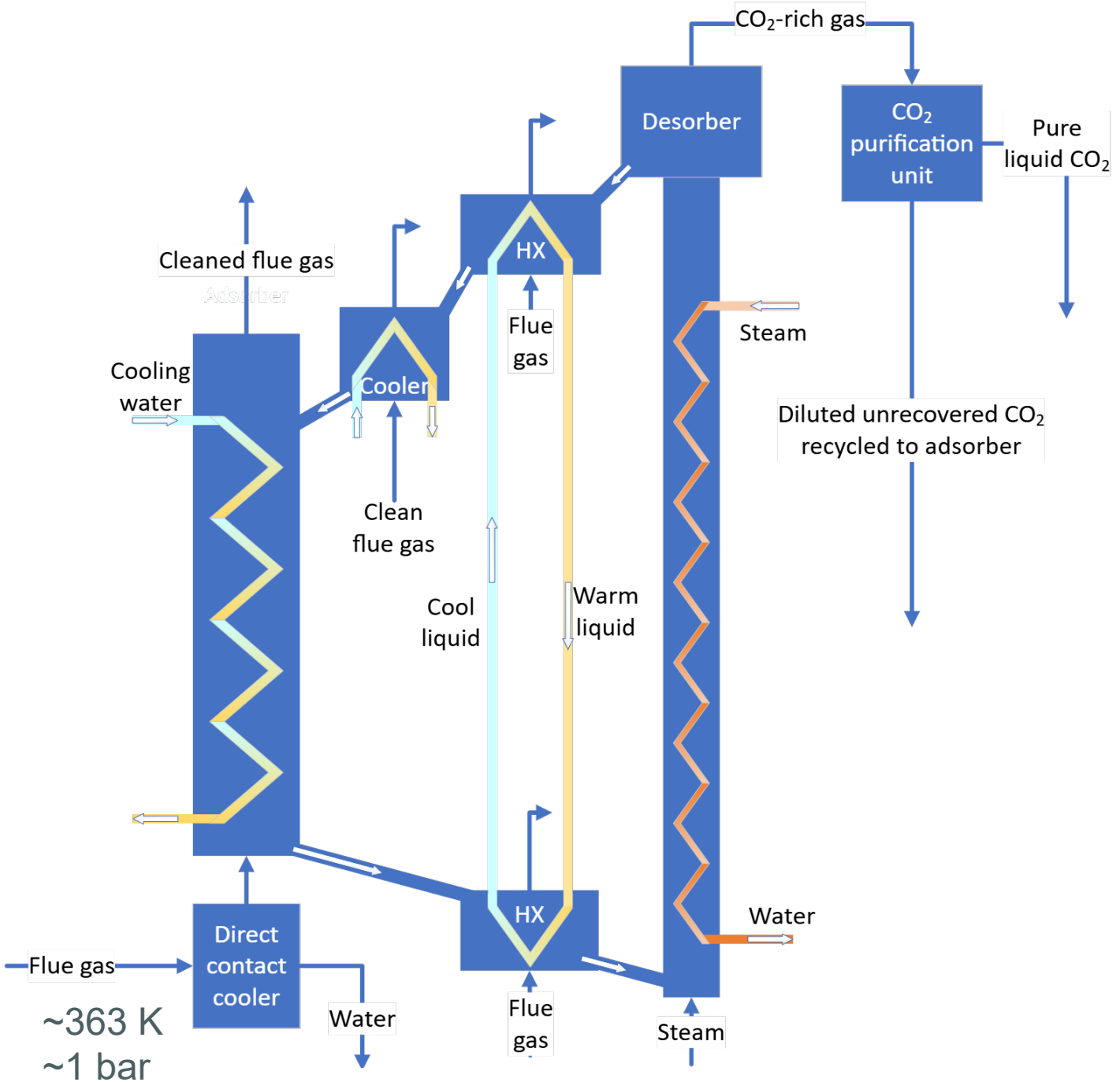
Introduction

- Capturing CO_2 is essential to mitigate climate change and meet global decarbonization goals.
- CO_2 in flue gas is dilute (~5%), making capture a technical challenge.
- Reducing CAPEX and OPEX are key to make CO_2 capture economically viable.
- Use of adsorption-based process could be of potential interest.
- The steam-assisted TSA process is used to assess the performance of “ideal” adsorbents, with the potential to reduce overall operational costs.

Fluidized bed TSA process

- Natural gas combined cycle power plant.
- Temperature swing driven by steam extracted from the power plant.
- Indirect recuperative heat exchange with a circulating heat transfer fluid.
- Direct contact cooler for flue gas drying before the adsorber.
- CO_2 purification unit for pure liquid CO_2 production after the desorber.



