

# Capture of CO<sub>2</sub> from flue gas streams with zeolite 13X by vacuum-pressure swing adsorption

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**Abstract** Vacuum swing adsorption (VSA) capture of CO<sub>2</sub> from flue gas streams is a promising technology for greenhouse gas mitigation. In this study we use a detailed, validated numerical model of the CO<sub>2</sub>VSA process to study the effect of a range of operating and design parameters on the system performance. The adsorbent used is 13X and a feed stream of 12% CO<sub>2</sub> and dry air is used to mimic flue gas. Feed pressures of 1.2 bar are used to minimize flue gas compression. A 9-step cycle with two equalisations and a 12-step cycle including product purge were both used to understand the impact of several cycle changes on performance. The ultimate vacuum level used is one of the most important parameters in dictating CO<sub>2</sub> purity, recovery and power consumption. For vacuum levels of 4 kPa and lower, CO<sub>2</sub> purities of >90% are achievable with a recovery of greater than 70%. Both purity and recovery drop quickly as the vacuum level is raised to 10 kPa. Total power consumption decreases as the vacuum pressure is raised, as expected, but the recovery decreases even quicker leading to a net increase in the specific power. The specific power appears to minimize at a vacuum pressure of approximately 4 kPa for the operating conditions used in our study. In addition to the ultimate vacuum level, vacuum time and feed

time are found to impact the results for differing reasons. Longer evacuation times (to the same pressure level) imply lower flow rates and less pressure drop providing improved performance. Longer feed times led to partial breakthrough of the CO<sub>2</sub> front and reduced recovery but improved purity. The starting pressure of evacuation (which is not necessarily equal to the feed pressure) was also found to be important since the gas phase was enriched in CO<sub>2</sub> prior to removal by vacuum leading to improved CO<sub>2</sub> purity. A 12-step cycle including product purge was able to produce high purity CO<sub>2</sub> (>95%) with minimal impact on recovery. Finally, it was found that for 13X, the optimal feed temperature was around 67°C to maximize system purity. This is a consequence of the temperature dependence of the working selectivity and working capacity of 13X. In summary, our numerical model indicates that there is considerable scope for improvement and use of the VSA process for CO<sub>2</sub> capture from flue gas streams.

**Keywords** Vacuum swing adsorption · CO<sub>2</sub> capture · Simulation

## 1 Introduction

With the concern over global warming, CO<sub>2</sub> capture and sequestration has been widely and intensely studied over the last decade. In particular, the technologies of capturing CO<sub>2</sub> from fossil fuel combustion using adsorption processes has been widely studied (Kikkinides et al. 1993; Chue et al. 1995; Siriwardane et al. 2001; Park et al. 2002; Na et al. 2002; Chaffee et al. 2007; Zhang and Webley 2008). Depending on the availability of adsorbents, PSA can be adapted to a wide range of temperatures and pressures

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(Ko et al. 2003; Reynolds et al. 2005). However, the actual operation of a PSA system with multi-beds, PID control, non-isothermal behaviour, etc. can be challenging to simulate and hence difficult to design and optimize. Some of the design and operating parameters of the PSA process can be optimized through experimental means but there are many PSA variables (e.g. bed diameter, bed length, particle size, etc.) which are difficult and time consuming to assess through experimental means only. For this reason there is a need for a reliable, validated numerical model to evaluate and estimate the performance of various PSA cycle designs, adsorbent materials, and process conditions of temperature and pressure on plant performance, as measured by parameters such as product purity, recovery and power consumption. Our numerical model (MINSAs) was built on the basis of mass and energy balances using a variety of adsorption isotherm models, kinetic models and heat transfer models as described earlier (Webley and He 2000 and Todd et al. 2003). The kinetic model contains a discrete pellet version implementing the Dusty Gas Model to describe mass transfer within porous materials. We have described this in detail in previous work (Todd and Webley 2006). Parameters required are dimensionless coefficients for Knudsen flow ( $C_K$ ), viscous flow ( $C_v$ ) and molecular flow ( $C_m$ ). Pressure drop in the adsorption bed is calculated with Ergun equation. We have used our numerical simulator extensively over the past decade to evaluate air separation systems and help guide experiments (Todd et al. 2001, 2006).

