

Retrofitting a CO₂ Capture Unit with a Coal Based Power Plant, Process Simulation and Parametric Study

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Abstract—In this work flowsheet simulation of a coal fired power plant retrofitted with a CO₂ capture unit has been carried out in the AspenPlus process simulator platform. The simulation is an attempt for the detailed process involved in CO₂ capture starting from generation of flue gas, CO₂ capture by monoethanolamine (MEA) and regeneration of solvent using unit operation models available in Aspen Plus and appropriate calculator blocks wherever necessary using FORTRAN codes. The parametric study includes effect of absorber column height, regenerator pressure, on reboiler heat duty and power plant efficiency. Parametric study such as energy penalty on the power plant, reboiler duty of the capture unit, evolution of energy requirement has been done and presented. The contribution of desorption energy is about 47% of the total capture energy and the power plant penalty is about 30% lower when low pressure steam has been utilized to supply heat energy to reboiler.

Index Terms—CO₂ capture, MEA, absorption, coal-fired power plant, simulation.

I. INTRODUCTION

One of the most serious problems facing the human civilization today is global warming, climate change and consequential damage to the environment of this blue planet, the habitat of *homo sapiens*. Hence, one of the most challenging issues confronting the international community in this century is how to simultaneously attain economic growth, poverty mitigation and energy security without deteriorating earth's environment further. Currently, fossil fuels (coal, oil, and natural gas) supply over 85% of the world's commercial energy, account for 65% of the world's electricity and 97% of the energy for transportation. As world population multiplies to about 9 billion in 2050 and demand for energy to sustain economic growth increases exponentially, energy supply projections point to the fact that abundant, affordable fossil fuels will have to be used to fuel economic growth well beyond 2030.

The production and use of fossil fuels contribute to 64% of anthropogenic greenhouse gas (GHG) emission worldwide, and fossil fuel based power generation currently accounts for over one third of global annual CO₂ emissions. Although among the green house gases (GHGs) such as CH₄, N₂O, halogens, CO₂ and water vapor, CO₂ is the least potent GHG on a molecular basis, given its sheer abundance and increasing emission levels, the threat of global warming is the highest from the emission of CO₂.

Manuscript received October 10, 2015; revised February 10, 2016.

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Large point sources of CO₂ include fossil fuel based energy facilities, natural gas processing, ammonia manufacture, oil refining operations, cement manufacture, ethylene production, and the aluminium, iron and steel industries. Because fossil fuel based electric power plants produce about one third of all CO₂ emissions worldwide, these along with the other large point sources such as natural gas processing plants and ammonia plants, are the prime targets for CO₂ capture and sequestration. Historically, coal has been the most significant fuel for electricity generation. The use of coal as a power source has steadily been rising since 1950. Natural gas use also increased, while petroleum combustion has remained fairly stable.

Another important factor to consider is the efficiency of fuels for power production. The efficiency is directly related to the amount of fuel necessary to produce the required quantum of electricity, and thus the amount of CO₂ produced. Of the three main plant types, natural gas-fired plants are the most efficient (55 to 60%) and the cleanest burning in terms of carbon, producing 0.45 kg CO₂/kW-hr. Power production from petroleum fuels gives 0.80 kg CO₂/kW-hr. Coal-fired plants produce the most CO₂, approximately 0.96 kg CO₂/kW-hr and are only 40 to 45% efficient. Hence, it is clear that the largest potential application for CO₂ capture is coal-fired power plants, and next to that are natural gas processing, ammonia manufacture and other point sources of CO₂. Although, amine solvent based absorption processes have been widely practiced for several years, capturing substantial amounts of CO₂ from the flue gas from a coal fired power plant using amine absorption technology requires large amount of energy, mostly in the form of heat. Although there are many new and patented technologies coming now days, monoethanolamine (MEA) based absorption process is still considered to be a feasible option that can be deployed in power plants.

