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Prime Solvent candidates for next generation of PCC plants

IEA GREENHOUSE GAS R&D PROGRAMME

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PRIME SOLVENT CANDIDATES FOR NEXT GENERATION OF POST-COMBUSTION CO_2 CAPTURE PLANTS

KEY MESSAGES

The primary goal of the study is to review prospective prime solvents and process designs to accelerate the deployment of CO_2 capture technologies. IEAGHG commissioned Khalifa University, United Arab Emirates (UAE) to conduct a comprehensive assessment of promising aqueous and water-lean PCC solvents. This study identifies and characterises prime solvent candidates for the next generation of post-combustion carbon capture (PCC) technology. The solvent comparison was carried out against a benchmark 30 wt.% monoethanolamine (MEA) aqueous solution and the IEAGHG benchmark system (IEAGHG 2019/09).

- Based on the collected data and their detailed analysis, no single amine was identified to have an overriding superior performance in terms of capital and operating costs. Most of the amines spanned between slightly better and poorer performance compared with MEA in terms of both capital and operating expenditures. The most promising amines were found to be 2-(isopropylamino) ethanol (IPAE), aminoethylethanolamine (AEEA), 2-methyl piperazine (2-MPZ), 2-(ethylamino) ethanol (2EAE), 2-amino-1,3-propandiol (2APD), 3-(methylamino) propylamine (MAPA), piperazine/2-amino-2-methyl-1-propanol (PZ/AMP) and monoethanolamine/ethylene glycol (MEA/EG).
- The solvent properties that have the most influence on the capital cost are the absorption capacity, reaction rate, absorption enthalpy (heat of absorption) and the liquid viscosity.
- In terms of process configurations, the most promising modifications include absorber inter-cooling, rich solvent split, stripper overhead compression, split flow, and lean vapour compression as per the reduction in the specific reboiler duty.
- The sensitivity analysis has shown that the CO_2 gas concentration is a predominant determinant of the cost of capture. Therefore, it is cheaper to capture CO_2 from higher concentration sources. The cost of capture increases linearly (slight slope) for capture rate of about 85%, but exponentially increases for capture rates of > 95% on a conventional process.
- A solvent database has been developed in this study, codenamed CO_2SOLV which hosts a large number of the most relevant solvents for PCC. An equilibrium-based process model that is integrated with the CO_2SOLV database has been developed. This model serves to analyse the data and deduce conclusions in terms of technical and economic performance of the solvents and process configurations.
- As more solvents are being proposed for the application of PCC, rapid screening of solvents becomes a necessity. A decision tool has been developed that offers high throughput screening of solvents inclusive of technical and economic indicators. Further, solvents can be assessed on a comparable basis under the same operating conditions.

BACKGROUND OF STUDY

Research, development, demonstration, and deployment of advanced solvents is at the forefront of decarbonising the fossil fuel combustion sectors with the aim of making CO_2 capture more competitive in a net zero economy. Considering the extensive research in solvent design and development, a rapid and reliable screening protocol is imperative for new solvents and process configurations to be ranked against existing systems.

Acid gas recovery using alkanolamines is a well-established technology and this technology is projected to play an important role in the decarbonisation of fossil fuel combustion facilities across the world. In spite of the decarbonising potential of reactive absorption with amines, its commercial deployment in hard-to-abate sectors, and fossil fuel power plants, has been lethargic to date. Only one commercial power plant equipped with carbon capture, usage, and storage (CCUS) remains in operation at the time of this reporting, i.e., the Boundary Dam Project. The other, Petra Nova, has discontinued its CCS operations due to falling oil prices and no date has been confirmed on when it will resume operations. One of the key challenges for the commercial deployment of amine capture plants are the high capital and the operating costs of the plant, and the cost of the solvent. Capturing CO_2 from clusters of industrial installations (including existing fossil fuel fired generation plant) and using shared infrastructure hubs for the subsequent CO_2 transportation and storage, is increasingly seen as the preferred approach to drive down unit costs across the CCUS value chain. There are in 2021 four such hubs in operation and 29 under active consideration according to the Global CCS institute. Further, the technical, economic, and environmental limitations of the solvent must be addressed to reduce the cost of operating an amine capture plant via improved chemical solvents and innovative process designs. To address the need for improvement, this study developed a decision tool for screening solvents and process configurations for PCC. This enables the user to perform techno-economic analyses by modifying process parameters as well as performing sensitivity tests on the economic parameters such as interest rates and duration of the project.

SCOPE OF STUDY

This study assesses promising PCC solvents, providing an analysis of their enhancement and their potential functionality under standardized metrics to measure the solvents performance and their impact on capture costs including both capital expenditure (CAPEX) and operational expenditure (OPEX). The classes of solvent considered in this study include aqueous amine solvents, solvent blends, water-free/water-lean solvent and biphasic solvents. A user-friendly excel front-end structure that allows ease of accessibility houses the wide-ranging solvents that has been designed and populated manually, through collecting references from the different sources. Further, this study developed a decision-matrix-tool to enable the comparison of the different solvents and processes based on Key Performance Indicators (KPIs). A detailed review of the most relevant chemical absorption processes and equipment designs are also presented in this study. This includes multi-modifications in a single process, which is a combination of the individual process modifications. The standard process for PCC employs an aqueous solution of 30 wt.% monoethanolamine (MEA), which is the benchmark defined in this study for comparison with novel process modifications and novel solvents. A detailed review of degradation and corrosion studies exhibited by the solvents, along with process emissions, amine consumption and solvent management, is also presented. Finally, the best performing PCC solvents and processes were ranked based on technical and economic indicators.

FINDINGS OF STUDY

The exhaustive literature survey of solvents for PCC led to the creation of a solvent database named CO_2SOLV which comprises of 842 entries of various type of solvents (see Figure 1). It contains detailed properties of >107 solvents plus several process configurations and modifications. This database includes publicly available information on installations testing solvents (at large, pilot and lab scale) for PCC, in addition to solvents reported in scientific publications and patents. A thorough review of the chemical absorption process and equipment designs at different scales for PCC was also embarked on.

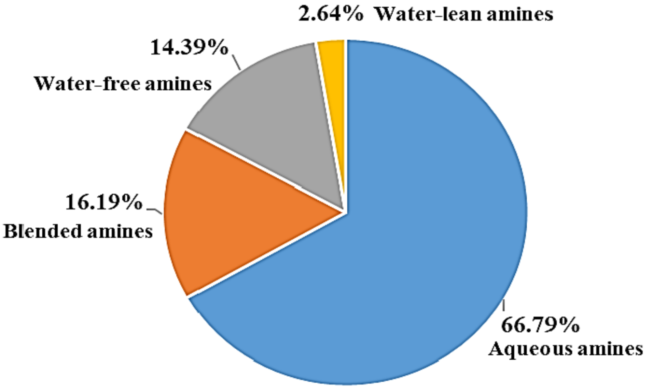

Figure 1. Distribution of types of solvents (from 842 entries) included in the Solvent Screening Tab in the CO_2SOLV Database

The study consisted of seven key tasks summarised below

Task 1: Review of emerging aqueous and water-lean PCC solvents.

CO_2SOLV, a codename ascribed to a database was developed in this study that hosts an exhaustive collection of available information on solvents for PCC (including traditional aqueous amines, novel aqueous amines, blended amines, water-free amines, and water-lean amines). CO_2SOLV offers access to the reported information on:

- Solvent type, components, and composition
- Testing scale (industrial vs lab-scale), conditions and applications
- Enhancement exhibited using the solvent

Figure 2 gives an illustrative example for the applicability of the CO_2SOLV database. The CO_2 absorption isotherm at 40°C for different solvents, as directly plotted from the information in the database offers an ease in the solvent screening capability based on desired parameters to be assessed.

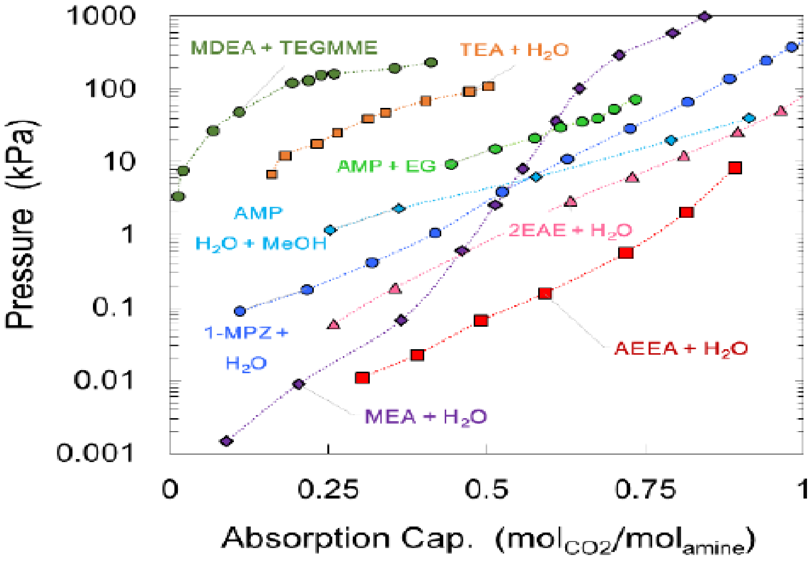

Figure 2. Absorption isotherms of selected solvents from CO_2SOLV

Task 2: Review of PCC processes and equipment design.

Task 2 reviewed the findings of the process modifications based on pilot and commercial plants, however, a dearth of data from some plants due to intellectual property (IP) sensitive matters, have resulted in several process simulation results. Most results from process modifications offer some form of reduction in the solvent regeneration energy requirement but in most cases at the expense of increased overnight expenditure. Figure 3 presents a summary of reported changes of specific reboiler duty for different solvents and process modifications. The green and red circles depict decrease and increase in the specific reboiler duty (SRD) respectively. Lean vapour compression (LVC) was observed to be the most studied for different solvent types and delivers up to 30% decrease in the SRD with reference to the conventional process of the probed solvent. However, this process modification results in an increase in the CAPEX due to the increase in the number of units, mainly the compressor (or steam ejector). Yet, due to the decrease of the condenser and reboiler duties, their sizes decrease, and which incurs less CAPEX and OPEX. Further analysis is important to close the knowledge gap with regards to how this process modification impacts on electricity consumption. Vacuum stripping (VS), compression heat integration (CHI) and multi-pressure stripper (MPS) (all with MEA) were observed to increase the SRD. Most process modifications were observed to reduce the SRD within a range of 10 to 20%, consequently reducing the energy impact levied on the parent power plant.

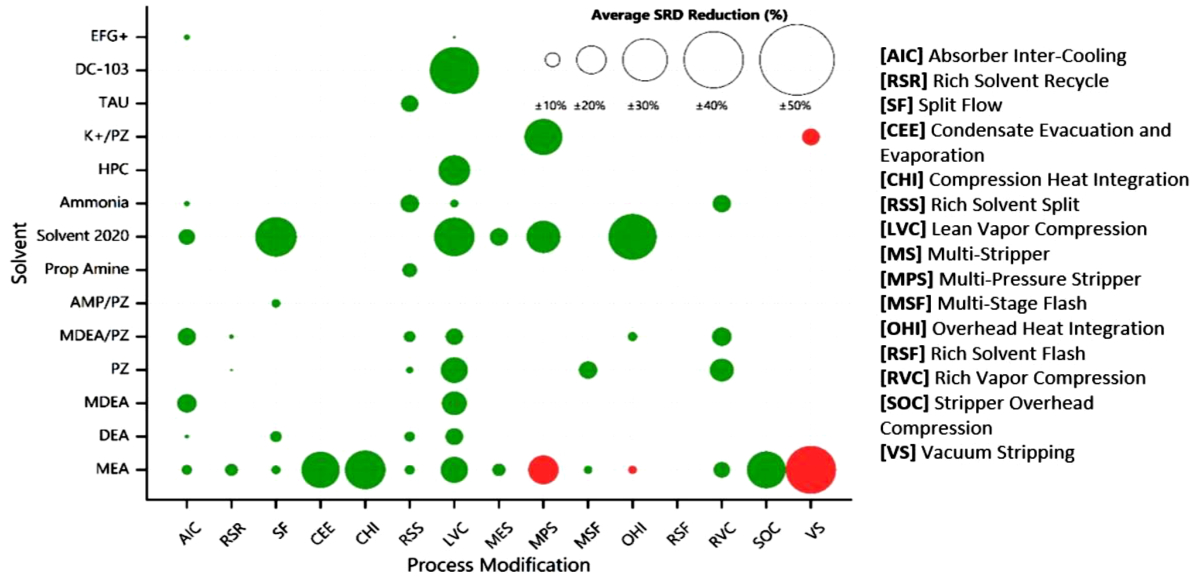

Figure 3. Summary of average percent reductions of specific reboiler duty of selected solvents and individual process modifications available in the literature.

Note: The reference baseline is the conventional process of the concerned solvent. Green circles depict a reduction in the SRD, while red circles imply an increase. ‘Solvent 2020’ is a hypothetical solvent similar in properties to MDEA/PZ.

Further, this study also evaluated the integration of two or more process configurations with respect to the SRD. Figure 4 presents the reduction of the SRD for an integrated process modifications against the conventional design of 30 wt. (%) MEA.

As observed, a combination of process configurations delivers a reduction in SRD within the range of about 5 to 40% as compared to the base case scenario. Absorber inter-cooling (AIC)/LVC/condensate evacuation and evaporation (CEE) was observed to reduce the SRD by almost 40%. This demonstrates that with the right combination of process modifications, the SRD can potentially be significantly reduced. However, the implication on the overnight and running costs need to be further assessed. The integration of more than three modifications were seldom encountered in the literature and were mostly found in patents perhaps due to the complexity of the process and investment cost burden. The interactions between modifications need to be thoroughly assessed as some modifications can impose detrimental effects and lack of compatibility in the process. For example, the multi-pressure stripper (MPS) operates at a low pressure at the bottom of the desorber column which makes integration with LVC an inefficient option because it requires high-pressure lean stream. Conversely, when AIC is coupled with rich solvent recycle (RSR), a positive interaction is produced as AIC increases the working capacity of the solvent but at the expense of the kinetics. Under this condition the RSR compensates and returns some of the solvent for increased contact time.

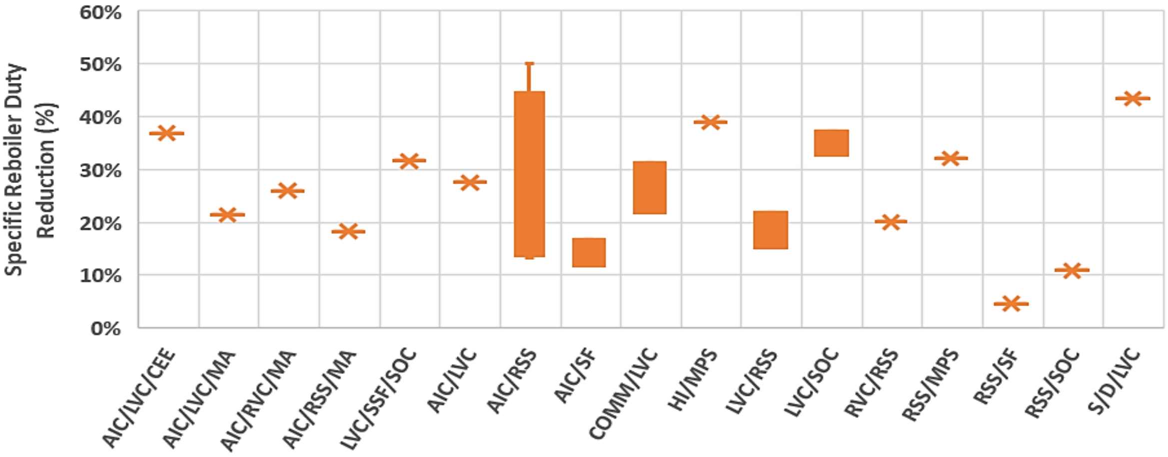

Figure 4. The SRD vs the combined process modifications

Task 3: Review of degradation, corrosion, and process emissions

This task presents a comprehensive review of the solvent degradation, emissions and corrosion studies exhibited by the solvents in Task 1. Solvent degradation has been identified as one of the most important challenges in acid gas recovery. Thermal degradation accelerates above 130°C.[1] This finding was based on the backdrop of the study by Rochelle at al., 2009 who established that MEA degrades at a pace of 2.5% to 6% weekly when held at 135°C. Whereas oxidative degradation induces dioxygen-enthused breakdown (irreversible chemical reaction into unwanted compounds that is triggered in the presence of oxygen). Furthermore, a study carried out by Goff and Rochelle has estimated that about 0.29 to 0.73 kg MEA/tCO_2 captured is consumed in the oxidation of amine solvent.[2] Thermal and oxidative degradation normally occurs in the PCC regions described in Figure 5.

The rate at which thermal degradation occurs is influenced by the residence time of the solvent in the regeneration column sump, reboiler temperature, CO_2 loading in the rich solvent, and amine concentration, with their increase resulting in an increased thermal degradation rate. The thermal degradation products reported in the literature for the main amines employed in industry are MEA, DEA, MDEA, AMP, and PZ. In oxidative degradation, the degradation rate is influenced by the concentration and type of impurity present in the flue gas, CO_2 loading in the rich stream, absorber temperature, amine concentration, and presence of metal ions that catalyses the degradation reaction. The impact of these parameters has been initially identified and examined on the standard benchmark solvent to date. The total loss of amine, determined from several pilot plant test campaigns, was in the range of 0.3 – 1.5 kg MEA per tonne of CO_2 captured, with more than 60% of these losses being attributed to oxidative degradation. Test campaigns over a long term (over 10,000

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[1] Degradation and Emission Results of Amine Plant Operations from MEA Testing at the CO_2 Technology Centre Mongstad. Energy Procedia Volume 114, July 2017. (https://www.sciencedirect.com/science/article/pii/S1876610217315643)

[2] Degradation of amine solvents used for co2 removal from flue gas with high co2 concentration. The Silesian University of Technology. 2021. (https://www.exeley.com/exeley/journals/architecture_civil_engineering_environment/14/1/pdf/10.21307_ACEE-2021-011.pdf)

hours) is critical to continued understanding of the mechanism of solvent degradation which has been established to be plant specific and changes with modifications of the CO_2 capture process conditions.

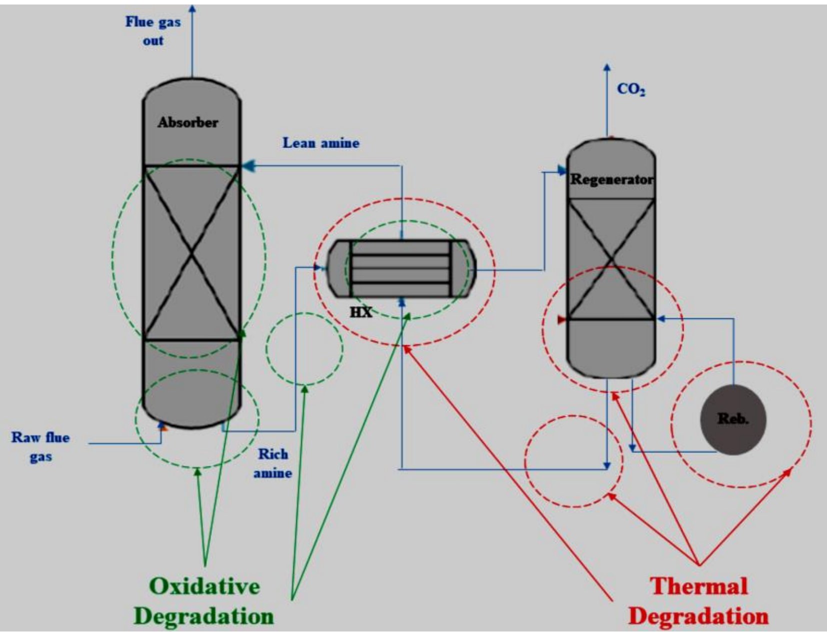

Figure 5. Location of oxidative and thermal degradation in a PCC unit

The CASTOR project was embarked on at the Esbjergværket power station in Denmark, where quantification of solvent consumption was carried out during a 500-hour test. During the MEA campaign, 720 kg of MEA was consumed during a 500-hour test, capturing 503 tons of CO_2, which resulted in 1.6 kg MEA consumed per ton of CO_2 captured. Findings from a 1,960-hour test at the Technology Centre Mongstad in 2015 reported 1.5 kg MEA consumed per ton of CO_2 captured. A 5,000-hours test campaign at Niederaussem pilot plant in Germany reported 0.3 kg of MEA per ton of CO_2 captured but more recently, an 18-month test campaign over a period of 13,000 hours at the same plant reported solvent consumption of about 0.5 kg per ton of CO_2 captured. The OCTAVIUS project aimed at understanding solvent degradation from three pilot plants namely: TNO's CO_2 capture plant at Maasvlakte; EnBW's CO_2 capture plant at Heilbronn; and ENEL's CO_2 capture plant at Brindisi, found that degradation rates are influenced by the different flue gas quality and dissolved oxygen concentrations. These test results advance the understanding in terms of studying solvent degradation from the lab-scale studies to pilot-scale campaigns. The results also reveal that the degradation profile is plant specific. These studies further underscore the importance of solvent management and design to limit the solvent depreciation, solvent degradation and emissions resulting from the degradation processes.

Information of value is generated from pilot-scale testing facilities because it analyses solvents under realistic conditions and over a prolonged period of operational time. However, due to the extended period of time that it takes to run these tests, an advanced laboratory rig was designed (which simulates the absorber/stripper configuration) by SINTEF Materials and Chemistry to study solvent degradation. Over the course of 14 weeks of test campaigns with 30 wt. (%) MEA, the formation of nitrosamine and nitramine were found to be highly reduced by elevated stripper temperature.

Corrosion is a key challenge in amine-based carbon capture installations and could increase the OPEX as well as the CAPEX of the solvent-based CO_2 capture plant (SCCP). Corrosion mechanisms occur in the form of wet acid corrosion and corrosion by amine solutions (formed from the reaction between amine and CO_2).

Pilot-scale test campaigns established that over the period of 48 months, carbon steel material at the stripper outlet lost over 80% of its initial weight due to a high corrosion rate. The corrosion behaviour of other amines examined in the literature found that the corrosion rate decreases in the order of monoethanolamine (MEA) > 2-amino-2- methyl-1-propanol (AMP) > diethanolamine (DEA) > piperazine (PZ) > methyldiethanolamine (MDEA).

The primary objective of the PCC technology is to curb CO_2 emissions, however, associated secondary emissions, that include ammonia, amine, nitrosamine, nitramines, volatile organic compounds (VOC) and particulate matter (PM), are potentially released into the atmosphere. The most critical of these emissions (e.g., nitrosamine and nitramine, formed from amine degradation) are carcinogenic. Though the amount released into the atmosphere is influenced by the size of the plant, operating conditions, flue gas composition and type of solvent. Online monitoring devices, and auxiliary units to capture these secondary emissions or their precursor towards their formation, is required in effect adding to the CAPEX of the plant.

Solvent management is key to maintaining the performance of the solvent and curtailing against solvent degradation, corrosion and emissions which are in effect precursors to operational challenges. These include, but are not limited to, solvent deactivation, corrosion, increased atmospheric emissions, fouling and foaming. A number of management strategies are thus employed to maintain the functionality of the solvent and include the following:

1. Solvent selection and optimization of process conditions
2. Inhibitors for degradation and corrosion and
3. Additional processing units for solvent reclamation.

Task 4: Identification of parameters for performance evaluation

These tasks identify the most important process parameters to evaluate the performance of the solvents and processes reviewed with regards to the impact on CO_2 capture cost in terms of CAPEX and OPEX. Factors to evaluate performance of PCC were identified and include technical, economic, and environmental parameters. The parameters considered for solvent screening include CO_2 cyclic capacity, heat of absorption, CO_2 absorption rate, solvent viscosity, solvent tension, degradation, toxicity, foaming, corrosivity and cost.

A modelling tool was developed for the CO_2 capture process to enable solvent screening using the available data hosted in CO_2SOLV database. Every sub-model of the capture process including the absorber, stripper or reboiler, incorporates cost equations based on the design equations and solvent properties (density, viscosity, surface tension, heat of absorption) that impacts the process performance were included in the model. Thereafter, the model was validated against a published study based on the CASTOR project pilot plant. The equilibrium-based process model integrated with CO_2SOLV database has successfully predicted the performance of mass transfer process of CO_2 separation using amines. It was reported that both the absorber and desorber columns accounts for about 70% of the CAPEX whereas the solvent regeneration cost accounts for about 70% of the OPEX. Results have shown that the total annual cost (TAC) of the capture process is US$57 per tonne of CO_2, which gives the total cost of the CO_2 capture at US$76 per tonne of CO_2 when the costs of CO_2 compression and dehydration are included.

Task 5: Development of standardised metrics to evaluate PCC performance

A set of standard metrics was developed in relation to the main parameters from Task 4 to appraise the performance of the solvents reviewed in Task 1. In order to define the standard metrics to appraise the performance of the solvents, the screening model developed in Task 4 was used to perform a sensitivity analysis (based on 30wt (%) MEA as the benchmark for comparison) to assess the impacts of different properties on design and process costs.

To evaluate the impact of physico-chemical properties on column design, sensitivity studies were conducted on the properties of gas and liquid phase density, viscosity, and diffusivity. These parameters varied from -30 to +30% against the benchmark (MEA) case. Deviation of the gas phase density, and viscosity of the liquid phase, impacted the pressure drop of the column as presented in Figure 6. The design column diameter was also shown to be more sensitive to the deviation of the gas phase density than the liquid phase property. The increase of gas phase viscosity decreases the CO_2 mass transfer through the gas film and accordingly decreases the overall mass transfer of absorption process. Thus, higher packing is required to attain the required CO_2 capture efficiency.

Deviation in liquid viscosity by +15% and -15% reflects on the variation of the column height by +12.9% and -13.1% respectively. In general, the CO_2 mass transfer through the liquid film increases with increases in density and diffusivity but decreases with increases in viscosity and surface tension as reflected in Figure 6.

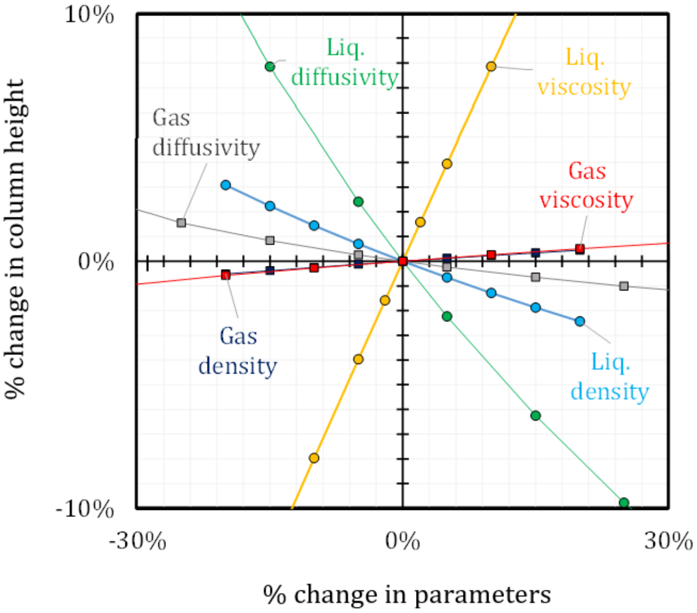

Figure 6. Sensitivity analysis of the impact of fluid properties on the percentage deviation of the column height.

The influence of the fluid property on the annual capital cost was assessed. The properties that have the greatest impact on the capital cost are the heat of absorption and liquid phase viscosity as presented in Figure 7. Deviation of +15% of the absorption enthalpy (heat of absorption) and liquid viscosity was found to affect the annual capital cost by +7.5% and +3.5% respectively. Whereas impacts on the viscosity and density of the gas phase was deemed to be mild.

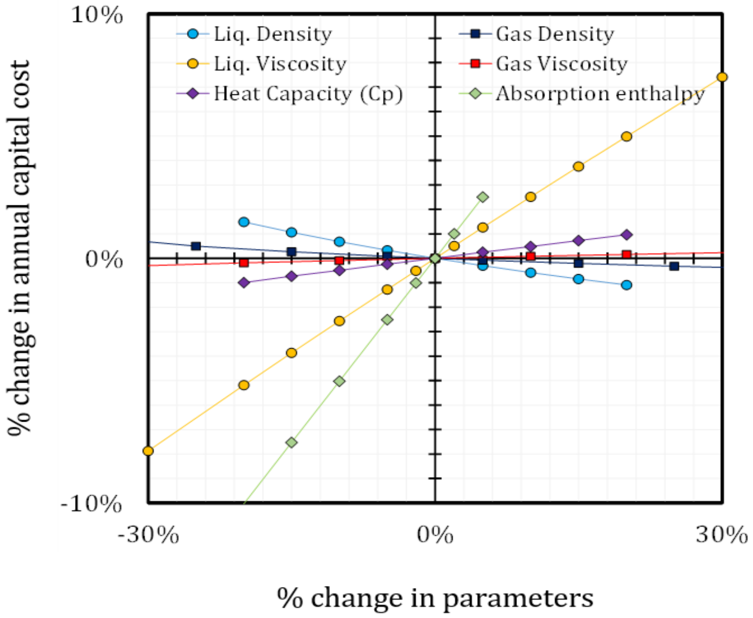

Figure 7. Sensitivity analysis of the influence of the fluid properties on the percentage deviation of the annual capital cost

The relationship between the CO_2 concentration, CO_2 capture efficiency and cost per tonne of CO_2 captured for 30wt (%) of MEA demonstrates that the partial pressure of CO_2 in the flue gas is a greater determinant of the cost of CO_2 capture than the degree of capture as depicted in Figure 8. The implication of this observation is that the concentration of CO_2 has the biggest influence on capture cost. Sensitivity analysis has shown that the TAC increases minimally up to 85% and exponentially for capture rates > 95% for varying CO_2 concentrations from 1 to 40% using 30 wt % MEA. The TAC begins to noticeably increase from 85 to 95% capture efficiencies. More solvent is utilised, absorption column height increased, or other process optimisation schemes employed to accommodate for the increased capture efficiency, consequently adding to the cost of carbon capture. At about 15 vol (%) of CO_2 (i.e., ~ the concentration of CO_2 in a coal fired power plant flue gas) the TAC (see Figure 8) was observed to increase from < US$50/t to > $US50/t.

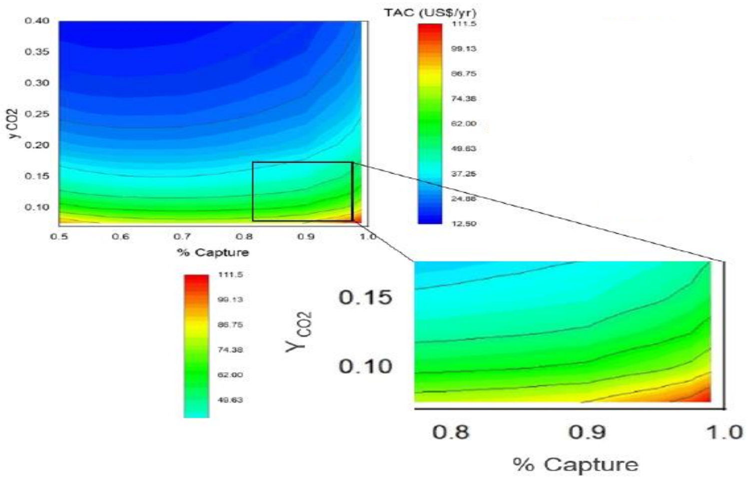

Figure 8. Cost of CO_2 captured per tonne as a function of percentage CO_2 capture and CO_2 concentration for 30wt (%) MEA.

Task 6: Critical evaluation of solvents and processes performance

Based on the prospective solvents and process identified in Tasks 1 and 2 respectively. The standardised metrics developed can be employed to evaluate the performance of enhanced CO_2 capture processes, and the potential for cost reduction, adding value to the next generation of capture technologies. A preliminary list of the most promising systems can be obtained from the results presented in Figure 9. The graph is methodically categorised into four quadrants. The most promising solvents are easily distinguished based on the quadrant they appear in. Amines with high CO_2 cyclic capacity, and lower heat of absorptions, are required to reduce costs and energy needed in PCC units. Therefore, the solvents located in the lower right quadrant in Figure 9a possess these qualities. PZ, MDEA and AMP have been observed to display better performance compared to MEA under the influence of the conditions studied, and as previously reported in the IEAGHG 2014 report. Other amines, that include 2-(ethylamino) ethanol (2EAE) and Aminoethylethanolamine (AEEA), can reach higher CO_2 loadings than MEA with lower heats of absorption and similar absorption rates.

Furthermore, critical assessment was carried out in this study in order to find out if the increase in CO_2 capture performance affects increases in the capital cost of the absorber units. The height of the absorption reactor was discovered to be more closely related to the viscosity of the liquid phase than the CO_2 capture rates (cyclic capacity), for example. Liquid viscosity deviation of +/-15% was observed to impact the capital cost by about +/-3.5%. Solvents can be selected based on the quadrant they fall into to establish if they could attract a high levelized cost of the absorber unit as depicted in Figure 9b.

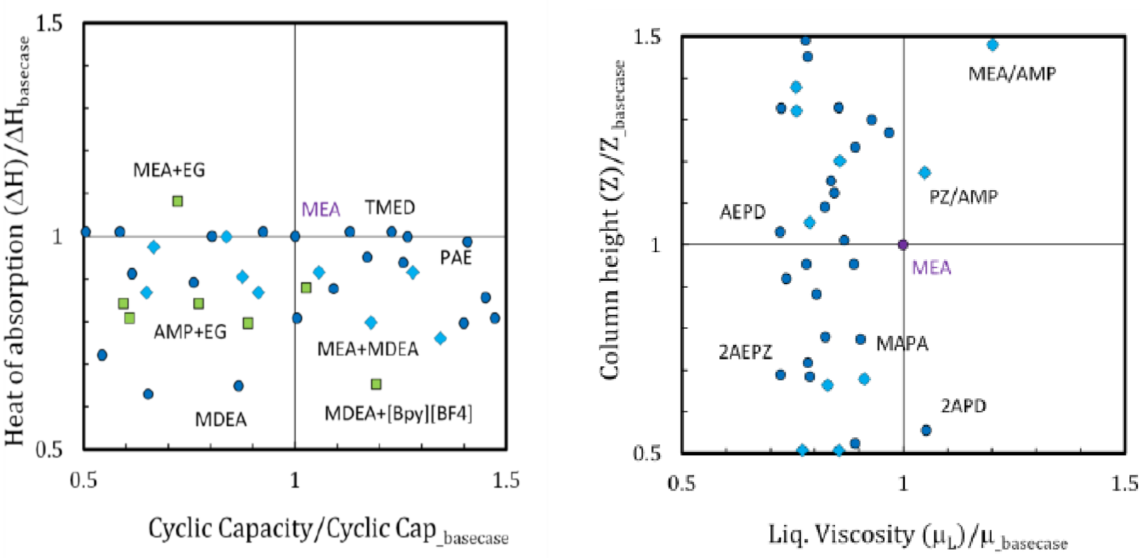

Figure 9. Solvent performance, (a) Heat of absorption as a function of cyclic capacity and (b) column height as a function of liquid viscosity.
*Aqueous MEA (purple), aqueous amine (dark blue), blends (light blue) and water-free/water-lean solvents (light green).

Based on the information for alternative solvents hosted in the CO_2SOLV database, 2APD was found to be the lowest in terms of the cost of CO_2 capture based on input parameters for the CASTOR plant at US\$46/tCO_2. Whereas MEA was found to be US\$51/tCO_2 IEAGHG's 2019-09 report estimated the costs for MEA, KS1 and Econamine FG Plus solvents at US\$45, US\$37, and US\$30 per tonne CO_2 avoided respectively.

Task 7: Development of a decision tool matrix for the design of PCC systems:

A decision model was developed to support the design of the solvent-based CO_2 capture system by selecting operating conditions for the absorber and stripper.

The input parameters consist of the following:

1. CO_2 capture efficiency, flow gas flow rate and CO_2 concentration in the flue gas
2. Temperature and pressure of the absorber and desorber.

The output parameters from the model include:

1. Total energy needed to operate the CO_2 capture system
2. Size of the separation unit e.g., absorber column size (diameter and height)
3. The CAPEX, OPEX and TAC

An important decision tool of this model is not only to modify process parameters but also perform sensitivity analyses (from the CO_2SOLV database) with regards to economic parameters. Figure 10 presents a sensitivity analysis result with respect to the TAC as a function of varying CO_2 capture efficiencies. The TAC was observed to attain its lowest value at 95% CO_2 capture efficiency and increasing the capture efficiency to 99% increases the TAC for all solvents studied. 30 wt. (%) IPAE and 40 wt. (%) PZ-AMP were observed to deliver the lowest total annual cost.

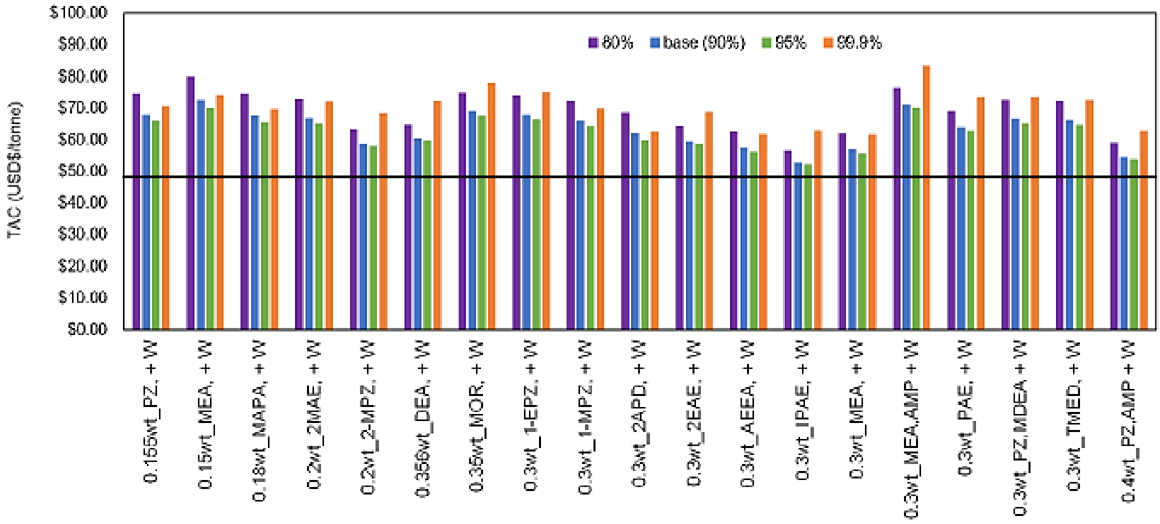

Figure 10. Total annual cost per tonne of CO_2 as a function of different solvent types (based on varying capture efficiency)

The findings of this study have identified piperazine/2-amino-2-methyl-1-propanol (PZ/AMP), 2-(isopropylamino) ethanol (IPAE), aminoethylethanolamiine (AEEA), 2-methylpiperazine (2-MPZ), 2-(ethylamino) ethanol (2EAE), 2-amino-1,3-propandiol (2APD), 3-(methylamino)propylamine (MAPA), lean monoethanolamine/Ethylene glycol (MEA/EG) as the prime solvents for the next generation PCC technologies in terms of monetised and non-monetised KPIs. These findings act as an initial vetting campaign. More optimisation studies are required for each solvent to verify where additional reductions are achievable.

A critical feature integrated into the decision-making tool is the ability to potentially account for benefits based on a particular process configuration/modification. Lean Vapour Compression (LVC), Rich Solvent Split (RSS), Absorber Inter-Cooling (AIC) and Split Flow (SF) were assessed and the LVC was found to yield more benefits with regards to the SRD and OPEX over other assessed process modifications. As more solvents are developed, this study provides an all-inclusive platform to not only compare its performances against publicly accessible solvents but assess how they fair in different process modifications against key monetary and non-monetary KPIs.

EXPERT REVIEW COMMENTS

- One reviewer noted that the study indicated only limited cost reductions over the standard MEA process and questioned if that was because the model used was based on MEA and extrapolations of MEA performance. The reviewer thought that it was important for the authors not to narrow their view around this deduction.
- Another reviewer had hoped for little more information on how the operating parameters of the process were translated into tower height and diameter. More information should have been given on how chemical kinetics and viscosity impacted the column sizing, CAPEX, and \$/tonne of CO_2. The same reviewer finally pointed out that it was commendable that the process performance, energy, OPEX, CAPEX and \$/tonne of the amines were compared in terms of process improvements as well as impact on CO_2 concentrations in the flue gas. M ore information on the new benchmark solution that include the concentration, name, developed/tested by, was required, and should be adequately referenced.
- This study did not discuss the tolerance of reviewed solvents with regards to NOx and SOx. Further comment from the same reviewer questioned the rationale behind why 'commercial' amine-based solvents such as MHI's KS-1^{TM} (older) and their newer KS-21^{TM} were hardly mentioned aside from a brief cost comment on KS-1^{TM}. Concerned as to the commercial outlook of the study was also raised because according to the reviewer without supplier/OEM input or direction the work is more of academic interest and not of project developer interest. However, there may be propriety constraints on the release of solvent properties.
- Environmental and human health impacts, due to solvent and degradation products emissions to the biosphere, could have been covered in greater depth as these aspects are important to address in the deployment of post-combustion capture projects. Further, considerations on control of emissions to air could have been included and corrosion and material selection discussed further. This aspect potentially has a significant impact on CAPEX, OPEX and solvent degradation rate. Although a detailed assessment of these impacts was not included in the project specification they should be investigated further.

CONCLUSIONS

- CO_2SOLV, a database of a large number of solvent types sourced from journal publications, patents, conferences, company reports etc for PCC has been methodically assembled and collated in an EXCEL front-end structure. CO_2SOLV is populated with 842 entries for a variety of solvents including traditional aqueous amines, novel aqueous amines, blended amines, water-free amines, and water-lean amines. The database also includes detailed properties of 107 solvents and several process configurations and modifications.
- A process model was developed based on the data hosted in CO_2SOLV, and which enables the assessment of technical and economic performance of the solvents and processes. The top promising solvents from the analysis include IPAE, AEEA, 2-MPZ, 2EAE, 2APD, MAPA, PZ/AMP, and MEA/EG (most promising water-lean solvent). The solvent properties that have the most influence on the capital cost, together with the absorption capacity and reaction rate, are the absorption enthalpy (heat of absorption) and the liquid phase viscosity.
- The CO_2 partial pressure in the flue gas was observed to be a more influential cost determinant than the degree of capture. The cost of capture increases marginally up to about 85% but increases exponentially at >95% under conventional process.
- In terms of process configurations, the most promising modifications include absorber inter-cooling, rich solvent split, stripper overhead compression, split flow, and lean vapour compression as per the reduction in the specific reboiler duty. However, a techno-economic analysis is needed to account for the possible trade-off in the capital costs.

- Integration of two or more process modifications can potentially induce positive interactions and synergy in maximizing effects and mitigate offsets. Dual process integration showed various impacts on the overall process with a reported reduction of the SRD ranging from 11% to 39% when simulating MEA. Further study to evaluate the behaviour of other emerging solvents under the influence of multiple process modifications is expected to yield lower SRD. However, new research is expected to reveal the extent of savings in terms of the relevant indicators like SRD.
- An increase in the solvent price only has a marginal effect on the capture cost when very low solvent losses of below 0.5 kg/tCO_2 captured occurs. This is due to the minimal cost component of replacing the solvents as compared to the total operating cost. The capture costs do not vary significantly between expensive and inexpensive solvents.
- Based on the collated data and the screening analysis carried out, it was observed that no single amine has an outright superior performance in terms of capital and operating expenditures. Most of the amines were observed to be either slightly better or worse in terms of the KPIs considered in this study when compared to MEA. It is worth noting that MEA is one of the most corrosive amines when compared to secondary or tertiary amines, which inevitably has an impact on both capital and operating cost of the CO_2 capture technology. Further optimisation is required to establish the potential benefits of the most promising solvents.