In addition to our numerical simulation work described below, we have built and operated a three-bed VSA system (Zhang and Webley 2008). Data from that system have been used to validate and improve our numerical simulator. In this study we examine the effect of a range of VSA parameters such as feed temperature, vacuum pressure (starting and ending) and step times on PSA performance. Our goal is to identify important variables and assess their impact with the target in mind of producing a CO<sub>2</sub> stream of purity greater than 95% and recovery greater than 70%.

Our simulations and experimental work are based on adsorbent 13X (PSAO2 HP Molsiv™ adsorbent (zeolite 13X, 8X12 mesh, bulk density of 641 kg/m<sup>3</sup>, bed voidage of 0.37 and pellet voidage of 0.6). An average intrapellet pore diameter of 1 μm, and tortuosity factors of 3.00 for molecular, Knudsen and viscous flow were used. This results in mass transfer parameters  $C_K = 0.083$ ,  $C_v = 0.061$ ,  $C_m = 0.166$  which were confirmed by comparison to breakthrough data and uptake data from our uptake apparatus. Isotherms for CO<sub>2</sub>, N<sub>2</sub> and O<sub>2</sub> on this adsorbent were measured at 20, 70 and 90°C on our volumetric apparatus from 0 to 1000 mmHg and represented with the Dual-Site Langmuir isotherm—the parameters are included in Table 1. The real binary and ternary data may differ from pure component data at the same partial pressure of CO<sub>2</sub>, but the adsorption loading of CO<sub>2</sub> is much higher than those of N<sub>2</sub>

**Table 1** Dual-Site Langmuir isotherm constants for CO<sub>2</sub>, N<sub>2</sub>, and O<sub>2</sub>

Item	CO <sub>2</sub>	N <sub>2</sub>	O <sub>2</sub>
$m_1$ (mol/kg)	2.808	2.0197	0.01260
$m_2$ (mol/kg)	2.4975	0	0
$b_0$ (1/kPa)	$4.7308 \times 10^{-7}$	$2.0364 \times 10^{-6}$	$1.619 \times 10^{-3}$
$Q_1$ (J/mol)	32194.3	14875.2	1297.8
$d_0$ (1/kPa)	$3.3005 \times 10^{-8}$	0	$2.119 \times 10^{-4}$
$Q_2$ (J/mol)	32176.7	0	4979.5

$$n_i = \frac{m_1 b_i P_i}{1 + b_i P_i + b_j P_j + b_k P_k} + \frac{m_2 d_i P_i}{1 + d_i P_i + d_j P_j + d_k P_k};$$

$$b_i = b_{oi} \exp\left(\frac{Q_{1i}}{RT}\right); \quad d_i = d_{oi} \exp\left(\frac{Q_{2i}}{RT}\right)$$

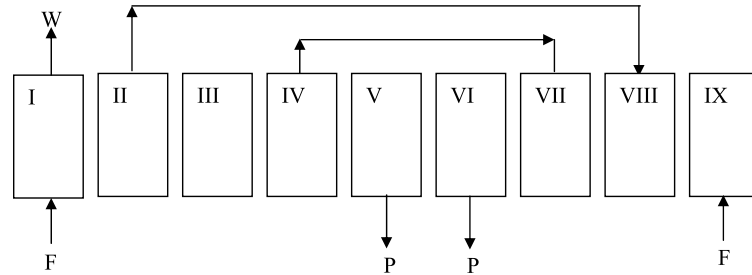
and O<sub>2</sub>. We expect the effect of N<sub>2</sub> and O<sub>2</sub> on CO<sub>2</sub> loading to be quite small. However, it is likely that the effect of CO<sub>2</sub> loading on N<sub>2</sub> and O<sub>2</sub> loading is quite large. Although IAST can be used to estimate this, it is known that IAST is not reliable for zeolitic systems which are highly heterogeneous. In the absence of experimental data therefore, it is difficult to quantify this error. Our intention in this study is not to provide high level accurate design simulations but rather establish trends and approximate performance. It should be noted however that although we are using pure component data in our simulations, our results are in reasonably good agreement with our experimental data from our pilot plant. Our experimental VSA system consists of three adsorption beds which are constructed from 3 mm thick stainless steel with an internal diameter of 50 mm. Each bed is packed to a height of 1 m with 1.32 kg of 13X adsorbent. The feed to our VSA system is CO<sub>2</sub> blended with dry air to produce a stream containing 12% CO<sub>2</sub>, 69.5% N<sub>2</sub>, 18.5% O<sub>2</sub>.

