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Modeling, Simulation and Optimization of a Carbon Capture Process Through a TSA Column

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ABSTRACT

By capturing carbon dioxide from biomass flue gases, energy processes with negative carbon footprint are achieved. Among carbon capture methods, the fluidized temperature swing adsorption (TSA) column is a promising low-pressure alternative, but it has been developed on small scales. This work aims to model, simulate and optimize a fluidized TSA multi-stage equilibrium system to obtain a cost estimate and a conceptual design for future process scale up. A mathematical model described adsorption in multiple stages, each with a heat exchanger, coupled to the desorption operation. The model was based on elementary macroscopic molar and energy balances, coupled to pressure drops in a fluidized bed designed to operate close to the minimum fluidization velocity, and coupled to thermodynamics of adsorption equilibrium of a mixture of carbon dioxide and nitrogen in solid sorbents (the Toth equilibrium isotherm was used). The complete fluidized TSA process has been optimized to minimize costs, considering equilibrium in each stage. The optimal configuration for heat exchangers was determined and a unit cost for carbon dioxide capture was estimated. It was found that a small number of stages is required to meet captured carbon specification at 95% molar purity, while process cost per metric ton of CO_2 was within range of other capture technologies. These findings show that the methodology developed here is useful for guiding the conceptual design of fluidized TSA process for carbon capture.

Keywords: Technoeconomic Analysis, Carbon Dioxide Capture, Adsorption, GAMS, Optimization, Modelling and Simulations.

INTRODUCTION

Motivation

The Paris Agreement is a legally binding international treaty adopted in 2015 by 196 countries. Its goal is to limit global warming to below 1.5°C, by reducing greenhouse gas emissions [1]. In the context of global decarbonization efforts, carbon capture and storage (CCS) technologies are often emphasized as a necessary pathway to limit global warming [2]. Bioenergy CCS (BECCS) is particularly promising due to its potential for achieving negative emissions, as it captures and permanently stores CO_2 that was originally removed from the atmosphere during biomass growth.

However, most optimization studies to date on the BECCS field focus on linear spatial and temporal analysis of networks of plants, farms and transportations, instead of diving into operational details and process variables in each site [3,4]. Process simulations and optimizations could provide key insights into relatively new CO_2 capture technologies in order to scale up processes and make them more mature.

Among recently developed CO_2 capture technologies that could benefit from such insights is the fluidized temperature swing adsorption (TSA) column, where a solid adsorbent flows countercurrent to an upward CO_2-rich gas [5,6]. Some works in the literature have already explored packed-beds TSA simulations [7,8], but fluidized TSA process optimization works remain scarce and limited to small scales [9,10]. This process is a suitable CO_2 capture method due to its high selectivity, reusability of solid adsorbents, and lower energy consumption

compared to conventional absorption-based methods. Adsorption-based methods using solid sorbents, such as zeolite 13X binder free, offer higher CO_2 selectivity and lower regeneration energy requirements [6].

Objective

The study aims an optimization-based design of fluidized TSA systems for large scale CO_2 capture from biomass-derived flue gases. This simulation study integrates process modeling and optimization techniques to improve fluidized TSA performance under realistic operating conditions, to develop basic guidelines to process scale up, in order to enhance process efficiency and minimize operational costs. This objective aligns with the need (highlighted in a previous study) to obtain a cost estimate for CO_2 capture through fluidized TSA process [5]. It also aligns with the Sustainable Development Goals set by the United Nations for 2030, including 7: Affordable and Clean Energy; 9: Industry, Innovation and Infrastructure; and 13: Climate Action [11].

MATERIALS AND METHODS

Hypothesis and parameters

The fluidized TSA system consists of two fluidized columns—one for adsorption and another for desorption—with continuous adsorbent recirculation. Each column has a heat exchanger at the gas inlet in the bottom, and each bed in each column also has a heat exchanger to optimize temperature. The recirculating solid adsorbent also passes through a heat exchanger between the columns. The number of adsorption stages should be optimized based on CO_2 purity targets and energy efficiency considerations. Our initial simplified simulations indicated that a small number of adsorption stages (as low as 3-5) suffices to obtain CO_2 at over 90%v/v purity [12]. Table 1 presents the hypothesis for the process modeling, while Table 2 presents the values and units for several parameters assumed for the optimization.

