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Modelling and Analysis of Direct Air Capture Systems in Different Locations

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Direct air capture is an important negative emission technology with the aim to reduce carbon dioxide emissions in the atmosphere and to face the current environmental problems such as global warming and climate change. This emerging technology can be based on an adsorption system affected by the used sorbent (physisorbents or chemisorbents). Efficiencies can be measured through the use of key performance indicators that allow a comparison among different processes.
An independent analysis was conducted in our previous research to evaluate key performance indicators (total cost, energy consumption, environmental impact and capture capacity) for a direct air capture system based on adsorption using different sorbents (three metal organic frameworks and two amine functionalized sorbents).
In this research, the same analysis was extended to several Countries around the world, changing the ambient air temperature according to the yearly average value of the location.
Results show that by increasing the air temperature, the adsorption capacity decreases, in a more significant way for metal organic frameworks compared to amine functionalized sorbents. An opposite effect is for energy consumption. Moreover, by increasing the ambient air temperature, a higher environmental impact (in terms of climate change) is present. A trend with the air temperature was not found for total costs. Overall, locations with lower ambient air temperatures are preferred due to a lower environmental impact and energy consumption.

1. Introduction

Carbon dioxide (CO_2) emissions in the world were more than 33 Gton in 2018 (IEA, 2020). Studies have confirmed that mitigation actions, meaning the reduction of CO_2 emissions, might be not enough to achieve what is defined in the International Environmental Agreements. Instead, the removal of CO_2 has been suggested by researchers through the use of Negative Emission Technologies (NETs) also known as Carbon Dioxide Removal (CDR) technologies (Lackner, 2015). Among these, due to particular advantages, much attention has been focused on Direct Air Capture (DAC), as underlined by the increasing research papers of these last years. In DAC, CO_2 is captured from the air with several methodologies. Absorption and adsorption are the most investigated in the literature and important DAC companies are based on them (e.g. Carbon Engineering and Climeworks use respectively absorption and adsorption processes) (Sanz-Pérez et al., 2016).
The adsorption process exhibiting modularity is characterized by a simpler process scheme compared to the absorption system also with the possibility to exploit low grade heat for the regeneration stage. For these reasons, this work was focused on the DAC adsorption. In the literature, several research works have been conducted changing the operating parameters (Schellevis et al., 2021; Miao et al., 2021) or proposing new regeneration methods (van Schagen et al., 2022) and adsorbent beds (Drechsler and Agar, 2019). However, most studies are about the evaluation of capture capacities, energy consumptions, costs and environmental impacts, as the most important Key Performance Indicators (KPIs) investigated in the literature for this process.
In Fasihi et al. (2019), the electrical energy consumption for systems based on amine functionalized sorbents has been reported between 150 and 300 kWh_{el}/tCO_2 while, processes based on Metal Organic Frameworks (MOFs) can have an electrical energy consumption up to 1420 kWh_{el}/tCO_2. Thermal energy consumptions for chemisorbent based systems have been evaluated between 1170 and 2000 kWh_{th}/tCO_2.

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A wider range for total costs up to 1000 \$/tCO_2 has been reported (House et al., 2011). On the other hand, other studies based on different assumptions for input and output conditions suggested total costs of a few hundred dollars (Zhang et al., 2014; Sinha et al., 2017; Kulkarni and Sholl, 2012).
In Kulkarni and Sholl (2012) a cost of CO_2 capture between 43 and 494 \$/tCO_2 has been reported, while Zhang et al. (2014) suggested a cost between 91 and 227 \$/tCO_2 but without considering capital costs. Sinha et al. (2017) evaluated a lower cost of capture between 60 and 190 \$/tCO_2 but cash flows were not discounted.
In order to verify the KPI ranges suggested in the literature, an independent analysis has been conducted in Leonzio et al. (2022a,b) for an adsorption process capturing CO_2 from the air and designed according to the Climeworks plant. Costs, adsorption capacities, energy consumptions and environmental impacts were evaluated for different systems based on different sorbents, such as two amine functionalized sorbents (SI-AEATPMS ([N-(2-aminoethyl)-3-aminopropyl]trimethoxysilane (AEATPMS) grafted on silica gel) and APDES-NFC-FD (3-aminopropylmethyldiethoxysilane (APDES) on nanofibrillated cellulose (NFC)) and three MOFs (MIL-101, MOF-177, MOF-5). In this work, the previous independent analysis was extended to several Countries around the world with the aim to find the best location for the DAC plant at different ambient air temperatures. The comparison was conducted evaluating the total cost, adsorption capacity, thermal and electrical energy consumptions and global warming.