It is important to note that real flue gas streams are invariably wet and can contain up to 10% water depending on the temperature. We are currently studying the simultaneous separation of water and CO<sub>2</sub> in a single VSA process (Li et al. 2008).

## 2 Numerical simulation and PSA cycle design

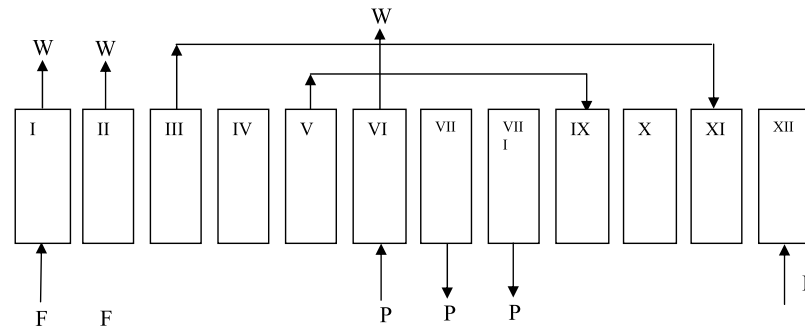
In our numerical model, boundary conditions for all the steps are based on flow through a valve (mimicking our plant operation). Thus source/sink pressures across the valves determine the flow rates. Application of control loops within our simulation leads to a constrained CSS (cyclic steady state) solution which satisfies the design specifications, that is, some dependent variables in the PSA system are forced to reach their preset target values at CSS by adjusting those

**Fig. 1** Nine step pressure swing adsorption cycle



Where F – feed flow; P – product flow (CO<sub>2</sub>); W – waste flow

**Fig. 2** Twelve step pressure swing adsorption cycle



Where F – feed flow; P – product flow; W – waste flow

parameters with PID (Proportional Integral Derivative) algorithms. This procedure is exactly that used in our VSA pilot plant operation. Power calculations are based on single stage adiabatic compression calculations assuming an isentropic efficiency of 70%.

### 2.1 Cycle design

Two separate VSA 3-bed cycles have been designed in this simulation; a nine—step cycle and a twelve-step cycle. The nine step cycle was designed to investigate effects of starting and ending vacuum pressures, vacuum time and feed temperatures. This design only involves four major phases; adsorption, equalisation, desorption and re-pressurization (Fig. 1). Two equalisation steps are included since these act as a co-current depressurisation (for the bed providing pressure equalisation gas) and permit a variety of starting vacuum pressures to be investigated.

In the first phase (adsorption step I), feed gas containing 12% CO<sub>2</sub> enters the bottom of the bed and exits to the atmosphere through the top of the bed. This step causes the preferentially adsorbed species (CO<sub>2</sub>) to be selectively adsorbed from the bulk gas to the solid phase. The second phase (step II) is the first equalisation. Thereafter an idle step is inserted to permit scheduling. The second phase of equalisation is continued through an additional equalisation (step IV). The third phase is counter-current evacuation (steps V and VI) which is the primary step removing

adsorbed CO<sub>2</sub> (and co-adsorbed N<sub>2</sub>) and the fourth phase is repressurisation (firstly with gas from the corresponding equalisation step) with feed gas.

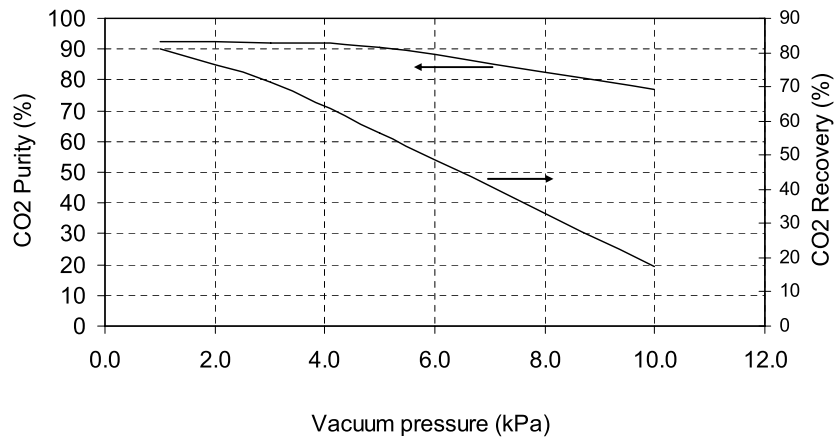
The twelve step cycle is based on the nine-step cycle described above with the inclusion of a CO<sub>2</sub> product purge step—step VI (Fig. 2). The purge step permits further adsorption of CO<sub>2</sub> by increasing the partial pressure of CO<sub>2</sub> and displacing N<sub>2</sub> to be released into the gas phase and then out the top of the bed. In our simulation (and our experimental work), a fixed percentage of product gas is used to purge the bed after the equalising step (V). The net result of the product purge step is that more concentrated CO<sub>2</sub> gas can be generated in the following evacuation steps (VII and VIII). If the exhausted stream from the purge step contains a high concentration of CO<sub>2</sub>, this gas flow can be recycled to the feed tank by a compressor for the next cycle.

