



Research Article

Modelling and Optimisation of Industrial CO₂ Production Process

Dauda Ibrahim, Babagana Gutti, Aliyu A. Bello

Department of Chemical Engineering, University of Maiduguri, P.M.B. 1069 Maiduguri,
Borno State

*Corresponding author's Email: didauda@yahoo.com, doi.org/10.55639/607.161514

ARTICLE INFO:

ABSTRACT

Keywords:

CO₂ capture,
Beverage-grade CO₂,
Operating condition,
Modeling,
Optimization

To improve profitability and avoid emitting residual CO₂ (Carbon dioxide) in beverage production plants, an insightful understanding of operating conditions having significant impact on CO₂ recovery is required. This research investigates the operating conditions that significantly impacts CO₂ recovery in addition to proposing a new procedure for techno-economic optimisation of food-grade CO₂ production process in beverage plant. The methodology applied in this research starts by collecting process data, followed by the development of a CO₂ production process model in Aspen HYSYS. Lastly, the model is used to set up a case study and conduct optimisation studies. Numerical results show that by independently optimizing lean MEA (monoethanolamine) temperature, operating pressure, lean MEA flow rate, and lean MEA composition, CO₂ yield increases by 0.3 %, 0.8 %, 0.8 % and 4 % respectively. Additionally, applying the optimum operating conditions simultaneously on the process increases CO₂ yield by 10.20 %. Optimizing lean MEA composition independently has the highest impact on CO₂ recovery compared with other operating conditions. Overall, the optimised process indicates an increase in benefit equivalent to 10,487 ₦/h, i.e., ₦ 7,550,640 per month.

Corresponding author: Dauda Ibrahim, **Email:** didauda@yahoo.com

Department of Chemical Engineering, University of Maiduguri, Borno State, Nigeria

INTRODUCTION

Soft drinks are enormously popular beverages consisting primarily of carbonated water, sugar, and flavourings (Avizienis, 2014). Carbonated water constitutes up to 94% of a soft drink. Carbon dioxide (CO₂) contained in carbonated water adds that special sparkle and bites to the beverage and also acts as a mild preservative. Carbon dioxide is a uniquely suitable gas for soft drinks because it is inert, non-toxic, and relatively inexpensive and easy to liquefy (Avizienis, 2014). A modern approach to carbon dioxide purchase suggests that industrial users can no more be dependent on gas manufacturer but has to install their own CO₂ production facility to get relevant economic benefits (cost saving from in-house production) and strategic advantages – complete carbon dioxide availability without any logistic problem or shortage in times of most demand (Fermi, 2011). Technology used for production of food-grade CO₂ in beverage industry is based on combustion of de-sulphurised fuel gas or liquid oil. The controlled combustion of fuel gas in generator-reboiler produces a flue gas rich in CO₂. The flue gas is delivered to absorption tower in which MEA solution selectively absorbs CO₂. The solution rich in CO₂ is pumped to a stripper where heat is used to facilitate release of CO₂ (Fermi, 2011). Products from stripping column containing CO₂, water vapour and entrained MEA (monoethanolamine) is condensed and majority of the liquid is separated. The final CO₂ product is delivered to the compression section where it is dried, compressed through a multi-stage compressor and liquefied. However, a loss of CO₂ in the overhead product from the CO₂ absorber has been observed from an existing CO₂ plant, with some valuable CO₂ products slipping into the off-gas which is undesirable. Therefore, additional revenue can be generated by the process if recovery of CO₂ is improved. Moreover, improved CO₂ product recovery will

also minimize greenhouse gas emissions released into the atmosphere.

The conventional method used to maximize yield of food-grade CO₂ in an existing production plant involves a “try-and-see method”, i.e., one equipment/ operating condition is adjusted at a time and the effect of changing the process variable on CO₂ yield is recorded before adjusting another equipment/ operating condition. This method is time-wasting and cost ineffective. There is a need for an alternative method (or solution) that improves the recovery of CO₂ in the existing CO₂ production plant as well as minimizing total overhauling time and cost.

The enhancement of CO₂ recovery in an existing process has drawn attention with much research progressing in this area. This results from the global concern on CO₂ emission and also growing market of CO₂ which is used as a preservative in beverages. Grégoire *et al.*, (2011) modelled a post-combustion CO₂ capture process with amine as solvent for carbon dioxide capture. In their work, the CO₂ capture process with monoethanolamine (MEA) is modelled using the simulation tool in Aspen Plus. Two different modelling approaches were studied and compared: the equilibrium and the rate-based approaches. An optimization of key process parameters is performed and process modifications are studied with the objective of improving the global process energy efficiency. Although the discussion of Grégoire *et al.* (2011) has taken into account some important operating condition that directly impact on CO₂ recovery, in their work only energy efficiency was improved; improvement in CO₂ recovery is not considered. Kim *et al.* (2004) optimized a CO₂ absorption process with MEA solution as solvent. In their work, they simulated the CO₂ absorption with MEA (mono-ethanolamine) solution to evaluate the operating condition of the bench-scale, continuous CO₂ absorption apparatus located in the Korea Institute of

Energy Research. Their main objective was to determine the most energy-effective process in the regenerator through the simulation of various operating conditions of CO₂ absorption. Kim *et al.* (2004) varied the flow rate of flue gases and MEA solution from 35-80 /min and 1.0-3.0 /min, thereby determining the regenerating process operating conditions of maximum CO₂ separation efficiency for the simulation with the change of reboiler heat duty and number of stages. Their work only focuses on determining the operating conditions those results to an energy-effective process. Ying *et al.*, (2013) modelled CO₂ absorption and desorption by aqueous monoethanolamine solution with Aspen rate-based model. They simulated nineteen data sets of CO₂ absorption by aqueous monoethanolamine solution obtained from a recent pilot plant at the University of Kaiserslautern with Aspen rate-based model. Their simulation study was performed with both the rigorous rate-based model and the traditional equilibrium stage model. Results from their studies shows that the rate-based model yields reasonable predictions on all key performance measurements including CO₂ removal percentage in the absorber, temperature and CO₂ concentration profiles in the absorber and the desorber, and the desorber reboiler duty; in contrast, the equilibrium-stage model fails to reliably predict these key performance variables. The author's effort was to identify the appropriate model for CO₂ absorption process. However, improvement in CO₂ yield was not considered in their work.

