

Direct Air Capture: Effects of Low-Purity CO₂ and Geological Depths on Post-Capture Compression Energy and Storage

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ORIGINAL RESEARCH

Abstract- Direct air capture and storage (DACS) has the potential to capture from innumerable random, mobile and immobile small-scale carbon-emission sources and safely store in the subsurface. However, the relatively high level of impurities in the CO₂ stream poses challenges to energy requirements and operating costs in post-capture operations like compression, cooling and carbon mineralization. In this study, compression energy and storage levels of impure CO₂ stream from Direct Air Capture (DAC) were investigated, using ASPEN and PHREEQC software. Findings show that isentropic compression work increases as the mole fraction of CO₂ decreases in the stream. At the same depth of sequestration, compression power requirement increases by 20% to sequesterate a 10% CO₂ stream compared to pure CO₂. Also, sequestration at deeper geological layers further raises the power cost of the compression by approximately 14% from 1000 to 1500m and by almost 32% from 1500m to 2500m depth, for pure CO₂. This increases to around 34% for storage at 2500m with 50% CO₂ mole fraction and 36% for 20% CO₂ fraction at the same depth. Similarly, the cost of cooling compressed CO₂ increases in proportion to the reduction in CO₂ mole fraction in the gas stream. It was shown that the subsurface solution density increases as the impurities level rises while pH falls in the presence of N₂ and O₂.

Keywords- Carbon, Compression, Direct Air Capture, Mineralization, Storage.

1 INTRODUCTION

The continuous emission of greenhouse gases into the atmosphere is setting a pathway to difficult climate conditions with consequences on ecological displacement and shift. This trend is already aggravating the state of global warming. Fossil fuel consumption and transformation generates 13 gigatonnes of CO₂ annually (IAEA, 2013). Substantial reduction of emission is needed to keep within and below the 2°C. This requires emissions reduction of about 37Gt/yr till 2050 or removal of the atmospheric incremental of 1 Gt CO₂ per year (Haszeldine *et al.*, 2018). This shows the enormity of the tasks required to remediate the climate and safeguard the planet.

Among the existing emission reduction technologies, Direct Air Capture and Storage (DACS) is a promising option, owing to the possibility of tackling innumerable random, mobile and immobile small-scale carbon-emission sources that account for half of the global GHG emissions, which are simply impossible to neutralize by conventional CO₂ capture applications (Seipp 2017). The other options are simply expensive and restricted in scope. For example, bio-sequestration by microbes, plants, oceans, rock weathering and so on, has been on for ages but at a rate that is not in step with the emission rate since industrial revolutions (Goepfert *et al.*, 2012). Even the popular carbon capture and sequestration (CCS), carbon capture and utilization (CCUS), cryogenic carbon capture (CCC) and so on are far too expensive and technically costly to operate.

DAC is advantageous in that it can be engineered to consume less space and avoid toxic solvents for capture while continuously looping to sense and scrub the atmosphere of carbon (Haszeldine *et al.*, 2018). Thus, Direct Air Capture and Storage (DACS) provides the lifeline to deal comprehensively with the menace of unceasing emissions from these innumerable sources, including vehicular emissions (Oloruntoba and Okediji, 2021). Thus, the use of DACS is pivotal to attaining the target CO₂ concentration in the atmosphere. However, the presence of impurities in the CO₂ captured by The Direct Air Capture (DAC) system has been a source of concern over time, because of the dilute nature of gases in the atmosphere (Broehm *et al.*, 2015; Goepfert *et al.*, 2012; Lackner, 2009). To be completely satisfactory, effective and sustainable DAC technology must be of lower cost and promotes environmental safety, among others. Also, the technology must be all-pervasive to cover many distributed outlets of emissions in different localities with a view to meeting the target of limiting global warming below 2 °C by the end of this century (Brethomé *et al.*, 2018). But, the challenge of purity in the CO₂ stream emanating from DAC system is difficult to overcome. Therefore, emphasis has to be placed on the effects of these impurities on the performance of the DAC systems owing to the unique compositions of gases available for this system, vis-a-vis its effects on the economy of the technology and the mineralization or permanent storage of the stored carbon.

Currently and in the near future, the DAC economy will be reckoned by factors such as Cost/tCO₂, Energy/tCO₂, space/unit DAC, Capture capacity and so on. Right now, DAC technology is reckoned with significant cost reduction potential (Keith *et al.* 2018; Fasihi *et al.* 2019) while overall efficiency in extracting CO₂ is comparably high (Fuss *et al.* 2018). Companies like Carbfix (Iceland) had embarked on open-air installation of this technology and started to capture carbon, creating large-scale Direct Air Carbon Capture and Storage (DACCS) or CO₂

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Section D- MATERIALS/ CHEMICAL ENGINEERING & RELATED SCIENCES

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utilization (Direct Air Carbon Capture and Utilization-DACCU). Application of the captured carbon can be found in transport fuels, including in marine, aviation and chemical industries (Haegel *et al.* 2019).