From both our experimental and simulation work, we have found that the beginning pressure of the evacuation process significantly affects product purity. Therefore, we studied this effect independently using a very simple four-step cycle with a single bed. The four steps are adsorption, pressure reduction, desorption and re-pressurisation.

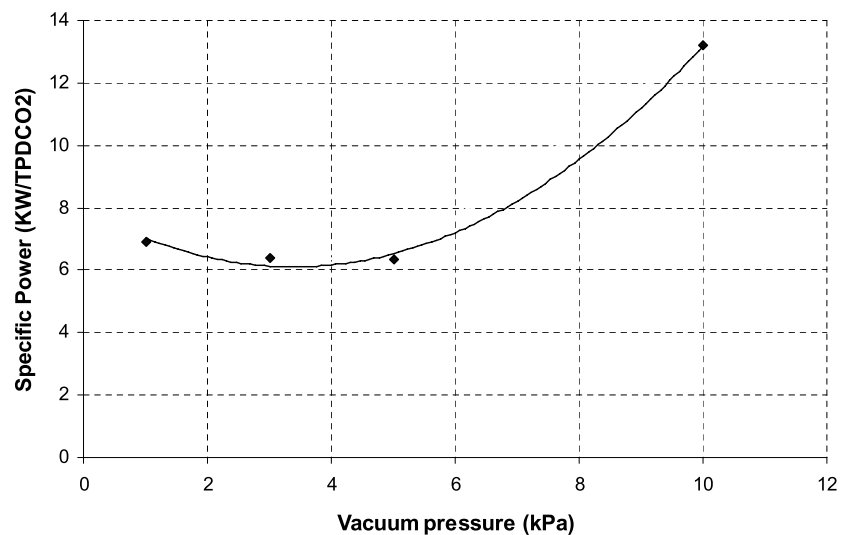
### 2.2 Parameters studied and operating conditions

Since flue gas streams from conventional power plants are invariably at low pressure (<0.1 bar gauge), we used a

**Fig. 3** Effect of vacuum pressure on CO<sub>2</sub> product purity and recovery for 9 step cycle (adsorption time = 60 s, desorption time = 100 s,  $P_{\text{high}} = 1.2$  bar,  $T_{\text{feed}} = 45^\circ\text{C}$ )



**Fig. 4** Effect of vacuum pressure on VSA specific power consumption for 9 step cycle (adsorption time = 60 s, desorption time = 100 s,  $P_{\text{high}} = 1.2$  bar,  $T_{\text{feed}} = 45^\circ\text{C}$ )



CO<sub>2</sub>/air mixture to simulate the flue gas stream at the pressure of 1.2 bar (absolute). This pressure can be accomplished from a flue gas stream with blowers. The feed temperature was set to range from 25 to 80°C since it is known that this spans the range of typical flue gas temperatures and is also the range over which 13X shows excellent performance. The pressure at the end of desorption (evacuation) ranged from 1 kPa to 10 kPa and a feed flow rate of 120 l/min was used. The step times for the adsorption (feed) step and evacuation step were studied as well as the purge/product ratio. All simulations are conducted to cyclic steady state as determined by bed profiles and closure of mass and energy balances.