2. Mathematical modelling

2.1 Adsorbent bed and model equations

The adsorbent bed design was based on the Climeworks plant located in Switzerland (Hinwil), consisting of 18 unit beds placed in 3 rows of 6 beds working simultaneously capturing and releasing CO_2 from the air. In this work, only a single adsorption bed was modelled with an area footprint excluded options of 20 m^2, a height of 3.2 m and treating 2.86 m^3/s of air with a CO_2 concentration of 400 ppm. The operating principle of the bed is based on the Temperature Swing Adsorption (TSA): the regeneration stage is ensured by increasing the temperature at 110 °C for the system using the silica gel based sorbent and 100 °C for systems using all other sorbents. The working adsorption temperature is set by the air temperature. Thermal and electrical energies are supplied by a Municipal Waste Incinerator (MWI), as for Climeworks. Some assumptions were considered to develop the mathematical model: ideal conditions for the gas phase, isothermal conditions for the bed neglecting radial gradients, negligible nitrogen (N_2) and water (H_2O) adsorption, linear driving force (LDF) for the adsorption kinetic. The mathematical model used to describe the single adsorbent bed has gas phase and adsorbed phase material balance equations respectively as a partial differential equation and ordinal differential equations. Maple software was used for its resolution and its detailed description has been reported in Leonzio et al. (2022a). Langmuir adsorption equilibrium isothermals were used for MOFs, the Toth model was used for the APDES-NFC-FD sorbent, while for SI-AEATPMS a regression of the adsorption equilibrium isothermal was made from literature data in order to have an expression as a function of temperature. Different locations around the world were considered for the DAC plant changing the ambient air temperature according to the yearly average value of the location as follows: Finland (2.52 °C), China (7.1 °C), Austria (7.25 °C), USA (7.63 °C), Poland (8.85 °C), UK (9.07 °C), Germany (9.63 °C), The Netherlands (10.4 °C), Japan (11.13 °C), France (11.69 °C), Italy (12.81 °C), Spain (13.93 °C), Australia (21.94 °C), India (24.68 °C), Denmark (8.76 °C), Brazil (25.51 °C), Slovenia (9.58 °C) and Switzerland (6.08 °C) (ListFit, 2021).

2.2 Energy consumption, economic and environmental analysis

While the adsorption capacity was obtained by solving the mathematical model, electrical (to move fans) and thermal (for the regeneration stage of the bed) energy consumptions were evaluated by Equations 21-22-23 of Leonzio et al. (2022a).The economic analysis was conducted estimating operating (OPEX) and capital (CAPEX) costs as detailed explained in Leonzio et al. (2022a), considering a cost for electrical and thermal energies respectively of 0.1 \$/kWh and 0.024 \$/kWh. A location factor was considered starting from the literature data (Perry, 1999; Towler and Sinnott, 2012) and it was updated with the current exchange rates (PoundSterlingLive, 2021) for all Countries: Finland (0.88), Switzerland (0.94), China (1.12), Austria (0.85), USA (1), Denmark (0.85), Poland (0.95), UK (0.76), Slovenia (1.01), Germany (0.86), The Netherlands (1.19), Japan (1.46), France (0.73), Italy (1.14), Spain (0.83), Australia (1.04), India (0.8), Brazil (1.14). The environmental analysis according to the principle of the life cycle assessment (LCA) was carried out in SimaPro software as explained in Leonzio et al. (2022b), considering a cradle-to-gate analysis for the DAC process that uses a MWI for the energy need. The impact category climate change (kgCO_{2eq}/tCO_2 captured) was measured and compared in all Countries.

