



# Guidelines for Techno-Economic Analysis of Adsorption Processes

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Techno-economic analyses (TEAs) of CO<sub>2</sub> capture technologies have risen in popularity, due to growing interest in meeting CO<sub>2</sub> emissions reduction targets. Adsorption processes are one of the technologies proposed for CO<sub>2</sub> capture, and although difficult, standardization of TEAs for adsorption should be attempted. The reason is that TEAs are often referred to as input data to other forms of modeling, to guide policy, and to act as summaries for those unfamiliar with adsorption processes. Herein, we discuss the aspects that should be considered when conducting TEAs for CO<sub>2</sub> adsorption processes, and we present the implications of choices made at the TEA stage and offer guidance on best practice. Our aim is to make TEAs of adsorption processes widely accessible to the adsorption community, and more generally to communities engaged in the evaluation of CCS technologies.

## OPEN ACCESS

**Keywords:** adsorption, CO<sub>2</sub> capture, costing, process design, separation, techno-economic analysis

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### Specialty section:

This article was submitted to  
Separation Processes,  
a section of the journal  
Frontiers in Chemical Engineering

**Received:** 04 September 2020

**Accepted:** 14 December 2020

**Published:** 20 January 2021

### Citation:

Danaci D, Webley PA and Petit C  
(2021) Guidelines for Techno-  
Economic Analysis of  
Adsorption Processes.  
*Front. Chem. Eng.* 2:602430.  
doi: 10.3389/fceng.2020.602430

## 1 INTRODUCTION

Adsorption based separation processes have been applied at an industrial scale since the 1960s for the purification of hydrogen (Wagner, 1967; Stöcker et al., 1998). Since then, additional applications such as gas and liquid dehydration, air separation, landfill gas upgrading, isomer separations, CO recovery, and pollutants removal (SO<sub>x</sub>, NO<sub>x</sub>, organic sulfur, cyanides, acid vapours, heavy metals, and VOCs) (Bart and von Gemmingen, 2005). Adsorption also finds applications in water treatment as well as, fine- and bio-chemical, and pharmaceuticals production (Bart and von Gemmingen, 2005). With increasing interest in CO<sub>2</sub> emissions abatement and efficiency improvement in industrial processes, adsorption-based processes have gained significant attention in the research community over the last ≈30 years.

Adsorption-based technologies have potential applications in each of the CO<sub>2</sub> capture categories: post-combustion capture, pre-combustion capture, oxy-combustion, natural gas sweetening, and negative emissions (i.e., direct-air capture). In the case of post-combustion capture, a fuel is combusted in air and produces a flue gas consisting mainly of N<sub>2</sub>, CO<sub>2</sub>, and H<sub>2</sub>O. The CO<sub>2</sub> is then separated from this low-pressure mixture for sequestration or utilization. Aside from the overt

**Abbreviations:** ASME, American Society of mechanical engineers; BECCS, bio-energy with carbon capture and storage; CCS, carbon capture and storage; CEPCI, chemical engineering plant cost index; COF, covalent organic framework; CPI, chemical process industry; CRF, capital recovery factor; C<sub>v</sub>, flow coefficient; DAC, direct-air capture; DACCS, direct-air carbon capture and storage; EAC, equivalent annual cost; HVAC, heating, ventilation, and air-conditioning; IPCC, intergovernmental panel on climate change; IBL, inside battery limits; MOF, metal-organic framework; NET, negative emissions technology; NMR, nuclear magnetic resonance; NPV, net present value; OBL, outside battery limits; PFG, pulsed field gradient; POP, porous organic polymer; PSA, pressure swing adsorption; TAC, total annualized cost; TEA, techno-economic analysis; TPD, tonnes per day; TRL, technology readiness level; VOC, volatile organic compound; VSA, vacuum swing adsorption.

applications in power generation, post-combustion capture can also be applied to industrial processes such as cement, and steel production. The main advantage of post-combustion capture is that it can be retrofit to existing processes with minimal process modifications.

Pre-combustion capture involves the gasification of a fuel to produce syngas, which is then processed further by means of a water-gas shift reaction to produce a mixture of  $H_2$ , and  $CO_2$ . The  $CO_2$  is separated and the  $H_2$  is used as a fuel producing  $H_2O$  upon combustion. The separation is undertaken at moderate pressures of 10–50 bar. Interest in pre-combustion capture is growing due to the increased enthusiasm towards a hydrogen economy.

In an effort to circumvent the separation of  $CO_2$  from a mixture, oxy-combustion was proposed. In this case, a fuel is combusted in  $O_2$  that is diluted with re-circulated flue gas, which is required to maintain a safe combustion temperature. The flue gas is a mixture of  $CO_2$ , and  $H_2O$ , the latter of which can be easily condensed to produce  $CO_2$ . For oxy-combustion the separation effort is required in producing  $O_2$  for combustion.

Natural gas can contain many impurities, and when the levels of acid- ( $CO_2$ ) or sour- ( $H_2S$ ) gas are above acceptable limits they must be removed. This is currently already undertaken, with the  $H_2S$  converted to elemental sulfur and sold, and the  $CO_2$  either vented or used for enhanced oil recovery (Kohl and Nielsen, 1997). The inclusion of  $CO_2$  capture in this process is to avert the  $CO_2$  emission completely by either sequestration or utilization.

Negative emissions technologies (NETs) have gained popularity since the IPCC published their Special Report about limiting global warming to 1.5 °C (IPCC, 2018). The two NETs which involve engineered solutions are bio-energy with CCS (BECCS) and direct-air CCS (DACCS). BECCS falls into the category of post-, pre-, or oxy-combustion capture, as conventional technologies are retrofit to utilize biomass as the fuel. Direct-air capture (DAC) of  $CO_2$  was first proposed by Lackner et al. (1999) and since then, potential processes based on absorption (Baciacchi et al., 2006), and adsorption have been proposed (Kulkarni and Sholl, 2012). At the time of writing, the only continuously operating DAC demonstration plants are based on adsorption technology.

In each of the aforementioned applications, adsorption-based separations could be employed. Adsorption refers to the adhesion of molecules (adsorbate) to a solid surface (adsorbent) and is classified as either physical adsorption (physisorption) governed by van der Waals forces, or chemical adsorption (chemisorption) characterized by the formation of a covalent bond. In terms of physisorption, adsorbates have differing levels of attraction to an adsorbent depending on the strength of the electrostatic interactions. For molecules of interest to CCS, a typical order may be  $H_2O > CO_2 > N_2 > O_2 > H_2$ . This difference gives rise to preferential adsorption (selectivity), and this is exploited to undertake a separation of a mixture. Chemisorbents can be highly selective as the adsorption site typically only forms a covalent bond with the corresponding adsorbate, however, their overall selectivity can be hampered by physisorption of non-reacting species.

Conventionally, adsorbents are formed into beads or extrudates and packed in a vertical bed. A gas mixture is

exposed to the adsorbent to allow components from the mixture adsorb, and the raffinate passes through. The adsorbent will eventually become saturated and require regeneration prior to re-use. This adsorption/regeneration procedure gives rise to the cyclic nature of adsorption processes. There are two main categories of adsorption process, namely pressure swing adsorption (PSA), and temperature swing adsorption (TSA). In PSA processes, the adsorbent is regenerated by reducing the pressure which shifts the equilibrium and causes the adsorbate to desorb. PSA processes are further characterized by adsorption above atmospheric pressure, and regeneration at (or above) atmospheric pressure. A sub-category of PSA is vacuum swing adsorption (VSA) where adsorption takes place close to atmospheric pressure and regeneration at sub-atmospheric pressures. TSA employs an increase in temperature to regenerate the adsorbent, as adsorption is an exothermic process. Combinations of these processes are also possible, i.e., pressure-vacuum swing adsorption (PVSA), and temperature-vacuum swing adsorption (TVSA), where vacuum is included to further enhance the regeneration.

