

# Optimisation of Pressure Swing Adsorption (PSA) Process for Producing High Purity CO<sub>2</sub> for Sequestration Purposes

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Fixed bed adsorption processes such as pressure swing (PSA) and temperature swing (TSA), unlike other chemical engineering separation processes, are dynamic processes which do not produce a continuous or steady flow of either the adsorbate or lean (non-adsorbed) phase. Instead, they operate with multiple vessels in a cyclic operation. These processes, therefore, pose additional challenges which include a much larger array of input parameters that control the individual steps within each PSA or TSA cycle. This work proposes an Aspen Adsorption™ based Multi-Objective Optimisation (MOO) framework for PSA systems. The PSA systems can be optimised against different step times and process parameters such as, blow down pressure, feed pressure, valve co-efficients etc. The proposed framework is demonstrated by considering an example of a PSA based Carbon Capture and Sequestration (CCS) unit, for the removal of CO<sub>2</sub> from an entrained flow gasifier synthesis gas stream, downstream of the Water Gas Shift Reactors. The two objective functions maximise the CO<sub>2</sub> capture rate and minimise the specific energy penalty associated with CO<sub>2</sub> capture. A novel feature of this study is the purification of the CO<sub>2</sub> produced by the PSA by condensing it, thereby, allowing it to be pumped up to a pressure of 100 bar. The off-gas from the separation has been constrained to have the same composition as that of the feed, which may be recycled to the PSA process or used for a different purpose. The MOO Pareto curves provide information on the most important variables for both the PSA and the refrigeration system.

## 1. Introduction

A typical PSA or TSA usually has several beds operating in a cyclic manner. Switching from one bed to another is done to optimise the purity of the two product streams, whilst minimising the total volume of adsorbent required in each bed. There is a large array of inputs that need to be specified for each step of the cycle. These specifications may include: step times and process parameters such as, blow down pressure, feed pressure, valve coefficients etc. It is for this reason that optimisation of a PSA process is often a challenging task. Optimisation of a PSA process may also often involve multiple, conflicting objectives. In such situations, a PSA operator may want to examine the trade-offs involved between such objectives. There have been only a few studies that have focussed on Multi-Objective Optimisation (MOO) of PSA processes. A brief summary of these works is given in the following paragraph.

Ko and Moon (2002) used a modified Summation of Weighted Objective Functions (mSWOF) method to simultaneously maximise O<sub>2</sub> recovery and purity while separating O<sub>2</sub> from air. Sankararao and Gupta (2007) applied a modified version of the aJG adaptation of Multi-Objective Simulated Annealing (MOSA-aJG) to maximise the recovery and purity of different product stream produced during separation of air by a PSA. Fiandaca and Fraga (2009) used a custom Multi-Objective Genetic Algorithm (MOGA) to optimise a PSA process, involving air separation, to simultaneously maximise N<sub>2</sub> purity and recovery. Cacas et al. (2013) studied the MOO of a PSA process from the point of view of maximising H<sub>2</sub> and CO<sub>2</sub> recovery from a binary mixture of H<sub>2</sub> and CO<sub>2</sub>. They considered different step times as decision variables. Liu and Sun

(2013) used a meta-model to approximate the performance of a PSA process involving separation of air. Beck et al. (2013) recently reported using a meta-model of the PSA system instead of an accurate and computationally expensive full scale model.

This work proposes a generalised Aspen Adsorption™ and Microsoft Excel based MOO framework similar to the one proposed by Sharma et al. (2012). This framework accesses the Aspen Adsorption™ flowsheet variables through an object of ACM (Aspen Custom Modeler™) application. The proposed framework is demonstrated with the help of a PSA based Carbon Capture and Sequestration (CCS) unit for the removal of CO<sub>2</sub> from an entrained flow gasifier synthesis gas stream, downstream of the Water Gas Shift Reactors. The objectives that have been considered are maximising CO<sub>2</sub> capture rate and minimising the corresponding specific energy penalty. Nondominated Sorting Genetic Algorithm (NSGA)-II, proposed by Deb et al. (2002), is used as the optimisation algorithm. A typical problem associated with using PSA process for carbon capture from synthesis gas is that the H<sub>2</sub> mole fraction in the CO<sub>2</sub> stream is typically high. The solution to this problem has usually been confined to the introduction of additional steps into the PSA cycle. A common solution to this problem is to follow the adsorption step by a high purity CO<sub>2</sub> stream reflux (Sircar (1979)). Chou et al. (2013) used a two stage PSA system to achieve the same goal. In this case, syngas was first passed through a modified activated carbon bed to produce an H<sub>2</sub> product stream with desired purity. A higher purity CO<sub>2</sub> stream was then produced in the second stage with the help of a zeolite 13X-Ca bed.