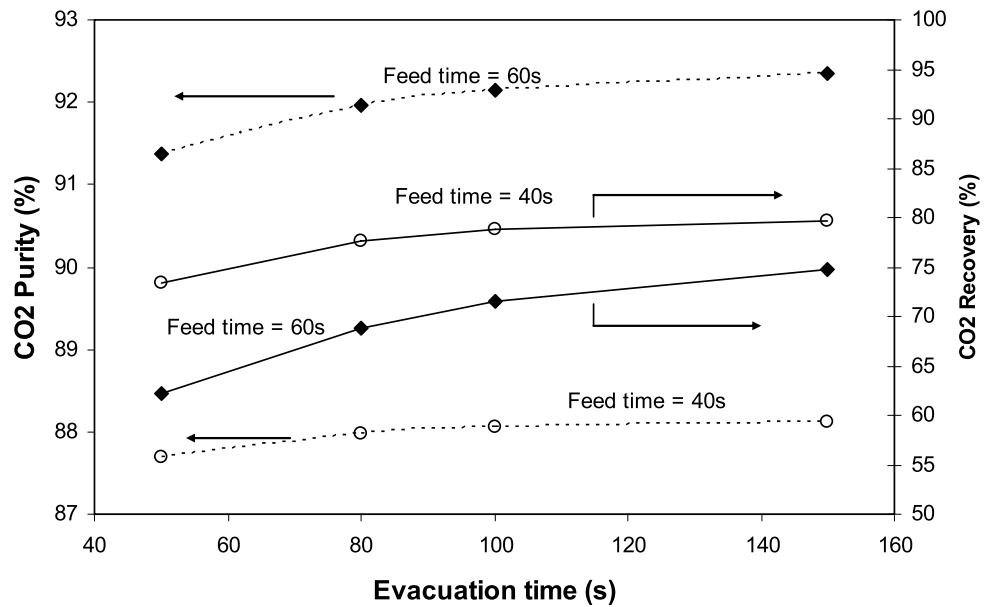
### 3 Results and discussion

#### 3.1 Effects of the vacuum pressure and time on performance

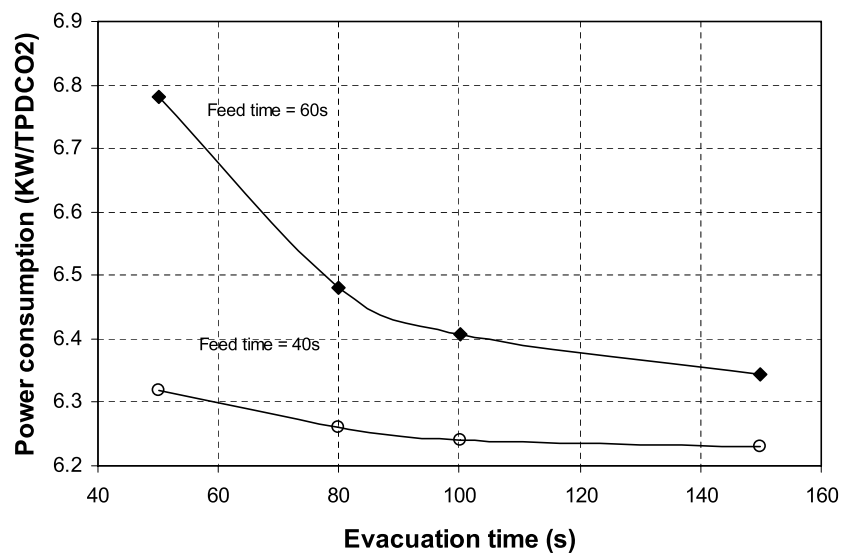
For this study, the feed temperature was 45°C, the feed step time was 60 s and an evacuation time of 100 s was used.

Figures 3 and 4 show the effect of vacuum pressure at the end of the vacuum step on CO<sub>2</sub> product purity, recovery and power consumption for the 9-step cycle. The CO<sub>2</sub> product purity drops rapidly when the evacuation pressure increases from 5 to 10 kPa, but the change is quite small between 1 to 5 kPa. This is a consequence of the isotherm for CO<sub>2</sub> which is very steep at low pressures. In contrast, the recovery of CO<sub>2</sub> is strongly dependent on vacuum level. Figure 3 shows that a drop from 80% to 15% occurs when the vacuum pressure increases from 1 to 10 kPa. This has important and serious implications for application of VSA to CO<sub>2</sub> capture by adsorption. Any pressure drop (as much as 1–3 kPa) in the vacuum line and/or bed can result in a significant effect on process performance. Figure 4 shows that specific power consumption in the VSA cycle decreases when the evacuation pressure increases from 1 to 4 kPa and then increases when the evacuation pressure increases continuously. Although the CO<sub>2</sub> productivity has decreased by increasing the vacuum level from 1 to 4 kPa (due to recovery and purity decline), the total vacuum power consumption has also decreased since the pressure ratio across the vacuum pump has

