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COMBINED FLUE GAS CLEANUP PROCESS FOR SIMULTANEOUS REMOVAL
OF SO_x, NO_x, AND CO₂—A TECHNO-ECONOMIC ANALYSIS

BY

AMIT NARENDRASING HAJARI

A THESIS

Presented to the Faculty of the Graduate School of the
MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

In Partial Fulfillment of the Requirements of the Degree
MASTER OF SCIENCE IN CHEMICAL ENGINEERING

2017

Approved by

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ABSTRACT

Flue gas cleanup often requires the removal of SO_x, NO_x and CO₂ in separate units before atmospheric emission. The step-wise treatment process currently in place incurs significant cost and energy penalty. A single-step adsorption process based on pressure swing adsorption (PSA) by which these impurities are removed is envisioned as an efficient means of flue gas cleanup that can be applied relatively easily. In this study, the technological and economic feasibility of a single-step separation process in which SO_x, NO_x and CO₂ are simultaneously removed from flue gas streams are assessed. Capital and operating costs are estimated based on sizing the equipment items and utilities needed and the potentials for increased energy efficiency are determined in relation to the required PSA performance. The energy saving potential for the adoption of 2-bed and 4-bed PSA cycle is compared to conventional FGD, SCR and CO₂ capture units needed to cleanup flue gas in a step-wise fashion. The results show that energy savings can be expected when the PSA removal efficiency is greater than 90%. In the case of a 550 MW coal-fired power plant, the energy savings can be as high as 30% depending on PSA removal efficiency and cycle time. This high value can be reached when the PSA cycle time is on the order of 2 min. Overall, the PSA process is expected to lower the cleanup costs for both retrofitted and new-build power plants. This techno-economic assessment shows that the integrated single-step system can be an attractive technology when compared to multi-step systems for the removal of flue gas impurities.

ACKNOWLEDGEMENTS

Firstly, I would like to express my sincere gratitude to my advisor Dr. Fateme Rezaei for the continuous support through my MS study and related research, for her patience, motivation, and immense knowledge. Her guidance has helped me during all of the time of research and writing of this thesis. I could not imagine having a better advisor and mentor for my work.

Secondly, I would like to thank the rest of my thesis committee: Dr. Ali Rownaghi and Dr. Glenn Morrison for their insightful comments and encouragement, as well as the hard questions which incited me to widen my research to various perspectives.

Additionally, I would thank my fellow lab mates for their continued support throughout my research, for the sleepless nights we were working together before deadlines, and for all the fun we have had in the last two years. Finally, I would like to thank my family supporting me spiritually throughout this journey.

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NOMENCLATURE**SYMBOL DESCRIPTION**

AD - Adsorption

PE - Pressure equalization

BD - Blow down to low pressure

PR - Purge with light product

F - Feed at high pressure

PE - Pressure equalization

BD - Blow down to low pressure

PR - Purge with light product

p - Pressure drop,

L - Height of the bed,

μ - Gas viscosity,

ϵ - Void space of the bed,

u_0 - Gas superficial velocity,

d_p - Particle diameter,

C_i - Gas phase concentration for component i ,

D_{Li} - Axial dispersion coefficient for component i ,

ρ - Density of gas,

- a_p - Particle external surface area to particle volume ratio ($=3/r_p$),
- C_{Vg} - Gas mixture heat capacity,
- C_{Ps} - Adsorbent particle heat capacity,
- H_s - Fluid/solid heat transfer coefficient,
- λ_g - Gas mixture thermal conductivity,
- λ_s - Solid phase thermal conductivity,
- P - Gas pressure,
- q_i - Amount adsorbed for component i ,
- q_i^{eq} - Equilibrium capacity for component i
- k_s - Mass transfer coefficient
- p_i - Partial pressure for component i ,
- b_i - Langmuir isotherm parameter
- t - Time,
- T_g - Gas temperature,
- T_s - Solid temperature,
- v_g - Superficial gas velocity,
- x - Axial distance coordinate,
- ΔH_i - Enthalpy of adsorption for component i , (heat of adsorption)

ϵ_b - Bed voidage (void fraction)

ϵ_t - Total voidage

ρ_g - Gas density,

ρ_b - Bed packing density,

1. INTRODUCTION

Flue gas from natural gas and coal power plants contain harmful gases which can cause serious environmental and health problems.¹ The major toxic components of flue gas emitted into the atmosphere during fossil fuel combustion are nitrogen, sulfur oxides (SO_x), nitrogen oxides (NO_x) and carbon dioxide (CO₂).² Many technologies and ideas have been proposed to capture these acidic gases. The current state of art technology for SO_x removal is flue gas desulfurization. NO_x is removed by selective catalytic reduction. Finally, CO₂ is removed by Amine scrubbing.³⁻⁹ Flue gas is the first process for SO_x removal in the FGD unit followed by NO_x removal in SCR unit. In the final step, CO₂ is removed in an absorber column and clean gas is released into the atmosphere. The complete process flow diagram is shown in Figure 1.1. These conventional processes are often multi-step and complex. Furthermore, they require large land space and high capital cost.^{4,10-14} Finally, these processes encounter a variety of operational problems.

Cleanup cost and removal efficiency of a process are the key factors to be considered for a power plant. However, state of the art technology incurs a high-energy penalty. One possibility to improve the efficiency and reduce the cleanup cost is to integrate two or more separation processes into a single-step process for the simultaneous removal of CO₂, SO_x, and NO_x from flue gas.

Among several alternative gas separation technologies, adsorptive removal is most efficient and has been identified as a potential alternative for the current state of the art technology due to its smaller environmental footprint and low cost incurred when compared to absorption and membrane separation technologies.^{2,6} Some common solid adsorbents include but are not limited calcium-based materials, zeolites, activated carbons,

metal oxides, metal-organic frameworks (MOFs) and organic-inorganic hybrid materials. These materials have been used successfully in many studies for adsorbing CO₂, SO₂ and NO_x. Unfortunately, most past studies primarily focus on single-component adsorption,^{15–22} and only a few studies have addressed the simultaneous removal of the aforementioned gases.^{23–27} The key factor for the proposed single-step cleanup process is the adsorbent material. The adsorbent should be effective in simultaneous removal of all acidic gases at without the loss of capacity. Among the various solid adsorbents investigated so far, Mg-MOF-74,^{28,29} K-NaX³⁰ and secondary amine-based solid adsorbents^{31,32} have been shown theoretically and experimentally to be promising candidates capable of removing the three aforementioned gases from the respective flue stream.

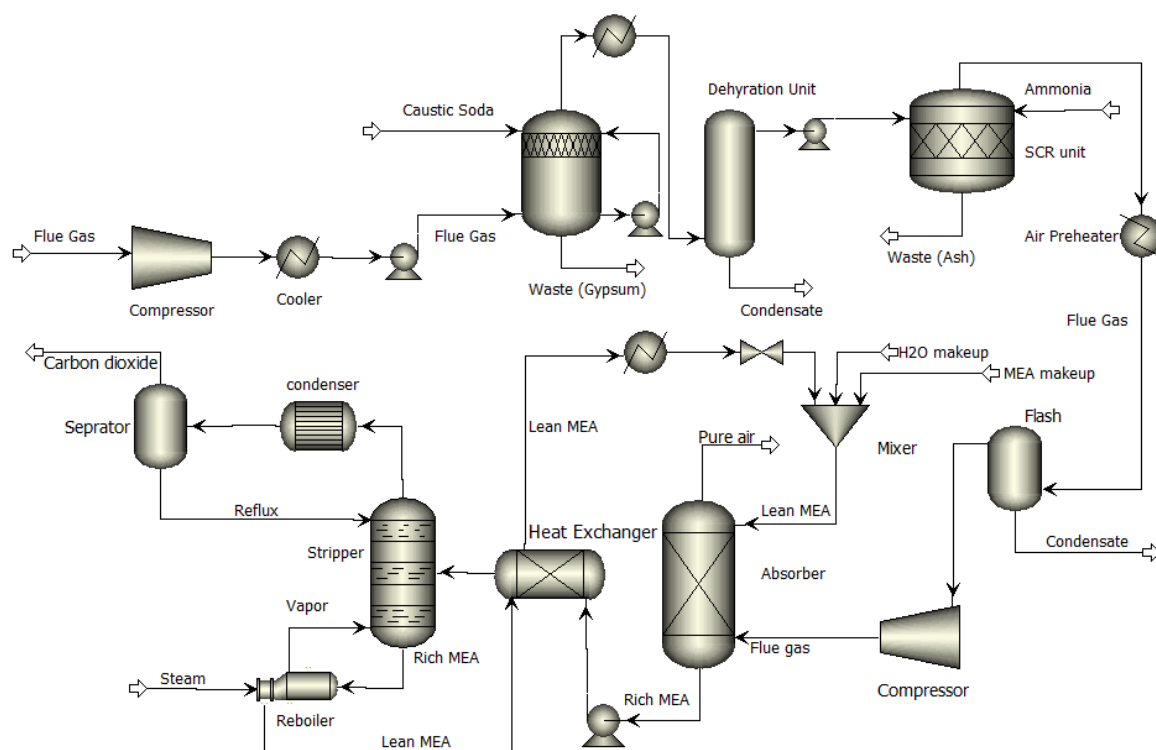


Figure 1.1: Process flow diagram of FGD, SCR and CO₂ capture units.

Therefore, such a conceptual design is not far from reality, with the advancement of materials science and development of highly efficient adsorbents with long-term stability. In this study, to evaluate the potential of the full-scale system, techno-economic analysis of a PSA system for CO₂/SO₂/NO_x removal from flue gas was developed and compared with current technologies to assess the potential implementation of the proposed system along with identifying the possible operational challenges. We have considered the specific energy and capital requirements associated with building and implementing the PSA system as well as the impact of different design choices. Based on energy balance equations and stream tables, an Aspen Plus flowsheet model has been generated to establish the technological and economic feasibility of the process. The parameters examined include adsorbent working capacities, overall capture efficiency, and process cycle. Additionally, the energy penalty of the system and its implications on retrofitted and new power plants has been determined. Often times, the biggest impediment to the implementation of lab-scale technologies on the commercial scale is correlating cost. This current study seeks to provide evidence that low-cost flue gas cleanup is possible with the use of single-step PSA system capable of simultaneously capturing CO₂, SO₂ and NO_x.

1.1. AMINE SCRUBBING-CO₂ REMOVAL

In the United States alone, approximately 300,000 MW of power, about 50% of the electricity requirement, is generated by coal fired power plants³³. These power plants contribute to approximately 30% of all CO₂ emissions. Typically, a flue gas contains 10-15% of CO₂³⁴, however, the concentration may vary according to the type of coal used in the power plant³⁵. A wide variety of technologies have been implemented for CO₂ capture. CO₂ removal by absorption and stripping with aqueous amine is a well-understood and

widely used technology. CO₂ is absorbed from the flue gas near ambient temperature into an aqueous solution of amine. Then CO₂ rich amine is regenerated in a stripper with the high-temperature stream (100-120°C)³⁶. Pure CO₂ is then compressed to 100-150 bar for sequestration^{37,38}.