An adsorption cycle consisting solely of adsorption and regeneration steps is rare, as other intermediate steps are usually included to optimize the process. These enhancements (or complications) are centered around improving the purity and recovery of the product gas, by implementing forms of rinse, purge, and recycle steps. For more detailed information regarding adsorption, and adsorption processes we refer the reader to a range of works (Ruthven, 1984; Yang, 1987; Rodrigues et al., 1989; Ruthven et al., 1994; Basmadjian, 1996; Do, 1998; Thomas and Crittenden, 1998; GPSA, 2004; Rouquerol et al., 2014; LeVan and Carter, 2018).

The use of adsorption processes for pre-combustion capture has a significant head start due to the extensive experience in using PSA for conventional hydrogen production. The implication of this is that the other classes of  $CO_2$  capture are in the earlier stages of development, and thus receive more attention from the academic research community. PSA and VSA are also used extensively for the production of  $O_2$ , however their scales are generally limited to  $\leq 500$  TPD $O_2$  and as such are uneconomical for large-scale oxy-combustion purposes. Although, improving their throughput is a current research goal.

To gauge the maturity of new technologies, technology readiness levels (TRLs) were proposed by NASA (2010). They have since been adapted to suit the needs of other industries, and in the case of CCS range from one (preliminary idea/concept) to nine (commercialisation). It should be noted that the TRL applies to the overall process in its intended application and not individual sub-components, i.e., the individual equipment items required to construct a CCS plant may all have a TRL of nine, however, the process overall may be TRL 6–7. This is why although adsorption processes for  $H_2$  purification are commercialized, adsorption processes for post-combustion  $CO_2$  capture are not considered as commercialized. There are some key points along the TRL scale which are seen to have greater hurdles. For example, progression from three (proof of

concept in lab tests) to five (lab scale plant) requires research funding, and progress beyond five requires significant financial investment or commercial interest (Bui et al., 2018). This is one area where techno-economic analyses (TEAs) are of importance, as demonstration of the technical viability, and process economics are required when seeking financial investment.

Commercialization ambitions aside, TEAs also have a role in comparing technologies, or guiding technology selection during the early stages of a process or system design. The outcome of TEAs are highly dependent on design decisions, techno-economic assumptions, and economic data sources, which can differ significantly between practitioners and as a result conclusions can vary widely. TEAs for adsorption processes are not as common as their absorption counterparts, however, a range have been published for packed-bed processes (Ho et al., 2008; Hasan et al., 2012; Leperi et al., 2015; Susarla et al., 2015; Khurana and Farooq, 2019; Subraveti et al., 2020), and some more recently for direct-air capture (Sinha et al., 2017; Azarabadi and Lackner, 2019; Fasihi et al., 2019; Sinha and Realff, 2019; Wijesiri et al., 2019; McQueen et al., 2020).

This paper is subdivided into two main sections, technical considerations (**Section 2**), and economic considerations (**Section 3**). In each, we discuss factors that can have significant impact on the outcome of TEAs which are sometimes overlooked. The technical and design guidelines presented here are applicable to all adsorption processes, however, some are applicable only for packed-bed processes. We have specified when this was the case. Most of the economics guidelines are also applicable to all adsorption processes, although some are directed specifically towards CCUS applications. We have also indicated these situations when relevant. Although a selection of TEA guidelines exist for CCUS in general (Rubin et al., 2013; van der Spek et al., 2019; van der Spek et al., 2020; Zimmermann et al., 2020), a set of guidelines specifically directed towards adsorption processes have not yet been proposed to the best of our knowledge. As a result we hope this paper will be useful to newcomers to the field, and those with experience in other areas who have not had significant exposure to adsorption processes. A short primer, as it were, on topics that are not widely discussed or readily accessible in one source.

## 2 TECHNICAL CONSIDERATIONS

### 2.1 Feed Flow Rates

Process simulations, and lab- and pilot-scale studies are generally carried out at nominal feed flow rates. This is of course sufficient for cycle design and adsorbent evaluation, however, there is a limit to which these results can be scaled up. We discuss these limitations below.

For packed-bed processes an upper limit is imposed on the flow rate based on the pressure drop across the bed. This is not in an attempt to minimize feed compression work, but rather to prevent the adsorbent being crushed from the additional force imparted by the pressure difference. The Gas Processors Suppliers Association (GPSA) recommends a maximum

pressure gradient of  $0.33 \text{ psi ft}^{-1}$  ( $7.5 \text{ kPa}\cdot\text{m}^{-1}$ ), and a maximum total pressure drop of 8 psi (55 kPa) (GPSA, 2004). These values are guidelines and are functions of the adsorbent, particle size, and particle shape, and are based on traditional adsorbents such as zeolites, silicas, and aluminas. Another factor to consider is fluidization of the bed, i.e., the gas velocity should not exceed the minimum fluidization velocity of the bed. The pressure drop (and velocity) can be reduced by increasing the bed diameter, however, the transport of the assembled vessel from manufacturer to plant site should be kept in mind. In general, this limits bed diameter to  $\approx 14 \text{ ft}$  (4.3 m), however, local regulations and transport options should be referred to as larger sizes may be viable on a case-by-case basis. This does not preclude beds being built in the field or larger diameter; however, this is at a considerably higher cost. Radial flow beds could also be deployed to overcome this limitation. They are commonly used in the front-end pre-purification units of cryogenic air separation plants where significant volumetric flow rates are processed. However, they are considerably more costly than an axial-flow vessel of the same size due to their more complex construction.

The implications of this are that beyond a certain feed flow rate, it is no longer possible to increase the size of the beds while meeting the above constraints. At that point beds must be replicated, as well as the associated equipment such as feed blowers/compressors, and vacuum pumps. Costing a pilot plant or scaling capacity using power laws will not capture these effects. Therefore, process design and economic evaluation should be carried out at the actual feed flow rate of the application in order to appropriately size and enumerate equipment items.

### 2.2 Cycle Time

The cycle time of an adsorption process is analogous to the period of a wave, i.e., the time it takes to return to the same point in a cycle. The start of the adsorption step is normally taken as the reference point for convenience. Consequently, cycle time has a direct impact on the productivity of the process. Productivity is defined as the amount of product obtained, per unit volume of adsorbent, per unit time ( $\text{kg}\cdot\text{m}^{-3}\cdot\text{h}^{-1}$ ). It is always desirable to increase the productivity of a process as this reduces capital costs. One approach may be to investigate whether a cycle with fewer beds can achieve equivalent purity and recovery, thus reducing the adsorbent inventory. However, the most common approach is to reduce the cycle time.

There is generally a lower limit imposed on cycle time by mass transfer, and these features are able to be captured by dynamic models. As the cycle time is reduced, the feed velocity is increased to utilize the full length of the bed. As the cycle time is reduced further, the bed is not able to be fully utilized due to mass transfer limitations. Low bed utilization can also be caused by purity-recovery constraints. For example, in the case of a heavy product cycle it may be necessary to have a short feed step time to reduce product loss, or short desorption step time to maintain the required product purity.