**Fig. 5** Effect of evacuation time on CO<sub>2</sub> product purity and recovery for two feed times for 9 step cycle ( $P_{\text{high}} = 1.2$  bar,  $P_{\text{low}} = 3$  kPa,  $T_{\text{feed}} = 45^{\circ}\text{C}$ )



**Fig. 6** Effect of evacuation time on VSA power consumption for two feed times for 9 step cycle ( $P_{\text{high}} = 1.2$  bar,  $P_{\text{low}} = 3$  kPa,  $T_{\text{feed}} = 45^{\circ}\text{C}$ )



reduced from 100:1 at 1 kPa to 25:1 at 4 kPa. The specific power therefore decreases. However, when the vacuum pressure is further increased, the CO<sub>2</sub> productivity drops quickly while the pressure ratio across the vacuum pump is reduced from 25:1 at 4 kPa to 10:1 at 10 kPa, The specific power therefore increases. Therefore, the optimal vacuum pressure for this case is 4 kPa.

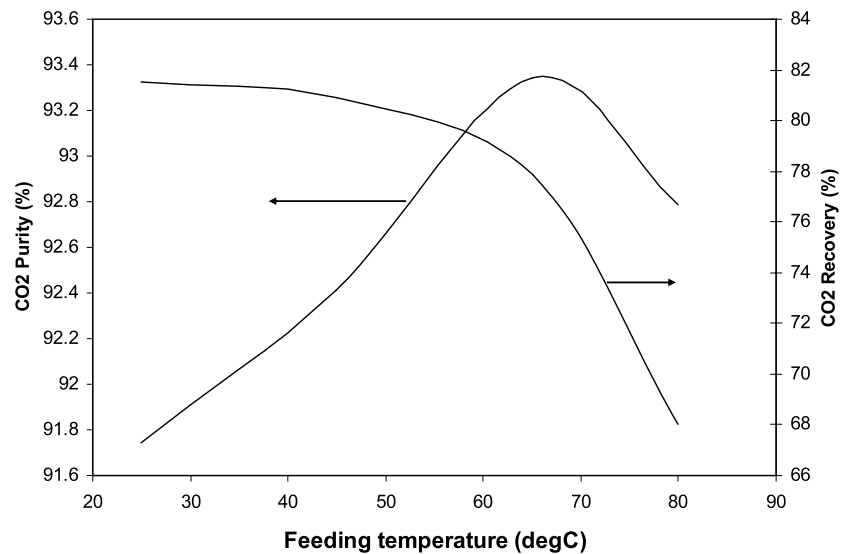
### 3.2 Effect of vacuum time and feeding time on VSA performance

Faster cycles lead to more throughput for the same amount of adsorbent, or alternatively, less adsorbent for a given throughput. Unfortunately, higher gas velocities are produced leading to higher pressure drop, higher power con-

sumption, and insufficient time for adsorption (mass transfer limitation). To test the impact of these high velocities on process performance, the simulation was run for feed step times of 40 s and 60 s separately, and desorption step times from 50 to 150 s. As before, the feed temperature was 45°C and a final vacuum pressure of 3 kPa was imposed. As expected, higher gas velocities are required for the 40 s feed step time and 50 s evacuation time.