Efficiency of CO₂ removal by amine scrubbing is around 60-65%, and it varies depending on the conditions³⁹. The reagent used in this process is cheap and readily available. Because of this, operating cost is low compared to other technology. However, stripping and regeneration of amine are complex processes and need a large capital investment. Along with this, the energy penalty is comparatively high. The cleanup cost for CO₂ using absorption technology is estimated to be \$53/ton of CO₂ removed⁴⁰. Detailed comparison is shown in result and discussion section (Table 5.2).

1.2. FLUE GAS DESULFURIZATION-SO_x REMOVAL

The flue gas derived from coal or natural gas fired powered plant contain sulfur dioxide as well. The amount of SO_x in flue gas varies according to the type of coal used in the power plant. The typical range of SO_x in flue gas varies from 200 ppm to 2000 ppm⁴¹. Various technologies are available for the removal of SO_x from flue gas. Every technology has its own advantages, disadvantages and removal efficiencies. Currently, the highest efficiency, above 90%, is achieved with wet scrubbing technology⁴². In wet scrubbing technology, the flue gas reacts with an aqueous slurry of adsorbent to produce calcium sulfite and carbon dioxide. Typically, the sorbent materials are limestone or lime. Limestone is inexpensive, however removal efficiencies for such systems are limited to approximately 60-90%. A Specially designed spray column is used for the reaction. To enhance the contact between the slurry and flue gas, different types of nozzles and injection

systems are designed and optimized. The advantages of using wet scrubbing technology are high removal efficiency, inexpensive and readily available reagents and reusable byproducts. Consequentially, the technology has some disadvantages including, high capital and operating costs, production of carbon dioxide, and a limitation on application of concentration greater than 2000 ppm.

The approximate capital cost for wet scrubbing technology varies from 100-250 \$/kW for a power plant greater than 400 MW capacity⁴³. The operating cost of the process varies according to the SO_x concentration in flue gas. On average SO_x cleanup cost has been estimated to be in the range of 200-500 \$/ ton of SO_x removed. The detailed analysis is mentioned in Table 5.1.

1.3. SELECTIVE CATALYTIC REDUCTION

Selective catalytic reduction is state of art technology used for removal of NO_x from the flue gas. SCR process chemically converts NO_x gases into nitrogen molecules and water molecules^{44,7,45}. For conversion, nitrogen base reagents such as urea or ammonia are injected into the reactor. Then, the flue gas reacts with the reagent at a particular temperature in the presence of catalyst and oxygen to convert NO_x gases into nitrogen and water molecules. The temperature, amount of reagent, catalyst and reactor design are the factors affecting NO_x removal efficiency. Advantages of using SCR technology are higher NO_x removal as compared to other processes, applicable to low NO_x concentration processes, low reaction temperature and no specific modification required. Unfortunately, there are also some disadvantages associated with SCR technology. These disadvantages include emission of unreacted ammonia (ammonia slip) and the requirement of large amounts of catalysts and reagents. Ultimately, this leads to an increase in capital cost and

operating cost for the process. Finally, this technology requires cleaning process downstream.

The approximate capital cost for SCR technology varies from 100-250 \$/kW⁴⁶ for a power plant with capacity greater than 400 MW. Additionally, the operating cost of the process varies accordingly with the NO_x concentration in the flue gas. Average NO_x cleanup costs have been estimated to be in the range of 3000-4000 \$/ ton of NO_x removed. The detailed analysis is mentioned in Table 5.1.

1.4 EPA STANDARDS

The Clean Air Act of 1970 enforces more stringent pollution control requirements on coal-fired power plants. Additionally, the act also accelerated the research on a “flue gas desulfurization unit”, or “scrubber.” Rather than trying to remove sulfur from coal before it was burned by washing it, which had little effect, scrubbers aimed at the “back end” of a power plant, trying to remove sulfur in the form of sulfur dioxide (or SO₂) from the flue gas exiting a coal boiler.

In 1977 a new Clean Air Act mandated that all new coal-fired power plants install scrubbers⁴⁷. In 2009, the EPA proposed new limits on sulfur dioxide emissions. The old limits measured sulfur dioxide concentration averages over 24-hour and one-year periods. The new rule would require one-hour measurements, such that a spike of emissions above a new limit between 50 and 100 parts per billion in one hour would no longer be acceptable⁴⁸. The NO_x emission limit for new electric utility steam generating units is 130 ng/J (1.0 lb NO_x/MWh) gross energy output regardless of the type of fuel burned in the unit. Compliance with this emission limit is determined on a 30-day rolling basis⁴⁸.

2. OBJECTIVES

The main objectives of this research work are

Objective 1: To design single step flue gas cleanup process for simultaneous removal of SO_x , NO_x and CO_2 from flue gas.

Objective 2: To optimize the process for removal efficiency of SO_x , NO_x and CO_2 greater than 90%.

Objective 3: To analyze the process economics, to calculate CAPEX (capital cost) and OPEX (operating cost)

Objective 4: To compare single step flue gas cleanup process with standard state of art technology in perspective of removal efficiency, cleanup cost and energy penalty.

Objective 5: To conduct sensitivity analysis for the best operating condition and cleanup cost by varying adsorption pressure, cycle time, purge flow rate and working capacity.

3. METHODOLOGY

3.1 SINGLE-STEP FLUE GAS CLEANUP PROCESS CONFIGURATION AND SIMULATION

The single step flue gas cleanup process that removes SO_x , NO_x , and CO_2 simultaneously is introduced and the schematic is shown in Figure 3.1. The process contains several components, such as a compressor, heat exchanger, flash separator, gas turbine and PSA unit. The PSA unit also contains an adsorption bed, desorption bed and a set of control valves. After removing the $\text{CO}_2/\text{SO}_x/\text{NO}_x$ impurities from flue gas, the concentrated stream is passed to the post-treatment process.

The concentrated stream of flue gas is used to produce the chemicals which have high value in the market, such as H_2SO_4 ⁴⁹ and HNO_3 ⁵⁰. The post-treatment method contains the scrubbing of SO_x and NO_x from concentrated stream of gas, enhances oil recovery and photo-bioreactor. The stream of $\text{CO}_2/\text{SO}_x/\text{NO}_x$ is first passed through water tank to scrub SO_x and NO_x from the flue gas. During this step, adsorbed acid gases (SO_x and NO_x) react with water to form corresponding acids such as, H_2SO_4 , H_2SO_3 , HNO_3 and HNO_2 . As CO_2 does not react with water at normal conditions, it proceeds without any chemical changes. In this manner, the acid gases are separated from the concentrated stream of gases. The next step is the utilization of the concentrated stream of CO_2 . There are some technologies which require a high concentration of CO_2 , such as, Photo-bioreactor and enhance oil recovery. First, the CO_2 stream is passed through the dryer to remove its water content and then it is fed to the photo-bioreactor to convert CO_2 into chemicals by algae⁵¹. Another use of the CO_2 stream is to enhance oil recovery (EOR)^{50,52}. During this process, a concentrated stream of CO_2 is compressed to high pressure (100-150 bar). Compressed

CO₂ is then injected into an oil well to recover more oil which leads to an increase in oil recovery of 20-40%.

The proposed post treatment that includes SO_x and NO_x scrubbing, photobioreactor and enhance oil recovery has little effect on the currently proposed process. Because of this, the techno-economic analysis study is mainly focused on compressor, heat exchanger and PSA unit.

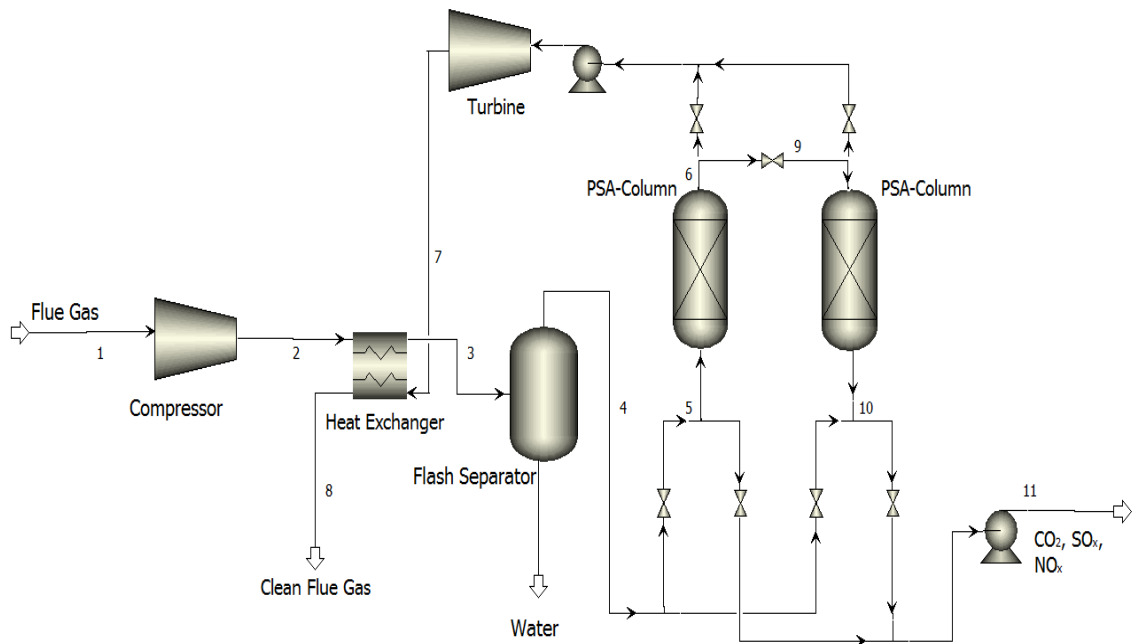


Figure 3.1: Schematic diagram of two-bed PSA system for flue gas cleanup.

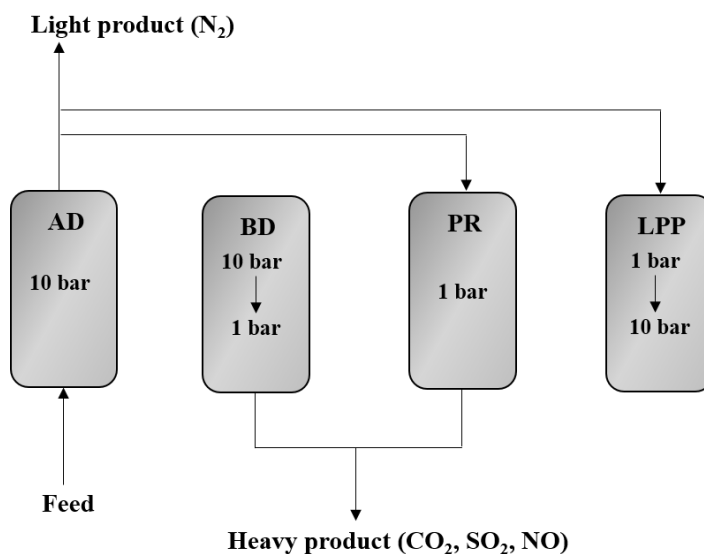
3.1.1 Process Description. The proposed process in this study is shown in Figure 3.1. First, the flue gas recovered from the coal powered power plant at 1 bar and 110⁰C is feed into the system at 670m³/s. The gas then passes through the compressor which

increases the pressure from 1 to 10 bar. As the gas is compressed to high pressure, the temperature of the flue gas increases to 365⁰C. Secondly, the gas is passed through a shell and tube heat exchanger where it is cooled from 365⁰C to the adsorption temperature of 35⁰C. The flue gas contains 7% of water vapor. To remove the water from the flue gas, the gas is processed in flash separator in step 3 for dehydration. At the end of the third step, the flue gas is completely dehydrated at 10 bar and 35⁰C. Under high-pressure conditions, the toxic components in the gas stream are captured by the adsorbent material. Afterword, the clean flue gas, mainly N₂ and O₂, leaves from the top (5→6). The clean flue gas is then sent to a heat exchanger to cool down before atmospheric emission (7→8). After the adsorption step, the bed is depressurized from the bottom (9→10). The desorbed gas during the purge step is collected from the bottom and sent to the post-treatment unit. The conventional two-bed, four-step design with cycle configuration, shown in Figure 3.1, is considered here to demonstrate the economic feasibility of using a pressure swing adsorption for simultaneous flue gas cleanup. Additionally, other complex and advanced cycle designs are possible to enhance the efficiency of the process. To demonstrate this, a 4-bed, 6-step cycle design was also considered and compared with the base case of the two-bed, 4-step cycle. The cycle configuration is shown in Figure 3.2 and Figure 3.3.