A novel and alternate way to achieve the same goal has been proposed in this work that involves partial condensation of the CO<sub>2</sub> product stream to produce a high purity liquid CO<sub>2</sub> stream which can then be pumped to supercritical conditions, required for sequestration. The remaining vapour, constrained to have the same composition as that of feed, may be recycled to the PSA process or used for a different purpose. The proposed strategy also offers an opportunity for energy integration with the rest of the process, for example, in ammonia production by coal gasification, where there is a similar refrigeration requirement.

## 2. Process Configuration

The PSA process under consideration consists of four adsorption beds filled with activated carbon. The PSA system is being operated in a cycle consisting of 12 steps. The PSA system and the time chart for the cycle are depicted in Figure 1 and 2.

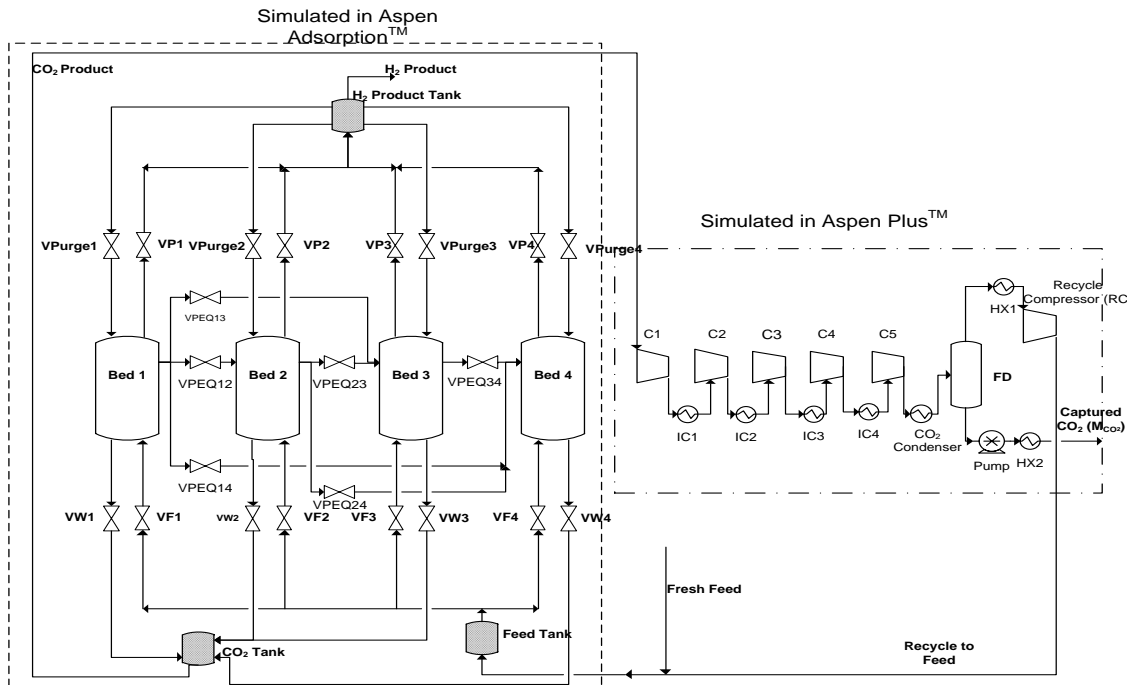


Figure 1: Flowsheet of the system being studied

PRES	AD	PED1	PED2	PED3	BD	PG	PEP1	PEP2	PEP3
PEP2	PEP3	PRES	AD	PED1	PED2	PED3	BD	PG	PEP1
BD	PG	PEP1	PEP2	PEP3	PRES	AD	PED1	PED2	PED3
PED2	PED3	BD	PG	PEP1	PEP2	PEP3	PRES	AD	PED1