Other limitations are generally not able to be accounted for easily. For example, very large processes such as those which

would be required for post-combustion capture, valve dynamics can limit minimum cycle time. In these cases geared motor-driven actuators may need to be used, as the valve and line sizes may be at least NPS 24/DN 600. These valves can take several minutes to complete a full stroke, and this time needs to be considered as it can become significant over the many steps of the cycle. Another consideration is the time required to redirect the feed flow between beds. For large processes, it is generally not possible to immediately switch the feed flow from one bed to another (i.e., perform a step change). Sudden changes in flow rate or direction can “bump” the bed, and cause damage to the brittle adsorbent. Repeated events can lead to significantly increased pressure drop, and abrasive adsorbent dust permeating the process equipment. In general, the flow should be gently introduced to the fresh bed and once the flow is stabilized, the feed to the saturated bed gradually reduced.

Unfortunately, there are not formally established or straightforward methods to account for this issue at the design or TEA stage. Estimations of valve dynamics (i.e.,  $C_v$  a function of time) could be incorporated into simulations, although accurate estimations of the stroke time are difficult *a priori*. Process flows would then be based on pressure difference and  $C_v$ , rather than specifying flow rates. An avenue for simplification may be to ramp the flow rate in place of imposing a step change. Furthermore, conventional cycle diagrams would need to be updated to reflect the crossover of steps between beds. A fundamental first order approach would be to ensure that the total step time is not shorter than two estimated valve stroke times.

For reference the shortest cycles are typically seen in O<sub>2</sub> PSA, where they are in the order of 1–10 min. This is achievable as the size of the plant is such that the aforementioned factors are negligible, and in some cases the slower diffusivity of N<sub>2</sub> is exploited to achieve the separation. Investigation of rapid cycles (<1 min) have gained interest, especially in the area of portable medical oxygen concentrators (where cycle times <5 s are common), and also other industrial separations (mostly H<sub>2</sub> PSA) (Sircar, 2001).

Furthermore, rapid cycles can also suffer from “switching” losses and inefficiencies. As the bed is frequently de-pressurised/evacuated, the feed gas in the bed void space is vented, which reduces recovery and increases specific energy consumption. Care should also be given to the relative volumes of the piping and vessel heads, to the adsorbent volume. The short step times can result in an effective shuffling of gas through these void spaces with little separation undertaken. Rapid de- and re-pressurization can also result in an unsteady flow to downstream equipment, which may affect plant operation.

To capture these effects in process simulation, the void volumes should be accounted for. The volume of the vessel heads can be readily estimated by assuming a torispherical head with a diameter of a the vessel. Assumptions will need to be made for the crown and knuckle radii, however, pressure vessel standards (Section 2.5) have recommended guidelines for these radii as ratios of the diameter. The void space due to piping is dependant on plant layout, however, estimates can be obtained by assuming a vessel spacing (i.e., one bed diameter between vessels)

and calculating the corresponding length of piping required to interconnect the beds.

## 2.3 Cycle Scheduling

In most cases adsorption cycles require more than one bed to undertake a separation. Cycle scheduling refers to the act of staggering or offsetting the cycle of each bed to meet certain objectives such as continuous feed flow, and matching any bed-to-bed flows. As the bed switches from adsorption to other cycle steps, another bed must be available to accept the feed to ensure continuous operation. More complex cycle steps such as purge, product pressurization, and pressure equalization all require one bed to provide gas, and another to receive it. As such, the duration of the step and the scheduling of those beds must align.

Depending on the cycle design, it is possible to meet one objective (aligning cycle steps) while not the other (continuous feed). In those cases, it may be simpler to duplicate the whole process and offset their operation. This is most commonly the case when the adsorption step times are much shorter than other cycle steps. In general, the more complex the cycle, or the smaller the fraction feed steps are of the total cycle time, the more beds that will be required. As such, improper consideration of these additional beds can have significant impact on a TEA.

The most common approach to determine the cycle schedule is the tabular or graphical method, and a demonstration can be found in Mehrotra et al. (2011). A mathematical approach is also available and may be useful for software integration (Mehrotra et al., 2010).

## 2.4 Vacuum Pump Curves

For adsorption processes with a vacuum regeneration step, i.e., VSA, PVSA, or TVSA, a vacuum source must be provided. One of the most convenient ways to do so industrially is *via* vacuum ejectors. These are generally not viable for adsorption applications as the product gas becomes mixed with the working fluid. As such, mechanical vacuum generation is used.

Vacuum pump curves depict the volumetric flow rate of gas that can be pumped at a given inlet pressure. They can normally be obtained from the technical literature provided by vendors and digitized and fit with a function for use in software. Care should be taken to the specified units of volume, as standard (Sm<sup>3</sup>, 15°C and 1 atm) or normal (Nm<sup>3</sup>, 0°C and 1 bar) volume will need to be converted to actual volume. The influence of vacuum pump curves in dynamic process simulation was investigated by Jiang et al. (2019), and impacts on attainable evacuation pressure and calculated energy consumption were significant. For TEAs, a vacuum pump should selected and its attainable pressure and flow rate considered during the process design. This will ensure a more accurate representation of the number of vacuum pumps needed.

A common issue in process simulation is the disagreement between simulation and plant energy consumption. A primary contributor to this is the vacuum pump performance, and efficiency. It has been standard practice to assume a constant isentropic efficiency for vacuum pumps (and compressors) in the range of 70–80%. As is known for compressors and liquid pumps,

this efficiency is not constant, and in the case of vacuum pumps can vary quite substantially. Vacuum pump efficiency data is scarce and work is required in this area by vendors to make this data available alongside pump curve data. The effects of vacuum pump efficiency and a proposed solution for use in process simulation are discussed by Maruyama et al. (2020).

When selecting an evacuation pressure, the pressure drop of the piping/ducting should be considered. It is difficult to estimate this without detailed design, as it is related to plant layout. However, an assumption on the order of 0.5 kPa may be sufficient for TEAs. Ludwig (1999) recommends sizing vacuum lines to limit pressure drop to 10% of the final pressure. The implications of this are that if 2 kPa is desired at the adsorbent bed,  $\approx 1.5$  kPa is required at the vacuum pump.

A side-effect of accounting for these factors is that for large CCS plants, the number of vacuum pumps and size of piping required can occupy significant area. It is possible that this area may be larger than any existing area set aside for plant expansion, and as such, costs for land may be prohibitive at some scales.

## 2.5 Mechanical Design

Although it is not feasible to undertake rigorous mechanical design of the adsorption vessels at the TEA stage, some attention should be given to vessel thickness. One of the common methods to estimate the cost of a vessel is based on the mass of steel required. In most cases, a thickness of 1.5 or 3 mm is assumed. Appropriate design guidelines should be followed to obtain a feasible design and a better estimate of the vessel mass.

For large beds, a wall thickness of 1.5 mm may not be able to withstand its own mass, let alone the mass of adsorbent, bed support and hold-down, and stresses from pressure and vacuum. Furthermore, the requirements for vessels subject to vacuum conditions are generally more stringent than those subject to pressure. There are a number of standards available to determine the required shell thickness of pressure vessels, including: ASME BPVC **Section 8**, Australian standard AS1210, British standard PD5500, European standard EN13345, and international standard ISO 16528. These pressure vessel standards also refer to vacuum designs, as vacuum operation is considered “external pressure.”

For TSA processes, the effect of temperature on the material of construction should be accounted for, i.e., reduction in the tensile strength. Attention should also be given to any isochoric cooling steps in the cycle as the pressure may reduce below atmospheric, requiring vacuum design.