3.1.2 Cycle Configuration. The PSA cycle is a crucial factor in perspective of purity recovery and throughput. In the next section, 2-bed and 4-bed PSA cycle configurations are explained with figures.

3.1.2.1 2-Bed configuration. The two-bed PSA cycle configuration considered here consists of 4-steps cycle with a duration of 400 s. The scheme and time schedule of this conventional PSA cycle is presented in Figure 3.2. The four steps are adsorption (AD)

at high-pressure (10 bar), countercurrent blowdown (BD) from 10 to 1 bar, countercurrent purge with the light product (PR) at low pressure (1 bar), and finally repressurization with light product (N_2) from 1 to 10 bar.

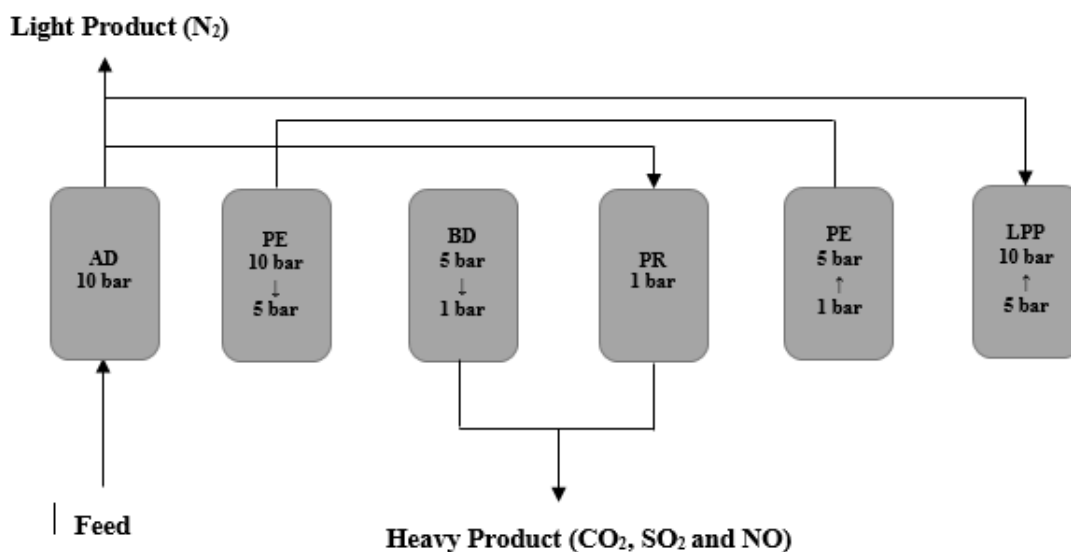


Bed 1	AD			BD	PR	LPP
Bed 1	BD	PR	LPP	AD		
	70 s	60 s	70 s	200 s		

Figure 3.2: Cycle scheme and time schedule for a 2-bed, 4-step PSA process.

3.1.2.2 4-Bed configuration. The 4-bed PSA cycle configuration considered here consists of 6-steps with a cycle duration of 400 s. The scheme and time schedule of this conventional PSA cycle is presented in Figure 3.3. The six steps are adsorption (AD) at high pressure (10 bar), pressure equalization (PE) from 10 to 5 bar, countercurrent

blowdown (BD) from 5 bar to 1 bar, countercurrent purge at 1 bar, pressure equalization (PE) from 1 to 5 bar, and finally repressurization from 5 to 10 bar.



Bed 1	AD			PE	PE	I	BD	PR	PE	PE	LPP
Bed 2	PE	PE	LPP	AD			PE	PE	I	BD	PR
Bed 3	BD	PR		PE			AD			PE	
Bed 4	PE	PE	I	BD	PR	PE	PE	LPP	AD		
Time	40	40	20	40	40	20	200 s				

Figure 3.3: Cycle scheme and time schedule for a 4-bed, 6-step PSA process.

3.1.3 Process Simulation. The process design calculations for this study were performed using Aspen Plus 8.6 software (Aspen dynamic), a commercial process simulator, coupled with an Aspen Adsim code for dynamic simulation of the PSA process. The explicit details are mentioned in the modeling tool and assumption section. The PSA

simulation was based on centered finite difference analysis. Finally, the thermodynamic method used in the model was based on Peng-Robinson equation of state (PR-EOS). Table 3.1 summarizes the process conditions used in the simulation obtained from a typical 550 MW coal-fired power plant.

Table 3.1: Flue gas feed stream conditions and composition

Target net power plant size (MW)	550
Volumetric flow rate (m ³ /h)	2.4×10 ⁶
Temperature (°C)	110
Pressure (kPa)	101.3
Removal efficiency (%)	90
Composition	
N ₂ (vol%)	75
CO ₂ (vol%)	13
O ₂ (vol%)	5
H ₂ O (vol%)	7
SO _x (ppm)	2000
NO _x (ppm)	2000

The system parameters and adsorbent properties for the PSA process are summarized in Table 3.2. Initially, a base pressure of 10 and 1 bar was assumed for the adsorption and desorption steps with a cycle time of 400 s. Also, a sensitivity analysis was

employed later to show the impacts of these parameters on the system economics. For our base case (Table 3.2), Mg-MOF 74 was considered for the selection of acidic gas impurities in the flue gas based on recent studies indicating that Mg-MOF-74 is a promising material for simultaneous CO₂, SO₂, NO_x removal.^{28,53} This material was demonstrated to show adsorption capacities of 7.95, 12 and 0.6 mmol/g for CO₂, SO₂ and NO, respectively at 25 °C and 1 atm. Additionally, the working capacities of the selected adsorbent were subject to sensitivity analysis to investigate their effect on the economic and technical performance of the process. Furthermore the PSA adsorber volume was estimated to be 92 m³ by taking into account a flue gas volumetric flow rate of 670 m³/s, a packing density of 75%, and a capture rate of 90%.

Table 3.2: System model parameters for 2-bed, 4-step PSA process analysis

PSA cycle	4-step cycle
Cycle time (s)	400
Adsorption pressure (bar)	10
Desorption pressure (bar)	1
Bed porosity	0.4
Purge flow rate (mol/s)	100
Adsorbent bulk density (kg/m ³)	960
Adsorbent porosity	0.4
CO ₂ , SO ₂ , NO working capacity (mol/kg)	6.3, 0.8, 0.8
Adsorbent particle diameter (cm)	0.75

3.2 PROCESS ECONOMIC ANALYSIS

3.2.1 Capital Cost Estimation. The capital cost of the combined flue gas cleanup process was determined using the module costing technique. This method relates the global cost to the purchase cost of the major units evaluated under base conditions.⁵⁴ The additional direct and indirect costs, such as instrumentation, piping foundations, construction overheads, and auxiliary facilities, are also incorporated into the total module cost. Based on this analysis, the bare cost of each module is estimated using

$$C_{BM} = C_p^0 F_{BM} \quad (1)$$

where C_p^0 and F_{BM} are, respectively, reference equipment cost and equipment unit bare module cost factor. The reference equipment cost was adjusted to the price level of 2015 using the chemical engineering plant cost index (CEPCI) with the value of 547.4 compared to 382 in 1996.⁵⁵ It should also be noted that the capital cost estimations are based on the assumption of the construction of a new plant, grassroots design, which can be broken into the following contributions. Total bare module cost, $\sum_i C_{BM,i}$, is the sum of the capital and installation costs of main equipment items. The contingency costs, C_C , include unexpected expenses related to the data cost uncertainty and flowsheet completeness and estimated at 15% of the total bare module cost ($C_C = 0.15 \sum_i C_{BM,i}$).^{45,56} The auxiliary facility costs, C_{AF} , take into account structures, services, and equipment not directly involved in the process⁵⁷ such as land purchase, utility systems, off-sites, and site development.^{57,58} There are two main classifications of auxiliaries, utilities, and services. For this study, they were assumed to be 35% of the total bare module cost ($C_{AF} = 0.35 \sum_i C_{BM,i}$). Total module cost,

C_{TM} , is computed using equation 2. Additionally, the overall grassroots cost was obtained by equation 3.

$$C_{TM} = \sum_i C_{BM,i} + C_C \quad (2)$$

$$C_{GR} = C_{TM} + C_{AF} \quad (3)$$

The time required for the construction of the plant was assumed to be 2 years with a finance distribution of 60% in the first year and 40% in the second year.

3.2.2 O&M Cost Estimation. Operation and maintenance, O&M, costs are typically estimated by considering all the expenses associated with manufacturing, labor, insurance and consumables. The O&M costs are broadly divided into two major categories, namely variable and fixed costs. Variable or direct costs consist of cost of consumables including raw materials (C_{RM}), utility costs (C_{UT}), operating labor fees (C_{OL}), and maintenance and repairs. In contrast, fixed or indirect O&M costs, include local taxes, insurances, storage, and plant overhead costs. Local taxes and insurances were taken as 3.2% of fixed capital cost (C_{GR}),⁵⁸ Plant overhead costs were taken to be 70.8% of operating labor cost plus 3.6% of fixed capital cost to cover the costs associated with operating auxiliary facilities that support the manufacturing process.⁵⁸ Maintenance and repair costs, which account for the costs of labor and materials associated with maintenance and repair, were assumed to be 6% of fixed capital cost. The total O&M costs are given by equation 4.

$$C_{O\&M} = C_{RM} + C_{UT} + C_{OL} + 0.13C_{GR} \quad (4)$$

The C_{RM} was estimated from the current prices listed in the chemical market report. The amount of adsorbent required per cycle was estimated from process material balance. The C_{UT} includes the costs of major utility such as electricity and cooling water. The utility requirement was obtained from simulation data. The Ulrich technique was used for

estimating the C_O .⁵⁴ According to this method, C_{OL} depends on the number of both the processing units (N_{np}) and operators (N_{op}) per shift. Assuming an annual operating salary of \$56,000 and three shifts per day, the C_{OL} can be calculated using equation 5.

$$C_{OL} = \$56,000 \times N_{op} (6.29 + 0.23N_{np}) \quad (5)$$

The overall plant cost (C_{OP}) was calculated by summing the total capital (C_{TC}) and O&M ($C_{O\&M}$) costs. The C_{TC} was given by $C_{TC} = C_{GR} + C_{land} + C_{work}$ where C_{land} and C_{work} are respectively, land cost (\$500,000) and working capital estimated as $C_{work} = 0.1(C_{GR} + C_{RM} + C_{OL})$. All assumptions used in the cost estimation are summarized in Table 3.3. The costs estimations were done using CAPCOST software.⁵⁸ Moreover, the cost of impurities capture was estimated using equation 6.

$$\text{Cost of cleanup} = \frac{C_{OP}}{CO_2/SO_2/NO_x \text{ avoided}} \quad (6)$$

Table 3.3: Assumptions for capital and O&M costs estimation

Base year	2015
Construction time period	2 years
Finance distribution	0.6 in first and 0.4 in second year
Cost estimation	Module costing technique
Contingency	15% of C_{BM}
Auxiliary facility costs	35% of C_{BM}
Operating hours	365 day \times 24 h
Electricity price	\$16.8/GJ

Table 3.3: Assumptions for capital and O&M costs estimation (cont)

Cooling water price	\$4.43/GJ
Adsorbent cost	\$20/kg
Maintenances and repair	6% of C_{GR}
Insurances	3.2% of C_{GR}
Operator wage	\$56,000/year
No of operating labor	8

4. MODELING TOOLS AND ASSUMPTIONS

4.1. ASPEN ADSIM

Aspen adsim is a process simulation software which deals with process modeling of adsorption and adsorptive reactions. It deals with a wide range of simulation and optimization processes involving industrial gas and liquid adsorption including reactive adsorption, ion exchange, and cyclic processes. Complete pressure swing adsorption modeling, vacuum swing adsorption modeling, and temperature swing adsorption modeling can be simulated and optimized for better configuration and performances.