CO_2= 4.6%
H_2O= 9.4%

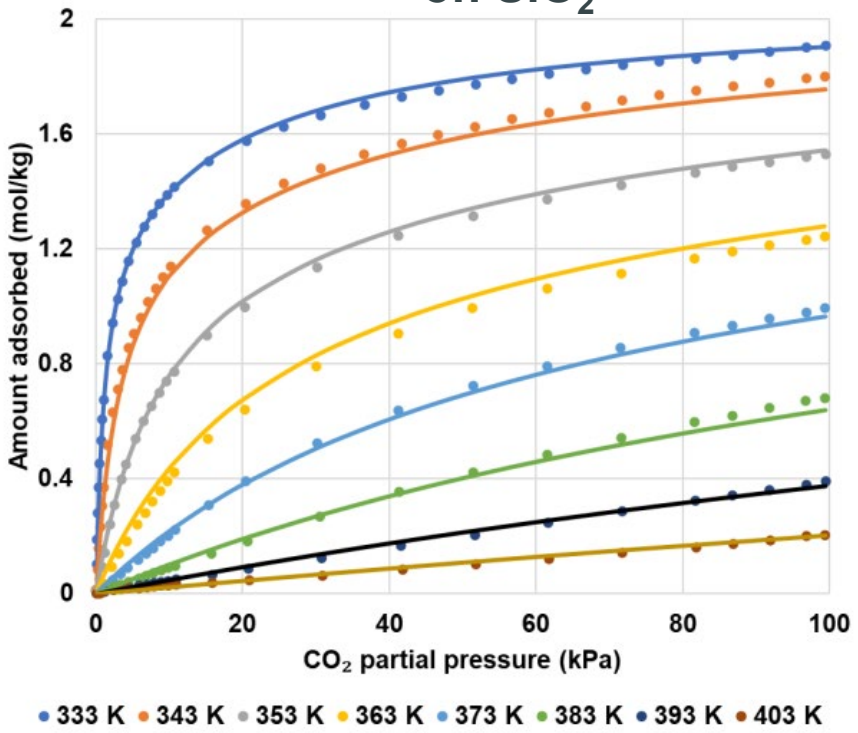
~363 K
~1 bar

The adsorbent case studies

Case 1- Chemisorbent

- Dual-site Langmuir for CO_2 and GAB model for H_2O
- Linear driving force kinetics

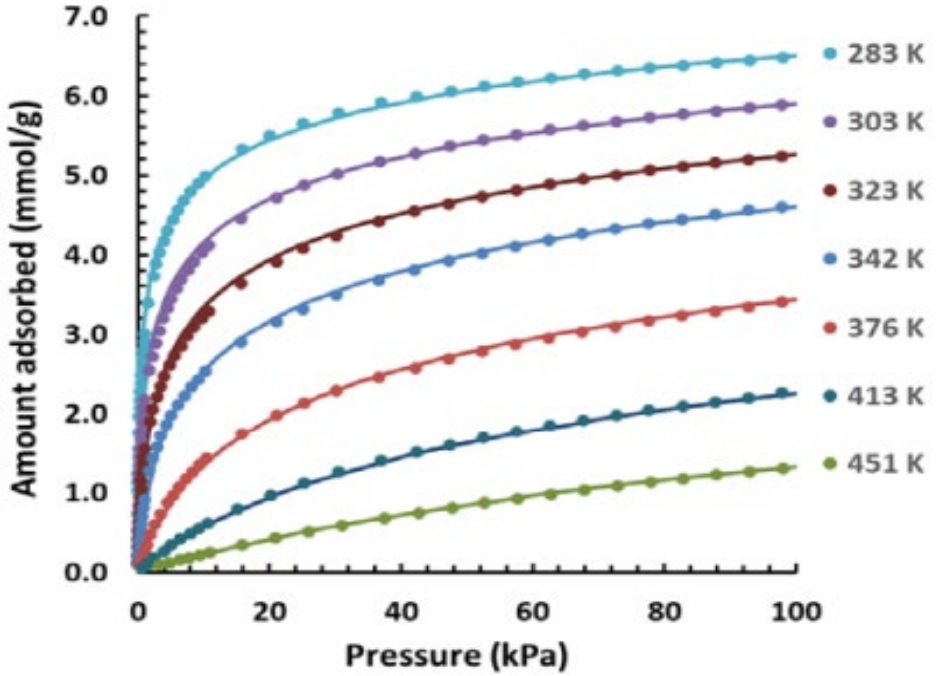
Epoxybutane-Polyethylenimine (EB-PEI) on SiO_2