Bed support is a critical feature of packed beds as it facilitates gas distribution, and immobilizes the adsorbent. This is normally achieved with a perforated steel plate, and bed support media. The bed support media serves two functions, to improve gas distribution, and act as a transition between the adsorbent particle size and the opening size in the support plate. The bed support media are commonly non-porous ceramic spheres which are layered in increasing size. For example, if the adsorbent size is  $1/8''$  and the openings in the support plate are  $1''$ , support media in sizes of  $2''$ ,  $1''$ ,  $1/2''$ , and  $1/4''$  are stacked in  $\approx 4''$  layers. This can add appreciable height to the bed and should be considered in the vessel length. For large beds, it is generally

not possible to support the plate only by its circumference and cross-members may be required.

Bed hold-down also becomes important for large beds, and rapid cycles (**Section 2.2**). Hold-down minimizes expansion and re-settling of the bed, bed bumping, and elutriation of adsorbent downstream. In some cases a segmented hold-down plate on top of the bed is sufficient. However, a more thorough approach would be to reverse the scheme used at the bottom of the bed, i.e., layers of bed support media in increasing size, followed by a segmented hold-down plate. This approach will also improve gas distribution for cycle steps with a top-down feed.

## 2.6 Heat and Work

It is fundamental to evaluate the energy requirements of the process, and in the case of TEAs, form comparisons between given processes (including other separation families). In the case of adsorption processes, heat input is seen during thermal regeneration steps for TSA, while work input is required for blowers and compressors, and vacuum pumps for VSA processes.

The quality of an energy source is related to the proportion of its total energy which can be recovered as work (energy to energy ratio). Electrical energy, chemical potential energy, and (macroscopic) kinetic energy can in theory be fully converted to work. On the other hand, thermal energy cannot, and its quality is proportional to its temperature. Therefore, the quality of an energy source should be taken into consideration when undertaking TEAs and process comparisons. The consistency of units ( $\text{MJ}\cdot\text{kg}^{-1}$ ) is a “red herring” in this regard.

There are two main options to deal with this issue. The first is to convert electrical energy requirements to a thermal equivalent by assuming a conversion factor of one-third, i.e.,  $1 \text{ MJelec} = 3 \text{ MJth}$ . This assumption is based on average efficiencies for thermal power plants. Shaft work requirements can be converted to electrical energy by using a motor and drive efficiency. These efficiencies are highly variable and are better for large systems, however, assumptions in the range of 70–80% are common.

The other approach is to convert the thermal energy to a shaft work equivalent (**Eq. 1**). This is done by assuming that the maximum work can be extracted from the thermal energy *via* the Carnot efficiency, and then applying an isentropic efficiency. The isentropic efficiency represents the hypothetical turbine undertaking this conversion. Again, values in the range of 70–80% are common.

$$W_S^{eq} = \eta_{isen} \cdot \left(1 - \frac{T_L}{T_H}\right) \cdot Q_{th} \quad (1)$$

where:  $W_S^{eq}$  is the equivalent shaft work (J),  $\eta_{isen}$  is the turbine isentropic efficiency,  $T_L$  is the temperature which the thermal energy is used down to (usually taken as ambient temperature) (K),  $T_H$  is the source temperature of thermal energy (K), and  $Q_{th}$  is the thermal energy requirement (J).

For example, an amine absorption process with a thermal energy consumption of  $3.7 \text{ MJ}\cdot\text{kg CO}_2^{-1}$  has a work equivalent of  $0.70 \text{ MJ kgCO}_2^{-1}$  assuming the heat is provided at  $125^\circ\text{C}$ , an ambient temperature of  $25^\circ\text{C}$ , and  $\eta_{isen}$  of 75%.

Both of these approaches allow a fair comparison between processes, and the ability to sum multiple energy inputs of a process to obtain its total energy requirement, i.e., blower work and regeneration energy in the case of TSA. It is also more than acceptable to report two energy requirement values, one for thermal energy, and one for electrical energy. Judgements should also be made on a case-by-case basis. For example, if a compressor is driven by a steam turbine then that should be attributed to thermal energy consumption, and if a TSA process is regenerated by resistive heating, that energy should be attributed to electrical energy consumption.

## 2.7 Milligrams to Kilotonnes

Adsorbent development has received significant attention over the last 25 years. This has been mostly driven by CO<sub>2</sub> capture, gas storage, alternatives to distillation for isomer and paraffin/olefin separation, and environmental remediation. It is often desired to evaluate the performance of these adsorbents to demonstrate their efficacy.

The most common evaluation method emerged to be simple isotherm analysis, i.e., the amount of CO<sub>2</sub> adsorbed at the feed conditions, or the ideal selectivity (Eq. 2). This likely resulted from modern adsorbents (such as MOFs, COFs, and POPs) typically having small batch sizes (mg scale), and isotherm measurement being the only feasible analytical technique.

$$\alpha_{ab} = \frac{n_a/y_a}{n_b/y_b}, \quad (2)$$

where:  $\alpha_{ab}$  is the ideal selectivity of component a over b,  $n_x$  is the amount adsorbed of component x [mol kg<sup>-1</sup>], and  $y_x$  is the mole fraction of component x in the feed.

It has since been demonstrated that simple metrics do not adequately assess an adsorbent's performance (Maring and Webley, 2013; Rajagopalan et al., 2016; Rajagopalan and Rajendran, 2018; Park et al., 2019; Burns et al., 2020; Danaci et al., 2020; Yancy-Caballero et al., 2020). Significant improvement over these metrics can be achieved by employing an equilibrium (or screening) process model (Maring and Webley, 2013; Joss et al., 2015; Subramanian Balashankar et al., 2019). The cost of this improved estimation is the measurement of additional isotherms, three for each of CO<sub>2</sub> and N<sub>2</sub>. Although more time consuming, it is more efficient as a first step than synthesizing multiple batches to undertake a multi-component breakthrough analysis. A potential issue with batch inconsistency can arise when combining multiple batches of material.

Care should be taken when scaling up designs based on such equilibrium models. As the mass transfer effects of the process are not considered, it is not possible to implement precise purity and recovery constraints. Furthermore, unless constraints on pressure drop or gas velocity are imposed, the bed size will be zero by definition. Therefore, equilibrium models should not be used for rigorous process design or cost estimation, but rather used for their intended purpose of adsorbent screening.

A promising outcome from equilibrium based models can justify scaling up for breakthrough analysis. The breakthrough

analysis will yield adsorption kinetics and multi-component selectivity information, which can then be used in dynamic process simulation. If dynamic simulation yields encouraging results, this could support further scale-up to lab-scale cyclic evaluation. Long term cyclic evaluation can then provide insight on the stability of the adsorbent.

A downside of the above pathway is that adsorbents which will perform best in a kinetic separation will not be identified by the equilibrium-based screening approach. In those cases, dynamic modeling is required in the first step and kinetic parameters can be obtained in two main ways (aside from breakthrough analysis). One is to perform zero-length column experiments (Gibson et al., 2016), and the other is rate of adsorption (ROA) measurements. ROA data can usually be obtained simultaneously with isotherm data on most commonly-available isotherm measurement apparatus. PFG NMR is also a valid alternative (Hwang and Karger, 2019; Baniani et al., 2020), however, it is currently not a readily accessible technique.

Lastly, assessing the ability of an adsorbent to achieve purity, recovery, and energy targets using the above techniques does not guarantee its commercial success. In addition, an adsorbent should display the following characteristics for practical use (Webley and Danaci, 2020): tolerance to impurities, tolerance to water, rapid mass transfer, ability to be formed, sufficiently high density, low cost, low environmental and safety impacts.

## 2.8 Direct-Air Capture

Direct-air capture of CO<sub>2</sub> (DAC) is gaining popularity both socially, and politically, as it offers potential for negative emissions and offsets for hard-to-abate sectors. Many of the points discussed above are equally applicable to direct-air capture systems, although they are typically not operated as packed-beds.