Aspen adsim has a number of options to choose from for various bed configurations including vertical bed, horizontal bed, and radial bed designs. It also includes axial dispersion, kinetics of reactions, isotherm fitting, energy balance and adsorptive reactions for more detailed modeling. Aspen adsim allows the customization and design of our own cycle configuration by allowing control with time as well as the adsorption bed condition.

4.2. MODEL ASSUMPTIONS

4.2.1. Adsorption Bed. In this study, 1-dimensional axial distribution is considered for its mass and the energy transport in the bed. Also, the mass and energy transport between gas phase and the adsorbent material, including the momentum balance in the bed which depends on the mass flow rate, is described. This model has an interface with different tabs including the design, fluid, wall, the isotherm, numeric and dynamics which allows the user to specify different parameters. This model comprises of several equations which are described below-

4.2.2. Mass Balance. The Convection with Constant Dispersion option is assumed. The dispersion coefficient is constant for all components throughout the bed. The

dispersion coefficient value is obtained by matching experimental result with the simulation result in the breakthrough experiment. The pressure differential is the driving force in the PSA column.

Material Balance (Convection with constant dispersion):

$$D_{Li}\varepsilon_b \frac{\partial^2 c_i}{\partial x^2} + \frac{\partial(v_g c_i)}{\partial x} + \varepsilon_i \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial q_i}{\partial t} = 0 \quad (7)$$

The mass balance for the adsorbed phase is given by:

$$\frac{\partial q_i}{\partial t} = ks(q_i^{eq} - q_i) \quad (8)$$

4.2.3. Energy Balance. The complete process is considered as non-isothermal. The heat of adsorption, heat capacity of gas, as well as material, heat transfer between material, gas and with the environment, are considered in this model. The equation is described as below:

Gas Phase:

$$-\lambda_g \varepsilon_b \frac{\partial^2 T_g}{\partial x^2} + C_{Vg} v_g \rho_g \frac{\partial T_g}{\partial x} + P \frac{\partial v_g}{\partial x} + C_{Vg} \varepsilon_t \rho_g \frac{\partial T_g}{\partial t} + H_s a_p (T_g - T_s) = 0 \quad (9)$$

Solid Phase:

$$-\lambda_s \frac{\partial^2 T_s}{\partial x^2} + C_{Ps} \rho_b \frac{\partial T_s}{\partial t} + \rho_P \sum_i \left(\Delta H_i \frac{\partial q_i}{\partial t} \right) - H_s a_p (T_g - T_s) = 0 \quad (10)$$

4.2.4. Momentum Balance. The static pressure drop is determined from the Ergun equation. The Ergun equation is valid in turbulent flow as well as laminar flow. The equation used in modeling is described as follows:

$$\frac{\Delta p}{L} = \frac{150\mu(1-\varepsilon_b)^2 v_g}{\varepsilon_b^3 d_p^2} + \frac{1.75(1-\varepsilon_b)\rho v_g^2}{\varepsilon_b^3 d_p} \quad (11)$$

4.2.5. Isotherm Model. In this process, simultaneous adsorptions of CO₂, SO_x, NO_x are considered. Adsorption of one gas will directly impact the adsorption capacity of the other material. As the process is non-isothermal, the effect of temperature change must be considered. To address this problem, temperature dependent Extended Langmuir isotherm is considered. The equation used in modeling is as follows:

Extended Langmuir Models (Temperature dependent):

$$q_i = \frac{q^{eq} b_i p_i}{1 + \sum_1^j b_i p_i} \quad (12)$$

5. RESULTS AND DISCUSSION

5.1 TECHNO-ECONOMIC EVALUATION

The suitability of the single-step flue gas cleanup process for a 550 MW power plant in terms of energy cost and capture efficiency is discussed below. For our base case, the capital cost components corresponding to each equipment are listed in Table 5.1. It was assumed that the equipment units were made of Nickel, to prevent corrosion from the SO_x/NO_x gases. The results show that the major portion of the capital cost comes from the flue gas compressor that is required to pressurize the feed to 10 bar. This cost makes up about 84% of the C_{GR} whereas, the cost of PSA adsorbers is only 9% of the C_{GR}. Thusly, a noticeable reduction in cleanup costs is observed.

Table 5.1: Capital cost data for major components in M\$ for the base case.

Equipment	Scaling parameter	C_{BM}	C_C	C_{AF}	C_{TM}	C_{GR}
Flue gas compressor	Pressure	66.23	9.93	23.18	76.16	99.35
Heat exchanger	Energy	0.42	0.06	0.15	0.48	0.63
Flash separator	Volume	5.36	0.80	1.88	6.16	8.04
Adsorption columns	Volume	6.75	1.01	2.36	7.76	10.13
Centrifugal pumps	Power	0.45	0.07	0.16	0.52	0.68

The techno-economic analysis of the single-step cleanup process for two-bed and four-bed PSA design configurations along with conventional FGD, SCR, and amine scrubbing as separate units are reported in Table 5.2. The cleanup cost using the proposed single-step process is \$56/ton of combined impurities avoided (CO_2 , SO_2 , NO). This will incur a 24% energy penalty to the power plant. In comparison, the published results suggest that for a typical 550 MW coal-fired power plant, a SO_2 removal cost of up to \$350/ton will be incurred for a \$400/kW FGD capital cost.^{40,59} Similarly, the retrofit of a SCR unit will incur \$300/kW capital cost and will expend about \$2000/ton to remove NO_x .^{40,59} Furthermore, the retrofit of a CO_2 capture unit based on the bench mark amine scrubbing technique with a removal rate of 90% will incur an operating cost of \$53/ton of CO_2 removal.^{60,61} Notably, the high cleanup cost of SCR and FGD units can be justified considering the low concentration of SO_x/NO_x gases in the flue gas in comparison with CO_2 . Furthermore, due to the high cost of ammonia and catalysts used in SCR process, the capture cost per ton of NO_x is much higher than that of SO_x with comparable concentrations.

The economic results for the 2-bed and 4-bed PSA systems are shown in Figure 5.1a-b and Figure 5.2 a-b. As evident from these figures, C_{TC} represents approximately 57% of C_{OP} which is M\$117.6 for 2-bed and M\$118.8 for the 4-bed PSA system. The results show that adding two additional beds to improve the capture performance of the combined process increases the C_{OP} only marginally. The breakdown of the $C_{\text{O\&M}}$ presented in Figure 5.1a reveals that the C_{UT} contributes to 81.4% of the $C_{\text{O\&M}}$ followed by maintenance and repair costs, plant overhead costs, tax and insurance, C_{RM} , and C_{OL} with 4.2, 8.0, 5.2, 4.2,

0.7, and 0.5% contributions to $C_{O\&M}$. As shown in Figure 5.1b for the 2-bed PSA system, the C_{TC} and $C_{O\&M}$ account for 60 and 40% of the overall plant cost (C_{OP}).

Table 5.2: Economic results for combined proposed process and comparison with individual unit operations.

	Recovery rate (%)	C_{TC} (M\$)	$C_{O\&M}$ (M\$)	Energy penalty (%)	Cleanup cost (\$/ton)	Year
2-bed PSA	>91 ^a	129.5	88.1	24	56	2015
4-bed PSA	90 ^b	138.2	88.3	24	59	2015
MEA scrubbing⁶²	90	-	-	30	53	2013
FGD²	90	96.2	2.7		350	2001
SCR²	90	0.6	1.65×10^{-2}		3500	1999

^a $CO_2/SO_2/NO$: 93/92/91 ^b $CO_2/SO_2/NO$: 90/90/90

5.2 SENSITIVITY ANALYSIS

5.2.1. 2-Bed System. Sensitivity analysis was performed on the 2-bed system in order to assess the effects of uncertainties in several key factors such as adsorption pressure, PSA cycle time, purge flow rate, and adsorbent working capacities on technological and economic performance of the single-step cleanup process with respect to recovery and cleanup cost of the impurity gases. For our sensitivity analyses, purity was not considered as a metric because of dealing with three impure gases instead of one.

5.2.1.1 Effect of adsorption pressure. Adsorption pressure is a crucial factor that affects purity, recovery and capture cost. The effect of adsorption pressure on capture cost