Case 2- Physisorbent

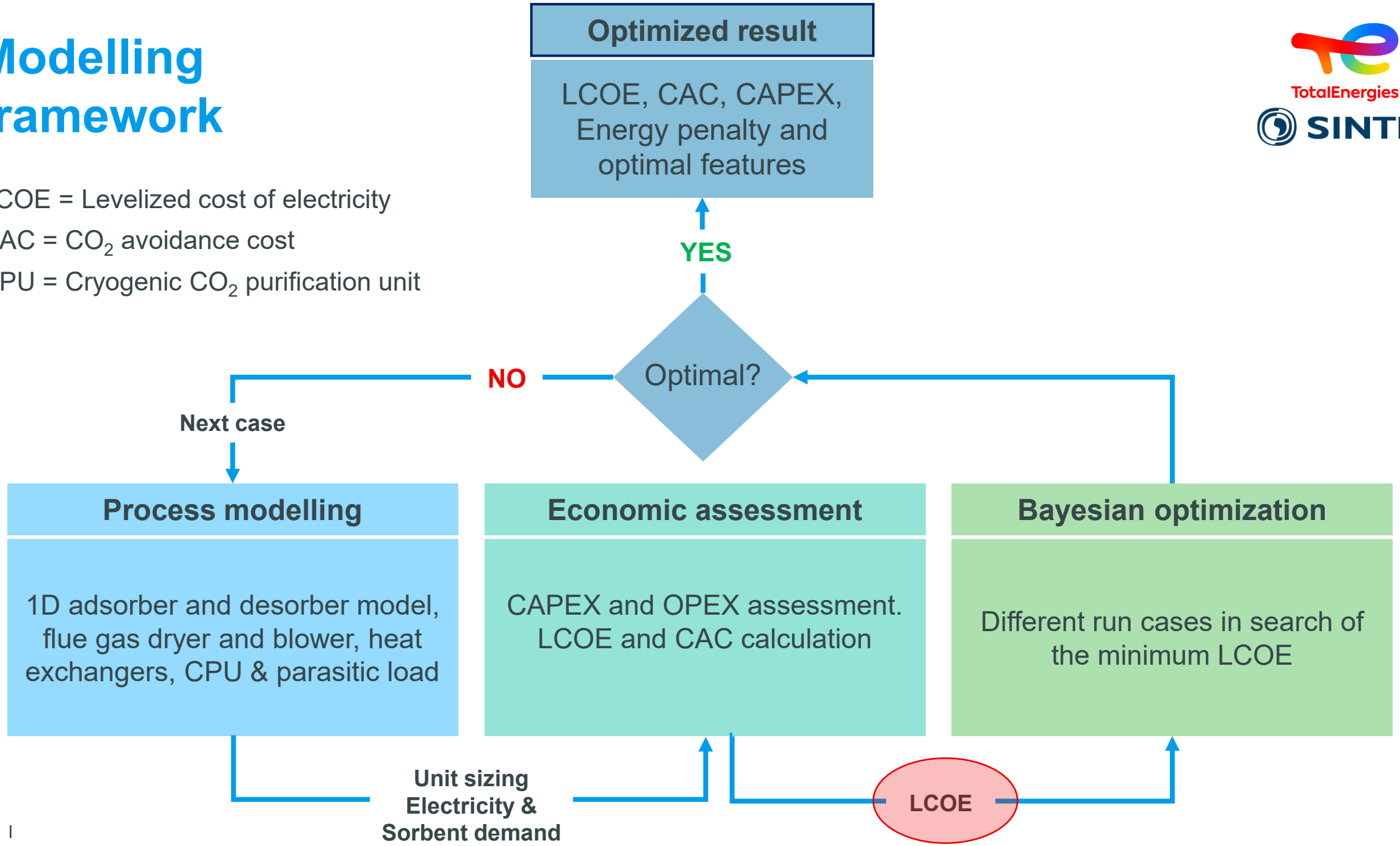
- Competitive Dual-site Langmuir for CO_2, H_2O and N_2
- Macropore mass transfer resistance

Zeolite 13X



Modelling framework

- LCOE = Levelized cost of electricity
- CAC = CO_2 avoidance cost
- CPU = Cryogenic CO_2 purification unit



Ideal sorbent assumptions

Progressively add ideal assumptions:

1. **Zero-cost sorbent:** No sorbent cost
2. **Fast kinetics:** Add fast kinetics to the previous case
3. **High capacity:** Add a high adsorption capacity (6 mol/kg) and low heat capacity to the previous case
4. **Perfect selectivity:** H_2O and N_2 and non-adsorbing relative to the previous case
5. **Ideal isotherm:** Add isotherm parameter optimization to the previous case, optimizing values of $q_b, q_d, b_0, d_0, \Delta H_b, \Delta H_d$

Process modelling

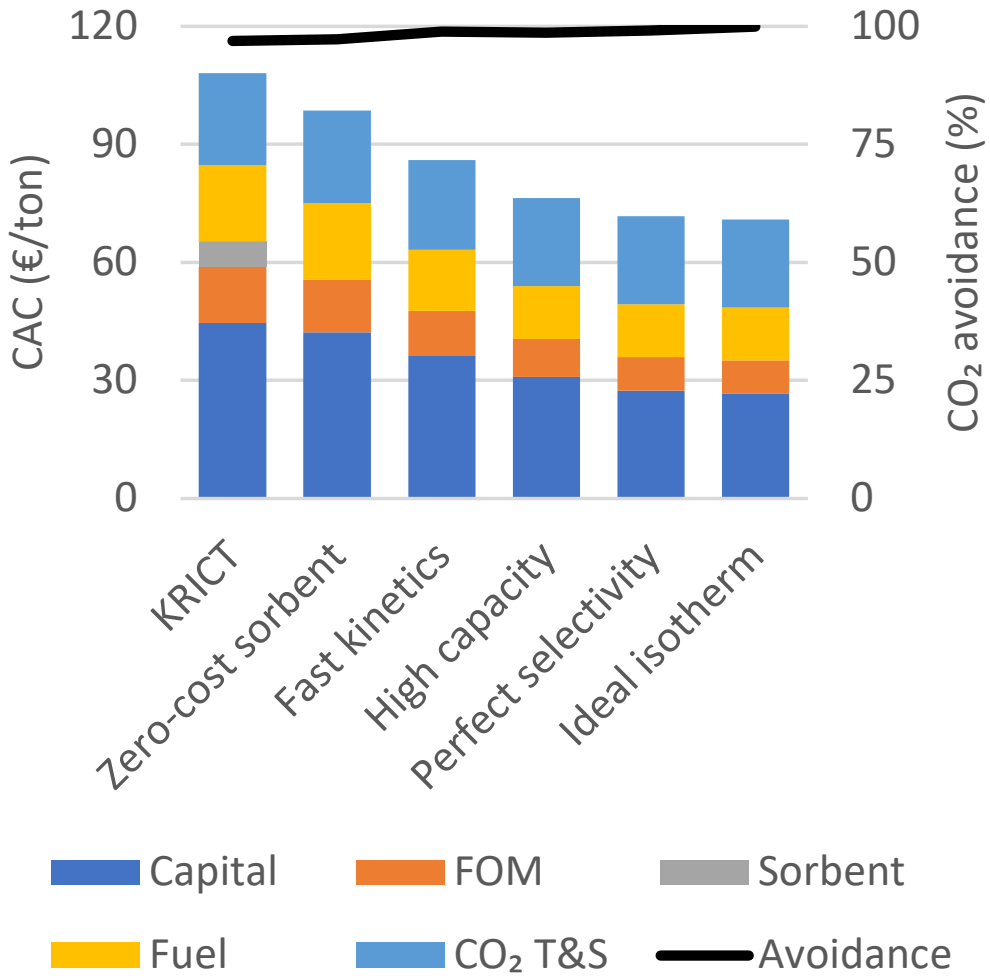
1D adsorber and desorber model, flue gas dryer and blower, heat exchangers, CPU & parasitic load