Table 1: Fluidized TSA modeling hypothesis.

No chemical reactions
No flue gas contaminants, only N_2 and CO_2
Ideal gases
No phase changes
Part of solid adsorbent replaced monthly
Equilibrium reached within each stage
No gradients within each stage
Spheric solid adsorbent particles
Air viscosity independent with respect to pressure
Startup cost is 10% of fixed capital investment [13]
Pressure drop due to stage heat exchangers neglected
Steady state

Table 2: Parameter values used in the GAMS code for modeling the fluidized TSA column.

Parameter description	Value
Flue gas molar flow	413 $mol.s^{-1}$
Flue gas molar composition	15%v/v CO_2 and 85%v/v N_2
Flue gas temperature	328 K
Flue gas pressure	1 bar
CO_2 max concentration after adsorption	0.5%v/v
Stage height *H*	1 m
Captured CO_2 min concentration	95%v/v
Zeolite 13XBF specific heat	880 $J.kg^{-1}.K^{-1}$ [14]
Zeolite 13XBF bulk density	1287 $kg.m^{-3}$ [6]
Zeolite 13XBF spheric particle diameter D_p	5.10^{-4} m [6]
Compressor efficiency	72% [15]
Overall heat transfer coefficient in each heat exchanger	170 $W.K^{-1}.m^{-2}$ [15]
Marshall & Swift index for late 2024	2500 [16]
Work hours per year	8000 $h.yr^{-1}$
Plant lifetime *t*	20 yr
Interest rate *i*	10%p.a.
Cost of land	0 USD
Cost of cold water	0.492 $USD.GJ^{-1}$ [17,18]
Cost of high-pressure steam	24.6 $USD.GJ^{-1}$ [17,18]
Cost of zeolite 13X BF	2 $USD.kg^{-1}$
Adsorbent monthly losses	10%

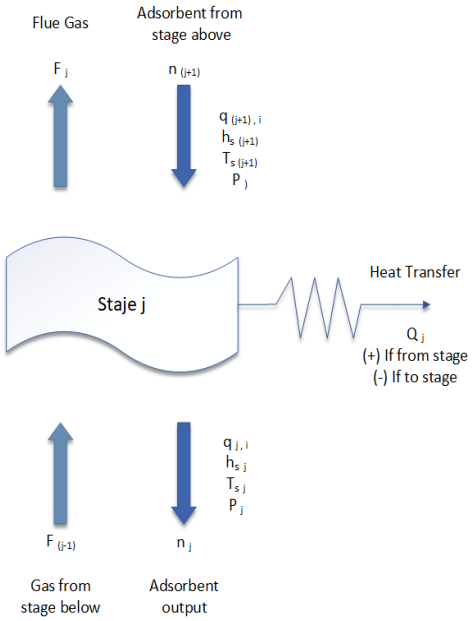

Figure 1. Modelling scheme of a generic equilibrium stage in the fluidized TSA column [6].

Modeling

A multistage fluidized bed receives an adsorbent stream from the upper side (solid phase inlet) and a biomass post-combustion flue gas stream at atmospheric pressure (1.01325 bar) from the lower side (flue gas inlet). The bed interior is subdivided into various stages; each stage receives the adsorbent and the flue gas from the neighboring stages. As each stage depends on the solution of other stages, an iterative solution is required. Figure 1 presents a sketch for a generic stage. A compressor is used at the bottom of the adsorption column to increase the flue gas pressure so it flows upwards.

The model is based on molar and energy balances of each gas component in each stage and in each external heat exchanger, coupled with thermodynamics of adsorption heat, according to previous studies where further details can be found [5,6] The Toth equation describes adsorption equilibrium within each stage, with model parameters from previous empirical results. For this study, based on our previous experimental results [6], we consider the heterogeneity parameter for N_2 to equal unity and not change with temperature.