Many researchers have reported MEA based absorption system for post combustion CO₂ capture (PCC). Wang *et al.* [1] presented a review report on PCC with chemical solvents. They emphasized that PCC is probably the first technology that will be deployed in the existing and new thermal power plants. Laura *et al.* [2] compared energy saving using different solvent with respect to PCC process by doing process simulation and configuration in Aspen platform. For their base line configuration in which 2.1053 kmol/h of CO₂ captured by 30 mass% MEA, they found that the reboiler heat duty was 187.5 kW. Cousins *et al.* [3] analyzed process flowsheet modification for energy efficient CO₂ capture from flue gases with aqueous solution of MEA. Their simulation results for 85% CO₂ capture from flue gas with a CO₂ purity stream of about 98% revealed that up to 19% energy can be saved by using vapor compression of lean solvent flashing.

Ho *et al.* [4] compared the MEA capture cost for low CO₂ emission sources in Australia. They reported that the capture cost depends on characteristics of industrial emission and it is similar for the PCC process from black coal pulverized coal power plants. Experimental pilot plant study of CO₂ capture using MEA absorbent has been reported by Badea and Dinca [5]. They also reported that the total thermal energy required for this process was 3.1 GJ/tonne CO₂ capture. Lawal *et al.* [6] presented dynamic rate based modeling of PCC process using MEA in a gPROM platform. Their simulation study showed that the normal behavior absorption and regeneration column operation could be maintained during load operation of flow rates of the flue gas and lean solvent. Cifre *et al.* [7] studied the simulation of a power plant with MEA based CO₂ capture and compression process.

Notz *et al.* [8] completely analyzed PCC process with MEA technology using a pilot plant study. They evaluated various energy contributions to the process such as heat of desorption, stripping steam requirement, heating of the solvent and heating of the condensate reflux and found that about 47% of the total energy goes to desorption of CO₂. In a similar work, Dash *et al.* [9] analyzed PCC process with new solvent consisting of aqueous solution of piperazine and 2-amino 2-methyl-1-propanol (AMP+PZ). For their simulation work, kinetic parameters and other properties were taken from [10]. Dash *et al.* [9] found that the contribution to the regeneration energy of this new solvent is comparable to that of MEA Technology.

In this present work, state-of-the-art process simulation tools are used to model coal combustion, steam cycle, and MEA absorption process in AspenPlus platform [11]. These disparate models are then combine to create a model of a coal-fired power plant with integrated CO₂ capture with the assumptions that, using the waste heat and low pressure steam from the power plant steam cycle to satisfy the heat requirements of the MEA absorption process. This base case simulation will have a scope to simulate power plant CO₂ capture using novel solvents based on sterically hindered amines, amine blends, and activated amines being developed in our lab and in the ongoing research work.

II. OVERALL PROCESS DESCRIPTION

This simulation work is an attempt to the detailed process involved in CO₂ capture starting from generation of flue gas in a coal-fired thermal power plant. This also includes the heat duty and the power requirements for the process units with an integrated steam cycle simulation determining the amount of steam required for the process. As commercial simulator has been used, only the outlines of the process are described here. The CO₂ recovery technology employed here is a solvent based absorption process. The simulations are so designed to make it relatively simpler to replace the MEA components with any alternate solvent available for CO₂ capture. This can be extended in comparing the efficiency of different solvents. The whole process can be divided into three sections, the coal combustion section, the steam cycle and power generation section and the CO₂ capture section from the flue gas generated. The CO₂ capture process includes absorption of CO₂ in alkanolamine solution and then

recovery of the used solvent in order to reuse it. The flue gas generated from the coal fired power plant is scrubbed to remove other acid gases present in the gas like SO₂, SO₃, HCl, HF, NO and NO₂ and fly ash (particulates). These if present results in high amine losses predominantly through the formation of aqueous acids that react with MEA to form amine salts that cannot be regenerated through the steam stripping processing.

The feed to the power plant is coal of known specifications (both proximate and ultimate analysis). The process specification for the complete combustion of the feed are calculated and modelled accordingly. The fundamental underlying principle for the absorption process is the exothermic, reversible reaction between a weak acid (CO₂) and a weak base (MEA) to form a soluble salt. The inlet gas to the absorber is contacted counter-currently with the 'lean' solvent (with respect to solvent content). Carbon dioxide is preferentially absorbed by the solvent. The enriched solvent with CO₂ is pre-heated before entering the stripping column where, the reaction is reversed by applying heat energy in the form of steam. From the bottom of the column, the lean solvent exchange heat with the rich solvent entering the column and is recycled back to the Absorber. From the top, a high-purity CO₂ is produced upon separation of CO₂ from steam in a flash drum.

