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*Proceeding Paper*

# Modeling and Simulation of Chemical Absorption Methods for $CO_2$ Separation from Cement Plant Flue Gases†

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**Abstract:** Climate changes; especially global warming; are observed due to greenhouse gases released on an industrial scale. For this reason; progress is being made around the world to reduce $CO_2$ emissions and transition to sustainable energy sources. One of the most matured methods of capturing $CO_2$ from flue gases in industrial sectors is chemical absorption. This work analyzed the absorption process in capturing $CO_2$ from the flue gases of a 1 Mt cement plant. The Aspen Plus modeling package was used to simulate the flue gas pre-treatment; absorption column; and regeneration unit. As a result of the modeling; optimal values of column sizes; heat duty; and solvent make-up that require the least capital and operational costs for capturing $CO_2$ in the flue gases of this plant were determined. When a 40% MEA solution is used and the $CO_2$ loading in the absorption-stripping process is 0.25 mol/mol; the reboiler heat duty is 4.06 MJ/kg $CO_2$.

**Keywords:** climate change; absorption; modeling; heat duty; flue gas; $CO_2$ capture

## 1. Introduction

Since the onset of the industrial revolution, human activities have had detrimental effects on the natural environment, resulting in widespread climatic alterations around the globe. The release of carbon dioxide ($CO_2$) gas into the atmosphere stands as one of the main contributors causing climate change [1]. Carbon capture, utilization, and storage (CCUS) technology including post, pre, and oxy-fuel combustion $CO_2$ capture methods has emerged as a very effective method for mitigating anthropogenic carbon dioxide ($CO_2$) emissions [2].

Currently, the amine-based chemical absorption method has achieved the highest level of maturity in post-combustion $CO_2$ capture [3]. Amine-based carbon capture technology has been effectively used for capturing $CO_2$ from flue gases with low $CO_2$ concentration [4]. This technology has found application in large-scale power plants, cement plants, and other sectors with significant carbon emissions [5]. Figure 1 illustrates the basic flow diagram of the absorption-based carbon capture process. In this process, the $CO_2$ present in the flue gas stream, which comes from cement plant, has a reaction with the solvent inside the absorption column. Subsequently, the solvent, which has been enriched with $CO_2$, is thermally regenerated within the stripper column. The lean loading solution, which is free from $CO_2$, is returned to the absorption column after a process of

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heat exchange with the rich-lean solution and subsequent cooling. The $CO_2$ stream with a high level of purity is conveyed to a process involving compression and subsequent usage or storage of the carbon. A flue gas stream that has undergone treatment is discharged into the atmosphere.

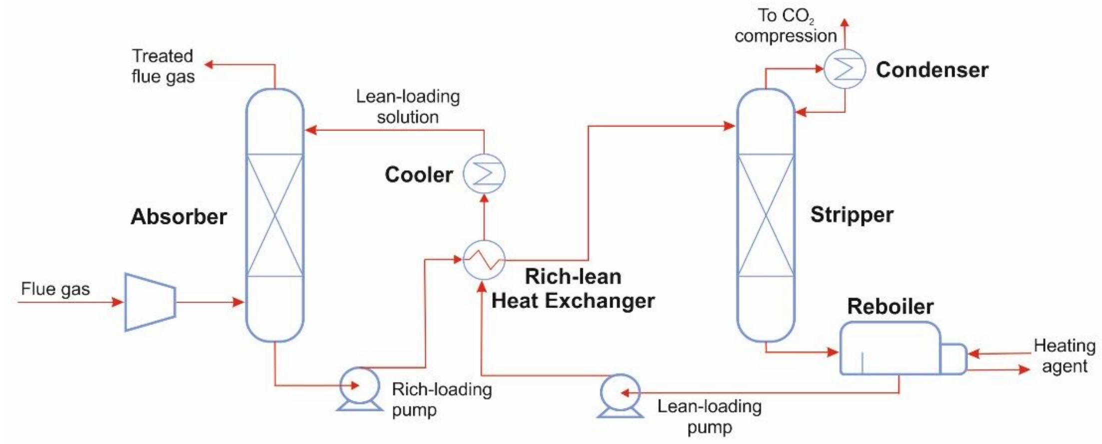


**Figure 1.** Flow diagram of a basic chemical absorption for $CO_2$ capture (Modified from [6]).

In this work, a modelling-based study of the "tail-end" chemical absorption method for $CO_2$ separation from cement plant (1 Mt production capacity annually) flue gases and determination of the best values in different configuration system cases are considered. This study is considered part of "Techno-economic evaluation of post-combustion $CO_2$ capture technologies for cement plant flue gases". Further future work will include comparative studies of this work as benchmark technology with other near or early stage post-combustion $CO_2$ capture technologies.