Three main stages of DAC technologies are contacting, capture by a sorbent, and separation of the CO₂ from the sorbent (Mostafa *et al.* 2022). Keith *et al.* (2018) reported the process of CO₂ capture from air using an aqueous KOH sorbent coupled to a calcium caustic recovery with a levelized cost from 94 to 232 USD/ tCO₂. Combining temperature and vacuum swing adsorption (TVSA), the authors successfully deployed DAC to achieve 95-100% vol CO₂ with an energy consumption of around 10kWh/kg. Economic improvement can be seen in the demonstration and proposition of High Hopes Lab in Israel, resulting in \$100-\$250 per ton, for the first stage and \$40-\$50 at the second stage.

Sustainable DAC requires sorbents with high CO₂ capacity, easily regenerable, favorable kinetics, ready availability and environmental compatibility. The solvent/sorbent cost should be ordinarily cheap or lowered through continuous improvement and innovation. These cheap and efficient sorbents and solvents will make DAC, not only reduce the cost of operation, but also overcome the lower net contribution of DAC to Carbon Dioxide Removal (CDR). The choice of solvent is another major factor that hampers the efficiency of DAC. Many solvents suffer from the problems of volatility, toxicity, costs and separation difficulty. There are cases of solvent hampering the successful conversion of captured carbon from DAC into methanol, owing to volatility issues, oxidative degradation, and notable toxicity, making them less suitable for DAC in a scaled-up process. Using waste minerals or industrial wastes as adsorbents may eliminate the recovery stage, saving energy, and project costs while also providing raw materials for other uses.

In addition, the DAC performance under different weather conditions and integration of DAC to systems with abundant waste heat needs to be demonstrated for overall sustainable energy performance, which will also bear down on cost. The flexibility of the sorbents and solvents under varying and extreme weather conditions is required to be checked for maintaining consistent performance (Kong *et al.* 2022). It is clear from the above that the relatively high level of impurities in the CO₂ stream poses challenges to energy requirements and operating costs in post-capture operations like compression, cooling and subsurface carbon mineralization. In this study, influences of impurities in the CO₂ stream and geological depths were analyzed in relation to the compression work requirement and subsurface storage levels of impure CO₂ stream, captured through the DAC system. Software- ASPEN and PHREEQC, were employed in the simulations. Questions answered include how the quality or compositions of captured carbon affects the post-capture processes of compression and cooling. How does the CO₂ stream impurity affect storage space in the aquifer? The use of cost and economy in this study is related to the compression work or energy required to treat the post-capture gas stream. It also relates to the storage space

required for injecting the compressed gas. These economic terms are used in this context.

2 METHODS

This study investigates the effects of the impure CO₂ stream captured from the Direct Air Capture (DAC) system on the post-capture compression energy and storage effectiveness in geological reservoirs. The analysis depends on ASPEN (version 10), and PHREEQC software. Parameters utilized in the simulations were listed in Tables 1 and 2. The hypothetical geological depths and associated conditions are listed in Table 1.

Table 1. Geological depths for gas storage in Anorthite- and Goethite-rich rock together with the associated conditions. (Tsuji *et al.*, 2021)

Geological Depth (km)	Temperature (°C)	Pressure (Mpa)
1.0	38	10
1.5	52.5	15
2.5	80	25

The conditions at each geological depth dictate that the captured stream of CO₂ will be necessarily compressed (Koohestanian and Shahraki, 2021) to similar pressure in order for effective storage to take place at such depth. This work chose reservoirs that are rich in Anorthite and Goethite minerals in order to understand how the chemistry of the subsurface will affect the storage effectiveness. Probable levels of impurities in CO₂ stream are adapted from the work of Tsuji *et al.* (2021). The mixes of impurities are shown in Table 2.

2.1 ASPEN

To analyze the compression work variation with different levels of CO₂ purity, the COMPR model in ASPEN software was used. This model computes the work required for compression together with the outlet stream temperature, phase condition and enthalpy. The head developed for a compressor to change from the inlet stream P1 to the outlet stream P2 is given by

$$Head = \int_{P_2}^{P_1} VdP \tag{1}$$

V is the molar volume of the gas. The actual enthalpy change per unit mole of gas for a compression process is calculated as

$$p\Delta h = \int_{P_2}^{P_1} VdP \tag{2}$$

where p is the isentropic or polytropic efficiency. The total enthalpy change in the stream is given as Indicated Horse Power (IHP)

$$IHP = F\Delta h \tag{3}$$

Where F is the gas flow rate. The IHP corrected for mechanical efficiency (η_m) is

BHP= IHP/ η_m). Net work required or produced is calculated as follows,

$$W_{out} = BHP + W_{in} \tag{4}$$

The network is positive if power is required and negative if power is produced.