Figure 2: Time chart for the PSA cycle. Steps are denoted as: PRES: Pressurisation; AD: Adsorption; PED1: First Pressure Equalisation (depressurisation); PED2: Second Pressure Equalisation (depressurisation); PED3: Third Pressure Equalisation (depressurisation); BD: Blow down; PG: Purging; PEP1: First Pressure Equalisation (pressurisation); PEP2: Second Pressure Equalisation (pressurisation); PEP3: Third Pressure Equalisation (pressurisation)

The CO<sub>2</sub> product stream generated by adsorption system is fed to a compression train to pressurise it to an intermediate pressure. The CO<sub>2</sub> is then condensed at this intermediate pressure in such a way that the vapour stream leaving the vessel (FD) has the same composition as that of feed. This vapour stream is then recycled to the PSA section. The high purity liquid CO<sub>2</sub> stream from vessel (FD) at intermediate pressure is then pumped to a pressure of 100 bar. By ensuring that the vapour stream from flash drum, FD has the same composition as that of feed, the computation time required to solve the system reduces significantly as the PSA system only needs to be solved once, because recycling the vapour effectively means scaling the PSA operation.

The adsorption system is simulated in Aspen Adsorption™ while the compression train and CO<sub>2</sub> condensation is simulated in Aspen Plus™. The stream data for CO<sub>2</sub> condenser, HX1 and HX2 are extracted (Harkin et al. (2012)) and the two stage refrigeration system is then optimised with the help of a separate algorithm. Figure 3 depicts the framework pictorially.

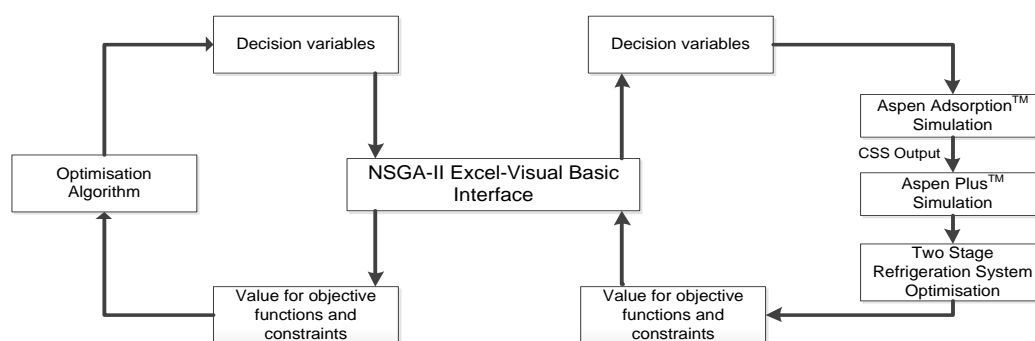


Figure 3: Proposed MOO framework (The details of the algorithm used to optimise refrigeration system can be found in Sharma et al. (2014)).

### 3. Adsorption model

The following simplifications have been made as part of the PSA model in Aspen Adsorption™:

- Isothermal operation
- The flow pattern has been assumed to be plug flow with axial dispersion only
- Concentration gradients in the radial direction have been neglected
- The overall mass transfer rate is assumed to be described by an overall lumped resistance

Table 1 lists the adsorbent and adsorption bed characteristics used in this work. The extended Langmuir Freundlich model is used to predict the multi-component adsorption equilibrium. A linear driving force (LDF) model has been used to estimate the rate of accumulation of adsorbate on the adsorbent. The extended Langmuir Freundlich model parameters and lumped mass transfer co-efficient values have been taken from Jee et al. (2001).

