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# Effects of Oscillating Injection Conditions of CO<sub>2</sub> onto its Adsorption Performance within a Packed-Bed Reactor

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**Abstract** – Carbon capture and storage (CCS) through adsorption onto activated carbon in packed-bed reactors is crucial for mitigating  $CO_2$  emissions. Optimizing these reactors' efficiency requires comprehensive exploration of various operational conditions. In this study, we investigated the influence of oscillating injection conditions, specifically periodic variations in temperature and pressure, on  $CO_2$  adsorption performance and associated energy efficiency. To achieve this, we employed a numerical model combining Computational Fluid Dynamics (CFD) with a Linear Driving Force (LDF) adsorption approach, enabling detailed simulation of heat and mass transfer within the reactor. Initially, sinusoidal and triangular waveforms were employed to evaluate the impact of periodic injection conditions on the adsorption dynamics. The results confirm that pressure fluctuations significantly affect adsorption performance while temperature fluctuations show negligible impact, highlighting pressure as the dominant injection parameter. Subsequently, the core analysis examined stepwise injection scenarios with variable holding times at high and low pressures to simulate practical industrial operating conditions. Results indicate that shorter holding times at high pressures reduce the overall adsorption efficiency due to insufficient contact time, while extended durations at elevated pressures significantly enhance  $CO_2$  uptake despite increased compression energy demands. Energy consumption analyses, incorporating compression and cooling metrics, demonstrated clear trade-offs between energy efficiency and adsorption performance under fluctuating conditions. Ultimately, our findings highlight that optimizing holding durations at elevated pressures in stepwise injection scenarios can substantially improve  $CO_2$  capture performance, offering crucial insights for the design of industrial adsorption systems.

Keywords: CO2 adsorption, Carbon capture, CFD, LDF, Oscillating conditions

## 1. Introduction

The escalating concerns over climate change have intensified the focus on carbon capture and storage (CCS) technologies, with adsorption-based methods emerging as a promising approach due to their energy efficiency and operational simplicity [1]. Packed-bed reactors employing solid adsorbents such as activated carbon have attracted considerable interest for post-combustion  $CO_2$  capture, as they provide a cost-effective solution with high adsorption capacity, ease of regeneration, and reusability, rendering them a sustainable option [2]. The performance of adsorption reactors relies heavily on the effective control of heat and mass transfer, underscoring the need for optimized operational strategies to enhance adsorption efficiency while reducing energy consumption [1].

In industrial settings, adsorption systems often face dynamic conditions, including pressure and temperature fluctuations caused by compressor cycling, feedstock inconsistencies, and operational disturbances. Understanding the impact of different oscillating patterns like sinusoidal, triangular, and pulsed is essential for designing resilient CO<sub>2</sub> adsorption systems that maintain efficiency under variable conditions [3]. Recent progress has highlighted the significant influence of operational parameters, particularly pressure and temperature, on adsorption system performance [4].

The impact of oscillatory gas flow on  $CO_2$  mass transfer has been thoroughly investigated in the literature. For instance, Hosseini et al. [5] explored the use of oscillating gas flow in a membrane gas-solvent contactor to enhance  $CO_2$  capture efficiency using an asymmetric polydimethylsiloxane membrane to study mass transfer behaviour. Their findings revealed a 19% improvement in overall mass transfer efficiency compared to steady-state conditions, with larger oscillation amplitudes further improving transfer rates. However, oscillation frequency had minimal influence beyond 2 Hz, suggesting that improved mixing, rather than oscillation speed, was the primary driver of enhanced  $CO_2$  transport.

In a separate study, Heidaryan et al. [6] explored the effects of oscillatory flow on  $CO_2$  capture at the reactor-scale using oscillatory baffled reactors (OBRs), which create periodic fluid motion to enhance mass transfer. They evaluated  $CO_2$ 

absorption in an oscillatory reactor with various solvents such as monoethanolamine (MEA), diethanolamine (DEA), and triethylamine (TEA). Results indicated that oscillatory flow significantly improved CO<sub>2</sub> absorption efficiency, particularly at low-flow conditions, by promoting better mixing and interfacial contact, achieving capture efficiencies of up to 99%. However, the study also highlighted increased energy consumption, emphasizing the need to optimize operating conditions to balance performance with energy efficiency.