Since particles in the present simulation are of Geldart group B and the system fluidizes readily (since minimum fluidization velocity and minimum bubbling velocity are similar) [19], air velocity was limited to twice the minimum fluidization velocity, which was calculated according to Equation 1 [20] where U_{mf} is the minimum fluidization velocity; g is gravity (9.80665 m.s^{-2}); μ is air viscosity; and ρ_g and ρ_p are respectively the gas and particle densities. The void fraction was calculated according to the semi empirical Ergun equation, which covers the entire range of flow rates as shown in Equation 2 [21], where ΔP is stage pressure drop; U is superficial air velocity; and ε is the bed void fraction. The pressure drop in each stage at the point of incipient fluidization was calculated according to the traditional Equation 3 [21], where ε_{mf} is the minimum fluidization void fraction.

$$U_{mf} = 0.0008g(\rho_p - \rho_g)D_p^2/\mu \quad (1)$$

$$\frac{\Delta P}{H} = \frac{150U\mu(1-\varepsilon)^2}{D_p^2\varepsilon^3} + \frac{1.75U^2\rho_g(1-\varepsilon)}{\varepsilon^3 D_p} \quad (2)$$

$$\Delta \mathrm{P} = gH(\rho_p - \rho_g)(1 - \varepsilon_{mf}) \quad (3)$$

The fixed capital investment (FCI) for the plant consisted in equipment, freight and installation cost for columns, heat exchangers and compressors. Correlations taken from the literature were generally in the form of Equation 4 [22], where K is an equipment constant; C is equipment capacity; $n \leq 1$ is a dimensionless scale factor; and F is a shape and material factor. The FCI was then annualized and then added to the yearly cost of utilities and startup cost according to Equation 5 [15]. The Marshall & Swift (*M&S*) index in Equation 4, which adjusts prices for inflation, was estimated as 2500 for late 2024 from values reported in the literature [16]. The utilities costs (cold water and high-pressure steam) were obtained from the literature for 2012 [17] and corrected for inflation [18] as shown in Table 2. Labor costs, taxes, depreciation, storage and transport costs, and revenues were not considered in this study, neither were carbon credits or other forms of subsidy.

$$FCI = \sum_{eqpts.} \frac{M\&S}{280} K(C)^n(F + 2.2) \quad (4)$$

$$\text{annualized cost} = \text{utilities yearly cost} + (FCI + \text{startup cost} + \text{cost of land}) \times \frac{i}{1-(1+i)^{-t}} \quad (5)$$

The balance, thermodynamic and Toth equations, along with equations for pressure drops, velocity, void fraction and costs (constraints), were implemented and solved in an environment within GAMS software (GAMS Software GmbH), release 48.2.0, using the non-linear programming solver CONOPT4 [23]. The model has 320 constraints (including inequalities) and 305 variables, with 95 definitional constraints. The objective function was to minimize the annualized cost defined in Equation 5 divided by yearly CO_2 capture (in mass units).

RESULTS AND DISCUSSION

As expected for a non-linear formulation, the problem convergence was heavily dependent on initial guesses and variable bounds. Pressure, temperature and Toth equilibrium parameters were therefore bound at the maximum and minimum theoretical values, and strictly positive initial guesses were applied to variables that would have cause undefinition errors if set to zero.

Low particle Reynolds numbers in each stage in adsorption and desorption, between 4 and 7, indicate the system readily fluidizes. It also indicates that viscous and kinetic energy losses during air flow past the particles are of similar order of magnitude, thus the use of both terms of the Ergun equation in Equation 2 is justified [21]. Calculated minimum fluidization porosity by the Ergun semi-empirical equation was about 0.42, similar to the 0.43 value reported in a previous study [6] and within the usual 0.40-0.45 range for spherical particles [21]. Stage pressure at the adsorption column was initially fixed at 1.8 bar in preliminary simulations, then set as a variable. Optimized results set the pressure between 1.42 bar (bottom stage) and 1.17 bar (top stage). It is worth mentioning that the simulated bed height had a conservative estimate (1 m, as shown in Table 2).