## 2. Methodology

### *2.1. Model development*

The core methodology for this research involves modeling and simulation using the Aspen Plus software. Our key targets and constraints are set as follows: $CO_2$ removal efficiency must be greater than 90%, $CO_2$ purity should be greater than 95%, and the occurrence of flooding in the absorption/stripper columns must remain below 75%. Aspen Plus process simulation software was chosen as the primary tool for modeling and simulating the selected $CO_2$ capture methods [7]. We developed simulation models that accurately represented the chosen chemical absorption methods. First, the absorber/stripper system were modelled and simulated on the open loop principle. Targets are accepted $CO_2$ removal in the flue gases, the purity of $CO_2$, and column packing flooding factor to build model. Packed column sizing is calculated for selected packing material [8]. The rate-based model is the most used approach based on two-film theory in the case of amine-based absorption. In the process of modeling, the following causes should be considered:

a) due to the high mole fraction of $CO_2$, a higher liquid/gas ratio is required for $CO_2$ molecules to absorb into the liquid phase. This causes more energy to be spent on solvent regeneration;

b) in order to reduce the column dimension, as well as to increase the gas/liquid transfer surface area, the selection of the packing material and the consideration of pressure drop and flooding are the most important requirements.

### *2.2. Case study scenarios*

Our research incorporated case studies to evaluate the performance of the selected chemical absorption methods under diverse operating conditions. These scenarios encompassed variations in solvent properties (30 and 40 % wt.) and $CO_2$ loading (0.134, 0.18, and 0.25 mol/mol) conditions (see Table 1). The composition of $CO_2$ in the incoming flue gas is consistent across all three cases, with a mole fraction of 0.1891. Examining these scenarios, we estimated acceptable reboiler duty in the stripper column and solvent make-up values in the absorption method of $CO_2$ capture in cement plant flue gas.

**Table 1.** Hydraulically design and packing internals for the absorption / stripping columns.

| | **Case 1** | **Case 2** | **Case 3** |
|---|---|---|---|
| | Absorption column | | |
| Packing diameter | 8.6 | 10 | 8.8 |
| Packing height | 35 | 45 | 35 |
| Packing type | RASCHIGPAK 250Y | IMTP | MELLAPAK 350Y |
| Flooding, % | 69 | 72 | 78.74 |
| | Stripping column | | |
| Packing diameter | 7.6 | 8.2 | 5 |
| Packing height | 25 | 30 | 20 |
| Packing type | PALL | BERL | MELLAPAK 128X |
| Flooding, % | 58 | 60 | 72 |

## 3. Results and discussion

Table 2 presents the results of modeling and simulation the process of separation of $CO_2$ in cement plant flue gases based on amine absorption. Each case provides information on the composition and the mass flows of various components, including MEA, $H_2O$, $CO_2$, $N_2$, and $O_2$. All the results fully satisfy the set targets and constraints.

**Table 2.** Modelling and simulation results.

| | **Case 1** | | **Case 2** | | **Case 3** | |
|---|---|---|---|---|---|---|
| | **Treated flue gas** | **$CO_2$ pipe** | Treated flue gas | $CO_2$ pipe | Treated flue gas | $CO_2$ pipe |
| | | | Mole Fractions (%) | | | |
| MEA | 0.047 | 0 | 0.05 | 0 | 0.04 | 0 |
| $H_2O$ | 31.407 | 3.149 | 30.5 | 3.16 | 30.51 | 3.149 |
| $CO_2$ | 1.603 | 96.731 | 1.758 | 96.7 | 1.76 | 96.68 |
| $N_2$ | 58.078 | 0.094 | 58.732 | 0.11 | 58.73 | 0.14 |
| $O_2$ | 8.865 | 0.027 | 8.96 | 0.03 | 8.96 | 0.03 |
| | | | Mass Flows (kg/h) | | | |
| MEA | 409.63 | 0 | 413.021 | 0 | 364.0955 | 0 |
| $H_2O$ | 80129.93 | 1287.60 | 81234 | 1291.54 | 76976.9 | 1278.431 |
| $CO_2$ | 9991.938 | 96629.89 | 10426.2 | 96321.52 | 10843.8 | 95786.71 |
| $N_2$ | 230414.5 | 59.561 | 230401 | 68.261 | 230385.4 | 88.64532 |
| $O_2$ | 40174.43 | 19.583 | 401168 | 27.2863 | 40165.02 | 28.98953 |