Figures 5 and 6 show CO<sub>2</sub> product purity, recovery and power consumption as a function of vacuum and feed step times for the 9-step cycle. Firstly, Fig. 5 shows that an increase in evacuation time (even though the same vacuum level has been reached) leads to an improvement in CO<sub>2</sub> purity and recovery while decreasing specific power, regardless of the step time used for the feed step. This is due to

**Fig. 7** Effect of feed temperatures on CO<sub>2</sub> product purity and recovery for 9 step cycle (adsorption time = 60 s, desorption time = 100 s,  $P_{\text{high}} = 1.2$  bar,  $P_{\text{low}} = 1$  kPa,  $T_{\text{feed}} = 45^\circ\text{C}$ )



the reduction in gas velocity resulting in lower bed pressure drop and hence improved CO<sub>2</sub> working capacity. The effect of the feed step time on CO<sub>2</sub> purity and recovery is revealing. Longer feed step times gives higher purity but lower recovery and vice versa. This is because longer feed step time has resulted in partial breakthrough of the CO<sub>2</sub> front during the feed step, “losing” CO<sub>2</sub> to the waste stream and reducing CO<sub>2</sub> recovery. However, allowing partial breakthrough has displaced remaining N<sub>2</sub> giving a slightly higher CO<sub>2</sub> product purity during the evacuation step since co-adsorbed nitrogen has been displaced. The behaviour suggests that feed step time may be a useful control parameter to control product purity. The increased power consumption for longer feed step times (Fig. 6) is a direct result of decreased CO<sub>2</sub> recovery.

### 3.3 Effect of feed temperature on VSA performance

A large number of simulations were conducted for feed temperatures ranging from 25 to 80°C at several vacuum pressures, vacuum and feed step times for the 9 step cycle. We show the results for the case of a 1 kPa vacuum level and an evacuation time of 60 s—other conditions gave similar trends. Figure 7 shows that the purity reaches a maximum for a feed temperature of 80°C and then decreases. The CO<sub>2</sub> recovery does not appear to reach a maximum but continually declines as temperature is increased. These observations are consistent with the behaviour of 13X as a function of temperature. The CO<sub>2</sub> purity is a sensitive function of adsorbent selectivity (ratio of CO<sub>2</sub> to N<sub>2</sub> adsorbed), and reaches a maximum at 80°C. The CO<sub>2</sub> recovery, however, is also a function of CO<sub>2</sub> working capacity which decreases as temperature increases. The net result is that recovery decreases with an increase in temperature. The decision on which tem-

perature to use must be based on economic considerations which include heat transfer considerations for the flue gas.

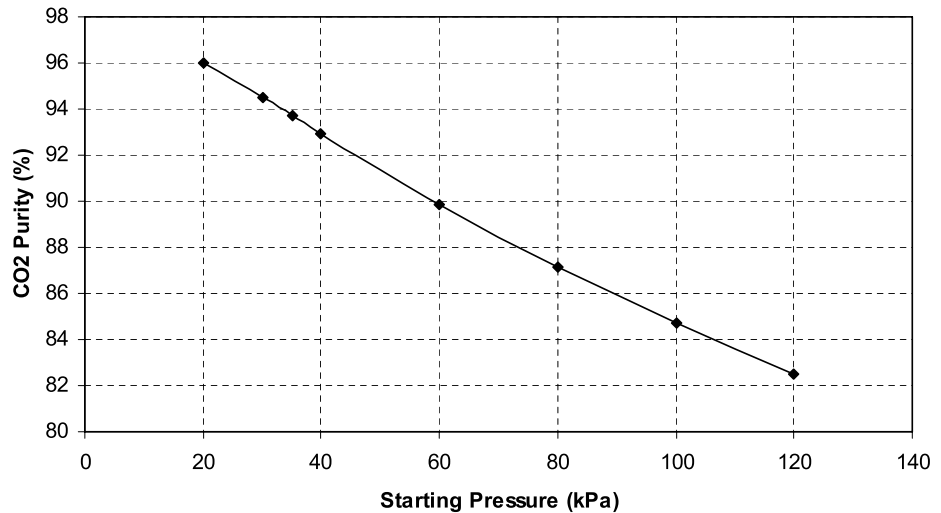
### 3.4 The effect of the starting pressure of the evacuation step on product purity

The pressure at which the evacuation step starts has an important effect on product purity. Typically, the evacuation step follows on from an equalisation step. The equalisation step is effectively a co-current depressurisation for the bed provide pressure equalisation gas. It therefore follows that more co-current depressurisation will lead to more release of CO<sub>2</sub>, displacing N<sub>2</sub> in the voids of the bed and improving the starting concentration of CO<sub>2</sub> in the bed. Subsequent evacuation of the bed leads to enhanced CO<sub>2</sub> product purity. To quantify this effect, we ran simulations for a feed temperature of 45°C, a vacuum time of 100 s and a vacuum pressure of 1 kPa with a single column for a 4-step cycle. Figure 8 shows that the CO<sub>2</sub> product purity drops from 96% to 82% when the starting pressure increases from 20 kPa to 120 kPa. However, there is very little effect on power consumption and product recovery. It is therefore advantageous to include a pressure equalisation step (or several) to reduce the pressure as much as possible prior to evacuation and recovery of CO<sub>2</sub>.