3. Results and discussion

Figure 1 shows the CO_2 capture capacity of DAC plants around the world and using different sorbents. By increasing the ambient air temperature, the amount of captured CO_2 decreases for systems based on MOFs. A DAC plant in Finland (air temperature of 2.52 °C) has a CO_2 capture capacity of 96.47, 80.42 and 81.74 $kgCO_2$/day if MOF-5, MOF-177 and MIL-101 are respectively used. On the other hand, a DAC plant in Brazil (air temperature of 25.51 °C) captures 68.29, 65.34 and 70.11 $kgCO_2$/day if MOF-5, MOF-177 or MIL-101 are respectively utilized. The decreasing trend of capture capacity with the increase of the air temperature is less significant for systems based on amine functionalized sorbents. Figure 2 reports the electrical energy consumption for the analysed processes in different places.

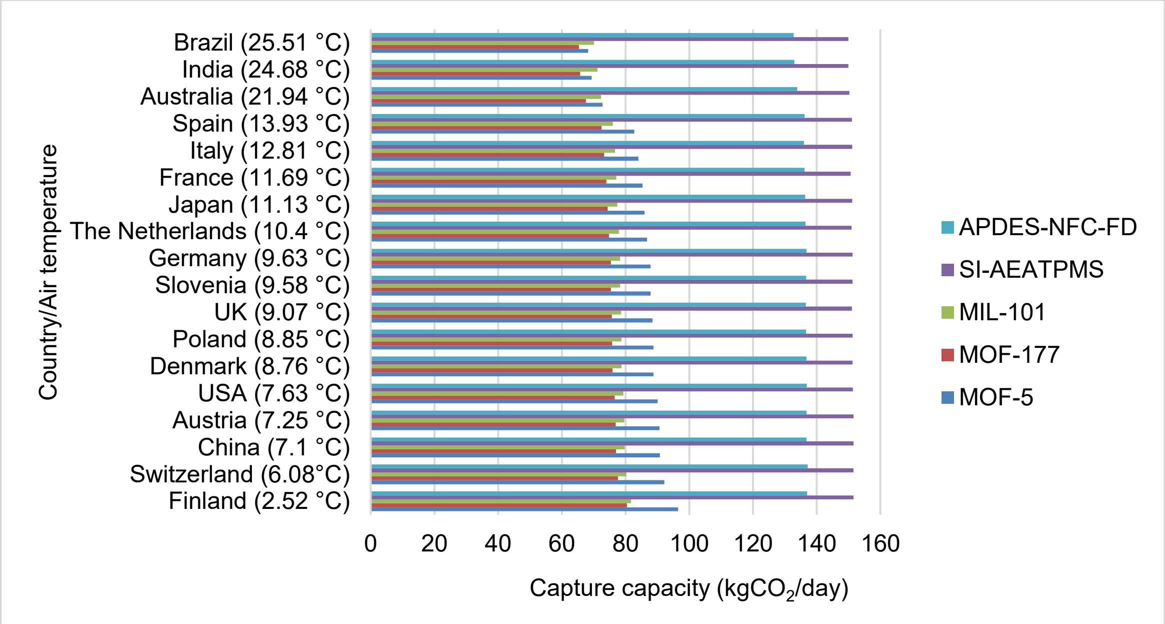

Figure 1 CO_2 capture capacity of DAC plants in different Countries

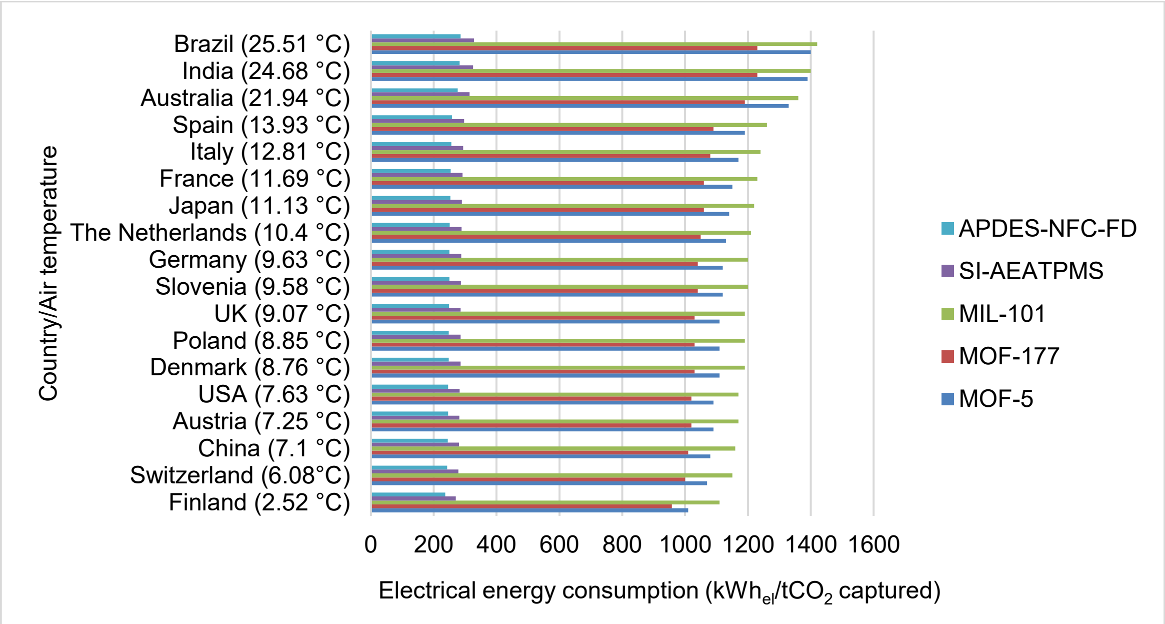

Figure 2 Electrical energy consumption of DAC plants in different Countries

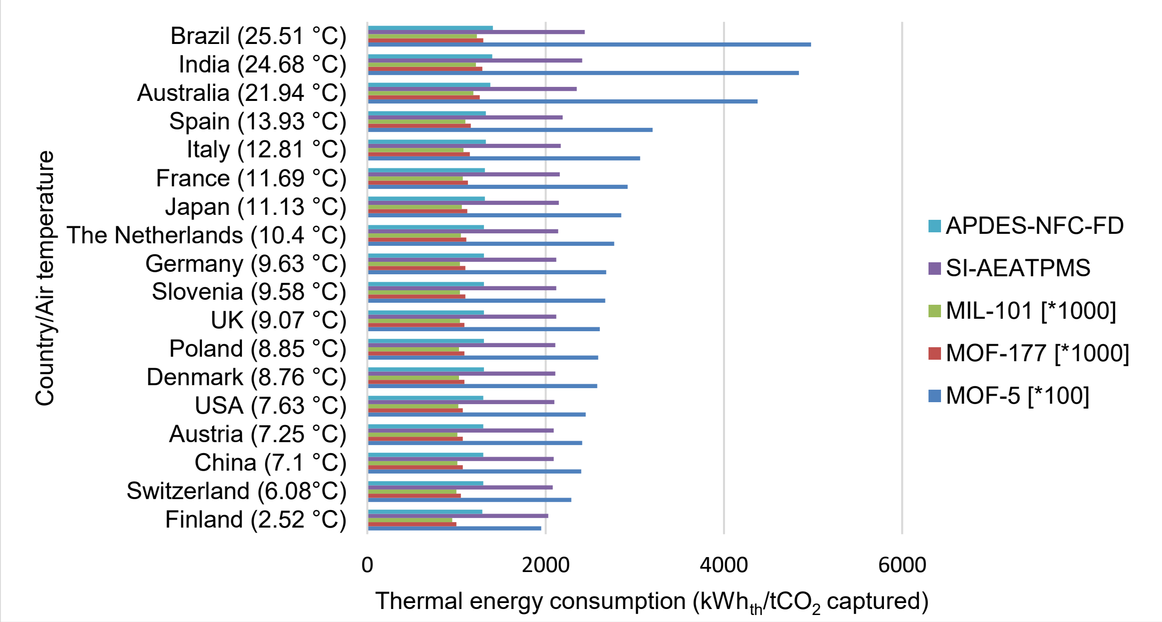

Figure 3 Thermal energy consumption of DAC plants in different Countries

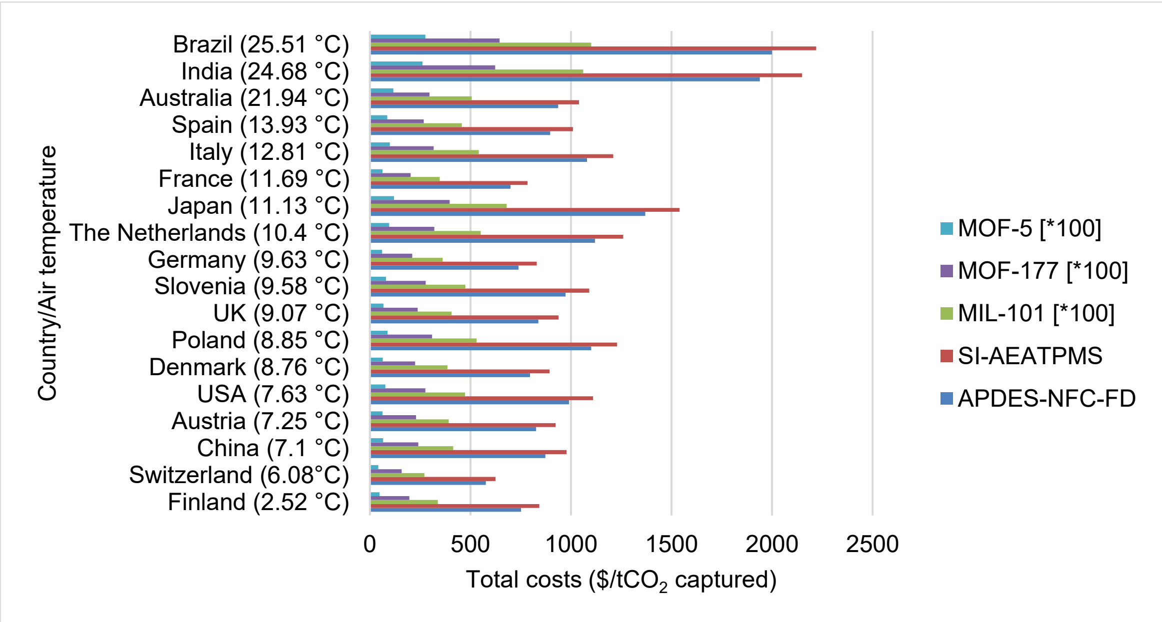

Figure 4 Total costs of DAC plants in different Countries

Regarding the electrical energy consumption of fans, it is evident that a greater amount of electricity is needed at higher air temperatures for both physisorbent and chemisorbent based systems, although a higher variation between the minimum and maximum air