RECOMMENDATIONS

In order to rationally screen, select and design solvents for the next generation PCC technologies, a whole system approach is important. The absence of such an approach to date has led to an over emphasis of CO_2 solubility in solvent selection and design, potentially limiting progress in this area. Only a systematic approach to solvent design, with all properties appropriately weighted, can lead to an optimal (or at least an improved) solvent design. On this basis, the following works are recommended:

- Process modifications usually deliver better energy savings but at the expense of capture costs. Test campaigns to determine the economic implication of improved process modifications, identified in this study, namely, absorber inter-cooling, rich solvent split, stripper overhead compression, split flow, and lean vapour compression is recommended with a focus on both overnight and running cost implications. Further, techno-economic assessment of integrating two or more process modifications that synergise together is recommended.
- Rotating packed bed (RPB) is an emerging solvent-based CO_2 capture technology that offers a reduction of 86% packing volume from a conventional amine capture plant. Running pilot trials of the most promising solvent on RPB is essential to examine the potential of the prime solvents under the influence of centrifugal force with the aim of gaining improvements on both technical and economic parameters.
- Trials of prime solvents on 3D printed dynamic polarity (DP) packing can potentially improve the value of CO_2 capture. DP packing has demonstrated improved mass transfer in absorber column and consequently, reduction in the absorber size (low capital expense), increase cyclic capacity and reduction in the solvent requirement. Employment of the most promising and emerging solvents on 3D printed DP is recommended to evaluate the improvement on the economics of PCC.
- Most of the information collected is from process simulation studies focused on existing aqueous alkanolamines and blends. Research examining process design and performance for emerging water-lean and water-free solvents is quite limited but highly desirable. Therefore, a pilot demonstration on the feasibility of water-lean and water-free solvents application in PCC is required to appraise the potential of these emerging systems.

- The cost of environmental mitigation and corrosion abatement measures of different solvents needs to be scrutinised in detail as part of future evaluations.

Prime Solvent candidates for next generation of PCC plants

Title:	**Prime Solvent candidates for next generation of PCC plants**
Content:	Final Report
Submission Date (revised):	22 February 2021
Principal Investigator	Prof. Lourdes Vega, Director Research Center on CO_2 and H_2 (RICH) Khalifa University
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PROJECT EXECUTIVE SUMMARY

Prime Solvent candidates for next generation of PCC plants [IEA/CON/20/265]

Background & Problem:

The removal of CO_2 through its absorption in aqueous alkanolamines is a well-established CO_2 capture technology industrially used to either mitigate anthropogenic CO_2 emissions or produce CO_2 for different industrial uses. However, to date, its full-scale deployment remains hindered by the capital- and energy-intensive solvent regeneration step, along with solvent degradation and evaporation losses. Subsequently, development of new chemical solvents and process designs are in progress to enhance the performance or mitigate issues associated with the established process with aqueous MEA. However, evaluating the emerging solvents/processes remains limited to overall characteristics such as the net power for regeneration and cost per tonne of CO_2 captured or avoided, and constrained to conditions far from typical process operating conditions with non-standardized measurements. Considering the vast amount of research in this area, a rapid and reliable procedure to screen new solvents/processes for CO_2 capture and rank them against processes currently in use is needed.

Project Objectives

The project goal was to identify the prime candidates for the next generation of PCC plants and compare them to the traditional 30 wt.% MEA aqueous solution and the IEAGHG benchmark system (IEAGHG 2019/09) under a standardized framework. The main objectives were: (O1) to summarize emerging solvents and process configurations promising to enhance the CO_2 capture performance; (O2) to develop a number of metrics to measure the solvents performance and its impact on capture costs; and (O3) to develop a decision-matrix-tool to choose the best solvent for a PCC plant. The project was conducted at the Research and Innovation Center on CO_2 and H_2 (RICH Center), at Khalifa University, being the Principal Investigator Professor Lourdes Vega, Director of the RICH Center.

Main results and deliverables

- The data obtained from a detailed literature review in terms of solvents, process configurations, solvents consumption and degradation and emissions has been included in the **CO_2SOLV database**, delivered as one of the outcomes of this project. The database comprises 842 entries for a variety of solvents for solvent screening, detailed properties of 107 solvents and several process configurations and modifications.
- Most of the **process modifications** found in the literature were part of simulation studies and a dearth of them were implemented experimentally. Generally, the absorber inter-cooling, split flow, and lean vapour compression are amongst the most studied process modifications in the literature. Solvents other than MEA are currently under assessment with modified processes, which allows for a rough

comparison between the expected benefits and solvent-process modification interactions, if they exist.

- A detailed review on literature studies focused on solvent degradation and corrosion, along with process emissions, amine consumption, factors determining process emissions, preventive measures, and their effectivity within a solvent management strategy has been included as part of this study.
- An **equilibrium-based process model** integrated with the **CO_2SOLV database** has been developed as a tool to analyse the data and extract conclusions in terms of technical and economic performance of the solvents and processes and validated versus experimental data. The model has the ability to predict the performance of mass transfer driven process of CO_2 separation with different solvents. It confirms that the column sizing and reboiler duty represent two important process parameters that can be used for fast comparative performance of solvents for CO_2 capture.
- The **solvent properties** that have more influence on the capital cost, altogether with the absorption capacity and reaction rate, are the absorption enthalpy (heat of absorption) and the liquid phase viscosity.
- According to the performed sensitivity analysis, the **CO_2 gas concentration** is a stronger determinant of the cost of capture than the degree of capture. This implies that for the same investment, it is economically preferable to capture CO_2 from higher concentration sources. The cost of capture increases linearly (small slope) for capture rates ~85%, but the marginal cost increases exponentially if rates above >95% are desired, when considering a conventional process.
- To perform the screening of the different solvents standardized metrics, factors, KPIs, and a model was developed as part of this study. The factors and KPI’s included monetised and non-monetised parameters/variables such as cyclic absorption capacity, heat of regeneration, solvent viscosity, enhancement indexing, heat capacity, degradability, surface tension, solvent cost, absorber sizing, reboiler temperature, among others. The **top promising amines** obtained from the analysis include IPAE, AEEA, 2-MPZ, 2EAE, 2APD, MAPA, PZ/AMP, and MEA/EG (most promising water-lean solvent). The benefits are projected by the total annualised cost compared to MEA 30 wt.% and compared under a variety of operational conditions (e.g. CO_2 concentration 5-25%).
- Due to the assumptions made in the model regarding the equilibrium stage model for the absorption and the monetised variables, it is advisable to perform more detailed optimised process simulations for each of the promising amines. The more detailed models should use rigorous absorption model (provided kinetic data is available) and conducting sensitivity analysis for the variables that were kept constant at this study (e.g. capture rate and solvent cost). Performing this detailed analysis was out of the scope of this study, more focused on developing a decision tool for screening.

- A **decision tool for the screening of solvents** and **processes** for PCC has been developed. The model used in the tool includes 50+ different amine co-solvent systems and different process configurations. It allows the user to perform a techno-economic study by modifying process parameters as well as performing sensitivity analysis in terms of economic parameters such as interest rate, duration of the project, etc.

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LIST OF ABBREVIATIONS/ACRONYMS

1A2P	1-Amino-2-propanol
1-MPZ	1-methyl piperazine
2APD	2-amino-1,3-propandiol
2EAE	2-(ethylamino)ethanol
2MAE	2-(methylamino)ethanol
2-MPZ	2-methyl piperazine
3A1P	3-Amino-1-propanol
ABS	Chemical Absorption Technologies
AE	Absorption Enhancement
AEEA	Aminoethylethanolamine
AEHEIA	N-(2-aminoethyl)-N’-(2-hydroxyethyl)imidazolidin-2-one
AEP	Aminoethylpiperazine
AIC	Absorber Inter-cooling
ALA	Alanate
AMP	2-amino-2-methyl-1-propanol
APDA	N-(3-aminopropyl)1,3-propanediamine
ASAP	Amine Screening Apparatus
BAE	Bis(aminoethyl)ether
BHEAE	Bis-(2-(2-hydroxyethylamino)ethyl)ether
BHEEDA	N,N’-bis(2-hydroxyethyl)ethylenediamine
BHEI	N,N’-bis(2-hydroxyethyl)imidazolidin-2-one
BHEOX	N,N’-bis(2-hydroxyethyl)oxalamide
BHEP	N,N’-bis(2-hydroxyethyl)piperazine
BZA	Benzylamine
C	Carbon
CANSOLV	Cansolv Technologies Inc.
CAPEX	Capital expenditures
CASTOR	CO_2, from Capture to Storage (EU funded project)
CCS	Carbon Capture and Storage
CCUS	Carbon Capture, Utilisation, and Storage
CEE	Condensate Evacuation and Evaporation
CESAR	CO_2 Enhanced Separation and Recovery Project
CH	Condensate Heating
CHI	Compression Heat Integration
CO	Carbon Monoxide
CO_2	Carbon Dioxide
CO_2SOLV	Database developed in this project (IEA/CON/20/265)
CO_3^{2-}	Carbonate
COE	Cost of Electricity
CORAL	Proprietary Solvent
CSIRO	Commonwealth Scientific and Industrial Research Organisation

Cu	Copper
DAB	Butane-1,4-diamine / putrescine
DBUA	dibutylamine
DC-103	Cansolv Solvent
DC-201	Cansolv Solvent
DEA	Diethanolamine
DECAB	A Phase Change Absorption Process
DEEA	N,N-Diethylethanolamine
DETA	Diethylenetriamine
DGA	Diglycolamine
DIPA	di-isopropanolamine
DMAE	N,N-(dimethyl)ethanolamine
DMEA	N,N-dimethylethylamine
DMP	N,N’-dimethylpiperazine
DMX-1	Proprietary Solvent
DOCA	dioctylamine
DOE	Department of Energy
DPRA	dipropylamine
EAE	2 (ethylamino)ethanol
EBUA	N-ethylbutylamine
ED	Electrodialysis
EDA	Ethylenediamine
EDTA	Ethylenediaminetetraacetic acid
EFG+	Econamine FG Plus™
EG	Ethylene glycol
ENEL	Italian Company
EO	Ethylene Oxide
EOR	Enhanced Oil Recovery
EPZ	N-ethylpiperazine
Fe	Iron
FPZ	N-formylpiperazine (FPZ)
H_2CO_3	Carbonic Acid
H_2S	Hydrogen Sulfide
HAO	N-2-[bis(2-hydroxyethyl)-amino]ethyloxazolidin-2-one
HAP	N-2-[bis(2-hydroxyethyl)-amino]ethyl-N’-(2-hydroxyethyl)piperazine
HCl	Hydrochloric Acid
HCO_3^-	Bicarbonate
HEA	N-(2-hydroxyethyl)acetamide
HEAEHEP	N-(2-hydroxyethyl)-N’-(2-(2-hydroxyethylamino)ethyl)piperazine
HEAEP	N-2-[bis(2-hydroxyethyl)-amino]ethylpiperazine
HEEDA	N-(2-hydroxyethyl)ethylenediamine
HEF	N-(2-hydroxyethyl)formamide

HEHEAA	N-(2-hydroxyethyl)-2-(2-hydroxyethylamino)acetamide
HEI	N-(2-hydroxethyl)imidazole
HEIA	N-(2-hydroxyethyl)imidazolidin-2 one
HEM	N-(2-hydroxyethyl)aziridine
HEMAEHEP	N-[2-2-hydroxyethylmethylamino)ethyl]-N'-(2-ydroxyethyl)piperazine
HEMAEMP	N-[2-(2-hydroxyethylmethylamino)ethyl]-N'-methylpiperazine
HEOD	N-(2-hydroxyethyl)oxazolidin-2-one
HEP	N-(2-hydroxyethyl)piperazine
HEPO	N-(2-hydroxyethyl)piperazin-3-one
HF	Hydrofluoric Acid
HHEA	2-Hydroxy-N-(2-hydroxyethyl)acetamide
HI	Heat Integration
HMDA	Hexamethylenediamine
HMP	N-(2-hydroxyethyl)-N'-methylpiperazine
HSS(s)	Heat Stable Salt(s)
IEAGHG	IEA Greenhouse Gas R&D Programme
IFP	French Institute of Petroleum
IMTP	INTALOX® Metal Tower Packing
IPAE	2-(isopropylamino)etanol
ITCN	International Test Center Network
i-THEDT	N,N,N',N'-tetrakis(2-hydroxyethyl)diethylenetriamine
KANSAI	Kansai Electric Power Company, Inc.
KEPCO	Korea Electric Power Corporation
Kgly	Potassium Glycinate
KM CDR	Shell Process for Carbon Capture
KOP(s)	Key Operating Parameter(s)
KPI(s)	Key Performance Indicator(s)
KS	KM CDR Process Solvent
KSAR	Potassium Sarcosine
L/G	Liquid-to-Gas Ratio
LCST	Low Critical Solution Temperature
LLSP	Liquid-Liquid Phase Separation
LVC	Lean Vapour Compression
MA	Multi-Absorber
MAE	N-methylethanolamine
MAPA	3-(methylamino)propylamine
MDA	1,8-p-methanediamine
MDEA	Methyl diethanolamine
MEA	Monoethanolamine
MHI ENG	Mitsubishi Heavy Industries Engineering
MM	N-methylmorpholine
MMEA	Methyl Monoethanolamine
MOR	Morpholine

MPS	Multi-Pressure Stripping
MPZ	N-methylpiperazine
MS	Multi-Stripper or Matrix Stripping
MSDS	Material Safety Data Sheet
MSF	Multi-Stage Flash Stripping
MTHEED	N-methyl-N,N’,N’-tris(2-hydroxyethyl)ethylenediamine
N	Nitrogen
Na_2SO_3	Sodiumsulphite
NaGly	Sodium Glycinate
NaOH	Sodium Hydroxide
$NaVO_3$	Sodium Metavanadate
NCCC	National Carbon Capture Center
NFPA	National Fire Protection Association
NH_3	Ammonia
NMP	N-methyl pyrrolidone
NOx	Nitrogen Oxides
NPV	Net Present Value
NTNU	Norwegian University of Science and Technology
O	Oxygen
O&M	Operation and Maintenance
O_2	Oxygen gas
OHI	Overhead Heat Integration
OPEX	Operating expenses
OZD	Oxazolidin-2-one
PCC	Post-Combustion Capture
PE	2-piperidineethanol
PM	Particulate Matter
PSR	Proprietary Solvent
PZ	Piperazine
RICH	Research and Innovation Center on CO_2 and H_2
RVC	Rich Vapour Compression
RSF	Rich Solvent Flash
RSR	Rich Solvent Recycle
RSS	Rich Solvent Split
S/D	Separator/Decanter
SARMAPA	3-(methylamino)Propylamine Sarcosine
SE	Stripping Enhancement
SEPPL	SEParation PLant (Austria)
SF	Split Flow
SIH	Stripper Interheating
SINTEF	Norwegian Company
SO_2	Sulphur Dioxide

SOC	Stripper Overhead Compression
soft-SAFT	Soft Statistical Associating Fluid Theory
SO_x	Sulphur Oxides
TAC	Total Annualised Cost
TAU	Taurate
TBAE	2-[(1,1-dimethylethyl)amino]ethanol
TBAP	1-[(1,1-dimethylethyl)amino]-2-propanol
TCM	Test Centre Mongstad
TEA	Triethanolamine
TEHEED	N,N,N’,N’-tetrakis(2-hydroxyethyl)ethylenediamine
TEHEU	N,N,N’,N’-tetrakis(2-hydroxyethyl)urea
TETA	Triethylenetetramine
THEDT	N,N,N’,N’-tetrakis(2-hydroxyethyl)diethylenetriamine
THEED	N,N,N’-tris(2-hydroxyethyl)ethylenediamine
TMA	Trimethylamine
USC PC	Ultra Supercritical Pulverized Coal
UT	University of Texas
VLE	Vapour-Liquid Equilibrium
VOC(s)	Volatile Organic Compound(s)
vol.	volume basis
VS	Vacuum Stripping
WP	Working Package
wt.	weight basis
WWC	Wetted-Wall Column

PROJECT DEFINITION

INTRODUCTION

BACKGROUND - MOTIVATION

Any new developed technology for CO_2 capture should aim at improving the conditions of the existing ones [1,2] in terms of technical, economic and environmental performance. Of particular interest, for practical implementations, is the need to reduce the CAPEX and OPEX, also taking into account safety and environmental considerations. Absorption (i.e. solvent scrubbing) is a well-established CO_2 separation approach industrially used to produce CO_2 for different uses in the market. However, to date, only few full-scale CO_2 capture facilities from flue gas have been built, or are under construction, for carbon capture, utilisation and storage (CCUS) at large scale. The Boundary Dam project in Canada, which is operating since 2014, is the first commercial post-combustion capture plant with 1 Mtpa CO_2 capacity [3]. The captured CO_2 is used for enhanced oil recovery (EOR) in the Weyburn oil field [4]. The Petra Nova project is claimed to be the largest carbon-capture retrofit at a coal-based power plant [5]. The large-scale facility operates with 1.4 Mtpa capacity with EOR as an end use of the captured CO_2. ROAD of Netherlands and Sinopec Shengli of China are two recent large scale projects operating at 1.1 and 1 Mtpa capacity, respectively, which started operation in 2017 [3]. One of the reasons for the slow implementation of carbon capture at large scale is the cost associated with this process. Although excellent separation performance can be achieved by absorption using aqueous MEA, the respective regeneration step is capital-intensive (to a lesser extent than absorption) and requires significant utility consumption during operation, especially in the regenerator column [6,7]. In addition, there are problems associated with the degradation and evaporation of the solvent. These limitations are magnified at the required CCUS large scale, which spans from 0.1 to 1.4 Mtpa for post-combustion capture plants [3]. The problem is more challenging when considering that the world's fossil-based CO_2 emissions reached an average of 9.4 ± 0.5 $GtC.yr^{-1}$ during 2010–2019 [8].

Because of the limitations associated with the classical aqueous amines solvents just mentioned, new chemical absorption solvents and process designs continue to be developed [9], with many vendors and patents claiming better performance than the established process with aqueous MEA. However, the evaluation of the solvent performance is usually limited to overall characteristics such as the net power for regeneration and cost per tonne of CO_2 captured or avoided. In addition, most measurements are performed far away from the process requirements in which they will ultimately be used; i. e., limited thermophysical properties, with non-standard measurements, are provided in some cases; the effect of the impurities is not evaluated, and even the conditions at which the data are presented are not the ones at which the capture/separation industrial process will take place. Moreover, while packed column absorbers may be optimal for aqueous solvents, the same may not be the case for water-lean solvents due to changes in physical properties along the column. Emerging modifications of the process design (as seen in IEAGHG 2013/TR5 [10]) significantly impact the overall process performance, which also affects the evaluation of novel solvents. In order to evaluate the emerging solvents and processes some testing facilities around the globe have been established, such as the Technology Centre of Mongstad (TCM), the International Test

Center Network (ITCN), the National Carbon Capture Center (NCCC), and Boundary Dam, among others, where research on the scalability of the absorption process is taking place.

Given the vast amount of published research in this area [11], a rapid and reliable procedure to screen new solvents for CO_2 capture and rank them against processes currently in use is needed. The solvents should meet the desirable characteristics for an absorbent to separate CO_2 from a stream: (i) a high selectivity and good adsorption capacity for the target gas component, (ii) fast absorption and desorption kinetics, (iii) good physical and chemical stability through the absorption/desorption cycles, and (iv) be regenerable by modest pressure or temperatures, to minimize operational energy costs. The absorbent must also show robust performance in the presence of contaminants in the gas feed to the separation treating unit. The cost of the solvent and the equipment and the environmental impact are further considerations to be taken into account.

New post-combustion capture (PCC) solvents and advanced processes were identified in the IEAGHG report 2014/TR4 [12] as main technologies to decrease the cost of CO_2 capture. Later, in the IEAGHG technical study 2019/09 [13], the new benchmark solution was announced. The parameter to select the new whole system was the reduction on the heat of absorption and the overall associated energy consumption. The enhancement of the new system compared to the previous benchmark solution (30% wt. MEA) was calculated through the cost of CO_2 captured and net power plant efficiency. The performance was analysed through modelling at thermodynamic and process scales, while the techno-economic analysis was done under the IEAGHG economic framework[1]. That new system is based on a 40 wt.% PZ (piperazine) + AMP (2-amino-2-methyl-1-propanol) solution (1:2 M ratio), combined with an advanced process configuration, including intercooling and rich-split arrangements. The PZ/AMP blend was tested as part of the CESAR project [14]. The selection of the solvent aimed to reproduce the current state of the art of commercial solvents and campaigns at large scale, with enhanced performance compared to the traditional MEA solution. The main objective of the IEAGHG technical study 2019/09 [13] was to reproduce the performance of commercial solvents based on the heat of absorption. However, other parameters were not taken into account. Operational and environmentally desirable properties, such as lower degradation, less volatility, being non-corrosive or non-toxic, more environmentally-friendly, exhibiting low viscosity, fast kinetic rate, or being non-foaming have also been presented as relevant factors. Additionally, the impact of those parameters on the cost of the CO_2 capture system (CAPEX and OPEX) is of high importance. Although the standard ISO 27919-1:2018 [15] covers PCC performance evaluation as a whole – "Performance evaluation methods for post-combustion CO_2 capture integrated with a power plant", it only touches upon solvent performance in a limited fashion via 'absorbent and chemical consumption'. Moreover, given the high CAPEX and OPEX associated with capturing CO_2, some studies are focusing on the design, integration of utilities and selection of key operating parameters (KOPs), using key performance indicators (KPIs), thus allowing to mitigate significant capital expenditure and energy demands associated with CO_2 capture plants [7].

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[1] The IEAGHG economic framework is the techno-economic and financial parameters common to all the IEAGHG techno-economic assessments.

Research and development on the optimal performance of new and existing technologies on the final CO_2 sources is needed before the deployment of several industrial projects becomes a reality. Hence, the aim of this study was to analyse in detail solvents, configurations, and their separate enhancement on the CO_2 capture process in order to identify the prime candidates for the next generation of PCC plants and compare those to the traditional 30 wt.% MEA aqueous solution and the recent new IEAGHG benchmark system under a standardized framework.

STUDY OBJECTIVES

The objectives of this study were: (i) to summarize emerging solvents and process configurations promising to enhance the CO_2 capture performance; (ii) to develop a number of metrics to measure the solvents performance and their impact on capture costs; and (iii) to develop a decision-matrix-tool to choose the best solvent for a PCC plant.

For this purpose, the defined specific objectives were:

1. Perform a detailed literature survey comparing the different emerging solvents and processes for CO_2 capture. The literature survey should explicitly include available information on large installations testing solvents (at large, pilot and lab scale) for PCC, in addition to scientific publications and patents.
2. Develop a number of metrics to assess the solvents performance and their impact on capture cost (CAPEX and OPEX).
3. Develop a modelling tool to allow the comparison of the different solvents and processes based on defined metrics or Key Performance Indicators (KPI). This includes the development of a detailed dynamic database, comparing the different alternative solvents for CO_2 capture at the same process operating conditions.
4. Assess promising aqueous and water-lean PCC solvents, providing an analysis of their enhancement and their potential under standardized metrics.
5. Quantify the technical and economic performance of the most promising selected solvents for PCC with the database and the developed modelling tool using as benchmark the available technologies (amine scrubbing). Use the proprietary soft-SAFT code for generating missing thermophysical data [16–20], and soft-SAFT combined with gPROMS or another process simulator for generating the process conditions when needed.
6. Based on the results from 1 to 5, develop a decision matrix tool and implement a software platform to integrate the materials screening of chemical (and/or physical) solvents for CO_2 capture, solvent characterization, process modelling and dynamic process integration (including the associated CAPEX and OPEX of the unit operations).

SCOPE

This study assesses promising aqueous and water-lean PCC solvents, providing an analysis of their enhancement and their potential under standardized metrics.

RESULTS

1. REVIEW OF EMERGING AQUEOUS AND WATER-LEAN PCC SOLVENTS (TASK1)

Objective: This task involves a detailed literature survey on the most relevant PCC solvents tested at industry- and lab-scale (including patents, publications, reports, etc.). The collected information is used for the development of a database (excel based), inclusive of:

1. Solvent type, components, and composition.
2. Testing scale (industrial vs. lab-scale), conditions and application (source of flue gas).
3. Enhancement showed by the use of this solvent.

1.1 SOLVENTS FOR POST-COMBUSTION CO_2 CAPTURE

The mitigation of the adverse effects of increased CO_2 emissions and global warming phenomena led to widespread developments on scientific, technological, and policy making levels. Among them, Carbon Capture, Utilisation, and Storage (CCUS) remains one of the most viable solutions to these global issues in the short- and medium-terms. CCUS relies on capturing CO_2 from large flue gas emitting facilities, and conditioning it, either for its utilisation in industrial application or for its storage in geological formations [21,22].

The carbon capture element is integral element to the CCUS chain and requires the availability of an efficient and economically viable CO_2 capture technology [23,24]. A variety of technologies have been explored over the past decades [25–28], yet, the separation of CO_2 through its chemical absorption using aqueous alkanolamine still remains the most mature solution nowadays at large scale. The advantage of chemical solvents for CO_2 capture, particularly monoethanolamine (MEA), relies on being an “end-of-pipe” technology already implemented for purification and separation in other industrial applications, that can be successfully applied to other areas such as carbon capture [27,28]. An additional advantage is that these processes can be integrated with power generation facilities without additional retrofitting, and in the case of capture process shutdown, the operation of the power generation facility will not be compromised. [27,28]. However, the process still suffers from various operational issues such as high solvent regeneration energy, solvent instability, and corrosion [23,26–28]. These drawbacks are directly linked to their thermophysical properties such as high CO_2 absorption enthalpy, low thermal and chemical stability, high vapour pressure, and corrosive nature, which can be mitigated with the addition of additives that can add to the operating costs of the process. However, the search for a solvent with attractive properties spurred significant progress over the past decades towards the synthesis and application of emerging solvents for PCC, which are reviewed in this section [29].

1.1.1. AQUEOUS AMINE SOLVENTS

As previously highlighted, chemical absorption of CO_2 using aqueous amines has been used in industry since the 1950s [30], primarily for gas-treating facilities, making it the most technologically developed CO_2 removal process.

The absorption of CO_2 in these amines within the context of PCC is typically performed at temperatures below 333 K and atmospheric pressure leading to the formation of weakly-bonded reaction products (carbamate and bicarbonate), while the reversal of the absorption (solvent regeneration) can be accomplished through heating the solution at temperatures generally higher than 373 K in a stripping column. Conventional alkanolamines for CO_2 capture are typically classified based on their molecular structure, having at least one hydroxyl group (-OH), and a varying degree of substitution on the central nitrogen, with single (-NH_2), double (-NH), and triple (-N) substitutions denoting, primary, secondary, and tertiary amines, respectively [25,31–33]. The presence of the hydroxyl group is responsible for the reduction in solvent vapour pressure and increased solvent solubility in water, while the amine group is responsible for providing the required alkalinity of the aqueous solution to promote the chemisorption of CO_2. The molecular structure of the alkanolamine dictates the solvent's CO_2 removal capabilities and reaction mechanism.

The overall reactions for the absorption of CO_2 can proceed by the formation of two primary reaction products (i.e. carbamate (**Reaction 2.1**) and bicarbonate (**Reaction 2.2**)). Carbamate formation is more favourable for primary and secondary amines such as MEA and diethanol-amine (DEA), respectively [34,35]. In contrast, the absorption of CO_2 proceeds through the formation of bicarbonate for some sterically hindered and tertiary amines such as 2-amino-2-methyl-1-propanol (AMP) and methyl-diethanol-amine (MDEA), respectively [36].

$$CO_2 + 2R_1R_2HN \leftrightarrow R_1R_2NH_2{}^+ + R_1R_2NCOO^- \tag{1.1}$$

$$CO_2 + R_1R_2R_3N + B \leftrightarrow R_1R_2R_3NH^+ + HCO_3{}^- \tag{1.2}$$

where, $R_1R_2R_3N$ represents amine and, depending on the type of amine, R_1, R_2, R_3 can be hydrocarbon groups or mobile protons, and B is any base existing in the solution such as amines, water or any other physical solvents.

MEA and diglycolamine (DGA) are among the most commonly employed primary alkanolamines. These solvents provide high chemical reactivity, faster kinetics, and medium to low absorption capacity, with acceptable levels of solvent stability depending on the process operating conditions. The promising aspect about utilization of alkanolamines is their long-standing operation mainly in natural gas sweetening applications. As such, chemical absorption technology is endowed with sufficient technical knowledge and experience garnered over more than 50 years of operation, for a successful transition and application as a carbon capture technology. However, their large-scale deployment for post-combustion CO_2 capture is still marred mainly by: (1) the cost intensive solvent regeneration energy requirements, (2) degradability, either at the high temperature regeneration conditions or in the presence of oxygenated compounds commonly found in flue gases, (3) solvent losses due to high solvent volatility, and (4) high corrosivity jeopardizing the structural integrity of processing facilities [23,26–28].

Secondary alkanolamines such as DEA and diisopropanolamine (DIPA), possess intermediate properties to primary amines and are being considered as an alternative to MEA. For example, DEA is more resistant to solvent degradation along with lower corrosion rates compared to

MEA, while DIPA has relatively lower energy of regeneration compared to MEA. Lastly, tertiary alkanolamines such as MDEA and triethanolamine (TEA), possess low absorption capacity and low reactivity, but high stability. The high reactivity of primary and secondary amines compared to tertiary amines is due to the formation of carbamate when the former react with CO_2 (**Reaction 2.1**). Alternatively, tertiary amines can only form a bicarbonate ion and protonated amine by the base-catalysed hydration of CO_2 (**Reaction 2.2)** due to their lack of the necessary N─H bond, which is slower than the direct reaction by carbamate formation and, hence, tertiary amines show low CO_2 absorption rates [13].

Novel alkanolamines have been developed to improve the enthalpy of absorption compared to conventional primary and secondary amines. These novel sterically hindered alkanolamines are formed from a primary or a secondary amine, in which the amine group is attached to a tertiary carbon atom, such as 2-piperidineethanol (PE), 1,8-p-methanediamine (MDA), and 2-amino-2-methyl-1-propanol (AMP) [25,31–33,37–40]. The chemisorption of CO_2 with these alkanolamines can proceed via either the formation of carbamate or bicarbonate (depending on the type structure of the alkanolamines); however, in the case of carbamate formation, their stability is intermediate to low, due to the steric hindrance. In this manner, high concentrations of free amines in the solution are present leading to a reduction in the energy consumption required for solvent regeneration, as compared to primary and secondary alkanolamines, up to 15% of total regeneration energy. Another advantage of sterically hindered alkanolamines, is that the carbamate formation for primary and secondary alkanolamines requires two amine molecules to capture one CO_2 molecule, while sterically hindered amines require only one amine molecule to capture one CO_2 molecule, hence, the maximum CO_2 absorption capacity of these alkanolamines is higher than those for conventional primary and secondary alkanolamines. However, this might be on the expense of reduced reaction kinetics, which has direct implications on the CAPEX of the absorption process.

Conversely, polyamines/multiamines (with multiple amine groups) have also demonstrated potential for CO_2 capture, wherein the presence of two amine groups can help accelerating the absorption rate and increase the absorption capacity of the solvent due to the presence of multiple amine groups within the structure [41].

Other novel amines recently developed include the secondary cyclic amine piperazine (PZ), with its attractive properties including fast kinetics, good thermal and chemical stability, lower volatility compared to MEA [42,43], which has been heavily tested using lab-scale and pilot-scale to fully examine its potential as a new benchmark solvent for PCC.

A wide number of works examined the performance of different amine structures (cyclic, polyamines, linear, *etc.*) for CO_2 capture. In a series of contributions, Singh *et al.* [44–46] conducted extensive screening tests to determine the relationship between the amine structure and its CO_2 absorption activity in terms of capacity and rate, examining different structural effects. It was established that increasing the chain length of the amine and different functional groups in the molecular structure increased the absorption capacity of the solvent on the expense of reduced absorption rate. Additionally, sterically hindered, and aromatic amines with side alkyl groups have increased capacity and absorption rate. Chowdhury *et al.* [47] also examined the effect of steric hindrance on secondary and tertiary amines, demonstrating the potentiality of some of the developed amines over conventional amines in terms of increased absorption capacity, and reduced enthalpy of absorption. In another contribution, Chowdhury *et al.* [48], developed a wide range of tertiary amines, with the goal of enhancing their absorption rates while preserving their low enthalpy and high absorption capacities. The study demonstrated the potentiality of some of the synthesized amines. Puxty *et al*. [30] conducted rapid screening tests on 76 different amines for their potentiality for CO_2 capture, determining that four primary amines, and two secondary amines had higher absorption capacities, and similar absorption rates to that of MEA. Similarly, El Hadri *et al*. [49] evaluated the performance of 30 aqueous amines, determining that a few tertiary amines and one secondary amine had the potential for CO_2 capture. A wide collection of works focused on the synthesis of new amines or the screening of a wide selection of amines to determine the ones with potential application in CO_2 capture [40,41,50–60].

Notwithstanding, it remains challenging to find a single solvent encompassing all attractive solvent requirement for PCC, such as fast kinetics, high CO_2 absorption, low enthalpy of absorption, etc. As such, taking advantage of the different properties of available single amine solvents, the formation of blends can be advantageous.

1.1.2 SOLVENT BLENDS

Another solvent formulation exploiting the advantages of some of the previously mentioned solvents is based on the formulation of blended aqueous alkanolamines, of at least two alkanolamines. For example, taking advantage of the higher stability and low regeneration energy for tertiary amines (MDEA and TEA), can be blended with primary and secondary aqueous amines, forming a solvent blend with enhanced overall characteristics such as low regeneration requirement and increased resistance to degradation [61–65]. Alternatively, solvents with faster reaction kinetics such as piperazine (PZ), and MEA can be added in small quantities as promoters to aqueous solutions with slow kinetic solvents such as TEA, and MDEA. The main advantages of blend formulations include: (1) improved thermodynamic absorption capacity, (2) enhanced solvent thermal and chemical stability, (3) flexibility in solvent operation as the composition can be optimised depending on the required absorption conditions, and (4) reduction in regeneration energy requirements.

1.1.3 NEW GENERATION PCC SOLVENTS

1.1.3.1 WATER-FREE/ WATER-LEAN SOLVENTS

The most integral hurdle towards the large-scale deployment of aqueous alkanolamines for PCC, is related to their solvent regeneration high energy consumption. This energy requirement adds a load on power-generation facilities to burn more fossil fuels, resulting in more CO_2 emissions to compensate for the energy consumed for solvent regeneration, in addition to dropping overall efficiency of these facilities by approximately 30% [23,28]. The regeneration energy (reboiler, stripper) for a conventional 30 wt.% MEA aqueous solution is 60-65% of the total energy consumption of a CO_2 capture plant [11–13,21–23]. A number of new generation solvents have been developed over the past decades focusing on making CO_2 chemical absorption a cost competitive technology through lowering the associated solvent regeneration energy.

The presence of water as a co-solvent in large quantities for single and blended aqueous alkanolamines is responsible for the large solvent regeneration energy, as water possesses a high heat capacity and enthalpy of vaporisation relative to other physical co-solvents [66]. The heat duty required to regenerate a conventional 30 wt.% MEA aqueous solution is approximately 180.3 kJ.mol^{-1} of captured CO_2, with 87.9 kJ required to desorb 1 mole of CO_2 absorbed into aqueous MEA, and an additional 92.4 kJ required to heat the solution and produce 2.1 mole of H_2O steam to remove 1 mole of CO_2 from the aqueous MEA solution [25,28]. Hence, more than 50% of the total heat duty required for solvent regeneration is directed at water heating and vaporization, due to its large amount in the solution and high thermal properties.

An alternative option to reduce this energy load is through the partial or full replacement of water as a co-solvent, with other physical solvents with lower heat capacities and enthalpy of vaporization relative to water, forming hybrid chemical-physical solvents such as water-lean and non-aqueous amine solutions. Physical solvents candidates for this application are 1-alkanols [67], glycols [27,31,32], glymes [33,68], ionic liquids [36,69], and other polar solvents [37,38]. In these hybrid solvents, most of the regeneration energy will be required to reverse the chemical reaction (heat of absorption) and release the absorbed CO_2 rather than that needed to heat and evaporate the co-solvent [70]. For example, Yu et al. [71] reported that regeneration of a non-aqueous MEA + methanol solution can be achieved at a temperature lower than 373 K, resulting in a regeneration energy of 110 kJ. mol_{CO2}^{-1} (2.5 GJ. t_{CO2}^{-1}) which is lower than that needed for aqueous MEA in the range of 146 – 218 kJ. mol_{CO2}^{-1} (3.3 – 4.9 GJ. t_{CO2}^{-1}), marking a 24 – 49% reduction in the consumed regeneration energy. Rivas and Prausnitz [70] demonstrated that a mixed solvent of MEA + N-methyl pyrrolidone (NMP) has a lower absorption capacity compared to aqueous MEA; however, it can be regenerated far easier than aqueous MEA at lower temperatures. The implications of lower regeneration temperatures for non-aqueous amines reflects itself in requiring substantially less steam for solvent regeneration and smaller number of trays in the stripping column, significantly enhancing the techno-economic viability of the process [70]. The main advantage of employing water-free/water-lean solvents is exhibited by the significant reduction in reboiler duty (almost 50%) and lower regeneration temperatures, due to the lower thermal properties of organic dilutants compared to water. However, this is on the expense of other trade-offs, such as, lower CO_2 absorption capacity, increased solvent viscosity, and slower reaction kinetics [72]. Another aspect to consider is that the lower vapour pressure of organic solvents compared to water, might require a modification in the stripper configuration to ensure efficient solvent regeneration.

Several works in the literature reported the formulation of novel water-free amine solutions. For example, the combination of two sterically hindered amines 2-[(1,1-dimethylethyl)amino]ethanol (TBAE) and 1-[(1,1-dimethylethyl)amino]-2-propanol (TBAP) were developed in references [38,61–65]. These amines reversibly bind CO_2 by nucleophilic attack of the electrophilic carbon in which the alcohol forms an ammonium alkylcarbonate zwitterion, which can be regenerated at lower temperature than aqueous MEA and DEA. The addition of a co-solvent such as methanol or ethylene glycol was needed as the zwitterionic carbonate formed in this reaction is a solid. Another non-aqueous solvent system under development [73,74] comprises AMP blended with other alkanolamines such as DEA, MDEA, MMEA, and DIPA, in organic co-solvents such as ethylene glycol, 1,2-propanediol, methanol, or ethanol, demonstrating 73−96% CO_2 absorption efficiency at equilibrium. A single amine system consisting of sterically hindered secondary amines like dipropylamine (DPRA), N-ethylbutylamine (EBUA), dibutylamine (DBUA), and dioctylamine (DOCA) has also been reported in the literature, showing promise in this class of solvents. The CO_2 binding mode for these amines is the conventional carbamate mechanism; however, significant amounts of zwitterionic carbonate species can form, resulting in a loading capacity greater than 50 mol %. Nevertheless, the challenges associated with these systems is their high viscosity for CO_2 rich solvents along with the possibility of precipitation and formation of solid carbamate, hence the need for modifications in the process.

Another type of water-free solvents for CO_2 capture are aminosilicones. The potentiality of these solvents are mainly due to the absence of water from their formulation, along with the hybrid nature of these solvents, allowing both physical and chemical absorption of CO_2. Of these solvents, GAP-0 and GAP-1 aminosilicones were developed with a CO_2-philic siloxane backbone and a CO_2 reactive amino group [75]. The absorption capacity of these compounds is higher than the theoretical of the selected amino group due to the physisorption phenomenon that occurs in this type of blends. However, the possibility of solid formation and the increase of viscosity during the absorption process making it necessary to use co-solvents in order to avoid the above-mentioned issues.

1.1.3.2 BIPHASIC SOLVENTS

In the last decades, it has been assumed that biphasic mixes generation during CO_2 amine-based capture processes becomes an operational issue in terms of liquid circulation and homogeneity of the solvents, especially in the regeneration step. However, recent studies support the new idea that a decrease in the energy requirements using biphasic solvents would be possible [34,35,76–78]. This argument is based on the optimization of the solvent volume treated in regeneration step, stripping only the CO_2-rich phase.

In recent years, polyamine compounds and blends have been studied in order to improve the CO_2 absorption capacity in CCUS technologies. A higher amount of amine functional groups, using water as a dissolvent, provides the polyamines higher absorption rates, but in spite of that fact, regeneration penalties and solvent circulation costs due to the high viscosity of this kind of compounds made unfeasible its application in pilot plants. Triethylenetetramine (TETA) using ethanol as dissolvent was tested by Zheng *et al.* [79]. In their work, solid generation occurred after the CO_2 reaction with TETA. Solid phase generated and separated, containing a total of 81.8% of the captured CO_2, allowed a lower cost regeneration process due to the fact that liquid phase can be recycled back to the absorption process without energy consumption. The precipitate formed after CO_2 absorption can be regenerated by heating to 363 K and returns to liquid phase TETA. This new solvent represents an alternative to the usual polyamine-water solvents although the high vapour pressure of ethanol must be considered in order to minimize evaporation losses. Other solvents exhibiting precipitation recently tested include water-free amines, and amino acids [72,80,81]. Karlsson *et al.* [33] examined the onset of precipitation form water-free solvents formed from AMP blended with a range of physical co-solvents, establishing that AMP + NMP water-free solvent has the potential to reduce reboiler duty. Moioli *et al.* [82] through process simulations and comparison with available commercial solvents demonstrated the potential for potassium taurate amino acid for CO_2 capture mainly due to the lower reboiler duty.

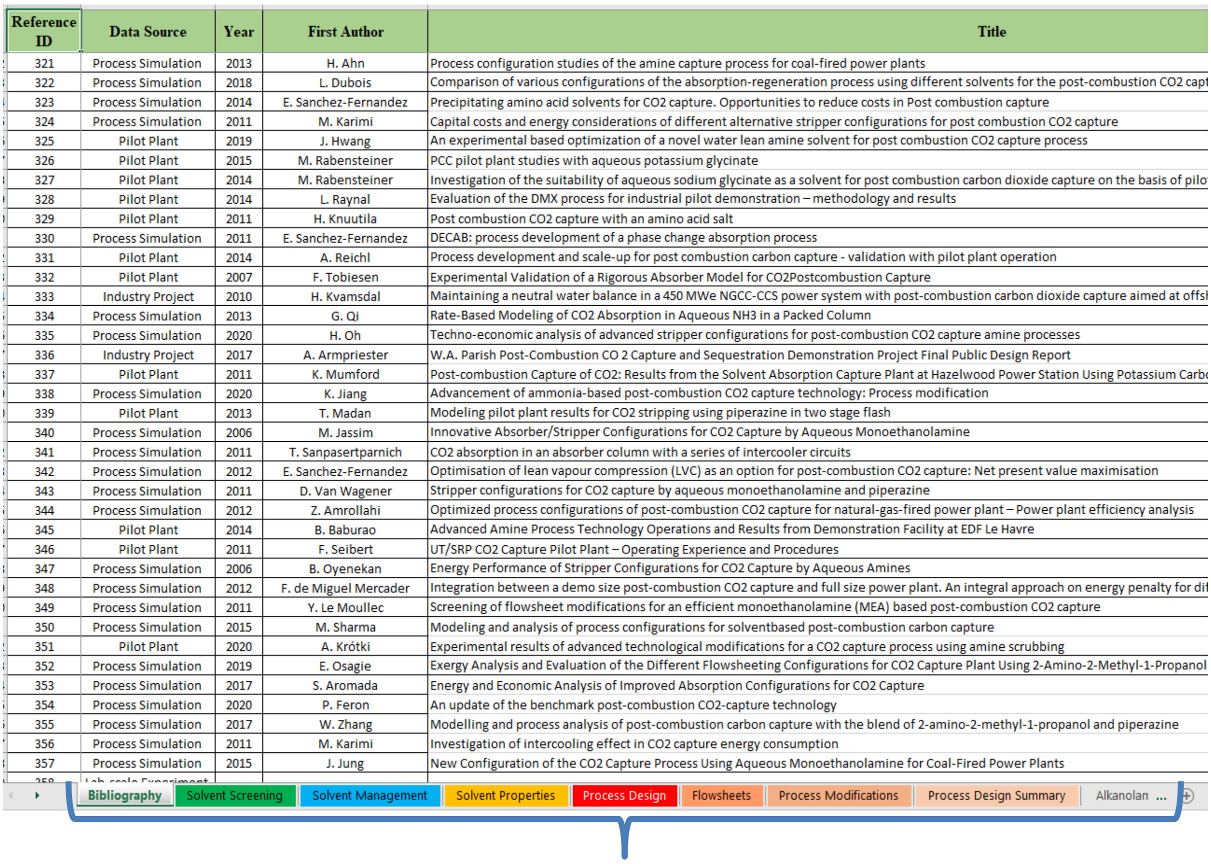
Recent studies showed that some types of blended amines have the property of forming two different liquid phases after reaction with CO_2 in the capture process such as 3-(methylamino)propylamine (MAPA) and 2-(diethylamino) ethanol (DEEA) blend [83]. This singularity of the solvent provides the possibility of performing a selective regeneration process, being only the rich amine treated inside the regeneration reboiler.