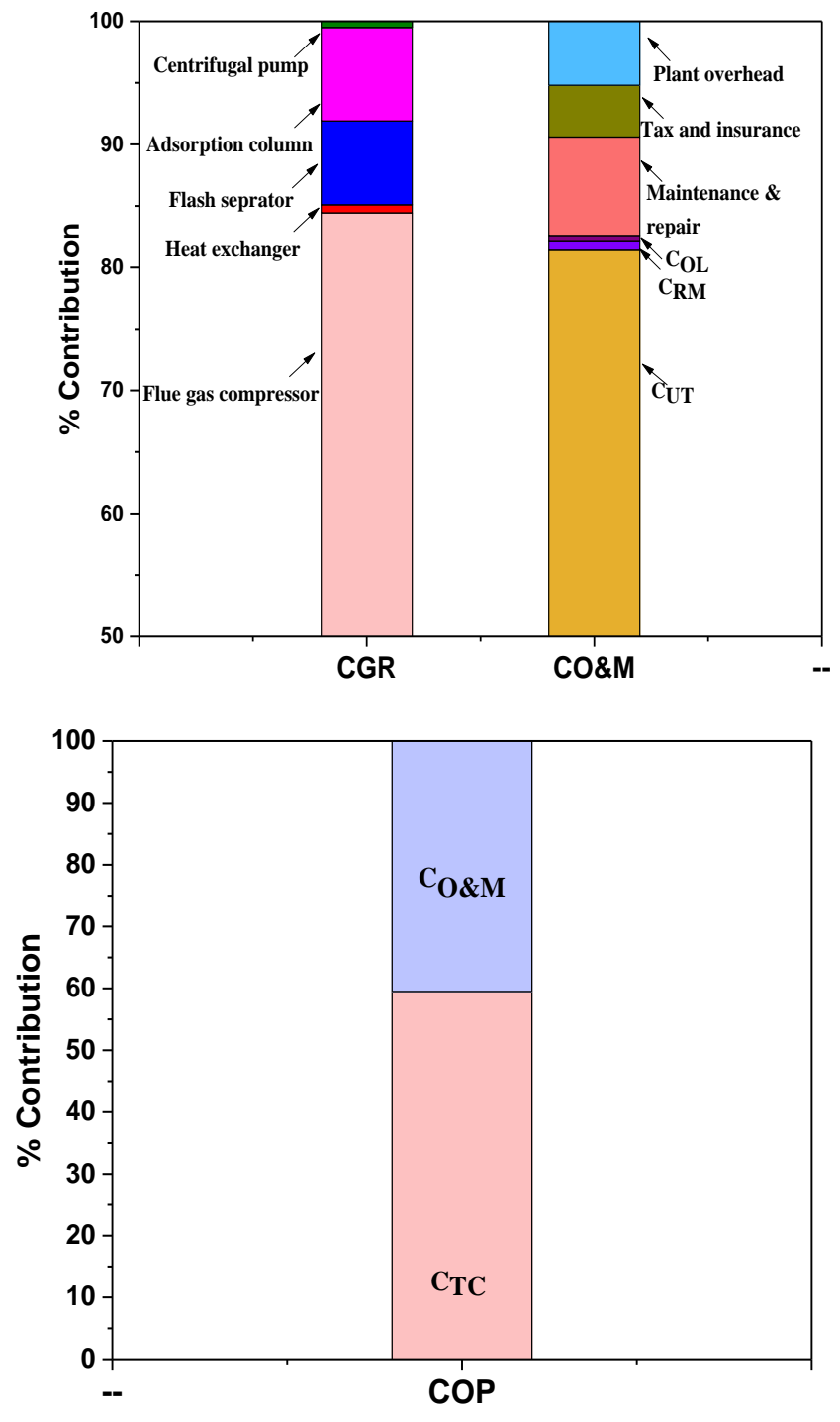


Figure 5.1: Economic analysis (a) Capital and O&M costs and (b) the overall plant cost of the 2-bed PSA process.

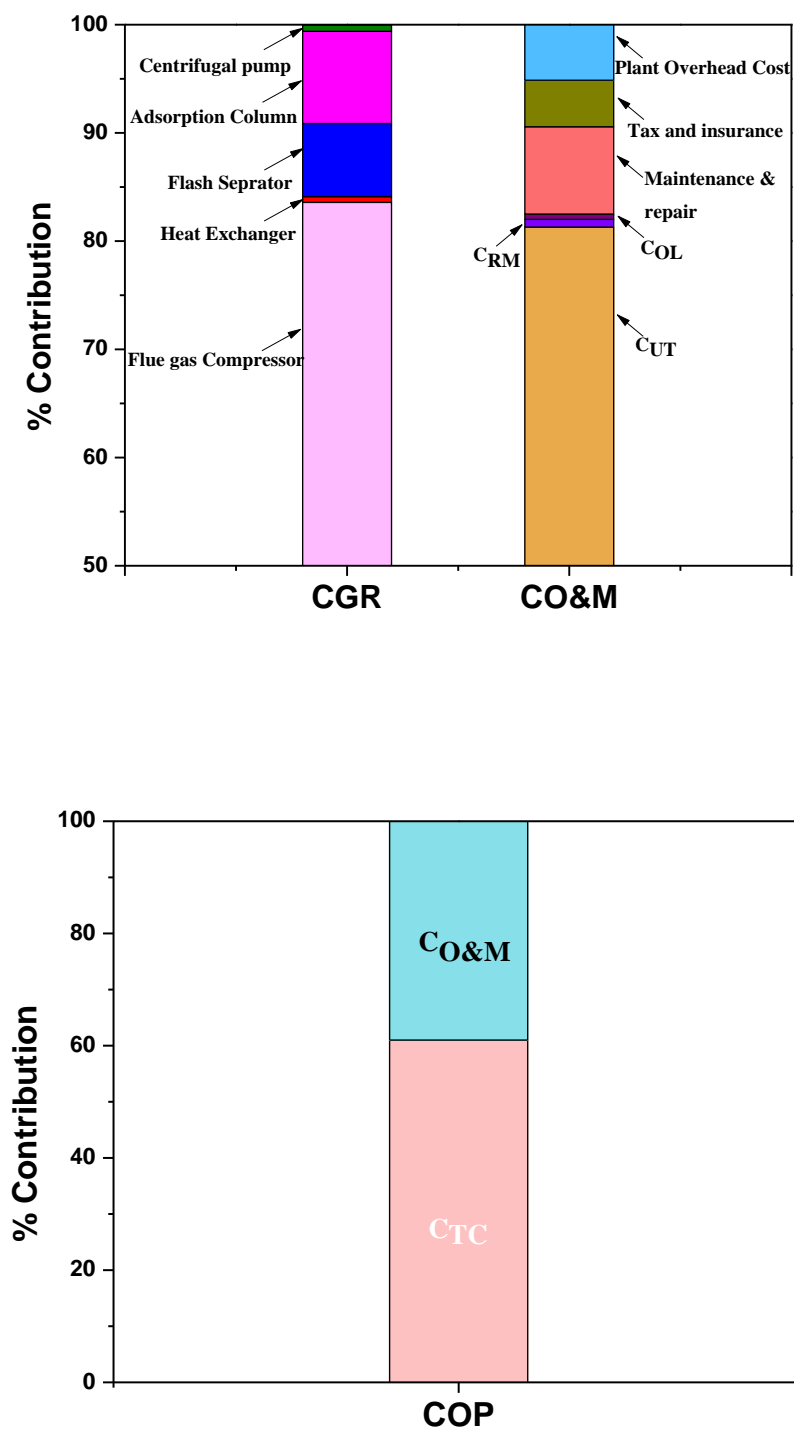


Figure 5.2: Economic analysis (a) Capital and O&M costs and (b) the overall plant cost of the 4-bed PSA process.

and recovery is shown in Figure 5.3 and its effect on throughput and purity is shown in Figure 5.4 using the pressure conditions of 5, 10, and 15. At 5 bar, the recovery of $\text{CO}_2/\text{SO}_x/\text{NO}_x$ is 55/56/55, and the cleanup cost is \$66 / ton of impurity. As pressure increases, gas recovery also increases. At 10 and 15 bar, material recovery increases to ($\text{CO}_2/\text{SO}_x/\text{NO}_x$) 93/92/92 and 96/95/95 while capture cost is \$57/ton of impurity for 10 bar and \$70/ton of impurity for 15 bar. Demonstrated in equation 6, capture cost depends on both capital cost as well as gaseous recovery. As adsorption pressure increases from 5 to 10 bar, the overall recovery of all three gases and capital cost is increases by approximately 70% and 45% respectively. Additionally, the resulting capture cost is reduced by \$9/ton of impurity. Reduction of capture cost can be attributed to the increased recovery of gases imparted by the pressure increase. Furthermore, when the adsorption to desorption ratio is high, more gases are recovered. Finally, the opposite trend is observed when pressure is increased from 10 bar to 15 bar.

In conclusion, the recovery of gases is increases along however, this causes the capital cost to increase drastically. Eventually, the capture cost will also increase. From the above discussion, it can be concluded that the capture cost is traded between the capital cost and recovery of gases. To combat this, an optimized adsorption pressure should be used for the lowest possible capture cost.

5.2.1.2 Effect of cycle time. The effect of cycle time on recovery and capture cost is shown in Figure 5.5. When cycle time was increases from 200 to 400 seconds, the recovery of gases ($\text{CO}_2/\text{SO}_x/\text{NO}_x$) also increases. However, when cycle time is changed from 400 to 600 seconds, the gaseous recovery is reduced.

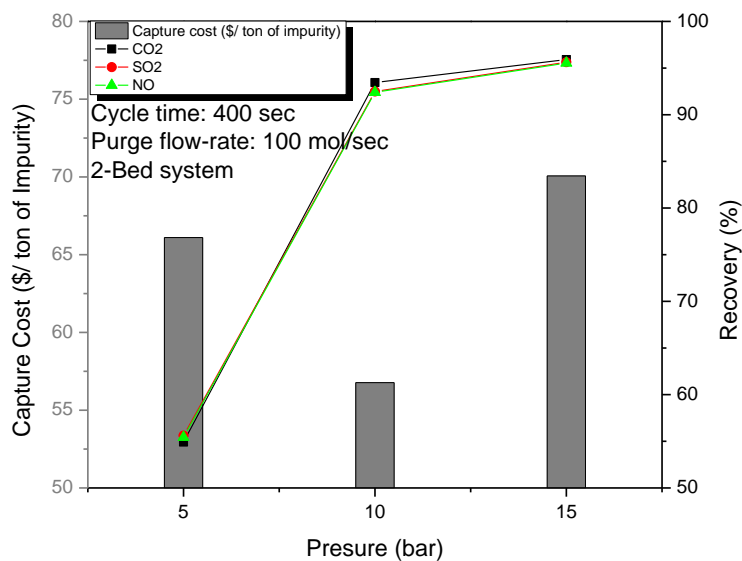


Figure 5.3: Effect of adsorption pressure on recovery and cleanup cost of the 2-bed PSA system.

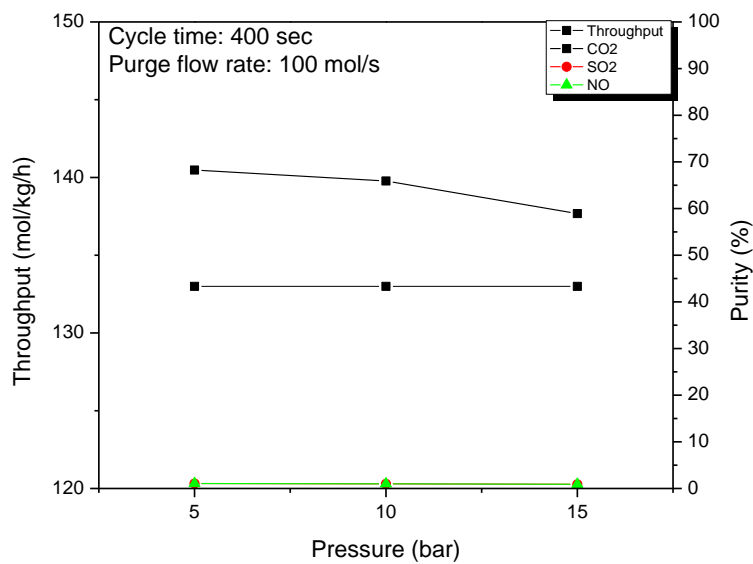


Figure 5.4: Effect of adsorption pressure on throughput and purity of the 2-bed PSA system.