There are currently no strict guidelines for the design and operation of these systems. However, previous work on the modeling of monolithic and structured adsorbents has been reported (Shuai et al., 1996; Rezaei and Webley, 2009; Rezaei and Webley, 2010). The main advantage of these structured adsorbents is the reduced pressure drop and increased throughput relative to packed-bed processes. This makes them promising candidates for the high volume of gas processing required for DAC.

The body of work on the process modeling aspect of direct-air capture is slowly growing, as the majority of the literature to date has been focused on adsorbent development. Some of these studies assume equilibrium, or that physisorption kinetics apply (Kulkarni and Sholl, 2012; Elfving et al., 2017; Sinha et al., 2017; Azarabadi and Lackner, 2019; Sinha and Realff, 2019). To date, these processes are based on amine functionalized adsorbents to which the CO<sub>2</sub> chemisorbs. The kinetics of chemisorption are poor at ambient temperature, and are also a function of reactant (CO<sub>2</sub>) concentration. Given the low concentration of CO<sub>2</sub> in DAC applications, the adsorption kinetics can be quite poor.

To obtain a reliable estimate of the CO<sub>2</sub> recovery, and productivity of the process, the adsorption kinetics of these systems should be accounted for. It will also lead to a more

accurate assessment of the process economics. The findings, which are currently popular amongst systems and integrated assessment modelers, would then have greater validity.

### 3 ECONOMIC CONSIDERATIONS

#### 3.1 IBL Costing Methods

In general, most techno-economic analyses are concerned with the inside battery limits (IBL) costs. The battery limits represent the main process equipment items involved with converting the feed to the final product. This is opposed to outside battery limits (OBL) equipment such as utilities generation, waste treatment, and product storage. In terms of IBL costs, process equipment in addition to the adsorption vessels should be considered. These can represent a significant proportion of costs and could include feed gas blowers/compressors and heat exchangers, buffer tanks, control valves, heat exchangers and compressors for bed-to-bed gas flows, and regeneration gas heaters and product gas coolers for TSA.

There are two main methods to estimate the IBL capital costs, extrapolating published cost data, and factoring purchased equipment cost data. The extrapolation method involves taking published cost data and scaling it based on capacity, location, and inflation. This method has an accuracy of  $\pm 50\%$ , and care should also be taken around scaling actual cost data vs. estimated cost data (Brennan, 2020). For CCS applications, this approach is currently not widespread as published cost data is not available.

Factored cost estimation methods are available in two main alternatives. The most popular by far is the Lang factor approach, whereby the purchase cost of all equipment items are summed and then multiplied by a Lang factor. Lang factors can range between three and four for total IBL cost (Gerrard, 2000; Peters et al., 2006; Brennan, 2020). The other alternative is to apply an installation factor, comprised of sub-factors, to the cost of each equipment item. This approach is known as the factorial cost estimation method, IChemE method, or ICI method. These sub-factors account for equipment erection, piping, instrumentation, electrical requirements, civil requirements, structures or buildings, and insulation. The sub-factors are functions of the required complexity and equipment purchase cost, and can be found in Gerrard (2000), Brennan and Golonka (2002), or Brennan (2020). Although not as straightforward as the Lang factor approach, this method is more comprehensive as the factors are tailored to each equipment item, and can yield an accuracy of  $\pm 30\%$ .

#### 3.2 Costing Data

To apply either of the factored cost estimation techniques, purchase costs of equipment items are required. The best approach would be to obtain quotes from vendors, however this is generally infeasible for academic studies. There are a selection of popular sources for such data (Garrett, 1989; Peters et al., 2006; Couper et al., 2012) and in cases where plots are provided in place of equations, these can be digitized and fit for use in software applications.

One drawback to most sources of published purchase cost data is the applicable equipment size range. This is primarily due to the age of the original data on which they are based. The maximum size of process equipment has increased over time, driven by a desire to reduce costs from economies of scale. Care should be taken if extrapolation of the data is required, and the cause for extrapolation investigated. For example, 100 MW centrifugal compressors are now available, but 4,000 m<sup>2</sup> shell and tube heat exchangers are still infeasible (both are outside the range of commonly available data). In cases where extrapolation leads to an exponential increase, or the size is impractical, the equipment should be parallelized.

Lastly, any equipment cost data should be converted to the current year with a cost index. The most common is the Chemical Engineering Plant Cost Index (CEPCI), published monthly by Chemical Engineering magazine. A reference CEPCI value is normally provided in the cost data source; in cases where it is not, the CEPCI for the year of (or before) its publication could be used.

#### 3.2.1 Novel Technologies

Although not novel in their own right, there are some technologies which are being considered for adsorption processes, such as fluidized beds for moving bed TSA, and rotary adsorbers for continuous TSA. These alternatives to the packed-bed configuration are being proposed to increase the productivity of TSA processes, to take advantage of the increased working capacity that TSA can offer relative to VSA.

Woods (2007) provides data on fluidized beds, reactors, and other solids processing equipment which may be useful for moving bed TSA processes. The concept of rotary adsorbers are based on thermal wheels, or regenerative heat exchangers, which then made their way into HVAC applications for desiccant based dehumidification. The modeling of these for adsorption processes has been touched on (Konrad and Eigenberger, 1994; Palfi, 2020), and some cost data is available for thermal wheels (Woods et al., 1976; Woods, 2007). An alternative approach to thermal wheels may be to cost the rotary adsorber as a rotating absorber (Sudhoff et al., 2015) and include the cost of adsorbent in place of packing. The mechanical implementation of this alternative may be more in-line with rotary adsorber technologies currently in the process of commercialization for CCS applications.

#### 3.2.2 Adsorbent

Estimating the bulk cost of an adsorbent which is not yet commercialized is a contentious area. If a novel adsorbent displays excellent performance and meets the other criteria for industrial suitability (Section 2.7), efforts will be made to scale its production. One argument is that its cost could be reduced to levels seen for currently commercialized adsorbents, simply due to economies of scale. However, this does not address the inherent difference in cost of feedstock. For example, activated carbons are lower in cost than silicas, and silicas are lower in cost than zeolites. Aside from feedstock, the organic ligands required for MOFs for example, may also have inherently lower yields also increasing the final cost.

A potential approach may be to use a commercialized adsorbent as a scaling reference. The cost of lab-prepared 13X can be calculated using the procedure and yield from a reputable source (Mintova and Barrier, 2016) and compared to commercially available 13X. This factor could then be applied to the lab-prepared cost for other adsorbents. This approach assumes the same factorial reduction can be achieved due to scale. This reasoning may not apply in cases where the cost of the raw materials is significantly more expensive and will not benefit in the same way from economies of scale. Furthermore, the same scale-up and manufacturing techniques may not be applicable for contemporary adsorbents.

In cases where the adsorbent cost is at best, an educated estimate, a sensitivity analysis should be carried out to identify the impact of this on final cost.

### 3.3 Other Capital Costs

In addition to IBL costs, other costs contribute to the total fixed capital investment of a project. These include land, start-up capital, working capital, vehicles, and OBL costs. These costs are difficult to determine as they depend on many factors. Approximations exist to estimate these costs as a percentage of total equipment purchase cost, or total IBL cost (Peters et al., 2006; Brennan, 2020). Although the inclusion of these costs are useful to gauge the total capital required, it may not be as useful when comparing alternate technologies, or projects with differing location. Therefore, excluding these costs may be best, or clear breakdowns of the total fixed capital provided.

### 3.4 Operating Costs

The primary contributor to operating cost for large plants is generally process utilities. Brennan (2020) provides costs for common utilities, while Ulrich and Vasudevan (2006) has a more comprehensive list. The cost of any raw materials or feedstocks would also be included here, however, the CO<sub>2</sub> is normally assumed to be free of charge for CCS applications.