A. Modelling of Individual Sections

Coal combustion unit: The simulation flow-sheet of coal combustion unit is as shown in the Fig. 1.

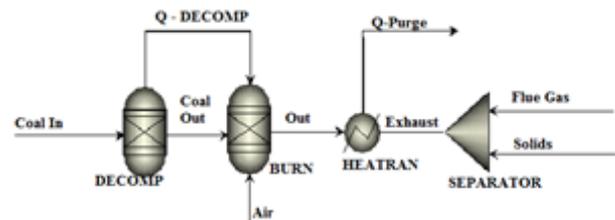


Fig. 1. Flow-sheet for coal-combustion unit.

This section has been modelled using appropriate unit operation blocks from the AspenPlus model library [11]. The description of these blocks is given later in this section. It is required to specify the components, i.e., reactants and products involved in the reaction process along with the property model that handles coal operation. Specification of streams and blocks depends on the block function and the charge to be handled. In this simulation-sheet there are some calculator blocks present such as air flow calculator, which calculates the air volume required for complete combustion of the coal. Normally all the properties of the coal are available on dry basis. To get actual coal composition it should be converted to wet basis that takes part in the combustion process. The coal considered in this work has ultimate, proximate and sulphur analysis given in Table I.

TABLE I: PROXIMATE AND ULTIMATE ANALYSIS OF COAL

Proximate analysis (% dry basis):			
Moisture	Volatile matter	Ash content	Fixed Carbon
5.98	20.7	38.63	34.64
Ultimate analysis (% dry):			
Carbon	H ₂	N ₂	S
41.11	2.76	1.22	0.41

Before simulating the process we need to convert the coal specification values into wet basis which is the actual composition of the coal that take part in the combustion reaction. To do this a calculator block *C-dec* is defined converting the mole fraction of each element to the same when moisture is included. The air flow required for the complete combustion of supplied coal can be calculated by introducing a calculator block *AIR-FLOW* wherein the required amount of O₂ is calculated for oxidation of carbon, sulphur, nitrogen and hydrogen present in coal. The summary of the blocks used and their descriptions are presented in Table II.

TABLE II: SUMMARY OF MAIN STREAMS AND BLOCK USED IN THE COAL COMBUSTION SECTION

Streams		
COAL-IN	The inlet coal flow rate, considering a 500MW power plant, is taken as 10 kg/sec.	
AIR	A simplified composition of air is taken which is nominally 78% N ₂ , 21% O ₂ , and 1% Ar. AIR flow rate is calculated such that there is 21% excess O ₂ in the burner.	
Blocks		
C-DEC	calculator	Converts the mole fraction of each element of coal to the same when moisture is included
Air flow	calculator	Calculate the air volume required for complete combustion of coal.
DECOMP:	RYIELD	decomposes the coal into a stream of component elements
BURN	RGIBBS	performs rigorous reaction based on Gibbs free energy minimization
HTRAN	HEATER	basically a heat exchanger where sensible heat of the burnt feed can be utilised

With the above specifications and block calculations the simulation was performed. Results from the simulation with respect to the composition of the flue gas generated from the coal burnt thermal power plant are presented in the result and discussion section.

B. CO₂ Absorption with MEA

The CO₂ capture process includes absorption of CO₂ in MEA solution and then recovery of the used solvent in order to reuse it. The fundamental underlying principle for the absorption process is the exothermic, reversible reaction between CO₂ and MEA to form a soluble salt. The inlet gas to the absorber is contacted counter-currently with the ‘lean’ solvent coming from the regenerator. Carbon dioxide is preferentially absorbed by the solution. The enriched solution with CO₂ is pre-heated before entering the regeneration column also known as stripping column where, through the addition of heat, the reaction is reversed. From the bottom of the column, the lean solvent exchange heat in a heat exchanger with the rich solvent entering the column and is recycled back to the absorber. From the top of the stripping column, a high-purity CO₂ is produced after flash operation. A representative flow sheet of this section is given in Fig. 2.

The description of the unit operation blocks are given in Table III.