Similarly, Lars *et al.* (2014) Optimized configurations for amine-based CO₂ absorption using Aspen HYSYS. The authors simulated different absorption and desorption configurations for 85 % amine-based CO₂ removal from a natural gas-based power plant using Aspen HYSYS. A standard process, split-stream, vapour recompression and different combinations thereof were also simulated. They

used the simulations as a basis for equipment dimensioning, cost estimation and process optimization. Results from their investigation shows that the simple vapour recompression case is the most cost optimum configuration. However, their investigation focuses only on minimizing capital cost of the CO₂ absorption process. Ahmed *et al.* (2003) studied the kinetics of the reactive absorption of carbon dioxide in high CO₂-loaded, concentrated aqueous monoethanolamine solutions. The authors investigated the kinetics of the reaction between carbon dioxide and high CO₂-loaded, concentrated aqueous solutions of monoethanolamine (MEA) over a temperature range from 293 to 333 K, MEA concentration range from 3 to 9M, and CO₂ loading from 0.1 to 0.49 mol/mol. Results from their studies shows that the developed termolecular-kinetics model for CO₂ reaction with MEA solutions, proves to be better than previously published kinetic models. Their model was comprehensive enough to describe for the first time the absorption of CO₂ in highly concentrated and high CO₂-loaded aqueous MEA solutions for a wide temperature range. No improvement of CO₂ recovery was considered in their work.

So far, however, there has been no attention paid to improvement of food-grade CO₂ recovery in the beverage industry. Additionally, none of the work in literature developed a handy approach that can be used by plant operators to conduct techno-economic optimisation of food-grade CO₂ production plant. The need to enhance the recovery of food-grade CO₂ in the CO₂ production plant is of great importance in order to add more value to the process. Similarly, greenhouse gas emissions could be reduced substantially. Unlike previous work discussed in literature, this work addresses improvement of food-grade CO₂ recovery in beverage industry, in order to overcome limitations of current practice involving a "try-and-see" approach which is time-wasting and cost ineffective.

Operators in food-grade CO₂ production plant can utilise the proposed methodology to improve plant performance.

This research work develops a stepwise method for improving the performance of industrial CO₂ production process. The methodology starts by collecting plant data supplemented by information from literature and investigation of process operating conditions that can affect CO₂ recovery. Followed by development of process model using process simulation software such as Aspen HYSYS, and lastly the model is used to conduct an optimisation study in order to maximise CO₂ yield as well as revenue. As discussed, the key process operating conditions affecting recovery of CO₂ discussed in the literature includes lean MEA temperature, operating pressure, lean MEA flow rate and lean MEA composition. These operating conditions are optimized separately to gain insights into the impact of each operating condition on CO₂ recovery. For each case, the operating condition is varied within a range that is set by the allowable operating conditions of the process equipment and the properties of the MEA solution. The range constitutes four different values of the operating condition, which are termed Case 1, Case 2, Case 3 and Case 4. Each case value is then applied on the CO₂ plant model in Aspen HYSYS, by adjusting the operating conditions. The resulting effect on the recovery of CO₂, fraction of CO₂ in off gas, reboiler duty and temperature are recorded. For each operating condition, the case that economically maximized the recovery of CO₂ is selected as the optimum operating condition.

The optimized operating conditions are then applied on the CO₂ plant model to obtain an overall optimized process. The CO₂ recoveries from the base case and optimized case are used to determine the revenue from the process, and the utility demand is used to determine the operating cost. The recent market price of CO₂ and each utility is used for estimating the revenue and operating cost. The net benefit is estimated by subtracting operating cost from revenue. The benefit from the base case and optimized case is compared, in order to provide insight into the significance of optimizing the CO₂ production plant.

This paper consists of three sections in addition to the introductory section. Section 2 describes the existing CO₂ production process and presents a stepwise procedure for modelling and optimizing the CO₂ production plant. In Section 3, optimization results from procedure outlined in Section 2 are analysed and discussed. Results from optimization of operating conditions (such as operating pressure, lean MEA temperature, lean MEA compositions and flow rate) on CO₂ recovery are examined. A comprehensive economic analysis is carried out to determine the benefit from the optimized process. Finally, conclusions on the optimization of CO₂ recovery, highlighting the benefit from the optimized process and recommendations for future work are presented.

MATERIALS AND METHODS

The method proposed to address the research goals presented in Section 1 comprises three main steps: data collection, process modelling, and process optimisation, (Figure 1).

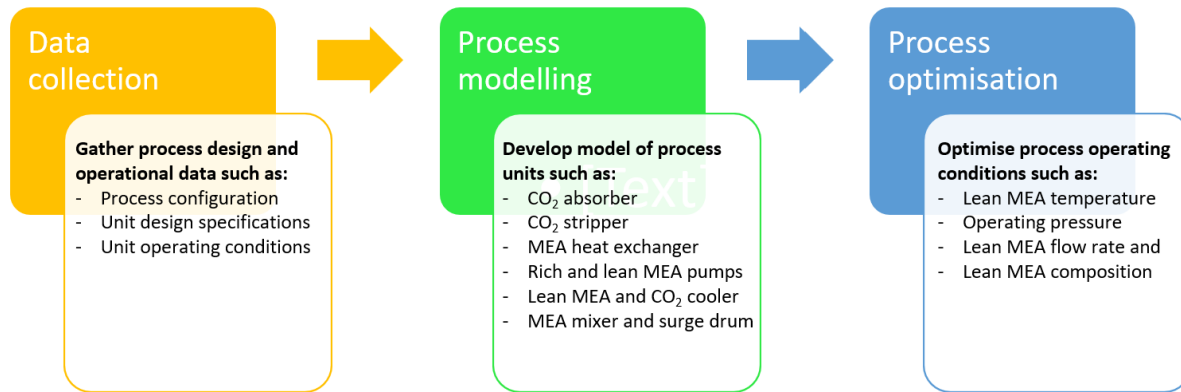


Figure 1: Proposed research methodology for modelling and optimisation of industrial CO₂ production process

First, information from an existing plant supplemented by data from literature was collected. This includes process configuration, unit design specification, and unit operating conditions. The collected information is used to develop a model of CO₂ production process in Aspen HYSYS. Lastly, the CO₂ plant model is used to optimise operating conditions and to evaluate the profitability of optimised case. Performance indicators used include CO₂ recovery and fraction of CO₂ in off gas. Amount of CO₂ recovered determines the revenue from

the process, whereas fraction of CO₂ in dry gas indicates lost CO₂ from the process.

Data collection

As shown in Figure 1, there are three essential information required to build a model of CO₂ production plant, namely: process configuration, unit design specification, and unit operating conditions. In this work, data were collected from an existing plant and from literature. The process flow diagram/process configuration of the existing CO₂ production plant is shown in Figure 2.