2.2 PHREEQC

The mineralization reaction of the impure CO₂ stream in anorthite and goethite minerals was simulated with PHREEQC software. The program assumes that there exists thermodynamic equilibrium among dissolved species and determines the unknowns for each species (Parkhurst and Appelo 2013). These unknowns include the activity, a_i , activity coefficient, γ_i , molality, m_i , and moles in solution, n_i . The governing equations for the activities of the aqueous species are shown below,

$$a_i = \gamma_i m_i \tag{5}$$

$$n_i = m_i W_{aq} \tag{6}$$

Where W_{aq} is the mass of solvent water in an aqueous solution. An isentropic compression turbine was used. Probable mole fractions of N₂-O₂-CO₂ stream in the DAC process are listed in Table 2.

Table 2. Mole fractions N₂-O₂-CO₂ stream in DAC process (Tsuji et al., 2021)

CO ₂	N ₂	O ₂
1	0	0
0.8	0.16	0.04
0.7	0.24	0.06
0.5	0.4	0.1
0.3	0.56	0.14
0.2	0.64	0.16
0.1	0.72	0.18
0.05	0.76	0.19
0	0.8	0.2

3 RESULTS AND DISCUSSIONS

The analysis of the results from the simulation of impure CO₂ stream in ASPEN and PHREEQC software are presented below. As shown in Figure 1, the compression work increases as the impurity level in the CO₂ stream increases. The isentropic compression work increases as the mole fraction of CO₂ decreases in the stream. At the same depth of sequestration, compression power requirement increases by 20% to sequester a 10% CO₂ stream compared to pure CO₂. Also, sequestration at deeper geological layers further raises the power requirement of the compression by approximately 14% from 1000 to 1500m and by almost 32% from 1500m to 2500m depth, for pure CO₂. This increases to around 34% for storage at 2500m with 50% CO₂ mole fraction and 36% for 20% CO₂ fraction at the same depth. Thus, the purity level of the gas stream poses a higher net power need on the carbon compression and eventual total capture and storage cost.

Furthermore, the energy for cooling compressed CO₂ imposes an additional burden on the total storage cost. This is because the compression is an exothermic process (Pei, et al. 2014), which makes the system require heat reduction before further processing. Figure 2 shows the heat duty required to cool the compressed CO₂, corresponding to various depths. In the figure, the amount

of heat needed to be removed increases as the purity of CO₂ reduces while also increasing with the depth of the storage domain.

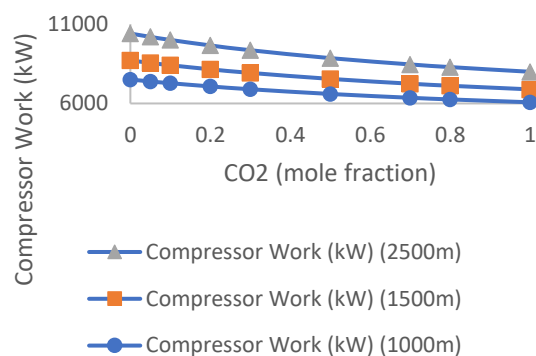


Fig. 1: Compressor Work at various CO₂ purity levels

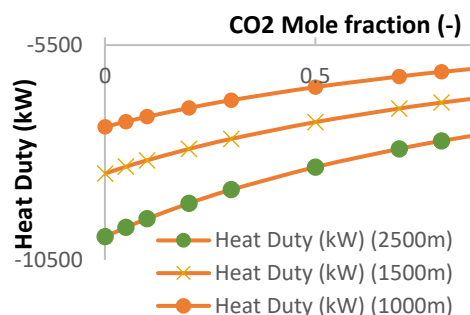


Fig. 2: Heat duty at various CO₂ purity levels. The heat duty is per unit mole of the compressed air. Negative implies heat removal

Pei et al (2014) propose waste heat recovery for the compression and intercooler of the gas stream in order to reduce the CCS operating cost. Apart from compression and cooling power requirement, Wang et al. (2011), Alnes et al. (2011) and Tsuji et al. (2021) found that the low-purity of CO₂ stream raised the operating cost of storage disproportionately, owing to density disparity. For example, at 1000m depth, low purity stream was found cost-ineffective owing to reduced density of the CO₂ at low purity. At 80% CO₂ purity, storage cost is doubled that of 90% CO₂ stream, bearing the costs of drilling and transport, which can be offset by situating the system near the injection site (Tsuji et al., 2021).