Despite these advancements, there is still a lack of research focusing on the effects of fluctuating injection conditions, particularly oscillatory pressure and temperature profiles, on adsorption dynamics in packed-bed reactors. Gaining insight into these effects is essential, given the variable operating conditions often encountered in industrial processes. Investigations into stepwise pressure variations and their impact on adsorption performance are especially limited.

This study aims to bridge this knowledge gap by systematically examining the influence of oscillating injection conditions on  $CO_2$  adsorption in packed-bed reactors. We developed a numerical model that combines computational fluid dynamics (CFD) with the Linear Driving Force (LDF) model to concurrently simulate heat transfer, fluid flow, and mass adsorption processes inside the adsorption reactor. Initially, we evaluate the effects of sinusoidal and triangular waveforms in both injection pressure and temperature to establish baseline behaviors. Next, we explore stepwise pressure variations with differing holding times to assess their impact on adsorption efficiency and energy consumption. Through this comprehensive analysis, we aim to provide insights into optimizing dynamic operational strategies for enhanced  $CO_2$  capture performance.

#### 2. Methods

In this study, we developed a coupled numerical model to simulate  $CO_2$  adsorption onto activated carbon within a packed-bed reactor. The model integrates CFD to analyse gas flow and temperature distribution within the bed, with the LDF adsorption model to simulate  $CO_2$  adsorption kinetics, with associated mass dissipation, and heat generation, effectively capturing the interactions among fluid dynamics, heat transfer, and adsorption kinetics.

## 2.1. Flow Dynamics within the Porous Medium

The gas flow inside the porous bed was assumed to be laminar, with the medium treated as homogeneous and isotropic. Neglecting viscous shear stresses and assuming local thermal equilibrium, gas flow was governed by Darcy's law [7]:

$$\boldsymbol{u} = -\frac{\kappa}{\mu_g} \boldsymbol{\nabla} \boldsymbol{P} \tag{1}$$

where  $\boldsymbol{u}$  is the gas velocity vector,  $\boldsymbol{\kappa}$  is the bed permeability,  $\mu_g$  is the gas dynamic viscosity, and  $\nabla \boldsymbol{P}$  is the gas pressure gradient inside the domain.

The permeability  $\kappa$  for the packed bed was determined using [8]:

$$\kappa = \frac{D_p^2 \varepsilon^3}{150 \ (1 - \varepsilon)^2} \tag{2}$$

where  $\varepsilon$  is the bed porosity and  $D_p = 70 \ \mu m$  is the average particle diameter [9].

The continuity equation accounting for compressible flow with mass adsorption is [9]:

$$\frac{\partial(\varepsilon\rho_g)}{\partial t} + \nabla . \left(\rho_g \boldsymbol{u}\right) = S_m \tag{3}$$

where  $S_m$  represents the mass sink due to adsorption, can be calculated as [9]:

$$S_m = -\frac{dq}{dt}\rho_{ac}(1-\varepsilon) \tag{4}$$

#### 2.2. Heat Transfer in the Porous Medium

Heat transfer in the porous matrix was solved simultaneously with the flow field using [9]:

$$(\rho C_p)_{eff} \frac{\partial T}{\partial t} + (\rho C_p)_g u. \nabla T = \nabla . \left( k_{eff} \nabla T \right) - S_m Q_{ad}$$
(5)

Here,  $(\rho C_p)_{eff}$  and  $k_{eff}$  are the effective heat capacity and thermal conductivity of the porous medium, respectively. The heat of adsorption per unit mass of the adsorbed activated carbon  $(Q_{ad})$  is used to calculate the term  $S_m Q_{ad}$  which represents the heat generation during the adsorption process.

The reactor container is modelled as stainless steel (type 316), enabling heat transfer via pure conduction.