Unit sizing
Electricity &
Sorbent demand

Economic assessment

KRICT EB-PEI comparison results

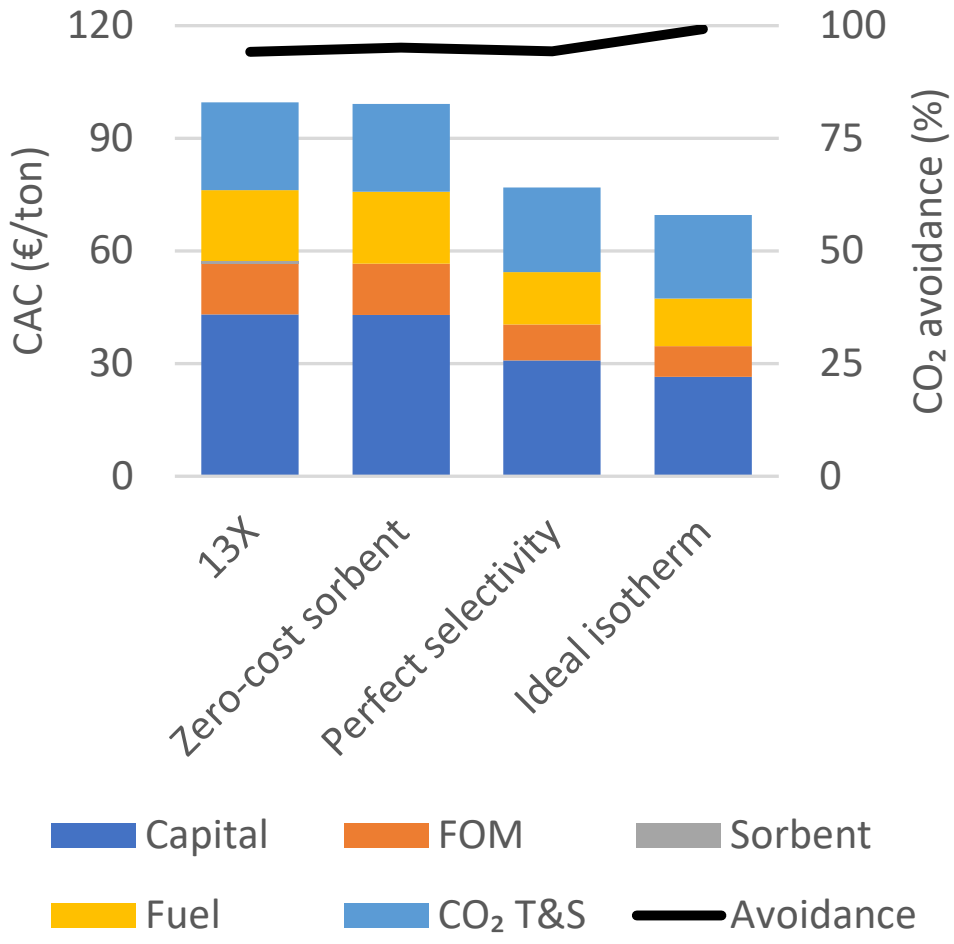
- **Reducing adsorbent cost** ↓ 10 €/ton
- **Reducing kinetic limitations** ↓ 13 €/ton
  - Smaller reactors
  - Avoids wider temperature swing
- **High adsorption capacity** ↓ 10 €/ton
  - Lower sorbent circulation rate
  - Lower sensible heat penalty
- **No H_2O adsorption** ↓ 5 €/ton
  - Avoids the need for flue gas drying
  - Avoids heat demand for H_2O desorption



FOM = Fixed operating and maintenance costs
Fuel = Extra natural gas consumption required for CO_2 capture, purification, and liquefaction
CO_2 T&S = CO_2 transport and storage (assumed to cost 20 €/ton)

13X comparison results

- **Reducing sorbent costs** –
  - Negligible effect because 13X is inexpensive.
- **Fast kinetics and high adsorption capacity** –
  - Already present in 13X and not considered
- **Perfect selectivity** ↓ 22 €/ton
  - Lower desorption temperature & sorbent circulation rate
  - No flue gas drying or heat demand for H_2O desorption
- **Isotherm optimization** ↓ 7 €/ton
  - TSA prefers a more temperature-sensitive sorbent