temperature is present for processes using MOFs. The highest electrical energy consumption (1420 kWh$_{el}$/tCO$_2$ captured) is for plant using MIL-101 located in Brazil. The lowest value of electrical need (237 kWh$_{el}$/tCO$_2$ captured) is obtained for the APDES-NFC-FD based system located in Finland. Overall, these values are comparable with those reported in the literature by Fasihi et al. (2019) and, as also reported in Leonzio et al. (2022a) MOF based systems are characterized by a higher electrical need. Thermal energy consumptions for DAC systems around the world are shown in Figure 3. As for the electrical energy consumption, a greater amount of heat is required at higher air temperatures in processes using physisorbents and chemisorbents. As found in Leonzio et al. (2022a) the use of MOFs requires a huge

amount of heat for the regeneration stage, due to a very low working capacity that makes impracticable these kinds of systems. The plant using MOF-177 and located in Brazil needs the highest value of thermal energy (1,300,000 kWh_{th}/tCO_2 captured). For amine functionalized sorbents values similar to those reported by Fasihi et al. (2019), Elfving et al. (2021) and Wijesiri et al. (2019) are obtained. In Brazil, the system using the silica gel based sorbent requires an amount of heat of 2,440 kWh_{th}/tCO_2 captured, while the process using the cellulose based sorbent needs 1,410 kWh_{th}/tCO_2 captured.