Other contributions exist and the most common are include: number of personnel, salaries and payroll overheads, consumables, depreciation, land tax, insurance, maintenance, and royalties (Brennan, 2020). As per Section 3.3, these are difficult to estimate and will also vary on a case-by-case basis. If inclusion of these is desired, cost breakdowns should be provided.

### 3.5 Unit Cost of CO<sub>2</sub>

The first step in determining the cost of CO<sub>2</sub> is to obtain the annual cost associated with the operating plant, accounting for both capital and operating costs. The most direct approach is to utilize a capital recovery factor (Eq. 3) which distributes the total capital cost over the life of the plant, and then add the annual operating cost to obtain the total annualized cost (Eq. 4).

$$CRF = \frac{i(1+i)^n}{(1+i)^n - 1}, \quad (3)$$

$$TAC = CRF \cdot CapEx + OpEx. \quad (4)$$

where: *CRF* is the capital recovery factor (year<sup>-1</sup>), *i* is the interest rate, *n* is the economic lifetime of the plant (years), *TAC* is the

total annualized cost (\$ year<sup>-1</sup>), *CapEx* is the total capital expenditure (\$), and *OpEx* is the annual operating costs (\$ year<sup>-1</sup>).

Another approach would be *via* the net present value (NPV) of the project. The reporting of NPVs for CCS projects is uncommon as there is no revenue source, although for CCUS applications it can be quite versatile. An advantage of the NPV method is that time-varying values can be accounted for, i.e., the investment of capital over a number of years, or variable operating costs. Once the NPV is determined, it can be annualized *via* the equivalent annual cost (Eq. 5).

$$EAC = NPV \cdot \frac{i}{1 - (1+i)^{-n}}, \quad (5)$$

where: *EAC* is the equivalent annual cost (\$), *NPV* is the net present value of the project (\$), *i* is the interest rate, and *n* is the length of the project (years).

Once the annual cost is obtained, the unit cost of CO<sub>2</sub> can be obtained. The two main approaches to report the cost of CO<sub>2</sub> are captured cost, and avoided cost. The captured cost is simply the annual cost divided by the amount of CO<sub>2</sub> captured per year. The avoided cost is the ratio of the difference in cost of a product, to the difference in CO<sub>2</sub> emissions of the system, with and without CCS. The costs of transport and storage must be included when reporting avoided costs, as the CO<sub>2</sub> emission is not avoided unless it is stored. The avoided cost is a truer representation of the cost for an individual project, and is useful when comparing technologies for a given CCS project. However, when investigating the application of a given technology to different CO<sub>2</sub> emission sources, the captured cost should be used. Each source will have its own baseline emissions, and the capture plant will have varying CO<sub>2</sub> emissions as they are a function of utilities consumption.

These costing approaches and others are discussed in further detail in Section 3.7.2 of IPCC (2005). The costing of CO<sub>2</sub> is also discussed by Rubin (2012) and Roussanaly (2019); the former focuses on power generation and the latter on industrial processes.

As with any cost estimation, the specifics should be stipulated, i.e., included costs, annualization method, cost of capital, operating life, capital cost correlations, and operating cost data. These have a heavy influence on the final outcome, and can improve the reproducibility and transparency of the work.

## 4 FINAL REMARKS

The growing interest in climate change mitigation pathways and policies call for reliable and detailed techno-economic data. Furthermore, the results can be and are used by systems, and integrated assessment modelers to guide government and policy-makers.

The standardization of techno-economic studies is not easily achievable, and differences in approach can make fair or accurate



comparisons between scenarios difficult. Although not a comprehensive guide, we have raised points for consideration as well as recommendations for undertaking techno-economic analyses of adsorption processes, one of the candidate technologies proposed for CO<sub>2</sub> capture.

## DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding author.

## REFERENCES

- Azarabadi, H., and Lackner, K. S. (2019). A sorbent-focused techno-economic analysis of direct air capture. *Appl. Energy* 250, 959–975. doi:10.1016/j.apenergy.2019.04.012
- Bacocchi, R., Storti, G., and Mazzotti, M. (2006). Process design and energy requirements for the capture of carbon dioxide from air. *Chem. Eng. Process: Process Intensification* 45, 1047–1058. doi:10.1016/j.cep.2006.03.015
- Baniani, A., Berens, S. J., Rivera, M. P., Lively, R. P., and Vasenkov, S. (2020). Potentials and challenges of high-field PFG NMR diffusion studies with sorbates in nanoporous media. *Adsorption*. doi:10.1007/s10450-020-00255-y
- Bart, H.-J., and von Gemmingen, U. (2005). *Ullmann's encyclopedia of industrial chemistry*. Weinheim, DE: Wiley-VCH Verlag.
- Basmađjan, D. (1996). *The little adsorption book*. Boca Raton, FL: CRC Press.
- Brennan, D. J. (2020). *Process industry economics*. 2nd Edn. Amsterdam, NL: Elsevier.
- Brennan, D. J., and Golonka, K. A. (2002). New factors for capital cost estimation in evolving process designs. *Chem. Eng. Res. Des.* 80, 579–586. doi:10.1205/026387602760312773
- Bui, M., Adjiman, C. S., Bardow, A., Anthony, E. J., Boston, A., Brown, S., et al. (2018). Carbon capture and storage (CCS): the way forward. *Energy Environ. Sci.* 11, 1062–1176. doi:10.1039/c7ee02342a
- Burns, T. D., Pai, K. N., Subraveti, S. G., Collins, S. P., Krykunov, M., Rajendran, A., et al. (2020). Prediction of MOF performance in vacuum swing adsorption systems for postcombustion CO. *Environ. Sci. Technol.* 54, 4536–4544. doi:10.1021/acs.est.9b07407
- Couper, J. R., Penney, W. R., Fair, J. R., and Walas, S. M. (2012). *Chemical process equipment: selection and design*. 3rd Edn. Waltham, MA: Butterworth-Heinemann.
- Danaci, D., Bui, M., Mac Dowell, N., and Petit, C. (2020). Exploring the limits of adsorption-based CO capture using MOFs with PVSA—from molecular design to process economics. *Mol. Syst. Des. Eng.* 5, 212–231. doi:10.1039/c9me00102f
- Do, D. (1998). *Adsorption analysis: equilibria and kinetics*. London, United Kingdom: Imperial College Press.
- Elfving, J., Bajamundi, C., Kauppinen, J., and Sainio, T. (2017). Modelling of equilibrium working capacity of PSA, TSA and TVSA processes for CO adsorption under direct air capture conditions. *J. CO<sub>2</sub> Util.* 22, 270–277. doi:10.1016/j.jcou.2017.10.010
- Fasihi, M., Efimova, O., and Breyer, C. (2019). Techno-economic assessment of CO direct air capture plants. *J. Clean. Prod.* 224, 957–980. doi:10.1016/j.jclepro.2019.03.086
- Garrett, D. E. (1989). *Chemical engineering economics*. New York, NY: Van Nostrand Reinhold.
- Gerrard, A. M. (2000). *Guide to capital cost estimating*. 4th Edn. Warwickshire, United Kingdom: RugbyIChemE.
- Gibson, J. A. A., Mangano, E., Shiko, E., Greenaway, A. G., Gromov, A. V., Lozinska, M. M., et al. (2016). Adsorption materials and processes for carbon capture from gas-fired power plants: AMPGas. *Ind. Eng. Chem. Res.* 55, 3840–3851. doi:10.1021/acs.iecr.5b05015
- GPSA (2004). *Dehydration-engineering data book gas processors suppliers association*. 12th Edn. Tulsa, OK: GPSA.
- Hasan, M. M. F., Baliban, R. C., Elia, J. A., and Floudas, C. A. (2012). Modeling, simulation, and optimization of postcombustion CO capture for variable feed concentration and flow rate. 2. Pressure swing adsorption and vacuum swing adsorption processes. *Ind. Eng. Chem. Res.* 51, 15665–15682. doi:10.1021/ie301572n
- Ho, M. T., Allinson, G. W., and Wiley, D. E. (2008). Reducing the cost of CO capture from flue gases using pressure swing adsorption. *Magn. Reson. Imaging* 47, 4883–4890. doi:10.1021/ie070831e
- Hwang, S., and Karger, J. (2019). NMR diffusometry with guest molecules in nanoporous materials. *Magn. Reson. Imag.* 56, 3–13. doi:10.1016/j.mri.2018.08.010
- IPCC (2005). *Prepared by working group III of the intergovernmental Panel on climate change-IPCC special report on carbon dioxide capture and storage*. Cambridge, NY: Cambridge University Press.
- IPCC (2018). *Global warming of 1.5°C. An IPCC special report on the impacts of global warming of 1.5°C above pre-industrial levels and related global greenhouse gas emission pathways, the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty*. Geneva, Switzerland: IPCC.
- Jiang, H., Ebner, A. D., and Ritter, J. A. (2019). Importance of incorporating a vacuum pump performance curve in dynamic adsorption process simulation. *Ind. Eng. Chem. Res.* 59, 856–873. doi:10.1021/acs.iecr.9b04929
- Joss, L., Gazzani, M., Hefti, M., Marx, D., and Mazzotti, M. (2015). Temperature swing adsorption for the recovery of the heavy component: an equilibrium-based shortcut model. *Ind. Eng. Chem. Res.* 54, 3027–3038. doi:10.1021/ie5048829
- Khurana, M., and Farooq, S. (2019). Integrated adsorbent process optimization for minimum cost of electricity including carbon capture by a VSA process. *AIChE J.* 65, 184–195. doi:10.1002/aic.16362
- Kohl, A. L., and Nielsen, R. B. (1997). *Gas purification*. 5th Edn. Houston, TX: Gulf Publishing.
- Konrad, G., and Eigenberger, G. (1994). Rotoradsorber zur Abluftreinigung und Lösungsmittel-Rückgewinnung. *Chem. Ing. Tech.* 66, 321–331. doi:10.1002/cite.330660305
- Kulkarni, A. R., and Sholl, D. S. (2012). Analysis of equilibrium-based TSA processes for direct capture of CO from air. *Ind. Eng. Chem. Res.* 51, 8631–8645. doi:10.1021/ie300691
- Lackner, K., Ziock, H.-J., and Grimes, P. (1999). “Carbon dioxide extraction from air: is it an option?” in 24th annual technical conference on coal utilization and fuel systems (Washington, DC: United States Department of Energy). Available at: <https://www.osti.gov/biblio/770509>.
- Leperi, K. T., Snurr, R. Q., and You, F. (2015). Optimization of two-stage pressure/vacuum swing adsorption with variable dehydration level for postcombustion carbon capture. *Ind. Eng. Chem. Res.* 55, 3338–3350. doi:10.1021/acs.iecr.5b03122
- LeVan, M. D., and Carter, G. (2018). “Adsorption and ion exchange,” in *Perry's chemical engineers' handbook*, Editors D. W. Green and M. Z. Southard (New York, NY: McGraw-Hill Education), Vol. 16.
- Ludwig, E. E. (1999). *Applied process design for chemical and petrochemical plants*. 3rd Edn. Houston, TX: Gulf Professional Publishing.