Comparing the work of these authors with the findings in this work shows that low-purity of CO₂ is generally problematic to DAC cost. However, the cost impacts of density disparity under different conditions can be ameliorated by choosing a higher depth to raise the density of the stream and consequently, the amount of CO₂ stored. The net increase in the cost of compressional and cooling can be offset by the storage quantity per unit space allocated at higher depths. The impurity or presence of a higher proportion of N₂ and O₂ decreases the CO₂ density and affects the effectiveness and cost of storage (Tsuji et al., 2021). Commonly, CO₂ possesses a much higher freezing point (-78°C) than many other components of the gas stream (Font-Palma et al. 2021). Presence of impurity will lead to reduced density of CO₂, as other components exist as mainly gas even under high pressure, unlike CO₂ which increases in density under pressure at pure conditions.

Some unclear deleterious and possibly advantageous effects of low purity CO₂ and high concentrations of N₂ may be complex to decipher. Ordinarily, owing to its high bond energy, N₂ requires high activation energy for the reaction to take place. To get the best yield of carbon adsorption for carbon mineralization, it is essential to reduce the level of competing molecules, like unreactive N₂, that can preferentially occupy the adsorption sites of the mineral adsorbents. Thus, it is essential to utilize a dehumidifier for the entering air to reduce moisture entry. Figure 3 shows that the density of the solution increases with impurities in the CO₂ stream.

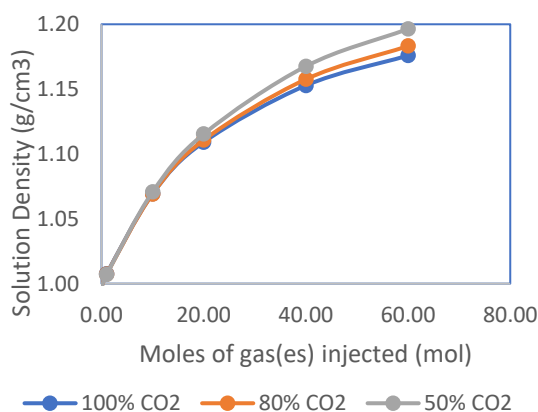


Fig. 3: Solution Density at 1km Depth

This is because the pH decreases in the presence of N₂ and O₂, which leads to increased mineral dissolution. The increase in solution density should not be confused with the density reduction of the gas stream, reported by Tsuji et al. (2021). The solution density increases as more minerals (anorthite and goethite) dissolve at low pH, in the presence of higher impurities.

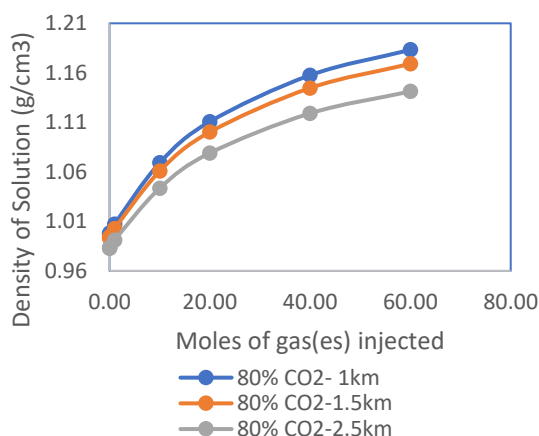


Fig. 4: Solution Density at Different Depths

Figure 4 shows that the solution density decreases with depth. This is because, though, pH increases with the depth of sequestration, mineral dissolution decreases, as a result of rising temperature at higher depths.

4 CONCLUSION

This study analyzed the effects of CO₂ purity, from Direct Air Capture (DAC), on the post-capture compression work before injection as well as on the subsurface mineralization process. The influence of this on the

effective storage at different geological depths was also discussed. Simulation results reveal the isentropic compression work increases as the mole fraction of CO₂ decreases in the captured stream of gas. At the same depth of sequestration, compression power requirement increases by 20% to sequester a 10% CO₂ stream compared to pure (100%) CO₂. Also, sequestration at deeper geological layers further raises the power cost of the compression by approximately 14% from 1000 to 1500m and by almost 32% from 1500m to 2500m depth, for pure CO₂. This increases to around 34% for storage at 2500m with 50% CO₂ mole fraction and 36% for 20% CO₂ fraction at the same depth. Thus, purity poses the net cost of the carbon compression and eventual total capture and storage costs. Similarly, the energy requirement of cooling compressed CO₂ will impose an addition on the total storage cost, as it increases in proportion to the reduction in CO₂ mole fraction in the gas stream. Also, the density of the solution increases with impurities in the CO₂ stream owing to mineral dissolution under low pH, in the presence of impurities. The results of these analyses are mainly valid for the stream compositions and conditions used in the simulations.

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