Lipophilic-amine-based thermomorphic biphasic solvents have shown potential advantages in CO_2 capture compared to conventional alkanolamines in terms of solvent regeneration and cyclic capacity. The improvements obtained using these types of solvent are based on their thermomorphic behaviour. This phenomenon consists of the generation of two liquid phases after heating inside the reboiler. According to Zhang *et al.* [78], these systems can be regenerated at lower temperatures than the conventional alkanolamine blends. This temperature reduction in the regeneration step allows a decrease of the energetic consumption in CO_2 capture processes.

1.2 THE CO₂SOLV DATABASE

A comprehensive analysis and comparison of available solvents for PCC requires the full characterization of thermophysical and transport properties of solvents, along with other considerations such as those related to operational problems (solvent degradation, corrosion, and losses) and environmental impact (secondary emissions). For this end, a solvent database has been developed in this project, named **CO_2SOLV *database***, housing a collection of available information on the plethora of solvents reported in recent years for PCC. The purpose of the database is to allow ease of accessibility to reported information on solvent properties and performance for CO_2 capture. Additionally, with this information, solvents can be compared under the same operating conditions and selection criteria to determine the most promising ones. As a way of keeping it flexible and user-friendly, an EXCEL front-end structure was used. The choice was due to the relative ease in which the database can be modified to cope with the information of new types of processes and materials as they are developed or made available in literature. Furthermore, it can also be used to generate reports and queries on the available information.

The solvents database was populated manually, through collecting references from the different sources (journal publications, patents, conferences, company reports, etc.), included in the “Bibliography Tab”. The information is categorized and collected in the different tabs for an easy identification and subsequent utilisation (see **Figure 1.1**).



Reference ID	Data Source	Year	First Author	Title
321	Process Simulation	2013	H. Ahn	Process configuration studies of the amine capture process for coal-fired power plants
322	Process Simulation	2018	L. Dubois	Comparison of various configurations of the absorption-regeneration process using different solvents for the post-combustion CO2 capt
323	Process Simulation	2014	E. Sanchez-Fernandez	Precipitating amino acid solvents for CO2 capture. Opportunities to reduce costs in Post combustion capture
324	Process Simulation	2011	M. Karimi	Capital costs and energy considerations of different alternative stripper configurations for post combustion CO2 capture
325	Pilot Plant	2019	J. Hwang	An experimental based optimization of a novel water lean amine solvent for post combustion CO2 capture process
326	Pilot Plant	2015	M. Rabensteiner	PCC pilot plant studies with aqueous potassium glycinate
327	Pilot Plant	2014	M. Rabensteiner	Investigation of the suitability of aqueous sodium glycinate as a solvent for post combustion carbon dioxide capture on the basis of pilo
328	Pilot Plant	2014	L. Raynal	Evaluation of the DMX process for industrial pilot demonstration – methodology and results
329	Pilot Plant	2011	H. Knuutila	Post combustion CO2 capture with an amino acid salt
330	Process Simulation	2011	E. Sanchez-Fernandez	DECAB: process development of a phase change absorption process
331	Pilot Plant	2014	A. Reichl	Process development and scale-up for post combustion carbon capture - validation with pilot plant operation
332	Pilot Plant	2007	F. Tobiesen	Experimental Validation of a Rigorous Absorber Model for CO2Postcombustion Capture
333	Industry Project	2010	H. Kvamsdal	Maintaining a neutral water balance in a 450 MWe NGCC-CCS power system with post-combustion carbon dioxide capture aimed at offs
334	Process Simulation	2013	G. Qi	Rate-Based Modeling of CO2 Absorption in Aqueous NH3 in a Packed Column
335	Process Simulation	2020	H. Oh	Techno-economic analysis of advanced stripper configurations for post-combustion CO2 capture amine processes
336	Industry Project	2017	A. Armpriester	W.A. Parish Post-Combustion CO 2 Capture and Sequestration Demonstration Project Final Public Design Report
337	Pilot Plant	2011	K. Mumford	Post-combustion Capture of CO2: Results from the Solvent Absorption Capture Plant at Hazelwood Power Station Using Potassium Carb
338	Process Simulation	2020	K. Jiang	Advancement of ammonia-based post-combustion CO2 capture technology: Process modification
339	Pilot Plant	2013	T. Madan	Modeling pilot plant results for CO2 stripping using piperazine in two stage flash
340	Process Simulation	2006	M. Jassim	Innovative Absorber/Stripper Configurations for CO2 Capture by Aqueous Monoethanolamine
341	Process Simulation	2011	T. Sanpasertparnich	CO2 absorption in an absorber column with a series of intercooler circuits
342	Process Simulation	2012	E. Sanchez-Fernandez	Optimisation of lean vapour compression (LVC) as an option for post-combustion CO2 capture: Net present value maximisation
343	Process Simulation	2011	D. Van Wagener	Stripper configurations for CO2 capture by aqueous monoethanolamine and piperazine
344	Process Simulation	2012	Z. Amrollahi	Optimized process configurations of post-combustion CO2 capture for natural-gas-fired power plant – Power plant efficiency analysis
345	Pilot Plant	2014	B. Baburao	Advanced Amine Process Technology Operations and Results from Demonstration Facility at EDF Le Havre
346	Pilot Plant	2011	F. Seibert	UT/SRP CO2 Capture Pilot Plant – Operating Experience and Procedures
347	Process Simulation	2006	B. Oyenekan	Energy Performance of Stripper Configurations for CO2 Capture by Aqueous Amines
348	Process Simulation	2012	F. de Miguel Mercader	Integration between a demo size post-combustion CO2 capture and full size power plant. An integral approach on energy penalty for di
349	Process Simulation	2011	Y. Le Moullec	Screening of flowsheet modifications for an efficient monoethanolamine (MEA) based post-combustion CO2 capture
350	Process Simulation	2015	M. Sharma	Modeling and analysis of process configurations for solventbased post-combustion carbon capture
351	Pilot Plant	2020	A. Krótki	Experimental results of advanced technological modifications for a CO2 capture process using amine scrubbing
352	Process Simulation	2019	E. Osagie	Exergy Analysis and Evaluation of the Different Flowsheeting Configurations for CO2 Capture Plant Using 2-Amino-2-Methyl-1-Propanol
353	Process Simulation	2017	S. Aromada	Energy and Economic Analysis of Improved Absorption Configurations for CO2 Capture
354	Process Simulation	2020	P. Feron	An update of the benchmark post-combustion CO2-capture technology
355	Process Simulation	2017	W. Zhang	Modelling and process analysis of post-combustion carbon capture with the blend of 2-amino-2-methyl-1-propanol and piperazine
356	Process Simulation	2011	M. Karimi	Investigation of intercooling effect in CO2 capture energy consumption
357	Process Simulation	2015	J. Jung	New Configuration of the CO2 Capture Process Using Aqueous Monoethanolamine for Coal-Fired Power Plants

Figure 1.1 A screenshot showing the structure of the **CO_2SOLV** *database using EXCEL.*

As shown at **Figure 1.1**, the CO_2SOLV database has 6 main tabs:

1. Bibliography: containing details on references included in the database. It gives flexibility of choosing the type of data (Lab-scale experiments, pilot plant, industry project, process simulation, or molecular simulation).
2. Solvent screening: containing information on screening tests conducted to assess performance of solvents mainly at a single condition (i.e. temperature, and CO_2 partial pressure). The information included in this tab is mainly on rich CO_2 loading at 313 K, cyclic capacity (assessed at different lean conditions), and heat of absorption.
3. Solvent management: containing information on the degradation and corrosion of examined solvents.
4. Solvent properties: containing references with available data on thermophysical and transport properties of PCC solvents at both rich and lean conditions. The actual data for each solvent is also tabulated in the database. This tab gives a quick summary of which type of data are available for a particular solvent along with the source of information.
5. Pilot-scale solvent testing: containing information on the conditions, type of solvents, and capacities of different campaigns.
6. Process design: containing information on available process configurations, conditions and performance for post combustion CO_2 capture. The data is mainly collected from

process simulation results in journal publications, pilot plant data, and a few industrial-scale plants from open access sources.

Moreover, the database includes additional tabs:

1. Flowsheets: containing screenshots of the process configurations and modifications related to the sources in the “Process Design” tab.
2. Process Modifications: containing a collation of data reflecting the different process modifications observed in the studies along with the associated key performance indicator(s).
3. Process Design Summary: containing the visualization of the “Process Modifications” tab using pivot table and chart. It also contains a rough estimation of the columns dimensions based on the reported values in the “Process Design” tab.
4. Alkanolamine list tab: containing a general list of alkanolamines and other details such as acronym, name, chemical formula, type, molecular weight, and CAS number.
5. Co-solvent list tab: containing a general list of co-solvents and other details such as acronym, name, chemical formula, type, molecular weight, and CAS number.
6. Solvent (xx) tab(s): containing all the data collected on rich and lean thermophysical and transport properties, and absorption isotherms, and kinetic data for each solvent included in the “Solvent Properties” tab.

Representative screenshots of these tabs are included in **ANNEX I** (Figure A1-Figure A4), while the list of solvents with detailed thermophysical and transport properties collected in the database are included in **ANNEX II**. The full **CO_2SOLV** database has been delivered to IEAGHG as one of the outcomes of this project.

Two tabs are of particular interest for solvent performance and properties, which are **“Solvent Screening”** and **“Solvent Properties”** tabs.

The **“Solvent Screening”** tab (see **Figure A1 in ANNEX I**), was populated with single measurements performed at single condition (T, P_{CO2}) for limited properties including rich solvent loading, cyclic capacity, and heat of absorption. These measurements are typically used for high-throughput solvent screening. This tab was populated with **842 entries** for a variety of solvents including traditional aqueous amines, novel aqueous amines, blended amines, water-free amines, and water-lean amines. The percentage distribution of type of solvents populated in this tab is shown in **Figure 1.2**, with the majority of the screening results focused on single aqueous amine solutions.

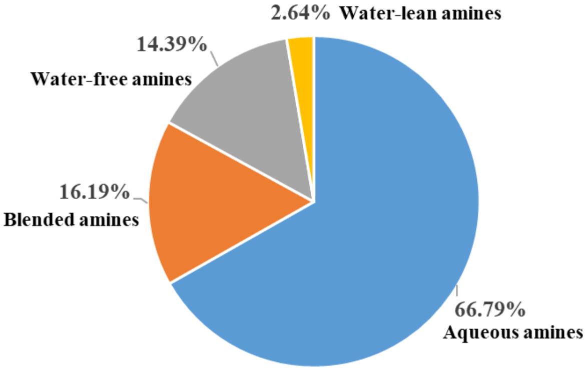


***Figure 1.2** Distribution of types of solvents (from 842 entries) included in the Solvent Screening Tab in the CO_2SOLV Database.*

However, the full reliance on this limited information for solvent selection can be misleading. A detailed account for the various trade-offs associated with these solvents requires a more comprehensive examination for various thermophysical and transport properties at rich and lean conditions. As such, the **"Solvent Properties"** tab hosts a detailed collection of available thermophysical and transport properties (at lean and rich conditions) for **100+ solvents** of different types (see **Figure A2 in ANNEX I**). The actual experimental data were also included in the ***CO_2SOLV database*** for further reference. With this tab, a quick summary is available for the type of data and solvents available in the database (see in **ANNEX II** the list of solvents with detailed thermophysical and transport properties collected in CO_2SOLV). The percentage distribution of type of solvents populated in this tab is shown in **Figure 1.3**, being the majority of the detailed properties those related to water-free amines and single aqueous amine solutions.

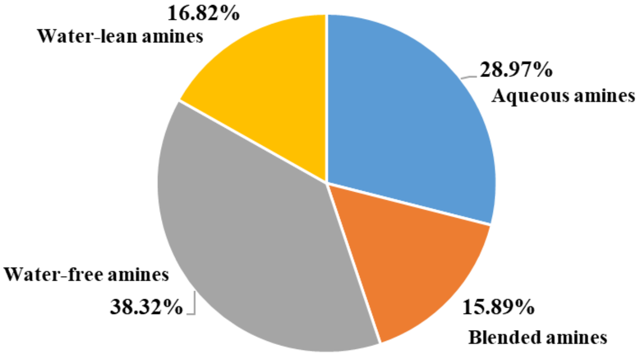


Figure 1.3 *Distribution of types of solvents (from 107 entries) included in the Solvent Properties Tab in CO_2SOLV Database.*

The "**Process Design"** tab, shown in **Figure A3** in **ANNEX I**, summarizes the findings of process simulations, pilot plants, and few industrial-scale demonstrations pertaining to process configurations and modifications to the conventional MEA process. This tab contains the reported process conditions including descriptions of the absorber and stripper conditions.

1.3 EXAMPLE OF APPLICATIONS OF THE CO_2SOLV DATABASE

We present next two examples where the efficacy of employing the **CO_2SOLV** database is highlighted. Firstly, the **CO_2SOLV** allows an analysis of the collected information on available solvents for PCC, leading to the identification of several observation and gaps, such as:

1. For **water-free/water-lean solvents**, AMP has been the alkanolamine of choice for the majority of the solvents reported in literature, due to its higher absorption capacity and lower heat of regeneration compared to other alkanolamines.
2. The data collected on solvent rich loading and cyclic capacity (in the "Solvent Screening" tab), along with the absorption isotherms for the solvents (in the solvent properties tab) were reported in the literature in **different units due to the lack of a standardized methodology** on reporting them (mol CO_2/mol amine, mol CO_2/L solution, mol CO_2/ kg solution, etc.). This has been homogenised in the database for fair comparisons based on the choice of performance metrics and their standardization (in **WP2** of this study, **Tasks 4** and **5**).

3. The reporting of the **cyclic capacity** of the examined solvents is discrepant between different studies in terms of rich and lean temperature and pressure conditions. This has been homogenised based on the choice of performance metrics and their standardization.
4. For the detailed properties of solvents summarised in the “Solvent Properties” tab, the majority of these properties are lean solvent density, lean solvent heat capacity, lean solvent viscosity, and absorption isotherm.

Secondly, as an illustrative example for the efficacy of the database, we present in **Figure 1.4** the CO_2 absorption isotherm at 40°C for different solvents, as directly plotted from the available information in the database[2]. Furthermore, the data presented in the “Solvent (xx)” tabs are automatically updated in the “Solvents Screening” tab according to the desired rich and lean conditions, in order to identify and rank promising systems based on selected KPIs.

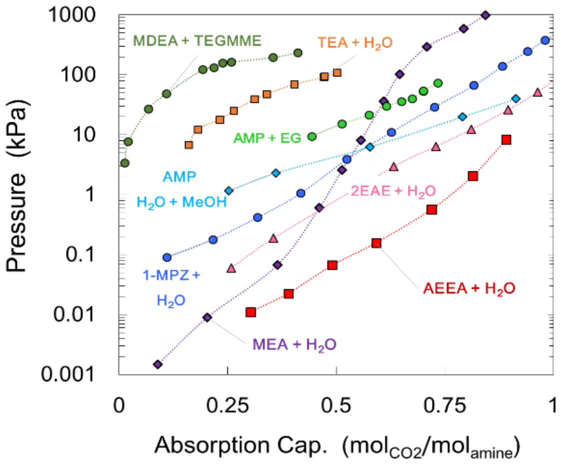


Figure 1.4 *Absorption isotherms of selected solvents collected in the “Solvent (xx)” tabs on the* CO_2*SOLV database.*

The initial screening of the solvents was done using information collected in the “Solvent Screening” tab, as an initial assessment of the gaps in available data, and identification of trends for promising solvents, compared to benchmark 30 wt% aqueous MEA. The entries were updated to remove any repetitive data on the performance of the same solvent.

It can be seen in **Figure 1.5**, that for P_{CO2} = 5 – 35 kPa, at least 30% of the data have a rich loading higher than the benchmark MEA.

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[2] *The units were homogenised in the database for all the data collected on solvent rich loading and cyclic capacity, along with the absorption isotherms for the solvents (in the “Solvent Properties” tab) for fair comparisons.*

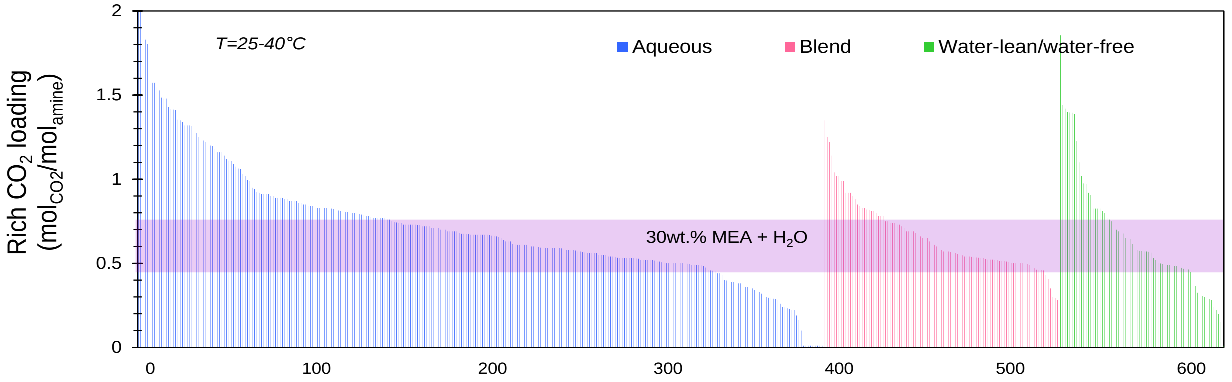


***Figure 1.5** Screening results of alternative solvents available in the* **CO_2SOLV** *database in terms of absorption (rich) capacity for a temperature range between 298 – 313 K.*

1.4 Collected data from Large-Scale Facilities

The inclusion of information gathered from large-scale or pilot-scale facilities is of vital importance, as they help in bridging the gap between the industrial commercialization of chemical solvents and their lab-scale testing. Several chemical solvents have been tested at pilot-plant scales and they are summarised in **Table 1.1** and **Figure 1.6**.

The performance of MEA in pilot plants is typically used as a benchmark for CO_2 capture, usually evaluated for a 90% capture rate with CO_2 purity of 95%. The performance of benchmark 30 wt.% MEA at those conditions, entails a 3.6 $GJ.t_{CO2}^{-1}$ total reboiler duty consumption, resulting in an 80% increased cost of electricity (COE), once integrated with a power plant. This is reported from process simulations on the scale of the SaskPower Boundary Dam Power Station [84]The current targets on novel amines and processes aim at lowering the cost of electricity due to power plant integration with carbon capture units to be below 35% [22,85,86].

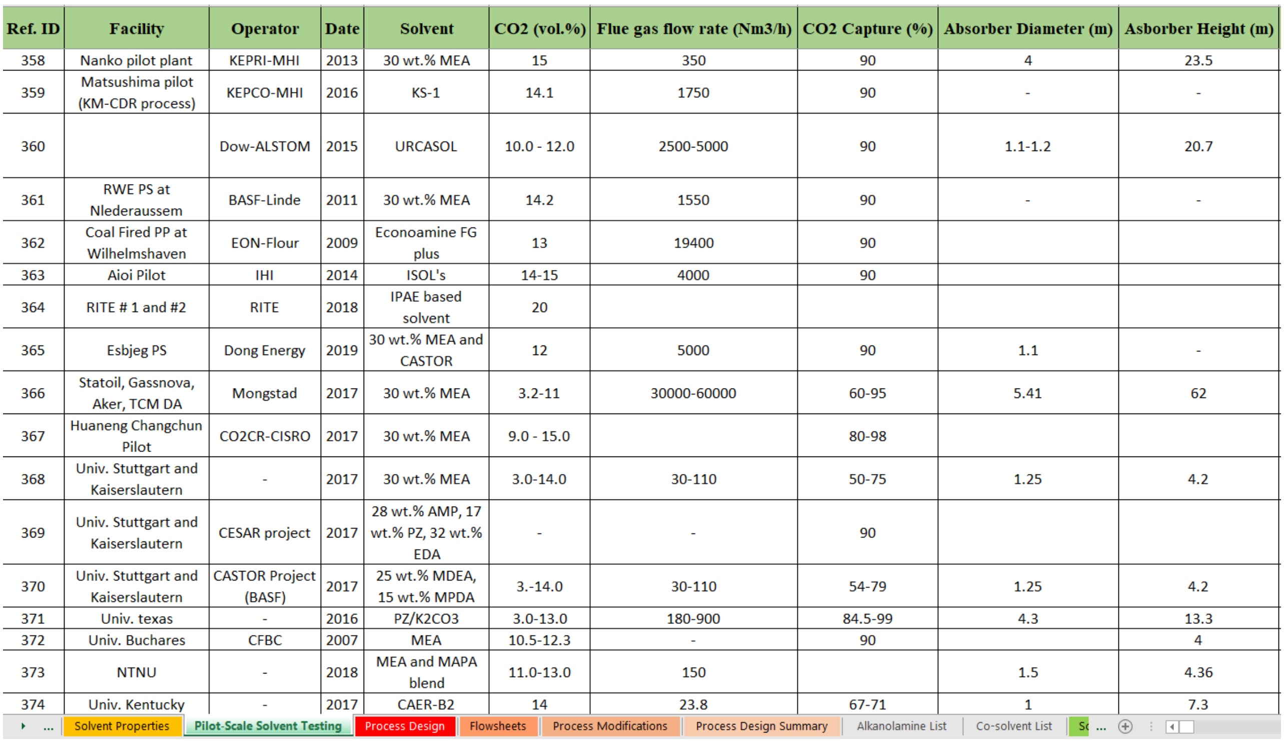
At this stage, the utilisation of **novel amines** such as **PZ** or **AMP** has established their potential as next generation PCC solvents, with the new benchmark solvent being a blend of AMP + PZ as identified in IEAGHG technical study 2019/09 [13]. In the case of PZ, aside from its faster absorption rate and higher loading capacity compared to MEA, pilot plant testing indicated its high thermal stability, and a 0.3% total amine losses due to degradation and other operational issues, which is 10 times lower than that experienced with MEA [57,87–92]. Still some operational problems exist such as its oxidative degradation and precipitation at high concentrations. Conversely, the sterically hindered amine (AMP) established its potential due to its high absorption capacity and low energy of regeneration compared to MEA; however, its reaction kinetics are slower than that of MEA. This led to its employment in several patented blended solvents, to take advantage of its positive characteristics. Patented solvents include the KS series (see **Section 2.4.2**), which were claimed to be energy effective, have less solvent loss and degradation without the requirement of additives and inhibitors. It has been reported that by using KS-1 [93], 40% solvent circulation rate and 20% regeneration energy can be saved with 90% less degradation, 90% less solvent loss and 65% less corrosion compared to MEA. Other blended amines have been tested at pilot scale showing great promise such as the CESAR series (blends of PZ and AMP) [94–96] and CANSOLV (blend of PZ with tertiary amine) [97,98] demonstrating high oxidative stability, reduced solvent regeneration energy and circulation rates. A detailed description of the commercial solvents used in pilot-plant testing processes can be found in **Section 2.4** in this report.

Table 1.1 *Summary of pilot plant testing of amine-based solvents for PCC.*

Solvent	Facility	Company	Source of Flue gas	Processing Capacity (tonne CO_2 per day)	Ref.
Advanced amine (Shell-Cansolv)	Boundary Dam Power Station	SaskPower, Canada	Brown Coal	4	[4]
MEA	Esbjergværket (ESV) pilot plant	Dong Energy	Coal	50	[93]
MEA	Loy Yang Power Station	CSIRO, Australia	Brown Coal, PCC	1	[99]
MEA	Tarong Power Station	CSIRO, Australia	Black Coal, PCC	2	[100]
MEA	Jilin Oil Field	PetroChina, China	Natural Gas	550	[93]
MEA	International Test Centre for CO_2 capture	SaskPower, Canada	Steam Boiler	1	[93]
MEA	Tokyo Electric Power Station	Hitachi, Japan	Coal	-	[93]
MEA	E. W. Brown Generating Station	Hitachi, Japan	Coal	15	[93]
MEA	Brindisi Power Plant	ENEL, Italy	Coal	54	[93]
Advanced amine (H3-1)	Tokyo Electric Power Station	Hitachi, Japan	Coal	-	[93]
Advanced amine (H3-1)	SaskPower, Shand Power Station	Hitachi, Japan	Lignite	120	[93]
Advanced amine (H3-1)	E. W. Brown Generating Station	Hitachi, Japan	Coal	15	[93]
Advanced amine (Cansolv-Shell)	Aberthaw	RWE, UK	Coal	50	[97,98]
Advanced amine (UCARSOL)	Dow Chemicals	Dow Chemicals, USA	Coal, PCC	5	[93]

Solvent	**Facility**	**Company**	**Source of Flue gas**	**Processing Capacity (tonne CO_2 per day)**	**Ref.**
Advanced Amine (CASTOR Series)	Esbjergværket (ESV) pilot plant	Done Energy	Coal, PCC	24	[101, 102]
Advanced amine (RS Series)	International Test Centre for CO_2 capture	SaskPowers, Canada	Steam Boiler	1	[103, 104]
Advanced amine (KoSol Series)	Boryeong Thermal Power Plant	KEPCO, Korea	Coal, PCC	2	[93]
KS-1	MHI Hiroshima R&D Center	MHI, Japan	Coal, PCC	1	[105]
KS-1	J-Power, Matsushima Thermal Power Station	MHI, Japan	Coal, PCC	10	[105]
KS-1	KEPCO, Nanko Natural Gas	MHI, Japan	Natural Gas	2	[105]
KS-1	Georgia Power Plant Yates	MHI and Southern Company, USA	Coal	-	[105]
KS-1	Plant Barry Power Station	MHI, Southern Energy, electric Power Research Institute, USA	Coal	410	[105]
Amine Mixture	Shidongkou	Huaneng, China	Coal	300	[106]
MEA/PZ/Carbonate	University of Texas/Separations Research Program	University of Texas, USA	Prepared flue gas	1.3-5.9	[92]
PZ (Concentrated)	University of Texas	University of Texas, USA	Prepared flue gas	-	[93]
PZ	Colorado Springs Utilities Drake #7	Neumann Systems Group, USA	PCC	-	[93]
MEA, GUSTAV2000	Niederaussem pilot plant	BASF	Coal	7.2	[107]
APBS	EON, Maasvlakte power plant	Carbon Clean Solutions	Coal	6.0	[108]
CDRmax	National Carbon Capture Center (NCCC) and	Carbon Clean Solutions	Natural gas	-	[109]

Solvent	Facility	Company	Source of Flue gas	Processing Capacity (tonne CO_2 per day)	Ref.
	CO_2 Technology Centre Mongstad DA, Norway				
Amine based solvent	NCCC	Linde-BASF	Coal	-	[110]
Advanced amine (H3-1)	NCCC	Hitachi	Coal	-	[111]
Advanced amine (T3 solvent)	NCCC	Chiyoda Corporation	Coal	-	[112]
Advanced amine (ION)	NCCC	ION Engineering	Coal	-	[113]
PZ	NCCC	URS Group and University of Texas at Austin	Coal		[114]



Ref. ID	Facility	Operator	Date	Solvent	CO2 (vol.%)	Flue gas flow rate (Nm3/h)	CO2 Capture (%)	Absorber Diameter (m)	Asborber Height (m)
358	Nanko pilot plant	KEPRI-MHI	2013	30 wt.% MEA	15	350	90	4	23.5
359	Matsushima pilot (KM-CDR process)	KEPCO-MHI	2016	KS-1	14.1	1750	90	-	-
360		Dow-ALSTOM	2015	URCASOL	10.0 - 12.0	2500-5000	90	1.1-1.2	20.7
361	RWE PS at Nlederaussem	BASF-Linde	2011	30 wt.% MEA	14.2	1550	90	-	-
362	Coal Fired PP at Wilhelmshaven	EON-Flour	2009	Econoamine FG plus	13	19400	90		
363	Aioi Pilot	IHI	2014	ISOL's	14-15	4000	90		
364	RITE # 1 and #2	RITE	2018	IPAE based solvent	20				
365	Esbjeg PS	Dong Energy	2019	30 wt.% MEA and CASTOR	12	5000	90	1.1	-
366	Statoil, Gassnova, Aker, TCM DA	Mongstad	2017	30 wt.% MEA	3.2-11	30000-60000	60-95	5.41	62
367	Huaneng Changchun Pilot	CO2CR-CISRO	2017	30 wt.% MEA	9.0 - 15.0		80-98		
368	Univ. Stuttgart and Kaiserslautern	-	2017	30 wt.% MEA	3.0-14.0	30-110	50-75	1.25	4.2
369	Univ. Stuttgart and Kaiserslautern	CESAR project	2017	28 wt.% AMP, 17 wt.% PZ, 32 wt.% EDA	-	-	90		
370	Univ. Stuttgart and Kaiserslautern	CASTOR Project (BASF)	2017	25 wt.% MDEA, 15 wt.% MPDA	3.-14.0	30-110	54-79	1.25	4.2
371	Univ. texas	-	2016	PZ/K2CO3	3.0-13.0	180-900	84.5-99	4.3	13.3
372	Univ. Buchares	CFBC	2007	MEA	10.5-12.3	-	90		4
373	NTNU	-	2018	MEA and MAPA blend	11.0-13.0	150		1.5	4.36
374	Univ. Kentucky	-	2017	CAER-B2	14	23.8	67-71	1	7.3

Figure 1.6 *Screenshot of the* **CO_2SOLV** *showing the "Pilot-Scale Solvent Testing", which includes the conditions, solvents, and capacities of different campaigns.*

2. REVIEW OF PCC PROCESSES AND EQUIPMENT DESIGN (TASK 2)

Objective: Perform a detailed review of the most relevant chemical absorption processes and equipment designs tested at large/lab scale for PCC. It comprises:

1. Solvent used, testing scale and conditions.
2. Application of the configuration/design (e.g. power/industrial scale or process simulations)
3. Definition of measurable parameters for enhancement of these processes over traditional configurations.

2.1 SUMMARY OF PUBLISHED PROCESS CONFIGURATIONS

The standard process for post-combustion carbon capture employs an aqueous solution of 30 wt.% monoethanolamine (MEA), which is the benchmark defined in this study for comparison with novel process modifications and novel solvents. The MEA-based process demands improvement as it suffers primarily from high regeneration energy requirement, adding a high load on the parent power plant. This section summarizes some of the latest advancements in process enhancement and the quest for novel solvents superseding MEA. Additionally, the information related to process and equipment design, and performance as defined for this task are populated in the **CO_2SOLV** database as shown in **Figure A3** in **ANNEX I**. The process modifications found in the literature were included in the "**Process Modifications**" tab, highlighting the reboiler duty reductions as a main KPI to compare between the different cases. Valuable information and trends can be extracted from this tab showcasing the solvents and trials that were scaled up in the PCC of CO_2 processes. It also provides approximate values to be used as inputs for the prominent process modifications into the CAPEX and OPEX analysis in **Task 7**. Some of the most relevant identified process configurations and their enhancement over the benchmark aqueous MEA are included in **Table 2.1**.

Table 2.1 *Summary of published process configurations and their performance enhancement.*

Solvents	Process Modification	Description	Merits/Effects	Ref.
MEA and Ammonia	Multi-Absorber (MA)	Two absorber columns operated in series or parallel	Flexible operation and possibility of using two different solvents	[115–118]
MEA, PZ/AMP, EFG+, and prop. amine	Absorber Intercooling (AIC)	Installing inter-stage coolers along the absorber to extract the excess heat	Lower solvent circulating rate, smaller units, and reduced reboiler duty	[119–128]
MEA, PZ, and MDEA/PZ	Rich Solvent Recycle (RSR)	Portion of the rich solvent is returned to the absorber	increase the loading of the solvent, and	[127,129]

Solvents	Process Modification	Description	Merits/Effects	Ref.
			possible cool down the solvent	
MEA and prop. amines	Multi-Stripper (MS)	Extra stripping column operating at a different pressure	Further strip the solvent and produce purer CO2 effluent	[130,131]
MEA and PZ	Multi-Stage flash stripping (MSF)	Stripper column(s) are replaced with flash separator(s)	High recovery of CO_2 at higher pressure. Reduced the compression needed for the stripper overhead	[89,91,127,132]
MEA and K^+/PZ	Multi-Pressure Stripping (MPS)	Operating the stripper at different pressures with the lowest at the bottom of the column	Reduction of load on the CO_2 compression train, higher CO_2 recovery and less reboiler duty	[89,122,133–135]
MEA and K^+/PZ	Vacuum stripping (VS)	Operating the stripper at sub-atmospheric pressures	Lower regeneration temperatures (low-grade steam can be used)	[89,127,133,136]
MEA and PZ	Stripping inter-heating (SIH)	Heat integration between semi-lean and lean solvents	Reduction of reboiler duty and reducing heat losses	[91,137]
MEA	Split-flow (SF)	Semi-lean solvent is drawn from the stripper and cooled by a split of the rich solvent before being introduced to the middle of the absorber	Reduction of the reboiler duty and enhancement of the absorption process by reducing the amount of lean solvent at absorber top	[120,122,125,134,138–140]
MEA, PZ, and MDEA/PZ	Rich solvent split (RSS)	Rich solvent is split before the rich/lean heat exchanger and introduced directly to the top of the stripper	Reduction of the rich/lean heat exchanger pinch, water consumption by the condenser, and reboiler duty	[127,129,133,139,141–144]
MEA	Rich solvent flash (RSF)	Rich solvent is flashed prior to the stripper to recover some CO_2 that is combined with the stripper overhead	Partial recovery of CO_2. No tangible effect on reboiler duty	[127,133]

Solvents	Process Modification	Description	Merits/Effects	Ref.
MEA, PZ, and MDEA/PZ	Rich vapour compression (RVC)	Rich solvent is flashed followed by compression of the resulting vapour and heat integration with liquid rich solvent before the stripper	Reduction of reboiler duty and potential reduction of condenser duty	[127,133]
MEA, PZ, PZ/AMP, MDEA/PZ, DC-103, and EFG+	Lean vapour compression (LVC)	Lean solvent from the stripper bottom is flashed and the vapour is compressed and used in the reboiler	Recovery of more CO_2 and reduction of reboiler duty, condenser duty (indirectly), sizes of reboiler and condenser	[97,121,122,125,127–129,133,134,137,144–147]
MEA	Condensate Evacuation and Evaporation (CEE)	Heat integration between the condensate and stripper overhead to produce saturated steam. The generated steam is compressed and fed to the stripper bottom	Reduction of steam requirement and reboiler duty	[122]
MEA	Condensate heating (CH)	Heat integration between the condensate and stripper overhead to produce heated water that is introduced before the reboiler	Slight reduction of the reboiler duty	[122]
MEA	Stripper Overhead Compression (SOC)	compressing the stripper overhead before the condenser and recovering the heat of the subsequent hot stream	Heat recovery from the compressed CO_2 and less external heat is required	[122,127,133,144]
MEA	Heat Integration (HI)	Various configurations are possible.	Recovery of dissipated heat	[122,134,135]

We provide next details on the standard MEA process, several key modifications that have been evaluated at pilot scale as well as some identified processes for novel amines and other novel solvents.

2.2 CONVENTIONAL PCC PROCESS

The standard process of the 30 wt.% MEA aqueous solvent for PCC of CO_2 from a flue gas employs a pre-treatment system, absorber, main rich/lean heat exchanger, stripper (with reboiler), flash tank, pumps, and coolers (**Figure 2.1**). MEA has been used commercially capturing up to 1000 t_{CO2}/day [3,13].

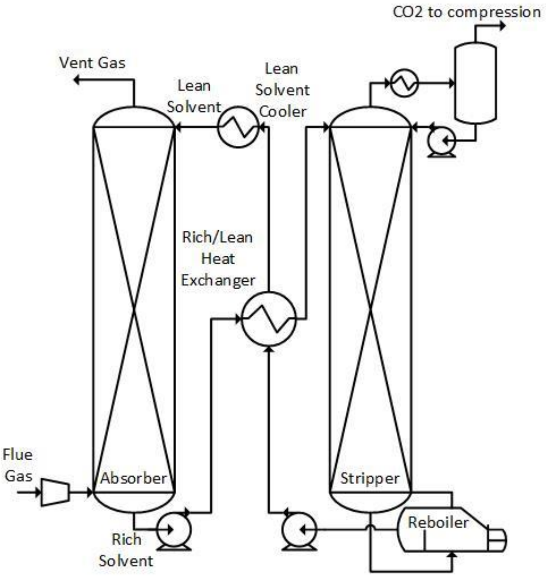


Figure 2.1 *Simplified process flow diagram for a conventional PCC process.*

2.3 PROCESS MODIFICATIONS TO THE CONVENTIONAL PROCESS

One way to mitigate the relatively high energy requirement of the conventional 30 wt.% MEA process is through modifications to the process flowsheet. These modifications aim to enhance the absorption, regeneration or heat integration of the overall process. There are many options available in the literature but most of them are yet to be experimentally verified. The aim of this task was to find process modifications in pilot- and large-scale plants but due to the dearth of real applications of such modifications (as it is IP-sensitive), results from process simulations were also included to complement the analysis of the most potential process modifications. There are multiple patents addressing process modifications to the CO_2 absorption process [143], but only a few were closely studied or implemented (simulation-wise or experimentally).

The categorization of process modifications can be challenging, especially with the propagation of effects of a particular modification on the whole process. Le Moullec *et al.* [127] classified the process modifications into absorption enhancement, heat integration, and heat pump. Here, the categorization of the process modifications is ought to follow a similar general trend; **absorption enhancement**, **stripping enhancement**, and **overall enhancement**. A process modification would belong to the first two categories if the scope were the absorber or the stripper column/process, respectively. The overall enhancement category encompasses multiple modifications. Noteworthy, these categories are not mutually exclusive when considering the effects of the process modification, in which a specific modification can entail multiple effects on different parts of the process (e.g. absorption modifications can lead to reduction in the reboiler duty). In addition, heat integration modifications that are not pertaining to a column (absorber or stripper) are usually associated to the regeneration process as reboiler duty savings are always sought, and these modifications were included in the stripping enhancement category in this section.

The absorber enhancement category includes absorber intercooling (AIC), multi-absorber (MA), and rich solvent recycle (RSR). The stripping enhancement category includes multi-stripper (or matrix stripper, MS), multi-pressure stripping (MPS), multi-stage flash stripping (MSF), vacuum stripping (VS), split-flow (SF), rich solvent split (RSS), stripper overhead compression (SOC), lean vapour compression (LVC), rich solvent compression (RVC), rich solvent flash (RSF), condensate evacuation and evaporation (CEE), stripper inter-heating (SIH), and heat integration (HI), the latter includes several possible configurations. Process modifications in the overall enhancement category are merely combinations of the individual modifications from the previous categories, which also includes solvents other than MEA. Trials with novel solvents will be discussed in the next section. As can be inferred, many modifications are directed towards the stripping process, which is a direct consequence of the high demand of thermal energy during this process, making up about 70-80% of the operating costs [148]. This entails the consideration of the reboiler duty reduction as a key performance indicator (KPI) to evaluate the efficiency of a given process modification, which is the case mostly found in the reviewed literature.

2.3.1 ABSORPTION ENHANCEMENT

Absorber intercooling (AIC) is frequently found in process flowsheets as a means of enhancing the absorption process (**Figure 2.3**). The gist of using inter-stage coolers along the absorber is to extract the excess heat which is caused by the exothermic reaction inside the absorber between the solvent and the rich flue gas [124], which reduces the temperature bulge in the column (**Figure 2.2** – IEAGHG 2014/08). This causes an increase of the solvent loading at the bottom of the reactor and the working capacity of the solvent, which eventually results in lower circulating rate, smaller units, and reduced reboiler duty [122]. However, the increase in CO_2 solubility comes at the expense of lower chemical kinetics and diffusivities as of the temperature decrease in the column. There are several factors affecting the performance of AIC including the position of the inter-stage cooler, lean loading, and split fractions [127,149]. Overall, studies have shown an advantage of introducing absorber intercooling on the reduction of the reboiler duty ranging from 2.5 to 24.9% using MEA evaluated via process simulation software [122–126,133,134]. The employment of absorber intercooling in pilot-scale pants has been reported in the literature [90,130,150]. Particularly, reboiler duty reductions of 4.5% and 4% were reported in pilot studies using MEA [120] and Fluor Econamine FG Plus™ (EFG+) solvents [121], respectively.

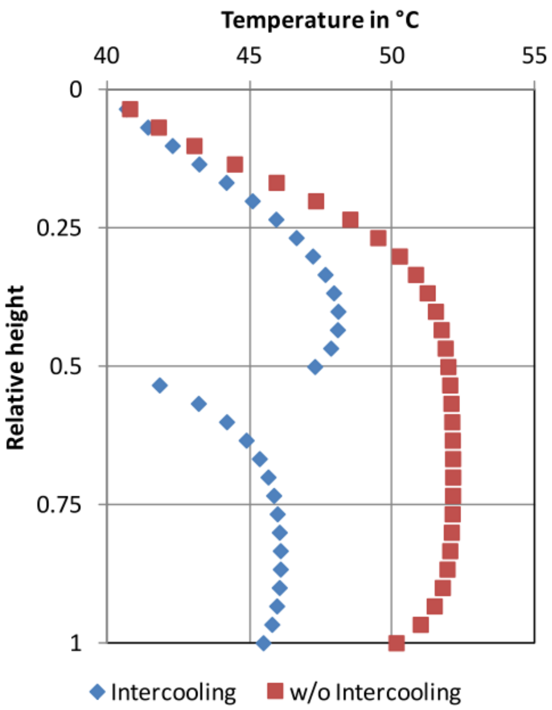


***Figure 2.2** Comparison of absorber's temperature profile with and without intercooling* [151].

The implementation of absorber intercooling would require an increase in the capital and complexity of the process due to the extra pumps and coolers needed along the column. Linde's gravity-driven interstage cooler design is claimed to mitigate these issues [119].

Multi-absorber (MA), multi-effect, or multi-stage absorption describes the process modification of adding an extra absorption column with the possibility of operating them in parallel or series, which also allows flexibility of operation, or when the available space is a constraint [116]. When operated in parallel, it is similar to having a single larger absorber with respect to capacities. Operating in series allows the incorporation of a cooler between the two absorbers as in CSIRO PCC pilot plant in the AGL Loy Yang power station, Australia [115], in which the flue gas enters the second absorber column then enters the bottom of the first absorber column. The lean solvent, in contrast, enters the first absorber column coming from the rich/lean solvent heat exchanger, and then exits to the second absorber column, in which it goes through a cooler. The rich solvent is then collected at the bottom of the first absorber and redirected to the rich/lean heat exchanger prior to the stripper column. Another possible configuration is a multi-stage absorber and dual stripper configuration, where two absorber loops can be initiated with one or two different solvents [127].

Rich solvent recycle (RSR) process modification aims at recycling part of the rich solvent from the bottom of the absorber back to the absorber column at different possible heights (**Figure 2.3**). This modification ought to further polish the flue gas, increase the loading of the solvent, and possibly cool down the solvent in the column as depicted in the AIC modification [127]. The degrees of freedom associated with the RSR include the split ratio, the height of introducing the recycled stream, and the temperature of the drawn solution [129]. Dubois and

Thomas [129] reported 1.9, 3.3, and 8.6% reboiler duty reduction with PZ, MDEA/PZ, and MEA solvents, respectively, when implementing an RSR modification through process simulation calculations.

Split-flow (SF) process modification is among the most studied configurations in the literature [127,139]. This configuration consists of splitting the rich solvent stream into two streams; one which enters the top of the stripper and exits from the middle (or elsewhere) (**Figure 2.3**).

