

# Modeling and Simulation of Chemical Absorption Methods for CO<sub>2</sub> Separation from Cement Plant Flue Gases <sup>†</sup>

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<sup>†</sup> Presented at the 4th International Electronic Conference on Applied Sciences, 27 October–10 November 2023; Available online: <https://asec2023.sciforum.net/>.

**Abstract:** Climate change, especially global warming, is observed due to greenhouse gases released on an industrial scale. For this reason, progress is being made around the world to reduce CO<sub>2</sub> emissions and transition to sustainable energy sources. One of the most mature methods of capturing CO<sub>2</sub> from flue gases in industrial sectors is chemical absorption. This work analyzed the absorption process involved in capturing CO<sub>2</sub> 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, the optimal values of column sizes; heat duty; and solvent make-up that require the least capital and operational costs for capturing CO<sub>2</sub> in the flue gases of this plant were determined. When a 40% MEA solution was used, and the CO<sub>2</sub> loading in the absorption-stripping process was 0.25 mol/mol, the reboiler heat duty was 4.06 MJ/kg CO<sub>2</sub>.

**Keywords:** climate change; absorption; modeling; heat duty; flue gas; CO<sub>2</sub> capture



**Citation:** Turakulov, Z.; Kamolov, A.; Eshbobaev, J.; Turakulov, A.; Norkobilov, A.; Boboyorov, R. Modeling and Simulation of Chemical Absorption Methods for CO<sub>2</sub> Separation from Cement Plant Flue Gases. *Eng. Proc.* **2023**, *56*, 142. <https://doi.org/10.3390/ASEC2023-15352>

Academic Editor: Simeone Chianese

Published: 26 October 2023



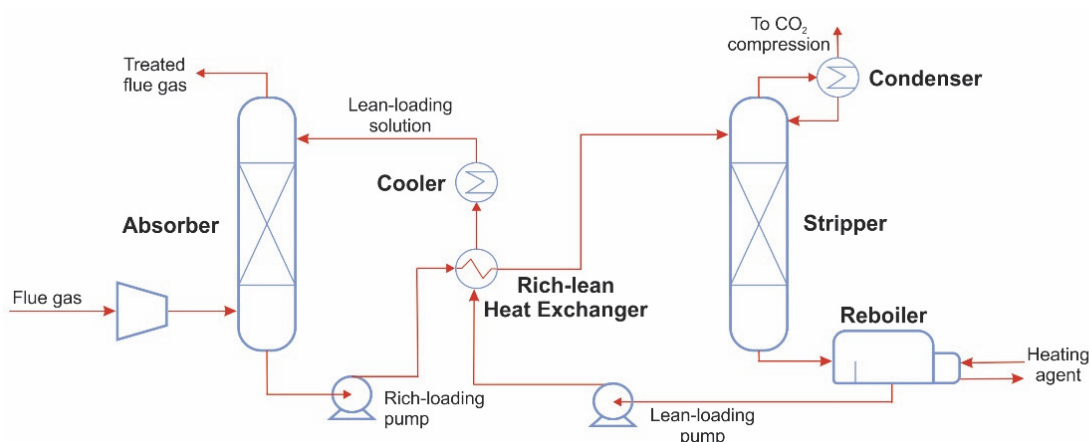
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## 1. Introduction

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<sub>2</sub>) 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<sub>2</sub> capture methods has emerged as a very effective method for mitigating anthropogenic carbon dioxide (CO<sub>2</sub>) emissions [2].

Currently, the amine-based chemical absorption method has achieved the highest level of maturity in post-combustion CO<sub>2</sub> capture [3]. Amine-based carbon capture technology has been effectively used for capturing CO<sub>2</sub> from flue gases with a low CO<sub>2</sub> 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<sub>2</sub> present in the flue gas stream, which comes from the cement plant, has a reaction with the solvent inside the absorption column. Subsequently, the solvent, which is enriched with CO<sub>2</sub>, is thermally regenerated within the stripper column. The lean-loading solution, which is free from CO<sub>2</sub>, is returned to the absorption column after a process of heat exchange with the rich-lean solution and subsequent cooling. The CO<sub>2</sub> stream with a high level of purity is

conveyed in a process involving the 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<sub>2</sub> capture (Modified from [6]).