An initial assessment of the influence of stage numbers in adsorption and desorption columns resulted in a small number of stages reaching the specified project constraints on separation and purity of Table 2. In fact, only 5 adsorption stages and a single desorption stage were enough to extract CO_2 from a 15%v/v composition

flue gas into a 0.5%v/v composition stream, while CO_2 captured and recovered was 95%v/v. This supports claims that capturing CO_2 at purities greater than 90% is physically as well as economically feasible [12]. This also confirms previous results from the authors [5,6], indicating that fluidized TSA column size is probably not an impediment for scaling up this CO_2 capture technology. Additionally, increasing the flue gas molar flow from 1.556 $mol.s^{-1}$ [5,6] to 413 $mol.s^{-1}$ showed economies of scale effects on the CO_2 capture cost per mass unit.

Figure 2 shows the optimized setup with five adsorption stages, indicating temperatures and process streams. It was also possible to confirm that not all stages in the columns needed heat exchangers, with some heat loads being set at zero during the optimization [5]. Figure 3 shows the heat load per heat exchanger for the entire process, and the heat exchanger between columns removes most of the heat applied in the desorption column.

Utilities are the main cost drivers, as shown in Figure 4, which highlights the importance of adequate energy efficiency management. Future studies might simulate a fluidized TSA process with a heat pump between the adsorption and desorption columns, which could render the heat exchanger for the recirculating solid obsolete. Figure 4 also shows that, from all equipment costs comprising the FCI, the compressor at the bottom of the adsorption column is the most expensive. In most conventional setups, flue gas is delivered at atmospheric pressure because its thermal and kinetic energy is largely expended during upstream processes. However, if these processes are optimized or even omitted, the inherent pressure drop in the system preceding the column can be minimized. Consequently, the flue gas could maintain a higher pressure from the combustion process to the TSA column. This elevated pressure at the column inlet would reduce or eliminate the necessity for a compressor, decreasing costs.

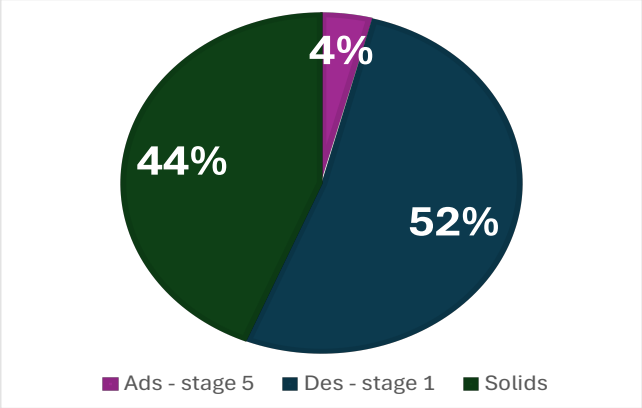

Figure 3. Heat loads per heat exchanger in an optimized fluidized TSA process.

The objective function value, the CO_2 capture cost per mass unit, was optimized at 84.6 $USD.t^{-1}$. This value falls within ranges reported in the literature for some technologies, and is significantly smaller than costs for direct air capture [2,30], as shown in Table 3. It is still, however, larger than amine-based absorption technologies [31], which are more mature despite their shortcomings. However, there is still room for fluidized TSA processes improvement before scale-up, such as development of new adsorbents as well as even greater economies of scale. For reference, the estimated market price of CO_2 at 96%v/v in Brazil is about 100 $USD.t^{-1}$, and