## AUTHOR CONTRIBUTIONS

DD conceived the work and authored the first draft of the manuscript. PW and CP contributed additional points for discussion. All authors contributed to the final manuscript and approved the submitted version.

## FUNDING

DD and CP are grateful to the EPSRC for providing the funding to undertake this work via the United Kingdom Carbon Capture and Storage Research Center (UKCCSRC, Grant No. EP/P026214/1).

- Maring, B. J., and Webley, P. A. (2013). A new simplified pressure/vacuum swing adsorption model for rapid adsorbent screening for CO capture applications. *Int. J. Greenhouse Gas Control*. 15, 16–31. doi:10.1016/j.jggc.2013.01.009
- Maruyama, R. T., Pai, K. N., Subraveti, S. G., and Rajendran, A. (2020). Improving the performance of vacuum swing adsorption based CO capture under reduced recovery requirements. *Int. J. Greenhouse Gas Control*. 93, 102902. doi:10.1016/j.jggc.2019.102902
- McQueen, N., Psarras, P., Pilorge, H., Liguori, S., He, J., Yuan, M., et al. (2020). Cost analysis of direct air capture and sequestration coupled to low-carbon thermal energy in the United States. *Environ. Sci. Technol.* 54, 7542–7551. doi:10.1021/acs.est.0c00476
- Mehrotra, A., Ebner, A. D., and Ritter, J. A. (2010). Arithmetic approach for complex PSA cycle scheduling. *Adsorption*. 16, 113–126. doi:10.1007/s10450-010-9211-8
- Mehrotra, A., Ebner, A. D., and Ritter, J. A. (2011). Simplified graphical approach for complex PSA cycle scheduling. *Adsorption*. 17, 337–345. doi:10.1007/s10450-011-9326-6
- Mintova, S., and Barrier, N. (2016). *Verified syntheses of zeolitic materials (synthesis commission of the international zeolite association)*. 3rd Edn. Caen: Synthesis Commission of the International Zeolite Association.
- NASA (2010). *Technology readiness levels demystified*. (Washington, DC: NASA). Available at: [https://www.nasa.gov/topics/aeronautics/features/trl\\_demystified.html](https://www.nasa.gov/topics/aeronautics/features/trl_demystified.html) (Accessed August 10, 2020).
- Palfi, E. A. (2020). Kinetic model of a CO recycling rotary adsorption wheel for gas turbine power plants with carbon capture. Engineering thesis. Edinburgh (United Kingdom): School of EngineeringThe University of Edinburgh.
- Park, J., Rubiera Landa, H. O., Kawajiri, Y., Realf, M. J., Lively, R. P., and Sholl, D. S. (2019). How well do approximate models of adsorption-based CO capture processes predict results of detailed process models? *Ind. Eng. Chem. Res.* 59, 7097–7108. doi:10.1021/acs.iecr.9b05363
- Peters, M., Timmerhaus, K., and West, R. (2006). *Plant design and economics for chemical Engineers*. 5th Edn. Boston, MA: McGraw-Hill.
- Rajagopalan, A. K., Avila, A. M., and Rajendran, A. (2016). Do adsorbent screening metrics predict process performance? A process optimisation based study for post-combustion capture of CO. *Int. J. Greenhouse Gas Control*. 46, 76–85. doi:10.1016/j.jggc.2015.12.033
- Rajagopalan, A. K., and Rajendran, A. (2018). The effect of nitrogen adsorption on vacuum swing adsorption based post-combustion CO capture. *Int. J. Greenhouse Gas Control*. 78, 437–447. doi:10.1016/j.jggc.2018.09.002
- Rezaei, F., and Webley, P. (2009). Optimum structured adsorbents for gas separation processes. *Chem. Eng. Sci.* 64, 5182–5191. doi:10.1016/j.ces.2009.08.029
- Rezaei, F., and Webley, P. (2010). Structured adsorbents in gas separation processes. *Separ. Purif. Technol.* 70, 243–256. doi:10.1016/j.seppur.2009.10.004
- Rodrigues, A. E., LeVan, M. D., and Tondeur, D. (1989). *Adsorption: science and technology*. Dordrecht, NL: Kluwer Academic Publishers.
- Rouquerol, J., Rouquerol, F., Llewellyn, P., Maurin, G., and Sing, K. S. W. (2014). *Adsorption by powders and porous solids: principles methodology and applications*. 2nd Edn. Oxford, United Kingdom: Academic Press.
- Roussanaly, S. (2019). Calculating CO avoidance costs of carbon capture and storage from industry. *Carbon Manag.* 10, 105–112. doi:10.1080/17583004.2018.1553435
- Rubin, E. S. (2012). Understanding the pitfalls of CCS cost estimates. *Int. J. Greenhouse Gas Control*. 10, 181–190. doi:10.1016/j.jggc.2012.06.004
- Rubin, E. S., Short, C., Booras, G., Davison, J., Ekstrom, C., Matuszewski, M., et al. (2013). A proposed methodology for CO capture and storage cost estimates. *Int. J. Greenhouse Gas Control*. 17, 488–503. doi:10.1016/j.jggc.2013.06.004
- Ruthven, D. M. (1984). *Principles of adsorption and adsorption processes*. New York, NY: John Wiley & Sons.
- Ruthven, D. M., Shamsuzzaman, F., and Knaebel, K. S. (1994). *Pressure swing adsorption*. New York, NY: VCH Publishers.
- Shuai, X., Cheng, S., and Meisen, A. (1996). Simulation of pressure swing adsorption modules having laminated structure. *Microporous Mater.* 5, 347–355. doi:10.1016/0927-6513(95)00070-4