Total costs of DAC plants in different Countries are reported in Figure 4: a trend with the ambient air temperature is not present, as they are related to the location factor. However, higher total costs are for processes based on MOFs, as found by Leonzio et al. (2022a). The use of MIL-101 can cause a cost of the process up to 110,000 $\$/tCO_2$ captured, underlining how physisorbents make the plant unfeasible from an economic point of view as well. Total costs of systems based on amine functionalized sorbents are in most cases in agreement with values reported in the literature (e.g. up to 1000 $\$/tCO_2$ captured). However, a higher cost is obtained for some locations (Brazil, India, Italy, Japan, The Netherland and Poland when APDES-NFC-FD is used and Brazil, India, Australia, Spain, Italy, Japan, The Netherlands, Slovenia, Poland, USA when SI-AEATPMS is used): the construction of a DAC plant here is not suggested. Switzerland is the most preferred place where to build an adsorption plant for CO_2 capture from the air, using the cellulose based amine functionalized sorbent: total costs are 577 $\$/tCO_2$ captured. This value is comparable with that suggested by the Climeworks company (e.g. 600 $\$/tCO_2$ captured) (Climeworks, 2020).
Figure 5 shows the values of climate change for DAC plants in different Countries and with different sorbents. A lower environmental impact is present at a lower air temperature, while only the APDES-NFC-FD sorbent ensures a negative value of climate change. Due to the huge energy consumption, systems with MOF sorbents are characterized by a significant value of climate change.

