UNIVERSIDAD DE INVESTIGACIÓN DE TECNOCLOGÍA EXPERIMENTAL YACHAY

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ADDITIVES TO IMPROVE THE CO_2 CAPTURE PROCESS USING CHEMICAL SOLVENTS: A REVIEW

Trabajo de integración curricular presentado como requisito para la obtención del título de Petroquímico

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This thesis is dedicated to my family, who supported me to achieve my goals with their unconditional help. Especially to my grandmother Laura, my parents Patricio and Geovanna who with their unconditional love guided me at all times and inspired me to give my best at all times. To my brother Ismael to show him that with a little effort it is possible.

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RESUMEN

Los solventes químicos empleados en el proceso de captura de dióxido de carbono (CO_2) han permitido un tratamiento adecuado a este gas de efecto invernadero. Sin embargo, debido a los problemas operacionales que acarrean se ha empezado a considerar nuevos solventes. Con el objetivo de mejorar la eficacia durante los procesos de captura es necesario llevar a cabo actividades de investigación entorno a los aditivos que mejoren el proceso de captura de CO_2 tratando de mantener la infraestructura industrial existente. Es por ello que se evidencia, la necesidad de generar una base de datos que permita identificar este tipo de aditivos. En este trabajo se presenta una recopilación bibliográfica de diferentes investigaciones que proponen solventes para mejorar el proceso de captura de CO_2. Se analizan diferentes solventes considerando aspectos cinéticos, termodinámicos o mejoras operacionales en la infraestructura, tales como la reducción de corrosión y la disminución en pérdidas de solventes por evaporación. Para la revisión bibliográfica se consideraron diferentes trabajos publicados entre el período 2000 y 2020 enfocados en (i) mejorar el proceso de captura, (ii) presentar datos de emisiones de CO_2 por sectores productivos, y (iii) mostrar los problemas e inconvenientes en equipamiento que acarrea el uso de solventes convencionales. La estrategia de búsqueda se definió en tres pasos. Primero, selección de bases de datos y palabras claves que más se ajusten al área de estudio. Segundo, recopilación de trabajos de investigación publicados relacionados a la captura de CO_2. Tercero, revisión y análisis de tendencias de los últimos 20 años entorno a los nuevos solventes, tipo de gas empleado en los procesos de captura, organización de aditivos según su naturaleza química y el tipo de mejora, cinética, termodinámica u operacional que brinden los aditivos. Se concluyó que, existe una evidencia suficiente para considerar que los compuestos que contienen un grupo amino, y especialmente alcanolaminas, son los aditivos más utilizados para procesos de captura de CO_2. Así mismo, ya que poseen un grupo hidroxilo en su estructura, éste facilita su disolución, y debido a la gran variedad de compuestos, estos exhiben mejoras cinéticas, termodinámicas y operacionales. Se espera que este trabajo permita desarrollar posteriores investigaciones enfocadas en la captura de CO_2 ya que no es solamente una problemática interna sino de interés internacional.

Palabras claves: CO_2, proceso de captura, aditivos, aminas, solventes químicos, revisión.

ABSTRACT

The current chemical solvents used in the carbon dioxide (CO_2) capture process have allowed an adequate treatment of this greenhouse gas; however, new solvents have being considered due to the operational problems that traditional solvents might cause. Research on chemical additives is needed to improve efficiency during the CO_2 capture process while keeping the existing industrial infrastructure and avoiding higher costs. For this reason, the need to generate a database gathering information on this type of additives is evident. The following work is presented as a bibliographic compilation of different researches that propose solvents to improve the CO_2 capture process. Different solvents are analyzed considering kinetic and thermodynamic aspects or operational improvements in the infrastructure, such as corrosion reduction and reduction in solvent losses by evaporation. In this review, different works published between 2000 and 2020 are considered that focus on (i) improving the capture process, (ii) gathering data of CO_2 emissions by productive sectors, and (iii) addressing the problems and inconveniences in equipment that entails the use of conventional solvents. The search strategy was defined in three steps. First, selection of databases and keywords that best fit the area of study. Second, a compilation of published research papers related to CO_2 capture. Third, review and analysis of trends over the last 20 years regarding new solvents, type of gas used in the capture processes, organization of additives according to their chemical nature, and the type of improvement, kinetic, thermodynamic, or operational that the additives provide. It was concluded that there is sufficient evidence to consider that compounds containing an amino group, and especially alkanolamines, are the most widely used additives for CO_2 capture processes. Since they have a hydroxyl group in their structure, they facilitate their dissolution, and due to the great variety of compounds, they exhibit kinetic, thermodynamic, and operational improvements. It is expected that this work will allow the development of further research focused on CO_2 capture since it is not only a domestic problem but also of international interest.

Keywords: CO_2, capture process, additives, amines, chemical solvents, review.

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CHAPTER I

1. INTRODUCTION

The scientific evidence is overwhelming for the proposition that global warming is due in great measure to the increase in CO_2 levels in the atmosphere, as is the fact that the increase in CO_2 concentration is due to human activity (Miguel & Arroyo M., 2020c). Global warming is evident in Ecuador. Recently, the glaciers of the Chimborazo, Cotopaxi, and Antisana volcanoes have decreased by about 40%; and to address this problem, there is a climate change strategy developed by the Ministry of Environment and socialized within the municipality since 2012. The plan includes adaptation, mitigation, and reduction of emissions (Miguel & Arroyo M., 2020a).

Carbon dioxide (CO_2) is one of the major waste gases from factory exhaust and industrial concerns, transportation, and electricity; these production sectors emit the most CO_2 employing fossil fuels (Babamohammadi et al., 2015; Nwaoha et al., 2017). Besides, a carbon capture strategy is required to prevent emissions from all possible sources (Alivand et al., 2020). Most CO_2-containing gases fall into typical gas mixtures, such as fuel gas (H_2 + CO_2), flue gas (N_2 + CO_2) and CO_2-containing gas mixtures that contain high concentrations (>15%) of CO_2 (and most times H_2S), for example, natural gas, biogas, landfill gas or alternative extraction gas (Amin et al., 2016; Y. Wang et al., 2013).

As concerns over increasing atmospheric concentrations of artificial greenhouse gases increase, effective CO_2 emission reduction strategies such as carbon capture and storage (CCS) are needed to counter this trend. The CCS consists of three basic steps. (1) CO_2 separation (CO_2 capture), (2) transportation, and (3) storage combustion post-capture. Technologies of CO_2 separation and purification in post-combustion capture can be employed as absorption, adsorption, membrane separation, and cryogenic distillation. Chemical absorption with aqueous solvents has been the most reliable and promising technology for CO_2 capture after large-scale combustion. (Alivand et al., 2020; M. Wang et al., 2011)

Chemical absorption consists of the reaction of CO_2 with chemical solvents to form weakly bonded intermediate compounds that can be regenerated with the application of heat to the original solvent and CO_2 stream (M. Wang et al., 2011). Amine solutions are generally employed as chemical solvents in the CO_2 capture process (Park et al., 2021). Two technological approaches usually accomplish the reduction of energy use for CO_2 solvent regeneration: (1) new solvent discovery, either using a new selective CO_2 solvent or mixing various solvents/additives; and (2) process optimization (Gusnawan et al., 2020).

In chemical absorption, amine-based systems, carbonate-based systems, aqueous ammonia, and ionic liquid-based systems are common systems for carbon dioxide capture (Koronaki et al., 2015). The capture process includes two units, the first column where absorption takes place in contact with the amine solution in countercurrent, and the second column releases the previously absorbed CO_2 and regenerates the amine solution, which can be used again to promote absorption in the first column (Gomes et al., 2015).

CO_2 capture from the combustion uses mixed amine solvents that have been thoroughly tested in laboratory-scale and pilot-scale to study the ability to achieve high absorption potential, cyclic loading and cyclic capacity, improved absorption rate, low solvent regeneration energy, decreased corrosion and degradation (Nwaoha et al., 2017). It is thought that the use of additives in the most widely used chemical solvents for the decomposition of carbon dioxide (mainly based on the use of alkanolamines in aqueous solution) has been considered an exciting option to improve overall performance. The effectiveness of several chemicals depends not only on their absorption capacity and efficiency, particularly the role of thermodynamics solution, but also on the kinetics (Gómez-Díaz et al., 2018; Jeon et al., 2013; Mathias et al., 2013).

In the research of chemical solvents, Altway et al., (2016) stated different types of amine solvents that have been extensively studied; those typically are monoethanolamine (MEA), diethanolamine (DEA), and N-methyldiethanolamine (MDEA). Besides, MEA is the foremost well-known and most customary solvent among the commonly accessible solvents (Babamohammadi et al., 2015). MEA is also considered an attractive solvent at a low partial pressure of CO_2 in the flue gas due to its rapid reaction rates compared to secondary and tertiary amines (Koronaki et al., 2015). Primary and secondary amines, contrary to tertiary amines, may have mobile hydrogen atoms on the nitrogen, allowing a better performance (Barth et al., 1986). Adding some chemical additive to the reaction fluid could efficiently separate CO_2 gas, such as ionic liquids, surfactants, and physical and chemical absorbers (Yue et al., 2019).

Hence, the objective of this state-of-the-art review of chemical solvents is to identify possible multiple additives/promoters to improve the CO_2 capture process. The present work has its basis on a line of research in CO_2 capture under development at Yachay Tech University to identify additives that can improve the CO_2 capture process. The classification process aims to obtain additives that reduce typical problems related to the amine usages, such as volatility, corrosion equipment (to reduce as much as possible unscheduled stops), high temperatures for regeneration, the high energy consumption they represent, and others. Also, try to find amine-containing compounds from natural sources, non-edible sources, or agro-industrial wastes that do not compromise the amines' performance.

This review's methodology consists of extensive and deep investigation of chemical solvents employed to improve CO_2 capture to establish the most effective options to choose possible additives to study afterward. Second, the classification of the obtained promoters according to technical aspects, like their performance and viability. Then, identify some characteristics when choosing different additives (as their efficiency might come from a kinetical or thermodynamical improvement) and analyze the actual tendencies within this investigation field.

1.1 Problem Approach

As Jimenez et al. (2019) stated, Ecuador is an oil-dependent country as the main export resource; however, its exploitation and other raw materials, among others, produce high levels of environmental degradation as CO_2 emissions in a more extensive group named greenhouse gases (GHG). At the end of 2017, 41% of the country's industries are located in Guayas, which houses 32,866 companies, followed by the Pichincha, with 25,995 companies. It means that 27% of the industries are located in the rest of the country (Remache et al., 2019).

Over the last few years, the penetration of clean energy sources has primarily been marketed as a promising option. It appears, though, that fossil fuels will still be a prevalent part of the global energy mix, prompting a more direct response (Koronaki et al., 2015). Promoting green energies and energy conservation is common for countries to achieve their energy and environmental targets and decarbonize and decontaminate in the potential energy matrix (Miguel & Arroyo M., 2020b).

The United Nations' goal No. 7 stated the Affordable and Clean Energy, due to this, Ecuadorian institutions of education have to undertake and engage their efforts to include this need to preserve the environment. According to the National Development Plan 2017 – 2021 in its goal No. 3: Look to guarantee nature's rights for current and future generations and in its policy No. 3.3 establishes "To promote good practices that contribute to the reduction of the contamination, the conservation, mitigation, and the adaptation climate change effects, and promote this practices in a world level." (Mendieta et al., 2019).

Capturing and storing CO_2 is seen as a key aspect of the plan to slow carbon-based climate change progress (K. Li et al., 2020). The carbon dioxide decomposition from a certain gas mixture using chemical absorption is a combination of chemical and physical processes. Chemical engineering aims to focus on getting in contact with the liquid and the gas phase, making the most efficient way of the chemical absorbent performance considering rates of a chemical reaction, chemical balance, solubility, heat capacity, viscosity, and how these structures differ in temperature (Puxty & Maeder, 2016). However, the main drawback of capturing and storing CO_2 implementation on an industrial scale is high energy consumption. Besides, amines with hydroxyl groups (alkanolamines), which are most often used in industrial applications, are known to be corrosive and require a high amount of energy to be recovered. This situation has led to an extensive empirical search for alternatives (Ma et al., 2015; Madeddu et al., 2018).

Extensive global work is taking place in developing new and enhanced post-combustion CO_2 capture technologies (Mathias et al., 2013). The desirable advancements by employing amine-based compounds center on solvents with a lower heat capacity, vaporization heat, or binding energy (Gómez-Díaz et al., 2018). Each advancement plays a role in determining the new absorbent's efficiency and setting the process's design and operation standards. (Puxty & Maeder, 2016). A few cases are natural co-solvents (Gómez-Díaz et al., 2018), surfactants (Bavoh et al., 2019), amino acid salt aqueous solutions (Gusnawan et al., 2020), ionic liquid-based solvents (Babamohammadi et al., 2015), antifoaming agents, and corrosion inhibitors (Mota-Martinez et al., 2014).

1.2 Objectives

1.2.1 General Objective

- To generate a state-of-the-art review on additives that improve the CO_2 capture process using chemical solvents, focusing on possible energetic, kinetic, and thermodynamic improvements.

1.2.2 Specific Objective

- To identify the last 20-years publication trends of chemical additives, which improves the capture process of CO_2.

- To identify typical gas mixtures currents employed in the capture process.

- To classify additives per their chemical nature according to the most employed groups and identify if there are some from natural sources.

- To catalog the additives improvements found in the study.

1.3 Keywords and Databases

At the beginning of the work, the search was focused on using keywords and databases centered on the study's objectives. Keywords are multipurpose tools that, together with specific engineering databases, limit the extent of information search.

The selection of the employed words in the research task is based on a mixture; as a consequence of this, the searches were made by mixing the base word plus another keyword, then adding one more to past results to narrow down the search criteria.

The study was performed and developed on thinking about how words employed can be organized. Then, looking deep some studies keywords can be separated into two groups:

- One of them was the main topic of this study, named specific words, as the most repeated word "CO_2". This word was used during all the searches that fulfill the purpose of the project.
- The other group was based on each chapter, named variable words. Due to the extent type of research made, each chapter has its characteristics, so the alternative words vary from one to another.

Each chapter developed in this work has the following keywords, as stated in **Table 1**:

Table 1: *Organization of keywords employed in each chapter*

Organization	Specific Words	Variable Words
Chapter II	CO_2 capture process	Adsorption, absorption, membranes, emissions, greenhouse effect, Ecuador, water-wash, amines, amine blends, industrial, chemical engineering
Chapter III	CO_2 capture amine	classification, handbook, mechanism, kinetics, formulated amines, amine blends, solvents, industrial problems, process, improvements, conventional, renewable
Chapter IV	CO_2 capture additives improvements	

The databases consulted during the development of this study, for a better development focused on the main topic, were:

- ACS Publications
- Google Patents
- OnePetro
- Science Direct

- Scopus
- Taylor & Francis Online

CHAPTER II

2. FUNDAMENTALS

2.1 Global Warming

According to the United States Environmental Protection Agency (EPA) (n.d.), climate change can affect air quality, and conversely, air quality can affect climate change. Climate change due to pollutant emissions affects local air quality due to air warming associated with climate change. Carbon dioxide (CO_2), tropospheric ozone, water vapor, and methane (CH_4) have increased their concentration due to human activity (Andino Enríquez, 2020).

Carbon dioxide is one of the most important anthropogenic greenhouse gas, contributes substantially to global warming and climate change, and the increase in CO_2 emissions (part of the greenhouse gases, GHGs), especially over the past 150 years, is determined by increased energy consumption from burning fossil fuels (Krótki et al., 2020). The largest cause of CO_2 pollution is flue gas from industrial and power plants (Choi et al., 2014). As established by the International Energy Agency (IEA), carbon capture and storage (CCS) is one of the feasible mitigation measures that will help achieve the emissions reduction goals by 2050 (Osagie et al., 2018).

Environmental authorities (EPA) define two primary types of pollution: one where the pollution is determined, called point-source pollution, and the other where it is not determined, named non-point-source pollution. The first-point source of pollution suggests it comes from a unique place: factories, power plants, oil refineries, paper mills, manufacturing plants, and municipal wastewater treatment plants. On the contrary, non-point-source pollution refers to pollutants released in a huge place, as pollution in a whole city, affecting environmental degradation (National Geographic, 2019).

Ecuador and other South American countries presented a positive relationship between economic growth and environmental degradation. These countries have a prominent cause of an environmental decline in supporting economic activity (Jimenez et al., 2019). In Ecuador on 26th July 2016, it was signed the Paris Agreement of Climate Change, despite being barely responsible for 0.15% of the world's pollution (Ministerio del Ambiente y Agua, 2016).

CO_2 emissions can be controlled in three ways (i) using non-carbon energy resources to replace fossil fuels, (ii) improving energy efficiency or reducing GHG emissions per unit energy consumption, and (iii) carbon capture and storage (Y. Wang et al., 2013). As Zhao et al. (2012) stated, CO_2 capture has become an important method for controlling and recycling CO_2 emissions from the flue gas after combustion (post-combustion processes).

2.2 CO_2 Emissions

Due to CO_2 and other greenhouse gas emissions, global warming in the 21st century is one of the biggest crises the world faces today. Carbon dioxide is the most important greenhouse gas emitted from various sources, such as refineries, oil and gas production sites, iron and steel production plants, fossil fuel-based cement, chemical plants, and thermal power plants for 78% of global GHGs. Its annual emissions increased by about 80% between 1970 and 2004 (Baca, 2014; De Souza Henriques et al., 2019; Hdom, 2019; Muchan et al., 2017; Yangyang Xu et al., 2020).

Ecuador's industrial sector accounts for 13 % of the national CO_2 emissions (Remache et al., 2019). One of the major risks that Ecuador has to face, among others, is the importance of climate change to society. Climate change mitigation and adaptation require cooperation and commitment between government entities as the decision-makers, executives as the industry, the population as the GHGs emitters, and academia as knowledge producers (Toulkeridis et al., 2020).

The data of CO_2 emissions of Ecuador in the year 2017 are shown in **Figure 1**. These data correspond to the metric tons of carbon dioxide equivalent ($MtCO_2e$), an amount of GHGs. As data is shown in percentages, the total amount of GHGs emissions during 2017 is 99.86 $MtCO_2e$. As we could observe in the figure, one of the main sectors that emit a significant amount of CO_2 is the energy sector, which corresponds to mainly industrial operations and transportation.

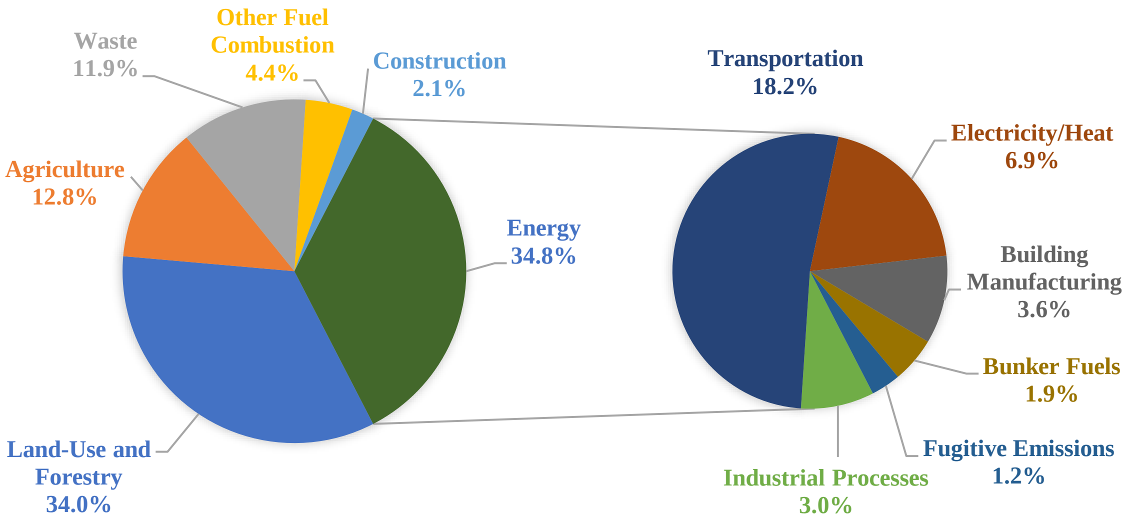

Figure 1: *Ecuador CO_2 emissions by sector in 2017*
Source: CAIT Climate Data Explorer - Climate Watch, 2021

2.3 Gases Types for CO_2 Capture

The treatment for post-combustion processes typically involves amines-based absorbents that are the most advanced technology in a process called amine scrubbing, which was first patented in 1930 to remove acid gases (CO_2 and H_2S) from natural gas (Chowdhury et al., 2013; Yuan & Rochelle, 2019). The isolation of CO_2 from different processes has always been one of the most crucial concerns, and it is vital to find a way to reduce CO_2 (Amin et al., 2016). The combustion methods are stated by Scibioh & Viswanathan (2018), where they significantly affect the selection of a suitable CO_2 removal technique. Currently, CO_2 capture technologies for fossil fuel-based power plants can be categorized into four techniques:

1. Post-combustion capture
2. Pre-combustion capture
3. Oxy-combustion
4. Chemical looping combustion

There are two ways to perform pre-combustion and post-combustion CCS. Before combustion, it is the separation of CO_2 from the CO_2 / H_2 mixture, and after combustion, it is the CO_2 capture from the CO_2 / N_2 mixture (Y. Wang et al., 2013). During this revision, we will consider the post-combustion capture and four possible sources from which the gases will be studied:

- Biogas (or simulated biogas): for example, simulated biogas 64.0 mol % CH_4 and 36.0 mol % CO_2
- Flue Gas: for example, a mixture of 15 % vol CO_2 and 85 % vol N_2
- Fuel Gas: for example, a mixture between H_2 and CO_2
- Pure Gas: for example, pure CO_2
- Other Sources: for example, natural gas, a mixture of various gas components

As discussed above, the separation of CO_2 from the various systems is important. Many experiments and methods have been carried out in this respect, such as absorption, adsorption, water-wash, and membrane separation (Amin et al., 2016).