#### 2.3. CO<sub>2</sub> Adsorption Modelling

The adsorption kinetics were modelled using the first-order Linear Driving Force (LDF) model [10]:

$$\frac{dq}{dt} = k(q_{eq} - q) \tag{6}$$

where q is the instantaneous adsorption capacity,  $q_{eq}$  is the equilibrium adsorption capacity, and k is the LDF rate constant calculated by [10]:

$$k = \frac{15 D_s}{R_p^2} \tag{7}$$

with  $R_p$  denoting average particle radius  $\binom{D_p}{2}$ , and  $D_s$  being the surface diffusivity of CO<sub>2</sub>, which follows an Arrhenius temperature dependence [9]:

$$D_s = D_{s,0} \exp(-\frac{E_a}{RT}) \tag{8}$$

where  $D_{s,0}$  and  $E_a$  are the pre-exponential factor and activation energy, respectively.

#### 2.4. Equilibrium Adsorption Model

The equilibrium adsorption capacity  $q_{eq}$  was determined using the D–A model [11]:

$$q_{eq} = q_0 \exp(-(\frac{A}{E})^n) \tag{9}$$

where  $q_0$  is the theoretical maximum adsorption capacity,  $q_0$  is the characteristic energy, and n is the heterogeneity factor.

The adsorption potential A was calculated as [12]:

$$A = RT \ln(\frac{P_{sat}}{P}) \tag{10}$$

where  $P_{sat}$  is the saturation pressure, and *P* is the partial pressure of CO<sub>2</sub>. Above the critical temperature of CO<sub>2</sub> (303 K), the pseudo-vapor pressure  $P_{sat}$  was estimated using [11]:

$$P_{sat} = \left(\frac{T}{T_c}\right)^2 P_c \tag{11}$$

Finally,  $q_0$  is related to the micropore volume  $W_0$  and the molar volume  $V_m$  of CO<sub>2</sub> by [11]:

$$q_0 = \frac{W_0}{V_m} \tag{12}$$

and the temperature dependence of  $V_m$  was given by [11]:

$$V_m = V_t \exp(\alpha(T - T_t)) \tag{13}$$

where  $V_t = 0.84858 \ cm^3/g$  is the specific volume of CO<sub>2</sub> at triple point and  $\alpha = 0.0025 \ K^{-1}$  is the thermal expansion coefficient.

### 3. Results and Discussions

The governing equations presented above were coupled and solved using COMSOL Multiphysics v6.3 on a twodimensional axisymmetric domain, which was used to represent the physical structure of the packed-bed reactor. The corresponding three-dimensional geometry, reconstructed from the 2D axisymmetric setup, is illustrated in Figure 1.a, showing the reactor packed with adsorbent material. Maxsorb III activated carbon powder, characterized by a porosity of 40%, was selected as the adsorbent. CO<sub>2</sub> gas was introduced into the reactor from the top boundary, while the bottom boundary was closed and thermally insulated. A cooling temperature of 5°C was applied along the side walls to facilitate thermal management. The reactor itself had an internal diameter of 20 mm, a height of 50 mm, and a stainless steel wall thickness of 0.5 mm. The entire reactor system was initialized with a uniform temperature of 20°C and a pressure of 1 bar prior to the injection of CO<sub>2</sub>.

To ensure the numerical results were independent of mesh density, a mesh sensitivity analysis was conducted. After several trials, a total of 1051 elements was selected using COMSOL's "fine" mesh setting, offering an optimal balance between computational efficiency and solution precision. The numerical model was then validated against experimental results obtained from a study by Assilbekov et al [9], where the adsorption behavior of CO<sub>2</sub> on Maxsorb III activated carbon powder was measured using a magnetically suspended balance (MSB-GS-100-10 M). In their experiments, a cylindrical SUS316 container with an inner diameter of 23.5 mm and a wall thickness of 0.2 mm was used, and adsorption tests were carried out under varying bed thicknesses, pressures, and temperatures. For validation purposes, a specific experimental condition, with a bed thickness of 0.9 mm, a pressure of 555.2 kPa, and a temperature of 30°C was selected and replicated numerically. As shown in Figure 1.b, the simulated adsorption uptake closely matches the experimental results over time, thereby confirming the accuracy and robustness of the developed model.