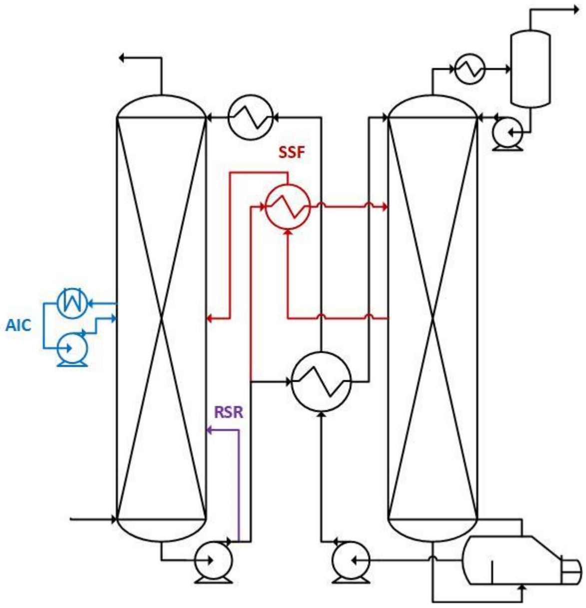


Figure 2.3 *Simplified process flowsheet of AIC, RSR, and SSF process modifications. The coloured portion of the flowsheet indicates the modification to the conventional case.*

This semi-lean solvent is then redirected to enter the middle of the absorber, after losing its heat to the rich solvent split, which initially entered the top of the stripper column. The second stream of the rich solvent is introduced to the middle of the stripper after heating in a second rich/lean heat exchanger, which then exists the bottom of the stripper as a lean solvent. The lean solvent stream flows through the second rich/lean heat exchanger (similar to the first case) followed by a cooler before being introduced to the top of the absorber column [125,138]. It can be considered as parallel arrangement of two stripping stages. This modification aims to reduce the load on the reboiler as less solvent reaches the bottom of the column. Also, the semi-lean solvent, which is introduced to the middle of the absorber column, increase its load by contacting with the concurrently flowing flue gas, and hence, reduces the load on the lean solvent at the top of the column and enhances the absorption process due to lower temperatures in the column [122]. As the thermodynamic driving force in the absorber is lowered, this modification is recommended for tertiary amines when compared to MEA [127]. Due to the changes of the solvent flow throughout the process, the solvent circulation rate would increase as the solvent working capacity decreases and the regeneration is downgraded, which leads to increased capital costs [122,138]. Many factors require optimization when incorporating split-flow modifications including split-ratios, stream positions (points of drawing/injecting), temperatures, and loadings [134]. Process simulation studies report 7 – 16.6% reduction of reboiler duty using MEA [122,125,134], while a real implementation of the split-flow modification in a pilot plant reported 5% reduction [120].

2.3.2 STRIPPING ENHANCEMENT

Multi-stripper (MS), multi-effect stripping or matrix stripping are all variations consisting of multiple strippers (mainly two) to further strip the solvent and produce purer CO_2 effluent (**Figure 2.4**). Multiple variations and configurations exist for such modification; one consists of operating two strippers at different pressures, in which the primary column operates as the conventional stripper (heat provided by the reboiler) while the secondary column, at a lower pressure, uses the heat of the exiting lean solvent from the primary stripper [127]. Another configuration by Oyenekan and Rochelle [131], double matrix, consists of two columns at 295 and 160 kPa, respectively. The rich solvent coming from the absorber is split and fed to both columns, in which the semi-lean solvent from the first column (295 kPa) is fed to the middle of the second column. The second column produces a lean and semi-lean solvents, in which the former is sent to the rich/lean heat exchanger and the latter exchanges heat with the feed of the second column. This matrix configuration is believed to reduce the energy consumption by 22% over the baseline performance.

The UKy-CAER PCC pilot plant at the Kentucky Utilities E. W. Brown Generating Station employed a two-stripper configuration using 30 wt.% MEA and two other proprietary amine-based solvents [130]. The extra column is shown to provide leaner solvent which is positively reflected on the performance of the absorber. Heat integration and absorber intercooling are also employed in the pilot plant. MEA trials at different conditions yielded 2.33 – 3.73 $MJ.kg_{CO2}^{-1}$ CO_2 reboiler duty compared to 2.1 – 3.5 and 3.32 – 3.87 $MJ.kg_{CO2}^{-1}$ for the other solvents at the same conditions. However, the capital cost of such modification needs to be critically evaluated as it requires extra units which might outweigh the merits of reducing the operating costs at a given project life.

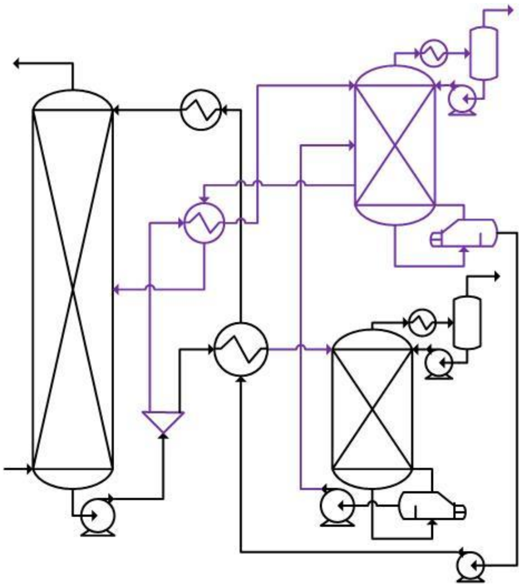


Figure 2.4 *Simplified process flowsheet of an MS process modification. The coloured portion of the flowsheet indicates the modification to the conventional case.*

Multi-Stage flash stripping (MSF) configuration replaces the stripper column(s) with flash separator(s). The rich solvent is flashed isothermally through each flash vessel. The flashed vapour, CO_2 and water, is collected from each stage and compressed while the bottom liquid, the lean solvent, is sent to the rich/lean heat exchanger [91]. This configuration is easier in operation and cheaper to construct compared to a conventional stripper column [127]. A process simulation of two-stage flash stripping was conducted for MEA and PZ solvents [91]. The MEA-modified stripping yielded 5.8% increase of the reboiler duty but with 1.7% reduction of the equivalent work (kJ/mol CO_2). In contrast, the PZ-modified case yielded 7.1% increase of the reboiler duty compared to the unmodified stripped using PZ; however, when compared to the MEA conventional flowsheet, there is a 12.4% reduction. This shows that the reboiler duty is not necessarily reduced when introducing the multi-stage flash stripping regardless of the used solvent. Similarly, this modification was considered the least effective among other stripper modifications [131]. A pilot-scale plant at the Separation Research Program at University of Texas, Austinwas operated using a two-stage flash stripping system along with absorber intercooler using PZ solvent [132]. The modelled process predicted an optimum performance of 32.6 $kJ.mol_{CO2}^{-1}$ equivalent work.

Multi-pressure stripper (MPS) is another modification of the conventional regeneration column. The gist of this modification is to strip the solvent at different pressures across the column. The reboiler ought to operate at the lowest pressure where the pressure is gradually increased up the column using integrated compressors (**Figure 2.5**). The compressed vapour of each stage acts as the stripping gas of the second stage. The temperature should be fixed to a maximum limit at the top of the column to avoid degradation of solvents [133]. Such modification reduces heat losses and consequently, reduces the total load. It also reduces the compression requirement for the following CO_2 compression train after exiting the stripper [89]. Multi-pressure strippers were mostly observed in process simulation studies [89,122,133–135] reporting 9.9-32.4% decrease in the reboiler duty. Very scarce to no studies were found on pilot-scale plants. A major challenge in this modification is the complexity of operation and increased CAPEX associated to the extra compressors. Yet, if complemented with the CO_2 compression train, a net positive impact can be sought.

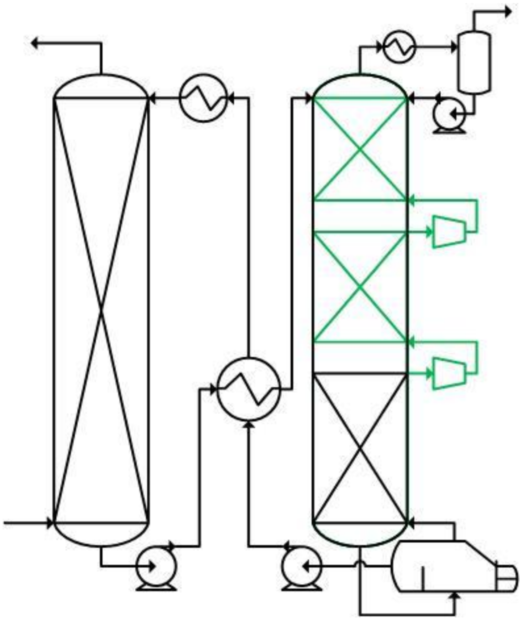


Figure 2.5 *Simplified process flowsheet of an MPS process modification. The coloured portion of the flowsheet indicates the modification to the conventional case.*

Vacuum stripping (VS), as the name infers, is operating the stripper at lower pressure (below atmospheric pressure), which entails operating the reboiler at lower temperatures. There are no extra units required; however, the size of the units can be affected [136]. The effect of operating at such conditions depends on the CO_2 heat of absorption of the solvent; if higher than the water heat of vaporization, more steam is required and vice versa [127]. The main drawback of vacuum stripping is the higher load put on the CO_2 compression train. Process simulation studies show 8.2-62% increase in the reboiler duty for MEA and K^+/PZ solvents [89,133].

Stripping inter-heating (SIH) is an analogy to the absorber inter-cooling, in which semi-lean solvent splits are taken from the column to exchange heat with the lean solvent coming from the reboiler, and then reintroduced again at different heights. A process simulation of SIH using PZ resulted in 10.7 and 27% reduction of the reboiler duty compared to the conventional configuration using PZ and MEA, respectively [91]. Another process simulation study reports 10.2% decrease in reboiler duty using 30 wt.% MEA [137].

Rich solvent split (RSS), or stripper staged feed, is similar to the split-flow configuration except that no semi-lean solvent is drawn from the stripper (**Figure 2.6**). The process modification only consists of a split of the rich solvent prior the rich/lean heat exchanger in which a bypass (cold strip) is directly introduced to the top of the stripper [129,139,144]. The other stream flows through the heat exchanger and then to a lower point than that of the cold bypass. This simple yet effective modification recovers the heat from the rising stripping gas and thus reduces the load of the condenser as less cooling water is needed [133]. The reboiler duty is also prone to reduction as the hot rich solvent is capable to flash more and produce more steam, reducing the load on the reboiler [152]. For MEA, PZ, MDEA/PZ solvents, process simulation predicted 3.2 – 12.1% [129,133,141,144], 4.8% [129], and 9.5% [129] reboiler duty reduction, respectively. Rich solvent split was employed in **Tarong pilot plant** and showed a 7% reduction in the required thermal energy and up to 60% reduction of the condenser duty [142].

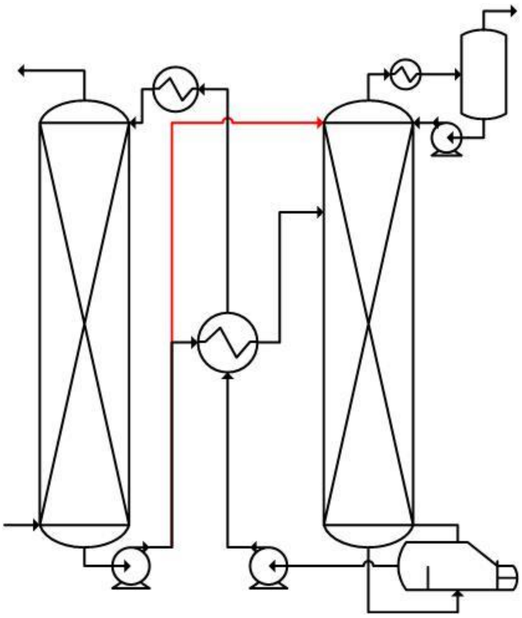


Figure 2.6 *Simplified process flowsheet of an RSS process modification. The coloured portion of the flowsheet indicates the modification to the conventional case.*

Rich solvent flash (RSF) process modification was not observed in many studies, more in patents [127]. It is aimed at flashing the rich solvent prior the stripper in which the vapour is merged to the stripper overhead while the liquid enters the stripper top. Through process simulation of MEA solvent, there was no tangible effect on the reboiler duty [133].

Rich vapour compression (RVSC) process modification targets the rich solvent by flashing it similar to the RSF modification. The vapour is then compressed and the liquid is pumped and to a heat exchanger where the vapour is cooled. Both streams are then introduced to the stripper column at different heights; the vapour to the bottom and the liquid to the top (**Figure 2.7**) [127]. Dubois and Thomas [129] tested RVC for MEA, PZ, MDEA/PZ solvents and yielded reboiler reductions of 12.2%, 16.2%, and 13.1%, respectively.

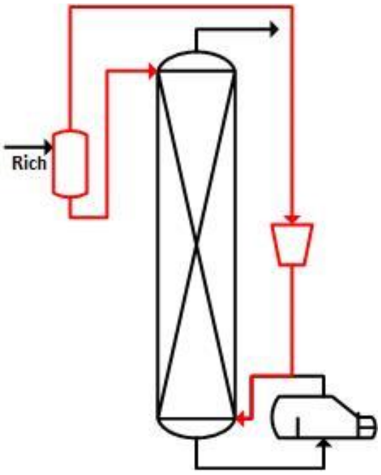


Figure 2.7 *Simplified process flowsheet of an RVC process modification. The coloured portion of the flowsheet indicates the modification to the conventional case.*

Lean vapour compression (LVC) process modification is among the most observed configurations in the literature. Its concept lies in flashing the hot lean solvent coming out of the stripper column and recompressing the vapour and feeding it back to the column, while the liquid is directed towards the rich/lean heat exchanger (**Figure 2.8**) [122,127,128,144,147]. This technique reduces the burden on the reboiler by stripping CO_2 during the flashing and by generating hot steam (mainly water) complementing the stripping gas [125,133,146]. Another positive effect is sought on the condenser as the lower flow rate of the lean solvent is being sent to the rich/lean heat exchanger which results in less heating of the rich solvent. This makes the feed to the stripper colder than the conventional configuration, and hence, the effects of the RSS become apparent and the condenser operates with less load [121,137]. However, this process modification results in an increase in the CAPEX due to the increase in the number of units, mainly the compressor (or steam ejector). Yet, due to the decrease of the condenser and reboiler duties, their sizes must decrease which incurs less CAPEX, and adds to the primary goal of reducing the OPEX [121]. Ultimately, a thorough economic analysis should be considered, which turned out positive to many studies with 1.4 –11.6% reduction of the load [127]. Process simulation studies on MEA, PZ, and MDEA/PZ with the LVC process modification showed 13.1 – 26.8% [122,125,129,133,134,137,141,144–147], 18.2% [129], and 11.6% [129] decrease in the reboiler duty, respectively.

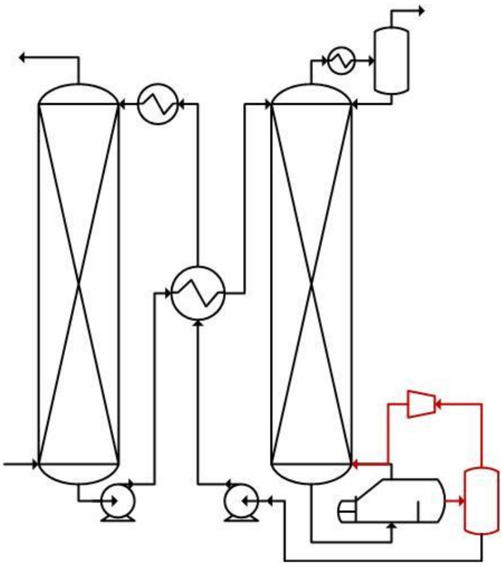


Figure 2.8 *Simplified process flowsheet of an LVC process modification. The coloured portion of the flowsheet indicates the modification to the conventional case.*

Condensate Evacuation and Evaporation (CEE) has a similar effect of the LVC as in generating more steam to aid the reboiler duty. The concept lies in a heat integration between the condensate and stripper overhead, in which the steam that is generated after the heat exchanger is compressed prior to its introduction to the bottom of the stripper [122]. A reduction of 26% of reboiler duty was calculated through process simulation using 30 wt.% MEA.

Condensate heating (CH) aims at recovering the heat of the stripper overhead the same as in CEE; however, the heating does not generate steam but heated water (close to saturation). The heated condensate is introduced before the reboiler, which places a higher load initially on the reboiler. That considered, the benefit of this modification is believed to be marginally reducing the reboiler duty due to the slightly colder overhead stripper produced [122].

Stripper Overhead Compression (SOC) has a similar modification and scope as the CEE, except that the order of the units is slightly different. The principle lies in compressing the stripper overhead before the condenser and recovering the heat of the subsequent hot stream [127]. There are multiple variations to the cold stream that is recovering the heat from the compressed stripper overhead. The main case is to provide the heat to the reboiler in order to directly reduce its duty [122,133]. Oh *et al.* [144] suggested two variants: heating the solvent before the reboiler, and heating the rich solvent before the stripper with the former reducing the reboiler duty almost twice as much as the latter (**Figure 2.9**). SOC was simulated with MEA and has shown 15.5 – 31.5% reboiler duty reduction. Some of the drawbacks to be considered when employing SOC is the increased mechanical (electrical) work for the compression step, which needs to be considered for a collective OPEX analysis [127].

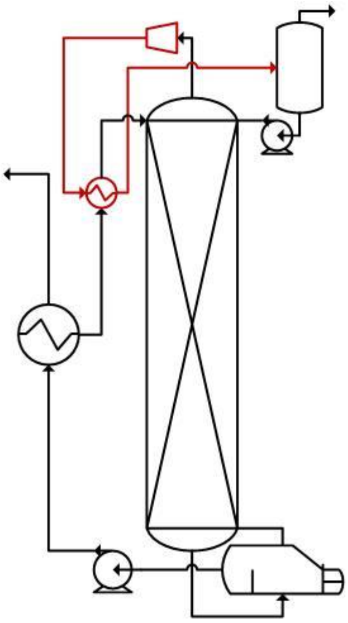


***Figure 2.9** Simplified process flowsheet of an SOC process modification variant. The coloured portion of the flowsheet indicates the modification to the conventional case.*

Heat Integration (HI) is usually present in most process modifications. When no substantial changes are done to the process flow sheet, and only heat recovery and heat loss reduction are sought, such modifications can fall in the HI category. However, the effect of such modifications, if implemented wisely, can substantially reduce the overall heat losses in the system and reduce the reboiler duty to a greater extent than more complicated process modifications. The ***overhead heat integration (OHI)*** and the ***compression heat integration (CHI)*** are two prime process modifications. The OHI is similar to SOC but it devoid of compression [122], in which the stripper overhead is heat-exchanged with the rich solvent leading to lower reboiler and condenser duties [153]. When the heat integration was employed before the main heat exchanger, the process simulation of OHI using MEA and DEA did not show tangible effects on the process performance as of the small difference in the stream's temperatures [154]. As an alternative configuration, the rich solvent could be split and only a small portion is heat-exchanged with the stripper overhead. The heated rich solvent split is then merged to the main rich stream exiting the main heat exchanger. Using process simulation and MEA as a solvent, this configuration showed 11.9% SRD reduction . Process simulation of MDEA/PZ yielded 6.4% SRD reduction compared to the MDEA/PZ conventional case [155]. In the IEAGHG 2014/08 report, a hypothetical solvent in an OHI-modified process achieved 29.0 and 35.6% SRD reductions for coal- and NG-fired flue gases, respectively [151]. The CHI makes use of the compressed CO_2 heat, in which a portion of the lean solvent taken before entering the reboiler is heat-exchanged [134]. Yet, such modification proved to be uneconomical due to the increase in investment and operating costs associated to the higher compression needed for subsequent streams after the heat integration modification. The same modification was suggested but with the removal of the knock-out drum at the stripper overhead, in which 4.6% reduction of the capture cost ($\$/t_{CO2}$ captured) was reported [135].

2.3.3 OVERALL ENHANCEMENT

This category encompasses multi-modifications in a single process, which is a combination of the individual modifications from the previous categories. There was always an off-set when using individual modifications that reduces the apparent enhancement of the targeted part of the process. Combinations of modifications can induce positive interactions and synergy resulting in maximizing effects and mitigating the off-sets.

Suggested ***Combinations of process modifications*** to the conventional process included duals such as AIC/SF [125,134], AIC/LVC [125,128], AIC/RSS [126,128,139,156], LVC/RSS [128,137,141,144], LVC/SOC [133,144], RSS/RVC [141], RSS/SF [157], RSS/SOC [144], RSS/MPS [133], and HI/MPS [135]. Combinations of three modifications included AIC/LVC/CEE [122], AIC/LVC/RSS [128], AIC/LVC/MA [117], AIC/RSS/MA [117], AIC/RSS/RVC [117], and LVC/SSF/SOC [144]. Combinations of more than three modifications were seldom encountered and where mostly found in patents [127], perhaps the complexity of the process and investment cost become a burden.

Dual combinations showed various effects on the overall process with a reported reduction of reboiler duty ranging from 11 to 39% when simulating MEA. RSS was coupled with AIC in a pilot plant using a propriety amine. The reboiler duty was reported to be reduced to half of that of the MEA conventional process [156]. RSS/SF combination was implemented in a pilot plant reporting 4.6% reduction of reboiler duty [157]. The interactions between modifications need to be thoroughly assessed as some modifications can impose deteriorating effects and lack of compatibility. For example, the MPS operates at a low pressure at the bottom of the stripper column, which makes LVC, for instance, an inefficient combination as it requires high-pressure lean stream [127]. On the contrary, AIC when coupled with RSR produced a positive interaction as AIC increases the working capacity of the solvent but at the expense of the kinetics; this is where the RSR compensates and returns some of the solvent for higher contact time [127].

2.3.4 REFLECTION ON PROCESS MODIFICATIONS

Most of the process modifications found in the literature were part of simulation studies and a dearth of them were implemented experimentally. Validation of the most promising process modification should be carried out and their integration and retrofitting to existing plants should be carefully assessed [158]. Extracting information and effects of the process modifications on the process KPI’s is still a challenge. Studies would usually assess a small group of modifications on one solvent or more, and the conditions of the process are different than other studies, which makes the generalization risky. However, there are some modifications that showed an apparent potential and benefits over a range of studies, including pilot-scale trials. Such pieces of information are valuable, yet they lack accuracy of the expected savings. The magnitudes of reboiler duty savings are sometimes surprisingly high in some studies. Another issue is that most studies report few KPI’s (mostly specific reboiler duty), which makes the comparison between other studies very limited. Making the case for a thorough assessment, all costs should be considered upon introducing a modification to the process as the conditions, sizes, and energy balances are prone to change. The full assessment of the CAPEX and OPEX can give a more vivid view of the actual effects of a certain process modification and its applicability for integration [134,147,159].

Figure 2.10 shows a summary of reported reductions of specific reboiler duty (averages of reported values) for different solvents and process modifications from the following studies [89–91,97,119–126,128–131,133–135,137,140–142,144–147,150,151,154,155,157,160–175]The SRD reductions (each bubble) is referenced to the SRD of the conventional process using the same solvent. As such, confounding effects of the solvent and the process modification are avoided.

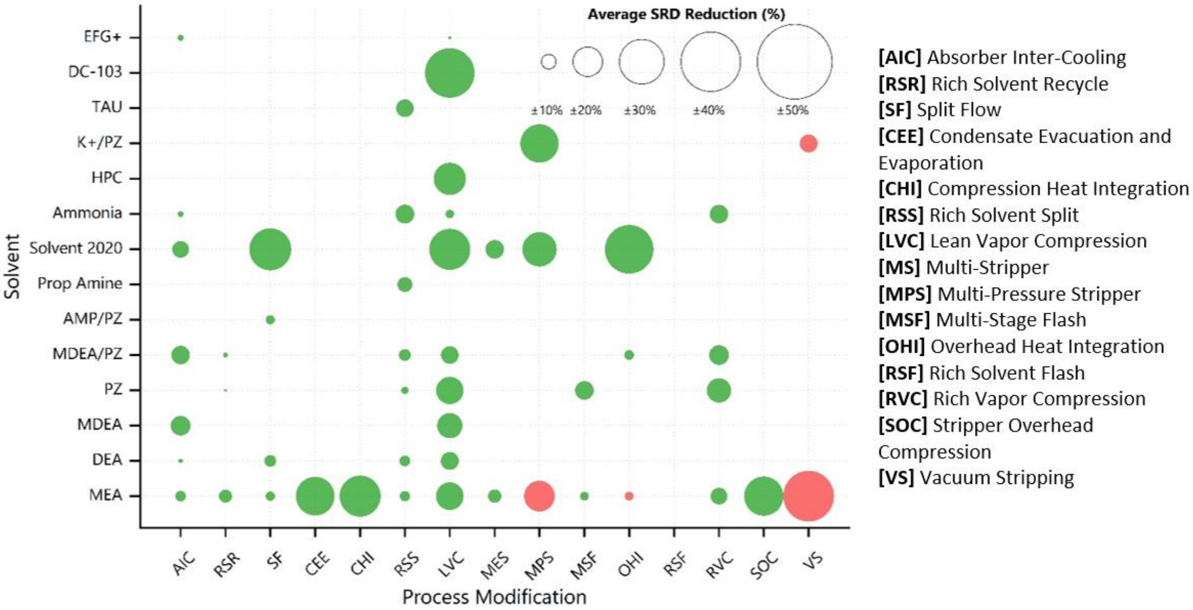


***Figure 2.10** Summary of average percent reductions of specific reboiler duty of selected solvents and individual process modifications available in the literature. The reference baseline is the conventional process of the concerned solvent. Green circles depict a reduction in the SRD, while red circles imply an increase.* ‘Solvent 2020’ is a hypothetical solvent similar in properties to MDEA/PZ [151]

Combinations of process modifications usually yielded high reduction of reboiler duty (**Figure 2.11)**. Some combinations were used more often than others with varying efficiencies, for example, AIC/RSS. Some individual process modifications appeared in combinations more than others as seen in **Figure 2.12**. LVC, RSS, and AIC were the coupled modifications in two- or three-element combinations.

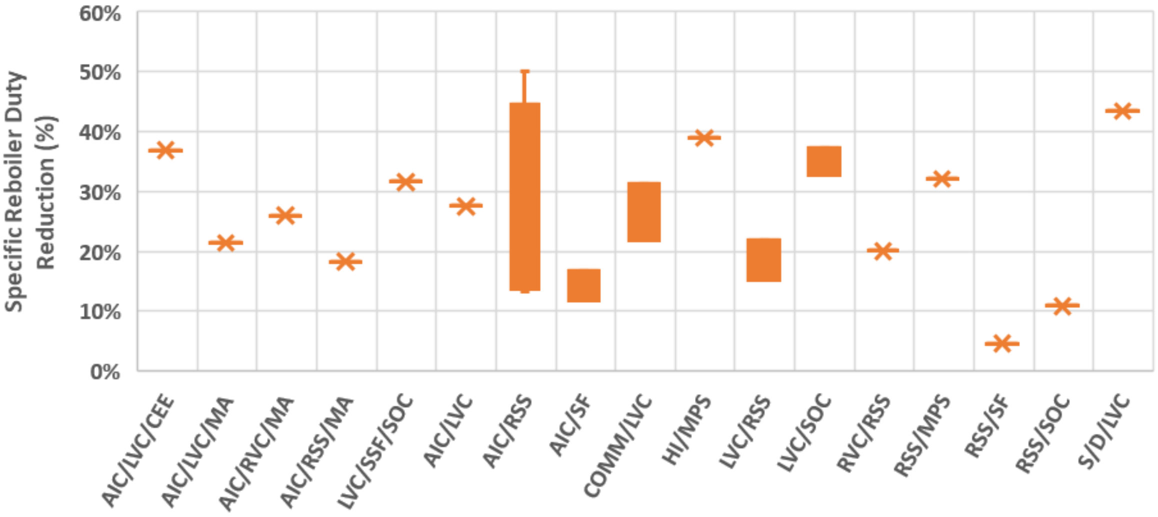


Figure 2.11 *Specific reboiler duty reduction against reported combinations of process modifications. Reference baseline is the specific reboiler duty of the conventional 30 wt.% MEA process (~3.7 MJ/kg$_{CO2}$).*

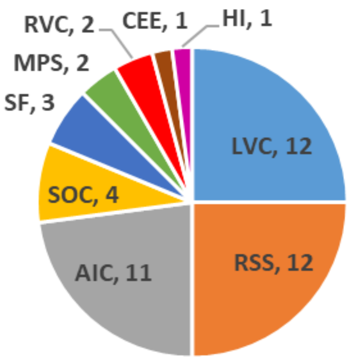


Figure 2.12 *Occurrence of individual process modifications in combinations of two or three.*

2.4 REVIEW OF COMMERCIAL TECHNOLOGIES AND SOLVENTS

2.4.1 CANSOLV®

Shell Cansolv commenced and operated the first commercial amine-based post-combustion carbon capture plant in 2014 at the **Boundary Dam power station**, which is owned by SaskPower [176]. The CCS facility, which installed in Unit 3 of the power station, has achieved 2,413 tonnes per day CO_2 capture rate as of November 2020 [177]. Shell Cansolv has implemented an LVC-modified line-up receiving aflue gas (CO_2 composition 9 –11 vol.%) from a gas-fired boiler (check figure 1 in [97]). The capture unit, which is situated at Lanxess, South Africa, is designed to handle 170 tonnes/day CO_2 captures, yet the working capacity is 120 tonnes/day [178].A pre-scrubber is installed in the upstream before the absorber and the water wash column. The amine-based Cansolv solvent is introduced at the top of the vertical multi-level packed-bed column and leaves as a rich solvent to a lean/rich solvent heat exchanger before entering the stripper. Since the Cansolv absorbent reacts reversibly with CO_2, multi-stage countercurrent contacting is used to achieve maximum loading of the carbon dioxide into the absorbent solution. The required heat in the regeneration column is provided by the reboiler and a mechanical vapour compressor, which compresses the water vapour collected from the flash tank of the lean amine. The condensate of the reboiler is collected, flashed, and routed to the compressor. The compressed vapour is introduced at the bottom of the regenerator to promote more stripping. During the time the absorption liquid is contacting the feed gas in the absorber, and due to the high heat of reaction of the CO_2 capture, small amounts of absorbent maybe vaporized and entrained by the gas. The water wash section serves to capture this entrained absorbent and return it to the solvent solution. Since the Cansolv absorbent has low volatility, the product CO_2 is washed with reflux water to ensure that losses of amine into the product CO_2 are as minimal as possible. The Cansolv DC-103 amine is prone to degradation, which produces unwanted products that need to be removed along with other contaminants present in the lean solvent. A thermal reclaimer unit collects the concentrated contaminants and undesired degradation products upon boiling off the water and amine, which is ultimately diluted with water prior to its disposal.

Moreover, in cases where the flowrates are extremely large, the absorber is expected to be constructed out of concrete and lined with an acid-resistant lining. This arrangement allows significant savings in terms of CAPEX compared to a stainless steel option. This process maintained an average CO_2 capture at 90% and a maximum of 98% capture was achieved, while CO_2 was produced at 98% purity. Also, the use of the mechanical vapour compressor (LVC process modification) can save up to 38% of the required steam for the regeneration column. The process was tested in pilot and testing **facilities such as Aberthaw and SaskPower**. Furthermore, a new solvent, DC-201, is on its way for commercialization. It is expected to reduce the regeneration energy as it requires 20% less steam relative to the DC-103 [98].

2.4.2 KS SOLVENTS

Another established amine-based process is the **KM CDR Process®** (KANSAI MITSUBISHI Carbon Dioxide Recovery Process), which was developed by Mitsubishi Heavy Industries Engineering (MHI ENG) and Kansai Electric Power Company, Inc. (KANSAI). The process utilizes an advanced sterically hindered amine solvent termed **KS-1, KS-2 and KS-3.** The novel KS solvents are reported to be superior to MEA as of less corrosivity, higher loading capacity of CO_2, and less susceptible to degradation (which reduces solvent makeup requirements). MHI claims that KM-CDR circulation rate is 60% of that for MEA, regeneration energy is 68% of MEA, and solvent loss and degradation are 10% of MEA. Although, unit cost of the solvent is higher by a factor of about five. The KS solvent also requires low levels of SO_x and NO_x (typically 1ppm) and therefore requires upstream polishing of flue gas to achieve these input requirements. **The process has been implemented as part of the Petra Nova Project, Texas** (currently, the largest operating PCC of CO_2 system for coal-fired flue gas) [179]. The CO_2 capture capacity of the plant is designed as 4776 tonnes/day, with a capture efficiency of 90%. The KM CDR Process® follows a typical process flow but with enhanced stripping operation. The regeneration is claimed to be enhanced using advanced heat integrations with the lean solvent and steam condensate. The steam consumption is 1.3 tonnes steam/t_{CO2} at 3 barg steam pressure [180].

2.4.3 FLUOR'S "ECONAMINE"

Fluor's Econamine FG Plus^{SM} technology is an advanced process that is claimed to the reboiler duty by 30% compared to a conventional process [3]. The Econamine GF Plus^{SM} process utilizes AIC, advanced solvent formulation, LVC, and heat recovery and integration to lower the overall energy consumption of the process [181]. A large-scale demonstration plant at WA Parish using EGF+ was successfully implemented with more than 4700 tonnes/day of CO_2 produced [182]. The LVC process modification was estimated to reduce the consumption of steam by 10-12%, while the AIC was estimated to achieve 5-10% energy savings. Reddy *et al.* [121] investigated the LVC process modification using Flour's Econamine FG Plus^{SM} process at Uniper's Wilhelmshaven coal power plant in Germany. The reboiler duty reduction was found to be between 2 and 8%. Shell Cansolv solvent DC-103 also tested the LVC using a mechanical vapour compression to recompress the lean vapour in which the steam consumption was reduced by 33 – 38% [97].

2.5 EMERGING AND NOVEL SOLVENTS

2.5.1 PILOT-SCALE PLANT TRIALS OF SELECTED SOLVENTS

Several solvents were suggested in lieu of MEA (see **Section 1** in this report) but few were experimentally tested in a pilot plant. Singh *et al.* [183] conducted a screening of solvents before testing them in **Shell's pilot plant A**mine **S**creening **Ap**paratus (ASAP) unit. A proprietary amine, AMP, AMP/PZ, and AMP/HMDA amine-based solvents were tested and compared to 30 wt.% MEA. The absorption was carried out at 313 K and 130 kPa with a varying CO_2 inlet concentration (5 and 10 %) while the regeneration was at 393 K and 200 – 220 kPa with 90% CO_2 capture efficiency. The new solvent (proprietary amine) exhibited the best performance measured by a reduction of the reboiler duty of almost half of that of MEA for both CO_2 inlet concentrations. The AMP/HMDA (26.7%/11.9%) blend also showed promising results with 21 – 29% reduction of reboiler duty. AMP and AMP/PZ achieved 9.7% and 19.4% reductions, respectively.

Harbou *et al.* [184] tested a proprietary amine (secondary amine) and AMP/EDA aqueous solution in a pilot plant as part of **EU-project CESAR**. The study optimised the process in terms of the L/G ratio that corresponds to the lower reboiler duty and compared the performance of the new solvents to MEA. With 4.1 $GJ.t_{CO2}^{-1}$ for the MEA process, the reboiler duty was reduced to 3.4 $GJ.t_{CO2}^{-1}$ and 3.7 $GJ.t_{CO2}^{-1}$ by the proprietary amine (L/G 1.6 kg/kg) and AMP/EDA solvent (1.4 kg/kg), respectively.

Aruno *et al.* [185] tested 3-(methylamino)Propylamine Sarcosine (SARMAPA) in a pilot plant with flue gas flow rate 150 Nm^3/h and capture capacity of 10 $kg_{CO2}.h^{-1}$. The amino acid-based solvent is reported to reduce the reboiler duty to half compared to MEA but with a lower absorption rate. Other amino acid salts, aqueous sodium glycinate (NaGly) and aqueous potassium glycinate (KGly), were also tested for PCC from hard coal flue gas in the CO_2 SEPPL pilot plant in Austria [186,187]. The reboiler duty required for the regeneration of these solvents scored 5 – 5.7 $GJ.t_{CO2}^{-1}$; more than 40% of the conventional 30 wt.% MEA process. Albeit the low absorption enthalpy compared to MEA, the regeneration energy requirement did not show the expected decrease. The authors attributed such observation to the low kinetics and low partial pressure of CO_2 at the top of the stripper. Similarly, 3.5 M potassium sarcosine

(KSAR) was tested in **SINTEF Lab Pilot Plant** scoring significantly higher energy requirements (~6.5 $GJ.t_{CO2}^{-1}$) compared to MEA [188].

2.5.1 CHILLED AMMONIA PROCESS

As an alternative to MEA, aqueous ammonia is a promising solvent for PCC of CO_2. Ammonia-based solvents require less regeneration energy than aqueous MEA reflected by the lower heat of absorption. Also, as the stripping process is conducted at higher pressure, smaller-sized units are needed, and the captured CO_2 would need less compression. The characteristics of the ammonia-based solvent allows for higher absorption capacity compared to MEA, an added advantage for the novel solvent. Additionally, the absorption operating temperature is lower, in which the flue gas is pre-cooled resulting in less volumetric flow rate. This allows operating with a smaller absorber and lower pressure drop. Further reduction of the energy required can achieves at locations with abundant cooling water [189].
From a solvent management perspective, ammonia is more tolerant than MEA as it does not degrade in the presence of oxygen and is generally cheaper. Yet, ammonia is more volatile and is less reactive than MEA, which can limit its applicability and economic feasibility [190]. These merits have enticed many companies and researchers to test the viability of aqueous NH_3 solvent in a pilot-scale plant. Alstom has been pioneering in the Chilled Ammonia Process (CAP), which has led to many pilot-scale implementations [191]. Alstom's Chilled Ammonia Process (CAP) is a carbonate/bicarbonate process, in which the absorber is operated at low temperatures (as low as 273 – 283 K) yielding a slurry of ammonium bicarbonate. This rich slurry is then regenerated at 200 – 400 kPa producing ammonium carbonate. The regeneration of the solvent primarily consists of the main stripper with a reboiler and a condenser. It is expected that the regeneration unit would be similar in principle to an amine desorption tower. The key assumption should be that there will not be carbonate solids present in the stripper and reboiler section. This is achieved by dissolution of the solids in a regenerative heat exchanger. Alstom process was implemented in the **Technology Centre of Mongstad** for PCC of CO_2 [192], which was designed to treat flue gas sourced from refinery operations in addition to a combined heat and power plant. The flue gas from the refinery off-gas and combined heat and power plant yielded a CO_2 composition of 12 – 13 vol.% and 3 – 4 vol.%, respectively. The total height of the absorber is 29 m with 3 main sections. The removal efficiency ranged between 80 and 87% with a 99.9% CO_2 purity. These preliminary tests validated the viability of the process and paves for further optimization of the process and economic analysis.

An aqueous NH_3-based PCC of CO_2 pilot plant was operated at the **Munmorah black coal-fired power station in Australia** [116]. The design of the pilot plant includes two absorbers (can be connected in parallel or series, see **Section 2.3.1** in this report), stripper, heat exchangers, and a pre-cooling system to serve the low temperatures of the absorbers. The process is essentially similar to Alstom's process. A direct contact cooler precedes the absorber columns, which brings the temperature to 288 – 293 K. The absorbers in this case are connected in parallel. Each absorber (2 – 3.9 m height) is equipped with its own washer column. The combined rich solvent stream from both absorbers enters the top of the stripper, which is heated by a steam-powered reboiler. The flue gas flow rate varies between 650 – 1000 $kg.h^{-1}$ with a CO_2 composition from 8.5 to 12 vol.%. The NH_3 concentration in the solvent is varied to a maximum of 6 wt.%. The absorption is carried out at 101 – 150 kPa with a 50 – 134 L/min solvent flow rate. The stripping is carried out at 363 – 423 K and 300 – 850 kPa. The pilot plant in operation achieved more than 85% CO_2 capture with 99-100% purity. Yet, the use of diluted NH_3 solvent resulted in an increase of the regeneration energy scoring 4 – 4.2 MJ. kg_{CO2}^{-1} CO_2 captured, which is higher than the typical reported values for the MEA process. The use of higher concentrations of ammonia in the aqueous solvent might yield better performance in regard to the required regeneration energy and might enhance the loading of the solvent in the absorbers.

Darde *et al.* [193] evaluated an aqueous ammonia process (10 wt.%) with an inlet CO_2 concentration of 12 vol.% and 45 kmol/h flue gas flow rate. The flue gas and lean solvent entering the absorber are both cooled down to 7°C. The process also includes a solid/liquid separator right after the absorber, where the rich solvent separates and yields 22 wt.% solid phase (ammonium bicarbonate). The liquid phase is merged with the lean solvent while the solid phase is heated to dissolve the ammonium bicarbonate prior to the main heat exchanger. With 10 bar stripping pressure and 90% capture, the regeneration energy was estimated to reach 2.07 MJ.kg_{CO2}^{-1} [193]; significantly lower than the conventional process.

A special combination of modifications was employed for a chilled ammonia process that incorporated a combined removal of $NOx/SO_2/CO_2$. This process employed a two-stage CO_2 absorption unit and an advanced flash stripping unit [194]. The regeneration energy was reduced by 42% while the CO_2 avoided cost decreased by 42.8%.

2.5.2 PHASE CHANGE SOLVENT PROCESS

Phase change solvents are emerging candidates to supersede typical MEA-like solvents due to their anticipated superior performance. These solvents undergo a phase change corresponding to a change in the process conditions, which allows the solvent to split to rich- and lean-CO_2 phases without the need of thermal intervention. As such, the amount of solvent is sent to the stripper is reduced; hence, the total regeneration energy is expected to drop. Many solvents are susceptible to yield two phases upon the absorption, including amine-based blends, ammonia, and amino acids [25]. After reacting with CO_2, ammonia and amino acid solvents can exhibit a solid-liquid phase change, in which the solid part is the rich part that can be separated via a cyclone or other separation units. The rich solid slurry would then be heated to dissolve it before it is sent to the rich/lean heat exchange and the stripper. The liquid lean phase would be merged with the lean solvent that is coming from the bottom of the stripper, which is then introduced to the top of the absorber. Liquid/liquid phase change, which is mostly encountered with amine-based blends, would essentially follow the same scheme of the solid-liquid phase separation. Yet, liquid-liquid phase is the closest for a retrofit solution in the existing amine-based facilities [195]. Modifications to the process appear to be minimal, as simple as adding a mechanical separation for the rich solvent, unlike a liquid-solid phase change, which is more complex to handle [195]. A liquid-liquid phase separation (LLSP) is desired to occur at higher temperature of the absorption, yet as close as possible to it. This suggests a phase separation unit to be placed after the lean/rich heat exchanger in a typical PCC of CO_2 amine-based process flow.

Phase change solvents are still under screening and bench-scale experiments. Some candidates managed to be tested in pilot-scale plants, such as the **DMX-1 solvent**, which is a blend of amines exhibiting a lower critical solution temperature (LCST) above the absorption temperature [196]A **DMX pilot plant** (ENEL at Brindisi) was developed by IFP Energies nouvelles (IFPEN), which showed a potential for scalability [197]. The process modification introduced a decanter after the rich/lean solvent heat exchanger prior to the stripper. The DMX blend yielded an LLSP temperature above 373 K and the desorption was conducted at a maximum temperature 423 K and 500 kPa. The reboiler energy consumption scored 2.5 $GJ.t_{CO2}^{-1}$, in which it could be improved to 2.3 $GJ.t_{CO2}^{-1}$ as per the theoretical calculations. The **D**MX^{TM} **D**emonstration in **D**unkirk (The “3D” project) was recently launched by 11 European stakeholders [198]. The industrial-scale process is expected to capture more than 1 million tonnes/year of CO_2 by 2025.

Pinto *et al.* [199] tested a 5M DEEA/2M MAPA mixture in the Gløshaugen **(NTNU/SINTEF) pilot plant**. This mixture forms two liquid phases upon the loading of CO_2. A separator was added after the absorber column to separate the phases in which the light phase (lean solvent) was sent to the absorber while the heavy phase (rich solvent) was sent to the rich/lean heat exchanger followed by the stripper. The new configuration with the novel phase change solvent reduced the reboiler duty from 3.7 $GJ.t_{CO2}^{-1}$ (for 30 wt.% MEA) to 2.2 – 2.4 $GJ.t_{CO2}^{-1}$ and a rich solvent loading of 1.04 mol_{CO2}/mol_{MAPA}, which is more than double that of MEA. The authors suggested to install a pre-cooler for a better control of temperature in the absorber and to replace the stripper with flash vessels as the CO_2 ought to strip easily from the heavy rich phase. Further pilot tests are required to assess the viability of scalability and confirm such promising findings.