In this process simulation, few alterations to the process can be made in optimizing the plant performance like introducing a flash column for the rich outlet stream as the absorber operates at high pressure or by heating a part of the stripper feed which considerably lowers the reboiler heat duty. Vapour can be compressed in the regeneration column and

send back to the reboiler which also will help for energy saving. The design variables of each unit depend on the plant’s output specifications which are a balance between the performance, availability and the cost of operation.

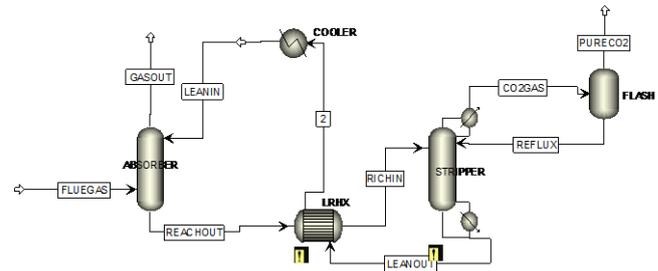


Fig. 2. Process flow sheet of the MEA absorption process.

TABLE III: DESCRIPTION OF THE ASPEN BLOCKS USED

Block Name	Block Type	Description
Absorber column	RadFrac	The <i>Absorber</i> column is simulated, considering four aspects of the units: column configuration, column type, internal geometry, and column pressure.
Stripper column	RadFrac	The <i>Stripper</i> has both a partial condenser and a conventional reboiler. The molar reflux ratio is varied to achieve a specified condenser temperature; the bottoms-to-feed ratio is adjusted such that the desired molar flow of CO ₂ in the distillate is obtained.
Blower	COMPR	The <i>Blower</i> is required to overcome the pressure drop in the cooler and the absorber.
MAKE-UP	MIXER	Adds MEA and H ₂ O to the process to exactly offset the small amounts that are lost from the top of the absorber and as a part of stripper distillate
H ₂ O Pump and Rich Pump	PUMP	For <i>H₂O Pump</i> , the pressure rise is effectively that required to overcome the pressure drop of the <i>Direct Contact Cooler</i> and the <i>Absorber</i> . For <i>Rich Pump</i> , the <i>rich</i> solvent pressure is increased, if required, to equal the <i>Stripper</i> pressure at the feed segment.
Cooler	HEATER	The <i>Cooler</i> cools the <i>lean</i> solvent to the desired <i>Absorber</i> inlet temperature (typically 40°C).

C. Method for Stand-Alone Simulation of CO₂ Capture Process

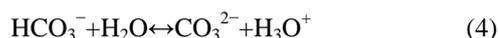
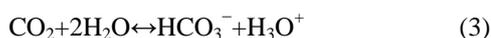
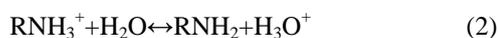
The flow sheet described in Fig. 2 is simulated by choosing appropriate unit operation models in AspenPlus Platform described in Table III. The thermodynamic property method is chosen to take into account the reaction kinetics and the intermediate products formed. Streams along with the process blocks are specified based on the block function and amount of charge handled. Modelling of the absorber and the stripper column calls for knowledge of the detailed mechanism involved in mass transfer. The mass transfer correlations are used as suggested by Aroonwilas *et al.* [12].

As a preliminary design to the heat exchangers we choose a constant heat transfer coefficient with a 5 °C temperature approach. Since the reactions involved are thermodynamically controlled, we limit the prevailing temperature (and hence pressure) inside the column. For efficient absorption of CO₂ in the absorber a concentration of 30 mass% aqueous solution of MEA is used which is maintained at each charge to the absorber. This is done by defining a calculator block which calculates and adds the amount of lost solvent in the stream. Lastly for a desired amount of CO₂ capture, the stream calculations are put into

loops to attain the design specifications (for each column) with an allowable error and are solved in order of their occurrence in the flow-sheet.

D. Specifying Properties

The solution chemistry of the absorption is a series of equilibrium reactions represented by (1)–(5).



The reactions are automatically generated in Aspen simulation with electrolyte NRTL property methods which have its limits of temperature up to 120°C and amine concentration up to 50%. Electrolyte NRTL being more flexible of the two is used in the simulation process.