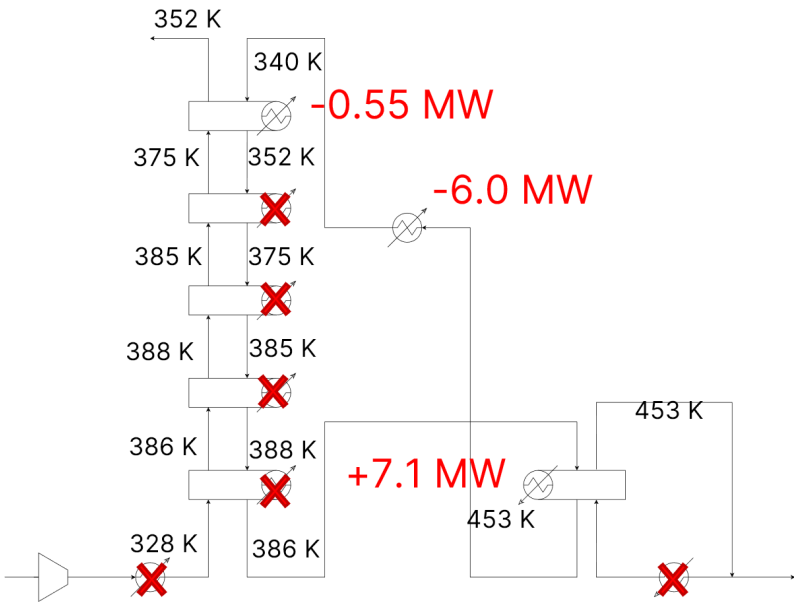

Figure 2: Fluidized TSA process schematics.

carbon credits for compliant industries sell as high as 50 USD.t^{-1} in some countries.

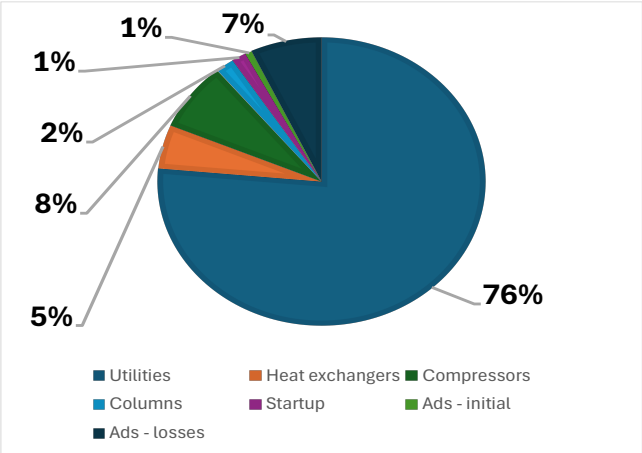

Figure 4. Main annualized cost drivers in an optimized fluidized TSA process.

Table 3: CO_2 capture costs reported in the literature.

Reference	CO_2 capture cost (USD.t^{-1})	CO_2 source
[2]	40-120	Industrial processes with diluted CO_2 streams
[2]	134-342	Direct air capture
[24]	25-190	BECCS
[25]	20-290	Several industrial processes
[26]	36-107	Industrial processes with diluted CO_2 streams
[27]	84-129	5-20%v/v CO_2
[28]	104-147	Wet flue gas, 15%v/v CO_2
[29]	88-288	BECCS
[30]	177-399	Direct air capture
[31]	31-45	Blast furnace gas

CONCLUSION

These findings show that the methodology developed here is useful for guiding the conceptual design of fluidized TSA processes for carbon capture. This study draws key conclusions based on modeling and optimization of a fluidized TSA process to capture CO_2 from biomass flue gases. Process-wide optimization is crucial for balancing CO_2 capture efficiency and energy consumption, particularly in large-scale implementations. The study identifies key design parameters, such as heat exchanger placements, that significantly impact process efficiency. The research establishes guidelines for scaling up TSA systems, emphasizing computational tools for process design refinement. This study thus contributes to the development of fluidized TSA systems for biomass-based CO_2 capture, supporting the bioenergy sector and global decarbonization efforts. Multi-scale integrated modeling approaches should be integrated into future process optimization studies to further assess residence time distribution, assist in temperature control, and improve energy efficiency.

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