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The potential of advanced sorbents to reduce CO2 capture cost capture via temperature swing adsorption

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Abstract

Adsorption-based CO_2 capture is gaining traction as an alternative to established solvent-based routes due to advantages regarding regeneration enthalpy, adsorption rates, and emissions control. However, solid sorbents are more challenging to circulate between adsorption and desorption reactors than liquid solvents. Thus, sorbent-based CO_2 capture is mostly carried out in fixed beds where the sorbent is kept in a single reactor vessel and alternatively exposed to adsorption and desorption atmospheres. Since a temperature swing is difficult to achieve in fixed bed reactors, such systems typically use a pressure swing to regenerate the sorbent, limiting their applicability to flue gases with higher CO_2 contents. However, if a temperature swing with sorbent circulation can successfully be implemented in adsorption-based CO_2 capture, the benefits of solid sorbents can be extended to flue gases with lower CO_2 fractions. Hence, the current work simulates a fluidized bed-based temperature swing adsorption (FBTSA) process for capturing CO_2 from the flue gas of a natural gas combined cycle (NGCC) power plant with only 4.6% (mol) CO_2 content.

Figure 1 shows that flue gas is fed to the adsorber, where it rises against a counter-current flow of cool and regenerated sorbent from the cooler. Internal heat exchange surfaces continuously extract heat generated by the exothermic adsorption reaction to maximize CO₂ capture. Once the sorbent is loaded with CO₂, it circulates to the bottom of the desorber where it is heated to release the captured CO₂. A small quantity of steam raised from waste heat in the process is fed directly to the bottom of the desorber, but desorber fluidization is achieved primarily via the desorbed gases. Since the amount of fluidizing gas will increase along the height of the desorber, a conical reactor body with a narrower cross-section at the bottom can be used to ensure uniform fluidization. After desorption, the hot sorbent at the top of the desorber falls into the cooler under gravity, where it is cooled before passing to the adsorber to minimize the equilibrium CO₂ partial pressure and, thereby, maximize the CO₂ capture ratio.

Sorbent circulation, which will be challenging to implement in practice, is kept as simple as possible by implementing a dilute desorber to create a pressure driving force for circulating particles from the bottom of the adsorber to the bottom of the desorber. Heat recuperation is carried out via indirect heating/cooling through a closed heat transfer circuit where a working fluid flows counter-current to the flow of the sorbent. This recuperator configuration is a practical choice that will simplify sorbent circulation,

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even though it will be less efficient than the conventional recuperative heat exchanger that can be implemented directly between the hot and cold streams in a solvent-based process.

The adsorber is assumed to consist of four stages separated by perforated plates that limit the axial mixing in the fluidized bed reactor. In this way, the good heat and mass transfer properties of a fluidized bed can be preserved without compromising the counter-current flow required to ensure high CO₂ capture ratios [1]. Axial mixing in the bottom of the desorber is limited in a similar matter to ensure good counter-current heat exchange performance with the hot working fluid from the cooler. After heat recuperation, the sorbent is further heated via a heat exchanger carrying steam extracted from the NGCC power plant to drive the endothermic desorption reaction.

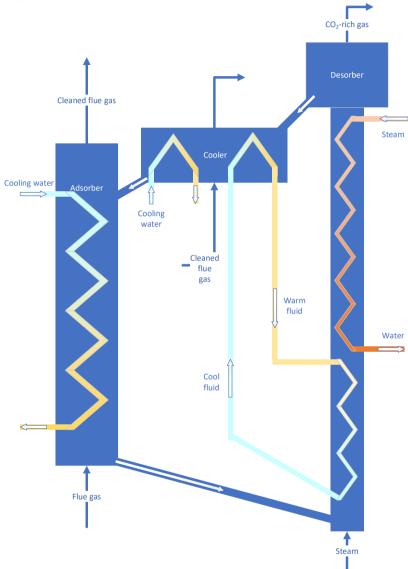


Figure 1: Schematic of the FBTSA process simulated in this work. The white arrows indicate the flow direction of the particles and the heat exchange fluids.

The reactors are simulated using conventional phenomenological fluidized bed reactor modelling [2] for physical phenomena such as bubble formation and growth, axial mixing, and mass transfer between dense and dilute phases. Heat transfer via the embedded heat exchange surfaces is modeled using a validated in-house model. A dual-site Langmuir (DSL) isotherm is used to describe adsorption equilibrium and a linear driving force approach for describing the adsorption rate.

The technical results from the model are directly coupled to economic estimates of capital and operating costs of the fluidized bed

system and surrounding equipment, including a flue gas blower and flue gas drying (via a direct contact cooler) upstream from the adsorber, a CO₂ liquefaction unit downstream from the desorber, cyclones and filters for fines handling downstream from both reactors, and capital costs and power losses related to steam extraction from the NGCC power plant. This full techno-economic model returns the levelized cost of electricity (LCOE) from the NGCC plant retrofitted with FBTSA CO₂ capture, assuming a 150 €/ton price on emitted CO₂. Other techno-economic metrics such as the CO₂ avoidance cost (CAC) and specific primary energy consumption for CO₂ avoidance (SPECCA) are also calculated.