To systematically assess the effects of oscillating injection conditions on CO<sub>2</sub> adsorption behaviour, we first define a baseline scenario in which both the injection pressure and temperature are maintained constant throughout the adsorption process. In the baseline case, carbon dioxide is injected at a pressure of 3 bar and a temperature of 20°C. Following this, to reflect common industrial operating patterns, we introduce two classical oscillating waveforms: sinusoidal and triangular fluctuations. These waveforms are applied simultaneously to both the injection pressure and temperature, allowing us to explore how smooth versus sharper periodic changes influence the adsorption dynamics. The injection temperature oscillates around  $20^{\circ}$ C with an amplitude of  $5^{\circ}$ C, and the injection pressure oscillates around 3 bar with an amplitude of 1 bar, both with a cycle period of 250 seconds.



Fig. 1: Schematic of the modelled reactor, with the dark region indicating the activated carbon powder located within the container (a). Comparison of CO<sub>2</sub> adsorption per unit mass of activated carbon, contrasting experimental data from Assilbekov et al [9] with the present numerical findings.

The mathematical expressions governing the oscillations of these waveforms are defined as:

$$T_{in}(t) = 20 + 5\sin(\frac{2\pi}{250}t)$$
(13)

$$P_{in}(t) = 3 + 1\sin(\frac{2\pi}{250}t)$$
(13)

For sinusoidal and

$$T_{in}(t) = 20 + 5 \arcsin(\sin(\frac{2\pi}{250}t))$$
 (13)

$$P_{in}(t) = 3 + 1 \arcsin\left(\sin\left(\frac{2\pi}{250}t\right)\right) \tag{13}$$

For triangular oscillations.

The adsorption behaviour of  $CO_2$  for the baseline, sinusoidal, and triangular fluctuation cases are displayed in Figure 2. Under the baseline condition, adsorption uptake smoothly increases over time and asymptotically approaches an equilibrium value without any oscillatory behaviour. In contrast, both sinusoidal and triangular oscillations introduce significant fluctuations in the adsorption uptake curve.

The sinusoidal case results in relatively smooth oscillations around the baseline adsorption trajectory, with gradual and symmetric rises and falls. While the triangular one induces sharper, more abrupt changes in adsorption behaviour, with a distinctly jagged pattern reflecting the sudden shifts inherent to the triangular profile. Over time, both sinusoidal and triangular fluctuating cases oscillate around the baseline's equilibrium value, indicating that although the mean adsorption amount remains comparable, transient instabilities are introduced into the system by oscillations. These instabilities could impact operational consistency and potentially energy efficiency.



Fig. 2: Comparison of CO<sub>2</sub> adsorption uptake per unit mass of activated carbon for baseline and fluctuating scenarios.

After establishing the effects of periodic fluctuations, we further isolate the independent effects of temperature and pressure oscillations individually to better understand their contributions. For this purpose, we conducted a set of simulations where only one parameter was allowed to oscillate while the other remained constant. Two amplitude levels of small and large amplitudes were studied for each variable. For temperature-only cases, the injection temperature fluctuated sinusoidally around 20°C with amplitudes of  $\pm 2^{\circ}$ C (small) and  $\pm 10^{\circ}$ C (large), while the injection pressure was kept constant at 3 bar. The resulting adsorption curves for both temperature amplitudes, shown in Figure 3, closely align with the baseline curve and exhibit no significant deviations. This confirms that, under the conditions studied, oscillations in injection temperature do not meaningfully influence the CO<sub>2</sub> uptake.



Fig. 3: Comparison of CO<sub>2</sub> adsorption uptake per unit mass of activated carbon for the baseline case and cases with isolated fluctuations in injection pressure and temperature.