In this work, a modeling-based study of the “tail-end” chemical absorption method for CO<sub>2</sub> separation from cement plant (with a 1 Mt production capacity annually) flue gases and the determination of the best values in different configuration system cases are considered. This study is considered part of the “Techno-economic evaluation of post-combustion CO<sub>2</sub> capture technologies for cement plant flue gases”. Further future work will include comparative studies of this work as a benchmark technology with other near or early-stage post-combustion CO<sub>2</sub> capture technologies.

## 2. Methodology

### 2.1. Model Development

The core methodology for this research involves modeling and simulation using the Aspen Plus V12 software. Our key targets and constraints are set as follows: CO<sub>2</sub> removal efficiency must be greater than 90%, CO<sub>2</sub> purity should be greater than 95%, and the occurrence of flooding in the absorption/stripper columns must remain below 75%. The Aspen Plus process simulation software was chosen as the primary tool for modeling and simulating the selected CO<sub>2</sub> capture methods [7]. We developed simulation models that accurately represented the chosen chemical absorption methods. First, the absorber/stripper system was modeled and simulated on the open loop principle. Targets accepted CO<sub>2</sub> removal in the flue gases, the purity of CO<sub>2</sub>, and the column packing flooding factor to build the model. Packed column sizing was calculated for the selected packing material [8]. The rate-based model was the most used approach based on the two-film theory in the case of amine-based absorption. In the process of modeling, the following causes should be considered:

- Due to the high mole fraction of CO<sub>2</sub>, a higher liquid/gas ratio is required for CO<sub>2</sub> molecules to absorb into the liquid phase. This causes more energy to be spent on solvent regeneration;
- 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<sub>2</sub> loading (0.134, 0.18, and 0.25 mol/mol) conditions (see Table 1). The composition of CO<sub>2</sub> in the incoming flue gas was 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<sub>2</sub> capture in cement plant flue gas.

**Table 1.** Hydraulic design and packing internals for 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

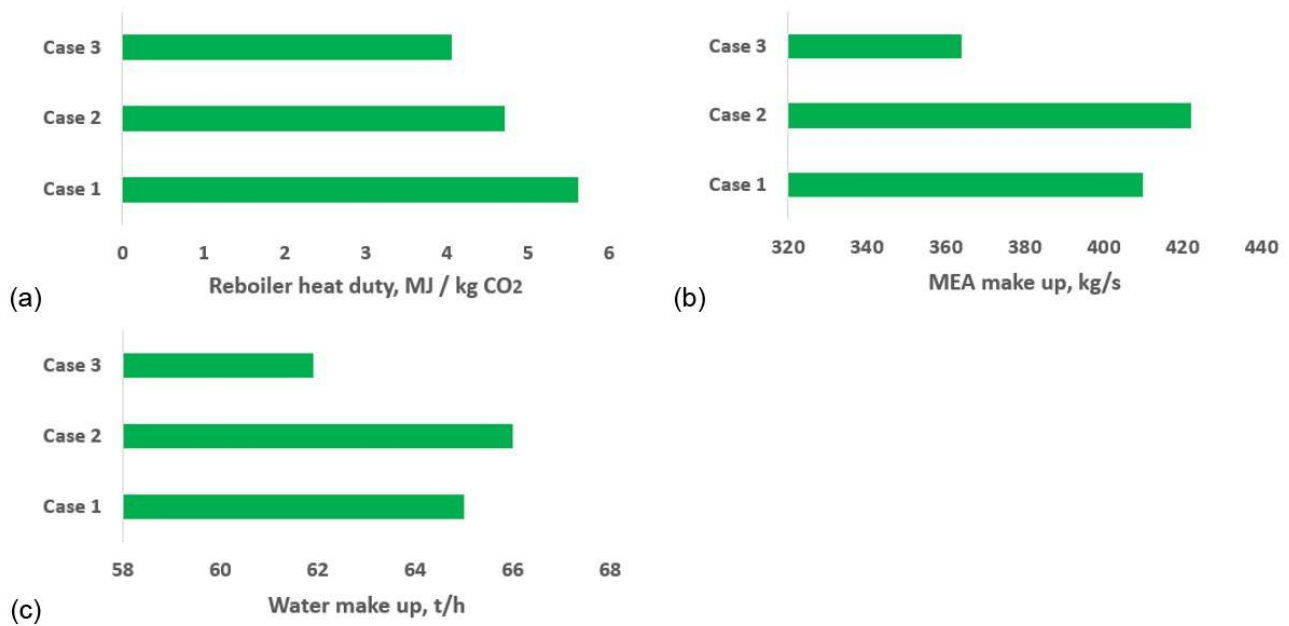
Table 2 presents the results of the modeling and simulation of the process of CO<sub>2</sub> separation in cement plant flue gases based on amine absorption. Each case provides information on the composition and the mass flows of various components, including MEA, H<sub>2</sub>O, CO<sub>2</sub>, N<sub>2</sub>, and O<sub>2</sub>. All the results fully satisfy the set targets and constraints.