2.4 Post-combustion CO_2 Capture Techniques

Post-combustion carbon capture currently employs solvent wet scrubbing, reversible capture, and CO_2 release using aqueous amine solvents. It is currently the frontline commercial technology in a cyclical process that implies carbon dioxide uptake and release in chemical absorbers (Conway et al., 2013; Ma et al., 2015). Splitting CO_2 from different gas sources is very important in terms of the cumulative impact of CO_2 emissions. Separation among various systems is fundamental (Amin et al., 2016).

2.4.1 Adsorption

Adsorption is a physical mechanism involving the binding of a gas or substance to a solid surface. The adsorbent is regenerated by the application of heat or by the removal of friction. Adsorbents for CO_2 capture include activated carbon, alumina, metal oxides, and zeolites. Even though actual adsorption systems are not available for their application on an industrial scale in gas treatment plants (M. Wang et al., 2011).

2.4.2 Physical Absorption

It includes the actual incorporation of CO_2 into a solution dependent on Henry's law. Absorption occurs at high partial CO_2 pressures. Physical absorption is also not economical for flue gas sources (M. Wang et al., 2011). Siani et al. (2020) stated that physical solvents could interact with CO_2 by weak forces (electrostatic interactions or dispersion interactions) without chemical reactions.

2.4.3 Membrane Separation

Membrane separation is one of the most effective and widely used methods in the field of CCS. However, it is controlled by certain restrictions, including selectivity, permeability, pore size, fouling, and high membrane costs. A great deal of work has been made over the last few years to prepare membrane materials consistent with a successful CO_2 capture operation's technological and economic specification. Some porous materials, such as metal-organic frames (MOFs), zeolites, and activated carbons, are inserted into the membranes to improve their CO_2 separation ability (Elhenawy et al., 2020; Janusz-Cygan et al., 2020).

2.4.4 Water Wash

Countercurrent water-wash, often used when upgrading biogas to vehicle fuel in sewage and biogas treatment plants, is a simple, efficient, and versatile method of treating corrosive compounds at relatively low cost. It is believed that water absorption is an effective upgrade, especially to treat CO_2, H_2S, and CH_4 (Rasi et al., 2008). In a typical absorption tower for post-combustion or industrial CO_2 capture, the flush system is intended to control gas-phase emissions (Majeed & Svendsen, 2018).

2.4.5 Chemical Absorption

Koronaki et al., (2015) agreed that chemical absorption (or reactive absorption) is a mechanism in which a liquid phase absorbs the gas through a mixture of reaction and absorptive mass transport. Specifically, for the capture of CO_2, chemical absorption involves the reaction of CO_2 with a chemical solvent forming a weakly bound intermediate compound, a mechanism that can be reversed by heating up and resulting in the original solvent and CO_2 source.

The chemical absorption process was initially carried out using an aqueous amine solution; the most mature and commercially applied amine is monoethanolamine due to its high absorption capacity. MEA is considered an attractive solvent at low partial pressures (Koronaki et al., 2015). Results of chemical investigations shortly with other advanced chemical solvents with improved energy performance will lead to faster absorption rates, smaller equipment sizes, reduced overall energy demand, and ultimately the identification of amines that can provide lower CO_2 capture cost (Conway et al., 2013; Gatti et al., 2020).

Chemical absorption relies on diverse techniques to produce novel chemical solvents with stronger properties than traditional solvents (Baltar et al., 2020). Due to its low cost and simplicity, it is perceived to be the most practical choice in many industrial situations than other approaches (Babamohammadi et al., 2015). The most widely used chemical solvents are based on amines (Mihaila et al., 2019).

Mathias et al., (2013) and Talkhan et al. (2020) showed that amine scrubbing is an already developed technology; many amine-based chemical solvents have been suggested and used in experimental demonstrations, probably be for the first time on a large scale. Complementary, amine solvent's desirable properties include rapid kinetics of absorption, desorption rate, maximum mass transfer rate, absorption capacity, high circulating loading, cyclic capacity, low amine loss due to depletion and volatility, high efficiency, a low melting power charge, and solvent regeneration (Nwaoha et al., 2017).

This review deals with chemical absorption processes focused on chemical solvents to improve CO_2 capture. This is an available technology used in Ecuadorian refineries such as the State Refinery of Esmeraldas.

2.5 CO_2 Capture Processes

There are many processes to carry out CO_2 capture, and this review classified them into processes made in small-scale and large-scale. Small-scale ones can be made in the laboratory like CO_2 scrubbing and hydrate formation, commonly performed within a reactor. Furthermore, large-scale processes are performed in industries such as refineries and pilot plants.

2.5.1 Small-Scale Processes

2.5.1.1 CO_2 Scrubbing

This system is based on an arrangement of various processes. First, the solution for CO_2 absorption (amine-based solvents) must be charged into the reactor for experimental purposes. It is recommendable to employ a water jacket around the reactor as an additional way to control the temperature of the operation. There must be a mass flow or flowmeter controller to adjust at desirable quantities the amount of CO_2 leaving the cylinder to the operational process. This leads to a glass filter to prevent impurities passed by to the inside reactor and control pressure; it is optional for the operative personal to employ a barometer to measure pressure out of the reactor. After the reactor has completed a test, it is recommendable to remove entrapped chemicals or precipitates in traps. The arrangement is shown in **Figure 2**, employees sulfuric acid trap and an ice-moisture trap. Finally, to analyze the amount of CO_2 obtained from the experiment, these apparatuses are commonly connected to computers to receive information about the process. (You et al., 2008)

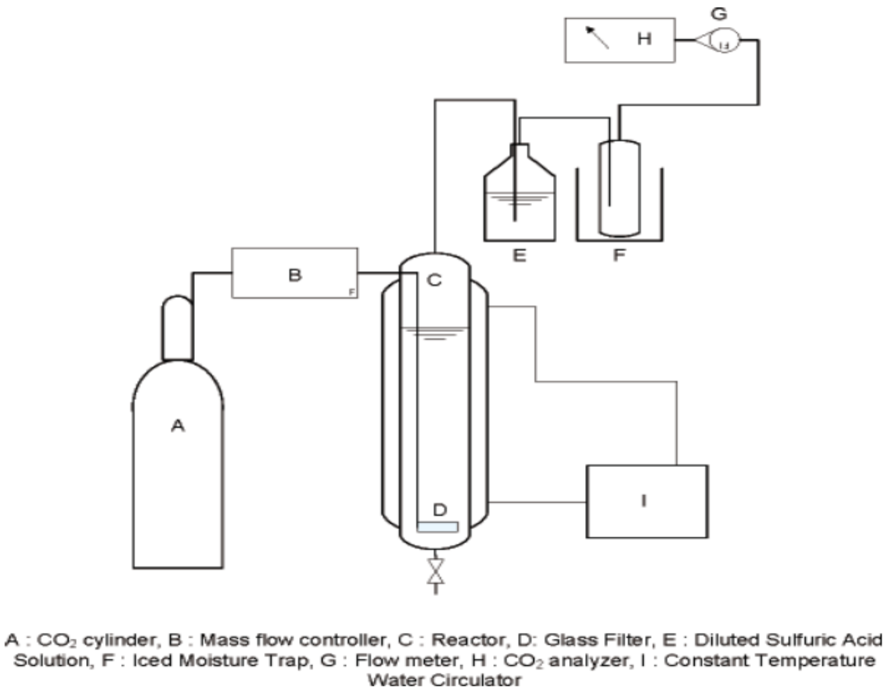

Figure 2: *Schematic diagram of an arrangement with a reactor system for testing CO_2 amine scrubbing*
Source: You et al., (2008)

2.5.1.2 CO_2 Hydrate Formation

Wang, Lang, and Fan (2013) widely studied gas separation technology as a promising option for CO_2 capture. The basis of the separation is the selective separation of CO_2 between the hydrate phase and the air phase. Hydrate-based CO_2 capture (HBCC) is high energy and easy to operate. Clathrate hydrates are solid crystalline compounds in which gas molecules (guests) are trapped in water cavities (hosts), consisting of water molecules hydrogen-bonded under suitable thermodynamic conditions (typically high pressure and low temperature). According to the hydrate principle, as gas hydrates are formed from a gas mixture, the concentration of these gasses in the hydrate and gas phases differs. As a result, the portion that formed hydrate could be more easily enriched in the hydrate phase.

According to **Figure 3**, two models are observed to these formations, model (a) where contains a recovery system of CO_2 after processing is completed, and model (b) where operators can dispose of CO_2 at their convenience.

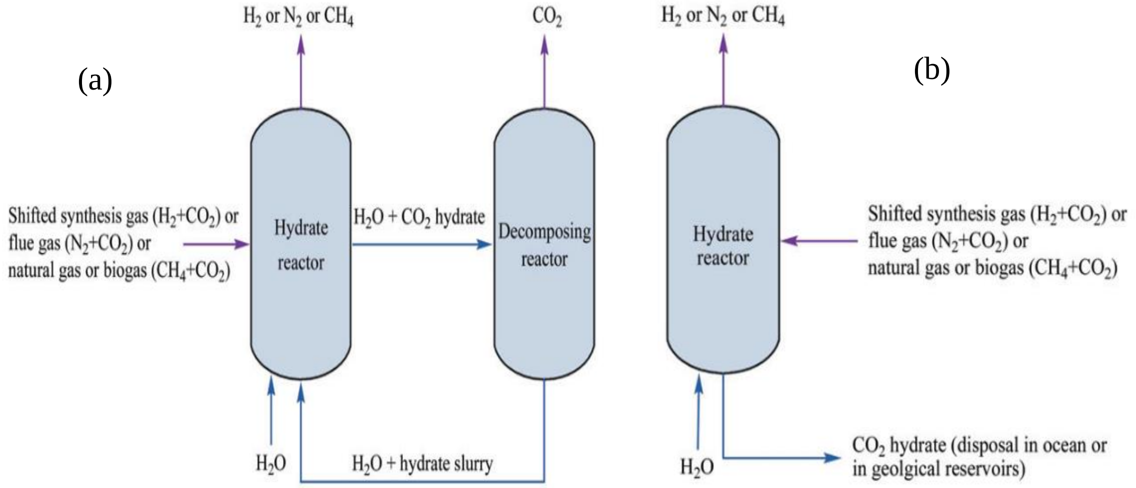

Figure 3: *CO_2 capture from shifted synthesis gas (a) Recovery System (b) CO_2 Disposal System*
Source: Wang et al. (2013)

As these arrangements are disposed of on a lab-scale, the disposition turns into a more complicated extension but maintains similar parts to the CO_2 scrubbing system shown in CO_2 scrubbing technology (see **Figure 4**).

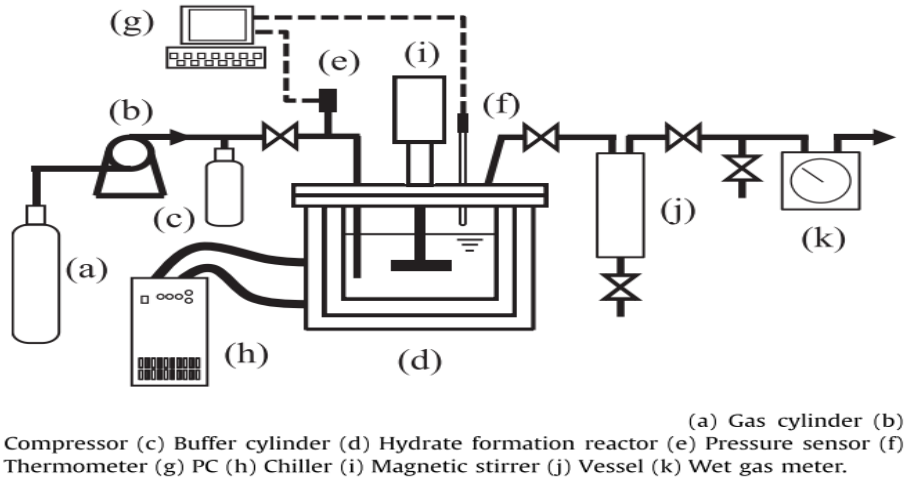

Figure 4: *Laboratory-scale reactor system for hydrate formation in CO_2 capture*
Source: Hashimoto et al. (2017)

The extension can be explained as this sophisticated arrangement employs valves to release and better control pressure in the system as the pressure in these processes is higher than in CO_2 scrubbing. Ricaurte et al., (2014) studied hydrate formation as a novel technology but found that the selectivity for CO_2 in the research is low compared to amine technologies.

2.5.1.3 CO_2 Bubble Column Reactor

Gómez-Díaz et al., (2018) studied the carbon dioxide chemical absorption of a bubble contactor. **Figure 5** shows the experimental setup and the characteristics of the bubble contactor. The working regime is continuous, and the reactor is a square bubble column reactor that makes contact with the gas phase through a five-hole sparger built-in Teflon.

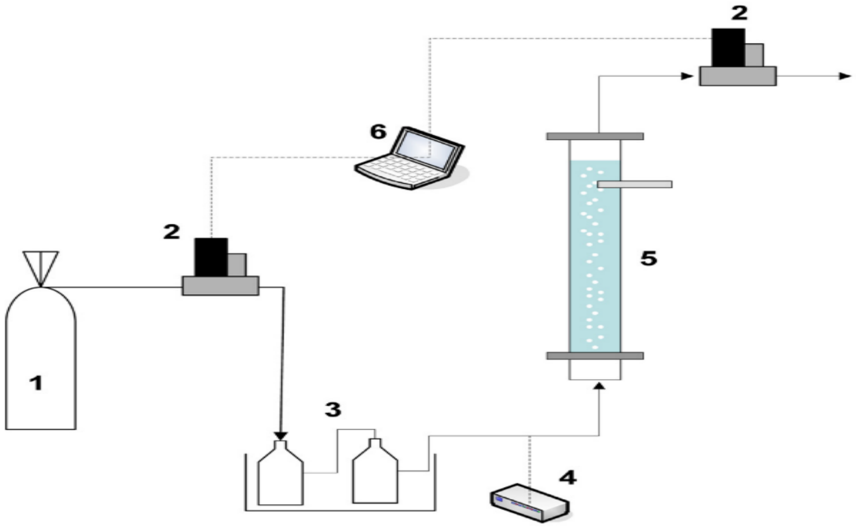

Figure 5: *Experimental set-up for a bubble column reactor, (1) Gas cylinder, (2) mass flow meter, (3) humidifier bath, (4) pressure gauge, (5) bubble column reactor, (6) PC*
Source: Gómez-Díaz et al. (2018)

2.5.2 Large-Scale Processes

2.5.2.1 Pilot Plant

The pilot plants' design comprises two units, the absorber and stripper columns which are packed columns. Internally are conformed by packed bed sections with a collector plate and redistributor between the beds (see **Figure 6**). The facility can process approximately 3 tons of CO_2 per day (M. Wang et al., 2011).

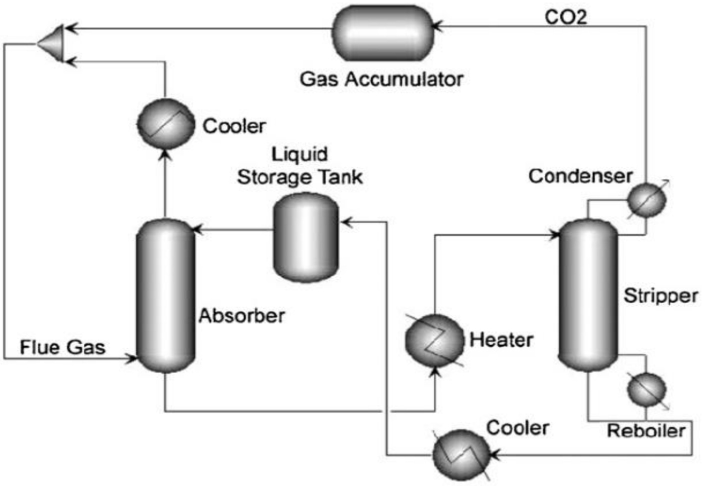

Figure 6: *Scheme of a pilot plant for CO_2 capture*
Source: M. Wang et al. (2011)

2.5.2.2 Industrial Plant

The mechanism of absorption of CO_2 typically involves the circulation of gasses through a packed or tray column. This technique has been around for a long time. It is still used in natural gas, syngas, synthetic ammonia, fossil fuel power plants, coal gasification, and gas treatment processes to remove CO_2 from gas streams in petrochemicals plants for operational, economic, and environmental reasons. (Babamohammadi et al., 2015). The natural gas industry's absorption of the amine has been used for more than six decades to extract CO_2 from natural gas and generate safe CO_2 for food and beverage industries. The absorption of amine closely resembles the process flow diagram seen in **Figure 7** (Scibioh & Viswanathan, 2018).

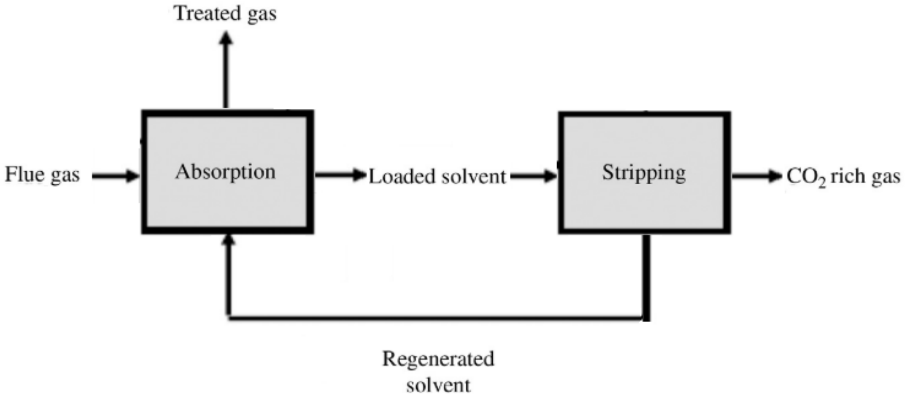

Figure 7: *Basic flow diagram of industrial post-combustion capture of CO_2 with chemical absorption*
Source: Scibioh & Viswanathan (2018)

Madeddu et al., (2018) established that the approach to designing absorption-desorption processes is based on sensitivity analyses. The column size and operating parameters vary within a certain range of values to obtain the desired final yield to the best technical performance. Analysis of column configurations is often overlooked. This fact can lead to columns not properly working, although the results at extreme levels, for example, product purity, duty, rejection rate, and others, are the mandatory results.

In acid gas extraction, an operational parameter is the solution loading, which is defined as the number of moles of acid gas extracted from the natural gas to the number of the substance's moles used for absorption. The loading of rich amine describes 1 mole of the solvent's capability in absorbing the acid gases (Sharif Dashti et al., 2015).