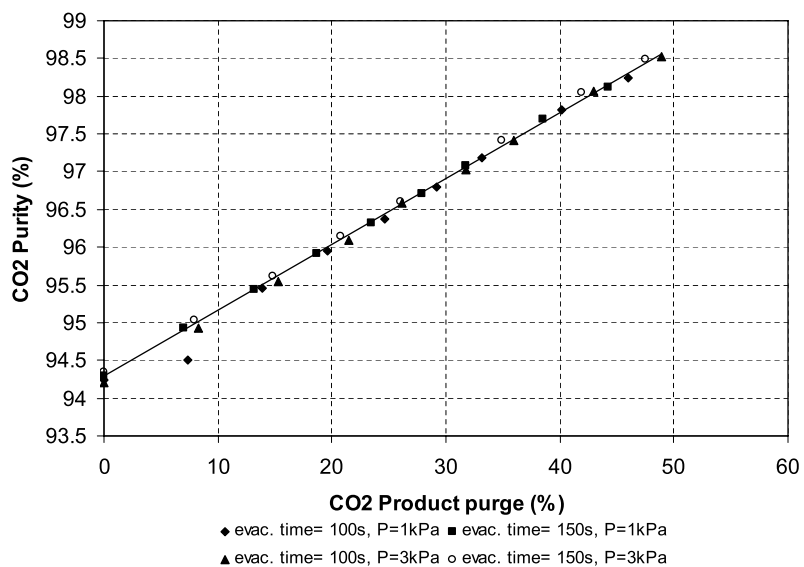
### 3.5 Effect of product purge on VSA performance

To enhance CO<sub>2</sub> product purity, a product purge step is typically added. A series of simulations were conducted at a feed temperature of 45°C, a feed time of 60 s, and a starting pressure of 35 kPa. Two vacuum pressures (1 and 3 kPa) and two evacuation times (100 and 150 s) were investigated for our 12-step cycle. Figure 9 shows that product purity correlates linearly with product purge. There is a small decline in

**Fig. 8** Effect of starting pressure during the period of evacuation on the CO<sub>2</sub> product purity for 9 step cycle (adsorption time = 60 s, desorption time = 100 s,  $P_{\text{high}} = 1.2$  bar,  $P_{\text{low}} = 1$  kPa,  $T_{\text{feed}} = 45^\circ\text{C}$ )



**Fig. 9** Effect of CO<sub>2</sub> product purge on CO<sub>2</sub> product purity for varying evacuation (desorption) time and vacuum pressures ( $P_{\text{high}} = 1.2$  bar, adsorption time = 60 s,  $T_{\text{feed}} = 45^\circ\text{C}$ )



CO<sub>2</sub> recovery with increase in CO<sub>2</sub> purge (not shown) and a subsequent small increase in specific power consumption with increase in product purge. It is interesting to note that a CO<sub>2</sub> product purity of over 95% is readily achieved.

#### 4 Conclusion

In this work, the effects of operating parameters on VSA performance were studied with our validated numerical simulator. The most important variables governing CO<sub>2</sub> purity, recovery and power consumption (all three of which impact on CO<sub>2</sub> capture cost) are vacuum pressure at the end of pump down, starting vacuum pressure level, amount of product gas used for purge, feed temperature, and rates of adsorption and desorption. We have found that a CO<sub>2</sub> product purity of greater than 95% is achievable with a recovery greater than 70% provided a vacuum pressure of at least

3 kPa is used, and a sufficient amount of purge gas is used. Use of high vacuum pressure levels such as 10 kPa lead to a dramatic drop in CO<sub>2</sub> recovery and purity. For 13X, an optimum feed temperature as regards product purity appears to be around 80°C although the actual optimal value depends on other economic factors. In summary, our numerical simulator is a powerful method for assessing the impact of a large number of variables on CO<sub>2</sub> VSA performance (some of which were reported here), ultimately reducing experiment time and assisting in cost-effective VSA design.

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