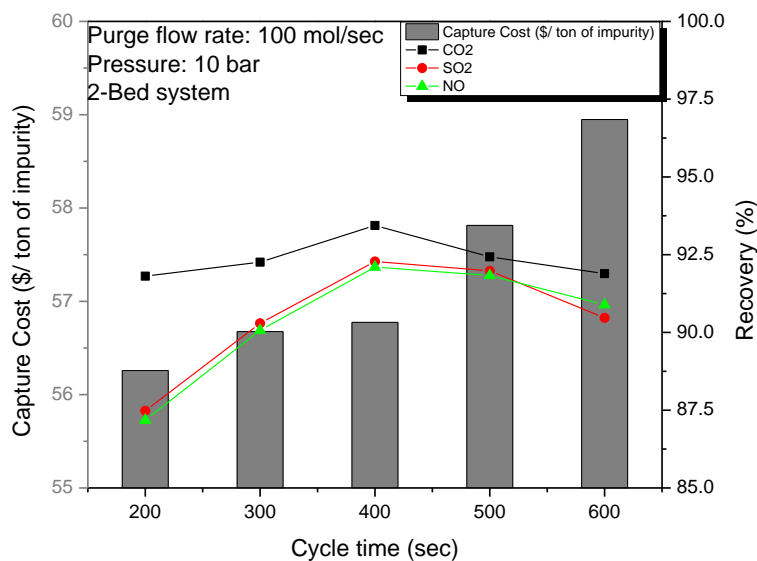


Figure 5.5: Effect of cycle time on recovery and cleanup cost of the 2-bed PSA system.

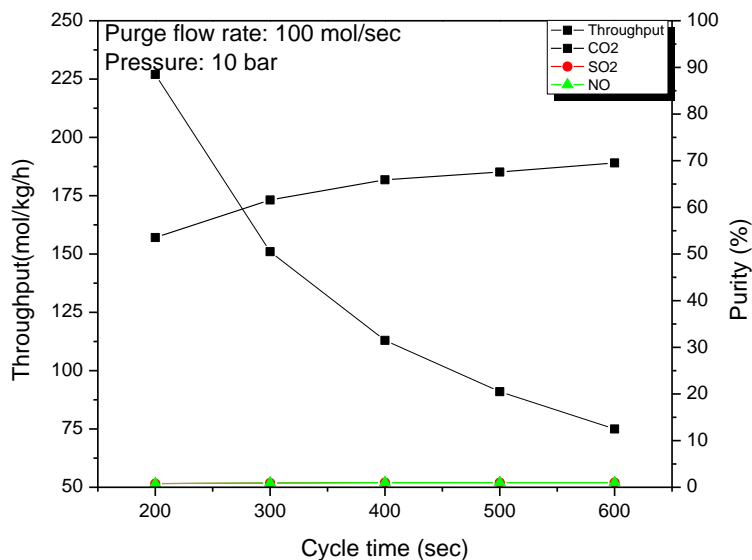


Figure 5.6: Effect of cycle time on throughput and purity of the 2-bed PSA system.

Cycle time directly affects the bed size and amount of adsorbent. As the cycle time changes, three times, from 200 to 600 seconds, the bed size and amount of adsorbent also

increases by a multiple of three. In turn, the capture cost increases along with the cycle time. The entire system is designed according to 400 seconds, and because of that, the highest recovery is observed at 400 seconds with a capture cost of \$57/ ton of impurity. The effect of cycle time on throughput and purity is shown in Figure 5.6. As cycle time increases, purity increases while throughput decreased. As the cycle time increased from 200 to 600 seconds, a smaller amount of material is processed, and for that reason, the overall purity is increased. Overall, the process gives a maximized purity result at 400 seconds.

5.2.1.3 Effect of purge flow rate. The recovery and capture cost relating to the change of purge flow rate are shown in Figure 5.7. The purge flow rate value is changed above and below the base condition given in Table 3.2. When the purge flow rate increased from 10 mol/sec to 900 mol/sec, the recovery of CO₂/SO_x/NO_x also increased from 93.3/92.3/92.2 to 95/93.2/93.2. Consequently, the capture cost reduces from \$56.8/ton of impurity to \$55.8/ton of impurity. When the purge flow rate is increased, more amount of pure gas is fed into the adsorption column for cleaning the adsorption bed. As a result, the partial pressure of CO₂/SO_x/NO_x are reduced and more gases are recovered. Eventually, the capture cost will be reduced. Because of the increasing purge flow rate, the purity of gases is decreases as more pure gas is mixed with adsorbent gas. Figure 5.8 shows the effect of purge flow rate on throughput and purity. In order to find the optimum purge flow rate, the effect of purge flow rate on recovery, purity, and capture cost should be considered.

5.2.1.4 Effect of working capacities. The effect of working capacity on recovery and capture cost is shown in Figure 5.9. Four sets of different working capacity values are

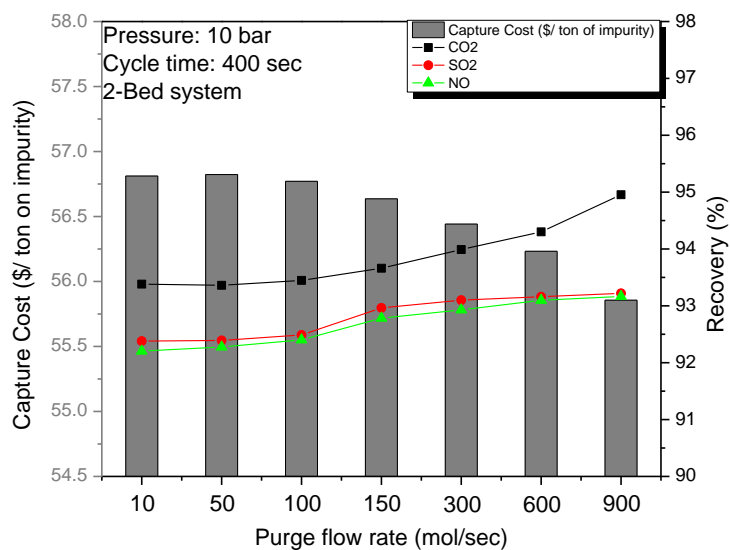


Figure 5.7: Effect of purge flow rate on recovery and cleanup cost of the 2-bed PSA system

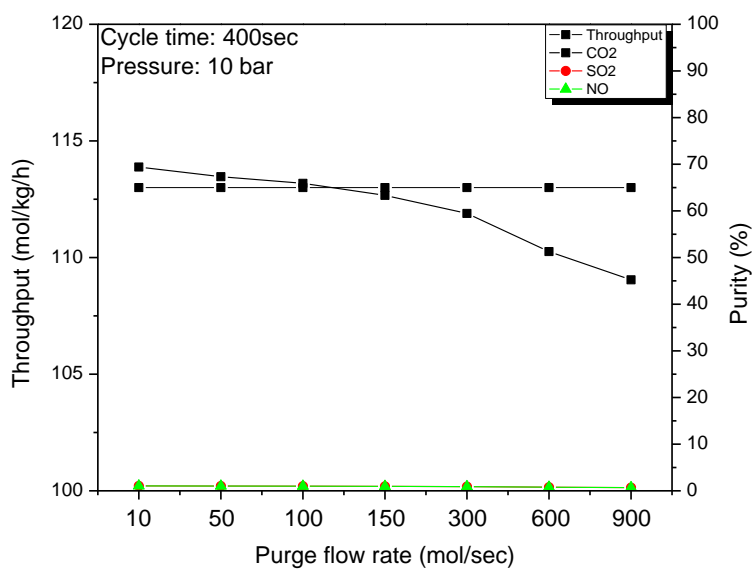


Figure 5.8: Effect of purge flow rate on throughput and purity of the 2-bed PSA system.

5.2.1.4 Effect of working capacities. The effect of working capacity on recovery and capture cost is shown in Figure 5.9. Four sets of different working capacity values are

considered. Two sets of values are below the base condition while one is above the base condition. Detailed values are mentioned in Table 5.3. As working capacity changes, bed size and amount of material required changes. Eventually, a change in capital cost and capture cost is inevitable. Similarly, working capacity reduces as the capture increases. In Figure 5.10 the effect of working capacity on throughput and purity of gases is demonstrated. As the working capacity increased, the throughput is increased. This result can be explained by the fact that as the working capacity increased, more amount of feed gas can be processed through the adsorbed bed. From the above observation, it can be concluded that an increase in working capacity will reduce the capture cost and the same trend is explained by Minh T.Ho⁶³

Table 5.3: Working Capacity Values

	CO₂ Capacity (mmol/g)	SO_x Capacity (mmol/g)	NO_x Capacity (mmol/g)
Set 1	2.5	0.4	0.4
Set 2	4	0.6	0.6
Set 3	6.3	1.3	1.3
Set 4	6.3	0.8	0.8

5.2.2. 4-Bed System. Sensitivity analysis was performed on the 4-bed system in order to assess the effects of adsorption pressure, PSA cycle time, purge flow rate, and adsorbent working capacities on technological and economic performance of the single-step cleanup process with respect to recovery and cleanup cost of the impure gases.

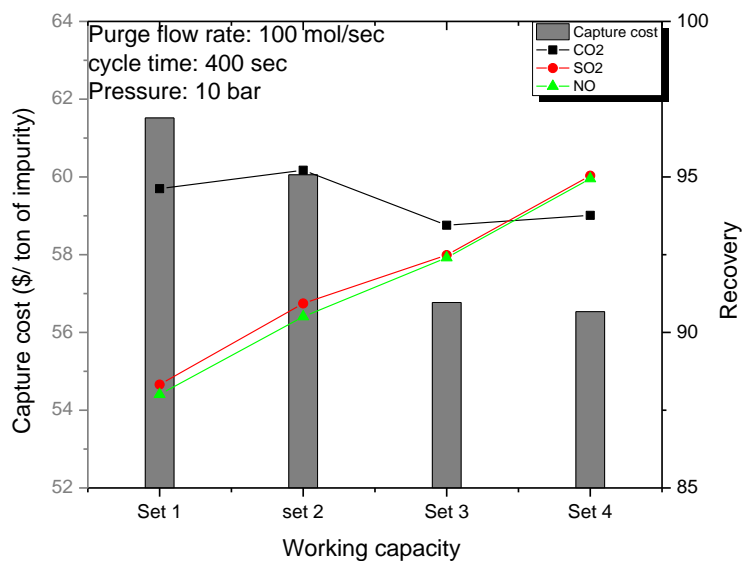


Figure 5.9: Effect of working capacities on recovery and cleanup cost of the 2-bed PSA system.

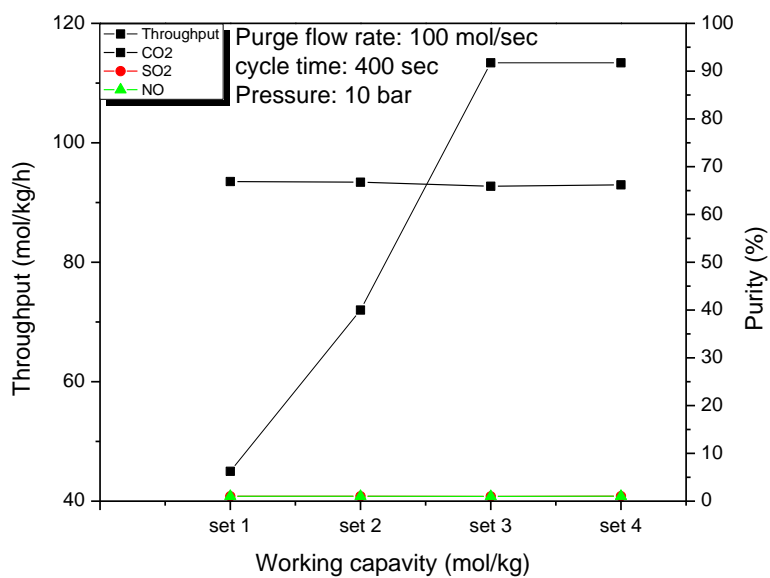


Figure 5.10: Effect of working capacities on throughput and Purity of the 2-bed PSA system.