The process flow diagram (PFD) presented in **Figure 8** is the most typical configuration in the absorption-desorption process. Flue gas at countercurrent comes into contact with the CO_2 lean aqueous amine solution (L-Amine), which flows down from the absorber (or contactor) to the top, and rich amine (R-amine) containing carbon dioxide from the bottom. Hence, the CO_2 mass transfer occurs from the gas phase to the liquid phase (Nwaoha et al., 2017). Here, the amine selection must be correct to avoid possible operational problems to perform technical and economic criteria better.

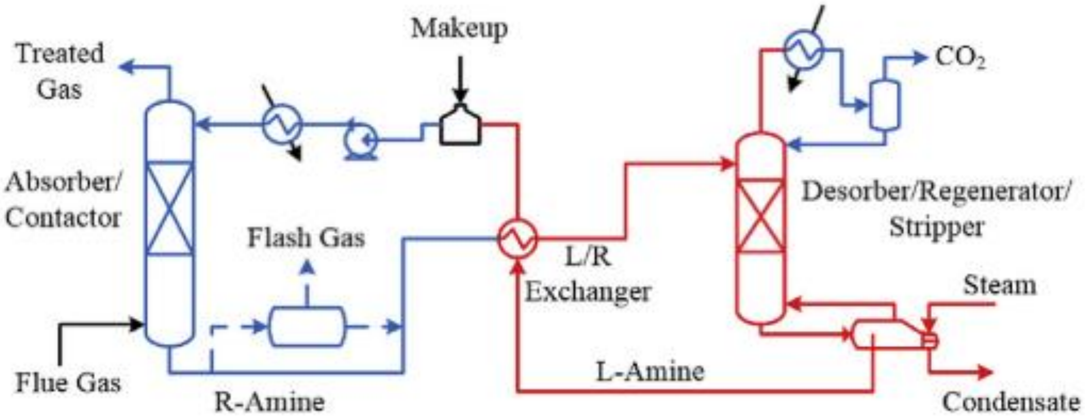

Figure 8: *Process Flow Diagram of CO_2 capture for chemical absorption*
Source: Nwaoha et al. (2017)

Generally, lean amine absorbs acid gases with primary and secondary amines more easily at a lower temperature. Lean amine temperature should be held 5 – 7 °C above the inlet gas temperature to avoid condensation of heavier fractions of hydrocarbon. In poor amine concentration, the number of molecules that have to be in contact with acid gases in the absorber would be fewer, which contributes to an inadequate absorption. At higher concentrations, the regeneration is more difficult, and it requires additional heat input. At higher concentrations, reboiler duty and corrosion rate rise in the long run (Sharif Dashti et al., 2015).

Complementary in **Figure 8**, absorption (blue) and desorption (red) processes are carried out at different temperatures wherein both can happen the amine degradation or evaporation. The rate of CO_2 desorption can vary from one amine to another. Flue gasses to the CO_2 absorber must be cooled between 45 and 50 ºC. Usually, the temperature inside the absorber is between 40 and 60°C. Then, the stripper will be regenerated at high temperatures typically from 100 to 130 ºC, and at a bit elevated pressure than atmospheric, which would be 1.5 – 2 atm (M. Wang et al., 2011).

CHAPTER III

3. CHEMICAL SOLVENTS

It is common to employ additives in small-scale and large-scale processes as amine-based aqueous compounds.

Namieśnik & Zygmunt (2005) stated that amines are chemical compounds extracted from ammonia in the same manner that alcohols and others are derived from water. Amines can be produced in the decomposition of larger molecules, i.e., amino acids and ammonia synthesis. It is also produced in animals' digestion and microorganisms and is found in animals' urine and feces. Short-chain aliphatic amines are released into the environment from waste incinerators, wastewater treatment plants, stock farming, tobacco smoking, and exhaust gases.

Complementary, amines abbreviations and compounds are found in **Appendix A**.

3.1 Amines Types

3.1.1 Amine Classification

As we can consider alcohols and ethers as organic derivatives of water, we can regard amines as ammonia derivatives. In any event, amines are not classified as alcohols. The distribution of alcohols is based on the number of groups involved in the carbon atom bearing, the hydroxyl groups. Amines are classified according to the number of alkyl (or aryl) groups attached to the nitrogen atom (Ouellette & Rawn, 2014). To sum it up, as an effect of this study, amines can be classified according to the number of atoms of radicals (carbon-chain or cyclic organic compounds) attached directly to the central nitrogen atom.

For this work, amines are considered into primary amines (with only one radical bonded), secondary amines (with two radicals bonded), and tertiary amines (with three radicals bonded), as shown in **Figure 9**. Additionally, other compounds can form cyclically; they are called heterocyclic amines, which will be studied in after parts.

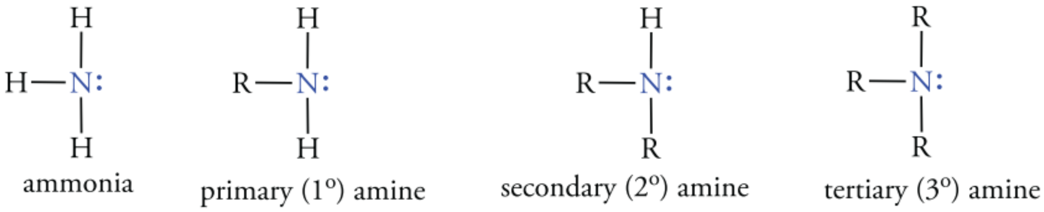

Figure 9: *Ammonia and amine classification*
Source: Ouellette & Rawn (2014)

A specially-named amine, alkanolamine, comes from the primary amines. This group is conformed by the bonding between three components, one hydroxyl group as a primary alcohol, one amino group as a primary amine, and an alkane backbone. Complementary through the wide group described before, two more categories, including secondary and tertiary alkanolamines, each composed of a secondary and tertiary amine, including one or more hydroxyl groups in its backbone. (Chowdhury et al., 2013; Kohl & Nielsen, 1997).

OH-group in alkanolamines reduces the instability and favors the solubility into water (Kidnay & Parrish, 2011). Consequently, during amine tests technologies, it is common that most amine-based chemical compounds and blends are employed with the use of deionized water (Liu et al., 2019), distilled water (Mei Wang et al., 2018), or deionized distilled water (Kierzkowska-Pawlak & Kruszczak, 2017).

At this point, it is desirable a brief explanation of the effects of primary, secondary, tertiary, hindered, and formulated amines in the CO_2 capture process. The typical utilization of amines in refining industries is as chemical solvents. It is expected that amines are used in water solutions at concentrations ranging from roughly 10 to 65 wt% (Kidnay & Parrish, 2011). According to Mokhatab et al., (2015), the typical concentrations of different amines are found in **Table 2**. However, there is important to mention that in different processes, amines can vary their concentration in the function of the desired grade of capture, operational arrangements of the industrial plant, or even the characteristics of the gas current employed due to corrosion problems. Some of the CO_2 capture process points where corrosion is detected are absorber overhead, absorber bottom; stripper overhead; stripper bottom; absorber off-gas, CO_2 product (Kittel et al., 2009).

Table 2: *Typical amine concentrations in chemical absorption*

Type of Amine	Typical concentration (wt%)
Primary (i.e., MEA)	10 – 30
Secondary (i.e., DEA)	20 – 40
Tertiary (i.e., MDEA)	30 – 50

MEA: monoethanolamine; DEA: diethanolamine; MDEA: N-methyldiethanolamine

3.1.2 Heterocyclic Amines

Heterocyclic aromatic amines, or heterocyclic amines (HCAs), are mainly produced when proteinaceous foods such as meat and fish are cooked by baking or frying at temperatures above 150ºC. Some can be found in vitamins, cigarette smoke, and oil exhaust particles as well. In this review, HCAs are considered as compounds with at least one heterocyclic ring (John & Beedanagari, 2014).

Their reactivity in the capture process requires the absorption of the acid-free carbonic proton produced by the interaction between CO_2 and water. The amine-water reaction interaction due to its basicity (in virtually all amines) results in pH values higher than 8.5. As a consequence, it helps in faster CO_2 reactivity. Two examples of heterocyclic amines are shown in **Figure 10**.

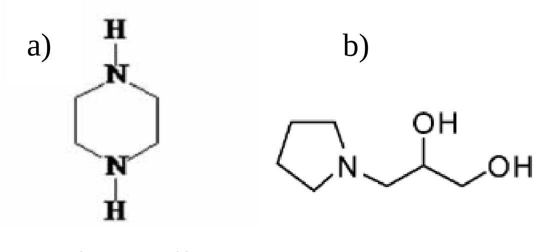

Figure 10: *Structures of two different heterocyclic amines (a) Piperazine (b) 3-piperidino-1,2-propanediol*
Sources: a) Bachelor & Toochinda (2012), b) Chowdhury et al. (2013)

3.1.3 Formulated Amines

In natural gas processing, acid gasses must be separated from the gas before transport. CO_2 separation technology should be regarded as a mature technology. When choosing amine for a combination of treatments, various factors need to be considered. This selection obeys enough volatility to be in the gas phase in the upside of the zone of condensation and condense along its zone. Success lies in the production of next-age solvents. "Engineered" or "formulated" amines are examples of the newest solvents that could be suitable for industrial applications (Chakma, 1999; Fearnside & Murphy, 2003).

A formulated amine can be generally defined as an amine explicitly formulated to perform simple tasks. Major solvent producers sell many patented solvents are based on formulated amines (Chakma, 1999). According to Koehler & Claffey (1999), the polyisobutene (PIB) – amine employment has been widely used as formulated amines. The enterprises have in their own the usage of each patent:

Table 3: *Representation of PIB-Amine yields from U.S. Patent literature*

U.S. Patent No.	Assigned To	Amine	PIB–Amine %
4,055,402	BP	AEEA	72.2 %
5,346,965	FERRO/KIEL	AEEA	72.0 %
3,869,514	TEXACO	AEEA	67.8 %
3,438,757	CHEVRON	EDA	31.0 %
3,753,670	SHELL	DMAPA	61.2 %

AEEA: 2-(2-aminoethyl-amino)ethanol; EDA: ethylenediamine; DMAPA: 3-dimetilaminopropilamina

In the study of formulated amines during the latest years, Chowdhury et al., (2013) make interest in the mixture of amine sorbents, especially primary and tertiary or secondary and tertiary amines; for example, MEA and MDEA or DEA and MDEA, respectively. These integrated components have a higher reaction rate than primary and secondary amine solvents proposed for industrial gas processing.

Linch (1953) proposed in their patent that, "In the case of formulated amines, it has long been known that aromatic amines tend to oxidize rapidly on contact with air, resulting in loss of aromatics and degradation due to contamination by oxidation products.” Amines that are consumed in industrial processes have become impractical. Storage deteriorated amines need to be cleaned before use, and it is too expensive due to amine loss through oxidation and additional losses in cleaning processes.

Another example of formulated amines is shown by Baburao et al., (2014), where UCARSOL^{TM} FGC-3000 is employed by Alstom Power and The Dow Chemical Company's authorization. Here, the amine solvent capture of CO_2 from flue gases produced by fossil fuel power plants is developed for minimal energy consumption and robust performance leading to cost-saving operational benefits. The amine solvent circuit is constructed from stainless steel materials to provide future options for working with other amine solvents, which may be more corrosive. Emissions of gaseous amines were low (a few ppmv). The behavior of the solvent shows good thermal and chemical stability.

Complementary, ExxonMobil and BASF have developed many formulated amines to support refineries and gas processors in today’s strict pollution regulations. The following can be highlighted Established OASE® sulfexx™, FLEXSORB™ SE, and FLEXSORB™ SE Plus technologies which allow low running costs and energy use, low capital costs, and environmental benefits (ExxonMobil, n.d.). INEOS Group (2021) developed a formulated amine-based on MDEA called Gas Spec, which is less corrosive than generic amines. All developed amines aim to separate in major quantity CO_2, better chemical stability, and a more extensive productive life under extreme conditions than MEA and DEA.

Additives as aqueous amine solvents contain either a single amine or several amines in a combination. While single amine solvents are still commercially used, amine blends and formulated amines tend to be rational alternatives in gas separation. Advancements in technology associated have proved to be superior to conventional technologies. Newly produced high-performance solvents are also based on amine blends (Chakma, 1999; Hwang et al., 2018). Many research aiming at discovering new mixed amine solvents have primarily focused on a laboratory scale (Hwang et al., 2018). Capturing and releasing CO_2 by a cyclical chemical absorption/regeneration mechanism is expected to result in more than half of the cost of capturing absorbent regeneration and reducing the energy consumption of absorbent regeneration (Chowdhury et al., 2013).

As stated before about formulated amines, those have a better performance than conventional amines, among others in economics and preserving installations by decreasing corrosion. Many research types at the vanguard look for conventional amines blends and/or additives to improve current industrial technologies' capture process. Formulated amines are not used all the time. Lee et al., (2013) and Nwaoha et al., (2017) develop strategies when selecting amine solvents considering each's market price. A huge contradiction as formulated amines is the best in the amines market. Thus, they would contain some restrictions, setbacks, or small print in contracts for the use of formulated amines.

According to Gas Technology Products LLC (2004) and Gulf Publishing Company (2012), various formulated amines are developed for specific processes. As expected, only the compounds' improvements are detailed in different chapters of treating gas processes, each explaining the improvements and advantages of the amines reviewed. However, it recognized that they follow a common pattern, including not publishing some (if there are) disadvantages of amines. The formulated compound comes not only as a chemical solvent; they include some specifically required operation units as pumps, tanks, and specific pipeline arrangements.

Summarizing the observations, it is proved that if an amine simply by being formulated implies a higher development and costs. A specific required additional technology is necessary to obtain a license for use. In practical aspects, this means that the average cost amount is aimed at increasing more than expected. Contradictory to the fact that the use and research of new additives do not need different industrial units than the existing ones to maintain production, energy, and licensing costs.

3.2 Reaction Mechanisms

The reaction of CO_2 with primary, secondary, and sterically hindered amines is generally described by the zwitterion process, whereas the base-catalyzed hydration of CO_2 describes the reaction with tertiary amines. Complementary, tertiary amines and sterically inhibited amines often do not form carbamates; their reactivity requires the absorption of the acid-free carbonic proton produced by the interaction between CO_2 and water (Conway et al., 2013; Vaidya & Kenig, 2007).

Alkanolamine solvents are widely used as a reactive absorbent in post-combustion capture due to their high performance and good recyclability. However, certain issues, such as a high-energy penalty for restoration and a propensity for decay, remain unanswered. Consequently, it is important to produce superior absorbents to replace current amino solvents (Xiao, Cui, Zou, et al., 2020).

The importance yields on the formation of certain intermediates that correlate the reaction that governs each mechanism, impacting economic investments, environmental and energetical consumption, operative technology, and control parameters as corrosion.

3.2.1 Zwitterion Mechanism

As stated before, we can describe the mechanism by which carbon dioxide reacts with amine-based (blended or not) compounds.

Vaidya & Kenig (2007) described step by step the reaction, where the reaction between the amine and carbon dioxide undergoes the formation of a zwitterion as intermediate:

$$CO_2 + AmH \rightleftarrows AmH^+COO^- \tag{1}$$

Where AmH can be a primary, secondary, or sterically hindered amine. After this, the intermediate is deprotonated by a base (or bases if there is more than one), to obtain the formation of a carbamate:

$$AmH^+COO^- + B \longrightarrow AmCOO^- + BH^+ \tag{2}$$

In the case where the base is the amine itself, Eq. (2) can be represented as:

$$AmH^+COO^- + AmH \longrightarrow AmCOO^- + AmH_2^+ \tag{3}$$

Eq. (1) and Eq. (3) describe a step-by-step process; due to this it is possible to transform them into an overall reaction stated in Eq. (4):

$$CO_2 + 2AmH \rightleftarrows AmCOO^- + AmH_2^+ \tag{4}$$

Additionally, if there is the presence of sterically hindered amines, the zwitterion reacts easily with water than amine, resulting in the formation of bicarbonate:

$$AmH^+COO^- + H_2O \longrightarrow HCO_3^- + AmH_2 \tag{5}$$

However, in sterically hindered amines, the carbamate that might take place can undergo hydrolysis, forming bicarbonates. This can be represented as:

$$AmCOO^- + H_2O \longrightarrow HCO_3^- + AmH \tag{6}$$

Increasing the formation of bicarbonates over carbamates in the reaction of sterically hindered amine. In kinetical terms, the momentum that defines the reaction rate is given by the formation of the zwitterion

3.2.2 Thermomolecular Mechanism

Suppose an amine interacts simultaneously with one molecule of CO_2 and one molecule of a base. The reaction proceeds in a single step through a coupled encounter complex as an intermediate. This may be described as:

$$CO_2 + AmH \cdots B \rightleftarrows AmCOO^- \cdots BH^+ \tag{7}$$

This complex can form reactant molecules, while a little fraction reacts with a second molecule of water or amine, producing ionic compounds. Resulting in a very similar form at the end regarding the zwitterion mechanism but without an intermediate compound (Vaidya & Kenig, 2007).

3.2.3 Base-Catalyzed Hydration Mechanism

It is suggested that tertiary amines cannot react as fast as primary or secondary amines with CO_2 because of steric hindrance. These amines have another mechanism, resulting in a base-catalytic effect on the hydration of CO_2.

$$CO_2 + H_2O + R_3Am \longrightarrow R_3N^+H + HCO_3^- \tag{8}$$

As shown in Eq. (8), tertiary amines include in the reaction the presence of water due to the sterically hindered tertiary amines as they have three radicals that might increase the hindered effect in the molecule (Vaidya & Kenig, 2007).

The main purpose of the mechanisms is to comprehend how to interact with carbon dioxide and how promoters/additives would improve the process. It is important to mention that bicarbonate formation in the presence of water can form a corrosive agent called carbonic acid in a very slow percentage but present during the chemical process. Kinetics and thermodynamic improvements yield an improvement on the mechanism and, in energy consumption, environmental impact, and industrial units involved. To sum up the mechanisms, it is suggested a general mechanism for carbon dioxide and amines is seen in **Figure 11**. According to this process, the bulk of the CO_2 trapped would result in bicarbonate production in the amine system's liquid presence. In aqueous media, 2 mol-amine/mol-CO_2 is needed to form stable bicarbonate compounds resulting in CO_2 capture (Yang et al., 2008).

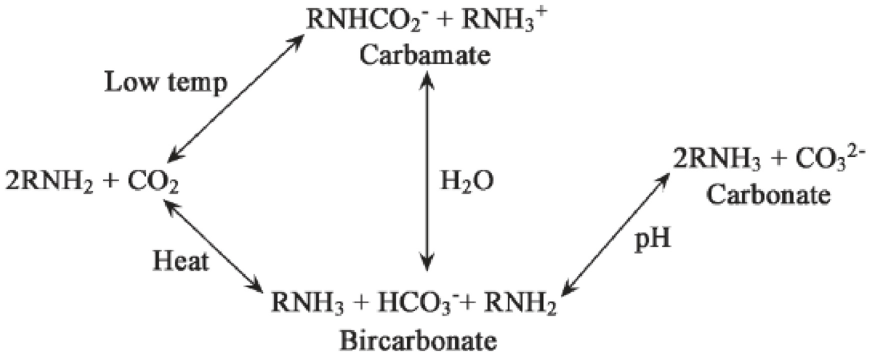

Figure 11: *General proposed reaction sequence of* CO_2 *chemical amine absorption*
Source: Yang et al., (2008)

3.3 Amine Challenges in the CO_2 Capture Processes

Amine concentrations are calculated by unit operating experience, taking into account solvent consistency, foaming propensity, corrosion rate, and unit efficiency. Higher concentrations can reduce the circulation of amines and increase the temperature of absorption and corrosion rate. Amine units can usually meet performance promises and have no operational issues in early service. However, device efficiency typically deteriorates with time, primarily due to the build-up of pollutants and impurities and lack of maintenance (Mokhatab et al., 2015).

The principal disadvantages of the types of CO_2 capture are:

- Adsorption devices may not be appropriate for use in large-scale flue gas treatment plants. At this size, the poor adsorption capability of most available adsorbents can pose major challenges.