- Sinha, A., Darunte, L. A., Jones, C. W., Realf, M. J., and Kawajiri, Y. (2017). Systems design and economic analysis of direct air capture of CO through temperature vacuum swing adsorption using MIL-101(Cr)-PEI-800 and mmen-Mg(dobpdc) MOF adsorbents. *Ind. Eng. Chem. Res.* 56, 750–764. doi:10.1021/acs.iecr.6b03887
- Sinha, A., and Realf, M. J. (2019). A parametric study of the techno-economics of direct CO air capture systems using solid adsorbents. *AIChE J.* 65, e16607. doi:10.1002/aic.16607
- Sircar, S. (2001). Applications of gas separation by adsorption for the future. *Adsorpt. Sci. Technol.* 19, 347–366. doi:10.1260/0263617011494222
- Stöcker, J., Whysall, M., and Miller, G. Q. (1998). *30 years of PSA technology for hydrogen purification*. Des Plaines, IL: UOP LLC).
- Subramanian Balashankar, V., Rajagopalan, A. K., de Pauw, R., Avila, A. M., and Rajendran, A. (2019). Analysis of a batch adsorber analogue for rapid screening of adsorbents for postcombustion CO capture. *Ind. Eng. Chem. Res.* 58, 3314–3328. doi:10.1021/acs.iecr.8b05420
- Subraveti, S. G., Roussanaly, S., Anantharaman, R., Riboldi, L., and Rajendran, A. (2020). Techno-economic assessment of optimised vacuum swing adsorption for post-combustion CO capture from steam-methane reformer flue gas. *Separ. Purif. Technol.* 256, 117832. doi:10.1016/j.seppur.2020.117832
- Sudhoff, D., Leimbrink, M., Schleinitz, M., Górak, A., and Lutze, P. (2015). Modelling, design and flexibility analysis of rotating packed beds for distillation. *Chem. Eng. Res. Des.* 94, 72–89. doi:10.1016/j.cherd.2014.11.015
- Susarla, N., Haghpanah, R., Karimi, I. A., Farooq, S., Rajendran, A., Tan, L. S. C., et al. (2015). Energy and cost estimates for capturing CO from a dry flue gas using pressure/vacuum swing adsorption. *Chem. Eng. Res. Des.* 102, 354–367. doi:10.1016/j.cherd.2015.06.033
- Thomas, W. J., and Crittenden, B. (1998). *Adsorption technology and design*. Oxford, United Kingdom: Butterworth-Heinemann.
- Ulrich, G. D., and Vasudevan, P. T. (2006). How to estimate utility costs. *Chem. Eng.* 113, 66–69.
- van der Spek, M., Fout, T., Garcia, M., Kuncheekanna, V. N., Matuszewski, M., McCoy, S., et al. (2020). Uncertainty analysis in the techno-economic assessment of CO capture and storage technologies. Critical review and guidelines for use. *Int. J. Greenhouse Gas Control*. 100, 103113. doi:10.1016/j.jggc.2020.103113
- van der Spek, M., Roussanaly, S., and Rubin, E. S. (2019). Best practices and recent advances in CCS cost engineering and economic analysis. *Int. J. Greenhouse Gas Control*. 83, 91–104. doi:10.1016/j.jggc.2019.02.006
- Wagner, J. L. (1967). *Selective adsorption process*. U.S. Patent No 3 430 418A. March 4, 1967.
- Webley, P. A., and Danaci, D. (2020). *Carbon capture and storage-chapter 5. CO capture by adsorption processes*. London, United Kingdom: The Royal Society of Chemistry.
- Wijesiri, R. P., Knowles, G. P., Yeasmin, H., Hoadley, A. F. A., and Chaffee, A. L. (2019). Technoeconomic evaluation of a process capturing CO directly from air. *Processes*. 7, 503. doi:10.3390/pr7080503
- Woods, D. R. (2007). *Rules of thumb in engineering practice*. Weinheim, DE: WileyVCH.
- Woods, D. R., Anderson, S. J., and Norman, S. L. (1976). Evaluation of capital cost data: heat exchangers. *Can. J. Chem. Eng.* 54, 469–488. doi:10.1002/cjce.5450540601
- Yancy-Caballero, D., Leperi, K. T., Bucior, B. J., Richardson, R. K., Islamoglu, T., Farha, O. K., et al. (2020). Process-level modelling and optimization to evaluate metal-organic frameworks for post-combustion capture of CO. *Mol. Syst. Des. Eng.* 5, 1205–1218. doi:10.1039/d0me00060d
- Yang, R. T. (1987). *Gas separation by adsorption processes*. Stoneham, MA: Butterworth Publishers.
- Zimmermann, A. W., Wunderlich, J., Müller, L., Buchner, G. A., Marxen, A., Michailos, S., et al. (2020). Techno-economic assessment guidelines for CO utilization. *Front. Energy Res.* 8, 5. doi:10.3389/fenrg.2020.00005

**Conflict of Interest:** The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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## GLOSSARY

**CapEx** total capital expenditure [\$]

**CRF** capital recovery factor [year<sup>-1</sup>]

**EAC** equivalent annual cost [\$]

**i** cost of capital or interest rate [-]

**n** lifetime, or economic life of project [years]

**n<sub>x</sub>** amount adsorbed of component *x* [mol kg<sup>-1</sup>]

**NPV** net present value [\$]

**OpEx** annual operating costs [\$ year<sup>-1</sup>]

**Q<sub>th</sub>** thermal energy [J]

**TAC** total annualized cost [\$ year<sup>-1</sup>]

**T<sub>H</sub>** high temperature source temperature [K]

**T<sub>L</sub>** low temperature sink temperature [K]

**W<sub>s</sub><sup>eq</sup>** equivalent shaft work [J]

**y<sub>x</sub>** mole fraction of component *x* in the feed [-]

**α<sub>ab</sub>** ideal selectivity of component *a* over *b* [-]

**η<sub>isen</sub>** Isentropic efficiency [-]