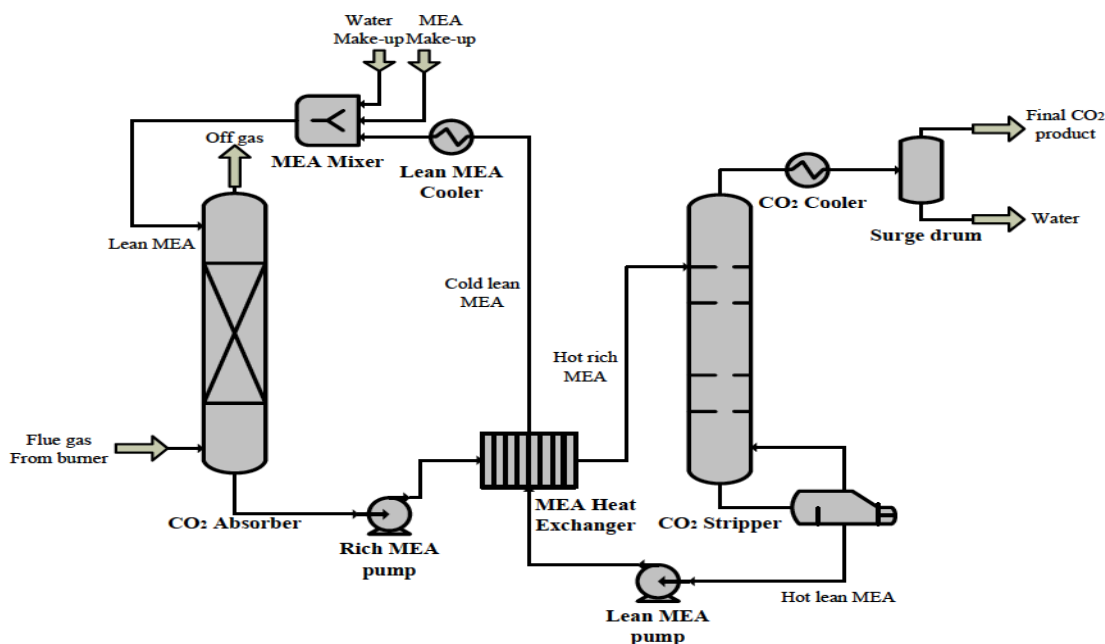


Figure 2: Base case CO₂ production process from an existing CO₂ plant

Figure 2 shows a simplified process flow diagram of the base case CO₂ production process, which is obtained from an existing CO₂ plant. The inlet flue gas passes up from the bottom of the absorber column; lean amine enters the top of the absorber column and distributes over the packing material. Lean amine in counter flow comes in contact with the gas and absorbs the CO₂ from the flue gas stream leaving the remaining gas to pass through the top chimney tray and into the absorber off-gas. The CO₂ rich amine is collected at the bottom of the absorber and pumped through a lean/rich MEA exchanger to near the top of the stripping column. A reboiler located near the bottom and connected to the stripper provides the heat necessary to strip out the CO₂ from the chemical solvent. Stripping steam produced from the reboiler passes upward through the stripper column. As the rich amine descends in counter flow, CO₂ is stripped out of the chemical solvent, in effect, reversing the solvent absorption reaction. The stripped lean amine accumulates in the bottom of the stripper column and reboiler where it exits to the lean/rich exchanger in order to utilize the lean amine heat from the regeneration process to preheat the rich amine prior to entering the stripper column, and at the same time, reduces the cooling load on the lean amine. From the top of the stripper column, CO₂ product, water vapour, and entrained amine enter the CO₂ condenser where the majority of the liquid is condensed, accumulated in the surge drum and returned back to the process. The final CO₂ product is delivered to the compression section where it is dried and compressed through a multi-stage compressor.

Process modeling

In this work, Aspen HYSYS process modelling software is used to develop a model of CO₂ production process. As shown in Figure 2, the production process consists of absorbers, stripper, coolers, heat exchanger, mixer and

pumps. Modelling the entire process at once can cause convergence problem; hence, the modelling is carried out one step at a time. The process modelling – performed using SI unit set

(a) Defining the simulation basis

Selection of an appropriate property package is crucial for accurate prediction of the thermodynamic, physical, and transport properties of a particular process (Yela, 2004). In general, property package is selected according to type of process, components, process temperatures and pressures etc. (Yela, 2004). The current process constitutes CO₂, O₂ (oxygen), N₂ (Nitrogen), MEA, and water. Hence, a sufficient property package for the simulation is Amine Property Package.

(b) Feed streams data

Feed streams are defined by specifying flow rate, composition and a minimum of two process conditions such as vapour fraction, temperature, pressure, heat flow etc. The unspecified stream conditions are then calculated by the software. The current simulation has two feed streams, which include flue gas and lean MEA.

(c) Installing and defining process equipment

To simulate the CO₂ absorber using the default “absorber model” in HYSYS, inputs required include number of stages and pressure at the column top and bottom. Note that the top and bottom temperature are optional inputs. Lean and rich MEA pumps are modelled by specifying key design parameter of a “pump model” such as pressure drop and outlet pressure as well as inlet and outlet stream conditions. Specifying two variables enables the software to estimate the remaining variables. CO₂ Stripper is modelled using the “reboiled absorber model”. Hence the required unit design parameters and product specification include number of stages, top stage pressure and temperature, boil-up ratio, and overhead product flowrate. Flash drum is modelled using a “two-phase separator”. Key design parameters include inlet pressure and

vapour outlet pressure, to determine flashing of the liquid stream. Typically, a two-phase separator is used for separating mixed liquid-vapour stream into liquid and vapour stream. Both inlet and vapour outlet pressure drops are set to 0 kPa. The inlet stream condition is known from CO₂ stripper simulation. MEA Heat Exchanger and Lean MEA cooler are modelled using “heat exchanger model” and “cooler model” with key design parameter such as pressure drop, temperature difference and heat duty in addition to inlet and outlet stream conditions. Specifying three variables enables the software to estimate the remaining unknown variables. For the current simulation, the outlet temperatures are specified together with pressure drop. The inlet stream condition is fully defined from the previous simulation. MEA mixer is modelled using the “mixer model” which has two parameter options namely ‘equalize all pressure’ and ‘set outlet to lowest inlet’. Therefore, the second option is used for the current simulation since all the inlet streams pressure is known. Recycle block compares the guess value (outlet) and the estimated value (inlet) during simulation and the block converges when the guess value equal estimated value. The inputs (guess values) used for the current simulation includes temperature, pressure and molar flow rate. Flow sheet convergence – the ‘recycled Lean MEA’ stream is connected to the inlet of the absorber column. Therefore, the recycle block re-iterates until convergence is attained; during the converging process, the CO₂ absorber and CO₂ stripper are all recalculated. Figure 3 shows the converged process flow diagram of the base case CO₂ production process.

Process optimisation

The process variables affecting CO₂ recovery discussed in Section 1 are used to develop four optimization case studies. Detailed procedure for optimizing each process variable is presented in the following sub-subsections. Note that each

operating condition consists of four cases and the case that leads to highest CO₂ recovery and economic benefit is selected as the best operating condition.