- Water wash cannot be afforded with very contaminated gas currents as they are needed to be purified before.
- Physical adsorption occurs at high partial CO_2 pressures. As such, the key energy requirements make the pressurization of flue gas very costly.
- In membrane separation, the high cost is the key drawback of using a membrane in carbon capture processes, and the method of synthesis of most separation ultimate membranes is very expensive, making them economically unfeasible.

Nevertheless, chemical solvents can also cause problems, less dangerous than other capture processes due to it is the most developed technology. Despiting that industrial damages are not only caused by amine blend solvent, but hydrocarbon waste can also be mitigated by keeping a temperature approach between the lean amine and feed gas, skimming hydrocarbons from rich amine flash drums and reflux drums, and regular improvements in particulate filters and carbon filters (Elhenawy et al., 2020; Mokhatab et al., 2015; Rasi et al., 2008; M. Wang et al., 2011).

Chemical absorption, high vapor pressure, corrosive nature, and high energy input are some drawbacks for the regeneration of amine-based solvents in sectors that are involved in CO_2 pollution (Babamohammadi et al., 2015). The drawbacks of the most common amine (MEA) employed in the capture process studied by Yang et al., (2008) include:

1. Low carbon dioxide loading capacity.
2. The high corrosion rate of the equipment.
3. Amine oxidation by SO_2, NO_2, HCl, HF, and oxygen in the flue gas.
4. High energy consumption during high-temperature absorbent regeneration.

The solubility of CO_2 in the liquid phase is very important for the proper measurement of absorption behavior. As a result, replacing water in amine solvents with organic co-solvents, such as alcohols, will also increase the physical solubility of CO_2 in solutions, improve the performance of solvent regeneration and reduce the cost of regeneration. However, the elevated level of volatility of co-solvents is a drawback for industrial applications. Besides, the higher viscosity of organic solvents such as amines may have detrimental effects on heat exchanger efficiency, absorption kinetics, and pumping costs (Ochedi et al., 2021).

CO_2 capture systems as amine-based chemical solvents are used in industrial processes, which by their chemical nature might corrode devices leading to bicarbonate and carbamate species. Some techniques have been implemented, such as incorporating corrosion inhibitors or the introduction of alternate absorption liquids. The electrochemical test checks must be carried out to clarify the potential harm incurred by the preceding evidence (X. Li et al., 2020). In comparison, mixed amine solvents can lead to a lower circulation flow rate, which means smaller equipment sizes and lower capital and operational costs (Ochedi et al., 2021).

Using an alkanolamine such as a liquid adsorbent makes variable debris and operative problems like corrosion, volatility, thermal degradation at 100 – 150 ºC, and makes it difficult to control. Therefore, the use of power and the cost are high and might increase in each absorption process (Siani et al., 2020). Thus, developing improved methods in the chemicals for the CO_2 capture process is required to prevent high temperatures and then mitigate negative effects (Baltar et al., 2020). To sum up, amine degradation activity can result in loss of solvents, accumulation of by-products, foaming, corrosion, which have a major effect on CO_2 capture efficiency (Xiao, Cui, Zou, et al., 2020).

3.3.1 Desirable and Typical Characteristics of Conventional Amines

As is well-known in industrial applications, a high grade of amine vaporization losses arise in the absorber when the sweet gas escapes saturated with water at a higher temperature. A single method cannot be selected only based on the solution flow rate in the employment of chemical solvents as amine-based compounds. The amine's proper selection will substantially reduce the regeneration energy demand and solution circulation rate (Sharif Dashti et al., 2015). Relative interest in selecting conventional and new searches of typical amines for the capture process responds to information published and literature concerning, as shown in **Figure 12**. Other operational problems include solvent corrosiveness and solvent chemical instability, which, as indicated in the studies, are more vulnerable to primary and secondary amines than tertiary amines (Idem et al., 2006).

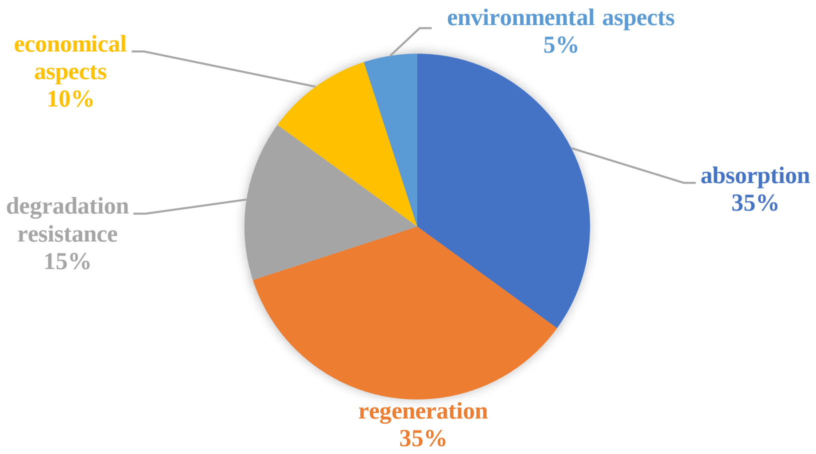

Figure 12: *Distribution of technical and economic studies for amine selection*
Source: Dubois & Thomas (2013)

As a consequence, it is important to guide the typical characteristics of conventional amines. As stated in **Table 2**, the comparative will be accurate to show the common characteristics of primary, secondary, and tertiary amines. First, the chemical solvents employed as aqueous amines have some advantages illustrated in **Table 4** (Zhao et al., 2012).

Table 4: *Advantages and disadvantages for CO_2 capture ammines*

Approach	Advantages	Barriers to application
Amines (MEA, DEA, MDEA, PZ)	• Less volatile • Good stability of absorbent • Enhancement role used as additives	• Absorption efficiency • High energy consumption for regeneration • Resulting in system corrosion

Next, including some of the typical solvents employed by Babamohammadi et al., (2015) in chemical absorption in **Table 5** without mentioning the improvements as they are going to be discussed in the next chapter.

Table 5: *Characteristics of some conventional solvents in CO_2 chemical absorption*

Chemical Solvent	**Specifications**
MEA	• Reactivity is high, and absorption is fast • Absorption of hydrocarbon is low • CO_2 loading limited by stable carbamates • Operational issues (foaming, increased corrosion, and viscosity)
DEA	• Reactivity is high, and absorption is fast • Less stable carbamate than MEA • CO_2 loading limited • Prone to certain corrosion and solvent degradation
MDEA	• CO_2 loading is higher than MEA and DEA due to bicarbonate formation • Regeneration is low as it interacts better with acid gases • Less degradation than MEA and DEA • Slow absorption kinetics with CO_2
PZ	• Reaction with CO_2 is much faster than MEA and DEA • Thermal degradation resistance up to 150º C • Volatility lower than MEA but its solubility in water is limited

CHAPTER IV

4. ADDITIVES TO IMPROVE THE CO_2 CAPTURE PROCESS

4.1 Research Approach

Several solvent solutions to the use of amines are being studied, but the ideal solvent has not been found. One of the most important factors is implementing a closed process that allows solvents to be reused at minimal environmental and economic costs. The implementation of new technology must always consider the overall effect of the whole process and how that technology can be tested to provide solutions on a local or global scale. (Varajas, 2021).

Ricaurte (2012) proposed in his work a literature review model that focused on the last 20-years and reviewed a variety of articles to improve hydrate formation. This work was based on that model as a template but to find chemical solvents (additives) to improve the CO_2 capture process. Once the articles have been analyzed, the respective resolutions to the work are presented.

4.2 Trends in Additives Research

The study's importance yields on the scientific community's interest to develop new strategies and improve actual ones without making changes in the current industrial infrastructure. Demonstrating that it is possible to formulate existent chemical compounds like additives that improve the capture process technologically, economically, and efficiently.

The research carried out as set out in **Appendix A** in a data matrix of additives was performed in the interest from the beginning of the 21^{th}-century to nowadays, as shown in **Figure 13**.

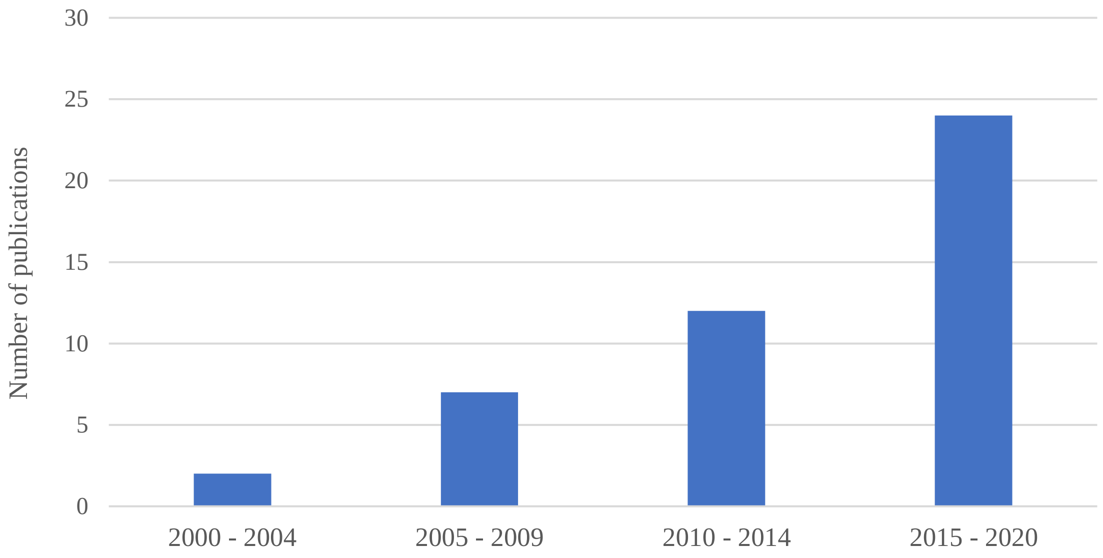

Figure 13: *Publication's trend of additives to improve* CO_2 *capture*

The graph establishes the research trend published in five years, starting at the beginning of the 21st century to 2020, where a clear tendency to increase chemical solvents' investigations. The graph reveals that the scientific community's interest in additives to improve CO_2 capture has evolved since the beginning of the century.

Also, it reflects that researches and works focused on finding additives that improve carbon dioxide capture tends to increase, this could be due to the increase in operational problems that conventional amines cause in their industrial use, such as technologies employed in natural gas, petroleum, coal-fuel fired thermal power plants and chemical process industrial units (Mukhtar et al., 2020). Furthermore, the high capital that must be invested to acquire permits and licenses for the use of formulated amines is confidential (Dotson, 2013).

There might be many causes that solve and prove this trend, but this study has proposed one. Suppose a chemical capture process undergoes amine-based blends composed of additives. In that case, the capture process rate might increase, helping industrial operation units prevent their main problems like corrosion and reducing maintenance costs and energetic ones, especially in countries that base their economics on oil and gas production.

It is important to mention that the available data of dates shown in **Figure 13** is related only to the Data Matrix in **Table B.1** in **Appendix B** of the present study and does not compile the basic information presented in the state-of-art work. It only collects additives reviewed with the correspondent date information, crucial to this study.

4.3 Additives Overview

The additives found during the literature review needed to be classified to manage the information better. For the present work's practical purposes, a classification based on the compounds' origin was taken, focusing on compounds' chemical nature as is stated in **Table 6**.

Table 6: *Abbreviations in the classification of additives*

Full Name	Abbreviation
Alcohol	Al
Alkanolamine	AAm
Amine Family	AF
Amino Acid	AmA
Antifoam Emulsion	AE
Catecholamine	CAm
Corrosion Inhibitor	CI
Cyclic Ester	CEs
Cyclic Ether	CEt
Heterocyclic Amine	HCA
Inorganic Compound	IC
Ionic Liquid	IL
Organic Salt	OS
Resin	R
Surfactant	S

This study culminated in extensive research of different chemical solvents, additives/promoters to improve the CO_2 absorption process. Additives are grouped according to the amine categorization, primary, secondary, and tertiary amine. Additional classifications correspond to other amine compounds with a different structure than primary secondary and tertiary as amino acids (containing a mixture). Additionally, some other compounds that do not contain amines in their chemical structure but keep being chemical solvents are also classified in other chemical nature compounds is located in **Appendix A**.

Chemical solvents additives are classified into families because it is necessary to manage the information efficiently. According to its chemical nature and engineering aspects, the criteria for their classification are conventional named products employed in the chemical capture process. On the other hand, this study has found that additives are not just closed to the kinetical or thermodynamical improvement. The additives can also control foaming production or protect the available equipment to avoid corrosion.

Hence, chemical solvents as additives/promoters to improve chemical absorption are in the front line of investigative applications nowadays, and the main benefit comes from that these chemical additives are already existent (purchasable) compounds. Its utilization is being tested, and the current infrastructure has no need to be transformed or adapted for its implementation. According to Alivand et al. (2020), various promoters have been successfully developed, including those in **Table 7**.

Table 7: *Some additives employed to improve chemical absorption*

Group	Additives	Reference
HCA	Piperazine	(Rochelle et al., 2011; Yuan & Rochelle, 2019)
	Benzotriazole	(Mota-Martinez et al., 2014)
AmA	Arginine	(Gusnawan et al., 2020)
	Histidine	(Vullo et al., 2012)
Al	Methanol	(Rashidi et al., 2020)
	Phenol	(Zhang et al., 2015)

CAm	Dopamine	(Vullo et al., 2012)
	Adrenaline	
OS	Tetrabutylammonium Chloride	(Hashimoto, Yamaguchi, Ozeki, et al., 2017)
	Tetrabutylammonium Bromide	(Yue et al., 2019)
IO	[Choline]Cl	(Yin Xu et al., 2015)
	3-Fluorophenol	(Zhang et al., 2015)
S	Sodium docecylbencene sulfolane	(Yue et al., 2019)
AE	VP 5371	(Hashimoto, Yamaguchi, Kinoshita, et al., 2017)
CI	CRO27005	(Mota-Martinez et al., 2014)

To overcome limitations presented in chemical absorption with amine-based solvents, the blended solvent is proposed, which is composed of an amine blend and some chemical additives. The benefits of amine blends are also limited to individual amines on the market (Chowdhury et al., 2011).

Gómez-Díaz et al., (2018) have studied the effect of primary amine (monoethanolamine, MEA), secondary amine (diethanolamine, DEA), and tertiary amine (triethanolamine, TEA) in the absorption with and without additives of CO_2 with a purity of 99.99%. They demonstrated that the main reaction is carbamate production when MEA and DEA are employed. The stability of DEA-carbamate is lower than that of MEA-carbamate due to the higher steric hindrance of DEA. So, it reduces the overall rate and confirms the lower absorption value. As TEA reacts differently with CO_2 and water, it will have a different value in the absorption process.

Gómez-Díaz et al., (2018) concluded that amines' absorption efficiency could be disposed of according to the next scale: DEA < MEA < TEA. Now, if an additive is added to the amines, its properties change. This scale might vary by adding different additives, as one main objective is to focus on added kinetic or thermodynamic additives to improve its properties. An example of kinetic and thermodynamic promoters is stated in MEA in the presence of sodium dodecyl sulfate (SDS), and tetra-n-butylammonium bromide (TBAB) can increase the mass transfer rate and the solubility in the presence of the additive, respectively (Mohammadpour et al., 2019).

Another study of conventional MDEA was made by Mei Wang et al., (2018), where a mixture of simulated flue gas of carbon dioxide and nitrogen was combined to perform this experiment, both with no further purification of 99.99% and the use of distilled water. It was made under two conditions, one of absorption and the respective desorption part. The amine additives are TETA and AEP, each employed with different compositions at vol%, one with the conventional amine and distilled water, the other with the amine, additive TETA and distilled water, and the final with MDEA, TETA, AEP, and distilled water at different compositions.

The experiment was carried out at 25 ºC and 1 bar of absorption and 100 ºC and 1 bar for desorption. It is observed that amine blends' viscosity increased as the additives were added and increased their concentration. The results reflected that absorption capacity increased as the additives were added to the amine base solution. These results also reflected that the activation effect of chemical solvents was much better than expected as MDEA < MDEA+TETA < MDEA+TETA+AEP. Similarly, the efficiency of desorption performance of additives was also improved as the solvents were added.

However, the negative effect reflected on the experiment was the increase of viscosity; due to this, it was confirmed an obvious increment of it while it was elevating the volume fraction of additives. Even if the experiment reveals no direct relationship between the absorption performance and the viscosity, an additional negative effect was evident in the desorption efficiency.

4.4 Additives Outcomes

After reviewing several articles that have the main topic of the CO_2 capture process with chemical solvents and additives, it is obtained additives' characteristics in a Data Matrix. These characteristics are obtained from the year of publication, chemical solvents, typical concentrations (provided by chemical houses and the employed in each experiment), type of gas employed in the capture process, relevant observations, and how they evaluate the efficiency of amine blends. Additional comments on the characteristics are stated in **Appendix B**.

4.4.1 Gases for CO_2 Capture Process

As a consequence, the information recorded and processed from the state-of-the-art work yielded the following. One of the observed common parameters in each research is the different utilization of gases in the capture process. As seen in **Figure 14**, the distribution of the different gases employed in the capture process reveals that flue gas is the most employed gas. This is due to the most efficient and low-cost processes are carried out in post-combustion capture processes.

Complementary, existing industrial plants can undergo this kind of process. It is relatively more efficient to develop a methodology to improve the efficiency in built plants than change all the industrial matrix of countries or creating new pre-combustion capture processes as it is the fuel gas (a mixture of $CO_2 + H_2$).

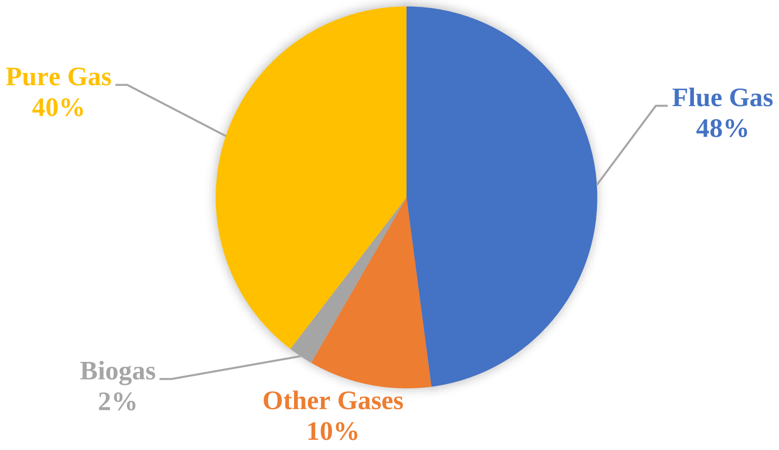

Figure 14: *Distribution of typical gas employed in the CO_2 capture process*

One of the most employed (gases) in small-scale processes is pure gas. Many types of research do not conveniently simulate other gas mixtures as their apparatus and systems are not certified and thus prepared for a gas mixture that might complicate the capture process. As stated before, corrosion in industrial scales is one main problem in the capture process, but if we take that to small-scale processes, the row of implementation new additives can break, and no further improvements would occur in the short term.

Biogas for CO_2 capture processes has a few examples, Yue et al., (2019) employed simulated biogas as the purpose of the investigation in the CO_2 capture and its posterior purification employing the hydration method (reviewed in Chapter II). The part of *other gases* must be included because many experiments include various gas mixes out of the common, that in general tries to simulate in a better way the industrial conditions:

- Some of these gases are pure methane (CH_4) as it has traces presented in natural gas for separation and after the capture process.
- Experiments show employees a complete mixture of gases as carbon dioxide, hydrogen sulfide, oxygen, oxide nitrates (NO_x) and dust, to maximize simulation as in real conditions.
- Others contain the components of flue gas but with one more component as nitrogen dioxide (NO_2).
- Other absorption systems are based on carbonic anhydrase, an enzyme that catalyzes carbon dioxide's rapid conversion.
- Natural gas is also tested for the CO_2 capture process.

It is also important to remark that the main part of flue gas, pure gas, biogas, and others are used in small-scale processes. Then, the proposed gases must be tested. Because laboratories must develop the closest simulation to prove the availability of a process, next, it is tested in pilot plants and if the tested evidence is rightful, it is suitable to implement it on an industrial scale. In contrast, final consent is one of the most difficult premises as industries have the strictest acceptance system. Despiting that, on a large scale as pilot plants, they employ flue gas, as it is the most similar gas current in comparison to the existing industrial gas capture plants.