The reboiler heat duty represents the amount of heat energy required to regenerate the MEA absorbent and release the captured $CO_2$. This value in Case 1 is 5.62 MJ per kg of captured $CO_2$. In Case 2, the reboiler heat duty is slightly lower at 4.72 MJ/kg $CO_2$. This indicates that Case 2 requires less energy to achieve the same level of $CO_2$ capture compared to Case 1. Case 3 has the lowest reboiler heat duty of 4.06 MJ per kg $CO_2$. This suggests that it is the most energy-efficient among the three cases for capturing $CO_2$ using MEA absorption.

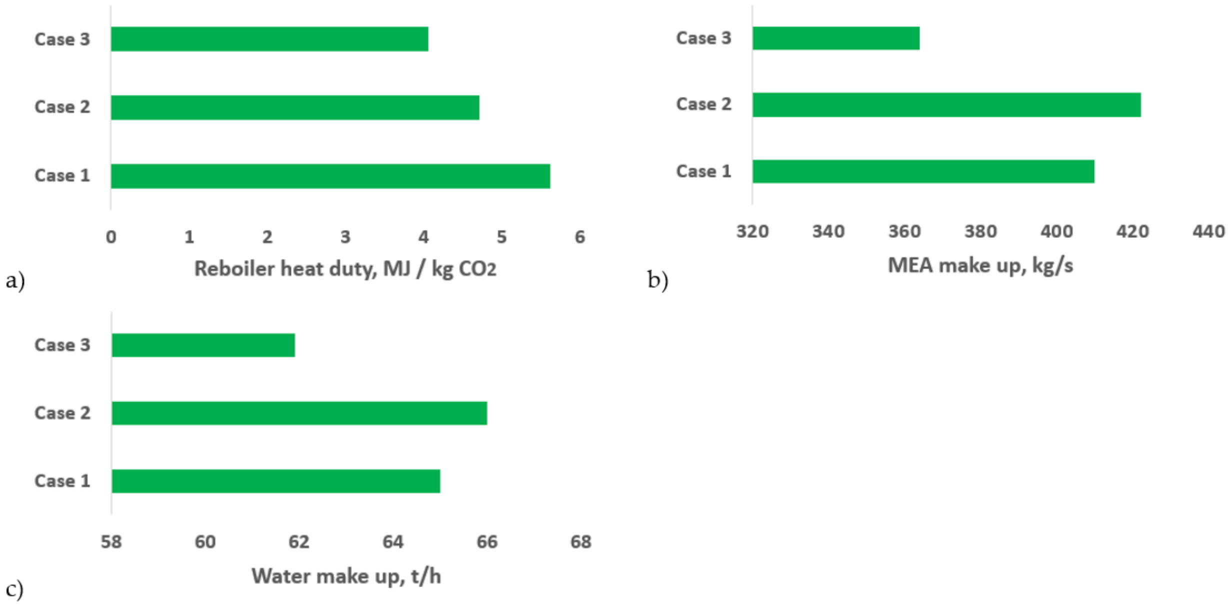


**Figure 2.** Case study scenarios results: a) reboiler heat duty; b) MEA make up; c) water make up.

In terms of MEA and water make up, Case 3 requires the lowest MEA and water makeup rate, which are 364 kg/s and 61.9 t/h, respectively. This implies that it consumes less MEA and $H_2O$ to achieve $CO_2$ capture compared to the other cases with smaller column dimension.

## 4. Conclusion

The study analyzed the $CO_2$ capture process in a 1 Mt cement plant using the Aspen Plus modeling software. The column sizes, heat duty, and liquid make-up values were determined using modeling and case study methodology to minimize capital and operational costs. The reboiler heat duty with 4.06 MJ/kg $CO_2$ in the stripper column was found to be the most energy-efficient among the three cases, with MEA 40% wt. and 0.25 mol/mol $CO_2$ loading condition, which is requiring the lowest MEA and water makeup rate, compared to other cases with smaller column dimensions.

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**Abbreviations**

| | |
|---|---|
| CCUS | Carbon capture, utilization, and storage |
| $CO_2$ | Carbon dioxide |
| MEA | Monoethanolamine |

| | |
|---|---|
| $H_2O$ | Water |
| $N_2$ | Nitrogen |
| $O_2$ | Oxygen |

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