(a) Lean MEA temperature

The tendency of a solvent to dissolve or absorb a solute depends on the solubility of the solute in the solvent. Solubility decreases with increase temperature (Smith, 2005). Decreasing temperature of lean-MEA solution during absorption increases the amount of solute dissolved and hence, improve CO₂ recovery. Therefore, the temperature range for the case is selected such that expensive utilities (both heating and cooling) are avoided, also high temperatures are avoided to prevent rise in lean-MEA vapour pressure which decreases gas solubility and results to loss of solvent during absorption. The temperature range used for the optimization includes 20 °C, 30 °C, 50 °C and 60 °C (Case 1, Case 2, Case 3 and Case 4 respectively); the base case lean-MEA temperature is 40 °C.

(b) Operating pressure

The operating pressure of an absorption process impacts directly on the solubility of the solute in the solvent. High solubility of solute in solvent is achieved at high pressure (Smith, 2005). Increasing the pressure in an absorber increases the partial pressure of the solute (Mehra, 1987) resulting in high recovery of solute. Operating at high pressure brings benefit to a process by enhancing recovery of solute. Moreover, while enhancing recovery in an existing process (revamp), the maximum increase in pressure is limited by the capacity of the existing equipment (Dean *et al.*, 2005) to avoid additional capital investment. Therefore, the operating pressure range is set according to the capacity limit of the existing process equipment. The operating pressure range used for the optimization includes 1.875 bar, 2.25 bar, 2.625 bar and 3.00 bar (Case 1, Case 2, Case 3 and Case 4

respectively); the base case operating pressure is 1.50 bar.

(c) Lean MEA flow rate (Circulation rate)

The flow rate of an absorbent has influence on the amount of absorbed solute. The liquid to vapour (L/V) ratio in an important design parameter for absorption processes (Smith, 2005). Increasing the flow rate of solvent increases the solute recovery (Mehra, 1986). The solvent used for CO₂ recovery in the CO₂ absorber contains a mixture of water and MEA at an appropriate proportion. The change in flow rate directly affects the liquid to vapour (L/V) ratio in the primary absorber; hence high CO₂ recovery is expected at high L/V ratio. Optimization of lean-MEA flow rate (circulation rate) is achieved by varying the stream flow rate in the range of 834855 kmol/h, 849970 kmol/h, 859365 kmol/h and 866026 kmol/h (Case 1, Case 2, Case 3 and Case 4 respectively); the base case flow rate is 831307 kmol/h. The flow rate range is usually set according to the capacity limit of lean-MEA pump (Haik, 2005).

(d) Lean MEA Composition

The chemical nature of lean-MEA solution is an important factor in CO₂ recovery due to the molecular interactions involved during the

$$R = \sum_i USP_i \times PF_i \quad (1)$$

Where R denotes revenue, USP_i denotes unit selling price of product i , and PF_i denotes flow rate of product i .

Step 2 determines the operating or utility cost required producing CO₂, seeing Equation 2 – the

$$O = \sum_i UPU_i \times QU_i \quad (2)$$

where O denotes operating cost, UPU_i denotes unit price of utility i , and QU_i denotes flow rate of utility i .

Step 3 determines the net production benefit, see Equation 3 – the net production benefit is calculated by subtracting the operating cost

absorption process. Lean-MEA solution used for CO₂ recovery contains water and MEA solution at a specific proportion. Hence, varying the flow rate of MEA solution affects the solvent performance, thereby affecting CO₂ recovery. Therefore, optimizing the lean-MEA composition is achieved by increasing the flow rate of make-up MEA solution in the range of 2131 kg/h, 2486 kg/h, 2841 kg/h and 3197 kg/h, which is represented as Case 1, Case 2, Case 3 and Case 4 respectively; the base case flow rate is 1776 kg/h.

Economic Evaluation of Cases

The economic evaluation involves determining benefit using selling price of CO₂ together with cost of process water, MEA solution and pump power demand. Benefit is determined and used for comparing the base case and the optimized case. The procedure used to perform the economic evaluation comprises three steps.

Step 1 determines revenue from product sales, see Equation 1 – the product from the process is CO₂ and corresponding flow rate of CO₂ is obtained from simulation while current market price of the CO₂ is used to determine net revenue.

utility required to produce CO₂ includes process water, pump power demand and MEA. Process water and pump power requirements for the cases are presented in the subsequent sections.

(determined in Step 2) from revenue (determined in Step 1). The benefit is evaluated for two cases, namely base case and optimized. Comparisons of benefits from base case and optimized case will provide general insights into which operating conditions/ parameters may be

optimized to maximized benefit in the CO₂ production process. Results of the optimization

$$B = R - O \quad (3)$$

where B denotes net production benefit.

RESULTS AND DISCUSSIONS

The optimisation results from case studies are presented, analysed and discussed. Figure 3 shows the converged process flow diagram of the base case CO₂ production process and results from the simulation shows that 1735.33 kmol/h (76371.39 kg/h) CO₂ is recovered from the process. Off gas flow rate is 19853.43 kmol/h (557325.66 kg/h), which contains 179.38 kmol/h

study are presented in section below.

(7894.29 kg/h) of CO₂. Thus, the CO₂ in off gas can be reduced by optimizing the operating conditions in the process, which in turns increase benefit. Recall, the case studies involve optimizing process operating conditions such as lean MEA temperature, operating pressure, lean MEA flow rate and lean MEA composition in the CO₂ production process.

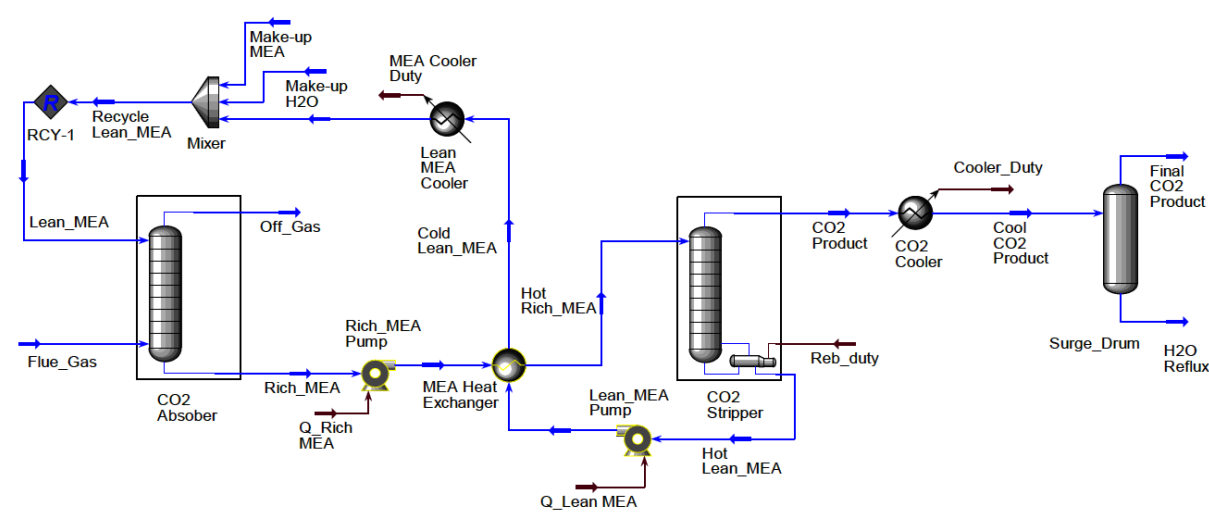


Figure 3: Simulation model of the base case CO₂ production plant showing various unit operations together with material and energy streams.