4.4.2 Additives Nature Classification

The present study of state-of-art is developed to investigate the premise of finding additives to improve the existing carbon dioxide capture process. Due to that, chemical solvents as additives/promoters are investigated during their completion. Many types of chemical solvents are observed during the progress of this study. All of them are defined in **Figure 15**. The percentage describes their frequency of employment as promoters in the chemical absorption of carbon dioxide.

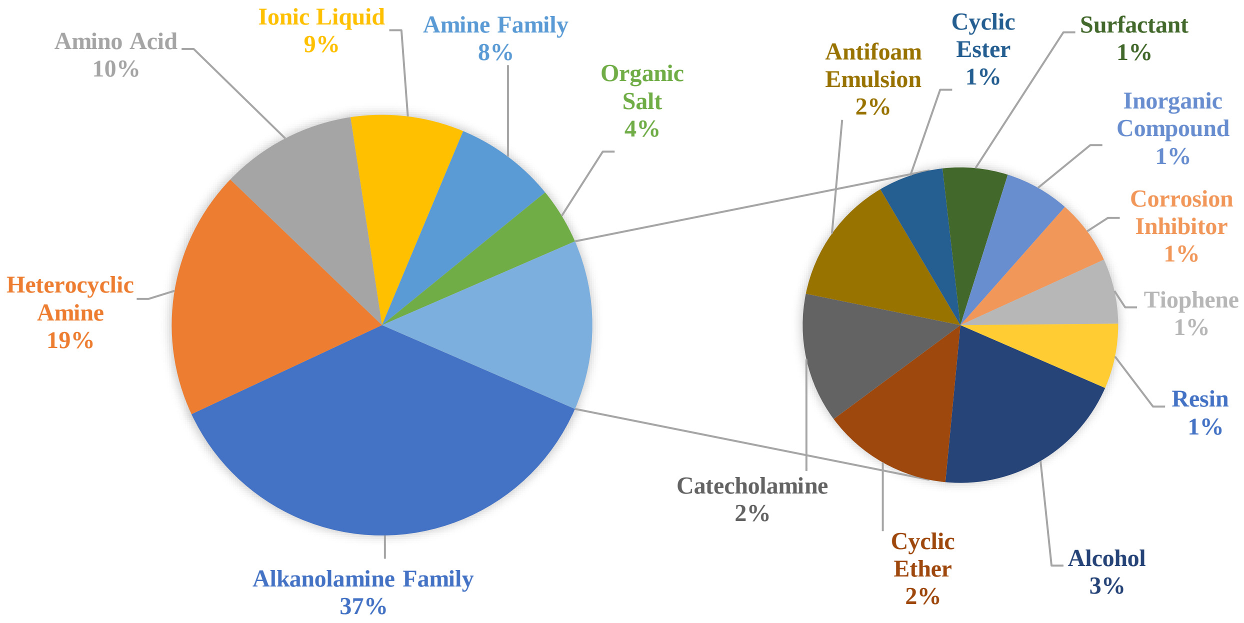

Figure 15: *Additives employed to improve CO_2 capture*

The compounds that have amine(s) in their structure are separated into four groups because of their nature; the remanent components are described as each one's chemical family. It is also important to clarify the compounds described in **Figure 15** are mostly used as promoters considering the employment of a base solution (no related with basicity) as the support or template of the chemical experiments and how the promoters show their improvements.

In terms of additives, compounds that contain amine-group in their structure are the most employed in carbon dioxide capture, as they represent 74% of the total compounds. As stated in section 3.1 of the present work, one of the additives employed is alkanolamines.

The major group is the alkanolamines; the group is formed mostly by the primary alkanolamines (composed between primary amine and primary alcohol). Other groups are the secondary and tertiary alkanolamines which are formed by a secondary and tertiary amine, respectively, and one or more hydroxyl groups. To unite all the alkanolamine groups, it was created the category of alkanolamine family. These are the most frequent additives employed to increase the capture process due to the alcohol group increasing their solubility, avoiding the blend's major viscosity problems.

Reciprocal alkanolamines are widely developed as promoters because of their facilities at the time of purchase and use; they are the most employed in industrial applications. As here lies the most typical amine MEA. Additionally, in this group are localized the most typical secondary and tertiary amines, which were already described, DEA and MDEA respectively. These amines are also considered as base solutions because of their current utilization in industries. Commonly, many types of research evaluate their possible improvements, like Liu et al., (2019) and You et al., (2008), where stated low energy regeneration has drawn a great deal of interest absorption than other traditional amine absorbents.

The second group is additives amine-cyclic-based compounds, the heterocyclic amines. Its name reveals the possible forms of them and their importance, mainly as kinetic promoters, which will be better explained below. Continuing this trend, amino acids appear, in the latest and closest years, many investigations have been carried out to justify their new importance as additives in the capture process, according to Bavoh et al., (2019) because of their chemical stronger interactions with water as zwitterion mechanisms, and as they can be more environmentally friendly.

The next group is the ionic liquids (IL), these compounds have the same characteristics as amino acids, which is the strong electronic interaction of the compounds and the CO_2, and its stability is also more prom than conventional additives. However, the difficulties yield on the synthesis of the ionic compounds as they need specific ambients and commercially are among the most expensive compounds to investigate (Haider et al., 2020). Additionally, the use of IL’s is proposed to be an exponential increase over time, as stated in the investigation of Haider et al., (2020).

Additionally, one of the big groups is the amine family. This group is only conformed of smaller families that only contain amine groups. The four smaller ones are monoamines conformed of compounds that only have one amine group; diamines conformed by two amine groups, triamines conformed for three amine groups, and tetramines conformed of four amine groups, despiting of if there is a primary, secondary or tertiary amine.

Alkanolamine family, heterocyclic amine, amino acid, ionic liquid, and amine family composed the top five employed additives. Those compounds are called big-five because they represent 83 % of the total additives considered in this study. In smaller percentages are stated compounds with no amine presence group, which might cause their use. Those are organic salts, alcohols, surfactants, catecholamines, antifoam emulsions, inorganic compounds, cyclic esters, cyclic ethers, corrosion inhibitors, thiophenes, and resins. Most of them can be directly related to additives that their efficiency is not focused on improving the in-situ capture process itself but rather on improving technical aspects of capture such as foam formation or one of the process's major problems such as corrosion.

It was established as a study objective to find chemical solvents from natural sources such as wastes from the agricultural or floricultural industry. However, no specific chemical compound was obtained that met the requirements established in the work. If the bibliographic review would be extended to include chemical solvents and natural compounds (such as algae or rose stems) that could improve the capture process, studies dealing with green additives should be found.

4.4.3 Additives Improvements

According to the data matrix and considering additives classification, the analysis proposed to this study reveals the different improvements of additives' different families. The results are shown in **Figure 16**. The final classification of additives can be divided into improvements that directly affect the capture process *per se* and others that involve improvements that prevent certain problems in the equipment and around the process.

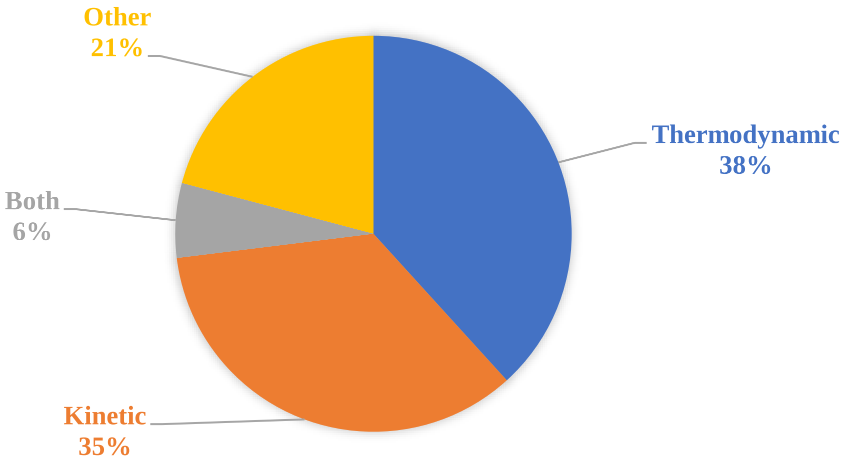

Figure 16: *Type of additives' improvement*

Thermodynamic improvements are directly related to those that affect the solubility, viscosity, evaporation, and physicochemical properties of additives in the blends. For example, You et al., (2008), employed different additives as AMP, AMPD, AEPD, and THAM (different types of alkanolamines) to prove their efficiency as thermodynamic promoters to avoid evaporation in the experiment and demonstrate it in different graphs of removal efficiency and quantify results in a scale of the weight loss. Complementary, Yin Xu et al., (2015), used different ionic liquids to prove their efficiency. The results are shown as the variation of CO_2 concentration for the different additives in the treated gas, also quantify the variation blends concentration in process and a comparative table of the total CO_2 capacity in blended solutions. That gives a final result of improvement in both experiments; thus, the thermodynamic improvement is confirmed.

Kinetic improvements are based on the reaction mechanism that macroscopically can be observed in the duration of the tests and absorption - desorption rate. Xiao et al., (2020), proved different amine compounds, an alkanolamine, two diamines, and one heterocyclic amine like DEEA, N,N-DM13PDA, N,N-DM12EDA, and 4-A1MPD, respectively. The evaluation was performed to observe the absorption curves versus carbamate formation rates, data of carbamate, bicarbonate concentrations versus CO_2 loading. Additionally, Mei Wang et al., (2018) studied the influence of TETA and AEP a tetramine and heterocyclic amine, respectively, in MDEA (tertiary amine). The data of CO_2 absorption capacity, the average CO_2 absorption rate, and absorption and desorption rates versus time were quantified. Both experiments result in an improvement of absorption rates; it is confirmed kinetic efficiency improvement.

At this point, few compounds may reflect both improvements, which are proved by analyzing different investigations or one that contains dual information. Yuan & Rochelle (2019), investigated the effects of piperazine (PZ) with different additives. The results reflected an improvement in viscosity and solubility at piperazine usage, which can be categorized as a thermodynamical improvement according to the present study classification. On the other hand, piperazine blends also exhibit an increment of CO_2 absorption rate capacity, cyclic capacity, and the average absorption rate, which in this study can be reflected as a kinetical improvement.

Finally, the other improvements are strongly related to the capture process's surroundings as, during this process, foam can be produced. To control this formation, antifoam emulsions are added. Mora-Martínez (2014) investigated some of them, who also studied the effect of corrosion inhibitors in the blends. Vullo et al., (2012) studied the effect of some additives as amines and amino acids that slightly improved the blends' kinetical parameters. This category is located in others because, at the time of analyzing the investigation results, the effects are proved in carbon anhydrase's enzyme catalytic processes. Thus, this process can be stigmatized to be on a very smaller scale than the ones that this study proposed. Additionally, the first study can reduce maintenance frequency in absorption – desorption equipment.

CONCLUSIONS AND RECOMMENDATIONS

- The extensive bibliographic review of the different articles and their subsequent classification according to the additives' characteristics made it possible to classify them according to their chemical nature. It has shown that amine compounds and specifically alkanolamines are the major group and the most employed additives due to their high percentage of use to improve CO_2 capture.

- The use of additives that improve industrial operability is very few compared to those that can improve kinetic and thermodynamic conditions. Both are the most desirable since they are the source of the most significant improvements, such as reducing additive volatility, decreased viscosity, or higher capture rate.

- It has shown that the scientific community considers the development of new carbon dioxide capture additives as essential as the number of investigations has increased since 2000.

- As a recommendation, it is proposed that further studies can use this work as a guide to select the best additives and implement them in the capture process using the current infrastructure of Yachay Tech University.

- Additionally, it is recommendable that this type of further study tries to focus more on finding compounds from natural sources such as agroindustry and waste that do not compromise food security to improve the carbon dioxide capture process.

- Finally, this work's development can be considered for future research on high-impact issues as it became evident that the increase of carbon dioxide is a global issue. Likewise, avoiding the change of current capture units by considering new additives does not affect the economy of industries and the environment.

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APPENDIX

APPENDIX A:

Additives Classification

Table A.1: *Additives classification – alkanolamine family*

Abbreviation	Additives' Name	CAS #	Improvement
AMP	2-amino-2-methyl-1-propanol	124-68-5	Thermodynamic
AMPD	2-amino-2-methyl-1,3-propandiol	115-69-5	Thermodynamic
AEDP	2-amino-2-ethyl-1,3-propandiol	115-70-8	Thermodynamic
THAM	tri(hydroxymethyl) aminomethane	77-86-1	Thermodynamic
MEA	monoethanolamine	141-43-5	Base Compound
DEEA	diethylethanolamine	100-37-8	Kinetic
AEEA	2-(2-aminoethyl-amino)ethanol	111-41-1	Thermodynamic
AEP	1,3-Diamino-2-propanol	616-29-5	Thermodynamic
DMEA	2-(dimethylamino)ethanol	108-01-0	Kinetic
DMA-1P	3-dimethylamino-1-propanol	3179-63-3	Kinetic
DEA-1P	3-diethylamino-1-propanol	622-93-5	Kinetic
DMA-2P	1-dimethylamino-2-propanol	108-16-7	Kinetic
DEA-2P	1-diethylamino-2-propanol	4402-32-8	Kinetic
DIPAE	2-(diisopropylamino)ethanol	96-80-0	Thermodynamic
DMA-2M-1P	2-(dimethylamino)-2-methyl-1-propanol	7005-47-2	Thermodynamic
DMA-2,2-DM-1P	3-dimethylamino-2,2-dimethyl-1-propanol	19059-68-8	Thermodynamic
4EMA-2B	4-ethyl-methyl-amino-2-butanol	26734-08-7	Thermodynamic
EDEA	N-ethyldiethanolamine	139-87-7	Thermodynamic
IPDEA	N-isopropyldiethanolamine	In lab	Thermodynamic
tBDEA	N-tert-butyldiethanolamine	2160-93-2	Kinetic
DMA-1,2-PD	3-(dimethylamino)-1,2-propanediol	623-57-4	Thermodynamic
DEA-1,2-PD	3-diethylamino-1,2-propanediol	621-56-7	Thermodynamic
TEA	triethanolamine	102-71-6	Base Compound
MDEA	N-methyldiethanolamine	105-59-9	Base Compound
DEAB	4-(diethylamino)butan-2-ol	5467-48-1	Thermodynamic
DEA	diethanolamine	111-42-2	Kinetic
MAMP	2-N-methylamino-2-methyl-1-propanol	In lab	Kinetic

EAMP	2-N-ethylamino-2-methyl-1-propanol	In lab	Kinetic
IPAE	2-(isopropylamino)ethanol	In lab	Kinetic
IBAE	2-(isobutylamino)ethanol	In lab	Kinetic
SBAE	2-(secondarybutyamino)ethanol	In lab	Kinetic
MMEA	2-(Methylamino)ethanol	109-83-1	Kinetic
NBMEA	mono-n-Butyl Ethanolamine	111-75-1	Kinetic
TBMEA	t-butylmonoethanolamine	4620-70-6	Kinetic
EMEA	ethylmonoethanolamine	110-73-6	Kinetic
DIPA	diisopropanolamine	110-97-4	Kinetic
AMPD	2-amino-2-methyl-1,3-propanediol	204-100-7	Kinetic
MAPA	3-methyl-amino-propyl-amine	6291-84-5	Thermodynamic
TEPA	tetraethylenepentamine	112-57-2	Thermodynamic
DGA	glycolamine	929-06-6	Kinetic
TIPA	triisopropanolamine	122-20-3	Kinetic
triMEDA	N,N,N′-Trimethylethylenediamine	142-25-6	Kinetic

Base Compound: compound employed as a template from which additives are employed.

In lab: compound synthesized in the laboratory.

***Table A.2:** Additives classification – heterocyclic amines*

Abbreviation	Additives' Name	CAS #	Improvement
PZ	piperazine	110-85-0	Both
NMP	N-Methyl-2-pyrrolidone	872-50-4	Base Compound
IMI	imidazole	288-32-4	Both
4-A1MPD	4-amino-1-methylpiperidine	41838-46-4	Kinetic
1-(2HE)PRLD	1-(2-hydroxyethyl)pyrrolidine	2955-88-6	Kinetic
PRLD-1,2-PD	3-pyrrolidino-1,2-propanediol	85391-19-1	Thermodynamic
1-(2HE)PP	1-(2-hydroxyethyl)piperidine	3040-44-6	Kinetic
3PP-1,2-PD	3-piperidino-1,2-propanediol	4847-93-2	Kinetic
1M-2PPE	1-methyl-2-piperidineethanol	in lab	Kinetic
3H-1MPP	3-hydroxy-1-methylpiperidine	3554-74-3	Thermodynamic
1E-3HPP	1-ethyl-3-hydroxypiperidine	13444-24-1	Thermodynamic
AEP	N-(2-aminoethyl) piperazine	140-31-8	Kinetic
1M-2PPE	1-Methyl-2-piperidineethanol	in lab	Kinetic
BTA	benzotriazole	95-14-7	Thermodynamic
H	Histamine	51-45-6	(-)
SRT	Serotonin	50-67-9	(-)
	2-Pyridyl-methylamine	3731-51-9	(-)
	2-(2-Aminoethyl)pyridine	2706-56-1	(-)
	4-(2-Aminoethyl)-morpholine	2038-03-1	(-)
NFM	N-Formylmorpholine	4394-85-8	Kinetic
PYR	pyrrolidine	123-75-1	Thermodynamic
DMP	N,N'-Dimethylpiperazine	106-58-1	Kinetic

Base Compound: compound employed as a template from which additives are employed.

Both: compound depending the use shows kinetic or thermodynamic effects on improvement.

In lab: compound synthesized in the laboratory.

(-): compound proposed to improve capture process without experimental test or lack of information.

Table A.3: *Additives classification – amino acids*

Abbreviation	Additives' Name	CAS #	Improvement
Arg	arginine	74-79-3	Thermodynamic
L-His	L-Histidine	71-00-1	(-)
D-His	D-Histidine	351-50-8	(-)
L-Phe	L-Phenylalanine	63-91-2	(-)
D-Phe	D-Phenylalanine	673-06-3	(-)
L-DOPA	L-Levodopa	59-92-7	(-)
D-DOPA	D-Levodopa	5796-17-8	(-)
L-Trp	L-Tryptophan	73-22-3	(-)
D-Trp	D-Tryptophan	153-94-6	(-)
L-Tyr	L-Tyrosine	60-18-4	(-)
D-Tyr	D-Tyrosine	556-02-5	(-)
4-amino-L-Phe	4-amino-L-Phenylalanine	2410-24-4	(-)

(-): compound proposed to improve capture process without experimental test or lack of information.

Table A.4: *Additives classification – ionic liquids*

Abbreviation	Additives' Name	CAS #	Improvement
[EMIM]BF4	1-butyl-3-methylimidazolium hexafluorophosphate	143314-16-3	Both
[EtOHMim][PF6]		444723-80-2	Thermodynamic
[EtOHMim][BF4]		374564-83-7	Thermodynamic
[EtOHMim]Cl		61755-34-8	Thermodynamic
[Choline][PF6]		1040887-91-9	Thermodynamic
[Choline][BF4]		152218-75-2	Thermodynamic
[Choline]Cl		67-48-1	Thermodynamic
2-PHEN	2-Fluorophenol	367-12-4	Thermodynamic
3-PHEN	3-Fluorophenol	372-20-3	Thermodynamic
4-PHEN	4-Fluorophenol	371-41-5	Thermodynamic

Both: compound depending the use shows kinetic or thermodynamic effects on improvement.