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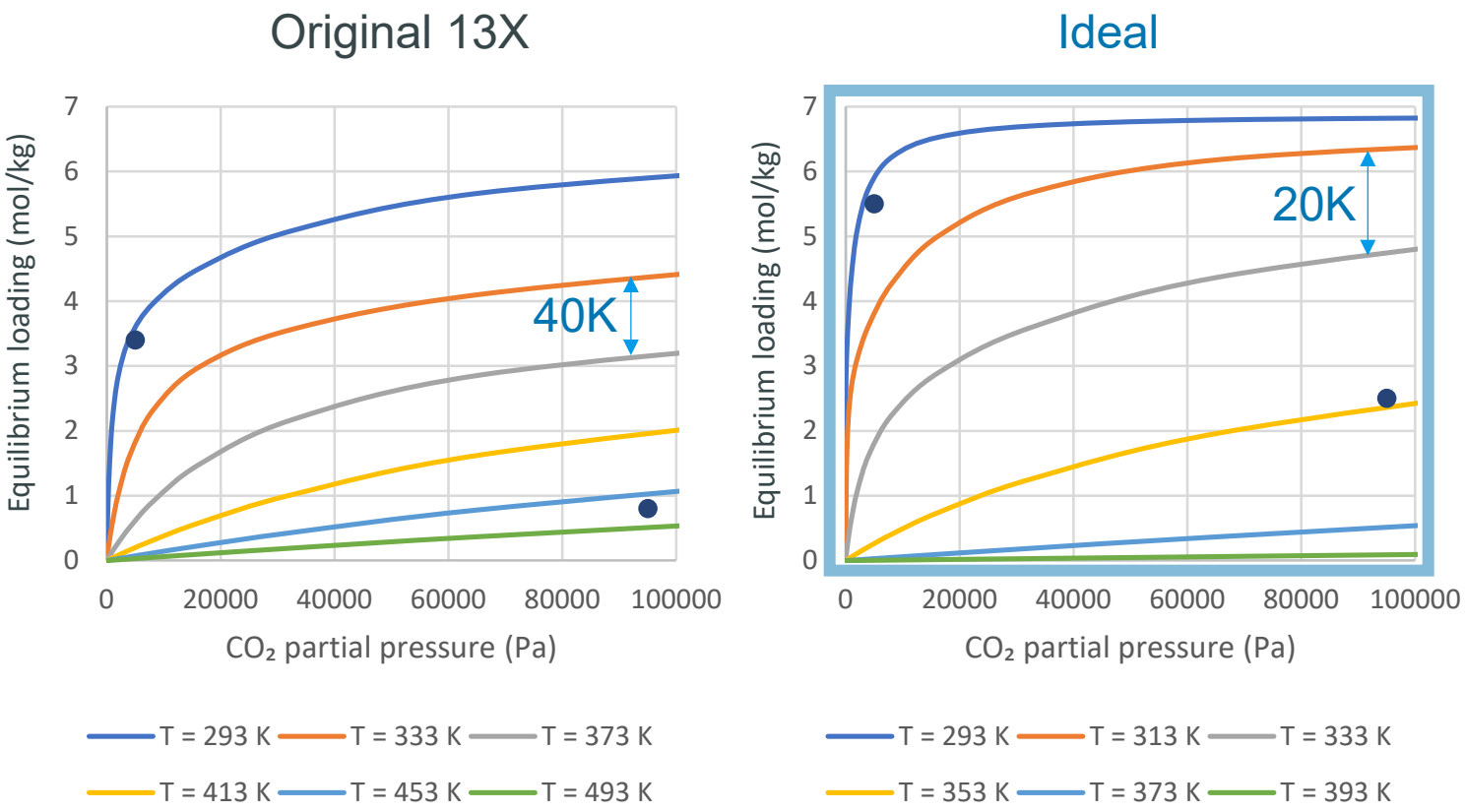
Zeolite13X vs ideal isotherm



- The ideal isotherm is much more **temperature sensitive**
- This comes at the cost of much higher desorption heat requirement (kJ/mol CO_2)
- Hence, a **larger quantity** of lower-grade **heat is needed**
- The amount of **sensible heat recuperation** required is **reduced**.
- Slight shift to left to **saturate at higher temperatures**.

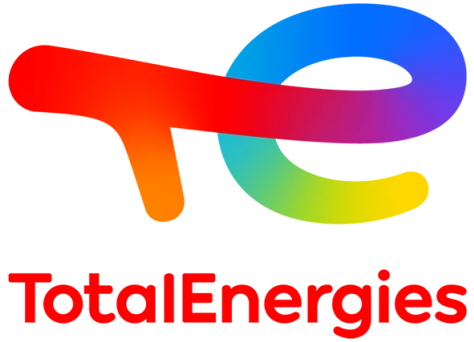
Conclusions

- Promising results as the **sorbent-based process using the KRICT sorbent can outcompete solvent technologies** due to lower energy demands and smaller reactors
  - CSAR (electrified FBTSA technology) is attractive against solvents for CHP applications [1]
  - CSAR and FBTSA return similar costs for coal-fired power plant retrofits [2]
- **This competitive edge would increase with significant sorbent improvements.** The most important handles for reducing CO_2 avoidance costs through sorbent development are:
  - Relative to a **chemisorbent** : Lowering costs, improving kinetics, and increasing capacity
  - Relative to a **physisorbent** : Reducing H_2O and N_2 competition and increasing temperature sensitivity