Optimizing lean MEA temperature entering the CO₂ absorber

The performance indicators from the optimization of lean MEA temperature are presented in Figure 4. From the results, increase in lean MEA temperature by approximately 10 °C from the base case temperature (baseline flowrate 76371.39 kg/h), decreases CO₂ recovery by 1.3%, while the CO₂ component in

off gas (baseline flowrate 7894.29 kg/h) is increased by 12%. Conversely, decrease in lean MEA temperature by approximately 10 °C from the base case temperature, increases CO₂ recovery by 0.3%, while the fraction of CO₂ in off gas decreases by 3%. Similar trends are observed at 10 °C increase or decrease in solvent temperature from the base case temperature.

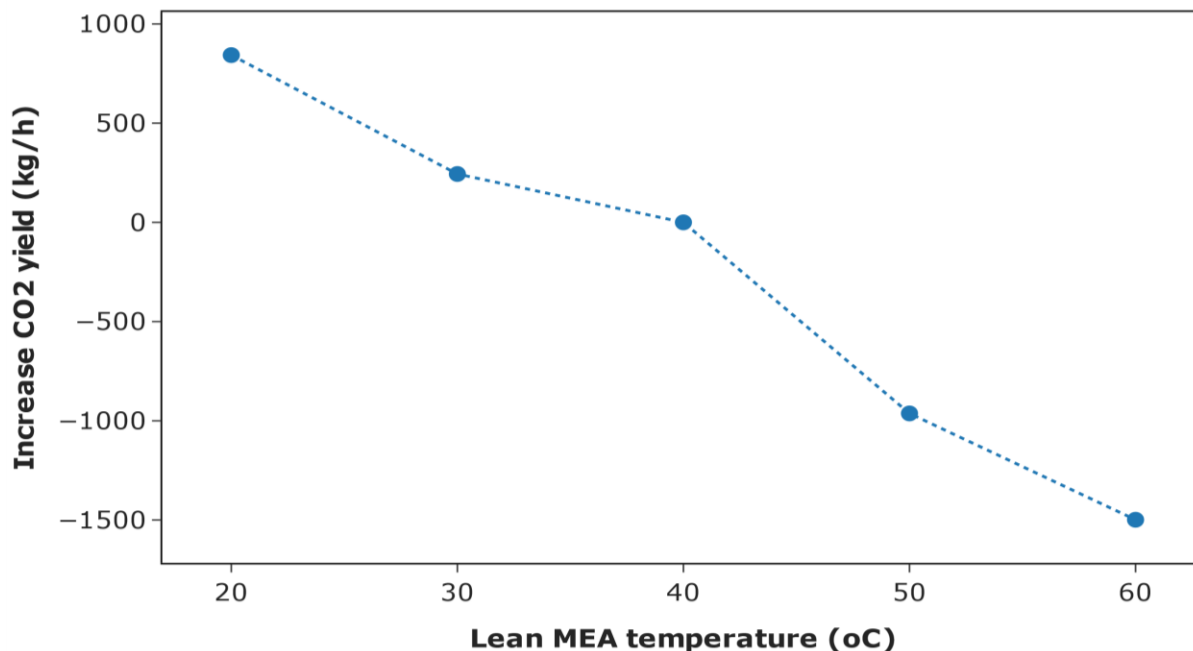


Figure 4: Amount increase/ decrease in CO₂ yield with lean MEA temperature

High CO₂ recovery and less CO₂ in off gas are observed at lower lean MEA temperature. For ΔT_{min} of 10 °C, operating at 20 °C requires chilled water at 10 °C, which will require a refrigeration system, therefore huge capital investment is required. On the other hand, operating at 50 °C and 60 °C requires ambient cooling medium, but decreases CO₂ recovery (Figure 4) and leads to high CO₂ in off gas. Thus, operating at low lean MEA temperature requires expensive utility, while high temperature reduces revenue (low CO₂ recovery); hence the optimum lean MEA temperature for the current study is 30 °C.

Optimizing process operating pressure

Figure 5 presents the case study results for optimization of operating pressure in the CO₂ production process. Increasing operating pressure by 0.375 bar (25% of base case pressure), increases CO₂ recovery by 1 % (baseline flowrate 76371.39 kg/h), while CO₂ in off gas is reduced by 9% (baseline flowrate 7894.29 kg/h). Similarly, increasing operating pressure by 0.75 bar (50% of base case pressure), increases CO₂ recovery by 2 %, while CO₂ in off gas is reduced by 18 %. Similar trends are observed at 1.125 bar and 1.50 bar increase of operating pressure.

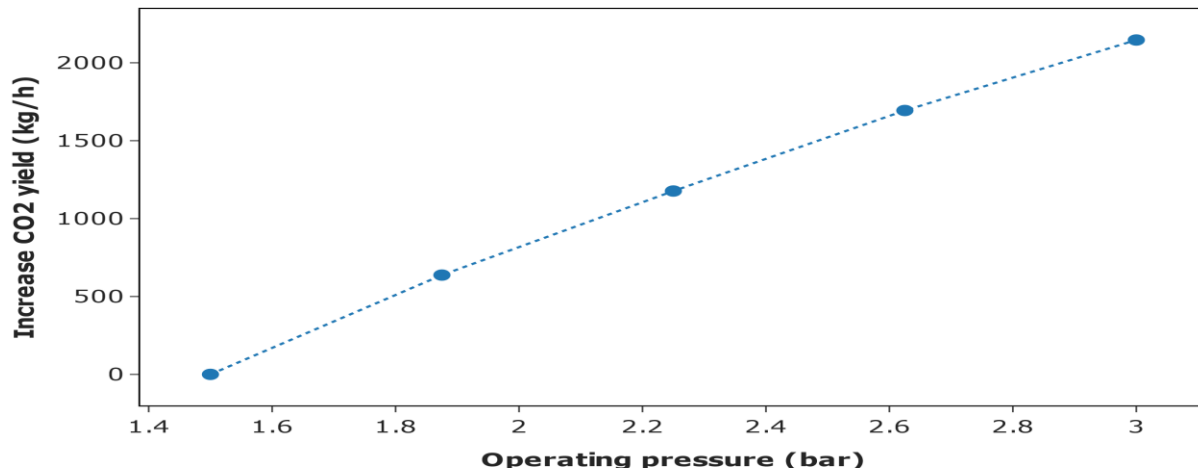


Figure 5: Amount Increase in CO₂ Yield with Operating Pressure

High operating pressure reduces lost CO₂ in off gas which in turns increases CO₂ recovery (Figure 5). In general, operating at high pressure improves recovery of CO₂ (increase revenue) and reduces lost CO₂ in off gas. Hence, the optimum operating pressure for the current study is 1.875 bar, corresponding to reboiler temperature of 122.15 °C, which is well below the degradation temperature of MEA (124 °C). Operating at a pressure above 1.875 bar results to degradation of MEA in CO₂ stripper reboiler, leading to loss of MEA strength and fouling of the reboiler.