Fernandez *et al.* [200] proposed the **DECAB process** for phase change solvents, which consists of a spray column before the absorber column. The concept is to react the solvent with CO_2 in the spray column and precipitate the insoluble slurry (rich) of the amino acid in which the flue gas is sent to the conventional absorption column for further capture. The potassium salt of taurine (6M) was simulated in the conceptual design of DECAB and achieved 3.2 $GJ.t_{CO2}^{-1}$ reboiler duty and 0.41$mol_{CO2}/mol_{Taurate}$ rich loading; a promising result compared to the conventional process. Further simulation results with aqueous solutions of potassium taurate (TAU) and potassium alanate (ALA) were conducted on DECAB and DECAB Plus processes, the latter which was complemented with LVC process modification [146]. With the LVC, TAU achieved 43.4% reduction of the reboiler duty showing the highest enhancement of the absorption process using phase change amino acid-based solvents.

2.5.3 WATER-LEAN SOLVENT PROCESS

Aqueous solvents pose a high energy requirement primarily due to the water content, which incurs a high regeneration energy and a great load on the reboiler. A plausible remedy is to substitute the water with co-solvents with lower heat capacities. The quest of finding suitable water-lean solvents requires a greater attention to the solvent chemistries, which can get complicated with the absence of water from the solvent matrix. Non-aqueous organic amine blends, aminosilicones, switchable carbamates, amino acids in organic solvents, and alkylcarbonates are among the prominent solvent systems investigated in the literature [201].

Still, water-lean solvents are in the development phase and are immature for a large-scale implementation.

A newly developed water-lean amine-based solvent, N-(2-ethoxyethyl)-3-morpholinopropan-1-amine (2-EEMPA), has been tested in a laboratory-scale continuous flow system to capture CO_2 from a flue gas simulant (15% CO_2 composition) [202]. The experimental system maintained 90% capture efficiency for the duration of 40 hours. Techno-economic analysis of the conventional process using 2-EEMPA have shown a specific reboiler duty of 2.27 $MJ.kg_{CO2}^{-1}$, which is around 30% less than MEA. Yet, as of the increased viscosity and circulation rate of the solvent, the capital costs are higher than MEA. A process simulation of a multi-modified process flowsheet employing LVC, rich solvent pre-heating, and SIH has shown the least specific reboiler duty estimated as 2.0 $MJ.kg_{CO2}^{-1}$ [202]. More water-lean solvents are expected to emerge. Process configurations/conditions can be modified to accommodate for the different behaviour of these solvents compared to the aqueous solvents. Some water-lean solvents can also undergo phase change, which should be also be incorporated in the process design.

2.6 REVIEW OF CAMPAIGNS OF DIFFERENT PROCESS DESIGNS

This section showcases pilot-scale campaigns of several process designs and commercial technologies. The process configurations, solvent used, application of the design, conditions of the testing campaign, CO_2 capture efficiency, and specific reboiler duty are all depicted in **Table 2.2**.

Table 2.2 *Pilot-scale campaigns of different processes configuration.*

Process Configuration	Source of Flue Gas	Flue Gas Flow Rate (kg/h)	CO_2 Feed Content (vol %)	Solvent	Absorption Conditions (°C/kPa)	Stripping Conditions (°C/kPa)	Rich CO_2 Loading (molar basis)	CO_2 Removal Efficiency (%)	Specific Reboiler Duty (MJ/kg CO_2)	Ref.
Advanced Amine Process	Hard Coal	2500-5000 (m^3/h)	10-12	UCARSOL™ FGC-3000	28-40	130		90%	2.60	[150]
AIC	Coal-fired power plant	4762.72	11-13.5	Amine	30-70/100	/160-340		85-95%	2.70	[119]
AIC	Hard coal fired power station	260-300	13.50	MEA (30 wt.%)	40-60	1105-108	0.42-0.50	80-88%	3.79-4.15	[120]
AIC	Hard coal fired power station	14000 (m^3/h)	13.10	Fluor Econamine FG Plus^{SM}				92%		[121]
MA	Brown-coal fired power station	90	10-11	MEA (30 wt.%)	33.68-55.42/103.05-105.34	106.49-113.41/103.05-151.77	0.1017 (mass basis)	92%	5.90	[115]
MA	Black coal fired power station	780-820	8.5-12	Ammonia (1.9-5.8 wt.%)	10-30/101-105	90-105/300-850	0.3-0.46 (mass basis)	45.2 - 87.9%	4-4.2	[116]

Process Configuration	Source of Flue Gas	Flue Gas Flow Rate (kg/h)	CO_2 Feed Content (vol %)	Solvent	Absorption Conditions (°C/kPa)	Stripping Conditions (°C/kPa)	Rich CO_2 Loading (molar basis)	CO_2 Removal Efficiency (%)	Specific Reboiler Duty (MJ/kg CO_2)	Ref.
MA	Coal-fired power plant	650-1200	8.5-12	Ammonia (0-6 wt.%)	10-30/101-150	90-150/300-850		85%		[118]
SF	Hard coal fired power station	260-300	13.50	MEA (30 wt.%)	40-60	109-110	0.48-0.53	85-89%	3.77-3.91	[120]
MSF				PZ (8m)		150	0.4			[132]
LVC (Cansolv)	Gas-fired boiler	4700	9-11	DC-103				90%	2.33	[97]
MS			12-16	MEA (30 wt.%)	40-50	65-75/150-350	0.48-0.52	90%	2.33-3.73	[130]
MS			12-16	Amine	40-50	65-75/150-350	0.44-0.51	90%	2.1-3.5	[130]

Process Configuration	Source of Flue Gas	Flue Gas Flow Rate (kg/h)	CO_2 Feed Content (vol %)	Solvent	Absorption Conditions (°C/kPa)	Stripping Conditions (°C/kPa)	Rich CO_2 Loading (molar basis)	CO_2 Removal Efficiency (%)	Specific Reboiler Duty (MJ/kg CO_2)	Ref.
RSS	Hard coal-fired power plant	285	13.34	MEA (30 wt.%)	40/130	109/130	0.53	88%	3.99	[157]
CAP Process (Alstom)	Combined Heat and Power Plant	47400 (m^3/h)	3-4	Ammonia		/2000		85%		[192]
Multi-Mod: RSS + Multi-Absorber Feed	Hard coal-fired power plant	285	13.37	MEA (30 wt.%)	40/130	109/130	0.53	90%	3.78	[157]
Multi-Mod: AIC + RSS	Coal-fired flue gas		14.00	ION (amine-based)	68			95%	2.50	[156]
Multi-Mod: RSS + SF	Hard coal-fired power plant	285	13.29	MEA (30 wt.%)	40/130	109/130	0.54	89%	3.81	[157]
PostCapTM, Lean Vapor Compression		230 (m^3/h)		Amino Acid/PostCap™				85-95%	2.70	[203]

Process Configuration	Source of Flue Gas	Flue Gas Flow Rate (kg/h)	CO_2 Feed Content (vol %)	Solvent	Absorption Conditions (°C/kPa)	Stripping Conditions (°C/kPa)	Rich CO_2 Loading (molar basis)	CO_2 Removal Efficiency (%)	Specific Reboiler Duty (MJ/kg CO_2)	Ref.
Separator Post-Absorber		88-90 (m^3/h)		DEEA/MAPA (5M/2M))	42.7-64.8/103.1-107.7	107-117/69.8-75.7	0.9-1.1		2.2-2.4	[199]
Separator Post-Absorber	Coal-fired power plant	10000 (m^3/h)	13.04	DMX		150/500		90%		[197]
Econamine FG Plus^{SM}	Hard coal fired power station	14010 (m^3/h)	13.10	Fluor Econamine FG Plus^{SM}				88%		[121]

3. REVIEW OF DEGRADATION, CORROSION, AND PROCESS EMISSIONS (TASK3)

Objective: Perform a detailed review of degradation and corrosion studies exhibited by the solvents included in **Task 1**, along with process emissions and amine consumption, focused on:

1. Degradation and corrosion mechanisms.
2. Factors determining process emissions and amine consumption.
3. Preventive measures and their effectivity within a solvent management strategy.

In line with the required information for **Task 3**, in this section, a summary on information collected on degradation, corrosion, and process emissions associated with utilisation of solvents, particularly aqueous amines, as well as factors or process conditions detrimental for the aforementioned solvent management components is presented. This information is populated in the **CO_2SOLV** database, as shown in **Figure A4 in ANNEX I**.

3.1 SOLVENT DEGRADATION: A SUMMARY

The degradation of solvents is among the most prevailing operational issues associated with the utilisation of alkanolamines for CO_2 capture and gas separation applications. With this phenomenon, the stability of the solvent is reduced, leading to its breakdown and transformation into products from which they are not easily regenerated. The occurrence of amine degradation reduces the solvent absorption capacity, increases solvent consumption, along with the occurrence of operational issues such as foaming, corrosion, increased solvent viscosity, fouling along with decreasing the operational integrity of the processing facility from the reaction of degradation products with the process equipment material [88,204–207]. Additionally, it is postulated that MEA makeup accounts for 10% of the total cost of CO_2 capture, with the major contributor being solvent degradation [208]. The mechanism for alkanolamine degradation occurs either through thermal or oxidative degradation, the location of each degradation type in a typical PCC process is depicted in **Figure 3.1**, while a summary of available information on amine degradation, testing scale, and purpose of the studies is provided in **Table 3.1**. The majority of the works available in the literature focused on the identification of degradation products for a variety of amines along with the proposition of a reaction mechanism explaining the pathway for the formation of these degradation products. The remaining works in the literature focused on the effect of degradation on the processing aspect.

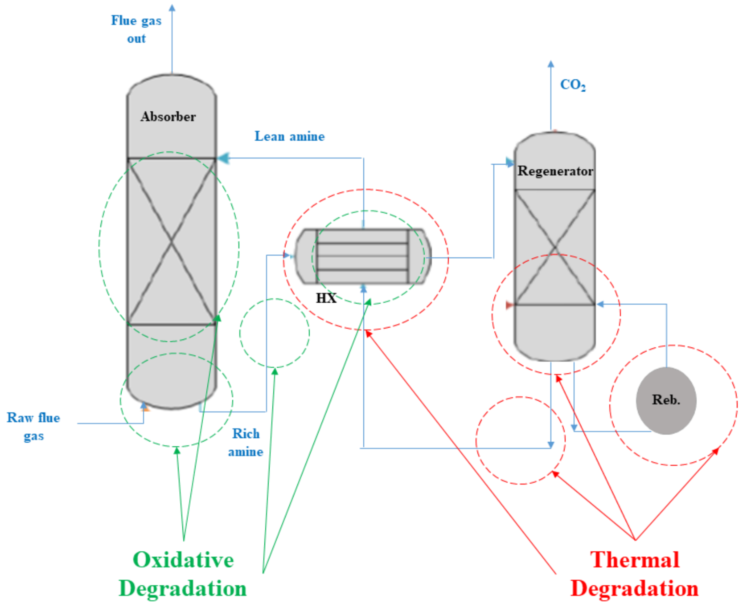


Figure 3.1 *Location of thermal and oxidative degradations in a typical PCC process.*

Table 3.1 *Summary of available published works on amine degradation related to PCC.*

Purpose	Solvents	Testing Scale	Type of degradation	Ref.
Identification of degradation products, reaction mechanism and kinetics	MEA, DEA, MDEA, AMP, PZ, DETA, MAPA, EDA, HEEDA, AEP, HEP, 1-MPZ, DGA, 2-MPZ, HMDA, MEA/PZ, MEA/DGA, MDEA/PZ, MEA/AMP, PZ/AMP, PZ/2-MPZ, HEP, BAE, DAB	Lab-Scale	Thermal and oxidative	[102,204–207,209–237]
Effect of process conditions on degradation	MEA	Process simulation	Thermal and oxidative	[238,239]
Monitoring of amine degradation and losses	MEA, KS-1, CANSOLV	Pilot-Scale	Thermal and oxidative	[102,240–244]

Thermal degradation of alkanolamines involves the breakdown of the carbamate form of the alkanolamine due to the exposure to high temperatures (373 K and higher) and high CO$_2$ partial pressures in the stripper during solvent regeneration, which elevates the kinetic rate of the degradation reactions otherwise suppressed during the low temperature absorption step [88,204–207,222,223,231,232]. Throughout the PCC process, thermal degradation primarily occurs in the regeneration column packing, sump, reboiler and solvent reclaimer (if utilised), along with the piping connecting the regeneration column and the cross-heat exchanger. Additional works established that the cross-heat exchanger is another possible location for thermal degradation as the temperature can increase up to 373 K. Several works are available in the literature on lab-scale testing on identifying main thermal degradation products, reaction mechanism, and kinetic rates of thermal degradation for several aqueous amines such MEA, DEA, MDEA, AMP, and PZ, along with several blended amines [88,218,221–223,229–232,243,245]. The literature remains limited with information on the degradation of novel alkanolamines such as water-free/water-lean solutions, as required before they can be implemented at large scale, being one of the identified gaps in this study.

Conversely, **oxidative degradation** involves a chemical reaction between the alkanolamine, and impurities commonly found in the raw flue gas stream, such as O_2, SO_x, NO_x, fly ash, metal oxides, HF and HCl [209,210,215–218,220,225,226,228,235–237]. The reaction between the amine and impurity results in the breakdown of the N-C bond in the amine and formation of O-C bond resulting in a number of degradation products that can react with each other, with O_2, or with the amine to produce additional degradation products. Depending on the type of impurity involved in the oxidative degradation reaction, different classes of degradation products can be formed, which have been mostly characterized for MEA. Oxidative degradation commonly occurs in the absorber sump, packing, piping leading to the cross-heat exchanger, and the cross-heat exchanger.

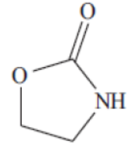
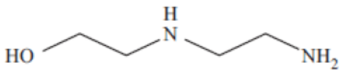
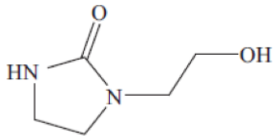
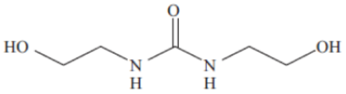
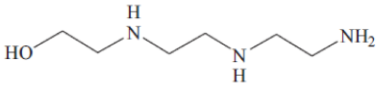
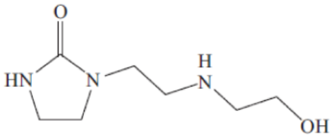
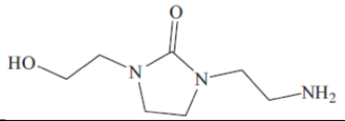
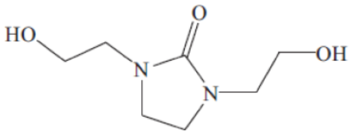
Lab-scale studies have demonstrated the effect of several **process parameters on the increase in degradation rates** [39,204,206,209–211,213,215–218,220,224–226,228,234–238,246]. In the case of thermal degradation, the rate is dependent on the residence time in the regeneration column sump, reboiler temperature, CO_2 loading in the rich solvent, and amine concentration, with their increase resulting in an increased thermal degradation rate. In the case of oxidative degradation, it was found that its rate is affected by the concentration and type of impurity present in the raw flue gas, CO_2 loading in the rich stream, absorber temperature, amine concentration, and presence of metal ions that catalyses the degradation reaction. Up to date, the effect of these parameters has been mainly identified and tested on the standard benchmark solvent (aqueous MEA) [210,213,214,240–242,245,246]. It was determined from several pilot plant testing that the total loss of amine under these conditions was in the range of 0.3 – 1.5 kg MEA per tonne of CO_2 captured, with more than 60% of these losses being attributed to oxidative degradation. However, the long term-effect on the process has not been explored [238,240–242,244].

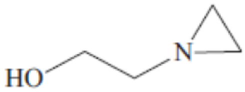
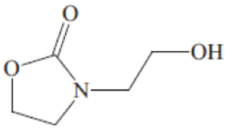
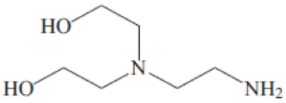
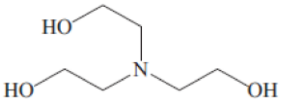
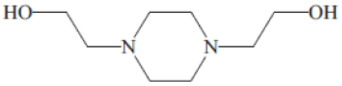
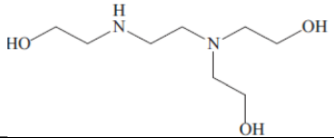
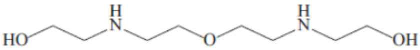
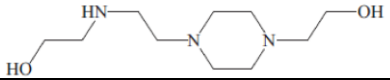
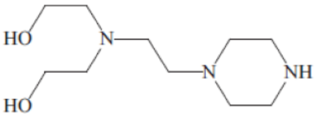
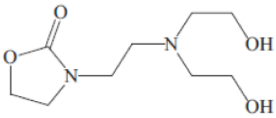
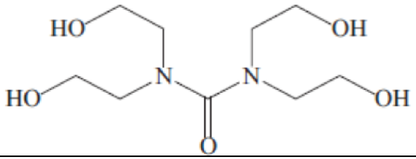
3.2 MECHANISM OF DEGRADATION OF ALKANOLAMINES

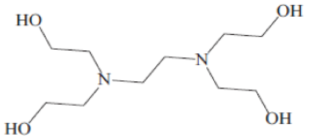
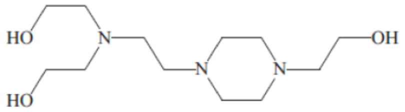
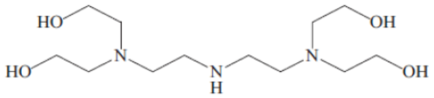
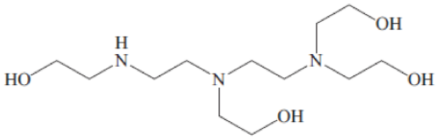
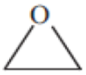
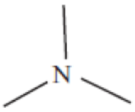
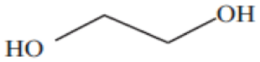
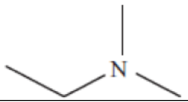
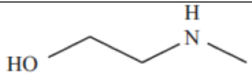
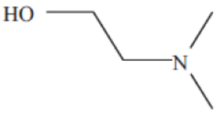
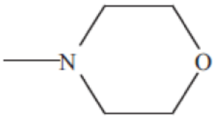
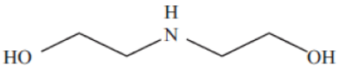
3.2.1 MECHANISM OF THERMAL DEGRADATION

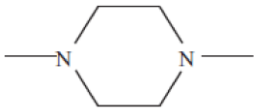
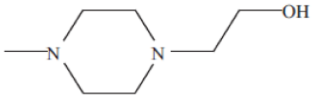
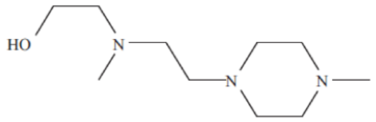
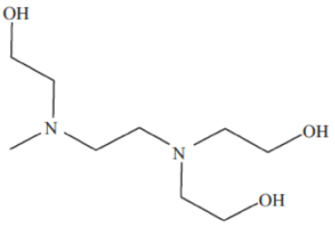
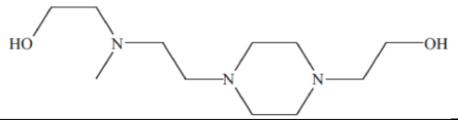
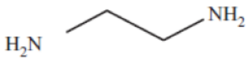
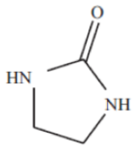
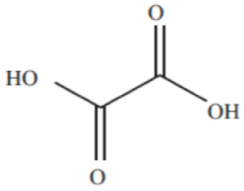
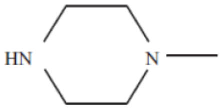
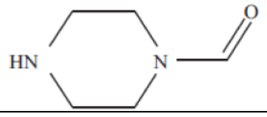
Among the wide variety of available alkanolamines, MEA remains the most widely studied alkanolamine for its thermal degradation, as it is an industry benchmark solvent. The majority of alkanolamine thermal degradation occurs in the stripper column of a typical PCC configuration (see **Figure 3.1**) due to the high temperature, which is a constant factor in studying thermal degradation [231,246]. The list of thermal degradation products identified in the literature for the main amines used in industry (MEA, DEA, MDEA, AMP, and PZ) is included in **Table 3.2**.

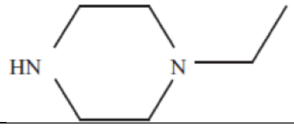
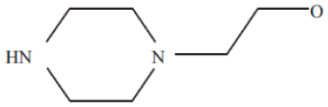
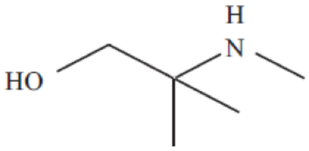
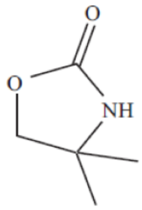
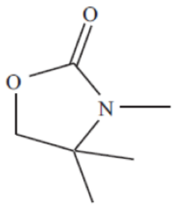
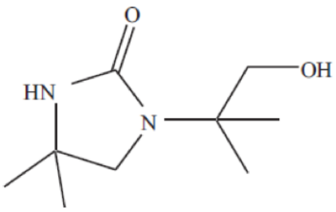
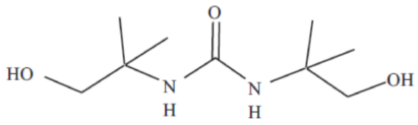
Table 3.2 *List of thermal degradation products for MEA, DEA, MDEA, AMP and PZ. References:* [88,204,209,211,215,221,223,225,228,231,232,245,246].

Solvent	Degradation Product Name	Degradation Product Chemical Structure
MEA	Oxazolidin-2-one (OZD)	
MEA	N-(2-hydroxyethyl)ethylenediamine (HEEDA)	
MEA	N-(2-hydroxyethyl)imidazolidin-2 one (HEIA)	
MEA	N, N'-bis-(2-hydroxyethyl)urea	
MEA	N-(2-hydroxyethyl)diethylenetriamine	
MEA	N-[2-[(2-hydroxyethyl)amino] ethyl] imidazolidin-2-one	
MEA	N-(2-aminoethyl)-N'-(2-hydroxyethyl)imidazolidin-2-one (AEHEIA)	
MEA	N,N'-bis(2-hydroxyethyl)imidazolidin-2-one (BHEI)	
DEA	Monoethanolamine (MEA)	
DEA	N-(2-hydroxyethyl)aziridine (HEM)	

Solvent	Degradation Product Name	Degradation Product Chemical Structure
		
DEA and MDEA	N-(2-hydroxyethyl)oxazolidin-2-one (HEOD)	
DEA	N,N-bis(2-hydroxyethyl)ethylenediamine	
DEA and MDEA	Triethanolamine (TEA)	
DEA and MDEA	N,N’-bis(2-hydroxyethyl)piperazine (BHEP)	
DEA and MDEA	N,N,N’-tris(2-hydroxyethyl)ethylenediamine (THEED)	
DEA	Bis-(2-(2-hydroxyethylamino)ethyl)ether (BHEAE)	
DEA	N-(2-hydroxyethyl)-N’-(2-(2-hydroxyethylamino)ethyl)piperazine (HEAEHEP)	
DEA	N-2-[bis(2-hydroxyethyl)-amino]ethylpiperazine (HEAEP)	
DEA	N-2-[bis(2-hydroxyethyl)-amino]ethyloxazolidin-2-one (HAO)	
DEA	N,N,N’,N’-tetrakis(2-hydroxyethyl)urea (TEHEU)	
DEA and MDEA	N,N,N’,N’-tetrakis(2-hydroxyethyl)ethylenediamine (TEHEED)	

Solvent	Degradation Product Name	Degradation Product Chemical Structure
		
DEA	N-2-[bis(2-hydroxyethyl)-amino]ethyl-N’-(2-hydroxyethyl)piperazine (HAP)	
DEA	N,N,N’,N’-tetrakis(2-hydroxyethyl)diethylenetriamine (THEDT)	
DEA	N,N,N’,N’-tetrakis(2-hydroxyethyl)diethylenetriamine (i-THEDT)	
MDEA	Methanol	H_3C-OH
MDEA	Ethylene Oxide (EO)	
MDEA	Trimethylamine (TMA)	
MDEA	Ethylene glycol (EG)	
MDEA	N,N-dimethylethylamine (DMEA)	
MDEA	N-methylethanolamine (MAE)	
MDEA	N,N-(dimethyl)ethanolamine (DMAE)	
MDEA	N-methylmorpholine (MM)	
MDEA	Diethanolamine (DEA)	

Solvent	Degradation Product Name	Degradation Product Chemical Structure
MDEA and PZ	N,N'-dimethylpiperazine (DMP)	
MDEA and PZ	N-(2-hydroxyethyl)-N'-methylpiperazine (HMP)	
MDEA	N-[2-(2-hydroxyethylmethylamino)ethyl]-N'-methylpiperazine (HEMAEMP)	
MDEA	N-methyl-N,N',N'-tris(2-hydroxyethyl)ethylenediamine(MTHED)	
MDEA	N-[2-2-hydroxyethylmethylamino)ethyl]-N'-(2-hydroxyethyl)piperazine (HEMAEHEP)	
PZ	Ethylenediamine	
PZ	Imidazolidin-2-one (2-Imid)	
PZ	Oxalic acid	
PZ	N-methylpiperazine (MPZ)	
PZ	N-formylpiperazine (FPZ)	

Solvent	Degradation Product Name	Degradation Product Chemical Structure
PZ	N-ethylpiperazine (EPZ)	
PZ	N-(2-hydroxyethyl)piperazine (HEP)	
AMP	N,2,2-trimethylethanolamine	
AMP	4,4-Dimethyloxazolidin-2-one	
AMP	N,4,4-trimethyloxazolidin-2-one	
AMP	4,4-Dimethyl-1-hydroxytertiobutylimidazolidin 2-one	
AMP	l,3-Bis-(2-hydroxy-l, l-dimethylethyl)urea	

A limited number of works in the literature examined solely the effect of high temperature on the thermal degradation of MEA (without the presence of CO_2), identifying the degradation of MEA through dealkylation, dimerization and cyclisation, however, no mechanism was proposed. The major MEA thermal degradation products under these conditions were ammonia and N-(2-hydroxyethyl) ethylenediamine (HEEDA) merely from the effect of high temperature [88,211,218,246].

The remainder of literature on thermal degradation products and mechanisms focused on the **dual effect of high temperature and high CO_2 partial pressure in the stripper column**, establishing the degradation of alkanolamines through the formation of successive degradation compounds. Focusing on the thermal degradation of MEA, the main degradation products identified under these conditions are: Oxazolidin-2-one (OZD), N-(2-hydroxyethyl) ethylenediamine (HEEDA), N-(2-hydroxyethyl)imidazolidine-2-one (HEIA), and N,N'-bis-(2-hydroxyethyl)urea, as summarised in **Table 3.2**. The proposed mechanisms for thermal degradation of MEA in the presence of CO_2 are shown in **Figure 3.2** [88,218,231,232,245,246]. As an initial step, MEA reacts with CO_2 to form a carbamate which occurs in the absorber column (Reaction 1), which is subsequently transformed into oxazolidin-2-one (OZD) (Reaction 2). Subsequently, OZD can react with another MEA molecule to form a diamine, particularly HEEDA (Reaction 3). This is followed by the formation of another carbamate from the reaction between HEEDA and CO_2, followed by formation of HEIA through intramolecular cyclisation (Reaction 4), which is a very stable degradation product that can accumulate in the solution. Lastly, minor degradation products such as urea can also be obtained through the reaction between carbamates and amines (Reaction 5).

The thermal degradation of another primary alkanolamine, AMP, though sterically hindered, was also defined through the same degradation mechanism for MEA shown in **Figure 3.2**. However, due to the steric hindrance of AMP compared to MEA, the limiting step is the carbamate formation as steric hindrance decreases carbamate stability [231–233]. Owing to this, studies suggest that AMP is less liable to thermal degradation than MEA.

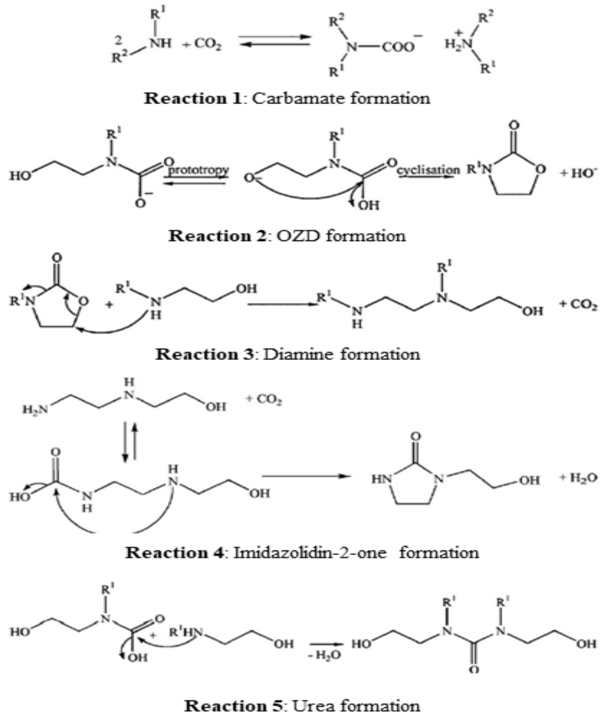


***Figure 3.2** Mechanisms for MEA thermal degradation* [204]**.**

DEA is another alkanolamine extensively examined for its thermal degradation products due to its utilisation in gas separation. It was reported that initial DEA solutions contained minor quantities of MEA (which is one of the possible degradation products of DEA through alkylation/dealkylation), hence, degradation products from MEA were also detected. The mechanisms for the thermal degradation of DEA and its major products are shown in **Figure 3.3** [204,224,225,246]. The initial step in the degradation of DEA is the formation of carbamate in the presence of CO_2, which leads to the formation of HEOD by intramolecular cyclisation (Reaction 1), followed by the formation of N,N,N-tris(2-hydroxyethyl)ethylenediamine (THEED) (Reaction 2-1). An alternative mechanism for the formation of THEED through an aziridium salt as intermediate (Reaction 2-2) was also proposed. Diamines such as THEED can form piperazines by intramolecular dehydration: producing N,N-bis(2-hydroxyethyl)piperazine (BHEP) (Reaction 3). Other minor degradation products were identified, for example, intermolecular dehydration of DEA leads to the formation of N-(2-hydroxyethyl)aziridine (HEM), which can react with another DEA molecule to form THEED; the reaction of two DEA molecule can produce Bis-(2-(2-hydroxyethylamino)ethyl)ether (BHEAE); intermolecular cyclisation of THEED carbamate produces an oxazolidin- 2-one (HAO), which upon reacting with DEA forms N,N,N,N-tetrakis(2-hydroxyethyl)diethylenetriamine (THEDT). The list of identified degradation products of DEA are provided in **Table 3.2**.

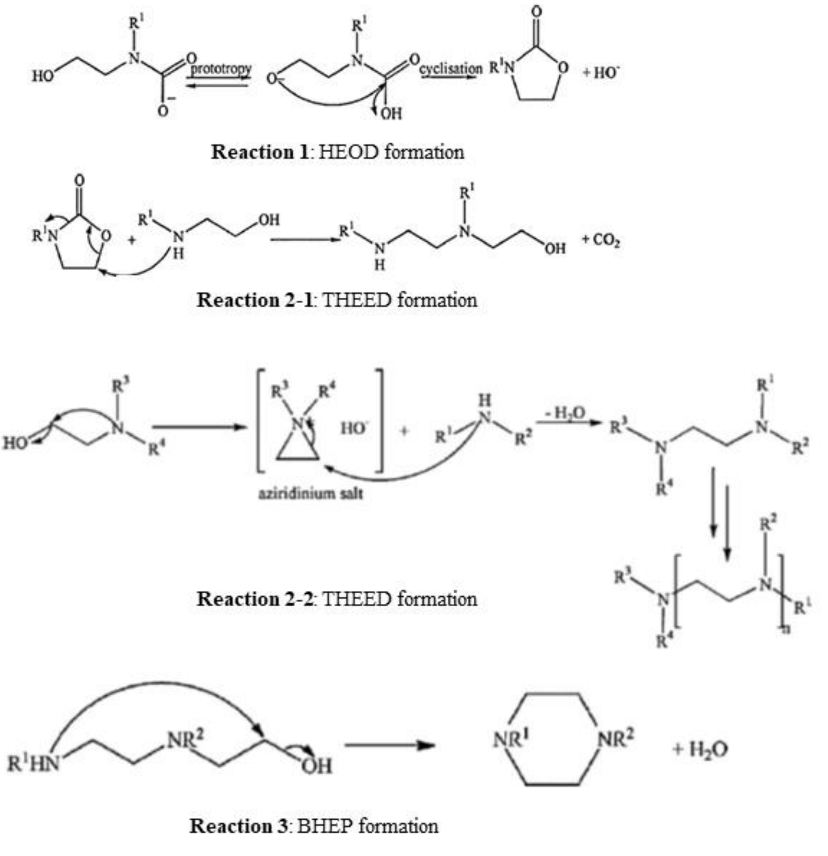
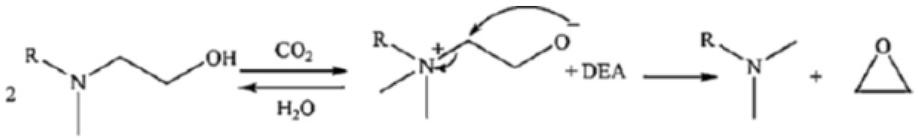
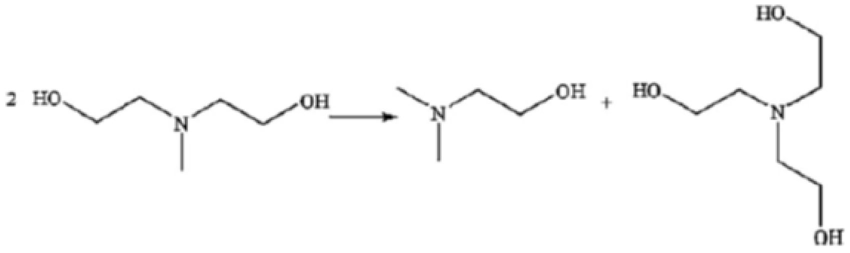


Figure 3.3 *Mechanisms for DEA thermal degradation* [204].

Lastly, MDEA is another alkanolamine studied for its thermal degradation mechanism, shown in **Figure 3.4**. Studies have identified that DEA is among the major degradation products of MDEA through Methylation of one molecule of MDEA and demethylation of another (Reaction 1) [215,237] and an ammonium intermediate which leads to N,N-dimethylethylamine (DMAE) and Ethylene oxide (EO) was proposed [88]. The formation of DMAE and TEA was also identified through the disproportionation of MDEA (Reaction 2). Other degradation products include N-methylmorpholine (MM) through cyclic dehydration, DMP formation from 2MAE molecules followed by cyclic dehydration, N-(2-hydroxyethyl)-N'-methylpiperazine (HMP) formation from DEA and MAE as starting materials, and N-methyl-N,N',N'-tris(2-hydroxyethyl)ethylenediamine (MTHEED) formation from MDEA and DEA as starting materials. It should be noted that PZ was also studied for its thermal degradation, identifying a range of possible products which are summarised in **Table 3.2**.



Reaction 1: MDEA Transamination



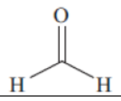
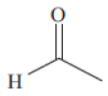
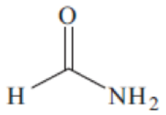
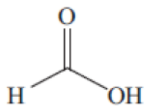
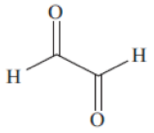
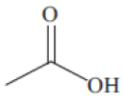
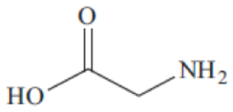
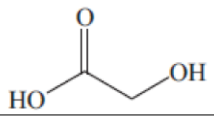
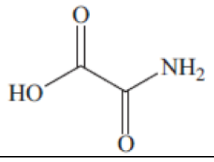
Reaction 2: MDEA Disproportionation

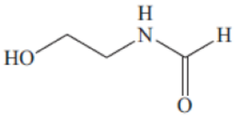
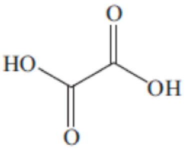
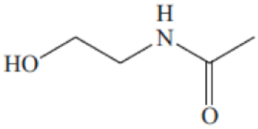
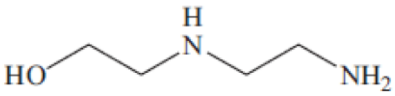
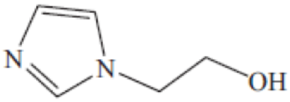
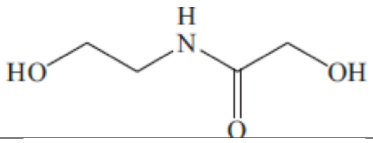
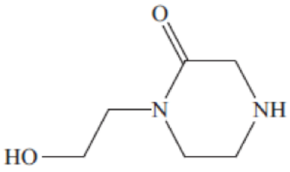
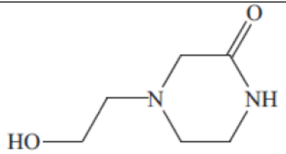
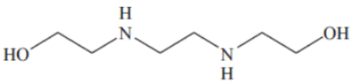
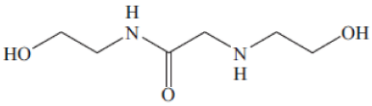
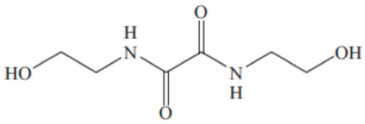
Figure 3.4 *Mechanisms for MDEA thermal degradation* [204]**.**

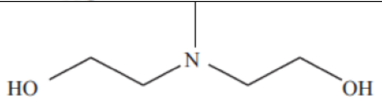
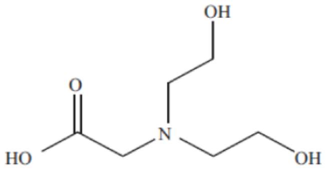
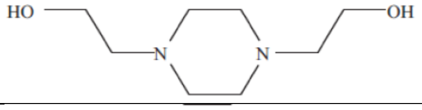
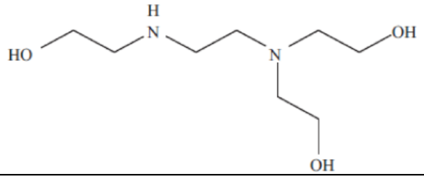
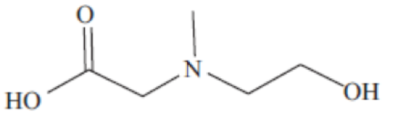
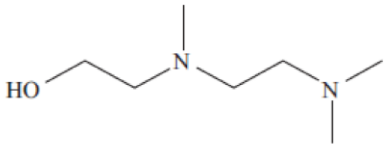
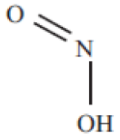
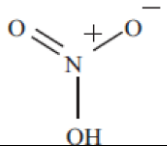
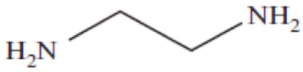
3.2.2 MECHANISM OF OXIDATIVE DEGRADATION

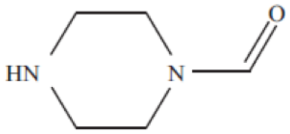
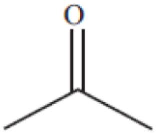
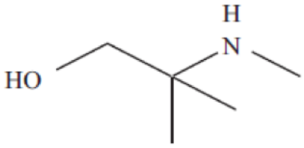
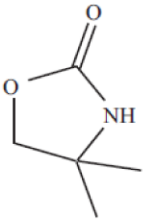
As previously highlighted, oxidative degradation of alkanolamines occurs mainly in the absorber column of a typical PCC process configuration. Similar to thermal oxidation, the effect of CO_2 presence was included in studying oxidative degradation. Yet again, MEA was the most widely studied alkanolamine for oxidative degradation. The major oxidative degradation products identified for MEA include: carboxylic acids, ammonia, ethylene oxide, N-(2-hydroxyethyl)ethylenediamine (HEEDA), and N-(2-hydroxethyl)imidazole (HEI). The list of oxidative degradation products identified for the major amines used for PCC is shown in **Table 3.3**.

Table 3.3 *List of oxidative degradation products for MEA, DEA, MDEA, AMP, and PZ. References:* [88,204,209,211,214,215,217,221,225,228,231–233,245,246].

Solvent	Degradation Product Name	Degradation Product Chemical Structure
MEA and AMP	Ammonia	NH_3
MEA	Formaldehyde	
MEA and MDEA	Methylamine	H_3C-NH_2
MEA and AMP	Acetaldehyde	
MEA	Formamide	
MEA/DEA/MDEA/PZ/AMP	Formic acid	
MEA	Glyoxal	
MEA/DEA/MDEA/PZ/AMP	Acetic acid	
MEA	Glycine	
MEA/DEA/MDEA/PZ/AMP	Glycolic acid	
MEA	Oxamic acid	

Solvent	Degradation Product Name	Degradation Product Chemical Structure
MEA	N-(2-hydroxyethyl)formamide (HEF)	
MEA/DEA/MDEA/PZ/AMP	Oxalic acid	
MEA	N-(2-hydroxyethyl)acetamide (HEA)	
MEA	N-(2-hydroxyethyl)ethylenediamine (HEEDA)	
MEA	N-(2-hydroxethyl)imidazole (HEI)	
MEA	2-Hydroxy-N-(2-hydroxyethyl)acetamide (HHEA)	
MEA	N-(2-hydroxyethyl)piperazin-2-one	
MEA	N-(2-hydroxyethyl)piperazin-3-one (HEPO)	
MEA	N,N’-bis(2-hydroxyethyl)ethylenediamine (BHEEDA)	
MEA	N-(2-hydroxyethyl)-2-(2-hydroxyethylamino)acetamide (HEHEAA)	
MEA	N,N’-bis(2-hydroxyethyl)oxalamide (BHEOX)	

Solvent	Degradation Product Name	Degradation Product Chemical Structure
DEA	Monoethanolamine (MEA)	
DEA	N-methyldiethanolamine (MDEA)	
DEA and MDEA	N-(carboxymethyl)diethanolamine (bicine)	
DEA	N,N_-bis(2-hydroxyethyl)piperazine (BHEP)	
DEA	N,N,N'-tris(2-hydroxyethyl)ethylenediamine (THEED)	
MDEA	2-[Methyl(2-hydroxyethyl)amino] acetic acid	
MDEA	N,N,N'-trimethyl-N'-(2 hydroxyethyl)ethylenediamine	
PZ and AMP	Nitrous acid	
PZ and AMP	Nitric acid	
PZ	Ethylenediamine (EDA)	
PZ	N-formylpiperazine (FPZ)	

Solvent	Degradation Product Name	Degradation Product Chemical Structure
		
AMP	Acetone	
AMP	N,2,2-trimethylethanolamine	
AMP	4,4-Dimethyloxazolidin-2-one	

The primary issue with the formation of carboxylic acids, volatile amines such as ammonia and methylamine is that these substances are **acid precursors** causing corrosion and fouling in pilot plants [211,238,246], along with increasing amine degradation leading to the **formation of Heat Stable Salts (HSSs)**, with the reaction mechanism shown in **Figure 3.5** [212,218]. It is important to point out that all acids are in HSSs form due to this reaction. HSSs are not regenerated in stripper conditions because carboxylic acids are more acidic than carbonic acid [210,219,228].