**Table 2.** Modeling and simulation results.

	Case 1		Case 2		Case 3	
	Treated Flue Gas	CO <sub>2</sub> Pipe	Treated Flue Gas	CO <sub>2</sub> Pipe	Treated Flue Gas	CO <sub>2</sub> Pipe
Mole Fractions (%)						
MEA	0.047	0	0.05	0	0.04	0
H <sub>2</sub> O	31.407	3.149	30.5	3.16	30.51	3.149
CO <sub>2</sub>	1.603	96.731	1.758	96.7	1.76	96.68
N <sub>2</sub>	58.078	0.094	58.732	0.11	58.73	0.14
O <sub>2</sub>	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 <sub>2</sub> O	80,129.93	1287.60	81,234	1291.54	76,976.9	1278.431
CO <sub>2</sub>	9991.938	96,629.89	10,426.2	96,321.52	10,843.8	95,786.71
N <sub>2</sub>	230,414.5	59.561	230,401	68.261	230,385.4	88.64532
O <sub>2</sub>	40,174.43	19.583	401,168	27.2863	40,165.02	28.98953

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

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<sub>2</sub>O to achieve CO<sub>2</sub> capture compared to the other cases with a smaller column dimension.



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

#### 4. Conclusions

This study analyzed the CO<sub>2</sub> 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 the modeling and case study methodology to minimize capital and operational costs. The reboiler heat duty with 4.06 MJ/kg of CO<sub>2</sub> 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<sub>2</sub> loading condition, which requires the lowest MEA and water makeup rate, compared to other cases with smaller column dimensions.

**Author Contributions:** Conceptualization, A.N. and Z.T.; writing—original draft preparation, Z.T. and A.K.; visualization, Z.T., J.E. and A.T.; writing—review and editing, Z.T., R.B. and A.N.; supervision, A.N.; Z.T. and A.K. contributed equally to this paper. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research received no external funding.

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** The data presented in this study are available on request from the corresponding author.

**Acknowledgments:** All authors acknowledge the members of the Department of Chemical and Biomolecular Engineering, University of Cantabria, for their guidance.

**Conflicts of Interest:** The authors declare no conflict of interest.

#### Abbreviations

CCUS	Carbon capture, utilization, and storage
CO <sub>2</sub>	Carbon dioxide
MEA	Monoethanolamine
H <sub>2</sub> O	Water
N <sub>2</sub>	Nitrogen
O <sub>2</sub>	Oxygen

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