Table 1: Adsorbent and adsorption bed characteristics

Diameter of adsorption bed	5.82 m
Length of adsorption bed	3 m
Adsorbent	Activated carbon
Average particle radius	0.00115 m (Jee et al. (2001))
Bed void fraction	0.433 (Jee et al. (2001))
Adsorbent particle density	850 kg/m <sup>3</sup> (Jee et al. (2001))

Table 2: Decision variable range for optimisation

Decision Variable	Range
$C_{VPurge_i}$	0.000278- 0.00174 ( $kmol/(s*bar)$ )
3.1 $F_{pi}$	0.5-8 ( $kmol/s$ )
$P_{BD}$	0.05-8 ( $bar$ )
$P_{cond}$	10, 20, 30, 40, 50 ( $bar$ )

#### 4. MOO problem formulation

The CO<sub>2</sub> capture rate ( $CR_{CO_2}$ , fraction of CO<sub>2</sub> being captured) and the specific energy (SE, energy penalty per unit CO<sub>2</sub> being captured) have been considered as the two conflicting objectives. Energy is consumed by CO<sub>2</sub> compressors, CO<sub>2</sub> pump, recycle compressor and refrigeration compressor.

$$\text{Maximise } CR_{CO_2} (\%) \text{ \& \textit{Minimise } } SE = \frac{\left(\sum_{i=1}^5 E_{Ci} + E_{RC} + E_{ref} + E_{pump}\right)}{M_{CO_2}} \quad (1)$$

w.r.t.  $C_{VPurge_i}$ ,  $F_{pi}$ ,  $P_{BD}$  and  $P_{cond}$

Where;

$CR_{CO_2}$  : CO<sub>2</sub> capture rate (%)

$E_{Ci}$  : Electrical power consumed by compressor  $C_i$  ( $kW$ )

$E_{ref}$  : Electrical power consumed by refrigeration compressor ( $kW$ )

$E_{RC}$  : Electrical power consumed by recycle compressor ( $kW$ )

$E_{pump}$  : Electrical power consumed by CO<sub>2</sub> pump ( $kW$ )

$M_{CO_2}$  : Amount of CO<sub>2</sub> captured ( $kmol$ )

$C_{VPurge_i}$ ;  $i = 1,2,3,4$ : Valve co-efficient for purging valves ( $kmol/(s*bar)$ )

$F_{pi}$ ;  $i = 1,2,3,4$  : Product flow rate during adsorption steps ( $kmol/s$ ) (i.e. flow through valves,  $VP_i$ )

$P_{BD}$  : Blow down pressure ( $bar$ )

$P_{cond}$  : Pressure at which CO<sub>2</sub> condensation is carried out ( $bar$ )

The range for the decision variables is given in Table 2.

#### 5. Results and Discussion

Figure 4(a) shows the approximate Pareto front obtained after 60 generations. The product flow rate and blow down pressure had the most significant effect on the final Pareto front. The  $F_{pi}$  and  $P_{BD}$  values corresponding to the Pareto optimum objectives is shown in Figures 4(b) and 4(c). The obtained Pareto

front can be thought to consist of two separate regions, i.e. from a CO<sub>2</sub> capture rate of ~50 to ~70 % (Region 1) and ~70 to ~95 % (Region 2).