Optimizing lean MEA flow rate entering the CO₂ absorber

Figure 6 presents the optimization results of lean MEA flow rate in the CO₂ production process. An increase in lean MEA flow rate by 3548 kg/h increases CO₂ recovery by 0.1 % (baseline flowrate 76371.39 kg/h) and decreases CO₂ lost to off gas by 0.5 % (baseline flowrate 7894.29 kg/h). Similarly, increasing lean MEA flow rate by 18662.7 kg/h increases CO₂ recovery by 0.6 % and decreases CO₂ lost to off gas by 6 %. Similar trends were observed for increase lean MEA flow rate by 28058 kg/h and 34719 kg/h

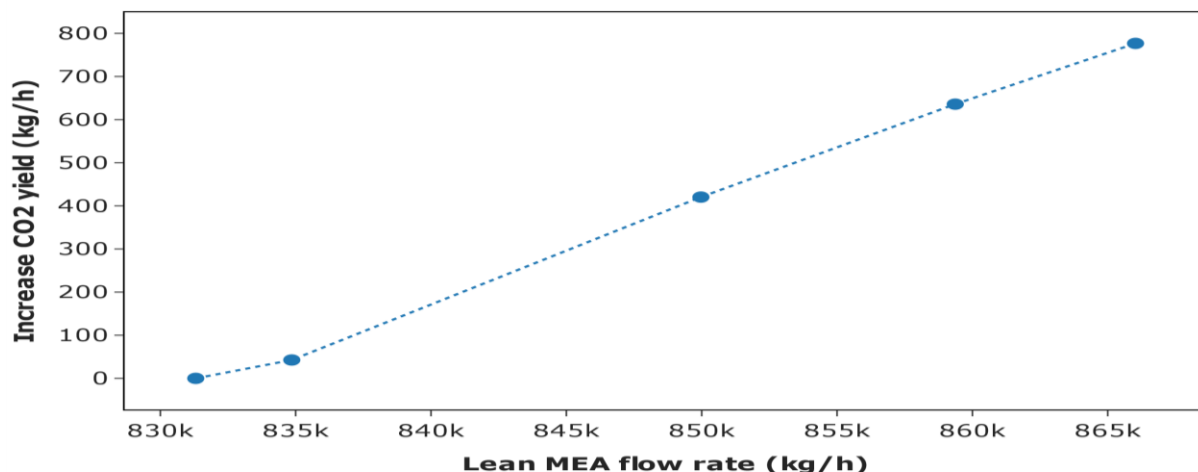


Figure 6: Amount increase in CO₂ yield with lean MEA flow rate

The lean MEA flow has less influence on CO₂ recovery in the CO₂ absorber, which is because the CO₂ recovery process is govern by chemical absorption rather than a physical absorption (Veawab, 2002). Therefore, 859365.45 kg/h is selected for optimum operation; flow rate beyond the optimum value results to less increase in CO₂ product as presented Figure 6.

Optimizing lean MEA composition

The optimization results of lean MEA composition on the recovery of CO₂ is presented in Figure 7. Increase in MEA make-up flow rate

by 355.20 kg/h (corresponding to 0.221 % MEA in lean MEA stream) increases CO₂ recovery by 0.14 % (baseline flowrate 76371.39 kg/h) and decreases CO₂ lost to off gas by 1.3 % (baseline flowrate 7894.29 kg/h). Similarly, increasing MEA make-up flow rate by 710.4 kg/h (corresponding to 0.224 % MEA in lean MEA stream) increases CO₂ recovery by 1.10 % and decreases CO₂ lost to off gas by 11.40 %. Similar trends were observed for increase MEA make-up flow rate by 1065.60 kg/h and 1420.80 kg/h.

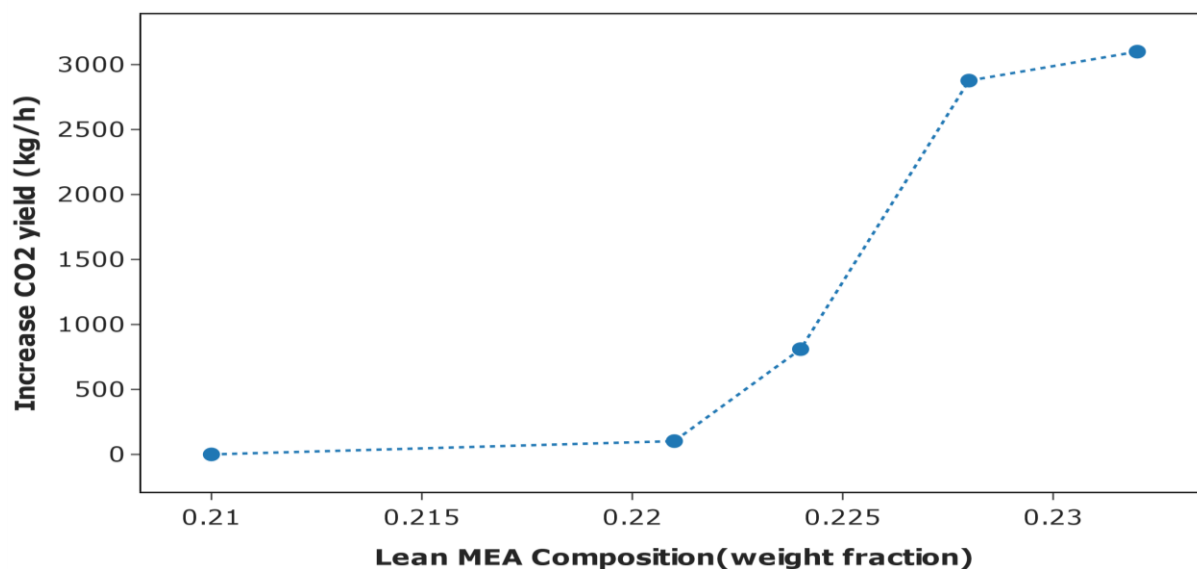


Figure 7: Amount increase in CO₂ yield with lean MEA composition

The change in MEA make-up flow rate (lean MEA composition) has high influence on CO₂ recovery in the CO₂ absorber because of the chemical nature of the absorption process (Veawab, 2002). High MEA make-up flow rate (high MEA composition in lean MEA stream) reduces lost CO₂ in off gas which in turns increases CO₂ recovery (Figure 7). Hence, the optimum MEA make-up flow rate (lean MEA composition) for the current study is 2841 kg/h

(corresponding to 0.228 % MEA). Therefore, operating beyond the optimum value increase operating cost (i.e. high chemical cost) and results to less increase in CO₂ product as can be seen in Figure 7.