Furthermore, the techno-economic assessment model is coupled with a Bayesian optimization framework for automated minimization of the LCOE via manipulation of 17 parameters, including the steam temperature, reactor dimensions, heat exchanger surface areas, degree of flue gas drying, and design parameters for the cyclones, filters, and CO₂ liquefaction unit.

This modelling framework is deployed in the present study to investigate the scope available for reducing costs via sorbent development by comparing the optimized economics of the FBTSA process using 1) an epoxybutane-functionalized polyethyleneimine (EB-PEI) sorbent developed by the Korean Research Institute of Chemical Technology (KRICT) [3] and 2) a hypothetical ideal sorbent with negligible cost, fast reaction rate, no water or nitrogen adsorption, high CO_2 adsorption capacity (6 mol/kg), low heat capacity (800 J/kg.K), and optimized DSL isotherm parameters. In simulations with the ideal sorbent, the optimizer was also allowed to manipulate the capacity distribution between the two DSL sites (q_b, q_d) alongside the pre-exponential factors (b_0, d_0) and desorption enthalpy (H_b, H_d) values in the DSL expression below. H_b and H_d are also used as the desorption heat demand in the model, ensuring that a more temperature-sensitive sorbent (which reduces the required temperature swing to use cheaper low-grade heat and limit the sensible heat penalty) will also require a larger amount of heat for desorption.

$$\begin{split} q_{CO_2}^* &= \frac{q_{b,CO_2} b_{CO_2} p_{CO_2}}{1 + b_{CO_2} p_{CO_2}} + \frac{q_{d,CO_2} d_{CO_2} p_{CO_2}}{1 + d_{CO_2} p_{CO_2}} \\ b_{CO_2} &= b_{0,CO_2} e^{\frac{\Delta H_{b,CO_2}}{RT}} \quad d_{CO_2} = d_{0,CO_2} e^{\frac{\Delta H_{d,CO_2}}{RT}} \end{split}$$

Results are summarized in Figure 2, where the first and most important conclusion is that there remains considerable scope for cost reduction via further sorbent development. The ideal sorbent reduces CO_2 avoidance costs by 46 ϵ /ton relative to the KRICT sorbent, partially by reducing capital costs and partially by reducing operating costs (mainly the energy penalty and sorbent replacement costs). The figure also shows that the optimizer chose high CO_2 capture ratios to minimize taxes on emitted CO_2 .

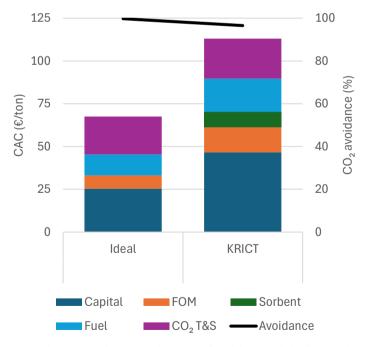


Figure 2: The optimized CO₂ avoidance cost breakdown and the degree of CO₂ avoidance for the ideal sorbent and the KRICT EB-PEI sorbent. FOM = fixed operating and maintenance costs, T&S = transport and storage.

An analysis of the importance of different elements of the ideal sorbent was also completed as outlined below, where the different

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factors are ranked from the largest to the smallest effect on reducing CO2 avoidance costs:

- The idealized assumption of negligible sorbent cost had the largest influence in comparison to the KRICT sorbent, which was assigned a relatively high cost of 20 €/kg (with a 2-year replacement period).
- The combined effect of a lower heat capacity and a higher adsorption capacity had the next-largest effect by reducing the sensible heat penalty and the required heat exchanger area in the recuperator.
- Higher adsorption rates had the third-largest effect by reducing the required reactor sizes and temperature swing required to approach equilibrium.
- Next, negligible water adsorption also had a significant effect by avoiding the need for flue gas drying as well as the heat demand and heat transfer surface area required for H₂O adsorption.
- Finally, optimized H-values and b-values minimize the energy penalty for CO₂ capture, but impact of optimizing these values was minor, indicating that the KRICT sorbent has a near-ideal isotherm shape for temperature swing adsorption.

The methodology presented here can be used in future work to assess the factors separating other promising sorbents from this hypothetical ideal, guiding sorbent developers to focus on the factors capable of achieving the largest reductions in CO₂ avoidance costs when commercialized. Even with the ideal sorbent, considerable costs remain due to the thermodynamic minimum energy required for CO₂ capture, the large adsorber needed for processing the dilute NGCC flue gas, and the desorption, CO₂ liquefaction, and CO₂ transport and storage infrastructure needed to handle the captured CO₂. Cost reductions in these areas may be pursued through process-related advances such as increasing the flue gas CO₂ content, standardizing the construction of CO₂ capture facilities, and establishing a cost-effective CO₂ transport and storage network.

References

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Keywords: CO₂ capture; temperature swing adsorption; sorbent development; techno-economic optimization; dilute flue gas. minimum 1 page, maximum 4 pages inclding diagrams and references.