E. Specifying Streams and Blocks

As a minimum, the conditions and flow rates of the three input streams, FLUE-BLO, H2O-PUMP and MAKE-UP, should be specified. For standalone simulation of the absorption process specifications to FLUE-BLO is required. For simpler process compilation and better convergence number of components in the flue gas is reduced to only N₂, CO₂ and H₂O. For the cooling tower, water (H2O-PUMP), at ambient temperature (25°C) and atm. pressure is used. The flow rate of the water is calculated to bring the hot flue gas stream to the inlet temperature of the absorber column. MAKE-UP stream adds MEA and H₂O to the process to exactly offset the small amounts that are lost from the top of the absorber and as a part of stripper distillate. The required flow rate of this stream can be calculated by introducing a calculator block before MIXER block. Temperature and pressure is assumed to be 25°C and 1 atm. respectively.

For simulating gas-liquid absorption and stripping columns AspenPlus provides RadFrac which is a rate based simulation [11]. It takes the column type and some geometry information as input from which it computes the coefficients, flow velocities, and hold-up times needed to calculate mass transfer. The Absorber and Stripper columns are modelled by considering four aspects of the units: column configuration, column type, internal geometry, and column pressure. For the *Absorber*, the flow is counter current so the inlets and outlets are connected to the top and bottom of the column. The *Stripper* has both a partial condenser and a conventional reboiler. The feed enters the column above the mass-transfer region. The molar reflux ratio is varied to achieve a specified condenser temperature of 40°C. The bottoms-to-feed ratio is adjusted such that the desired molar flow of CO₂ in the distillate is obtained. Both columns are modelled with sieve trays because they are commonly used and correlations exist for characterizing their hydrodynamic performance. For the column operation specifications, unknowns are the diameter

and the number of trays required. So as an initial estimate to the diameter of the column is taken as 20m with an entrainment flooding of 75%, tray spacing 192 in, and weir height 24 in. Increasing the pressure in the *absorber* would increase the reactivity of MEA in CO₂ but this comes with increased cost of pressurizing the flue gas. Therefore, the pressure at the top of the *absorber* is fixed at 1atm. In the case of the *stripper* increasing the pressure raises the column temperature. The temperature is limited to a maximum of 120 °C after which thermal degradation of 30 mass% MEA solution becomes intolerable. Therefore, in the process model, the pressure of the *stripper* reboiler is set such that the reboiler temperature does not exceed 120 °C. A *Blower* is used to overcome the pressure drop in the cooler and the absorption column and is implemented using the COMPR model. The specification includes the stream pressure rise and the performance characteristics. The pressure rise is initially set consistent with the initial pressure conditions in the *absorber*. The CO₂ Compressor (not shown in the figure) is required to compress the CO₂ for transportation via pipeline and is implemented using the MCOMPR model. Basically MCOMPR is a series of COMPR blocks interspersed with heat exchangers and is therefore suitable for modelling a multi-stage compressor with inter-cooling. This block requires the outlet pressure, compression performance, and the inter-stage temperatures to be specified. In this simulation the CO₂ is compressed to 110 bar at a temperature of 25°C. The water *Pump* and *Rich solvent Pump* are both modelled with the PUMP model. With all the above assumptions and initial approximation to the block parameters, compiler iteration decreases.

III. RESULTS AND DISCUSSION

For the successful simulation of the coal-combustion section, the flue-gas composition obtained can be studied with changing coal specifications. In general, the energy efficiency of a thermal power plant is about 40%, so for this low efficiency thermal power plants generally use a blend of low grade coal (mostly lignite and peat) for the combustion process. Tables IV and V present proximate and ultimate analysis respectively for three different coal compositions used in NALCO (National Aluminium Company) captive power plant at Orissa, India.

The simulation results for flue gas composition are presented in Table VI.