Table A.5: *Additives classification – amine family*

Abbreviation	Additives' Name	CAS #	Improvement
BEHA	bis(2-ethylhexyl)amine	106-20-7	Kinetic
N,N-DM13PDA	N,N-dimethyl-1,3-propanediamine	111-33-1	Kinetic
N,N- DM12EDA	N,N-dimethyl-1,2-ethanediamine	110-70-3	Kinetic
TMEDA	N,N,N',N'-tetramethyl-1,2-ethanediamine	110-18-9	Kinetic
TMPDA	N,N,N',N'- tetramethyl-1,3-propanediamine	110-95-2	Kinetic
TMBDA	N,N,N',N'-tetramethyl-1,4-butanediamine	111-51-3	Kinetic
EDA	ethylenediamine	107-15-3	Kinetic
DETA	diethylenetriamine	111-40-0	Thermodynamic
TETA	triethylenetetramine	112-24-3	Kinetic

Table A.6: *Additives classification – organic salts*

Abbreviation	Additives' Name	CAS #	Improvement
TBAB	tetrabutylammonium bromide	1643-19-2	Thermodynamic
TBAF	tetra-n-butylammonium fluoride	429-41-4	Thermodynamic
TBAC	tetra-n-butylammonium chloride	1112-67-0	Thermodynamic
TBPB	tetra-n-butylphosphonium bromide	3115-68-2	Thermodynamic
TBPC	tetra-n-butylphosphonium chloride	2304-30-5	Thermodynamic

Table A.7: *Additives classification – alcohols*

Abbreviation	Additives' Name	CAS #	Improvement
TEG	triethylene glycol	112-27-6	(-)
MeOH	methanol	67-56-1	Thermodynamic
PHEN	phenol	108-95-2	Thermodynamic

(-): compound proposed to improve capture process without experimental test or lack of information.

Table A. 8: *Additives classification – catecholamines*

Abbreviation	Additives’ Name	CAS #	Improvement
DA	dopamine	62-31-7	(-)
ADR	L-Adrenaline	51-43-4	(-)

(-): Compound proposed to improve capture process without experimental test or lack of information.

Table A.9: *Additives classification – antifoam emulsion*

Abbreviation	Additives’ Name	CAS #	Improvement
	SAG 7133		Thermodynamic
	VP 5371		Thermodynamic

Table A. 10: *Additives classification – cyclic ether*

Abbreviation	Additives’ Name	CAS #	Improvement
PEGDME	poly(ethylene glycol) dimethyl ether	24991-55-7	Kinetic
THF	tetrahydrofuran	109-99-9	Thermodynamic

Table A.11: *Additives classification – surfactants*

Abbreviation	Additives’ Name	CAS #	Improvement
SDBS	sodium dodecyl benzene sulfonate	25155-30-0	Both

Both: compound depending the use con show kinetic or thermodynamic effects on improvement.

Table A.12: *Additives classification – corrosion inhibitor*

Abbreviation	Additives’ Name	CAS #	Improvement
	CRO27005		Thermodynamic

Table A.13: *Additives classification – cyclic ester*

Abbreviation	Additives' Name	CAS #	Improvement
PC	propylene carbonate	108-32-7	Both

Table A.14: *Additives classification – inorganic compound*

Abbreviation	Additives' Name	CAS #	Improvement
AM	ammonia	1336-21-6	Base Compound

Base Compound: compound employed as a template from which additives are employed.

Table A.15: *Additives classification – resin*

Abbreviation	Additives' Name	CAS #	Improvement
	Amberlite IRA-402	52439-77-7	Both

Both: compound depending the use shows kinetic or thermodynamic effects on improvement.

Table A.16: *Additives classification – thiophene*

Abbreviation	Additives' Name	CAS #	Improvement
SUF	sulfolane	126-33-0	Both

Both: compound depending the use con show kinetic or thermodynamic effects on improvement.

APPENDIX B:

Data Matrix of Additives

Table B.1: *Data matrix of additives*

ID	Articles' name	DOI	Authors	Year	Chemcial Solvent Data					Type of Gas Current				Type of Data Analysis of Amines Efficiency	Observations and Comments
					Base Solution (BS)	Reactive	CAS Nº	Concentrations		Pure Gas	Other	Flue Gas	Biogas		
								Provided	Employed						
RW001	Influence of Additives Including Amine and Hydroxyl Groups on Aqueous Ammonia Absorbent for CO_2 Capture	https://doi.org/10.1021/jp711113q	Jong Kyun You, et. al.	2008	Ammonia Solution	Ammonia solution	1336-21-6	28 wt % - No Further Purification (NFP)	diluted with deionized water until 10 wt %			A mixed gas of 15 % vol CO_2 and 85 % vol N_2 at a rate of 970 mL/min		Table of removal efficiency (%) vs time (min) of aqueous ammonia and modified ammonia with the additives Weight loss of aqueous ammonia solution by evaporation before and during the CO_2 absorption reaction IR spectra of ammonia absorbents blended by additives before and after CO_2 absorption.	▪Strategies of capture: (1) decreasing the loss of ammonia and (2) maintaining or enhancing CO_2 removal efficiency of ammonia. ▪Salts were excluded as potential additives because they can strongly affect the solubility of CO_2 into the modified absorbent ▪Analytical comprobation made by FT-IR spectra and computational calculations ▪From the geometry of molecules, it was obtained molecular structures and binding energy.
						2-amino-2-methyl-1-propanol (AMP)	124-68-5	99% - NFP	Base Solution (BS) + 1 wt %						
						2-amino-2-methyl-1,3-propandiol (AMPD)	115-69-5	99% - NFP	BS + 1 wt %						
						2-amino-2-ethyl-1,3-propandiol (AEPD)	115-70-8	99% - NFP	BS + 1 wt %						
						tri(hydroxymethyl) aminomethane (THAM)	77-86-1	99% - NFP	BS + 1 wt %						
RW002	Combining Different Additives with TBAB on CO_2 Capture and CH_4 Purification from Simulated Biogas Using Hydration Method	https://doi.org/10.1021/acs.jced.8b01188	Gang Yue, et. al.	2019	Tetrabutyl ammonium bromide (TBAB)	Tetrabutylammonium bromide (TBAB)	1643-19-2	0.999 wt	0.05 wt	Pure CO_2 gas 99.9 mol %	Pure CH_4 gas 99.9 mol %		Simulated biogas 64.0 mol % CH_4/CO_2 (precise components)	Hydrates growth process in different periods pictures Hydrate formation equilibrium conditions of three gases at different temperatures, the kinetic study of CO_2 hydrate was carried out in the different additive solutions conditions as the changes of pressure vs time (min) and changes of temperature vs time(min)	▪This experiment will prove the effect on thermodynamic hydrate formation and the study of the CO_2 hydrate kinetic ▪CH_4 in simulated biogas increased from initial feeding gas 67−83.1 mol %. ▪The tolerable pressure of the reactor was 25 MPa and its volume was 246 mL. In the experimental procedure, the operation temperature was 277.15 K and the operational pressure 3.5 Mpa
						1-butyl-3-methylimidazolium hexafluorophosphate ([EMIM]BF4)	143314-16-3	0.999 wt	BS + 2000 ppm						
						propylene carbonate (PC)	108-32-7	-	BS + 0.1 wt						
						sodium dodecyl benzene sulfonate (SDBS)	25155-30-0	0.9 wt	BS + 0.005 wt						

RW003	Experimental, simulation and thermodynamic modelling of an acid gas removal pilot plant for CO_2 capturing by mono-ethanol amine solution	https://doi.org/10.1016/j.jngse.2019.103001	Hamid Reza Kalatjaria, et. al.	2019	Monoethanolamine (MEA)	Aqueous Monoethanolamine (MEA)	141-43-5	-	For high CO_2 gas feed 27 wt % (25, 30, 35 ºC) and 29 wt % (30, 40, 50 ºC)			For high CO_2 gas feed 0.995 mol % CO_2 and 0.005 mol % N_2		One of the simulation and modeling approaches was the parameters of the eNRTL activity coefficient function for the molecular and ionic species in the liquid solution were regressed using ASPEN PLUS DRS module. In addition to the modified eNRTL by Bishnoi and Gabrielsen's method, we used the other simulation approaches such as ASPEN PLUS default with its parameters. The other approach was given by the modified eNRTL by Bishnoi and Gabrielsen's method, we used the other simulation approaches such as ASPEN PLUS with the regressed parameters. The other approach was Gabrielsen's method that was applied so that the VLE calculations were simplified substantially. Hence, only one explicit equation was solved for the CO_2 partial pressure over the aqueous MEA solution.	▪The experimental procedure of the pilot plant is compared with Calculus in Simulated Model with Gabrielsen Model, in Aspen Plus Default, Simulated Model with Bishnoi Approach, and Aspen Plus with Regressed Parameters.
								-	For low CO_2 gas feed 25, 28, 30, and 33 wt % at 49ºC			For low CO_2 gas feed 0.05 mol % CO_2 and 0.95 mol % N_2			
RW004	CO_2 absorption rate and capacity of semi-aqueous piperazine for CO_2 capture	https://doi.org/10.1016/j.ijggc.2019.03.007	Ye Yuan, Gary T. Rochelle	2019	Piperazine (PZ)	Piperazine (PZ)	110-85-0	99.5%	5 m PZ (aq)	CO_2 pure 99.99%				Viscosity of 5m PZ in 1SUF/3water, 3SUF/1water, and 1IMI/1water was measured at different loadings at 20, 40, and 60 °C. The CO_2 absorption rate was measured at 40 °C in the wetted wall column (WWC) with 5m PZ in 1NMP/3water and 1TEG/2water. The CO_2 solubility in 5 m PZ in the different concentrations of the additives The cyclic capacity and the absorption average rate of 5 m PZ considering IMI and SUF additives	▪Molality (m) was used for the convenience of calculation, 5m PZ in 1 NMP/3 water means 5 mol PZ is mixed with 250 g NMP and 750 g water, and PZ is exactly 30 wt %. ▪The solvent was prepared by mixing chemicals gravimetrically. ▪Mol alkalinity was employed during this test at 20, 40, and 60 ºC
						N-Methyl-2-pyrrolidone (NMP)	872-50-4	99.0%	BS + 1 NMP/3water						
						Triethylene glycol (TEG)	112-27-6	99.0%	BS + 1 TEG/2water						
						Sulfolane (SUF)	126-33-0	99.00%	BS + 1SUF/3water BS+1SUF/1water						
						Imidazole (IMI)	288-32-4	99.0%	BS+ 1IMI/3water BS+1IMI/1water						

RW005	Experimental and theoretical studies on the influence of ionic liquids as additives on ammonia-based CO_2 capture	https://doi.org/10.1016/j.ijggc.2015.08.023	Yin Xu, et . al.	2015	Ammonia Solution	Ammonia Solution	1336-21-6	99%	2 mol/L			CO_2 + N_2 both 99.99% purity		Variation of CO_2 concentration in treated flue gas (%) vs time (s) for the additives with the choline cation and the additives with the EtOhMim cation Variation of the NH_3 concentration in treated flue gas during absorption (ppm) vs time (s) for the additives with the choline cation and the additives with the EtOhMim cation Table of comparative data of the total CO_2 capacity in blended solutions and pure aq. Ammonia Table of comparative data of the total NH_3 loss in the blended absorbents and pure aq. Ammonia solution during absorption	▪CO_2 and N_2 gas from cylinders were mixed to simulate typical flue gas with a CO_2 concentration of 15 vol%. With a mass flow rate at 1 L/min at 30ºC
						[EtOHMim][PF6]	444723-80-2	99%	BS + 0.2mol/L						
						[EtOHMim][BF4]	374564-83-7	99%	BS + 0.2mol/L						
						[EtOHMim]Cl	61755-34-8	99%	BS + 0.2mol/L						
						[Choline][PF6]	1040887-91-9	99%	BS + 0.2mol/L						
						[Choline][BF4]	152218-75-2	99%	BS + 0.2mol/L						
						[Choline]Cl	67-48-1	99%	BS + 0.2 mol/L						
RW006	CO_2 Capture from Flue Gas Based on Tetra-n-butylammonium Fluoride Hydrates at Near Ambient Temperature	https://doi.org/10.1021/acsomega.9b03442	Hidenori Hashimoto, et. al.	2020	tetra-n-butylammonium Fluoride (TBAF)	tetra-n-butylammonium Fluoride (TBAF)	429-41-4	0.84 mass fraction	0.10, 0.20, 0.30 in mass fraction			Flue Gas, in mole fraction was 0.151 CO_2 and 0.849 N_2		The obtained data for the total gas capture amount in the hydrate phase at the three different mass fraction of TBAF Data from the Single Crystal X-Ray Diffraction (SCXRD) on TBAF hydrates formed under CO_2 + N_2 gas pressure Data from the CO_2 capture amount in the hydrate phase	▪A batch-type gas separation process was employed under three different pressure levels, that is, 1, 3, and 5 MPa. ▪The inner dimension of the reactor is 80 mm in diameter, 155 mm in height, and 800 ± 20 cm3 in volume. ▪After experiments, all hydrates analysis were carried out under by X-Ray diffraction ▪Because the semiclathrate hydrates have a lot of advantages such as high melting temperatures and less hazardous and nonvolatile properties, gas separation for simulated flue gas, that is, CO_2 +N_2 gas, has been studied a lot. ▪TBAF aqueous solutions were gravimetrically prepared with the aid of an electronic balance (GX-6100, A&D Co., Tokyo) with 0.02 g of uncertainty with 95% reliability

RW007	Role of Mono- and Diamines as Kinetic Promoters in Mixed Aqueous Amine Solution for CO_2 Capture	https://doi.org/10.1016/j.ces.2020.116009	Min Xiao, et. al.	2020	Diethylethanol amine (DEEA)	Diethylethanolamine (DEEA)	100-37-8	99%	4 mol/L DEEA			CO_2 >99% and N_2 >99%		The data was observed into the CO_2 absorption curves at 40.0 °C for amine solutions with a total concentration of 4.0 mol/L while varies in composition Data of species concentration profiles as the carbamate concentration vs CO_2 loading and carbonate and bicarbonate total concentration vs CO_2 loading A comparison between observed CO_2 absorption and carbamate formation rates in the initial 30 min of absorption period Data of the CO_2 absorption performance using regenerated amine solution in terms of CO_2 absorption amount and initial absorption rate selecting a potentially selected group as kinetic promoters in tertiary amines	▪Dissolving the appropriate quantity of the amines in volumetric glassware and making up to volume with deionized water
						Monoethanolamine (MEA)	141-43-5	99%	4 mol/L MEA						
									MEA1:3DEEA MEA2:2:DEEA						
						N,N- dimethyl-1,3-propanediamine (N,N-DM13PDA)	111-33-1	99%	N,N-DM13PDA1:3 DEEA						
						N,N-dimethyl-1,2-ethanediamine (N,N-DM12EDA)	110-70-3	98%	N,N-DM12EDA1:3 DEEA						
						4-amino-1-methylpiperidine (4-A1MPD)	41838-46-4	97%	4-A1MPD1:3MEEA						
RW008	Experimental results of advanced technological modifications for a CO_2 capture process using amine scrubbing	10.1016/j.ijggc.2020.103014	Krótki, Aleksander et. al.	2020		Monoethanolamine (MEA)	141-43-5	-	-		CO_2 13.2 vol%, H_2O 7.3 vol %, O_2 8.7 vol%, Impurities SO_2 (100-200mg/m3), NO_x (200-400mg/m3), Dust (30mg/m3)			The disposal information of the effectiveness of the process is related in terms of corrosion advancements	▪Design of the pilot plant is based on the chemical post-combustion absorption process with several modifications. The designed pilot plant is a mobile unit, which allows its usage in various locations. ▪A simple 30 wt% monoethanolamine (MEA) water solution with the addition of anti-foam Silpian W-3 was chosen. ▪Parameters: Flue Gas Flow rate-285±7 kg/h, Temperature-up to 99ºC, Pressure-1bar(abs)
						2-amino-2-methyl-1-propanol (AMP)	124-68-5	-	-						
						piperazine (PZ)	110-85-0	-	-						
						2-(2-aminoethyl-amino)ethanol (AEEA)	111-41-1	-	-						
						1,3-Diamino-2-propanol (AEP)	616-29-5	-	-						

RW009	Experimental and modeling studies of bicarbonate forming amines for CO_2 capture by NMR spectroscopy and VLE	10.1016/j.seppur.2019.116097	Xiao, Min et. al.	2020		N,N,N',N'-tetramethyl-1,2-ethanediamine (TMEDA)	110-18-9	99%	2.0 mol/L			Simulated Flue Gas of CO_2+N_2 adjusting the CO_2 partial pressure to 15KPa		Calculations of pKa of TMEDA, TMPDA, TMBDA, as function of temperatures with a previous acid-base ratio using HCl Calculations of pKa vs the equilibrium CO_2 solubility to state a difference between the monoamine and the diamine	▪The CO_2 absorption was carried out in a continuous flow reactor. The overall flow rate of the mixed gas was 50 mL·min−1 CO_2 absorption experiment described above (CO_2 15 kPa, 298 K) ▪Nuclear Magnetic Resonance (NMR) spectroscopy was used to measure the chemical shift variation of carbon peaks during the protonation process.
						N,N,N',N'- tetramethyl-1,3-propanediamine (TMPDA)	110-95-2	99%	2.0 mol/L						
						N,N,N',N'-tetramethyl-1,4-butanediamine (TMBDA)	111-51-3	99%	2.0 mol/L						
						Hydrochloric acid solution (HCl)	7647-01-0	-	0.70M						
						Deionized water	Made in Lab	-							
RW010	Energy harvesting from amine-based CO_2 capture: proof-of-concept based on mono-ethanolamine	10.1016/j.fuel.2019.116661	Li, Kangkang et. al.	2020	Monoethanolamine (MEA)	Monoethanolamine (MEA)	141-43-5	-	NFP			CO_2+N_2 gas mixture 12 vol% CO_2		Modelling of the energy performance of Cu-based CO_2-regenerative amine-based battery (CRAB) cycles with the material balance in the CO_2 capture and electrochemical process	▪The experiment requires a Cu lean. The principle of CRAB is based on the dual ability of amines to reversibly react with CO_2 and to reversibly form metal-amine complexes in an aqueous solution. ▪UV–visible absorbance was measured by a Varian Cary 50 Bio UV–Visible Spectrophotometer. Solution conductivity was measured by an LCR meter
						Copper (II) nitrate CU(NO3)2	10031-43-3	-	NFP						
						Potassium Nitrate KNO3	7757-79-1	-	NFP						

RW011	CO$_2$ capture by tertiary amine absorbents: A performance comparison study	10.1021/ie400825u	Chowdhury, Firoz Alam et. al.	2013		2-(dimethylamino)ethanol (DMAE)	108-01-0	-				Gas (20% CO$_2$:80% N$_2$)		To determine the efficiency of the ammine it was observed experimental CO$_2$ absorption - regeneration profiles as, the CO$_2$ loading vs time (min) Data from the absorption rate versus pKa values for all the components, and the equilibrium solubilities of the partial pressures versus pKa values by calculating the absorption rate, desorption rate, and the cyclic capacity Data from absorption rates and heats of reaction of preferred absorbents The experiment was carried out at an aqueous solution 30% amine mass fraction	▪Water was purified with a water distillation apparatus and the process of a scrubbing test ▪MEA reacts with CO$_2$ faster than DEA, which reacts faster than MDEA. This indicates that the heats of reaction and absorption rates of the alkanolamines are dependent on the substituents attached to the nitrogen atom. ▪Additives are clasificated as amines (1−10), tertiary di- or trialkanolamines (11−16) and cyclic tertiary alkanolamines (17−23)], and alkyl substituents (e.g., methyl, ethyl, isopropyl, tert-butyl) around the amino group. ▪Gas scrubbing, VLE, and reaction calorimetry. experiments were conducted to obtain the absorption rates, CO$_2$ loadings, cyclic capacities, and heats of reaction for the absorbents.
						3-dimethylamino-1-propanol (DMA-1P)	3179-63-3	-							
						2-diethylaminoethanol (DEAE)	100-37-8	-							
						3-diethylamino-1-propanol (DEA-1P)	622-93-5	-							
						1-dimethylamino-2-propanol (DMA-2P)	108-16-7	-							
						1-diethylamino-2-propanol (DEA-2P)	4402-32-8	-							
						2-(diisopropylamino)ethanol (DIPAE)	96-80-0	-							
						2-(dimethylamino)-2-methyl-1-propanol (DMA-2M-1P)	7005-47-2	-							
						3-dimethylamino-2,2-dimethyl-1-propanol (DMA-2,2-DM-1P)	19059-68-8	-							
						4-ethyl-methyl-amino-2-butanol (4EMA-2B)	Synthesized in lab	96%							
						N-ethyldiethanolamine (EDEA)	139-87-7	-							
						N-isopropyldiethanolamine (IPDEA)	Synthesized in lab	99.4%							
						N-tert-butyldiethanolamine (tBDEA)	2160-93-2	-							
						3-(dimethylamino)-1,2-propanediol (DMA-1,2-PD)	623-57-4	-							
						3-diethylamino-1,2-propanediol (DEA-1,2-PD)	621-56-7	-							
						triethanolamine (TEA)	102-71-6	-							
						1-(2-hydroxyethyl)pyrrolidine [1-(2HE)PRLD]	2955-88-6	-							
						3-pyrrolidino-1,2-propanediol (PRLD-1,2-PD)	85391-19-1	-							
						1-(2-hydroxyethyl)piperidine [1-(2HE)PP]	3040-44-6	-							
						3-piperidino-1,2-propanediol (3PP-1,2-PD)	4847-93-2	-							
						1-methyl-2-piperidineethanol (1M-2PPE)	Synthesized in lab	98.0%							
						3-hydroxy-1-methylpiperidine (3H-1MPP)	3554-74-3	-							
						1-ethyl-3-hydroxypiperidine (1E-3HPP)	13444-24-1	-							
						N-methyldiethanolamine (MDEA)	Synthesized in lab	-							