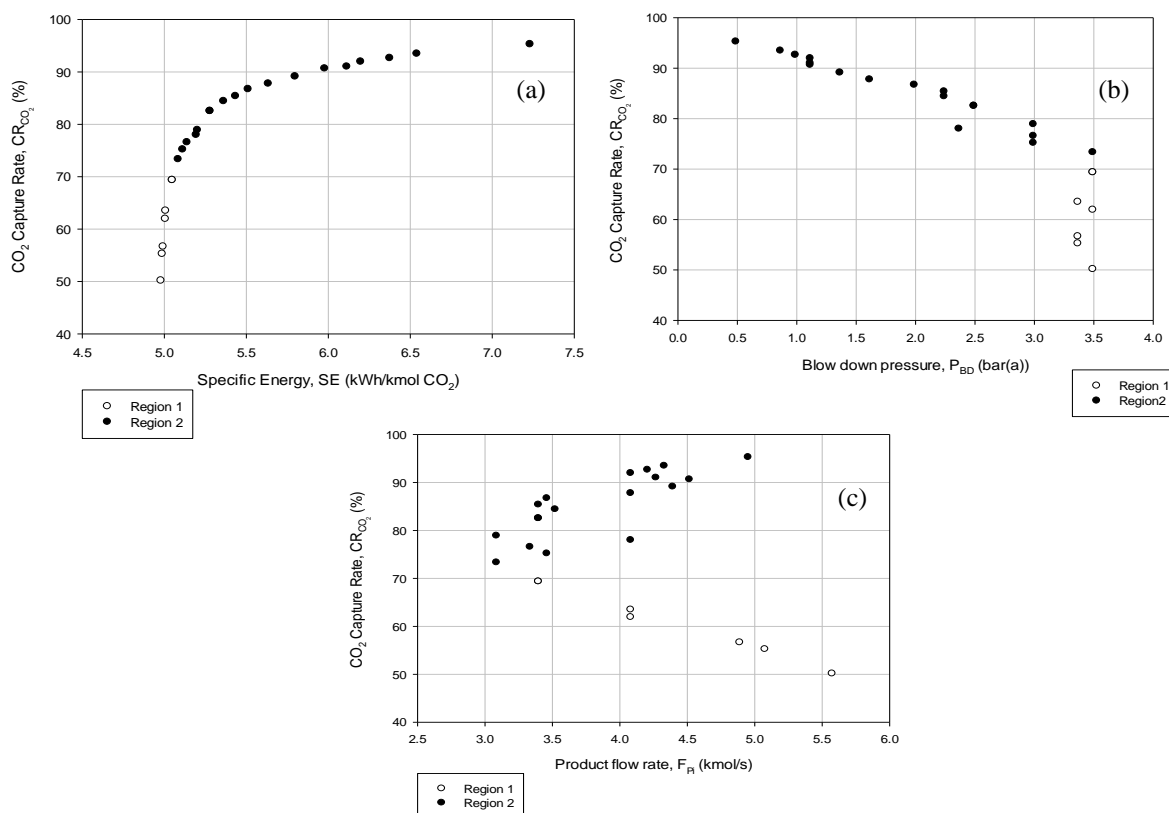


Figure 4: (a) Approximate Pareto front obtained after 60 generations of MOO run, (b) Product flow rate,  $F_{pi}$  (kmol/s), (c) Blow down pressure,  $P_{BD}$  (bar(a)) for the Pareto-optimal solutions depicted in (a)

The Pareto front in these two regions can be understood as follows:

Region 1:

In this region blow down pressure is approximately constant, as can be observed in Figure 4(b). The CO<sub>2</sub> capture rate, in this region, is increased by decreasing the product flow rate, thereby increasing the residence time of the syngas in the adsorber. This results in an increase in the extent of CO<sub>2</sub> adsorption thereby increasing the CO<sub>2</sub> capture rate at a constant blow down pressure.

Region 2:

In this region, the CO<sub>2</sub> capture rate cannot be further increased by decreasing product flow rate. Therefore, the blow down pressure needs to be lowered in order to desorb additional CO<sub>2</sub> from the adsorbent. Simultaneously, the product flow rate also needs to be increased as the working capacity of adsorbent has increased due to lowering in blow down pressure.

## 6. Conclusions

A generalised Aspen Adsorption<sup>TM</sup> and Microsoft Excel based MOO framework for optimisation of fixed bed adsorption processes has been proposed. The proposed framework has been demonstrated by optimising a PSA based Carbon Capture and Sequestration (CCS) unit for the removal of CO<sub>2</sub> from an entrained flow gasifier synthesis gas stream. A novel strategy has also been proposed to produce high purity CO<sub>2</sub> product stream for sequestration, which involves compression and partial condensation of the CO<sub>2</sub> rich stream produced from PSA system. This strategy also facilitates the pressurisation of CO<sub>2</sub> to supercritical conditions, required for sequestration. The PSA system has been successfully optimised against multiple process parameters.

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