In contrast, for pressure-only oscillation scenarios (temperature fixed at  $20^{\circ}$ C), the injection pressure varied sinusoidally around 3 bar with amplitudes of  $\pm 0.2$  bar (small) and  $\pm 2$  bar (large). The results clearly indicate that even small pressure oscillations induce noticeable fluctuations in adsorption uptake, and the effect becomes significantly more pronounced at higher amplitudes. These findings highlight that pressure plays a dominant role in modulating the adsorption kinetics and performance, whereas temperature fluctuations have negligible influence under the same conditions. Based on this observation, the subsequent investigation focuses solely on stepwise pressure waveforms—

where the high and low pressure levels alternate with varying holding times—to explore their impact on adsorption behaviour and energy efficiency in more depth.

To further investigate practical modulation strategies for CO<sub>2</sub> injection pressure, three distinct stepwise pressure profiles were examined: equal holding times between high and low pressure phases (SW-EH), extended high-pressure duration with shortened low-pressure intervals (SW-HL), and shortened high-pressure duration with extended low-pressure intervals (SW-HS). These scenarios were designed to assess how the distribution of time spent at elevated versus reduced pressures influences the adsorption behaviour and overall energy efficiency. Each profile alternates between a low pressure of 1 bar and a high pressure of 5 bar, but with differing durations spent at each pressure level. The case SW-EH maintains a 50%-50% distribution between high and low pressures. In contrast, SW-HL favours an 80%-20% distribution with longer durations at 5 bar, while SW-HS adopts the opposite, spending 80% of the cycle time at 1 bar and 20% at 5 bar.

According to Figure 4 and Table 1, the adsorption behaviour is highly sensitive to the duration spent at elevated pressures. SW-HL exhibits the highest  $CO_2$  uptake, reaching a total adsorption amount (2.36 g) higher than the base case. This improved performance can be attributed to the extended periods at 5 bar, allowing the system to approach local equilibrium more effectively before pressure drops. On the other hand, SW-HS results in a marked reduction in total  $CO_2$  uptake (1.61 g), as the system frequently resides at the low-pressure state, restricting adsorption capacity. SW-EH represents a balanced condition, with moderate uptake (1.95 g) and a strongly oscillating adsorption curve.



Fig. 4: CO<sub>2</sub> adsorption uptake curves under stepwise injection pressure conditions with equal holding (SW-EH), high-pressure long (SW-HL), and high-pressure short (SW-HS), compared to the base case.

Га	ble	1:	Energy	consump	tion	breakdov	vn and	l adsor	ption	performance	for ste	pwise	pressure i	njection	cases	and th	ie ba	seline
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Cases	В	SW-EH	SW-HL	SW-HS
Compression Energy (J)	37.13	353.56	338.48	258.63
Cooling Energy (J)	569.15	638.65	614.30	564.34
Total Energy (J)	606.28	992.21	952.78	822.98
Total adsorption (g)	2.10	1.95	2.36	1.61
Specific energy (J/g)	288.70	508.83	403.72	511.17

However, while SW-HL achieves a higher adsorption capacity than the base case, it does so at the expense of significantly greater energy consumption (952.78 J compared to 606.28 J in the base case), primarily due to the increased compression energy. This is reflected in the specific energy usage, where the base case remains the most efficient at 288.70 J/g, followed by SW-HL at 403.72 J/g. Both SW-EH and SW-HS perform less favourably, with specific energy values of 508.83 J/g and 511.17 J/g, respectively. These findings confirm that even though longer high-pressure durations can recover

adsorption capacity, they come at a steep energy penalty, underscoring the importance of balancing pressure intensity and energy efficiency in fluctuating strategies.

# 4. Conclusion

This study investigated the effects of fluctuating CO<sub>2</sub> injection conditions on adsorption performance in a packed-bed reactor through CFD-LDF modeling. After benchmarking against steady-state conditions, sinusoidal, triangular, and stepwise pressure oscillations were systematically evaluated. The results confirmed that pressure fluctuations significantly influence adsorption dynamics, while temperature oscillations have negligible impact. Stepwise pressure profiles, particularly with longer high-pressure durations, enhanced adsorption capacity but at the expense of higher energy consumption. Overall, maintaining stable or carefully modulated pressure conditions is crucial for optimizing both adsorption efficiency and energy performance in CO<sub>2</sub> capture systems.

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