Summary of optimization results

Table 1 presents a summary of optimum operating conditions for the industrial CO₂ production process studied.

Table 1: Summary of Optimization Results for CO₂ Production Process

Operating Condition	Base Case	Optimized Case	Difference
Lean MEA temperature (°C)	40	30	10
Operating pressure (bar)	1.5	1.875	0.375
Lean MEA flow rate (kg/h)	831307.45	859365.45	28058
Lean MEA Composition (wt frac.)	0.21	0.228	0.018

Compared to the base case, the optimized process results indicate 10.20 % increases in CO₂ product, which is accompanied by 99 % reduction of CO₂ lost in off gas (Figure 8).

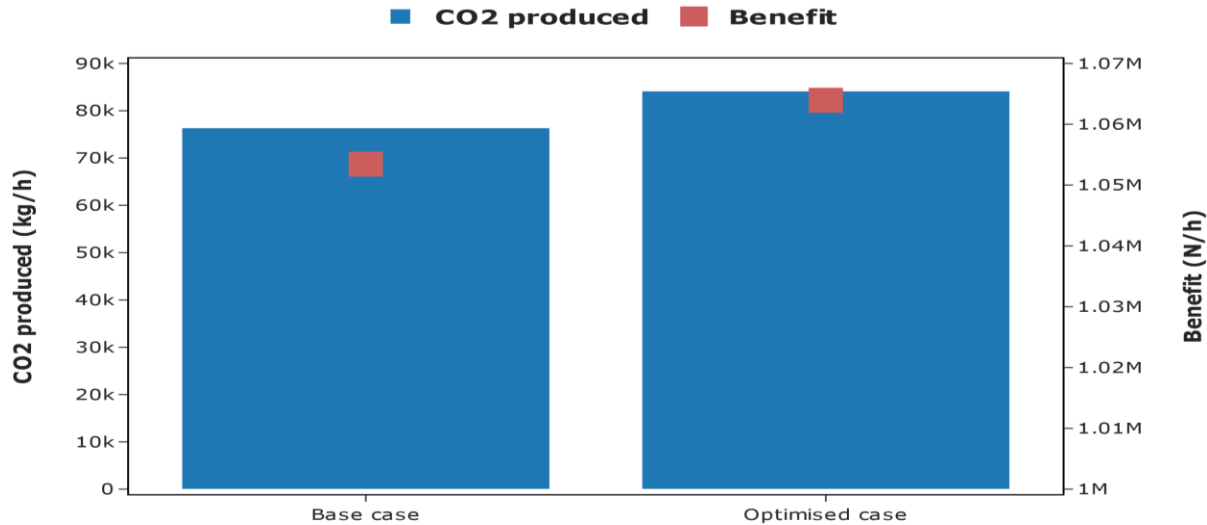


Figure 8: Production capacities for base case and optimized case and net production benefits for case study

The economic results obtained by applying the economic evaluation procedure is presented, analysed and discussed in this section. Thus, the analysis determines the benefit obtained from the optimized process compared with the base process. It should be noted that the current analysis determines only the operational benefit associated to the CO₂ production process. The utility cost is used together with net revenue to evaluate potential benefits as shown in Figure 3.6. Details of the calculation steps can be found in the appendix. As can be seen in Figure 3.6, the optimized case indicates an increase benefit of 1%, which is equivalent to 10,487 ₦/h. However, operating for a one-month period results to a net increase benefit of ₦ 7,550,640.00, which is largely contributed by the increase of CO₂ recovery in the process.

Overall, the following deductions can be drawn from the results, analysis and discussions presented in this section.

- Optimizing lean MEA temperature increases CO₂ yield by 0.3 % and decreases CO₂ lost in off gas by 3 %
- Optimizing operating pressure increases CO₂ yield by 0.8 % and decreases CO₂ lost in off gas by 9 %
- Optimizing lean MEA flow rate increases CO₂ yield by 0.8 % and decreases CO₂ lost in off gas by 9 %
- Optimizing lean MEA composition increases CO₂ yield by 4 % and decreases CO₂ lost in off gas by 57 %

From this analysis, optimizing lean MEA composition independently has the highest impact on CO₂ recovery compared with other

operating conditions. Applying the optimum operating conditions simultaneously on the process increases CO₂ yield by 10.20 % and decreases CO₂ lost in off gas by 99 %. It should be noted that: (i) no improvement of CO₂ recovery is observed with lean MEA temperature above the base case condition, but significant improvement is observed at low temperature, which requires expensive cooling medium, (ii) an increase in operating pressure improves CO₂ recovery, but the pressure increase is limited by the degradation temperature of MEA (124 °C). High operating pressure improves CO₂ recovery, but may lead to lost in MEA strength, (iii) CO₂ recovery may be enhanced by increasing lean MEA flow rate but the reboiler duty may also increase, (iv) optimizing lean MEA composition has the highest impact on CO₂ yield compared with other operating conditions.

CONCLUSIONS AND FUTURE WORK

This research proposes a stepwise approach for modelling and optimising an industrial process for production of beverage-grade CO₂. Key process operating conditions that can impact CO₂ recovery – obtained from literature – include lean MEA temperature, operating pressure, lean MEA flow rate and lean MEA composition. Investigation indicates that the optimum values of the aforementioned operating conditions correspond to 30 °C, 1.875 bar, 859365.45 kg/h and 0.228 weight fraction respectively, leading to CO₂ yield increases by 0.3 %, 0.8 %, 0.8 % and 4 % respectively. Applying the optimum operating conditions simultaneously on the CO₂ production process results to 10.20 % increases of CO₂ yield. It is worth mentioning that the current study considers a minimum cooling water supply temperature of 25 °C to avoid use of expensive utility to minimize utility cost; also, the changes in operating conditions used during the analysis are within equipment limits to avoid huge investment in major units. No improvement of

CO₂ recovery is observed with lean MEA temperature above the base case condition, but significant improvement is observed at low temperature, which requires expensive cooling medium. An increase in operating pressure improves CO₂ recovery, but the pressure increase is limited by the degradation temperature of MEA (124 °C). High operating pressure improves CO₂ recovery, but may lead to lost in MEA strength. CO₂ recovery may be enhanced by increasing lean MEA flow rate but the reboiler duty may also increase. Optimizing lean MEA composition has the highest impact on CO₂ yield compared with other operating conditions. Lastly, the successful application of the developed methodology to economically optimize CO₂ production process leads to 1% increase in benefit, which is equivalent to ₦ 10,487/h and/or net benefit of ₦ 7,550,640.00 per month. Important limitations of the current methodology include: (i) optimization of CO₂ recovery is achieved by adjusting the operating conditions independently. This approach limits the optimization of CO₂ recovery to the optimum value of only one operating condition, (ii) adjustment of operating condition to improve CO₂ recovery is limited to the design capacity of process equipment in the CO₂ production process, (iii) capital cost is not considered in the present work because the research focuses only on operational optimization.