5.2.2.1. Effect of adsorption pressure. As previously demonstrated, the adsorption pressure is a determining factor for purity, recovery and cleanup cost. The effect of pressure on cleanup cost and recovery is demonstrated in Figure 5.11. The effect on purity and throughput is shown in Figure 5.12. The pressure ranges of 5, 10 and 15 bar are chosen to demonstrate the effect of adsorption pressure on purity, recovery, throughput and cleanup. At 5 bar, 72/72/72 percent of recovery is obtained for CO₂/ SO_x/ NO_x, with a cleanup cost of \$49.75/ ton of impurities. Now, as the pressure increased from 5 to 10 bar, the recovery of flue gas also increased to 92/91/91 percent of CO₂/SO_x/NO_x. The same effect is observed in cleanup cost. The cleanup cost increased to \$57.70/ ton of impurities. The same trend is observed when the pressure increased from 10 to 15 bar. The recovery of CO₂/SO_x/ NO_x is increased to 94/93/93 and cleanup cost is increased to \$71.30/ ton of impurities. Additionally, the material has a high adsorption capacity at higher pressure. When pressure increased, the adsorption capacity of the material increased and, eventually, the recovery of the flue gas increased. However, as pressure increased a large compressor is required. In turn, this increased the capital cost and operating cost. As a result, the cleanup cost increased. When pressure increased from 5 to 10 bar, material recovery and capital cost increased. In consequence, the cleanup cost increased. The same trend is observed when pressure is increased from 10 to 15 bar.

The effect of pressure on purity and throughput is shown in Figure 5.12. As the pressure increased the purity of CO₂/SO_x/NO_x is decreased. At 5 bar, the purity of CO₂/SO_x/NO_x are 72/1.11/1.10 percent, and the throughput is 227 mol/kg/hr. As the pressure increased from the 5 to 10 bar, the gas purity decreased to 68/1.03/1.02 percent.

However, the throughput remained constant. The same trend is observed when pressure is increased from 10 to 15 bar.

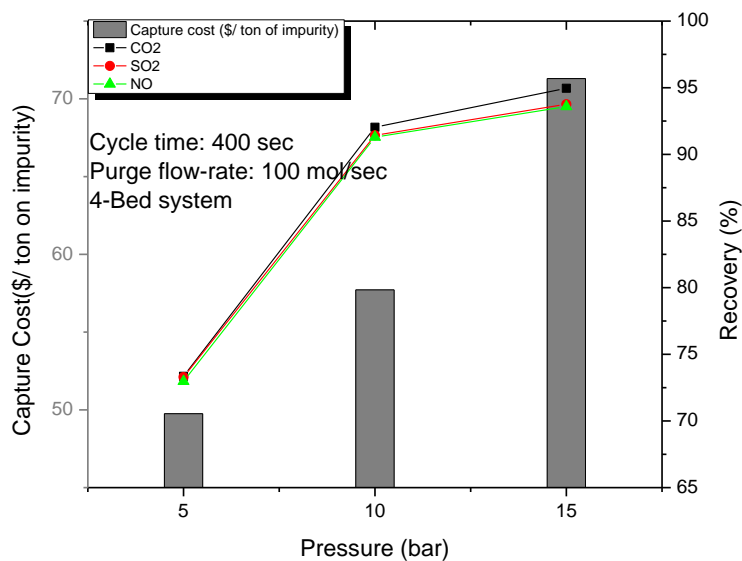


Figure 5.11: Effect of adsorption pressure on recovery and cleanup cost of the 4-bed PSA system.

As the pressure increased from the 5 to 10 bar, the gas purity decreased to 68/1.03/1.02 percent. However, the throughput remained constant. The same trend is observed when pressure is increased from 10 to 15 bar. The purity decreased to 62/0.95/0.94 percentage and throughput remain constant. Because the same amount of gas is getting processed in every pressure range, the throughput remained constant.

5.2.2.2. Effect of cycle time. PSA cycle time is one of the crucial factors that affects the purity, recovery, throughput and cleanup cost. The effect of cycle time on recovery and cleanup cost is shown in Figure 5.13. When cycle time was increased from 200 to 400

seconds, recovery of $\text{CO}_2/\text{SO}_x/\text{NO}_x$ increased from 90/88/88 to 92/91/91 percent and cleanup cost increased from \$56.51 to \$57.71/per ton of impurities removed.

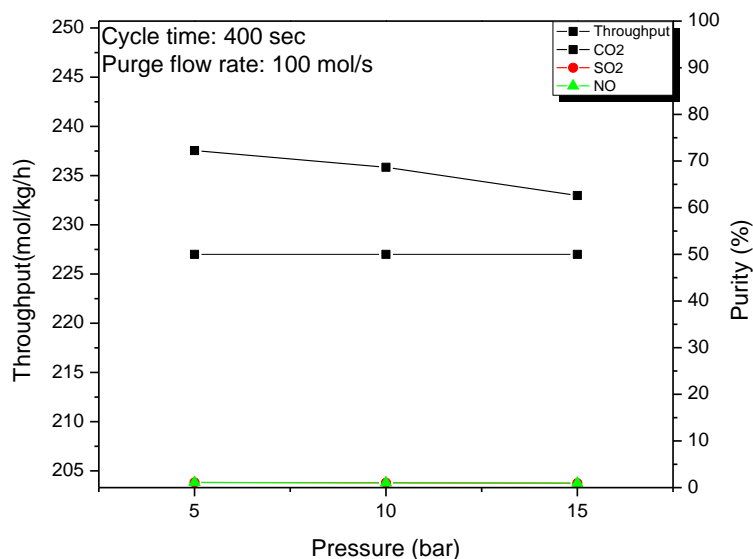


Figure 5.12: Effect of adsorption pressure on throughput and purity of the 4-bed PSA system.

However, the opposite trend is observed when cycle time is further increased from 400 to 600 seconds, i.e. the recovery of $\text{CO}_2/\text{SO}_x/\text{NO}_x$ dropped from 92/91/91 to 90/90/90 percent. However, the cleanup cost increased from \$57.71 to \$60.59 per ton of impurities removed. Cycle time affects the size of the adsorbent bed as well as the amount of adsorbent. When cycle time increased, the size of the adsorbent bed increased. As a consequence, the capital cost increased, and as cycle time increased, the amount of adsorbent also increased which contributed to operating cost. The same trend is observed in 2-bed system as well. The overall effect of cycle time on throughput and purity is shown

in Figure 5.14. As the cycle time was increased from 200 to 600 seconds, the purity of gases is increased and throughput is decreased.

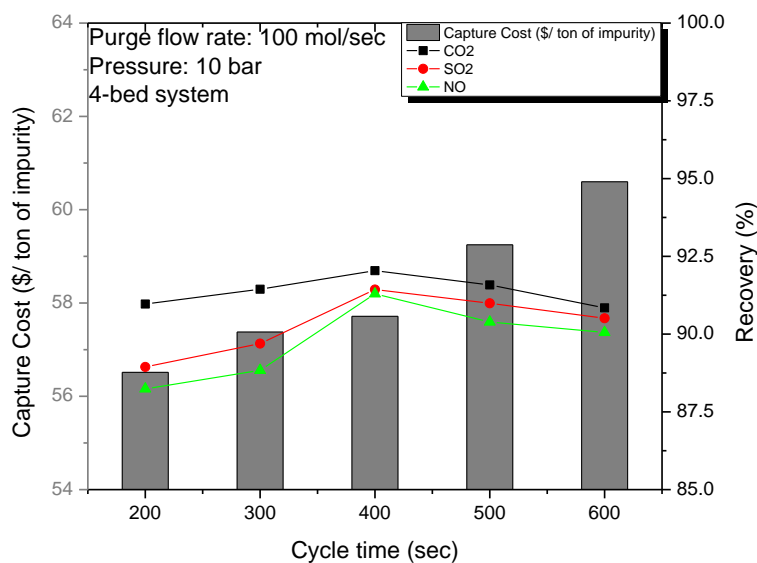


Figure 5.13: Effect of cycle time on recovery and cleanup cost of the 4-bed PSA system.

At cycle time 200 seconds, the purity of CO₂, SO_x and NO_x is 58/0.85/0.84 percent and the throughput is 453 mo/kg/hr. When cycle time increased three times to 600 seconds, the purity increased to 72/1.05/1.04 percent and the throughput decreased to 151 mo/kg/hr. When the cycle time increased, the individual step time increased causing the purity of gases to increase. When cycle time increased, a small amount of gas is processed in each cycle and the throughput decreased.

5.2.2.3. Effect of purge flow rate. The amount of gas used to purge the system affect the purity, recovery, and cleanup cost. The effect of purge flow rate on recovery and cleanup cost is demonstrated in Figure 5.15. 10 to 900 mol/sec purge flow rates are

considered for the analysis. The simulation is conducted at 10 bar and 400 seconds cycle time. When the purge flow rate increased from 10 to 900 mol/sec, the recovery of $\text{CO}_2/\text{SO}_x/\text{NO}_x$ increased from 91/89/88 to 94/94/93 percent. Cleanup cost is decreased from \$58.24 to \$56 per ton of impurities removed.

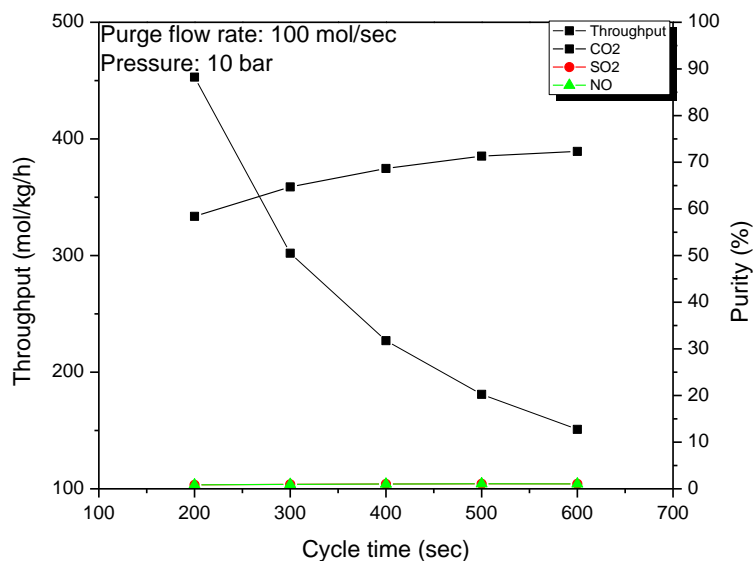


Figure 5.14: Effect of cycle time on throughput and purity of the 4-bed PSA system.

As the amount of purge gas is increased, more adsorbed gases strip out and more material is regenerated. Therefore, the recovery of gases is increased and, as a result, recovery is increased. Additionally, the cleanup cost decreased.