RW012	Better Choice of Tertiary Alkanolamines for Postcombustion CO$_2$ Capture: Structure with Linear Alkanol Chain Instead of Branched	10.1021/acs.iecr.9b02244	Liu, Sen. et. al.	2019		N-Methyldiethanolamine (MDEA)	105-59-9	99%				The CO$_2$ and nitrogen (N$_2$) gases with purity of 99.9 vol %		The introductory basic observation is layed into the view of the biphasic phenomenon of the fresh aqueous ammine, and the aqueous CO$_2$-loaded amine solution The main comparative of the amines in the work is seen into a graph where it was compared physical properties: boiling point and vapor pressure, both demonstrated into their experimental and predetermined values Additionally, to verify the basicity and the CO$_2$ solubility of amines, it was demonstrated into a comparison between the data of the pH of the fresh amine solution and in the loaded solution, and the equilibrium solubility as a function of the intramolecular hydrogen bonds To verify the kinetics of the amines it was determined the order of the reaction rate constants of CO$_2$ absorption into the fresh amine solutions. Finally, based on the cyclic capacity of amines at cyclic times of 30-90 min, the best-proposed amines are shown	▪Based on these researches, it can be concluded that the steric hindrance and electron-donating effect of alkyl group addition on the N atom can be in favor of CO$_2$ capture, while the addition of the hydroxyl group can decrease the basicity and reaction rate of amines. ▪The aqueous amine and CO$_2$ solutions were prepared by deionized water produced by a reverse osmosis ultra-pure water equipment ▪Afterward, it was used to measure the pH value of fresh amine solutions with a molar concentration of 0.05 M. ▪An absorption process was first performed at 313 K, and a volume of 0.3 L amine solution was bubbled by mixture gases of CO$_2$ and N$_2$, with a partial pressure of 15 kPa, and a total flow rate of 1 L/min. The absorption process was terminated when the reaction was close to the equilibrium. ▪Then, the desorption process was carried out with rich CO$_2$-loaded amine solutions produced by the absorption process, the temperature was constant at 353 K, and a stream of N$_2$ gas was bubbled into the solution with a flow rate of 0.85 L/min for CO$_2$ stripping.
						2-(Dimethylamino)-ethanol (DMEA)	108-01-0	99%							
						1-(Dimethylamino)-2-propanol (1DMA2P)	108-16-7	98%							
						3-Dimethylamino-1-propanol (3DMA2P)	3179-63-3	99%							
						3-(Dimethylamino)-1,2-propanediol (DM1-1,2-PD)	623-57-4	98%							
						2-(Diethylamino)-ethanol (DEEA)	100-37-8	99%							
						1-Diethylamino-2-propanol (1DEA2P)	4402-32-8	>98%							
						3-Diethylamino-1-propanol (3DEA1P)	622-93-5	>95%							
						3-(Diethylamino)-1,2-propanediol (DEA-1,2-PD)	621-56-7	97%							
						2-Dimethylamino-2-methylpropanol solution (DMA-2M-1P)	7005-47-2	>97%							
						4-(diethylamino)butan-2-ol (DEAB)	5467-48-1	94%							
						Deionized water									

RW013	Enhancement of CO_2 capture in the MDEA solution by introducing TETA or TETA-AEP mixtures as an activator	https://doi.org/10.1080/01496395.2018.1504797	Mei Wang, Na Rao, Yuqing Liu, Jiale Li, Qunpeng Cheng & Jianfen Li	2018	N-Methyldiethanolamine (MDEA)	N-Methyldiethanolamine (MDEA)	105-59-9	- NFP	-			CO_2 99.99% and N_2 99.99% with a flow rate of 100mL/min at atmospheric pressure		The data of amine's efficiency is shown in a table of CO_2 capture performance, where it was compared the CO_2 absorption capacity, the average CO_2 absorption rate, and the CO_2 desorption efficiency Tables of absorption rate (mmol/s) vs time (min) and desorption rate (mmol/s) vs time (min) and absorption capacity (mol/mol) vs time (min) Comparative graph of absorption capacity (mol/mol) vs the volume fraction of the activator (%) and average absorption rate (mmol/s) vs the volume fraction of the activator (%) and desorption efficiency (%) vs the volume fraction of the activator and viscosity (mpa/s) vs the volume fraction of activators (vol%)	Three categories including 10 kinds of absorbents were prepared: (30% MDEA + 70%H_2O), (x%MDEA + y1%TETA + 70% H_2O) and (x%MDEA + y1%TETA-y2%AEP + 70% H_2O), where the percentage value was vol.% ▪The absorption capacity significantly increased with the growing amount of TETA (4%–8%).
						Triethylenetetramine (TETA)	112-24-3	- NFP	-						
						N-(2-aminoethyl) piperazine (AEP)	140-31-8	- NFP	-						
						distilled water		-							
RW014	Choosing amine-based absorbents for CO_2 capture	http://dx.doi.org/10.1080/09593330.2014.934742	João Gomesa, Samuel Santos & João Bordado	2015		Monoethanolamine (MEA)	141-43-5		(10% (w/w))	CO_2 from a cylinder (99.99% Air Liquide)				Results for CO_2 absorption by aqueous amine solutions (10% (w/w)) using the precipitation method at different absorption times Comparison of the obtained results for CO_2 loading capacity over the absorption time for all the tested aqueous amine solutions Amine price versus CO_2 loading capacity of aqueous amine solutions.	▪Amines were prepared from pro-analysis Merck reagents in 10% concentration by weight in water: monoethanolamine (MEA), diethanolamine (DEA), diethylamine, ethylenediamine (EDA), N-methyldiethanolamine (MDEA), and piperazine (PZ) ▪Every 30 min, a sample of20mL was collected from the absorption column, to ascertain whether the solution was or was not saturated, through a sampling valve. ▪The pilot unit had a volume of 7 L. The flow rate of the aqueous amine solutions inside the absorption column was 24 L/h and the CO_2 stream entered the absorption column from the bottom with a flow rate of 20mL/min.
						Ethylenediamine (EDA)	107-15-3		(10% (w/w))						
						Piperazine (PZ)	110-85-0		(10% (w/w))						
						Bis(2-ethylhexyl)amine	106-20-7		(10% (w/w))						
						Triethylamine (TEA)	121-44-8		(10% (w/w))						
						N-Methyldiethanolamine (MDEA)	105-59-9		(10% (w/w))						
						Diethanolamine (DEA)	111-42-2		(10% (w/w))						

RW015	Structure-driven CO_2 selectivity and gas capacity of ionic clathrate hydrates	DOI:10.1038/s41598-017-17375-1	Hidenori Hashimoto, et. al.	2017		Tetra-n-butylammonium bromide (TBAB)	1643-19-2	≥0.99 on mass basis	0.200 mass basis and 0.320 mass basis			CO_2+N_2 mixed gas with ~0.15 and ~0.85 molar basis		It was performed gas separation test to observe optically morphologies of the hydrate crystals, single crystal X-Ray Diffraction, and Raman Spectroscopy	▪The test pressures were 1, 3, and 5 Mpa, employing CO_2 + N_2 mixed gases of which compositions were 0.1524 and 0.8476, 0.1502 and 0.8498 in mole fraction, respectively ▪Aqueous solutions were gravimetrically prepared using an electronic balance and a water bath made of polymethyl methacrylate (PMMA) ▪THF was employed in this study for Collecting Raman spectra of CO_2+N_2+THF to determine the hydrates structure form
						Tetra-n-butylammonium chloride (TBAC)	1112-67-0	≥0.97 in mass fraction	0.200 mass basis						
						tetra-n- butylphosphonium bromide (TBPB)	3115-68-2	≥0.98 in mass fraction	0.200 mass basis						
						tetra-n- butylphosphonium chloride (TBPC)	2304-30-5	≥0.96 in mass fraction	0.200 mass basis						
						Tetrahydrofuran (THF)	109-99-9	0.999 in mass fraction	-						
						Deionized water		Made in lab							
RW016	Gas separation of flue gas by tetra-n-butylammonium bromide hydrates under moderate pressure conditions	10.1016/j.energy.2017.04.074	Hidenori Hashimoto et. al.	2017		Tetra-n-butylammonium bromide (TBAB)	1643-19-2	>0.99 in mass fraction	Mass fraction in aqueous solution (w) = 0.20 and 0.32			CO_2 + N_2, without gas flow Carbon dioxide (0.1524) + nitrogen (0.8476) mixed gas, with continous gas flow Carbon dioxide (0.1342) + nitrogen (0.8658) mixed gas.		Gas separation without gas flow pressure trends during the hydrate formation with TBAB and THF; Pressure trends during the gas separation experiments P (Mpa) vs time (h); The CO_2 mole fraction of captured in the hydrate phase; The total amounts of gas captured in the hydrate phases Gas separation with the continuous gas flow with a large hydrate reactor is compared the separation factor with previous studies of ionic clathrate hydrate-based CO_2 + N_2 separation.	▪Two experimental systems: the gas separation experiments without gas flow and with the continuous gas flow with ≥0.0001 in mole fraction (GC) for both ▪After the supply of an aqueous solution, the reactor was sealed and purged by nitrogen gas and a vacuum pump. When the residual air was removed, we supplied CO_2 + N_2 mixed gas to the cell and started stirring for dissolution of the gas into the liquid phase for the stationary state.
						Tetrahydrofuran (THF)	109-99-9	>0.999 in mass fraction	w(TBAB) = 0.32 + w(mass basis, THF) = 0.188						

RW017	Synthesis and selection of hindered new amine absorbents for CO_2 capture	10.1016/j.egypro.2011.01.042	Chowdhury, Firoz Alam, et. al.	2011		Monoethanolamine (MEA)	141-43-5	- NFP	For all amines a 30wt% aqueous solution was used			20% CO_2 gas balanced with N_2		It is shown a preferred target into a graph of absorption rate vs reaction heat, then data of amines absorption are plotted into a typical example of screening tests of absorption amount (absorption and regeneration) vs time Table of experimental results for screening and heat reaction tests. VLE equilibrium stated in a graph of CO_2 partial pressure vs CO_2 loadings Experimental results of the heat of reaction stated in a histogram Final graph of the targets that fulfill the parameters demonstrated in the first graph of absorption rate vs reaction heat	▪The hindered new amino alcohols were synthesized in our laboratory by the alkylation reaction of amines and their corresponding alkylhalides. Synthesized amines purity and structure determination were established by GC and NMR spectroscopy. ▪A 250ml glass scrubbing bottle filled with 50ml of a 30 wt% was placed in a bath, after that the flow gas rate was supplied to the bottle at a flow rate of 700ml/min. After 60 minutes of CO_2 absorption, the bottle was moved to the other water bath which was controlled at 70 °C and CO_2 was regenerated from the solvent for 60 minutes. ▪It has been shown that the placement of functional groups within the amino alcohols affects the performance of the amino alcohols in CO_2 capture.
						2-amino-2-methyl-1-propanol (AMP)	124-68-5	- NFP							
						Diethanolamine (DEA)	111-42-2	- NFP							
						N-methyldiethanolamine (MDEA)	105-59-9	- NFP							
						2-N-methylamino-2-methyl-1-propanol (MAMP)	Synthesized amine absorbents								
						2-N-ethylamino-2-methyl-1-propanol (EAMP)									
						2-(isopropylamino)ethanol (IPAE)									
						2-(isobutylamino)ethanol (IBAE)									
						2-(secondarybutyamino)ethanol (SBAE)									
						2-(isopropyl)diethanolamine (IPDEA)									
						1-Methyl-2-piperidineethanol (1M-2PPE)									

RW018	CO_2-Alkanolamine Reaction Kinetics: A Review of Recent Studies	10.1002/ceat.200700268	Vaidya, Prakash D. & Kenig, Eugeny Y.	2007		Monoethanolamine (MEA)	141-43-5	- - - - - - - - - - - -	- - - - - - - - - - - -	CO_2				Comparative results of the different reaction rate constants	▪A complete review for the monoamines, diamines, and tertiary and substituted amines
						2-(Methylamino)ethanol (MMEA)	109-83-1								
						Mono-n-Butyl Ethanolamine (NBMEA)	111-75-1								
						t-butylmonoethanolamine (TBMEA)	4620-70-6								
						ethylmonoethanolamine (EMEA)	110-73-6								
						methyldiethanolamine (MDEA)	105-59-9								
						2-amino-2-methyl-1-propanol (AMP)	124-68-5								
						Diethanolamine (DEA)	111-42-2								
						diisopropanolamine (DIPA)	110-97-4								
						2-amino-2-methyl-1,3-propanediol (AMPD)	204-100-7								
						2-amino-2-ethyl-1,3-propanediol (AEPD)	115-70-8								
						Piperazine (PZ)	110-85-0								

RW019	Progress in carbon dioxide separation and capture: A review	10.1016/S1001-0742(08)60002-9	Yang, Hongqun, et. al.	2008		Monoethanolamine (MEA)	141-43-5	- - -	- - -	CO_2				The effectiveness of this work is the new industrial arrangements and advancements in the capture of the CO_2 process	▪Review with data of a selection of technologies for CO_2 separation and capture employing conventional amines
						Diethanolamine (DEA)	111-42-2								
						methyldiethanolamine (MDEA)	105-59-9								
RW020	New Amine Blends for Improved CO_2 Separation: A Study on Reaction Kinetics and Vapour-Liquid Equilibrium	https://dx.doi.org/10.1080/00986445.2017.1288620	Budhwani, Neha, et. al.	2017		N-ethyldiethanolamine (EDEA)	139-87-7	98%	2.0 - 2.5 M		Cylinders of CO_2, N_2, and N_2O with a purity of 99.95%			It is observed the order rate constant for the process and the dissociation constant Ka Dependence of absorption rates in blends on CO_2 partial pressure as the CO_2 absorption rates vs CO_2 partial pressure To evaluate the blends, it is studied the dependence of equilibrium partial pressure of CO_2 on loading capacity	▪A glass stirred cell reactor (inner diameter 9.7 mm), whose interfacial surface area and volume were 74 cm2 and 1210 cm3. ▪Every time, the reactor was flushed with N_2, evacuated using a vacuum pump, and filled with 400 cm3 of the amine blend. ▪They studied the rate of absorption by the results of aqueous blends
						N,N'-diethylmonoethanolamine (DEMEA)	100-37-8	98%	2.0 - 2.5 M						
						ethylmonoethanolamine (EMEA)	110-73-6	98%	0.1 - 0.5 M						
						Ethylenediamine (EDA)	107-15-3	98%	0.1 - 0.5 M						
RW021	Effect of Additives on the CO_2 Absorption in Aqueous MDEA Solutions	https://dx.doi.org/10.1021/ie503915k	Maria T. Mota-Martinez, et. al.	2014		methyldiethanolamine (MDEA)	105-59-9	-	45 parts of amine per 55 parts of water	CO_2				Experimental solubility of CO_2 in different amine solution, as the pressure vs temperature Effect of the CO_2 on the homogeneity of the liquid phase: at low pressure, the CO_2 has not reacted yet; the pressure is increased and the CO_2 starts reacting; a second liquid phase is observed in the top of the Caillet tube near the CO_2 bubble interface; at high pressure, all the CO_2 has reacted It is also showed a graph of the effects of additives on the bubble pressure of aqueous amine	▪The aqueous solution is the mixture of MDEA and benzotriazole
						Benzotriazole	95-14-7	-	1 part benzotriazole per 9 parts of water (10mass%), and 1 part of the solution per 19 parts of water						
						SAG 7133 antifoam emulsion									
						VP 5371 antifoam emulsion									
						CRO27005 corrosion inhibitor									

RW022	Carbon dioxide absorption into aqueous blends of methyldiethanolamine (MDEA) and alkyl amines containing multiple amino groups	10.1021/ie502434m	Choi, Song Yi, et. al.	2014		methyldiethanolamine (MDEA)	105-59-9	≥99%	30% (w/w)			CO_2 and N_2 gases with volume fractions of 0.9999 and 0.99999, respectively		The study reveals the CO_2 loading amount of aqueous blends of the amine at different temperatures; the CO_2 loadings amount of aqueous blends of the amine with absorption at different temperatures; the overall mass transfer coefficients Measuring the densities and viscosities of aqueous blends of amine	▪The total amine concentration of all aqueous blends of MDEA was fixed at 30% (w/w) including 20% (w/w) of MDEA with 10% (w/w) of activators. ▪CO_2 loading amounts of the aqueous blends of MDEA at 313, 333, and 353 K ▪The CO_2 loading amounts of absorbents were almost saturated after 200 min of absorption time at all three different temperature conditions, except for 30% (w/w) MDEA at 313 K. ▪They confirmed formations of primary carbamate, primary−primary dicarbamate, and primary−secondary dicarbamate ions from 13C NMR studies.
						Monoethanolamine (MEA)	141-43-5	≥99%	30% (w/w)						
						Diethylenetriamine (DETA)	111-40-0	≥99%	10% (w/w)						
						3-Methyl Amino Propyl Amine (MAPA)	6291-84-5	≥97%	10% (w/w)						
						Triethylenetetramine (TETA)	112-24-3	≥97%	10% (w/w)						
						Tetraethylenepentamine (TEPA)	112-57-2	technical grade	10% (w/w)						
RW023	Kinetics research on mixed solvents of MDEA and enamine in natural gas decarbonization process	10.1016/j.jngse.2014.04.014	Tang, Jianfeng, et. al.	2014	N-methyl-diethanolamine (MDEA)	N-methyl-diethanolamine (MDEA)	105-59-9	-	3 mol/L MDEA		Natural Gas			The absorption load and gas-phase pressure under different initial amine concentrations, as a graph of the combined partial pressure of CO_2, absorption load vs the absorption time The absorption rate of the process vs the absorption time; a comparison between the absorption rate under different amine concentrations as the calculated value vs the experimental values	▪For the single MDEA system, the absorption performance is best with 3.0 mol/L MDEA, and the optimal temperature was 50 ºC. In the mixed amine system, the absorption capacity is stronger when the dosage of DETA or TETA is larger. ▪The pressure in the stainless steel reactor which has a maximum volume of 765.2 mL can sustain at 15 MPa. The pressure in the reactor can be measured between the ranges of 0-13.8 MPa with an accuracy of ±0.075%. The reactor is linked to the gas storage cylinder with a pressure-reducing valve.
						Diethylenetriamine (DETA)	111-40-0	-	2.0mol/L MDEA+1.0mol/L DETA 2.3mol/L MDEA+0.7mol/L DETA 2.6mol/L MDEA+0.4mol/L DETA						
						Triethylenetetramine (TETA)	112-24-3	-	2.0mol/L MDEA+1.0mol/L TETA 2.3mol/L MDEA+0.7mol/L TETA 2.6mol/L MDEA+0.4mol/L TETA						