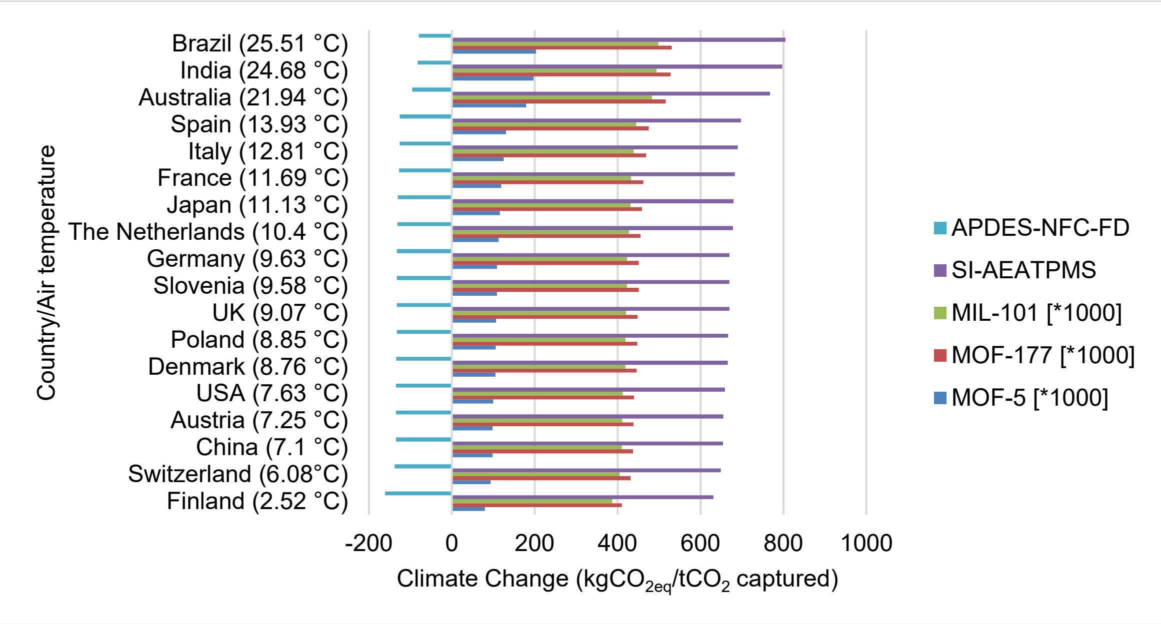

Figure 5 Climate change of DAC plants in different Countries

4. Conclusions

The analysis of a DAC adsorption process was conducted in different Countries around the world, changing the ambient air temperature according to the yearly average value of the considered location. A similar analysis has not been carried out in the literature before, underlining the novelty of this research about an emerging topic.
For the DAC system, using three MOFs and two amine functionalized sorbents, KPIs such as the adsorption capacity, thermal and electrical energy consumptions, total costs and climate change were evaluated.
Results show that locations with lower ambient temperatures are preferred due to a lower environmental impact and energy consumptions. For a DAC plant located in Finland (ambient air temperature of 2.52 °C) and using the APDES-NFC-FD sorbent, the climate change is -161 $kgCO_{2eq}/tCO_2$ captures, thermal and electrical energy consumptions are respectively of 1,290 kWh_{th}/tCO_2 captured and 237 kWh_{el}/tCO_2 captured, the adsorption capacity is 137.04 $kgCO_2$/day while total costs are 752 $\$/tCO_2$ captured.

Nomenclature

CDR – Carbon Dioxide Removal
DAC – Direct Air Capture
LCA – Life Cycle Assessment
LDF – Linear Driving Force
NET – Negative Emission Technology
TSA – Temperature Swing Adsorption

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