The effect of purge flow rate on purity and throughput is shown in Figure 5.16. As the purge flow rate is increased, gas purity decreased. In addition, the throughput remained constant, as the amount of gas processed in particular cycle remained constant. When the purge flow rate increased from 10 to 900 mol/sec, the purity of $\text{CO}_2/\text{SO}_x/\text{NO}_x$ decreased

from 76/1.6/1.4 to 38/0.56/0.56 percent. The main reason for this is, as more gas is used for system purging, the adsorbed gas becomes diluted and purity is decreased.

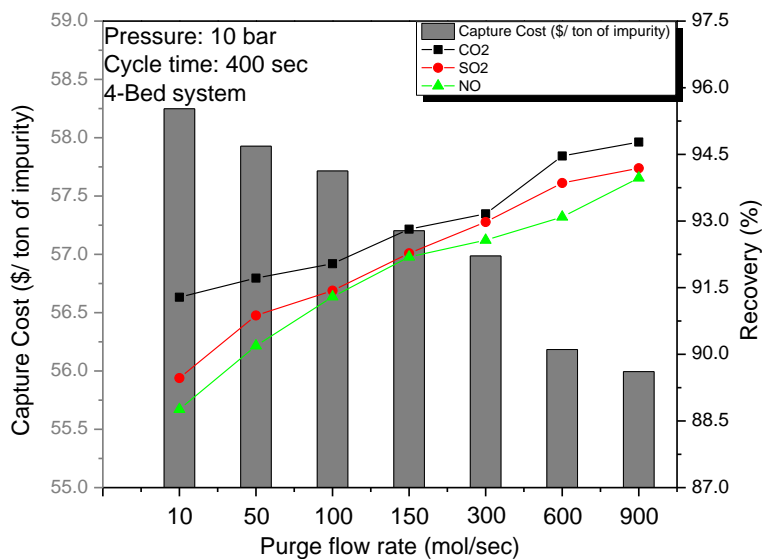


Figure 5.15: Effect of purge flow rate on recovery and cleanup cost of the 4-bed PSA system.

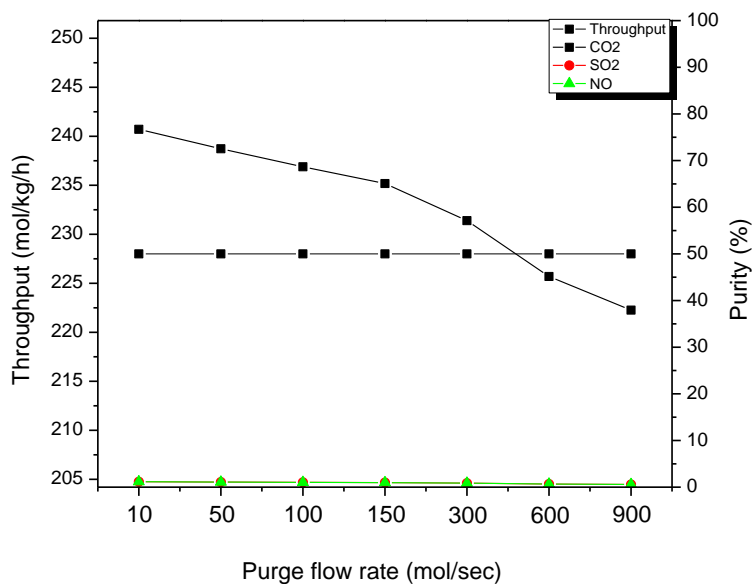


Figure 5.16: Effect of purge flow rate on throughput and purity of the 4-bed PSA system.

5.2.2.4. Effect of working capacity. Working capacity of adsorbent is one of the major factors that affect the purity, recovery, and cleanup cost. The same sets of values are used in the 4-bed system. The effect of working capacity on recovery and cleanup cost is shown Figure 5.17. As the working capacity changes, the size of adsorbent bed and amount of adsorbent used in bed is also changes. When adsorption capacity is high, the set value for cleanup cost is low. Similarly, when the adsorption capacity of 6.3/1.3/1.3 is used the cleanup cost is very low.

The effect of working capacity on purity and throughput is shown in Figure 5.18. There is not a lot of effect of working capacity on the purity. As the same amount of material is getting processed in each cycle, the throughput remained constant.

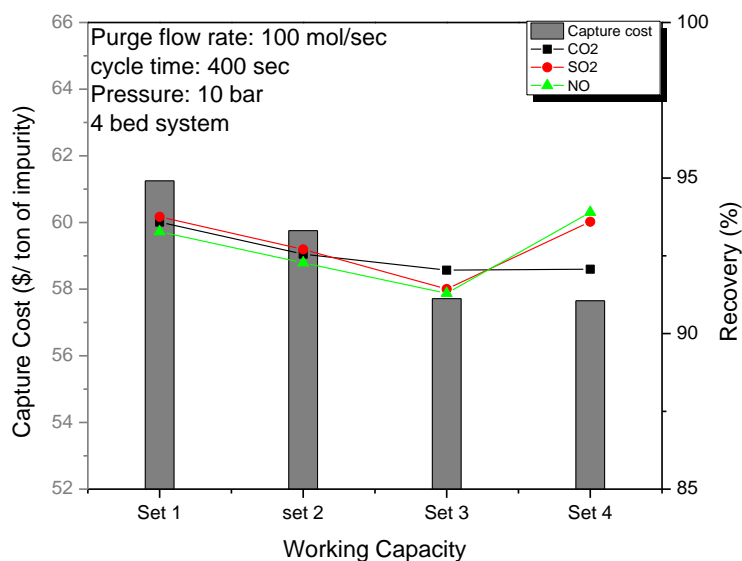


Figure 5.17: Effect of working capacities on recovery and cleanup cost of the 4-bed PSA.

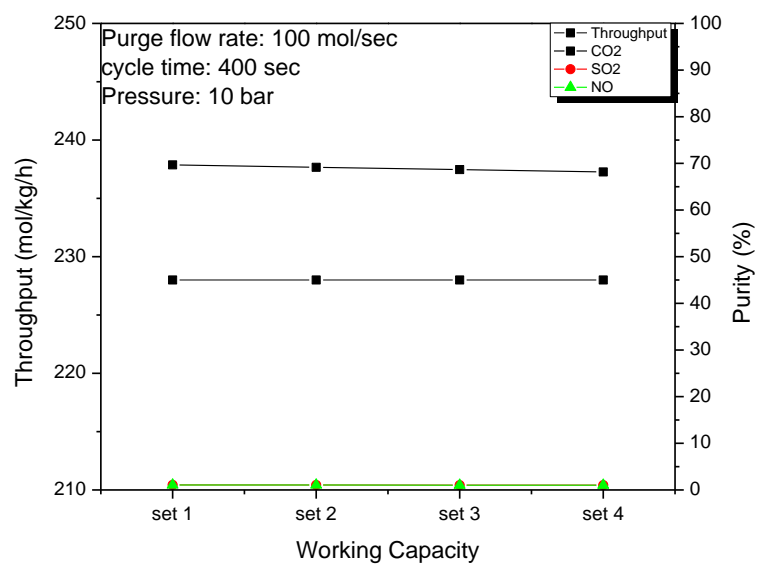


Figure 5.18: Effect of working capacities on throughput and Purity of the 4-bed PSA system.

6. CONCLUSION

The study has shown to fulfil all objectives. The single step process was designed and optimized as per the objectives. The economic analysis was conducted to find CAPEX and OPEX. An energy penalty was calculated for recovery above 90% for all three gases considering a 550 MW coal-fired power plant. The effect of adsorption pressure, cycle time, purge flow rate and working capacity were studied to find optimum conditions and cleanup cost.

6.1 OBJECTIVE 1

Objective 1 was to design single step flue gas cleanup process for simultaneous removal of SO_x, NO_x and CO₂ from the flue gas.

6.1.1. Objective 1 Conclusion. A single- step flue gas cleanup process based on 2-bed system and 4-bed system PSA process was designed to remove CO₂, SO_x and NO_x in a single step. The system consisted of a compressor, heat exchanger, turbine and pump. Aspen adsim model has been combined with aspen dynamic model to study the complete process.

6.1.2 Objective 1 Future Suggestions. A detail analysis can be performed on compressor, heat exchanger and adsorption column to get better understanding of process.

6.2 OBJECTIVE 2

Objective 2 was to optimize the process for removal efficiency of SO_x, NO_x and CO₂ greater than 90%.

6.2.1 Objective 2 Conclusion. 2-Bed, 4-step PSA cycle was designed with adsorption at high pressure, purge, blow down and light product pressurization steps.

Additionally, a 4-Bed, 6-step PSA cycle was designed with adsorption at pressure, pressure equalization, purge, blow down, and a light product pressurization step. In both configurations, recovery of all three gases was above 90%. Because the concentration of SO_x and NO_x released in to the atmosphere after treatment was less than 200 ppm, the process has not fulfilled the EPA requirements as mentioned in section 1.4.

6.2.2 Objective 2 Future Suggestions. Both 2-bed and 4-bed system were designed in this study. The number of beds and cycle confirmation are significant factors that affect purity, recovery and cleanup cost. Further study shall be conducted for a multibed system with different cycle configuration.

6.3 OBJECTIVE 3

Objective 3 was to analyze the process economics to calculate CAPEX (capital cost) and OPEX (operating cost).

6.3.1 Objective 3 Conclusion. The study was successfully conducted to find the CAPEX and OPEX of the process. The module costing technique was used to calculate bare module cost and the cost was adjusted to the year 2015 for economic analysis.

6.3.2 Objective 3 Future Suggestions. The post-treatment process of acidic gases was not considered in this study. Future research needs to be conducted to study the effect of post-treatment on capital cost, operating cost, and cleanup cost.

6.4 OBJECTIVE 4

Objective 4 was to compare the single step flue gas cleanup process with standard state of the art technology with respect to removal efficiency, cleanup cost, and energy penalization.

6.4.1 Objective 4 Conclusion. A single step flue gas cleanup process was compared with standard state the of art technology such as FGD, SCR, and amine scrubbing. A single step flue gas cleanup process incurred an energy penalty of 24 % with a recovery above 90 % for CO₂, SO_x, and NO_x to a 550 MW power plant. Notably, this is lower than the current individual unit operations. The cleanup cost associated with the 2 bed, 4s-tep and 4-bed, 6-step, processes was \$57/ ton of impurities and \$59/ton of impurities, respectively.

6.4.2 Objective 4 Future Suggestions. Post- treatment process can be studied for to see the effects on economic analysis.

6.5 OBJECTIVE 5

Objective 5 was to conduct a sensitivity analysis for the optimized operating condition and cleanup cost by varying adsorption pressure, cycle time, purge flow rate and working capacity.

6.5.1 Objective 5 Conclusion. Sensitivity analysis was conducted to study the effects of operating condition on recovery and cleanup cost and to find the best operating conditions with minimum cleanup cost. The optimum conditions for 2-bed and 4-bed systems were 10 bar adsorption pressure, 400 seconds of cycle time and 100 mol/sec of purge flow rate resulting in a cleanup cost of \$57 and \$59/ ton of impurities respectively.

6.5.2 Objective 5 Future Suggestions. Further study needs to be conducted to see the effect of the individual step time. The adsorbent material is an important factor for this process as well. Additional studies need to be conducted to determine the optimum material containing both a high working capacity and in addition to a longer life cycle.

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