RW024	Separation of CO_2 from Flue Gas: A Review	10.1081/SS-200042244	Douglas Aaron & Costas Tsouris	2005		Monoethanolamine (MEA)	141-43-5	-	-	This CO_2-rich solution				The effectiveness of the study yields in the new technologies of separation processes.	▪While this method is currently most promising, the development of ceramic and metallic CO_2 separation is liquid absorption using monoethanolamine (MEA). While this method is currently most promising, the development of ceramic and metallic membranes for membrane diffusion should produce membranes significantly more efficient at separation than liquid absorption.
RW025	Carbon capture and utilization technologies: a literature review and recent advances	https://doi.org/10.1080/15567036.2018.1548518	Francisco M. Baena-Moreno, et. al.	2019						CO_2				This review does not contain specific information on additives improvements	▪A pure gaseous component is considered in a supercritical state when its temperature and pressure exceeds its critical values, for CO_2 these are 304.1 K and 7.4 MPa, respectively
RW026	Absorption of CO_2 in aqueous blend of methyldiethanolamine and arginine	10.1002/apj.2460	Talkhan, Ahmed Gomaa, et. al.	2020		methyldiethanolamine (MDEA)	105-59-9	99%	2.0mol/L MDEA : 0.0mol/L Arg 1.97mol/L MDEA : 0.03mol/L Arg 1.95mol/L MDEA : 0.05mol/L Arg 1.9mol/L MDEA : 0.1mol/L Arg 1.8mol/L MDEA : 0.2mol/L Arg			Carbon dioxide (CO_2) and nitrogen (N_2) gases used in this work (both of purity 99.9%)		The effect of Arg concentration on the solubility of CO_2 and at different CO_2 partial pressures To verify data it is used the semiempirical vapor-liquid equilibrium to correlate the CO_2 solubility results	▪The experiment was carried out under different Temperatures, 303, 293, 313, 323 K, and under CO_2 partial pressure varying from 9 to 100 KPa
						Arginine (Arg)	74-79-3	99%							

RW 027	The first activation study of a bacterial carbonic anhydrase (CA). The thermostable a-CA from Sulfurihydrogenibium yellowstonense YO3AOP1 is highly activated by amino acids and amines	http://dx.doi.org/10.1016/j.bmcl.2012.08.088	Vullo, A. et. al.	2012	Human Isoforms Carbonic Anhydrase (hCA I)	L-Histidine	71-00-1	-	-		Carbonic Anhydrase			The effect of these additives (amine and amino acids) in the three base solutions can be reflected in the kinetic parameters for the activation of the enzymes for the CO_2 hydration reaction	•It might be possible to make SspCA an 'ideal molecule' in the CO_2 sequestration achieving a high reaction rate through the use of CAAs.
						D-Histidine	351-50-8	-	-						
						L-Phenylalanine	63-91-2	-	-						
						D-Phenylalanine	673-06-3	-	-						
						L-DOPA	59-92-7	-	-						
						D-DOPA	5796-17-8	-	-						
					Human Isoforms Carbonic Anhydrase (hCA II)	L-trp	73-22-3	-	-						
						D-trp	153-94-6	-	-						
						L-Tyr	60-18-4	-	-						
						D-Tyr	556-02-5	-	-						
						4-amino-L-Phe	2410-24-4	-	-						
						Histamine	51-45-6	-	-						
						Dopamine	62-31-7	-	-						
						Serotonin	50-67-9	-	-						
					extreme-α-Carbonic Anhydrase (SspCA)	2-Pyridyl-methylamine	3731-51-9	-	-						
						2-(2-Aminoethyl)pyridine	2706-56-1	-	-						
						1-(2-Aminoethyl)-piperazine	140-31-8	-	-						
						4-(2-Aminoethyl)-morpholine	2038-03-1	-	-						
						L-Adrenaline	51-43-4	-	-						
RW028	Development of low-cost amine-enriched solid sorbent for CO_2 capture	http://dx.doi.org/10.1080/09593330.2012.673014	Bachelor T. & Toochida P.	2012		Monoethanolamine (MEA)	141-43-5	-	-			$CO_2 + N_2$		According to previous investigations, it is stated that the data was established as CO_2 capture capacity of the amines It was established a table with the amine ratio information to provide data of the CO_2 capture performance of DEA-AEEA and MEA-AEEA	• They were then dried at atmospheric pressure and room temperature overnight. After that, they were dried in an oven at 333K for 30 min to remove methanol. Amounts of10 and 20% by weight of amine over sorbent mean that 10 or 20 g of single amine was loaded on 100 g of support, respectively • Additionally to prove the data it was made an IR test with recorded spectra at different intervals during the reaction
						Diethanolamine (DEA)	111-42-2	-	-						
						2-(2-aminoethyl-amino)ethanol (AEEA)	111-41-1	-	-						
						Piperazine (PZ)	110-85-0	-	-						
						Methanol	67-56-1	-	-						
						Sodium Hydroxide (NaOH)	1310-73-2	-	Supports with and without compound						

RW029	Kinetics of absorption of carbon dioxide into aqueous blends of 2-(1-piperazinyl)-ethylamine and N-methyldiethanolamine	doi:10.1016/j.ces.2008.12.034	Subham P., Aloke G & Bishnupada M.	2009		2-(1-piperazinyl)-ethylamine (PZEA)	140-31-8	96.75%				CO_2 and N_2O gas with purity of 99.99% for solubility and diffusivity measurements		The data obtained is stated as physicochemical parameters The kinetic data is stated as overall reaction rate constants of CO_2 with aqueous amine solutions Table of a comparison between the calculated rates to the experimental rates of absorption for CO_2 in aqueous solutions	• The total amine contents of the solutions were determined by acidimetric titration with standard HCl using an auto titrator • The experiments were performed at different temperatures employing a mixture of amines at different concentrations
						methyldiethanolamine (MDEA)	105-59-9	98%							
RW030	Thermodynamic analysis of CO_2 capture solvents	http://dx.doi.org/10.1016/j.ijggc.2013.09.001	Mathias, P. et al.	2013		methyldiethanolamine (MDEA)	105-59-9	-	-	CO_2				It is observed a graph of CO_2 partial pressure vs the enthalpy of solution of the different amines	• Thermodynamic models for the seven solvents are standard models from the AspenTechsupport Web
						Triethylamine (TEA)	121-44-8	-	-						
						2-amino-2-methyl-1-propanol (AMP)	124-68-5	-	-						
						Ammonia (NH3)	7664-41-7	-	-						
						Monoethanolamine (MEA)	141-43-5	-	-						
						Piperazine (PZ)	110-85-0	-	-						
						Glycolamine	929-06-6	-	-						
RW031	Aqueous piperazine as the new standard for CO_2 capture technology Gary	doi:10.1016/j.cej.2011.02.011	Rochelle, G., et al.	2011		Piperazine (PZ)	110-85-0	-	8 m			Flue Gas		Data from CO_2 solubility in some concentrations of PZ of different temperatures, additionally thermal degradation of the PZ with the loading of CO_2 and data of oxidative degradation of the amine	• Provided a second-generation electrolyte NRTL model of these data in Aspen Plus® (additionally m = gmol/kg-water, 40 wt%)
RW032	Kinetics of CO_2 desorption from aqueous N-methyldiethanolamine solutions	doi:10.1016/j.cej.2011.01.039	Kierzkowska-Pawlak, H. & Chacuk, A.	2011		methyldiethanolamine (MDEA)	105-59-9	99 wt%	10-30 wt%	CO_2 (L'Air Liquide, 99.995 vol% pure)				Treatment of desorption experimental data as the total pressure vs time (s); a Parity plot of experimental and calculated CO_2 desorption rates; the influence of the loading and temperature on chemical mass transfer coefficient for CO_2 desorption	• The common feature of absorption processes is that they are used absorber–stripper mode, requiring two separate steps in CO_2 separation. It is developed a mathematical mass-transfer model based on the film theory that includes all relevant chemical reactions in an acid gas–amine system to verify data.

RW033	Evaluation of MEA 5M performance at different CO_2 concentrations of flue gas tested at a CO_2 capture lab-scale plant Fernando	doi: 10.1016/j.egypro.2017.03.1760	Vega, F., et al.	2017		Monoethanolamine (MEA)	141-43-5	-	5M			Synthetic flue gas with similar composition from both a fossil fuel power plant and a cement plant on a lab-scale		Data to verify the efficiency of absorption is demonstrated into a graph of temperature profile absorber and temperature profile of stripper; additionally the CO_2 loading vs L/G ratio	• The experiment was carried out in a lab-scale plant
RW034	Fast screening of amine/physical solvent systems and mass transfer studies on efficient aqueous hybrid MEA/Sulfolane solution for postcombustion CO_2 capture	DOI 10.1002/jctb.6246	Hongxia, L. & Wu, Z. &Liang, Z.	2020	Monoethanolamine (MEA)	Monoethanolamine (MEA)	141-43-5	≥99%	MEA 30:70 H2O			99.9% N_2 and 99.9% CO_2		The data of the experiment is shown in graphs: absorption rate vs CO_2 loading for the additive amount of PC; The equilibrium solubility of CO_2 in the different hybrid solutions; The measurement of pH values for each hybrid solutions at a given temperature The absorption rate varies CO_2 loading for hybrid solutions: absorption rate versus CO_2 loading in mol CO_2/mol MEA Desorption rate varies CO_2 loading for hybrid solutions: desorption rate versus CO_2 loading in mol CO_2/mol MEA Finally, to adjust which additive is the best, it is stated comparison of cyclic CO_2 capacities of hybrid solutions for multiple screening processes.	• Composition [%(w/w)] - (MEA:additive:H_2O); Concentrations and compositions of the tested absorbents (each with total mass 250 g) • Additionally it was made a gas-liquid material balance for all tested hybrid solutions
						N-Methyl-2-pyrrolidone (NMP)	872-50-4	≥99%	30:20:50						
						propylene carbonate (PC)	108-32-7	≥99%	30:20:50 30:30:40 30:40:30 30:50:20						
						Polyethylene glycol dimethyl ether (NHD)	24991-55-7	average Mn250	30:20:50						
						N-Formylmorpholine (NFM)	4394-85-8	≥99%	30:20:50						
						Sulfolane	126-33-0	CP≥98%	30:20:50						
						Deionized water	-	-	-						
RW035	Absorption and regeneration studies of chemical solvents based on dimethylethanolamine and diethylethanolamine for carbon dioxide capture	DOI: 10.1002/aic.16770	Baltar, A., et al.	2020	DMEA and DEEA	2-Dimethylaminoethanol (DMEA)	108-01-0	>98%	-	CO_2 a purity of 99.998%				Data referenced at the influence of type amine; comparison between experimental values vs model values of absorbed molar flow rate of the amine; absorption rate kinetics after regeneration by stripping of amine + additives solutions. Data of absorption curve after three regeneration cycles using the amine + additives Data from the relation between acid dissociation constant and regeneration degree using the precipitation method for the amines + additives	• The solution was introduced into a three-necked flask
						2-(Diethylamino)ethanol (DEEA)	100-37-8	>99%	-						
						Calcium Hydroxide	1305-62-0	>96%	-						
						Amberlite IRA-402	52439-77-7	>98%	-						
						Sodium Hydroxide (NaOH)	1310-73-2	>98%	-						

RW036	Kinetics of absorption of carbon dioxide into aqueous solutions of 2-amino-2-hydroxymethyl-1,3-propanediol	doi:10.1016/j.seppur.2009.06.022	Subham, Paul, et. al	2009		2-amino-2-hydroxymethyl-1,3-propanediol (AHPD)	77-86-1	99.80%	-			CO_2 + N_2 certified purity of 99.99%		Comparison between the calculated rates to the experimental rates of absorption for CO_2. Table of kinetic data for the absorption of CO_2 into ($AHPD+H_2O$)	•The reaction involved in the process has its mechanism to interpret kinetic data using a wetted wall column absorber
RW037	Low-Viscous Fluorine-Substituted Phenolic Ionic Liquids with High Performance for Capture of CO_2	http://dx.doi.org/10.1016/j.cej.2015.03.052	Zhang, Xiao-Ming. et al.	2015	Phenol	Phenol	108-95-2	99 wt %	-	CO_2 with a minimum purity of 99.99 mol%				The effect of the ionic liquids (additives) and the base solutions in the capture process are developed in tables of densities, viscosities, and the absorption rate of CO_2	•The preparation of the studied Ionic Liquids is developed by a precise experimental procedure as the ionic liquids can not be bought in commercial sites •The ionic liquids prepared were characterized by 1H NMR, 13C NMR, FTIR, ESI-MS to figure out its structural properties and with this the physicochemical properties (densities, viscosities, and decomposition temperatures) •The CO_2 absorption mechanism is also proposed for these ionic liquids
						2-Fluorophenol	367-12-4	98 wt %	-						
						3-Fluorophenol	372-20-3	98 wt %	-						
						4-Fluorophenol	371-41-5	98 wt %	-						
						Tetrabutylphosphonium bromide	3115-68-2	98 wt %	-						
RW038	Kinetics of CO_2 absorption in aqueous N,N-diethylethanolamine and its blend with N-(2-aminoethyl)ethanolamine using a stirred cell reactor	http://dx.doi.org/10.1016/j.ijggc.2015.03.002	Hanna Kierzkowska-Pawlak	2015	DEEA	2-(Diethylamino)ethanol (DEEA)	100-37-8	≥ 99%	2M DEEA + 0.1M AEEA 2M DEEA + 0.2M AEEA 2M DEEA + 0.3M AEEA	CO_2 air-liquid at 99.995 vol% pure				The data presented in this article is referred to the CO_2 absorption rate into aqueous DEEA activated solutions with AEEA	•The experiments were carried out at three different temperatures 293K, 303K, 318K, and the enhancement factor that describes a chemical reactions' influence on the mass transfer calculated experimentally and theoretically
						2-(2-aminoethyl-amino)ethanol (AEEA)	111-41-1	≥ 99%							
						DDE water	prepared in lab								
RW039	Absorption of Carbon Dioxide into Aqueous Blends of Diethanolamine and Methyldiethanolamine	https://doi.org/10.1021/ie990850r	Rinker, Edward et. al	2000		methyldiethanolamine (MDEA)	105-59-9	-	10, 30, and 50 wt % Blends of DEA and MDEA (w/ varied molar ratios)	CO_2				The data treated is the reported product of the CO_2 absorption rate in the different wt %, the predicted data vs the obtained data	•The experiments were developed in a Laminar-Liquid-Jet absorber at 25º C
						Diethanolamine (DEA)	111-42-2	-							

RW040	Kinetics of absorption of carbon dioxide into aqueous solutions of 2-amino-2-methyl-1-propanol + monoethanolamine	https://doi.org/10.1016/S0009-2509(99)00303-6	Xiao, Jimmy, et. al	2000		Monoethanolamine (MEA)	141-43-5	99%	kmol/m-3 AMP + kmol/m-3 MEA 1.5+0.0 1.7+0.0 1.5+0.1 1.7+0.1 1.5+0.2 1.7+0.2 1.5+0.3 1.7+0.3 1.5+0.4 1.7+0.4	CO_2				The data presented to these experiments are developed in tables of densities, viscosities. It is also made an estimated solubility of CO_2 in the complex AMP+MEA+H_2O made under parameters of calculated solubility and diffusivity. Other tables reported are the kinetic data of absorption of the complex of AMP+MEA+H_2O	•The experiment proposes different models to calculate the variables involved in the CO_2 capture process at three different temperatures
						2-amino-2-methyl-1-propanol (AMP)	124-68-5	98%							
RW041	New processes for amine regeneration	http://dx.doi.org/10.1016/j.fuel.2014.06.067	García-Abuín, Alicia, et. al	2014		pyrrolidine (PYR)	123-75-1	> 99%	-	CO_2 99.99% pure				To show the efficiency of the compounds, three stages of absorption and regeneration are made, then the author quantifies the data obtained in each process to demonstrate which amine is better at the conditions of the operation. Finally, it was all exposed in a table of regeneration degree of amines aqueous solutions using calcium hydroxide.	•Two studies were performed, the first of them is a treatment of rich carbon dioxide amine with calcium hydroxide, the second was made under ion exchange operation •1H and 13C NMR spectroscopy was applied to investigate qualitatively the amines solutions loaded with carbon dioxide during the capture utilizing chemical absorption and regeneration processes.
						methyldiethanolamine (MDEA)	105-59-9	> 99%	-						
						triethanolamine (TEA)	102-71-6	> 99%	-						
						triisopropanolamine (TIPA)	122-20-3	> 95%	-						
RW042	Carbon dioxide capture with tertiary amines. Absorption rate and reaction mechanism	http://dx.doi.org/10.1016/j.jtice.2017.07.022	García-Abuín, Alicia, et. al	2017		methyldiethanolamine (MDEA)	105-59-9	≥99%	-	CO_2 gas phase 99.998% purity				The data presented was the influence of amine mole fraction upon the viscosity of aqueous solutions and surface tension of aqueous solutions of the tertiary amines at 298.15K There is also a graph of carbon dioxide loading values reached by different solvents	•The compounds were taken into account by the absorption rate experimental data and 13C and 1H NMR
						2-Dimethylaminoethanol (DMEA)	108-01-0	≥99%	-						
						2-(Diethylamino)ethanol (DEEA)	100-37-8	≥98%	-						
						triisopropanolamine (TIPA)	122-20-3	≥95%	-						
						Double Distilled Water									

RW043	Revised kinetics of CO_2 absorption in aqueous N,N-diethylethanolamine (DEEA) and its blend with N-methyl-1,3-propane-diamine (MAPA)	http://dx.doi.org/10.1016/j.ijggc.2016.12.019	Kierzkowska-Pawlak, Hanna & Kruszczak, Ewelina	2017	DEEA	2-(Diethylamino)ethanol (DEEA)	100-37-8	≥99%	2 M BS 1.95 M BS + 0.05 M MAPA 1.9 M BS + 0.1 M MAPA 1.8 M BS + 0.2 M MAPA	CO_2 air-liquid at 99.995 vol% pure				The data obtained were compared with similar data from previous works. The main results are plotted into a graph of CO_2 absorption rates into aqueous DEEA with the promoter. The additional data come from the contributions of the overall pseudo-first-order kinetic constant of the blended amine and a comparison between the relative enhancement factors	•The study was performed in a batch-operated stirred-cell reactor under a fast pseudo-first-order regime. It is also developed as a mechanism that should be followed by the elements
						N-methyl-1,3-propane-diamine (MAPA)	6291-84-5	≥98%							
RW044	Thermal degradation of aqueous DEEA solution at stripper conditions for post-combustion CO_2 capture	http://dx.doi.org/10.1016/j.ces.2015.02.033	Zhiwu Liang, Hongxia Gao, et. al.	2014	DEEA	2-(Diethylamino)ethanol (DEEA)	100-37-8	≥98%				CO_2 + N_2 with a purity of ≥ 99.9%		The data obtained is reviewed by the graph of the fraction of amine remaining for thermal degradation with and without CO_2. The effect of DEEA concentration on the fraction of DEEA remaining, its effect of degradation efficiency on the equilibrium solubility of CO_2 in the aqueous solution	•Thermal degradation experiments were conducted in a 600 mL stainless steel autoclave reactor. •The compounds were also characterized in comparison with the literature data in mass spectra and gas chromatography
RW045	New Amines for CO_2 Capture. I. Mechanisms of Amine Degradation in the Presence of CO_2	10.1021/ie900472x	Lepaumier, Helene. et. al.	2009		N,N-Dimethylethanolamine (DMEA)	108-01-0	-		Analytical-grade carbon dioxide supplied by Air Liquide (CO_2 99.9%, H_2O < 3 ppm, O_2 < 2 ppm, CnHm < 2 ppm, N_2 < 8 ppm, H_2 < 0.5 ppm)				The data obtained is classified in ethanolamines and ethylenediamines according to degradation rates of the different amines with temperature and CO_2 for a period of 15 days.	•The formation of different mechanisms are proposed to identify the way for each amine, and a general pathway to the ethanolamines and ethylenediamines
						methyldiethanolamine (MDEA)	105-59-9	-							
						N-Methylethanolamine (MAE)	109-83-1	-							
						Diethanolamine (DEA)	111-42-2	-							
						Monoethanolamine (MEA)	141-43-5	-							
						2-amino-2-methyl-1-propanol (AMP)	124-68-5	-							
						N-(2-Hydroxyethyl)ethylenediamine (HEEDA)	111-41-1	-							
						N,N'-Dimethylpiperazine (DMP)	106-58-1	-							
						N,N,N′,N′-Tetramethylethylenediamine (TMEDA)	110-18-9	-							
						N,N,N′-Trimethylethylenediamine (TriMEDA)	142-25-6	-							
						N,N′-Dimethylethylenediamine (DiMEDA)	110-70-3	-							