1. Prospects of the Novel CSAR Concept for Fully Electric or Flexible Electric–Thermal Hybrid CO2 Capture from CHP Plants, Schalk Cloete, Chaitanya Dhoke, Davide Bonalumi, John Morud, Antonio Giuffrida, Matteo Carmelo Romano, and Abdelghafour Zaabout, Energy & Fuels 2023 37 (16), 12030-12044
2. Heat pump-driven adsorption CO2 capture for simple and cost-effective retrofits of coal power plants, Schalk Cloete, Antonio Giuffrida, Matteo C. Romano, Abdelghafour Zaabout, Applied Thermal Engineering, 2024, 121456

Conclusions

- This work shows **potential for cost reduction** by enhancement of adsorbent properties. (30-40 €/ton cost reduction in the NGCC application simulated).
- **Trade-off** between physisorbent and chemisorbents due their unique properties and drawbacks.
- **Preferential adsorption of H_2O** and competitive adsorption of N_2 could potentially be manipulated in physisorbents (e.g. CALF20).
- In case of **chemisorbent**, room of improvement in terms of **adsorption capacity** and **kinetics**.
- **Bulk production** use of cheaper raw materials and simpler synthesis could bring down the adsorbent costs.



Thank you

Supplementary methodology slides

Isotherm parameters

Sorbent		KRICT	13X
Isotherm	CO_2	DSL	DSL-competitive
	N_2	-	DSL-competitive
	H_2O	$f(RH)$	DSL
Kinetics	CO_2	LDF	Macropore
	N_2	-	Macropore
	H_2O	Mass Tr.	Macropore

ZEOLITE 13X

	CO_2	$CO_{2,bin}$	N_2	H_2O
$q_{sb}(mol/m^3)$	3489.44	3125.7	6613.55	10468.60
$b_0(m^3/mol)$	8.65e-7	8.8e-8	2.50e-6	2.35e-7
$\Delta U_b(kJ/mol)$	36.64	38.15	15.82	55.72
$q_{sd}(mol/m^3)$	2872.35	1897.5	0	6434.50
$d_0(m^3/mol)$	2.63e-8	1.18e-9	0	7.99e-8
$\Delta U_d(kJ/mol)$	35.70	34.44	0	45.48

KRICT EB PEI

	CO_2
$q_{s1}(mol/kg)$	1.28
$b_{01}(1/Pa)$	1.04E-19
$\Delta H_1(J/mol)$	101800
$q_{s2}(mol/kg)$	0.79
$b_{02}(1/Pa)$	1.98e-17
$\Delta H_2(J/mol)$	78700

Reactor model

Process model

- 1D fluidized bed model for the adsorber and the desorber
- Two-phase theory where the bed is divided into dense and dilute phases with modelled mass exchange
- Reaction is modelled with a dual-site Langmiur isotherm and linear driving force kinetics

- Recuperators and coolers are modelled as heat exchangers with no reaction
- Correlations employed for:
  - Flue gas blower power
  - Cryogenic CO_2 purification unit power
  - Parasitic load on NGCC plant (due to steam extraction)
  - Direct contact cooler volume for a specified amount of flue gas drying

Economic model

- Bottom-up economic assessment built into the process model
- Capital cost estimate of all units
- Operating costs (fuel, sorbent)
- Levelized cost of electricity with and without CO_2 capture
- CO_2 avoidance cost calculated from LCOE and CO_2 intensity with and without CO_2 capture

Optimizer

- Bayesian optimization to minimize the LCOE
- Functions fitted through existing cases to decide where the next simulation should be run
- New cases are run until an optimization criterion is reached
- Usually requires around 500 automated runs with the 17 features of the FBTSA process

Optimized parameters

TotalEnergies

SINTEF

1D Adsorber and desorber model

- Steam temperature (°C)
- Sorbent circulation rate (kg/s)
- Adsorber & desorber HX fraction -
- Other HX area (m²)
- Cooler fraction -
- Effective adsorber & desorber diameter (m)
- Adsorber static bed height (m)
- Desorber diameter ratio -
- CPU parameter -
- Number of trains -
- Drying fraction -
- Adsorber & desorber cyclone & filter velocity (m/s)

Economic assessment

- Capital costs
- Fixed maintenance costs
- Fuel
- Sorbent costs
- Fixed transport and storage costs
- Fixed CO_2 taxes