TABLE IV: ^a PROXIMATE ANALYSIS

	Moisture content	Volatile matter	Fixed carbon	Ash content
Coal A	13.52	30.44	21.94	47.62
Coal B	18.59	46.88	33.54	19.58
Coal C	9.43	32.89	51.662	15.42

^aData obtained by personal communication

TABLE V: ^a ULTIMATE ANALYSIS

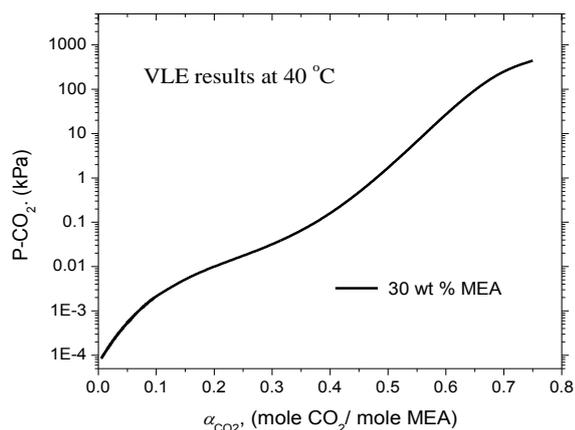
	H ₂	C	N ₂	S	O ₂	Ash
Coal A	3.49	39.07	0.4	0.75	11.67	47.62
Coal B	4.47	55.12	0.89	0.57	19.37	19.58
Coal C	4.593	65.00	1.126	0.6183	13.116	15.42

^aData obtained by personal communication

TABLE VI: SIMULATION RESULTS: (FLUE-GAS COMPOSITION OF MAJOR COMPONENTS)

Flue-gas composition	Coal A	Coal B	Coal C
N ₂	0.676	0.735	0.763
Ar	0.009	0.009	0.010
CH ₄	0.074	0.013	0.003
CO ₂	0.153	0.159	0.157
H ₂ O	0.074	0.074	0.074

From the above simulation results, it is found that the CO₂ composition in the flue gas stream is around 15% but normally the flue-gas composition in a coal fired power plant varies from 10–13%. Hence this simulation slightly over predicted CO₂ composition in flue gas but it may depend on the quality of coal used and the combustion process adopted. The simulated flue gas composition also includes trace amount of H₂, CO, SO₂ and NO₂ which are found quite noticeable in an actual power plant. Validation of experimental data with simulation results is quite important. The model predicted vapour liquid equilibrium of CO₂ over 30 mass% MEA is presented in Fig. 3 which has a well agreement with literature data. With respect to CO₂ capture, the results are not presented here, since the improvement of the simulation study is in progress. The results of the blocks and streams may be communicated in a later date.

Fig. 3. VLE of CO₂ in 30 mass% MEA.

The simulation and parametric study have been carried out with the condition that 90% of CO₂ removal from the flue gas and 98% pure CO₂ from the stripper column. The base case for the power plant is 500 MW. To supply heat to the reboiler, low pressure steam from power plant has been extracted and supplied to the regeneration column. As a result the power plant efficiency has decreased. The effect of regenerator pressure (pressure of CO₂ + steam + amine vapour) on the reboiler duty and power plant efficiency was investigated and the results are presented in Fig. 4. With a variation of regenerator pressure from 1 to 3 bar the reboiler duty has been computed. With variation of reboiler duty the steam drawn from the power plant changes and hence efficiency of the plant also changes. These effects are presented in Fig. 4. It is found from Fig. 4 that the reboiler duty is less at higher pressure which corresponds to higher temperature and the plant efficiency is also high at this condition. But at high temperature, special material of construction is required; again the corrosion and thermal degradation of the solvent become significant.

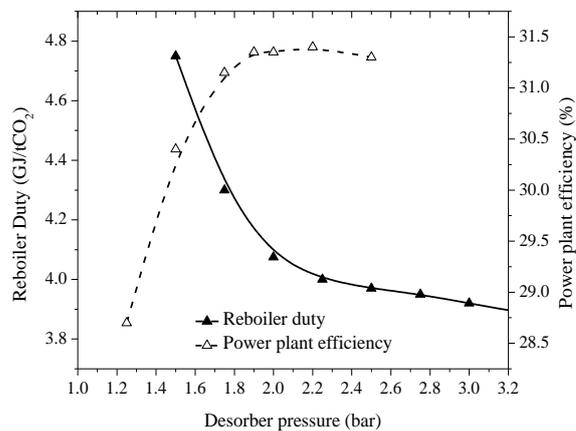


Fig. 4. Effect of regenerator pressure on reboiler duty and power plant efficiency (the base efficiency of the power plant is assumed as 45%).

The effect of height of the absorber column on reboiler duty and power plant efficiency is presented in Fig. 5. It is observed that the reboiler duty is decreases with increasing in the packing height. Again the power plant efficiency is also increases with the packing height.