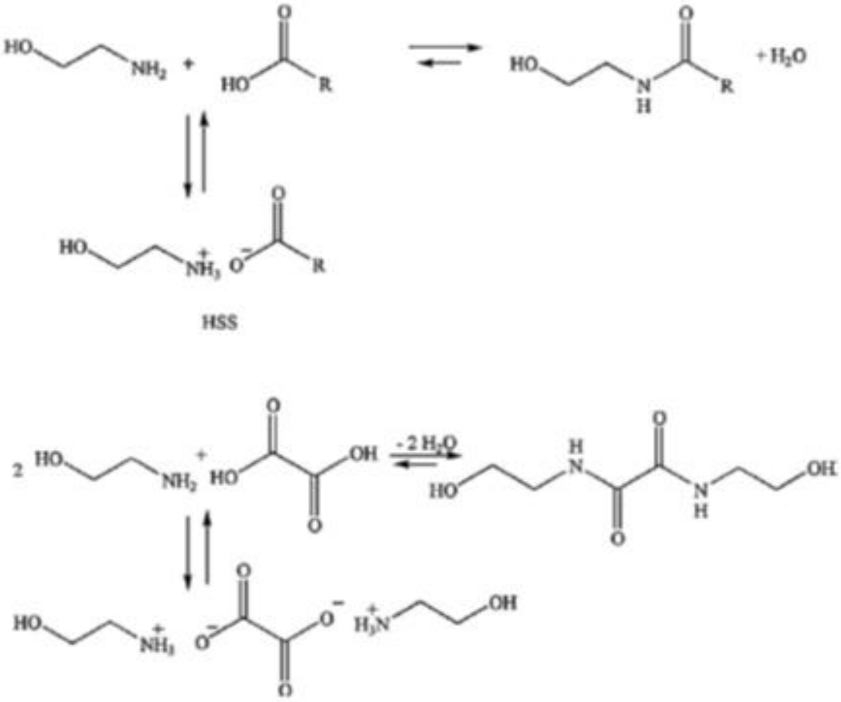


Figure 3.5 *Formation of amides and HSSs* [204].

3.2.3 FACTORS AFFECTING DEGRADATION

In the case of thermal degradation, the primary factor affecting the rate of degradation is temperature, with these reactions following a first order kinetics as a function of temperature, with increased degradation rate at higher temperatures. Additionally, various studies established the relevance of CO_2 and amine concentration, and the presence of other impurities in the flue gas stream. The more concentrated the amine solvent, and the higher the CO_2 partial pressure, the faster the rate of thermal degradation. Screening studies established that the highest thermal stability was observed for alkanolamines with no chains, followed by those with a higher chain length. Up to date, the most thermally stable alkanolamines identified include PD, Mor, PZ, BAE, AMP, and HMDA [247–250]. In this case, the temperature of the stripper column can be maintained at a level below the threshold for thermal degradation for the selected amine, however, this might be at the expense of efficient solvent regeneration. A collection of studies established that ideally amine concentration should not exceed 30 *wt.*% to ensure low solvent degradation, additionally, the operating temperature of the stripper is a governing factor in the solvent degradation, which should be within the range of 373 – 403 K, depending on the type of amine [204,224,244,251].

Nonetheless, a wide range of studies reported that the dominating form of amine degradation is through oxidation. The oxidative degradation is highly dependent on the concentration of O_2, however, temperature, CO_2 and presence of metal ions are also reported to catalyse the oxidation. For example, the oxidation of MEA and PZ is catalysed by Fe, and Cu cations, respectively [247]. Under similar condition, the oxidation of some amines can be ranked as follows: PZ < AMP < MDEA < DEA < MEA [245]. Oxidation of amine may also be affected by the blending it with another amine as oxidation of PZ is enhanced if it is blended with AMP [252]. Such cases make the solvent selection even difficult if one problem is solved on the expense of another problem created.

Pilot-scale testing of different amines under typical process conditions have been done over recent years. For example, the pilot plant at Esbjergværket power station operated four 1000-hr test campaigns as part of the CASTOR project [102]. The quantification of solvent consumption was done during 500-hr tests, through tracking decline in amine concentration and tracking amount of amine makeup. During the MEA campaign, 720 kg of MEA was consumed during the 500-hr test, capturing 503 tons of CO_2, resulting in 1.6 kg MEA consumed per ton of CO_2 captured. The low degradation rate of the solvent was attributed to the ow amount of SO_x in the flue gas inlet along with the utilization of fresh MEA solvent. Similar consumption ranges were obtained for CASTOR-1 and CASTOR-2 solvents. For all examined solvents, the major emissions detected were mainly ammonia resulting from oxidative degradation of MEA.

The technology centre Mongstad operated a test campaign in 2015 using MEA as a solvent with 1960 hours of operation [235]. During the testing campaign the amine consumption was determined to be 1.5 kg MEA per ton CO_2 captured. The formation of HSS was determined to be 1.5 wt.%, with the formation of ammonia as a degradation product accounting for 67% of the total MEA losses. In terms of emissions, MEA and alkyl amines were in part per billion ranges, while the formation of nitrosamine and nitramines were not detected.

Pilot plant at Niederaussem [241] carried out tests to understand the time dependency on MEA degradation. The solvent consumption was approximately 0.3 kg MEA per ton captured. Degradation samples during 5000 hrs of operation were mainly acetate, formate and oxalate from oxidative degradation.

Recently, an 18 month campaign using MEA at Pilot plant at Niederaussem [244] with almost 13000 hrs of operation. The major findings determined that MEA consumption can be as low as 0.5 kg per ton CO_2 captured when the degradation process remains stable within the linear degradation regime. The losses were 0.21 kg after 55 days of operation. This might be due to the observation that the major detected product were acetates and formats. Additionally, . , the detected levels of MEA emissions were very low, along with low aerosol concentrations.

A study within the OCTAVIUS project [240] focused on understanding solvent degradation from three pilot plants (TNO's CO_2 capture plant at Maasvlakte, EnBW's CO_2 capture plant at Heilbronn, and ENEL's CO_2 capture plant at Brindisi. The degradation rates between the different plants were different, attributed to the different flue gas quality, and dissolved oxygen concentrations promoting the formation of oxidative degradation products and ammonia emissions.

The UKy-CAER 0.7 MWe small pilot scale CO_2 capture facility underwent a campaign using MEA to test its degradation and emissions [242]. The overall solvent degradation was comparable to the results of other published pilot studies using MEA under similar coal flue gas conditions and pilot operating hours. Heat stable salts and polymeric amine formation showed a linear behaviour over the time which indicates that these compound were not involved in competing secondary reactions in the time frame measured. Nitrosamine were not observed above the detection limits calculated during this MEA testing campaign. Solvent oxidation in the form of heat stable salts and amine polymeric compounds were the main degradation products.

The information obtained from pilot-scale testing facilities are valuable as they test the solvent under realistic process conditions and prolonged operation times. However, such operation is time consuming. SINTEF Materials and Chemistry has designed an advanced laboratory test rig for studies of solvent degradation [253], which emulates the process conditions observed in an absorber/stripper configuration designed for CO_2 capture. During a 14-week test campaign with degradation of 30 wt.% MEA identified the formation of nitrosamines. Results indicate that the degradation of nitrosamines and nitramine in the solvent is highly temperature dependent, and that the levels of total nitrosamines and MEA-nitramine are significantly reduced by elevated stripper temperature. The results show that the SDR results give a realistic picture on the solvent degradation to be expected in a real CO_2 capture plant; degradation products formed in the SDR MEA solvent reflects those previously found in pilot plant studies.

3.3 SOLVENT CORROSION

Corrosion is another aspect of operational problems associated with amine utilisation for PCC. The occurrence of corrosion has a direct influence on the operational integrity of the processing facility, along with the capital and operating costs of the processing facility [254]. Corrosion in PCC can occur due to two possible mechanism which are wet acid corrosion, and corrosion by amine solutions [206,245,247,249,254,255]. Wet acid corrosion occurs due to the presence of aqueous solutions with high concentrations of acid gases such as CO_2 and H_2S and other oxidizing acid species such as NO_x and SO_x. In aqueous environments, these gases convert into acids that react with the material used in the equipment. This type of corrosion can occur at different parts of the processing facility which comes into contact with strong acidic solutions. They may be observed primarily at the inlet of the absorption column or cooling vessels in CO_2 compression units.

Corrosion by amine solutions occurs due to the corrosive nature of the products formed from the reaction between amine and CO_2, which alternative to the aforementioned type, can occur in different parts of the processing facility, primarily in the absorber and regeneration column sumps, cross-heat exchanger, and the reboiler.

The degree and extent of corrosion depends on the type of material used for equipment, for example it is established that the use of carbon steel has a higher tendency to corrode compared to stainless steel; however, this is at the expense of capital cost as stainless steel is six times more expensive than carbon steel [255–261]. An important preventive measure to counteract the effect of corrosion is the proper selection of materials for PCC design, which in turn depends on the chemistry of the amine system. Additionally, process operating conditions have an influence on the rate of corrosion, such as high operating temperatures, rich and lean amine loading, ratio of acid gas in inlet flue gas, amine type and concentration, along with presence of amine degradation products [262–268]. Other available corrective measures are the use of corrosion inhibitors to minimize corrosion, and the instillation of online corrosion monitoring [245,261,269–272].

The body of the work on corrosion has focused on the identification of corrosion mechanism and conditions, testing of material suitability under various process conditions, along with corrective measures to either inhibit or monitor corrosion, which are summarised in **Table 3.4**.

Table 3.4 *Summary of available works on corrosion in PCC.*

Purpose	Testing Scale	Ref.
Corrosion mechanism, effect of operating conditions, corrosion inhibitor testing	**Lab-Scale**	[245,247–250,252,254–256,258–260,263,264,266,267,269,271–286]
Corrosion monitoring, testing of corrective measures	**Pilot-Scale**	[94,256,257,261,262,265,266,268,270,282,285,287,288]

As previously mentioned, the two major forms of corrosion in amine-based gas treatment units are wet CO_2 corrosion and amine-solution corrosion. The mechanisms and factors affecting these forms of corrosion are highlighted below.

3.3.1 WET CO_2 CORROSION

In general, corrosion involves the simultaneous oxidation of a metallic surface leading to the production of electrons, and a reduction reaction that consumes those electrons, known as redox reactions [245,248,281]. These redox reactions require the presence of anode, cathode, and electrolyte solution. In the case of PCC processes, the electrolyte solution is CO_2-dissolved solvent, with which electrons from the anode (corrosion sites on the metal) will be released and transferred to the cathode. The tendency of a metal to corrode depends on the type of the metal and the pH of the electrolyte solution.

In amine-based plants, typically, amine solvents (which are basic in nature) hinder the process of corrosion; however, at low concentration or in the absence of amines, the dissolution of CO_2 in water leads to the formation of a highly acidic and corrosive solution [245,248,281,286,288]. This type of corrosion can occur in absorber's feed gas bottom and stripping column overhead sections due to high water saturation. The chemical reactions involved in this form of corrosion, initiates with the dissolution of CO_2 in water, which reacts with water leading to the formation of carbonic acid (H_2CO_3) (**Reactions 3.1** and **3.2**). The further dissociation of the carbonic acid leads to the formation of an acidic solution (**Reaction 3.3**). At the anode, the iron undergoes an oxidation reaction leading to its dissolution (**Reaction 3.4**). At the cathode side, the reduction reactions lead to the formation of hydronium and bicarbonate ions (**Reaction 3.5 – 3.7**). Subsequently, the redox reactions lead to two overall reactions, which are formation of ferrous hydroxide and ferrous carbonate (**Reactions 3.8 and 3.9**).

$$CO_2(g) \rightarrow CO_2(aq) \tag{3.1}$$

$$CO_2(aq) + H_2O \leftrightarrow H_2CO_3 \tag{3.2}$$

$$H_2CO_3 \leftrightarrow H^+ + HCO_3^- \tag{3.3}$$

$$Fe \rightarrow Fe^{2+} + 2e^{-} \tag{3.4}$$

$$2H_3O^{+} + 2e^{-} \leftrightarrow 2H_2O + H_2(g) \tag{3.5}$$

$$2HCO_3{}^{-} + 2e^{-} \leftrightarrow 2CO_3^{2-} + H_2(g) \tag{3.6}$$

$$2H_2O + 2e^{-} \leftrightarrow 2OH^{-} + H_2(g) \tag{3.7}$$

$$Fe^{2+} + 2OH^{-} \rightarrow Fe(OH)_2 \tag{3.8}$$

$$Fe^{2+} + 2CO_3^{2-} \rightarrow FeCO_3 \tag{3.9}$$

The primary factors affecting the rate of this type of corrosion are temperature and concentration of free CO_2 in the solution. A possible remedy is the utilisation of amine sprays at the overhead of the regenerator or amine wetting at the absorber bottom to increase the pH of the solution at these locations and prevent CO_2 induced corrosion. Alternatively, changing the material is another possible option using stainless steel which has a demonstrated resistance to corrosion, although more expensive that carbon steel, as already mentioned.

3.3.2 AMINE SOLUTION CORROSION

Aqueous solutions of amines are not corrosive in nature due to their high alkalinity. However, the formation of carbamate/bicarbonate from the reaction of amine with CO_2 (**Reaction 3.10 and 3.11**) creates an acidic environment that leads to corrosion. The amine-CO_2 corrosion has a different pathway than wet CO_2 corrosion that is not yet fully understood. The formation of carbamate/bicarbonate results in hydrogenated amine ions ($R_2NH_2^{+}$ and R_3NH^{+}) which are acidic in nature and provide protons for the corrosion reaction leading to the dissociation of iron into its cations (Reactions 3.12 and 3.13) [245,248,252,255,281].

$$CO_2 + R_3N + H_2O \leftrightarrow R_3NH^{+} + HCO_3^{-} \tag{3.10}$$

$$CO_2 + 2R_2HN \leftrightarrow R_2NH_2{}^{+} + R_2NCO_2^{-} \tag{3.11}$$

$$Fe + 2R_3NH^{+} \leftrightarrow 2R_3N + Fe^{2+} + H_2 \tag{3.12}$$

$$Fe + 2R_2NH_2{}^{+} \leftrightarrow 2R_2HN + Fe^{2+} + H_2 \tag{3.13}$$

It was postulated that carbamate are strong oxidizing agents leading to corrosion, hence, the higher corrosion rate observed with primary and secondary amines, as tertiary amines are incapable of forming carbamate.

Amine solution corrosion occurs mainly in piping sections of the rich solution, the rich amine side of the lean-rich solution heat exchanger, at the bottom of the absorber to the regenerator, and at the hot bottom part of the regenerator. Its severity is dependent on several factors, such as type and concentration of amine, CO_2 loading, temperature, presence of degradation products and other contaminates such as oxygen and others. The severity of corrosion and increased corrosion rates were connected with high CO_2 partial pressure, high amine concentration, increased CO_2 loading in rich solvent, high temperature, and the presence of degradation products (i.e. formic acid, oxalic acid, acetic acid, etc.) which act as corrosion agents [206,263,264,272]. Among these factors, it was established that temperature has a mild effect on increasing the corrosion rates, while the highest effects were due to CO_2 loading and amine concentration. In the case of increased amine concentration, the amount of CO_2 absorbed in the solvent, which increases the amount of hydronium ions present in the solution, resulting in increased corrosion rates. In the case of CO_2 loading, such an increase in corrosion rates is expected as corrosion starts with the dissociation of CO_2 and its subsequent reaction with the amine and the metal surface.

A number of studies in the literature examined the amine solution corrosion effects [206,252,255,263,264,269,270,272–274,277,278]. Among the variety of alkanolamines, MEA is the most corrosive, with its corrosivity being affected by its own concentration, CO_2 loading capacity, and the operating temperature. Pilot plant tests established that over the duration of 4-years, carbon steel material used at the outlet of the stripper underwent a high corrosion rate resulting in an 80% loss of its initial weight [256]. The corrosion behaviour of other amines was examined in the literature, establishing a decreased corrosion rate in the order of MEA > AMP > DEA > PZ > MDEA.

3.4 PROCESS EMISSIONS

The primary advantage of PCC systems is to help curb the increasing level of atmospheric CO_2 emissions. However, similar to any industrial processes, secondary emissions with environmental and health risks are associated with the operation of PCC systems. Up to date, major secondary emissions from the operation of amine-based PCC systems have been identified [289–305]. These emissions include, amine losses due to evaporation, degradation products from oxidative degradation particularly ammonia, nitrosamines and nitramines, volatile organic compounds (VOCs), ammonia resulting from degradation, particulate matter (PM), along with fugitive emissions [289–305].

The most alarming of these emissions are those generated from amine degradation due to their adverse effects on human health, being carcinogen compounds. The amount of these emissions significantly varies depending on the plant size and operating conditions, flue composition, and type of solvent utilised [298,306,307]. Particular attention has been paid over the past years to the formation of nitrosamines and nitramines [245]. These hazardous carcinogenic substances are formed due to the presence of nitrosating agents such as nitrate and nitrite, with the organic amine. The formation of nitrosamines is not typically formed from primary amines such as MEA, however, it was established that the presence of secondary and tertiary amines as impurities in industrial grade MEA, is a possible precursor for the formation of nitrosamine through disproportionation reactions [299]. Another precursor for nitrosamine formation is the presence of NO_x, mainly in the form of nitric oxide (NO), and traces of nitrogen dioxide (NO_2), and nitrous oxide (N_2O). This can be appropriately handled in facilities integrated with selective catalytic reduction (SCR) or selective noncatalytic reduction (SNCR) to reduce NO_x emissions and satisfy regulatory requirements. While the formation of these hazardous substances might not significantly contribute to increased solvent consumption, it remains that their atmospheric release has serious implication on human health and ecological system.

For the remaining types of possible emissions, available options to counteract secondary emissions include online monitoring [298], and installation of auxiliary units to capture any released gases or remove any precursor toward their formation [289,293,297,307]. Emissions associated with CO_2 capture processes are generated from two potential sources, which are: (1) point of discharge, (2) fugitive emissions, and (3) aerosol emissions. These types of emissions are further discussed in upcoming sections.

3.4.1 POINT OF DISCHARGE EMISSIONS

For point of discharge emissions, they are intentional emissions that can be quantified and predicted based on the operating conditions of the process. These emissions are released from the top of the absorption column and from wastes due to solvent reclamation or other purification processing units.

The first type of point of discharge emissions is the treated gas, which is mainly composed of the flue gas with a reduced CO_2 content and other gases from the process solutions, which are continuously released from the top of the absorber column to the atmosphere. The type of gases released to the atmosphere depends mainly on the composition of the feed flue gas. These gaseous substances include carbon monoxide (CO), NO_x, SO_x, and HCl. Additionally, traces of metals can also be released with the purified flue gas such as lead, cobalt, nickel, cadmium, arsenic, and chromium. Despite the adverse impacts of these emissions on human health, still, they are not considered major contributors to any environmental impacts due to CO_2 capture processes integrated with power plants. This is because these substances are originally produced from the combustion of fossil fuels, irrespective of the installation and operation of a CO_2 capture unit.

The emissions attributed to the operation of CO_2 capture processes are those related to vapours from the capture solutions. These emissions significantly depend on the type of chemical solvent (vapour pressure of solvent) used for CO_2 capture along with process operating conditions. These emissions include vaporized chemical solvent, water vapour, along with degradation and corrosion products such as ammonia, acetone, butanone, formic acid, and 1-propanamine (from MEA's degradation). These releases easily leave with the treated flue gas from the top of the absorption column, and they are a function of the solvent volatility, concentration and absorption temperature. The release of degradation or corrosion inhibitors are negligible due to their low vapour pressure. It is estimated that evaporative losses of MEA, as an example, were up to 1.6 kg MEA for 1 tonne of captured CO_2 from a gas-fired flue gas [235]. The severity of these emissions to human health and environment depends on the level of toxicity of the chemical solvent and level of exposure, which is dependent on environmental, atmospheric and geographic conditions, influencing the distribution and dispersion of the pollutants.

The other type of point of discharge emissions are those associated with wastes from the process solutions. These are associated with the general practice adopted from gas treatment facilities, in order to purify the solvent and remove any contaminants to maintain the quality of the solvent at a pre-determined level. As such, wastes from solvent purification are disposed of through incineration and landfills, with the former leading to the production of ashes of both degradation products and additives along with amine vapours, which can be harmful to human health and environment.

3.4.2 FUGITIVE EMISSIONS

In the case of fugitive emissions, they are unintentional releases from the equipment and piping of the process during operation, which can contribute to the environmental impact of operating a carbon capture unit. These emissions are typically occurring at random, with intermittent quantities in an unpredictable fashion. These releases include process fluids escaping the capture unit through leaks due to deterioration of processing facility from corrosion, impact damage, and others. Additionally, these fugitive emissions can occur from various equipment such as pumps, valves, flanges, sampling connections, vents, drains, pressure relief devices, and others. Apart from leakage losses, working and breathing losses also account for some fugitive emissions. Working loss occurs when the storage tanks of absorption solution are being filled. The quantity of solution vapour released from the tanks depends on temperature, vapour pressure of the solution, and pumping rate. Breathing losses are caused by thermal expansion of the solution vapour in the tanks as a result of temperature increase during the daytime. Regardless of their sources, fugitive emissions release certain amounts of process fluids and materials, including untreated flue gas, treated gas, absorption solvents, corrosion inhibitors, degradation products, and chemical additives

3.4.3 AEROSOL EMISSIONS

Another type of emissions recently reported from typical PCC pilot plants are aerosol-based emissions [302]. These emissions can lead to significant environmental hazards along with increased solvent losses. The primary issue with these emissions is their larger magnitude compared to vapour emissions, along with the inability of conventional countermeasures such as water washing or installation of demisters in reducing these emissions.

The formation of aerosol is governed by the degree of saturation which is the ratio between the total pressure of all the condensing components and their equilibrium partial pressure at the same composition and temperature, and requires two steps, (1) aerosol nucleation, and (2) aerosol growth [302]. The nucleation of aerosols can be initiated either through homogenous nucleation of molecules of condensable components, or heterogeneous nucleation of fine particles in the gas phase. Subsequently, the aerosol particle growth either through coagulation or condensation. The extent of the aerosol formation and emission is dependent on a variety of factors such as lean solvent temperature, pH, CO_2 concentration, presence of impurities, and others. A primary method to mitigate the formation of aerosol is the careful selection of plant operating conditions. Pilot-scale testing and process modelling were extensive employed to examine the parameters affecting formation of aerosol [293,296,302,306,308].

3.5 SOLVENT MANAGEMENT

As previously highlighted, solvent degradation, corrosion, and emissions are among the negative outcomes associated with utilisation of amines for CO_2 capture. These issues are precursors for other operational problems such as solvent deactivation, corrosion, increased atmospheric emissions, fouling, and foaming, among many others, which are cost intensive in terms of solvent replacement and equipment maintenance. Various options are available for solvent management in order to maintain appropriate solvent quality and reduce associated emissions for PCC processes. These strategies can be divided into: (1) Solvent selection and optimization of process operating conditions, (2) chemical additive for degradation and corrosion inhibition, and (3) additional processing units for solvent reclaiming.

3.5.1 SOLVENT SELECTION AND OPTIMAL PROCESS CONDITIONS

Among the simplest options for proper solvent management and mitigation of solvent degradation, corrosion, and associated process emissions, is merely through an appropriate solvent selection. This would entail choosing a solvent that possesses high thermal and chemical stability, low corrosivity, and low volatility, that also possesses the necessary process performance characteristics like high absorption rate and capacity, low viscosity and low energy requirement for regeneration. However, such a solvent encompassing the full range of desired properties still has to be found.

Another simple option for solvent management is the choice of optimal process operating conditions. This necessitates a comprehensive understanding of the primary factors affecting these operational issues, which are cross-linked in most cases. However, adjustments of operating conditions to avoid operational issues might also be on the expense of optimal process performance. For example, reducing stripping temperature might protect the solvent from thermal degradation; however, this might lead to a reduction in efficient solvent regeneration and limited release of captured CO_2. Such cases make the solvent selection and optimization of safe operating conditions rather difficult, requiring a comprehensive detailed view of the chosen solvent and process to account for all possible trade-offs.

3.5.2 CHEMICAL ADDITIVES FOR DEGRADATION AND CORROSION INHIBITION

Employing chemical additives to either mitigate or inhibit degradation and corrosion is another possible option for solvent management. With this approach, a chemical additive is added to the process stream to prevent the propagation of reactions associated with degradation and corrosion.

The use of degradation inhibitors has been mainly focused on reducing the extent of oxidative degradation, with the inhibitor substances either acting as scavengers for oxidative species or chelating agents for radicals. The most widely used inhibitor is Ethylene-diamine-tetra-acetic acid (EDTA), which is an excellent chelating agent for Cu and Fe cations, preventing them from O_2 exposure and initiation of oxidative degradation [205,213,217,245]. A variety of other inhibitors has been tested in the literature such as sodium sulphite, formaldehyde, ascorbic acid and many others [218]. Similarly, a variety of substances has been examined for their use as inhibitors for corrosion particularly added to lean amine solutions. Of such inhibitors, sodium metavanadate ($NaVO_3$) and sodiumsulphite (Na_2SO_3) have demonstrated their effectiveness in protecting metals from corrosion even with small quantities [263,269,278,286].

The use of degradation or corrosion inhibitors requires identification of optimal inhibitor concentration, which is the primary factor affecting the efficacy of their utilisation. An increase in inhibitor concentrations above the optimal value increases the degradation and corrosion rates, making them ineffective, along with additional issues such as eroding and plugging [218].

Although the use of degradation inhibitors has a potential of reducing the rate of degradation, still some operational issues were related to the use of inhibitors either for reduction of corrosion or degradation. For example, EDTA showed degradation issues, promoted Fe formation and acted as catalyst for activating intermediate peroxide and hydroxyl radical formations [218]. The utilisation of inhibitors requires a detailed identification of degradation products and reactive pathways to ensure their safe utilisation without further promoting/ catalysing the degradation reaction.

3.5.3 SOLVENT RECLAIMING

Once the degradation of the solvent and corrosion has taken place, additional processing units are included in the process to recover and separate these degradation and corrosion products from the circulating solvent. The most common methods for controlling the level of contaminants in amine solutions include purging, neutralization, and amine reclamation [309].

In solution purging, a portion of the contaminated solvent is removed and replaced with fresh solvent to reduce the level of degraded species; however, losses of useful solvent and increased disposal costs are among the operational issues of this strategy. For neutralization, a strong base is added to the amine solution to raise the pH of the system and convert HSSs to inorganic salts. In this manner, the amine trapped by the HSSs is released for CO_2 removal again. However, with this approach, the acid anions cannot be removed from the system and the addition of these solutions increased the solvent viscosity and corrosivity. As such, these strategies though useful as a temporary solution, are ineffective for long-term solvent management [309].

A more effective option is amine reclaiming, which has been extensively used to manage solvent degradation and corrosion through separating the impurities from the amine solvent. Amine reclaiming includes thermal reclamation, ion exchange, and electrodialysis.

3.5.3.1 THERMAL RECLAMATION

Thermal reclamation purifies the amine solvent through the addition of heat to evaporate the amine solvent from the higher boiling point degradation products. Typically, the distillation is performed on a small side stream, usually 1%–3% of the circulating lean solution, leaving the stripper reboiler and fed to a steam-heated or direct fired kettle or reclaimer [309]. Subsequently, the purified distillate is returned to the process through the overhead vapour line. Additionally, the contaminated solvent is mixed with a strong base such as caustic soda or soda ash to liberate the amine from HSSs, which is typically added prior to entering the thermal reclaimer.

The operating conditions of thermal reclamation are at the maximum allowable temperature prior to solvent thermal degradation, which is dependent on the solvent type. However, as the thermal reclamation. As the reclamation process is operated within the range of temperatures for thermal degradation, the occurrence of additional thermal degradation of the solvent is possible On the other hand, the operating pressure of the reclaimer can be either at vacuum conditions, atmospheric pressure or at the stripper pressure, for example, MEA reclaiming is often carried out at the stripper pressure. Mitsubishi Heavy Industries [310] provided a patent reclaiming apparatus, which includes a packed bed in which the absorbent is brought into gas–liquid contact with steam. The reclaiming apparatus further includes an absorbent distributing unit that extracts and distributes a part of the absorbent stored in the absorbent reservoir. Shell [311] has a patent distillation process that comprises at least two stages. In the first step, more than 95% of the water originally present is removed from the aqueous amine in a film-type evaporator. In the second step the aqueous amine is further purified in an agitated-film evaporator, which is operated at a temperature in the range of 120–200°C and a pressure in the range of 2 to 10 kPa. A pilot plant experiment showed that 96% di-isopropanolamine (DIPA) can be recovered from spent aqueous DIPA and approximately 90% HSSs were removed by applying a simple two step distillation process, if the sample was treated with stoichiometric amounts of NaOH prior to the first step.

The primary issue with thermal reclamation is its energy intensive nature, at which significant amount of heat is needed to increase the temperature of the solution (containing amine and water). It was reported that energy consumption associated with thermal reclaiming is approximately 0.3 GJ/t_{CO2} for an USC PC (ultra-supercritical pulverized coal) boiler reference case [312]. However, this can be reduced if the overhead vaporous from the reclaimer are fed to the stripper, to efficiently use the energy spent on solvent reclamation. Other disadvantages include (1) the tendency of the process to lose undegraded amine either through inducing its degradation under the reclamation operating conditions or with the waste stream, and (2) low separation efficiency as not all the degradation products are removed.

3.5.3.2 ION EXCHANGE

Ion exchange is a reversible exchange of ions between a solid (ion exchange material or resin particle) and a liquid, without the occurrence of substantial change in the solid structure. The typical ion exchange process involves two steps, the loading step to remove ionic species from the solution, and the regeneration step to remove the HSS anions from the resin by replacing them with caustic. However, ion exchange resins are not capable of removing uncharged contaminants like those produced from amine thermal degradation.

Although the basis of the process seems relatively simple, combining optimal HSSs removal with less chemical and energy consumption [313], still this strategy is faced by several technical and operational challenges. For instance, previous ion exchange processes used in amine systems are ineffective and produce large quantities of diluted waste, which requires neutralization and disposal. Poorly designed and/or operated ion exchange systems have caused significant amine losses that makes the waste untreatable in wastewater plants in some cases [313]. Additionally, the thermal degradation of ion exchange resins at high temperature limits efficiency.

Although the ion exchange process might be acceptable in natural gas treating services, the process alone cannot be considered an optimum solution for CO_2 capture application, particularly from flue gases [314]. In CO_2 capture, the high acid gas loading or high level of CO_3^{2-} and HCO_3^- in the amine solution could interfere and compete with HSS anions in the resin leading to reduced effectiveness of the HSS removal. This can be addressed through processing the lean amine solution rather than the rich solution. Dow and Alstom [315] have a patent process involving a stripper or flash drum for inexpensive, efficient and reliable removal of residual CO_2 from contaminated amine solution before the absorbent is fed to the amine reclaimer for separation of HSSs.

However, in the case of CCS application, amine degradation products and HSSs are almost in equivalent ratio in terms of importance [314], with the former being difficult to remove with ion exchange.

3.5.3.3 ELECTRODIALYSIS

Electrodialysis (ED) uses a direct current and ion-permeable membranes to remove ions from one solution chamber to another [314–316]. The separation of ionic degradation products from amine solutions by ED is done with a typical process setup consisting of a stack of alternating cation-selective and anion-selective membranes located between two electrodes. Commercial ED cells can contain hundreds of stacked membranes. When a current is applied across the two electrodes, the cations and anions move toward their opposite electrodes and through the selective-ion membrane. The net effect is to remove both cations and anions from the feed stream and collect them in a concentrated waste stream. As with ion exchange, the ED process is only capable of removing ionic contaminants, neutral amine degradation products would be left in the amine solvent. Some of the carbamate anions, and/or the protonated amine could be transferred and therefore lost.

Due to temperature sensitivity and limitation of the ion-exchange membranes, ED is best conducted on cold lean solvent. Thus, downstream of the lean amine cooler would be the best location to extract the slipstream. Additional cooling may be required to reduce the input temperature to around 40°C. Neutralization with a neutralizing agent or caustic and microfiltration are usually used upstream of the unit. The filtration step could cause a loss of amine solution. The presence of dissolved iron, hydrocarbons or suspended solids can result in fouling on the membrane surface, which increases the stack resistance and reduces the process efficiency [316].

3.5.4 COMPARISON OF SOLVENT CLEANING STRATEGIES

A variety of reclaiming options are now available for amine purification [316–318]. The use of purging or neutralization is unlikely to be sufficient to maintain amine purity in PCC systems. Other options, such as vacuum distillation, ion exchange, and electrodialysis, have matured and improved over the last two decades and are available as mobile service or permanent installations throughout the world.

Distillation is only appropriate for amines that are sufficiently volatile and stable at the temperatures that are required to distil the amine. Thermal reclaimers are operated at the PCC pilot plant using MEA or MEA blends as absorbents. However, no detailed performance data of the reclaimers is available. For high-boiling point amines, distillation exposes the amine to high temperature and, hence, results in potentially further solvent degradation and higher energy requirement, which is particularly significant for PCC where energy efficiency is of paramount importance. In contrast, ion exchange and electrodialysis do not require high temperature and thus reduce the possibility of further thermal degradation. However, these two options cannot remove non-ionic contaminants. It is likely that vacuum distillation is best suited for applications where solvent degradation is an issue.

Ion exchange is ideal if the HSS concentration is low. However, higher HSS concentrations and total solution flow rates are likely to be present in a PCC scenario, and thus the equipment costs and scale become prohibitive. Electrodialysis has an advantage of lower chemical and water usage than ion exchange. However, even a small quantity of CO_2 in MEA solution can decrease the process effectiveness and increase the waste fraction. Specific energy consumption is linearly increased with the increasing CO_2 loading. In addition, the currently high costs associated with manufacture of selective membranes that are resistant to both high pH and amine solvents limit the application of ED in PCC systems. More work is required to match the membrane chemistry to the contaminated amine solution being treated.

4. IDENTIFICATION OF PARAMETERS FOR PERFORMANCE EVALUATION (TASK4)

Objective: Identifying the main parameters such as cyclic absorption capacity, heat of regeneration, solvent viscosity, enhancement indexing, heat capacity, degradability, surface tension, solvent cost, absorber sizing, reboiler temperature, and others, to evaluate the performance of solvents and processes reviewed in Tasks 1 – 3, along with their influence on the CO_2 capture cost in terms of CAPEX and OPEX.

4.1 GLOBAL INDICATORS FOR PCC EVALUATION

Main parameters/indicators have been identified for the evaluation of emerging PCC solvents and processes. The choice of these parameters was conducted by detailed literature survey, experts' opinion, and available information from the facilities database to evaluate the direct impact on CO_2 capture outcomes [15,319–324]. Parameters focused on the overall productivity of the process, energy consumption and associated capital and operating costs. The list of parameters is summarised in **Table 4.1** in a schematic manner, divided by technical, economic and environmental aspects.

Table 4.1 *List of identified global parameters (indicators) to evaluate performance of PCC systems* [15,319–324].

Identified outcomes for performance	
Parameter	**Units**
Technical	
Recovery (removal, capture efficiency)	$t_{CO2\_captured} \cdot t_{CO2\ feed}^{-1}$ (target > 90%)
Purity $CO_{2\ captured}$	$t_{CO2\_captured} \cdot t_{gas\ captured}^{-1}$ (target > 95%)
Energy intensity	$GJ \cdot t_{CO2\ captured}^{-1}$
Energy consumption (if retrofitted to an industrial plant)	$GJ \cdot t_{CO2\ captured}^{-1}$
Efficiency reduction (if retrofitted to an existing power plant)	%
Economic	
OPEX	$US\$ \cdot t_{CO2\_captured}^{-1}$
Maintenance ratio	$hr_{maintenance} \cdot hr_{operation}^{-1}$
CAPEX	$US\$ \cdot t_{CO2}^{-1}$
Environmental	
CO_2 emissions avoided	$t_{CO2\_captured} \cdot t_{solvent}^{-1}$

Identified outcomes for performance	
Parameter	**Units**
Solvent emissions	$kg_{sol} \cdot t_{CO2}^{-1}$
Safety	
Solvent toxicity, others	0 – 4

Definitions of the indicators/parameters:

- Recovery is defined as the amount (flow rate) of CO_2 truly captured and separated (mass basis) per unit amount of CO_2 fed to the capture process. This represents the simplest way of thinking about a CO_2 capture metric. It is a dimensionless ratio and is mostly expressed as a percentage. The higher the percentage, the higher the removal of CO_2 in the capture process. In practice, typical CO_2 recoveries are between 80% and 95%. The exact recovery choice is an economic trade-off, a higher recovery will lead to a taller absorption column, higher energy penalties and hence increased costs.
- The CO_2 energy intensity indicator is defined as the net amount of energy required per unit amount of CO_2 captured (mass basis). It includes both thermal and electrical requirements, and is a measure of the energy efficiency of the technology or process to capture CO_2.
- The energy consumption is defined as the additional energy required (mass basis of CO_2 captured) for the operation of a PCC system when retrofitted to an existing industrial plant (i.e. cement industry, steel manufacturing, etc.), as the operation of PCC systems increases the global energy requirements. This is defined as the difference between the energy consumption for industrial plant with PCC and the original energy consumption of the industrial plant without PCC, relative to the amount of CO_2 captured.
- The efficiency reduction is defined as the percentage loss in power plant energy production once retrofitted with a PCC system, due to the energy requirements for PCC system operations. It should be noted that this indicator is relatively similar to the aforementioned energy consumption; however, the efficiency reduction is solely applied to power plants integrated with PCC.
- The total annualised cost of CO_2 captured is the sum of several terms encompassing the large capital costs associated with the capture plant, operating, and maintenance costs over the whole duration of the plant lifetime.
- The cost per tonne of CO_2 (OPEX) metric is the sum of annualised operating costs of the utilities relative to the amount of CO_2 captured and separated. It includes fixed and variable operating costs (US\$ yr^{-1}), capacity factor (# hours maintenance in a typical year), the cost of additional resources (i.e., makeup) needed to compensate for the efficiency reduction, among others. The cost of CO_2 compression should be also included.

- Capital cost (also known as investment cost, CAPEX) is a widely used, albeit incomplete, metric of the cost. It is often reported on a normalised basis according to the plant capacity (e.g., cost per kW installed in a power plant). For CO_2 capture systems, the capital cost is generally assumed to represent the total expenditure required to design, purchase and install the system of interest. It may also include the additional costs of other plant components not needed in the absence of a CO_2 capture device, such as the costs of an upstream gas purification system to protect the capture device. In addition, different organizations employ different systems of accounts to specify the elements of a capital cost estimate. The terms used to report capital costs might disguise such differences and lead to misunderstandings about what is and is not included. For example, power plant cost studies often report a value of capital cost that does not include the cost of interest during construction or other so-called 'owners costs' that typically add at least 10-20% to the 'total capital requirement' of a system. Only if a capital cost breakdown is reported can such omissions be discovered. Studies that fail to report the year of a cost estimate introduce further uncertainty that may affect cost comparisons. Moreover, since several of the parameter values may change over the operating life of a facility (such as the capacity factor, solvent cost, or variable operating costs), the cost also may vary from year to year. To include such effects, an economic evaluation would calculate the net present value (NPV) of discounted costs based on a schedule of year-to-year cost variations. However, most engineering-economic studies only calculate a single value of 'levelised' cost over the assumed life of the plant.
- CO_2 Avoided Emissions is referred to the amount of CO_2 emissions reduction per unit amount of solvent in the process ($t_{CO2\_captured} \cdot t_{solvent}^{-1}$). It is defined per tonne of solvent used for a fair comparison between different solvents and processes. Note that large-scale facilities and pilot-plants usually report the amount of CO_2 captured per year.
- Solvent Emission: The level of amine emission is an important parameter to manage in order to prevent any operational, environmental, health and safety issues. Usually, fresh virgin amine solutions tend to emit less than a regenerated amine solution, in which degradation products have built up. Several reduced amine emission strategies can be applied including acid washing and more efficient mist elimination.
- Safety Metric: The relative safety and environmental benefits metric is a composite assessment of the raw materials and processing conditions, including any environmental benefits, of the new process relative to those of any existing process for the same product. The metric assessment is either improved, no change, or reduced. The relative safety ranking uses the National Fire Protection Association (NFPA) Standard 704 "fire diamond" category hazard values, which range from 0 to 4, with 0 meaning no hazard and 4 meaning severe hazard.

4.2 MAIN PARAMETERS FOR SOLVENT AND PROCESS EVALUATION

Although the heat of absorption is considered the key parameter to compare emerging solvents [13], other key parameters have been extracted from the testing. We provide here a list of main parameters for the evaluation of the performance of emerging solvents and processes, and how those affect the CO_2 capture cost (CAPEX or OPEX).

The identified parameters are divided into those for solvent evaluation and for process evaluation. The list of parameters is provided in **Table 4.2**. To ensure that the examined solvents and processes are compared under the same conditions and criteria, a standardisation of performance metrics has been performed, with defined units also provided in **Table 4.2**.

***Table 4.2** List of identified parameters for solvent and process evaluation.*

For Solvent Evaluation		For Process Evaluation	
Parameter	**Units**	**Parameter**	**Units**
Rich loading	$kg_{CO2} \cdot t_{solvent}^{-1}$	Flue gas flow rate	$tonne \cdot h^{-1}$
Lean loading		CO_2 concentration	%
Heat of absorption	$kJ \cdot mol_{CO2}^{-1}$	Electrical power consumption	$kWh \cdot t_{CO2}^{-1}$
Heat of evaporation		Thermal reboiler duty	$GJ \cdot t_{CO2}^{-1}$
Lean solvent viscosity	cP	Reboiler temperature	K
Enhancement factor relative to MEA based on kinetic or indexing	Dimensionless	Solvent makeup rate	$kg_{sol} \cdot t_{CO2}^{-1}$
Lean solvent heat capacity	$kJ \cdot mol^{-1} \cdot K^{-1}$	Solvent corrosiveness	mm/yr
Lean solvent vapour pressure	Pa	Foaming factor	$Pa^{0.5}$

The framework used to assess the impact on CO_2 capture is based on the material and energy flows needed to produce a unit of product. These parameters for both solvents and processes, help identifying expected outcomes such as purity of captured CO_2, amount recovered and costs of CO_2 avoided and captured for the final assessment and ranking, part of the standardised metrics to evaluate their performance for PCC, as explained in **Section 4.1**.

4.3 FACTORS TO BE CONSIDERED FOR SOLVENT EVALUATION

Factors to consider when conducting solvent screening for conventional and emerging PCC process are: (1) CO_2 loading (cyclic capacity), (2) heat of absorption, (3) CO_2 absorption rate, (4) solvent viscosity, (5) surface tension, (6) solvent degradation, (7) solvent toxicity, volatility, foaming and corrosivity, and (8) solvent cost. Definitions and details for each of them are provided next:

1. CO_2 capacity: The ultimate capacity of the absorbent for capturing CO_2 is determined by the phase equilibria relationships between the absorbent and CO_2 as a function of temperature, solvent composition, and CO_2 partial pressure. This is related to the solvent flow rate required and the sensible heat requirement. Higher CO_2 absorption capacity would require lower solvent flow rate and subsequent less regeneration energy demand.

Due to the formation of bicarbonate, tertiary amines tend to have higher absorption capacities than primary or secondary amines. The cyclic loading of the solvent is the difference between lean and rich CO_2 loading, usually reported in terms of mole of CO_2 per mole of amine. For a fair comparison with water-lean and water-free systems (and others), we determine it is better to report it in mass basis terms (e.g., $t_{CO2} \cdot t_{solvent}^{-1}$). A high cyclic loading will result in lower solvent circulation flow rate in the plant, which will influence the dimensions of the solvent heat exchanger, the amine pumps, the reboiler, the absorber and piping. High cyclic loading will also lower the electricity consumption of the pumps and the energy required for solvent heating. In addition, a smaller absorber will lower the flue gas blower energy requirements and dimensions.