Bayesian optimization

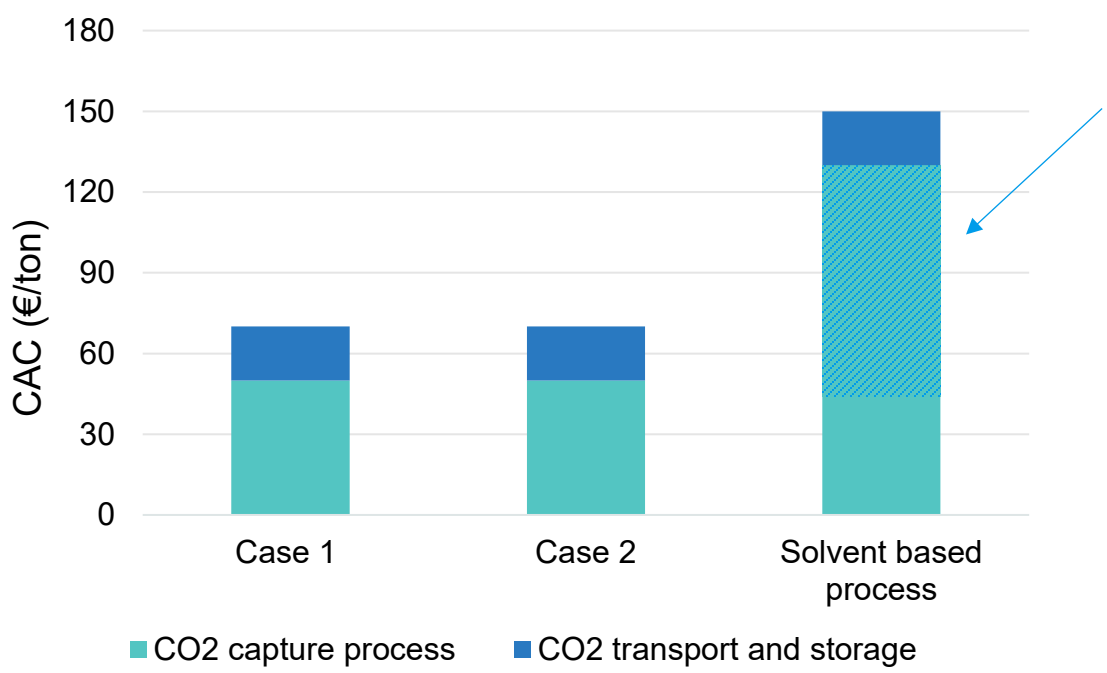
Levelized cost of electricity

$$\mathrm{LOCE}\ (€/\mathrm{MWh}) = \frac{ACC + FOM + Fuel + Sorbent + T\&S + Tax}{P \cdot 8766 \cdot CF}$$

CO_2 avoidance cost

$$CAC\ (€/ton) = \frac{LCOE_{CCS} - LCOEref}{e_{ref} - eCCS}$$

Conclusions



44-86 €/ton
+
20 €/ton Transport and storage costs

1. Heat pump-driven adsorption CO2 capture for simple and cost-effective retrofits of coal power plants, Schalk Cloete, Antonio Giuffrida, Matteo C. Romano, Abdelghafour Zaabout, Applied Thermal Engineering, 2024, 121456
2. The cost of CO2 capture and storage, International Journal of Greenhouse Gas Control, Edward S. Rubin, John E. Davison, Howard J. Herzog, Volume 40, 2015, Pages 378-400

Features for optimization

- **Desorption steam temperature.** Higher temperatures will achieve a higher CO_2 capture ratio at the expense of a higher energy.
- **Sorbent circulation rate.** Higher values increase CO_2 capture but also increase the sensible heat transfer requirement
- **Heat exchanger areas in the adsorber, desorber, recuperators, and cooler**. Higher heat exchange areas increase capital cost narrow the approach between the bed and heat exchange fluid temperature.
- **Cross sectional areas of adsorber and desorber.** Lower values reduce reactor costs but reduce conversion due to shorter gas residence time.
- **Adsorber bed height.** Lower values reduce reactor costs but reduce conversion due to shorter gas residence time. The desorber height is 5 m higher than the adsorber height to allow for sorbent circulation.
- **Desorber diameter ratio.** The desorber is designed as a truncated cone with a smaller cross section at the bottom to ensure good fluidization as the volume of desorbed gas increases along the reactor height.
- **CPU optimization.** Energy demand and capital cost of the CPU increase with the percentage of CO2 recovery, creating a trade-off that requires optimization.
- **Number of reactor trains.** The very large flue gas steam requires multiple parallel reactor trains.
- **DCC drying.** More drying increases DCC costs but reduces the amount of water fed to the adsorber.
- **Adsorber and desorber cyclone and filter velocities.** Higher velocities reduce capital costs at the expense of greater pressure drop.
- **In case of the ideal sorbent.** The six sorbent parameters discussed in the next slide.