Future work should focus on addressing: (i) optimization of CO₂ recovery has been achieved by adjusting each operating conditions independently and the corresponding improvement of CO₂ recovery are monitored. The approach provides insight into which operating conditions have high influence on CO₂ recovery. Therefore, considering the optimization of two or three operating condition simultaneously could provide an improved performance. It is proposed that research be carried out using similar procedure to the current work, but should consider optimizing two or

more operating conditions simultaneously; therefore, the combine best performance of the two operating conditions in question could be determined; (ii) in the current study, it has been noticed that the flue gas stream from the burner provides a heat source, with high potentials for steam generation and heat recovery. Integrating the flue gas stream with other units in the CO₂ production plant that are overall heat sinks (e.g. boiler) would enable transfer of considerable amount of heat or steam between the two units. Future work could consider enhancement of CO₂ recovery simultaneously with heat recovery between the CO₂ production plant and boiler/

heat recovery steam generator (HRSG). Also, the design of heat exchanger network for heat recovery in the process could be considered; (iii) the current research is limited to optimizing CO₂ recovery in the CO₂ production plant, without exceeding the capacity limit of equipment. It is recommended that research be carried out that will explore optimization more widely, to search for more potential benefits. The proposed work would consider process revamps, and require more detailed capital cost analysis, in addition to optimization of operating conditions to improve CO₂ recovery.

REFERENCES

- Alibaba. (2014, January 8). *99.5% Ethanolamine CAS NO 141-43-5/Monoethanolamine 99.5%*. Retrieved July 20, 2014, from: http://www.alibaba.com/product-detail/99-5-Ethanolamine-CAS-NO-141_1175921515.html
- Augsten, D. (1989). *A model for vapor-liquid equilibria for acid gas-alkanolamine-H₂O systems*. Austin: University of Texas.
- Austell, J. M. (2005). CO₂ for Enhanced Oil Recovery Needs – Enhanced Fiscal Incentives. *the Oil & Gas Review*.
- Avizienis, A. (2014, January 1). *Advameg, Inc.* Retrieved July 11, 2014, from Advameg Web site: <http://www.madehow.com/Volume-2/Soft-Drink.html>
- Chakma, A. (1987). *Degradation of Aqueous DEA Solutions in a Heat-Transfer Tube*. Canada: Canadian Journal of Chemical Engineering.
- Chapel, D. (1999). *Recovery of CO₂ from Flue Gases: Commerical Trends*. Saskatchewan, Canada.: Canadian Society of Chemical Engineers.
- Dean, C. F., Golden, S., & Rich, P. (2005). Increasing FCC propylene yield. *Saudi Aramco Journal of Technology*, 44-51.
- Doty. (2013, May 16). *Doty Energy*. Retrieved July 20, 2014, from http://www.dotyenergy.com/Economics/Econ_Physical_CO2_Market.htm
- Fermi. (2011, January 1). *TECNO PROJECT INDUSTRIALE*. Retrieved July 11, 2014, from <http://www.tecnoproject.com/ENG/CO2-Production-Plants-from-fuel-combustions.asp?target=2>
- Goff, G. (2005). *Oxidative degradation of aqueous monoethanolamine in CO₂ capture processes*. Austin: University of Texas.
- Goff, G. (2004). Monoethanolamine degradation: O₂ mass transfer effects under CO₂ capture conditions. *Industrial & Engineering Chemistry Research*, p. 6400-6408.
- Kohl, A. (1997). *Gas Purification*. New York: Elsevier.
- Metz, B. (2005). *IPCC Special Report on Carbon Dioxide Capture and Storage*. Editors.
- ntg. (2013, January 1). *Nigeria Technology Guide*. Retrieved July 2014, 20, from Nigeria Technology Guide: <http://www.naijatechguide.com/2013/06/new-electricity-tariff-cost-phcn-abuja.html>
- Pitt, M. (2013, January 8). *ICHEME Education Subject Group*. Retrieved July 2014, 1, from IChemE Education Subject Group.: <http://ed.icheme.org/costutil.html>
- Reddy, S. D. (2008). *Fluor's Econamine FG Plus Technology for CO₂ Capture at*

- Coal-fired Power Plants*. Baltimore: Mega Symposium.
- Reddy, S. J. (2003). *Fluor's Econamine FG Plus Technology: An Enhanced Amine-Based CO₂ Capture Process*. Alexandria, VA.: National Conference on Carbon Sequestration.
- Ringo, S. M. (2001, January 1). *Food Safety Magazine*. Retrieved July 31, 2014, from Food Safety Magazine: <http://www.foodsafetymagazine.com/magazine-archive1/december-2000january-2001/international-society-of-beverage-technologists-carbon-dioxide-guidelines/>
- Rochelle, G. S. (2001). *Research Needs for CO₂ Capture from Flue Gas by Aqueous Absorption/Stripping*. Austin: University of Texas.
- Ronald, P. (2001). *Kirk-Othmer Encyclopedia of Chemical Technology*. Wiley.
- Rushing, S. A. (2012, November 16). *Carbon dioxide: key to boosting revenues and limiting emissions from biofuels and allied ventures*. Retrieved July 31, 2014, from <http://www.biofuelsdigest.com/bdigest/2012/11/16/carbon-dioxide-key-to-boosting-revenues-and-limiting-emissions-from-biofuels-and-allied-ventures/>
- Smith, R. (2005). Chemical Process Design and Integration. In R. Smith, *Chemical Process Design and Integration* (pp. 181-184). Chichester: Wiley.
- Supap, T. R. (2001). Kinetics of the oxidative degradation of aqueous monoethanolamine in a flue gas treating unit. *Industrial and Engineering Chemistry Research*, p. 3445-3450.
- Treybal, R. E. (1981). Mass-Transfer Operations. In R. E. Treybal, *Mass-Transfer Operations* (pp. 275-282). Singapore: McGraw-Hill.
- Veawab, A. (2002). Identification of oxidizing agents in aqueous amine-CO₂ systems using a mechanistic corrosion model. *Corrosion Science*, p. 967-987.
- Yela, S. (2009). *Framework for Operability Assessment of Production Facilities: An Application to a Primary Unit of a Crude oil refinery*. Unpublished.