2. Heat of absorption: This is an important factor affecting the reboiler heat duty. Lower heat of absorption will require less regeneration energy input to reverse the chemical reaction and release absorbed CO_2. A low value often comes together with a low reactivity towards CO_2 and, similarly, a high absorption rate is normally accompanied by a high binding energy.
3. CO_2 reaction kinetics: The rate of reaction determines the required liquid residence time and hence the size of the contactor equipment. This determines the rate at which CO_2 will be captured. Fast reaction kinetics is essential for an intensified PCC process since the residence time is very short. Slow reacting absorbents may require large contact areas and residence times to achieve the target level of CO_2 removal, leading to large and expensive columns. Primary and secondary amines tend to react the fastest with CO_2 as they form a stable carbamate. Tertiary and hindered amines catalyse the hydrolysis of CO_2 to form a bicarbonate ion and protonated amine. The formation of bicarbonate is slower compared to carbamate formation.
4. Viscosity: Increasing viscosity will lead to thicker fluid layers on the packing bed and longer residence times, as well as an increase in the pump work to circulate the solvent between the absorber and regenerator. Moreover, since the diffusion coefficient is inversely proportional to viscosity, the mass transfer coefficient will decrease accordingly. The viscosity of the solvent typically increases with the increasing molecular weight of the amine, with increasing amine concentration and with decreasing temperature.
5. Surface tension: The surface tension of a liquid seeks to minimise the surface area of the fluid. Liquids that have strong intermolecular forces also have high surface tensions. The surface tension of a fluid is an important consideration as it affects the distribution of liquid over packing surfaces, liquid hold-up and the formation and breakup of foams. For high surface area packing materials, reduced surface tensions could increase the packing effective area, thought to be due to removal of capillary phenomena. Lowering the surface tension of fluids via surfactant addition, however, can have deleterious effects, like resulting in significant foam formation.
6. Solvent degradation: This is related to solvent stability, operational issues and environmental impact and need to be evaluated when selecting solvents. Solvent degradation (which may be controlled by having high stability against oxygen and thermal stress) and corrosion will cause an increase in operation and maintenance (O&M) costs by making up solvent and reducing the lifetime of the equipment. Formation of degradation products are thought to play an important role in the corrosion. Reducing

the degradation rate will thus result in lowering the OPEX and the CAPEX of the critical parts in the CO_2 capture plant as well as the environmental impact. Amines undergo irreversible reactions that will consume the solvent, create deposition layers especially on the reboiler heat transfer surfaces that must be periodically cleaned [e.g. heat stable salts] and must be removed, or they may spontaneously leave with the gas streams increasing the emission of toxic materials. The nature and extent of chemical stability is determined by the nature of the solvent and the operating parameters and must be studied carefully. The impact of chemical stability and the possible emission of by-products may not be fully understood until the solvent in question is run for extended periods. As amines with high concentration are likely to form higher concentrations of acidic degradation products, there are maximum concentration recommendations for most common absorbents in order to limit corrosion. However, there are benefits in using higher concentration absorbents, such as reduced absorbent and energy requirements. Hence, many proprietary solutions use higher absorbent concentrations, but will also include corrosion inhibitors. An example is the Fluor Econamine FG Plus utilizing a higher concentration of MEA coupled with proprietary corrosion inhibitors (see Section 2.4.1.3).

7. As corrosion rates tend to increase with an increase in CO_2 loading, highly loaded absorbents will suffer from greater corrosion effects. Inhibitor choice needs to be made carefully as inhibitors can affect plant operation (e.g. through increased foaming), and increase oxidative amine degradation, potentially increasing corrosion rates. The use of inhibitors can allow the use of lower grade, cheaper metals for construction (see Section 3.3). For instance, the absorber columns at both the **Test Centre Mongstad (TCM)** and the **Boundary Dam CO_2 capture plant** use ceramic lined concrete towers for their absorber columns (cheaper method of constructing a corrosion-resistant column).
8. Furthermore, evaporative losses and associated health and environmental risks are becoming increasingly important. Environmental impacts deserve serious attention when judging the potential of a solvent since causing secondary pollution while capturing CO_2 is not a scenario the public would be willing to take.
9. High cost and limited availability of potential solvents at commercial scale could contribute to limitations of the process feasibility.

4.4 FACTORS TO BE CONSIDERED FOR PROCESS EVALUATION

Factors to be considered for the process evaluation include:

1. The flue gas flow rate. It will determine the size of the absorber and the absorber represents a sizeable contribution to the overall cost. For a given system, the solvent flow rate will be fixed by the size of the absorber and the chosen CO_2 concentrations within the lean and the rich solutions.

2. CO_2 content in flue gas. Since flue gas is usually at atmospheric pressure, the partial pressure of CO_2 will normally be below 25%.

3. The energy consumption of the process, which is mainly related to the thermal energy needed to regenerate the solvents and the electrical energy required to operate liquid

pumps and the flue gas blower or fan. The thermal reboiler duty is one of the most influential parameters, since it has been estimated to be 15-30% of the net power production of a coal-fired power plant. Moreover, energy is also required to compress the CO_2 recovered to the final pressure required for transport and storage. Such energy load would reduce the output of the power plant and reduces its efficiency. For instance, the CO_2 capture plant in Unit 3 at the Boundary Dam Project reduces the output from 150 MW to 115 MW, corresponding to 23.3% drop in net power [325].

4. The reboiler temperature, which is important to avoid amine degradation. For the same reboiler temperature, lower lean loading can be achieved at a lower regenerator operating pressure. Hence, the minimum circulation rate necessary to achieve 90% CO_2 removal will be lower at a lower regenerator operating pressure.
5. Cost of the solvent. Because the cost of the makeup flow of solvent is one component of the total capture cost, to keep total capture costs at reasonable values, the makeup costs cannot be excessive. For instance, MEA loss rate is estimated around 1.5 $kg \cdot t_{CO2}^{-1}$ (from degradation and emission) [235], which corresponds to about 5-10% of the OPEX.
6. Absorber operating temperature plays a vital role in increasing solvent capacity and, in turn, reducing overall energy consumption. Cooling is needed to bring the flue gas and solvent temperatures down to temperature levels required for efficient absorption of CO_2. From the solvent/CO_2 phase equilibrium curve, it is well understood that at constant partial pressure of CO_2, lower solvent temperatures increase the equilibrium CO_2 loading and hence the potential absorption capacity. However, lower solvent temperature also reduces the reaction rate and requires longer residence time (packing height) to absorb CO_2. Therefore, it is essential to determine the optimum operating temperatures in the absorber system to maximize solvent capacity as well as minimizing column height and energy consumption. Bringing the absorption temperature closer to the desorption temperature will decrease the costs of the solvent heat exchanger. Nevertheless, for specific solvents, lowering desorption temperature will mean a higher lean CO_2 loading and thus a smaller cyclic loading. Counteracting this with higher solvent concentrations is not always possible, due to the corrosive nature of amine-based solvents.

4.5 DEVELOPMENT AND VALIDATION OF A SCREENING MODELLING TOOL FOR COST ESTIMATION

Previous works from our team and others have demonstrated that molecular modelling combined with macroscopic thermodynamics is a useful tool to screen solvents based on their cyclic capacity and heat of regeneration [9,17,18]. Although a priori desirable, rigorous process modelling might not be recommended during screening to evaluating how these solvents perform in terms of process-based metrics and cost; only the most promising ones should be rigorously evaluated.

To provide decision makers with a systematic method for solvent screening, we have developed a modelling tool for the process design including the examination of CAPEX and OPEX performance obtained using a simplified approach with the available data collected in the **CO_2SOLV** database. An equilibrium-based model to study the absorption of CO_2 in amines was used for this purpose. **Figure 4.1** shows a schematic representation of the evaluated system. The model comprises a blower absorption column, rich and lean solvent pumps, rich/lean heat exchanger, cooler, stripper, reboiler and condenser. Each of these sub-models incorporates standard cost equations based on the design equations, with the key equations and other model details presented in **ANNEX III**. The following solvent properties that can affect the process performance of the carbon capture were included in the model: density, viscosity, surface tension, heat capacity, heat of absorption, which might inherently include the heat of reaction in the case of reactant solvents, and CO_2 solubility.

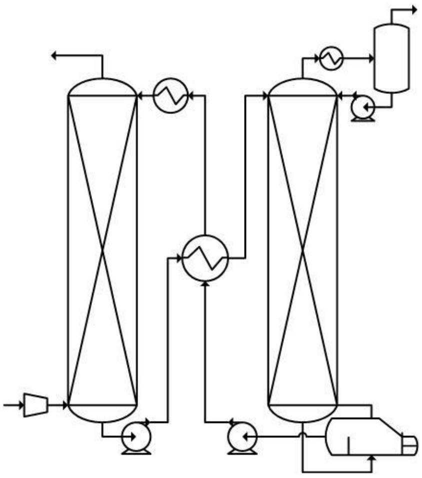


***Figure 4.1** Schematic diagram of the simulated model, showing the blower, absorber column, pumps, rich/lean heat exchanger, cooler, and solvent regeneration process (stripper, reboiler and condenser).*

The model was initially validated against published works on post-combustion CO_2 capture from a power plant, using the process specifications for the **CASTOR project pilot plant** as shown in **Table 4.3** [2]. The solvent selected was aqueous 30 %wt. MEA, as the benchmark against which all other CO_2 capture processes are compared. The validation of the absorption model was done by comparing the simulation results from the model with experimental data. The capture rate was set to 90% of the carbon emitted by the power plant.

***Table 4.3** Specifications of CASTOR project pilot plant* [2].

Specifications	
Plant capacity	7738 tonne of CO_2 per year
Lean solvent	23 m^3/h at 58.8°C (30.4 wt.% MEA)
Inlet flue gas	4915 Nm^3/h at 47.3°C (11.86 mol.% CO_2)
Absorber pressure	101.3 kPa
Stripper and reboiler pressure	181 kPa
Degree of capture	90%
Columns diameter	1.1 m

IMTP 50mm specific surface area (a_p)	107.1 m^2/m^3

The results of the validation are presented in **Table 4.4**. Lower prediction of absorber height might be due to lower degree of capture obtained with the integrated model as compared to experiments [2]. In terms of KPIs highly significant to the regeneration of amines (i.e. the reboiler duty), our study gives a reasonable validation.

Table 4.4 *Model prediction in comparison with CASTOR project pilot plant data.*

	Experiment [2]	**Model result**	**% relative error**
Absorber height (m)	18	15.8	12.2%
Lean solvent loading (mol CO_2/mol MEA)	0.28	0.30	7.1%
Rich solvent loading (mol CO_2/mol MEA)	0.46	0.514	11.7%
Reboiler duty (GJ/t_{CO2})	3.897	3.468	11.0%

From this analysis, it is obtained that the columns (absorber and stripper) account for about 70% of the equipment installation cost (CAPEX), while the amine regeneration cost (in reboiler) covers about 70% of the equipment operating cost (OPEX). This result is in close agreement with the findings of Abu-Zahra [2], and Al Hajaj *et al.* [326] and indicates that the column sizing and reboiler duty represent two important process parameters that can be used for fast comparative performance of solvents for CO_2 capture.

The results show that the TAC of the capture process is \$57 per $tonne_{CO2}$, which gives a total cost of the CO_2 capture of \$76 per $tonne_{CO2}$ once the costs of CO_2 compression and dehydration are accounted for [327]. This is in line with current projections of the cost of carbon capture on an industrial scale for example, the **Petra Nova Carbon Capture Project**, whose cost has been estimated to be \$70 per $tonne_{CO2}$ [328].

In summary, the equilibrium-based process model integrated with the **CO_2SOLV database** has the ability to predict the performance of mass transfer driven process of CO_2 separation using amines. After validating the model, a sensitivity analysis has been performed to determine the aftermaths of varying each of the properties on the size and annualised CAPEX, OPEX and TAC of the carbon capture plant in order to define the standard metrics and prioritize them. Results from the sensitivity analysis are presented and discussed in the next section.

5. DEVELOPMENT OF STANDARDISED METRICS TO EVALUATE PCC PERFORMANCE (TASK5)

Objective: to develop a set of standard metrics, in conjunction with the main parameters from **Task 4**, to evaluate the performance of the solvents reviewed in **Task 1**. The task includes:

1. Definition of standard metrics such as kinetic rate, heat of absorption, absorption capacity, ease of desorption, degradation, volatility, corrosion, toxicity, viscosity, and foaming capacity amongst others.
2. Definition of units of the standard metrics
3. Selection of valid measurement techniques

5.1 PROCEDURE FOR THE DEFINITION STANDARD METRICS

In order to define and prioritise the standard metrics to evaluate the performance of the solvents, the screening modelling tool developed in this project and validated in **Section 4.5** was used to perform a sensitivity analysis in order to quantitatively evaluate the impacts of different properties on the design and cost of the process. **Table 5.1** shows the values for some of the metrics for the base case (MEA 30 wt.%). Several studies have focused on novel solvent materials, process optimisations and techno-economic analysis. However, the systematic analysis of the property impacts on the PCC process has rarely been conducted [329].

***Table 5.1** Description of selected metrics values for the base case (MEA 30 wt.%).*

Property	Value
Liquid Viscosity	0.0018 kg/m.s
Liquid Density	1009.2 kg/m^3
Gas Density	1.22 kg/m^3
Gas Diffusivity	1.7e-5 m^2/s
Heat Capacity	3.6 kJ/kg.K
Absorption Enthalpy	84 kJ/mol
Absorber height	15.8 m
Total Annualised Cost	\$57 per tonne$_{CO2}$

The addressed questions to perform the sensitivity analysis are:

- What are the processes that are most sensitive to the properties of the solvent?

- What are the property impacts on the absorber design/CAPEX/OPEX?

The sensitivity analysis was performed based on a 30% wt. MEA aqueous solution, selected throughout this project as the benchmark for comparison. To assess the impact of properties on the column design, sensitivity studies were conducted regarding the properties of gas and liquid phase density, viscosity and diffusivity, which were varied from -30 to +30% of the initial values (the MEA benchmark case). Every property has been individually screened by varying its value within sensible ranges that were selected based on typical values of solvents. Different properties impact the column design. The overestimation of the gas flux is the result from overestimations of the gas and liquid densities and viscosity of the liquid phase.

As shown in **Figure 5.1**, deviations of the gas phase density and the density and viscosity of the liquid phase cause variations in the pressure drop of the column, which further affects the capacity parameter and the gas flux at flooding. The design column diameter is more sensitive to the deviation of the gas phase density than the liquid phase properties. The increase of gas phase viscosity decreases the CO_2 mass transfer through the gas film. Correspondingly, the overall mass transfer of the absorption also decreases. Thus, to achieve the same target of CO_2 recovery rate, higher packing height is needed. When the viscosity deviates +15% and –15%, the height shows variations of +12.9% and -13.1%, respectively. In addition, when the surface tension deviates +/-15%, the height variations are +/-2.7%, respectively. In general, the CO_2 mass transfer through the liquid film increases with the increases of the density and diffusivity but decreases with the increases in the viscosity and surface tension. The chemical reaction occurs in the liquid phase and it is represented by the enhancement factor, which is inversely affected by the diffusivity of CO_2 in the liquid phase. Although, the diffusivity directly affects the mass transfer through the liquid film, its inverse effect on the enhancement factor is more significant for the packing height calculation.

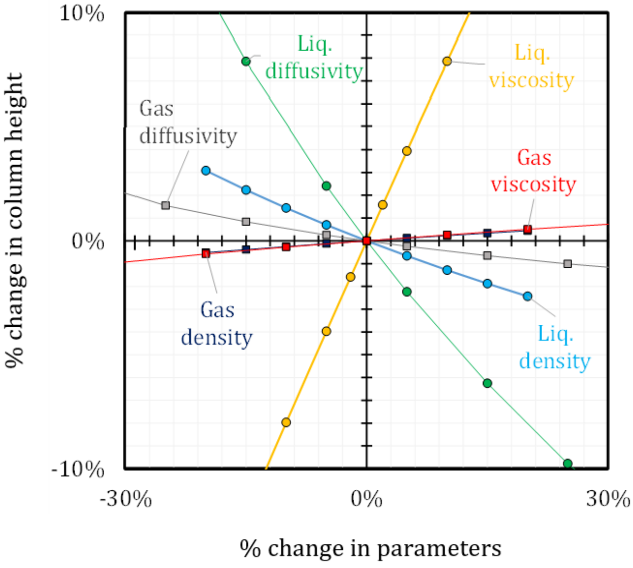


Figure 5.1 *Sensitivity analysis of the impact of the fluid properties on the percentage of deviation of the column height.*

The impacts of the **property deviations on the annual capital cost** are shown in **Figure 5.2**. The two properties that have more influence in the capital cost, altogether with the absorption capacity and reaction rate, are the absorption enthalpy (heat of absorption) and the liquid phase viscosity. +/-15% under/overestimation of the absorption enthalpy and liquid viscosity can vary the capital cost by +7.5% and +3.5%, respectively. Moreover, it was found that the impacts of the viscosity and density of the gas phase are less significant.

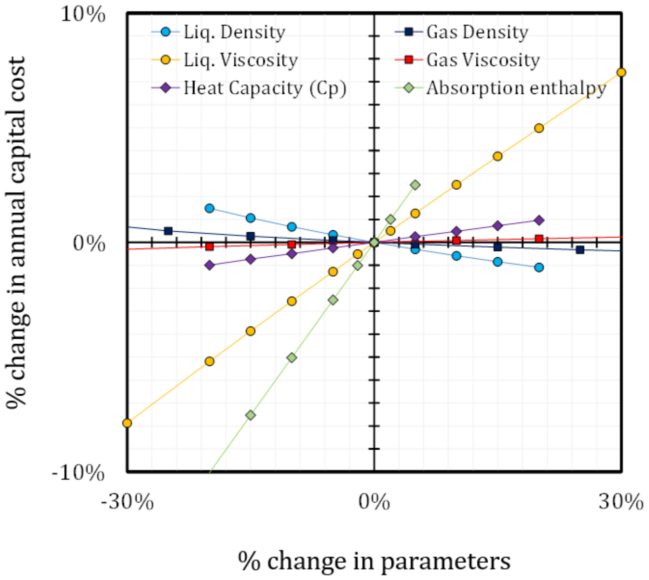


Figure 5.2 *Sensitivity analysis of the impact of the fluid properties on the percentage of deviation of the annual capital cost.*

Higher values of **viscosity** increase pump power because of changes in the hydraulic behaviour of the solvent associated with a higher friction factor and pressure drop, thus increasing the operational challenges. However, the cost related to the electric requirements represents 5% of the total OPEX of the process. Thus, an increase in plant electricity requirements for liquid pumping does not correspond to a significant increase in process costs. The **heat capacity** is the only property that has a pronounced effect on both the CAPEX and the OPEX. Higher values of heat capacity of the solvent result in higher heating and cooling requirements, *i.e.*, in the OPEX. As a result, larger contact areas are required in the heat exchangers, upon increasing the CAPEX. We found that varying the **thermal conductivity** and the **surface tension** of the solvents has a minor effect on the overall cost of the carbon capture plant compared to the effect of the properties investigated above. Having said that, the surface tension is expected to play a more important role in the case of non-reactive solvents [330].

There are **associated uncertainties** with the **material unit cost** and replacement rate as well as the mechanical efficiencies. Hence, it is imperative to investigate the influence of the variation in the material and equipment parameters on the performance of CO_2 capture and compression process plant using the monetised KPIs. Results show that there is a significant variation in the total cost of CO_2 capture and compression with change in material cost. Similarly, process cost could be reduced (although much lower as compared to with change in unit cost) by the development of less degradable materials with lower replacement rate (longer material lifetime).

The cost per tonne of **CO_2 captured as a function of % CO_2 capture and CO_2 concentration** for a 30 wt.% MEA solvent is presented in **Figure 5.3**, confirming that gas concentration is a stronger determinant of the cost of capture than the degree of capture. This implies that for the same investment, it is economically preferable to capture CO_2 from higher concentration sources. Based on a sensitivity analysis including monetised and non-monetised KPIs, the figure depicts contour plots of the total annualised cost as a function of capture rate and lean loading, for different concentrations of CO_2 being captured, from 1-40%, with 30% aqueous MEA. It was observed that cost increases linearly (with small slope) for capture rates ~85%, but the **marginal cost increases exponentially if rates above >95% are desired.**

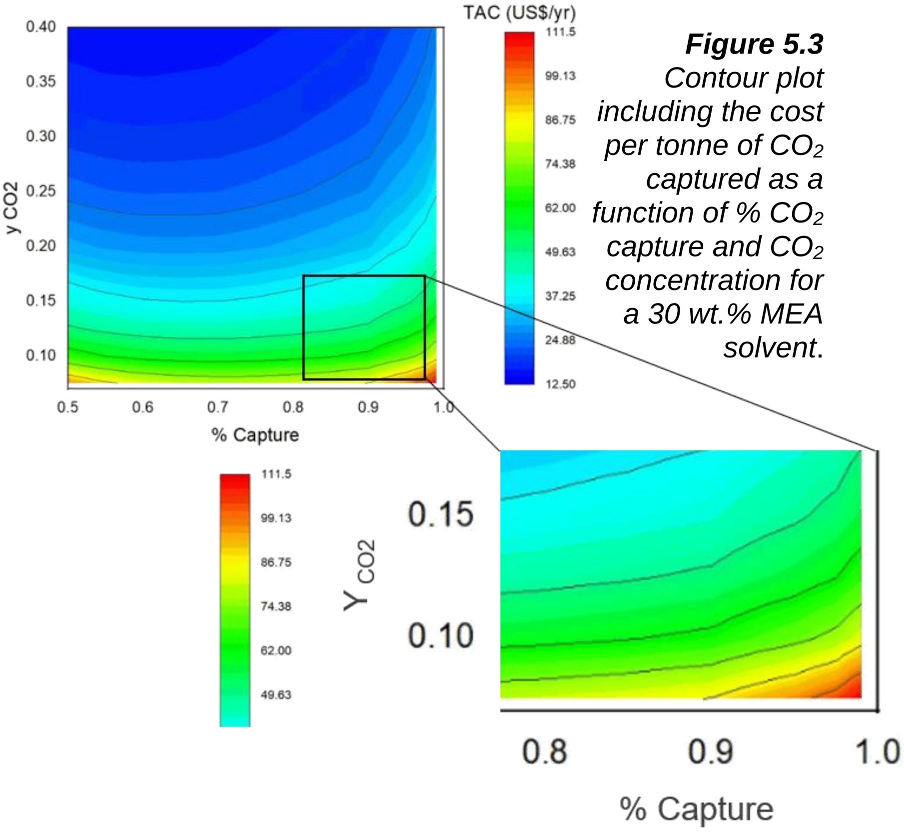


Figure 5.3 *Contour plot including the cost per tonne of CO_2 captured as a function of % CO_2 capture and CO_2 concentration for a 30 wt.% MEA solvent.*

5.2 STANDARD METRICS AND EVALUATION METHODS FOR PCC PERFORMANCE

According to the previous analysis on the impact of the solvent properties variation on the process and cost, we have summarised in **Table 5.2** a criteria for evaluating solvent properties based on their relative importance on a scale of 0 to 10, with 10 being the most important property. The choice of the first 4 parameters, which are related to the efficiency of the absorption and regeneration processes, pertains to the core of the process. These properties dictate the overall efficiency of the process and they can be considered as *necessary* constraints. The solvent cost has been placed in the middle as not to abandon competitive solvents just because their current cost is not favourable for its implementation at a large scale. On the other hand, it can still be a show-stopper if the cost is drastically high compared to the current used solvents. Note that the secondary parameters (less important) are related to expected operating issues with the examined solvents such as stability of the solvent, volatility, corrosiveness, toxicity and foaming tendency. Such properties can be considered as *sufficient* constraints. Further experimental data is required for a more detailed assessment of each of them.

Table 5.2 *Ranking of importance for the evaluation of solvent properties based on a scale of 0 to 10 (10 most important), together with their evaluation methods.*

Metrics	**Units**	**Importance**	**Potential show-stopper**	**Evaluation methods**
Absorption (cyclic) capacity	$kg_{CO2} \cdot t_{solvent}^{-1}$	10	Yes	Calculated from phase equilibria measurements at specified conditions
Heat of absorption	$kJ \cdot mol_{CO2}^{-1}$	10	Yes	Calorimetry measurement, calculation from phase equilibria measurements
Viscosity (loaded)	cP	8	Yes	Viscosimeter
Reaction kinetics	$mol.L^{-1}.s^{-1}$	7	Yes	Wetted-wall column (WWC) or similar
Solvent cost	$\$.kg^{-1}$	6	Yes	Vendor
Toxicity	LD_{50}	6	Maybe	Material safety data (MSDS)
Degradation	$kg_{sol} \cdot t_{CO2}^{-1}$	5	Maybe	Laboratory test and pilot plant rigs
Corrosivity	pH	5	Maybe	Laboratory test
Volatility	kPa (relative to vapour pressure)	4	Maybe	Laboratory test
Foaming	ml	4	Maybe	ASTM D892

6. CRITICAL EVALUATION OF SOLVENTS AND PROCESSES PERFORMANCE (TASK 6)

Objectives: Based on the most promising solvents and processes identified in **Tasks 1** and **2**, the evaluation metrics developed from **Tasks 3 – 5**, will be used to assess the performance of the most promising systems in terms of enhanced CO_2 capture performance and potential in reducing costs/adding value in future decarbonized plants.

6.1 IDENTIFIED GAPS FOR SOLVENT SCREENING

In order to rationally screen, select and design solvents for chemical processes in general, and CO_2 capture in particular, a whole system approach is necessary. Otherwise, it is impossible to fully assess the impact of solvent thermophysical properties on process performance and therefore costs. The absence of such an approach to date has led to an over emphasis of CO_2 solubility in solvent selection and design, potentially limiting progress in this area. Only a systematic approach to solvent design, with all properties appropriately weighted, can lead to an optimal (or possibly even improved) solvent design.

As previously mentioned, after the review of emerging aqueous and water-lean PCC solvents (**Task 1**), more than 800 entries were incorporated in the **CO_2SOLV** database at single conditions of temperature and partial pressure of CO_2, and more than 100 systems were incorporated with additional thermophysical information, including absorption isotherms, density, and viscosity. Moreover, the information in the solvent screening tab and solvent properties tab have been standardised with the same units of measurements, based on the performance metrics presented on **Task 5** (**M2**).

Based on the identified essential parameters for performance evaluation (**Task 4**), we have found that the reported properties such as absorption capacity and cyclic capacity of the examined solvents is discrepant between different studies in terms of rich and lean temperature and pressure conditions. Therefore**, 50+ different solvent systems were identified with enough data at typical process conditions** (e.g., rich loading, density, absorption enthalpy and viscosity at 313 K and P_{CO2} < 25 kPa in the feed stream, and at higher temperatures for desorption), and were evaluated in a techno-economic assessment, by utilising the model previously validated for MEA in **Tasks 4** and **5**. Furthermore, integration of the system to be used as a decision tool can be found in the next section (**Task 7**).

Additional identified gaps include:

- Most of the information collected is from process simulation studies focused on existing aqueous alkanolamines and blends. Works examining process design and performance for emerging water-lean and water-free solvents is quite limited but highly desirable.
- The reporting of the cyclic capacity is scarce and varies depending on the evaluated conditions (rich and lean temperature and pressure conditions) on each study.

- The information (e.g., thermodynamic properties) of the commercial solvents used in some of the large PCC facilities is confidential and, hence, non-available. Additionally, available data on solvent properties are limited to those at lean conditions.

6.2 SOLVENT SCREENING AND CRITICAL ANALYSIS

We present here the results obtained by using the modelling tool to screen the alternative solvents based on the standardised metrics defined in tasks 4 and 5 applied to 50 solvent systems. The approach followed for the selection of alternative amines was based on the evaluation of parameters specifically selected to assess their performance with respect to the reference MEA. The study focused on the critical analysis of the effect of using new solvents with improved solvent working capacity, concentration and regeneration properties. It also examines the effect of heat integration, novel stripper designs and lower capital costs.

An initial list of the most promising systems can be extracted from the results presented in **Figure 6.1**, according to the standard metrics developed for the solvents performance (**Task 5, M2**), using the typical reported relation between absorption at the rich and lean conditions, and the required energy for regeneration (i.e., heat of absorption) [331]. The **case study** presented is for absorption at 15kPa (313 K) and desorption at 100 kPa (393 K), with values been normalised with MEA. Since a previous screening was made from the database based on on-point values, only systems with similar or lower heat of absorption than MEA are plotted.

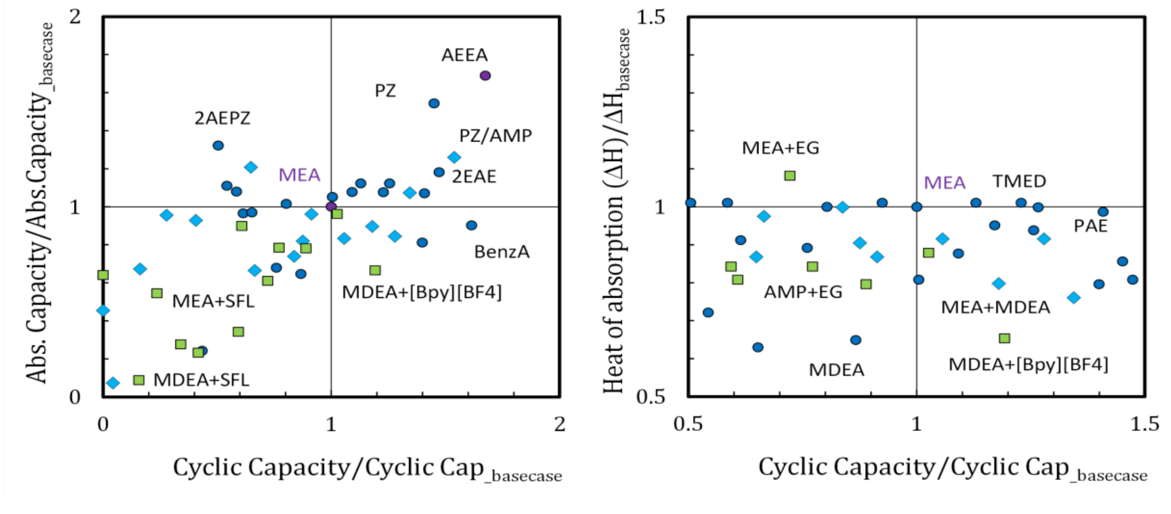


Figure 6.1 *Solvent performance in terms of absorption capacity, cyclic loading and heat of absorption, for aqueous MEA (purple), aqueous amines (dark blue), blends (light blue), and water-free/water-lean solvents (light green).*

The figures are divided in four quadrants, and the most promising systems appear depending on the required stipulation. For instance, to reduce the costs and energy requirements, amines with high CO_2 cyclic capacity and low heats of absorptions are needed. As can be seen, several systems can achieve higher CO_2 loadings and lower heat of absorption than that of MEA, as shown by the amines contained in lower-right quadrant in **Figure 6.1b**. In fact, **PZ, MDEA** and **AMP** have shown a superior performance to MEA under the investigated conditions, as previously mentioned in the IEA GHG 2014 Report [12], and tests have been performed already on pilot-plant to large-scale facilities, as previously mentioned during this report. PZ, one of the most promising molecules appear right next to its blend with MDEA. Other amines such as 2-(ethylamino)ethanol (2EAE) and Aminoethylethanolamine (AEEA) are able to reach higher CO_2 loadings than MEA, with lower heats of absorption and comparable absorption rates.

Nevertheless, it should be mentioned that additional properties and KPIs previously identified in **Task 5** must be also be evaluated, in order to completely verify if the enhancement in the absorption is not impacted by a higher consumption, or larger equipment sizes. As shown in **Figure 6.2**, the absorption column height is more strongly correlated with the **viscosity** of the liquid than with the amount of CO_2 captures (i.e., the cyclic capacity). Nevertheless, in both cases, similar systems can be identified as promising according to a reduction in the levelised cost of the absorber, being the best performers in terms of viscosity: APDA and IPAE; best performers in terms of cyclic capacity: APDA, ZAPD and PZ. *See acronym list for identification of the solvents.*

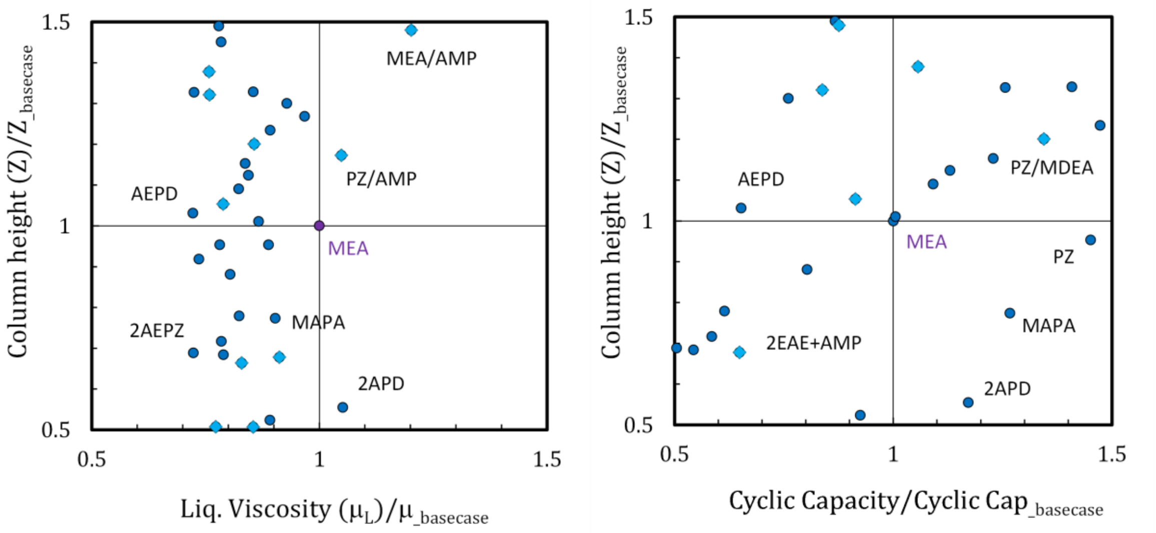


Figure 6.2 *Column height requirements for evaluated PCC systems under the conditions presented in* ***Task 4****. Values normalised with 30 wt% MEA.*

To have a global picture of the different associated costs of each equipment and utilities, **Figures 6.3 – 6.5** present an abatement curve for the levelised total cost and the OPEX. The list of solvents is arranged as aqueous amines first (on the left), followed by aqueous blends and water-free/water-lean amines on the right hand side of the figures. From these figures, it is clear that over **15 of the evaluated system can achieve similar values than the benchmark 30 wt.% aqueous MEA**. However, it is important to highlight that each solvent has a different optimal operating condition, which must be reached by using more complex/sophisticated modelling techniques and design configurations. **The results of the analysis in this report serve as an indicative and a first screening.** Further process optimisation is required for each system to confirm where reductions are achievable.

Using the available information for alternative solvents included in the CO_2SOLV database, the lowest cost of CO_2 capture (using the input parameters for the **Castor plant**, presented in **Task 4)** has been estimated to be is US$46/$t_{CO2}$, for 2APD as amine (and US$51/$t_{CO2}$ for MEA). In a previous report, the IEAGHG [13] estimated the costs for MEA, KS1 and Econamine FG Plus solvents to be US$45, US$37 and US$30 per tonne CO_2 avoided respectively. The capture cost estimated in this study is comparable to the other estimates, taking into account differences in both the economic and processing assumptions used. Details of the assumptions used in these studies can be found in **ANNEX III**.

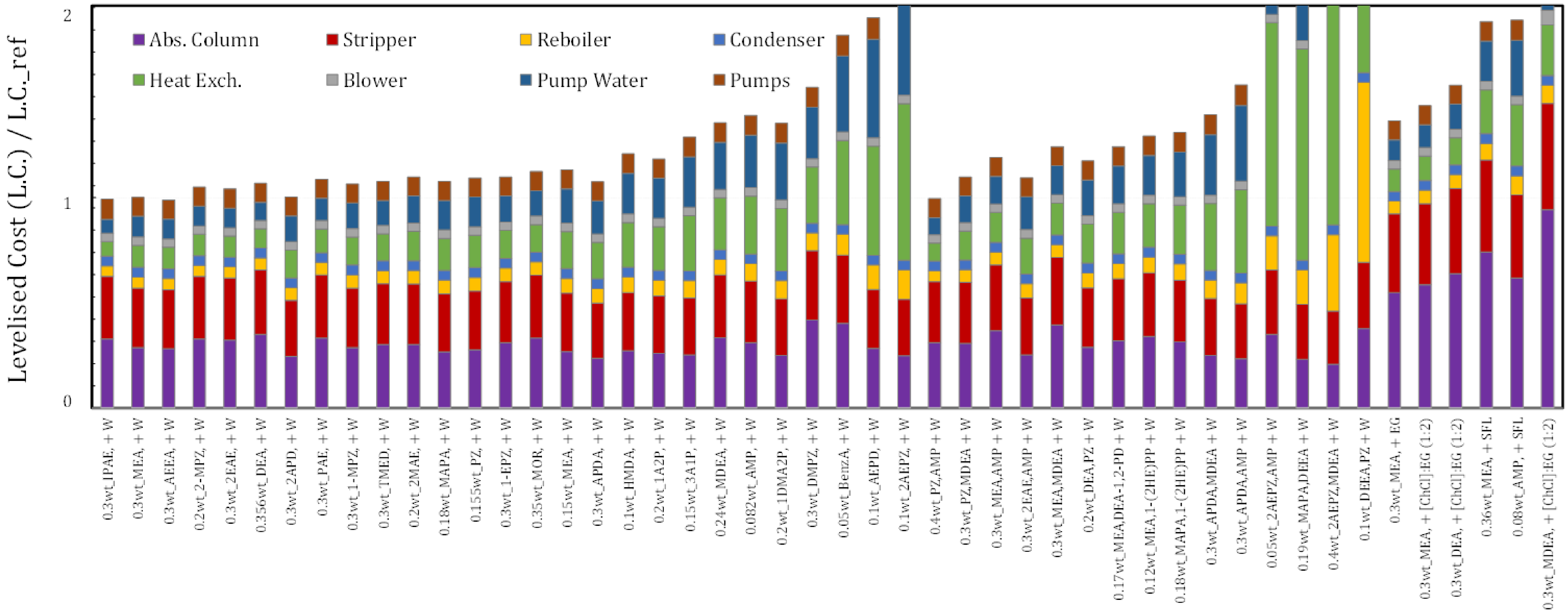


Figure 6.3 *Cost participation on the levelised capital cost, discriminated for each of the 50 evaluated amine-based system. Values normalised with 30 wt% MEA.*

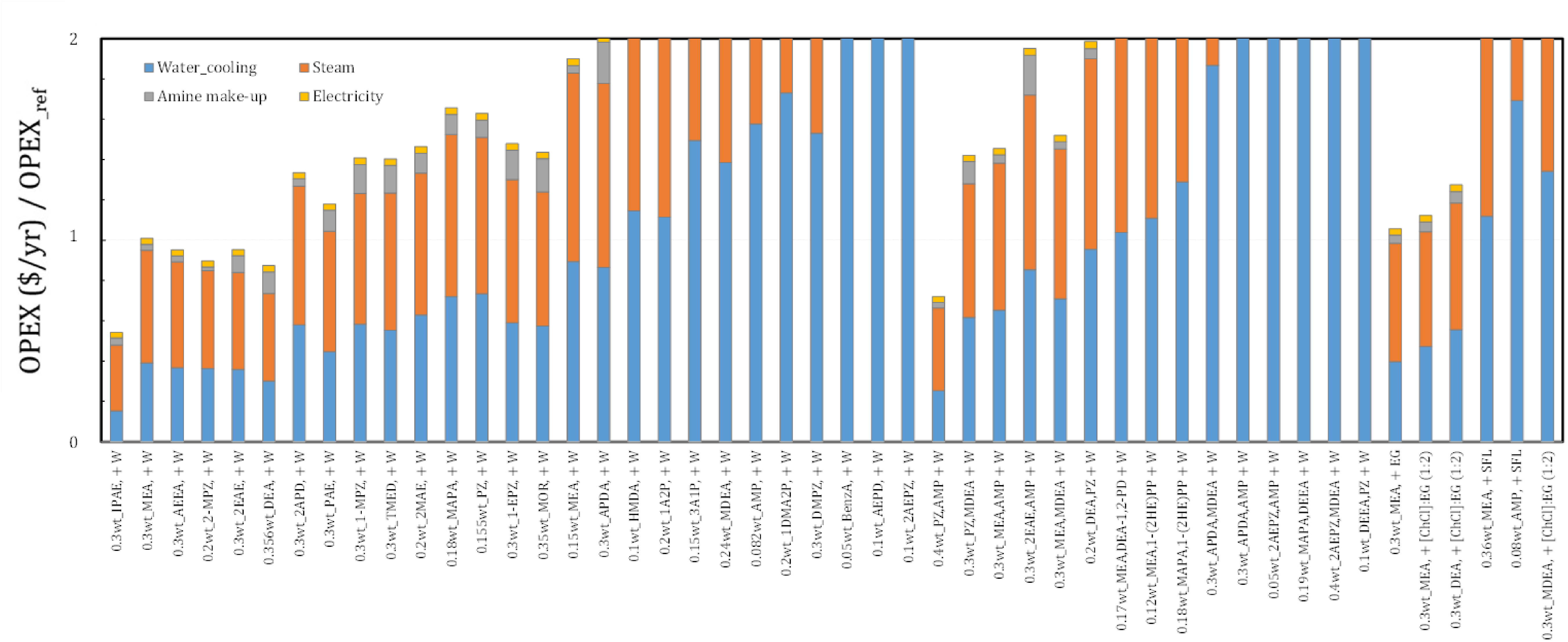


Figure 6.4 *Cost participation on the operating costs, discriminated for each of the 50 evaluated amine-based system. Values normalised with 30 wt% MEA.*

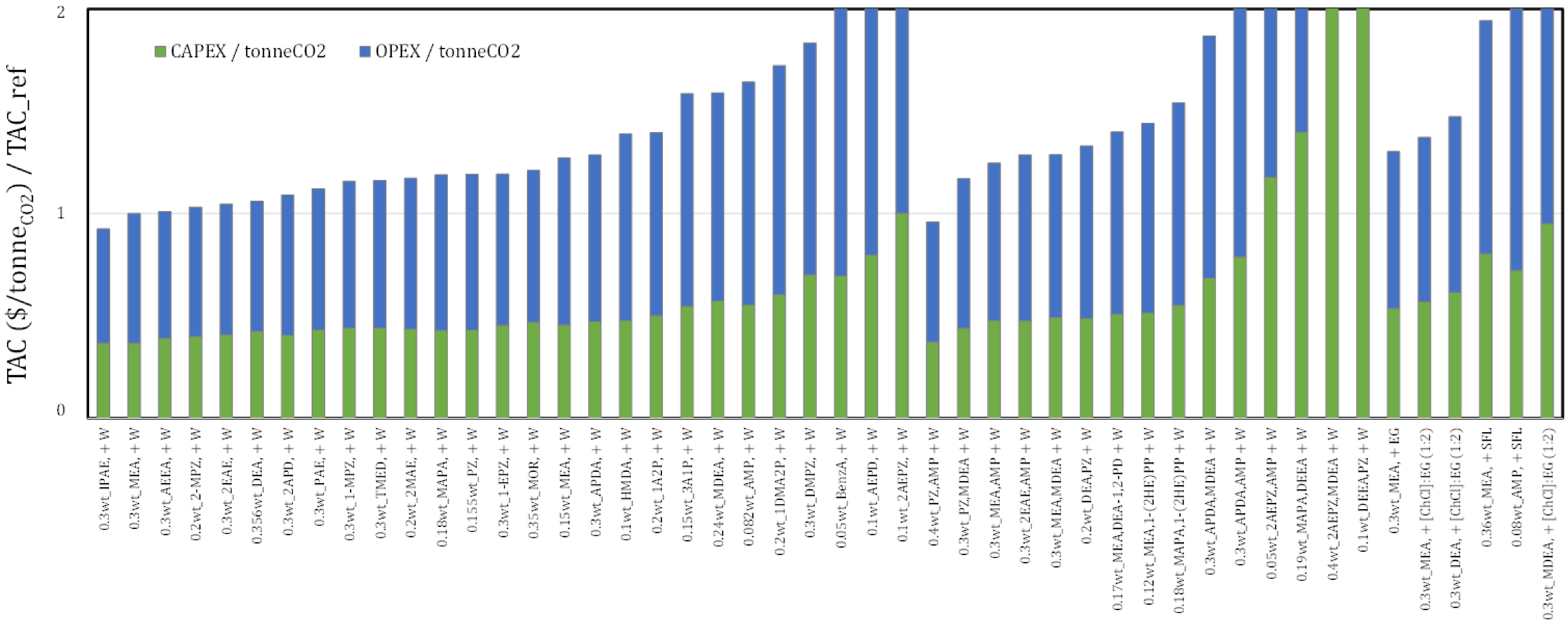


Figure 6.5 *Cost participation on the total annualised costs, discriminated for each of the 50 evaluated amine-based system. Values normalised with 30 wt% MEA.*

As previously observed [2], the absorption column accounts for around 30-40% of the total levelised costs, while the steam required for heating and desorbing the CO_2 in the stripper is the main contribution in the operation costs.