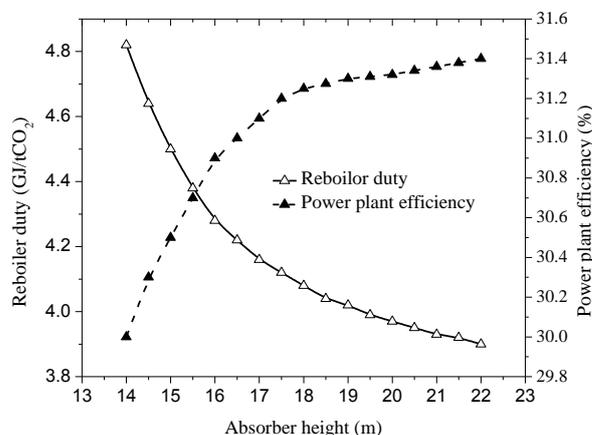


Fig. 5. Effect of absorber column height on reboiler duty and efficiency of the power plant.

This is due to the increase of mass transfer area in the column which favours more absorption of CO₂ in the column. But increasing the column height also increases the capital cost and, hence an overall economic analysis is required to choose the optimum column height.

The energy requirement for the regeneration of the solvent can be split up into four contributions as suggested by Notz *et al.* [8]. These contributions are i) energy has to be supplied to reverse the CO₂ reaction (heat of desorption), ii) to generate additional stripping steam, iii) heating of the rich solvent and iv) heating of the condensate reflux. Of course there may be slight mismatch of these quantities in an actual plant due to foaming behavior as reported by Chen *et al.* [13]. This splitting of the energy requirement for 30 mass% MEA is shown in the Fig. 6. It is found that 47.12% of total energy is utilized towards desorption of CO₂ i.e., reversing the carbamate reactions and 35.19% of energy goes to generate steam required for stripping. The contribution towards sensible heat i.e., heating the solvent and reflux are 15.11% and 2.58%, respectively. The heat of desorption of MEA is found to be slightly greater than that of heat of desorption of (AMP+PZ) blended solvent reported by Dash *et al.* [9].

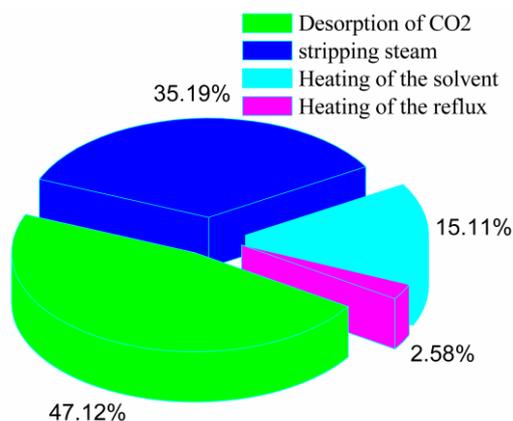


Fig. 6. Contribution to the regeneration energy for the MEA solvent.

The contribution of different energy has been compared with the work of Notz *et al.* [8]. It is observed that these results are in comparable with the results of Notz *et al.* [8].

IV. CONCLUSION

As a summary, the above simulation and parametric study is part of an integrated thermal power plant wherein the simulation of the flue gases generated is discussed thoroughly without going detail into the energy produced or the power required by the unit. So far, considering the power plant as a whole, a steam cycle has been coupled with the unit i.e. basically using steam as the working fluid for productive energy transformations and simulations has been done for optimizing the power load on different heat transfer units. The performance of the MEA based solvent has been carried out. Among the various parameters such as column pressure, temperature and height; solvent flow rate (liquid to gas ratio), reboiler heat, lean and rich solvent concentration etc., the solvent flow rate is important as it contributes the three out of four energy requirement. This relates to the reboiler heat duty calculation. The reboiler duty with column height, column pressure and power plant efficiency has been analyzed.

The simulation can further be modified and extended to account for the different plant configuration such as vapour recompression and interstate cooling of the absorber. With a wide variety of solvents available for CO₂ absorption, the model can also be used for comparing the performance of each with varying temperature and pressure. Further sensitivity analysis can be done for studying the optimum loading for a particular solvent with varying column specifications of the absorber and the stripper.

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