The parameters for **KS1** and **Econamine FG Plus**, which are hindered amines, are proprietary and hence there is insufficient information in the public domain that would enable the determination of solvent flowrates and mass transfer rates. Hence, these solvents are not included in the decision tool in **Task 7**. Conversely, other non-proprietary solvents beside their good performance have inherent disadvantages. For example, AEEA [41,332] has extreme corrosion properties and the ammonia-carbonate solids are difficult to regenerate. In addition, there is limited information published to evaluate mass and energy balances. However, based on the information available, it was possible to estimate the capture cost the different systems in the database.

An important feature of the analysis performed in this work is the **effect of the degradation** in the global performance and cost of the plant. Low solvent losses are already achievable using development solvents such as KS1 or PSR with reported losses at 0.35 kg and 0.5 kg per t_{CO2} respectively [204,225]. As observed from our calculations, **at very low solvent losses (below 0.5 kg/t_{CO2} captured), an increase in the solvent price only have a marginal effect on the capture cost**. This is because the cost of replacing these chemicals only makes up a small component of the operating cost, and the capture costs do not vary significantly between inexpensive and expensive solvents. In addition, we have assumed that the highest price for the novel solvents is to be US$3.5/kg, and even with this price, there is not much change in capture cost whether degradation is high or low, mostly due to the impact of other factors. Note that today some of the solvents under exploration may be more expensive that the assumed cost, as they are still at lab validation stage, hence, for detailed studies of specific solvents the actual cost should be considered. In addition, for corrosive systems, if corrosion inhibitors are added to the solvent without increasing its cost to more than US$2/kg, increasing the solvent concentration in isolation without improving other solvent properties will not result in any observable capture cost reductions.

6.2 SENSITIVITY ANALYSIS IN TERMS OF THE CO_2 COMPOSITION IN THE FLUE GAS

Figures 6.6 - 6.8 present a comparison between **global process indicators and economic process indicators** for the separation of different concentrations of CO_2 in the inlet flue gas. The sensitivity analysis showed that the capture cost could be lowered from US$46 to US$24 per tonne CO_2 avoided when the concentration of carbon dioxide is varied from 11% to 25% in the flue gas. By having a more concentrated CO_2 in the flue gas, both the capture cost and energy demand decreases (as previously showed in **Task 5**). This occurs because as the solvent cyclic capacity increases, the amount of solvent needed to absorb the CO_2 decreases. By decreasing the solvent flowrate, the amount of energy required in the regeneration process to vaporise and liberate the CO_2 also decreases, as well as the energy for pumping, while the size of the required equipment is also reduced.

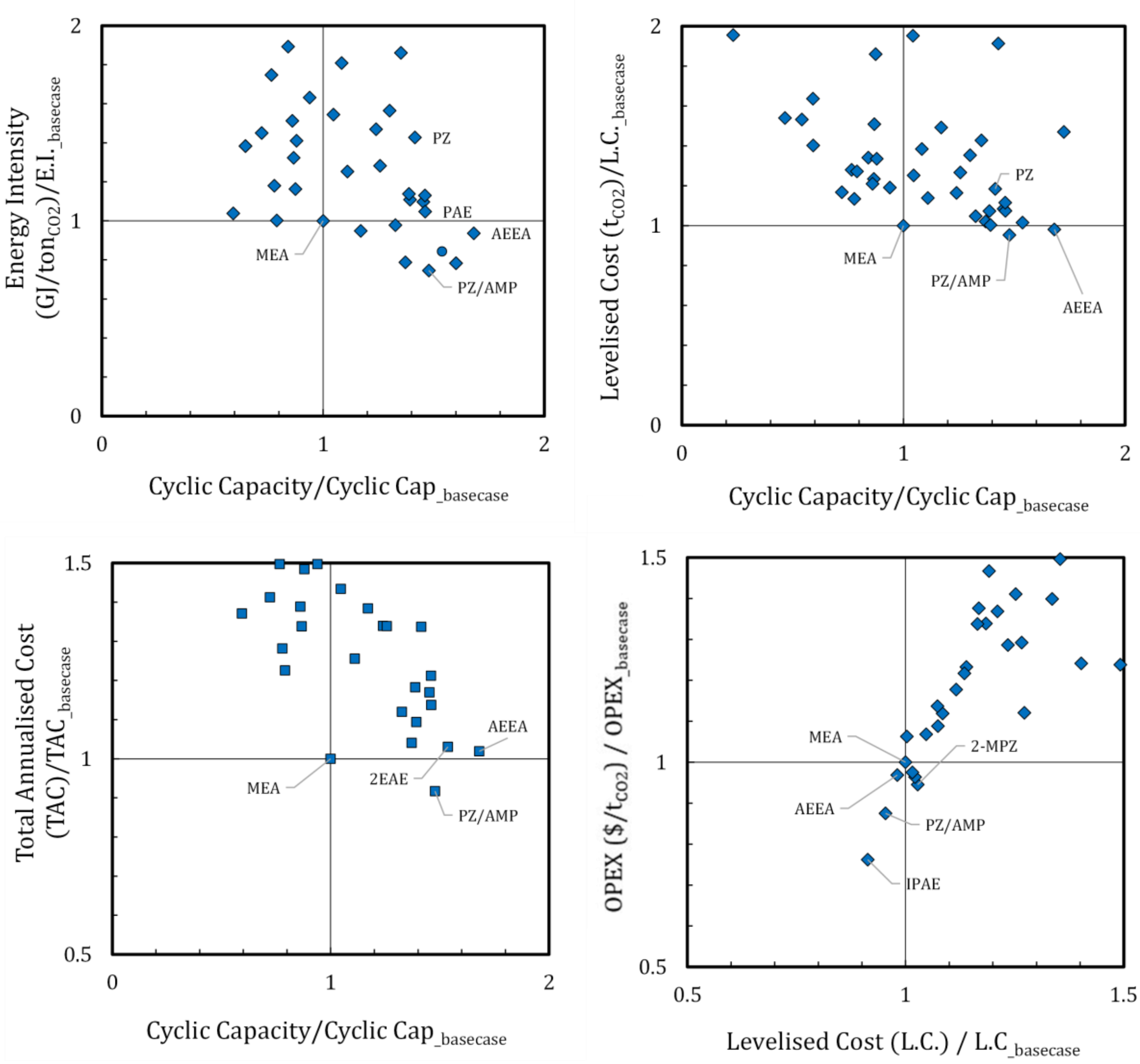


Figure 6.6 *Comparison of monetised and non-monetised KPIs for the different solvents evaluated. CO_2 composition in the inlet gas was fixed at 25%. Colour code: purple for MEA, dark blue for aqueous amines, light blue for aqueous blends and light green for water-free/water-lean absorbents. Values normalised with 30 wt% MEA.*

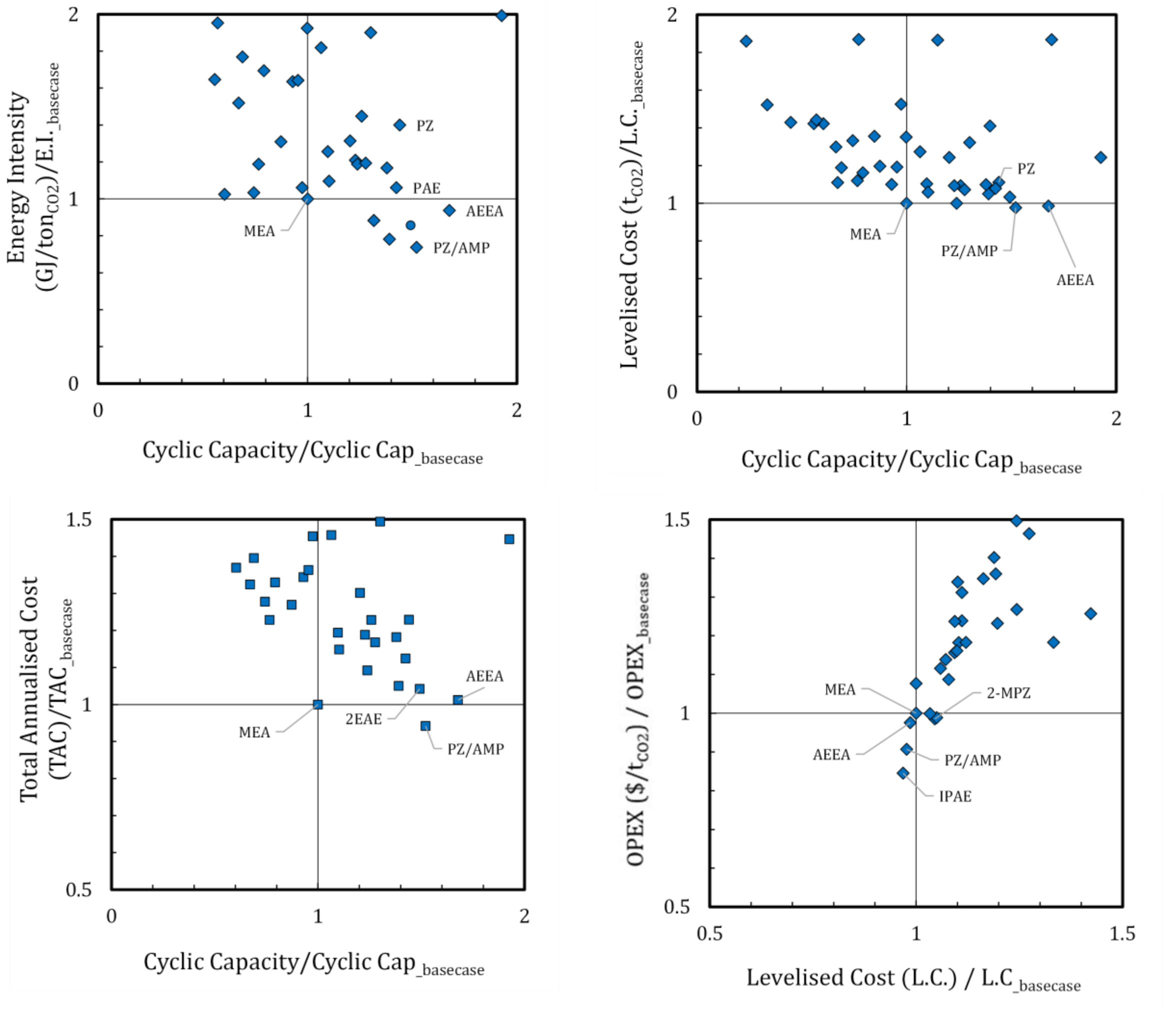


Figure 6.7 *Comparison of monetised and non-monetised KPIs for the different solvents evaluated. CO_2 composition in the inlet gas was fixed at 15%. Colour code: purple for MEA, dark blue for aqueous amines, light blue for aqueous blends and light green for water-free/water-lean absorbents. Values normalised with 30wt% MEA.*

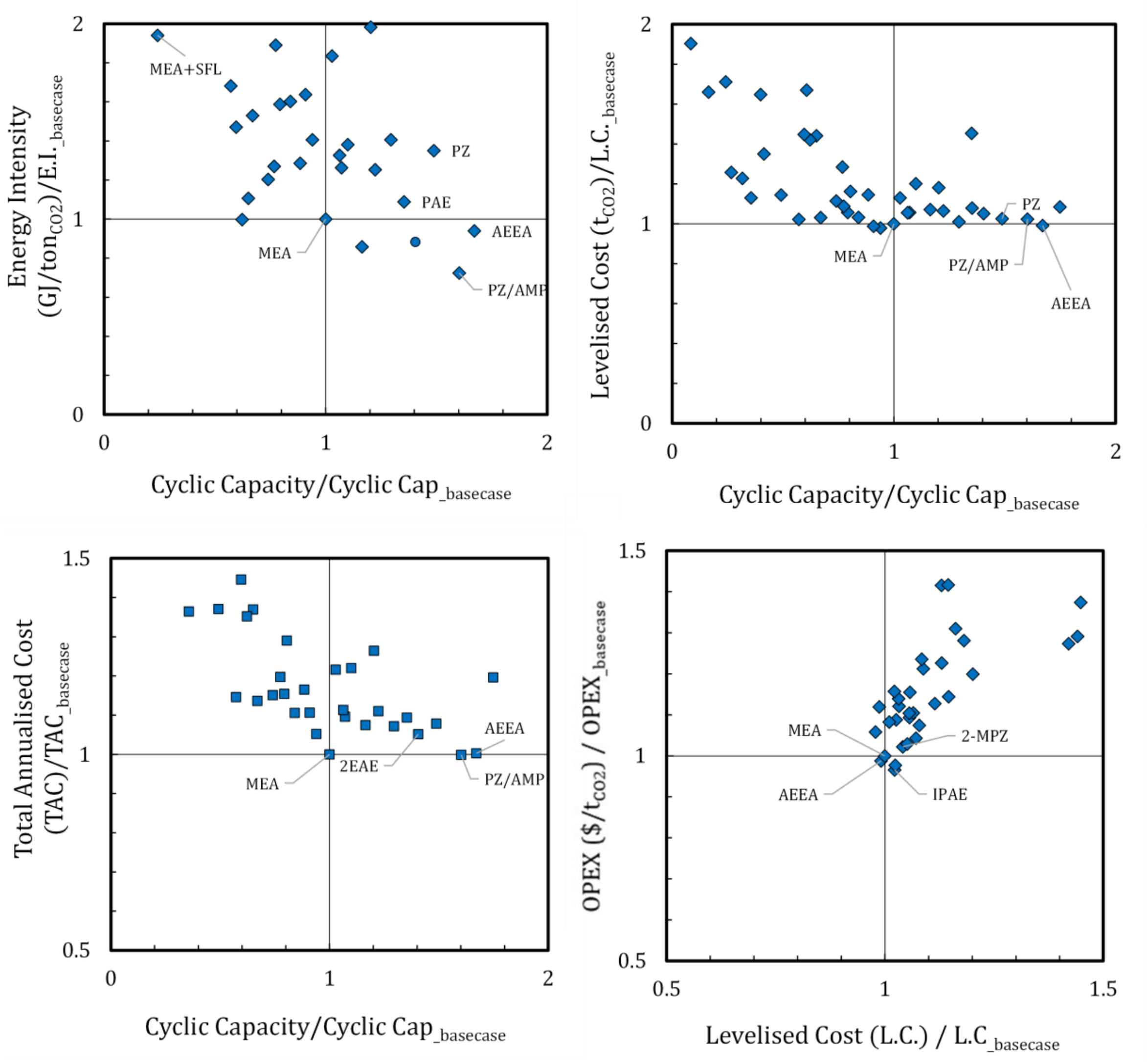


***Figure 6.8** Comparison of monetised and non-monetised KPIs for the different solvents evaluated. CO_2 composition in the inlet gas was fixed at 5%. Colour code: purple for MEA, dark blue for aqueous amines, light blue for aqueous blends and light green for water-free/water-lean absorbents. Values normalised with 30wt% MEA.*

It is observed that, although there is a broader distribution for the different systems in terms of non-monetised KPIs such as cyclic capacity and energy intensity, when it comes in terms of economic aspects, these differences are reduced, as also inferred from the sensitivity analysis of the different properties affecting both the height of the absorber column and the total annualised cost, performed in **Task 5**.

6.3 LIST OF BEST PERFORMING PCC SOLVENTS (M1)

By recapitulating the results from **Figures 6.3 – 6.8**, it is observed that the same amines appear as promising options to reduce costs and/or increase capture rate compared to MEA. Therefore, a **ranking with the most promising materials** (**Milestone M1**) was identified in terms of the KPIs defined in **Tasks 4 and 5**. The top promising amines are: **piperazine/2-amino-2-methyl-1-propanol (PZ/AMP), 2-(isopropylamino)ethanol (IPAE), aminoethylethanolamiine (AEEA), 2-methylpiperazine (2-MPZ), 2-(ethylamino)ethanol (2EAE), 2-amino-1,3-propandiol (2APD), 3-(methylamino)propylamine (MAPA), lean monoethanolamine/Ethylene glycol (MEA/EG).**

PZ/AMP has been labelled as the new benchmark solvent for PCC according to IEAGHG 2019/09 [13]. **IPAE** is a sterically hindered amine with competitive properties compared to MEA [54]. At the same solvent concentration (30 wt.%), IPAE has achieved comparable absorption rates to MEA (5.21 and 5.39 $g_{CO2}/L_{solution}$.min, respectively) and 3.4 fold higher absorption capacity [47]. **AEEA** is a linear diamine with primary and secondary amine groups, showing relatively high absorption rates and cyclic capacity [41]. The reaction rate constant was estimated to range around 1.19-3.46 kmol/m^3 [333]. **2MPZ,** from the piperazine (PZ) family, is a common building block used in organic synthesis. It has higher reaction rate than MEA (25 folds higher), but slower than that of PZ at the same amine concentration (36 folds less) [334]. **2EAE** is a linear secondary amine that has a small corrosion rate, even at higher concentrations (MEA corrodes 3 times faster than 2-EAE at 10 m concentration) [335]. In addition, it requires less energy for regeneration (14% lower than MEA) [49]. **2APD,** is a sterically hindered primary amine (also known as serinol), which should reduce the carbamate formation and be beneficial for CO_2 absorption capacity and regeneration performance. **MAPA** is a linear diamine with a primary and a secondary amine groups. The promising aspect of this solvent is attributed to its high cyclic capacity and relatively high reaction rate. **Lean MEA/EG** is a water-free hybrid solvent formulated from the chemical MEA and physical ethylene glycol. Even though water-free solvents exhibit a depressed carbamate formation, their low total energy of regeneration positions them as attractive solvents.

These systems have shown better results in terms of both monetised and non-monetised KPIs, with reductions up to 5-10% compared to the benchmark 30.wt% monoethanolamine under the same conditions. Although many of the new solvents are currently being investigated or marketed as possible reduced costs in operation compared to MEA, opportunities still exist to further improve the solvent characteristics and achieve a lower capture cost.

7. DEVELOPMENT OF A DECISION TOOL MATRIX FOR THE DESIGN OF PCC SYSTEMS

Objective: Develop a decision tool matrix (Excel based) to assist in the design of PCC systems inclusive of key parameters such as type of flue gas, regional contexts, standard solvent parameters, and others, linked to the database designed in **Tasks 1 – 3**. This allows screening materials/processes with the most promising performance, for particular flue gas conditions, available heat and work, and others. The screening of the systems can be done based on factors such as amount of CO_2 captured or avoided, and amount of energy expended.

7.1 SUMMARY OF DECISION MATRIX TOOL FOR DESIGN OF PCC SYSTEMS (DELIVERABLE 4)

After finishing the review of emerging aqueous and water-lean PCC solvents (**Task 1-3**), a decision modelling tool was developed based on the included systems with additional thermophysical information, comprising absorption isotherms, density, and viscosity. The model includes 50+ different amine co-solvent systems, used in the assessment presented in **Task 6**. The decision tool developed in this project has been configured to allow the user to select the operating conditions for the absorber and stripper.

The **input parameters** from the model include:

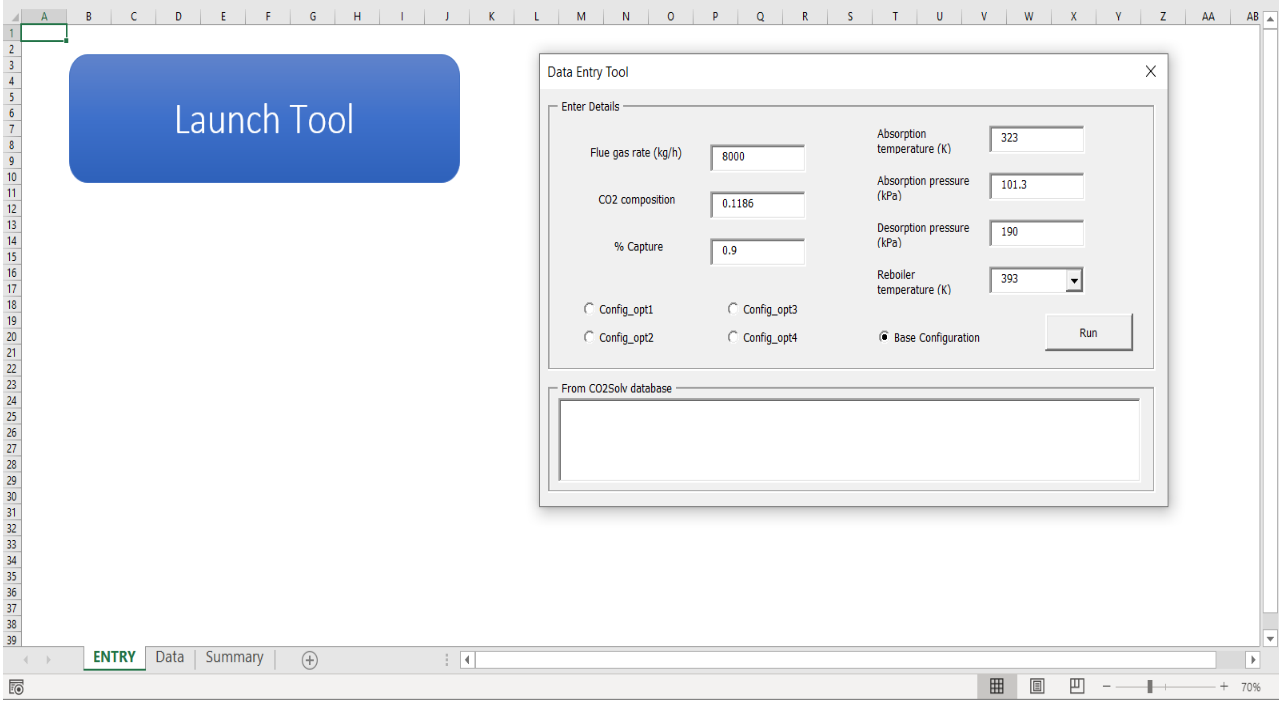
1. Capture percentage, flue gas flow and CO_2 composition.
2. Temperature and pressure of absorption and regeneration.

The **output parameters** from the model include:

1. Total energy required to operate the CO_2 capture system, as this describes the additional energy.
2. Size of the separation equipment, such as the area required for heat exchange, absorber size (diameter and height of the column).
3. CAPEX, OPEX, TAC.

In case of insufficient information for some of the solvents, the properties were assumed to be the same as for MEA. In specific, this approach was followed for most of the lean conditions in water free / water-lean absorbents because of the absence of experimental data.

The initial interface for the user when opening the decision tool has the following appearance, showed in **Figure 7.1.** After filling all the required information, the “Data” tab provides information related to the thermodynamic properties and the KPIs of the different assessed systems. The “Data” tab includes calculated values of column diameter and heights (both absorber and stripper), areas for the heat exchangers and coolers, required pumping work, levelised costs per equipment, operative costs for each specific utility, and finalises with The Total Annualised Cost (TAC), which is the sum of CAPEX (US\$/t_{CO2}) and OPEX (US\$/t_{CO2}). Then, according to the required information, the required column can be filter to rank the different solvents in a clear and direct way. Additionally, the “Summary” tab presents a brief report comparing the different KPIs, with most of the information already presented in **Task 6**. The primary advantage of the decision tool is that allows the user to modify not only process parameters (as the one already mentioned), but also to perform a sensitivity analysis in terms of economic parameters such as, for example, interest rate, duration of the project, etc.



Data Entry Tool

Enter Details

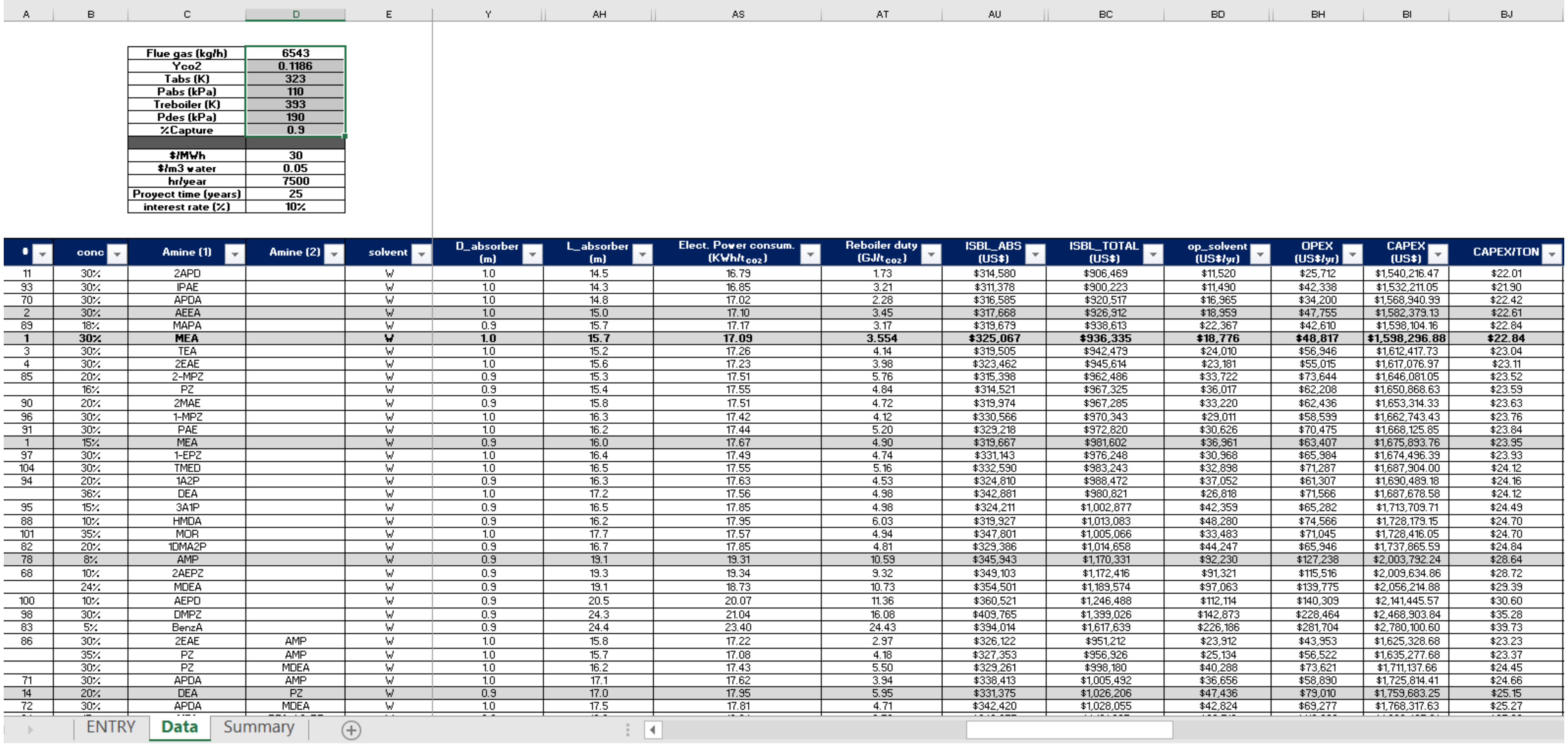
Flue gas rate (kg/h): 8000
CO2 composition: 0.1186
% Capture: 0.9
Absorption temperature (K): 323
Absorption pressure (kPa): 101.3
Desorption pressure (kPa): 190
Reboiler temperature (K): 393

○ Config_opt1
○ Config_opt2
○ Config_opt3
○ Config_opt4
● Base Configuration

From CO2Solv database

Figure 7.1 *Sample Information required in the decision tool developed in this study.*

While, as previously mentioned, many factors inherent to the solvent contribute to the variation in the reported cost of capture, according to Rao and Rubin [208], the parameters that have the most significant impact include the plant capacity factor, the project life, the plant operating capacity and the fixed charge or discount rate. For instance, increasing the discount rate by 20% will increase the capture cost by ca. 8%. In addition, although the length of the expected project life and plant capacity factor impact the capture cost, they only have a large effect if the project life is less than 80% of the nominal value (or less than 20 years) and if the plant capacity is operating at or near maximum capacity (100%).



Flue gas (kg/h)	6543
Yco2	0.1186
Tabs (K)	323
Pabs (kPa)	110
Treboiler (K)	393
Pdes (kPa)	190
%Capture	0.9
$/MWh	30
$/m3 water	0.05
hr/year	7500
Proyect time (years)	25
interest rate (%)	10%

#	conc	Amine (1)	Amine (2)	solvent	D_absorber (m)	L_absorber (m)	Elect. Power consum. (KWh/t_{co2})	Reboiler duty (GJ/t_{co2})	ISBL_ABS (US$)	ISBL_TOTAL (US$)	op_solvent (US$/yr)	OPEX (US$/yr)	CAPEX (US$)	CAPEX/TON
11	30%	2APD		W	1.0	14.5	16.79	1.73	$314,580	$906,469	$11,520	$25,712	$1,540,216.47	$22.01
93	30%	IPAE		W	1.0	14.3	16.85	3.21	$311,378	$900,223	$11,490	$42,338	$1,532,211.05	$21.90
70	30%	APDA		W	1.0	14.8	17.02	2.28	$316,585	$920,517	$16,965	$34,200	$1,568,940.99	$22.42
2	30%	AEEA		W	1.0	15.0	17.10	3.45	$317,668	$926,912	$18,959	$47,755	$1,582,379.13	$22.61
89	18%	MAPA		W	0.9	15.7	17.17	3.17	$319,679	$938,613	$22,367	$42,610	$1,598,104.16	$22.84
1	**30%**	**MEA**		**W**	**1.0**	**15.7**	**17.09**	**3.554**	**$325,067**	**$936,335**	**$18,776**	**$48,817**	**$1,598,296.88**	**$22.84**
3	30%	TEA		W	1.0	15.2	17.26	4.14	$319,505	$942,479	$24,010	$56,946	$1,612,417.73	$23.04
4	30%	2EAE		W	1.0	15.6	17.23	3.98	$323,462	$945,614	$23,181	$55,015	$1,617,076.97	$23.11
85	20%	2-MPZ		W	0.9	15.3	17.51	5.76	$315,398	$962,486	$33,722	$73,644	$1,646,081.05	$23.52
	16%	PZ		W	0.9	15.4	17.55	4.84	$314,521	$967,325	$36,017	$62,208	$1,650,868.63	$23.59
90	20%	2MAE		W	0.9	15.8	17.51	4.72	$319,974	$967,285	$33,220	$62,436	$1,653,314.33	$23.63
96	30%	1-MPZ		W	1.0	16.3	17.42	4.12	$330,566	$970,343	$29,011	$58,599	$1,662,743.43	$23.76
91	30%	PAE		W	1.0	16.2	17.44	5.20	$329,218	$972,820	$30,626	$70,475	$1,668,125.85	$23.84
1	15%	MEA		W	0.9	16.0	17.67	4.90	$319,667	$981,602	$36,961	$63,407	$1,675,893.76	$23.95
97	30%	1-EPZ		W	1.0	16.4	17.49	4.74	$331,143	$976,248	$30,968	$65,984	$1,674,496.39	$23.93
104	30%	TMED		W	1.0	16.5	17.55	5.16	$332,590	$983,243	$32,898	$71,287	$1,687,904.00	$24.12
94	20%	1A2P		W	0.9	16.3	17.63	4.53	$324,810	$988,472	$37,052	$61,307	$1,690,489.18	$24.16
	36%	DEA		W	1.0	17.2	17.56	4.98	$342,881	$980,821	$26,818	$71,566	$1,687,678.58	$24.12
95	15%	3A1P		W	0.9	16.5	17.85	4.98	$324,211	$1,002,877	$42,359	$65,282	$1,713,709.71	$24.49
88	10%	HMDA		W	0.9	16.2	17.95	6.03	$319,927	$1,013,083	$48,280	$74,566	$1,728,179.15	$24.70
101	35%	MOR		W	1.0	17.7	17.57	4.94	$347,801	$1,005,066	$33,483	$71,045	$1,728,416.05	$24.70
82	20%	1DMA2P		W	0.9	16.7	17.85	4.81	$329,386	$1,014,658	$44,247	$65,946	$1,737,865.59	$24.84
78	8%	AMP		W	0.9	19.1	19.31	10.59	$345,943	$1,170,331	$92,230	$127,238	$2,003,792.24	$28.64
68	10%	2AEPZ		W	0.9	19.3	19.34	9.32	$349,103	$1,172,416	$91,321	$115,516	$2,009,634.86	$28.72
	24%	MDEA		W	0.9	19.1	18.73	10.73	$354,501	$1,189,574	$97,063	$139,775	$2,056,214.88	$29.39
100	10%	AEPD		W	0.9	20.5	20.07	11.36	$360,521	$1,246,488	$112,114	$140,309	$2,141,445.57	$30.60
98	30%	DMPZ		W	0.9	24.3	21.04	16.08	$409,765	$1,399,026	$142,873	$228,464	$2,468,903.84	$35.28
83	5%	BenzA		W	0.9	24.4	23.40	24.43	$394,014	$1,617,639	$226,186	$281,704	$2,780,100.60	$39.73
86	30%	2EAE	AMP	W	1.0	15.8	17.22	2.97	$326,122	$951,212	$23,912	$43,953	$1,625,328.68	$23.23
	35%	PZ	AMP	W	1.0	15.7	17.08	4.18	$327,353	$956,926	$25,134	$56,522	$1,635,277.68	$23.37
	30%	PZ	MDEA	W	1.0	16.2	17.43	5.50	$329,261	$998,180	$40,288	$73,621	$1,711,137.66	$24.45
71	30%	APDA	AMP	W	1.0	17.1	17.62	3.94	$338,413	$1,005,492	$36,656	$58,890	$1,725,814.41	$24.66
14	20%	DEA	PZ	W	0.9	17.0	17.95	5.95	$331,375	$1,026,206	$47,436	$79,010	$1,759,683.25	$25.15
72	30%	APDA	MDEA	W	1.0	17.5	17.81	4.71	$342,420	$1,028,055	$42,824	$69,277	$1,768,317.63	$25.27

Figure 7.2 *Sample Information presented in the "Data" tab in the decision tool developed in this study.*

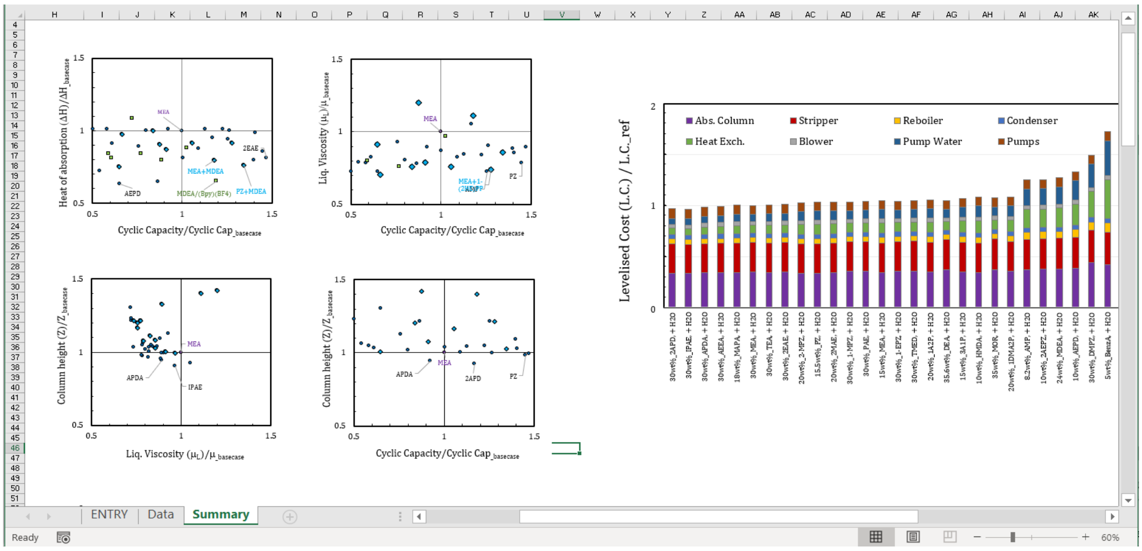


__Figure 7.3__ Sample of the outcomes obtained in the "Summary" tab of the decision tool developed in this study.

It should be mentioned that **solvent degradation** has been included in the model in terms of makeup rate. Nevertheless, the parameters seem to be less important when compared to other capital costs in the process. Notice that he comparison made here assumes that all the studied solvents have reached a competitive price in the market to be used in a large-scale facility.

7.2 SAMPLE SENSITIVITY ANALYSES USING THE CO2SOLV DATABASE

The developed CO$_2$SOLV database and the accompanying decision tool where designed to be flexible to perform various sensitivity analyses. **Figures 7.4**, **7.5**, **7.6**, and **7.7** depict the sensitivity analysis results with respect to the inlet concentration of CO$_2$, capture efficiency, solvent cost, and electricity cost. These three variables where fixed for the screening of this study. It can be seen that decreasing the inlet CO$_2$ concentration in the feed flue gas results in an increase in the TAC for all solvents. This effect on the TAC is expected as it gets harder to capture infinitesimal amounts of CO$_2$.

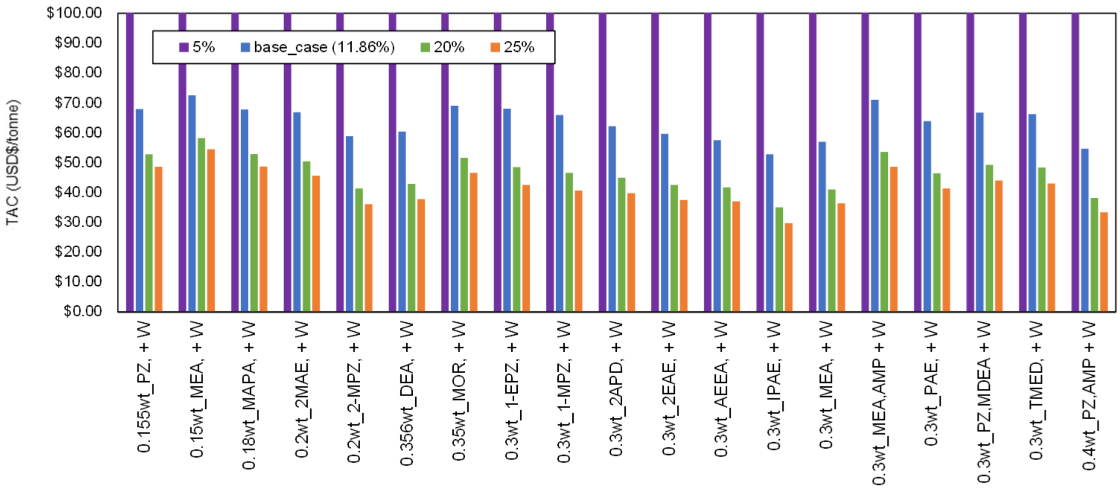


__Figure 7.4__ Sensitivity analysis of the inlet concentration of CO$_2$ using the CO$_2$SOLV Database. The base case (11.86%) refers to the conditions of the CASTOR plant.

The effect of changing the capture efficiency (%) is aligned with the IEAGHG 2019/02 [336]. The TAC achieved a minimum at 95% capture efficiency; comparable to the base case of 90%. Increasing the capture efficiency to 99.9% increases the TAC for all solvents, yet, some solvents exhibited lower values at 99.9% compared to 80% efficiency.

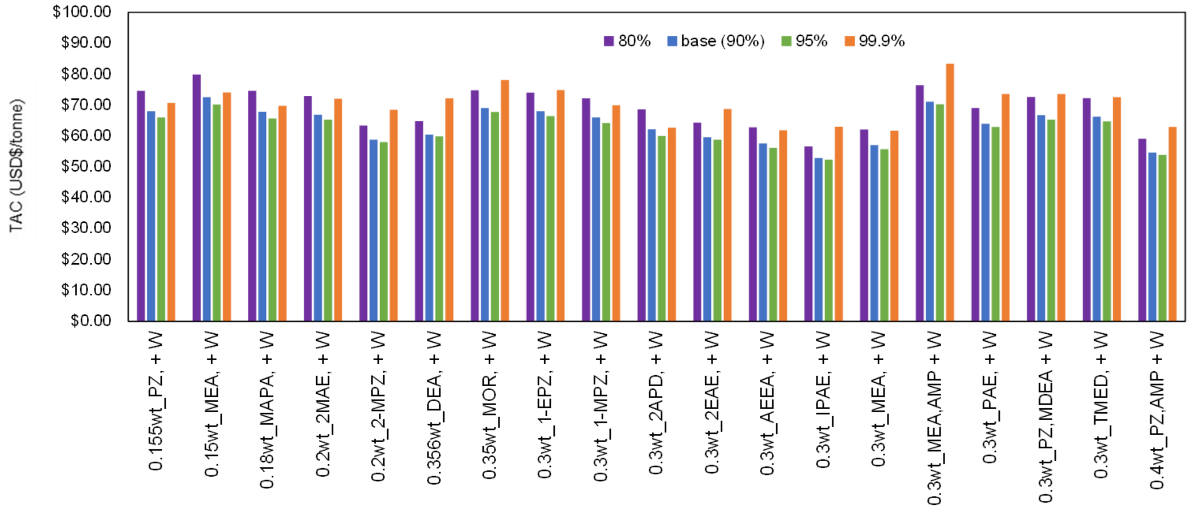


Figure 7.5 *Sensitivity analysis of the CO_2 capture efficiency (%) using the CO_2SOLV Database.*

As mentioned earlier, this study implemented the screening using a capped cost of solvent at $3.5/kg. The sensitivity analysis in **Figure 7.6** shows that increasing the cost of the solvent to $21/kg increases the TAC for all solvents. Yet, some solvents are more resistant to the change than others. For instance, the PZ/AMP formulation appears to be more stable than a MEA/AMP formulation. Such analysis backs up the assumption of fixing the solvent cost for the screening and proves that it has a marginal effect on the economics of the process.

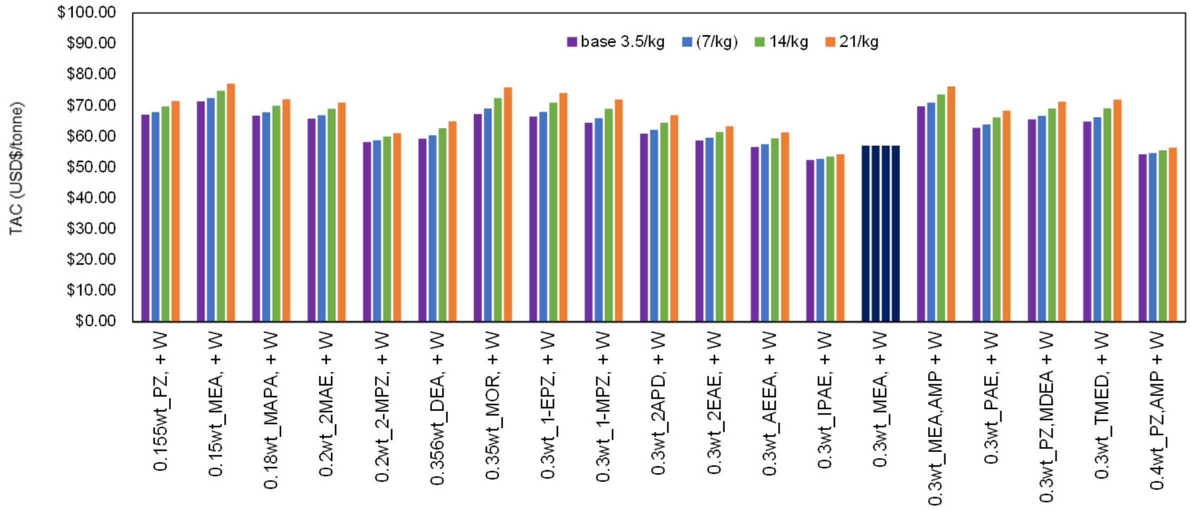


Figure 7.6 *Sensitivity analysis of the solvent cost using the CO_2SOLV Database.*

Increasing the cost of electricity, as a means to accommodate different regional contexts, appeared to minimally affect the TAC for all solvents, as depicted in **Figure 7.6**. With other monetary values kept constant, this suggests that a given solvent employed in a capture plant in UK ($0.244/kWh [337]) would incur the same cost compared to the same solvent employed in Canada ($0.088/kWh [337]), as reflected by the change in the cost of electricity.

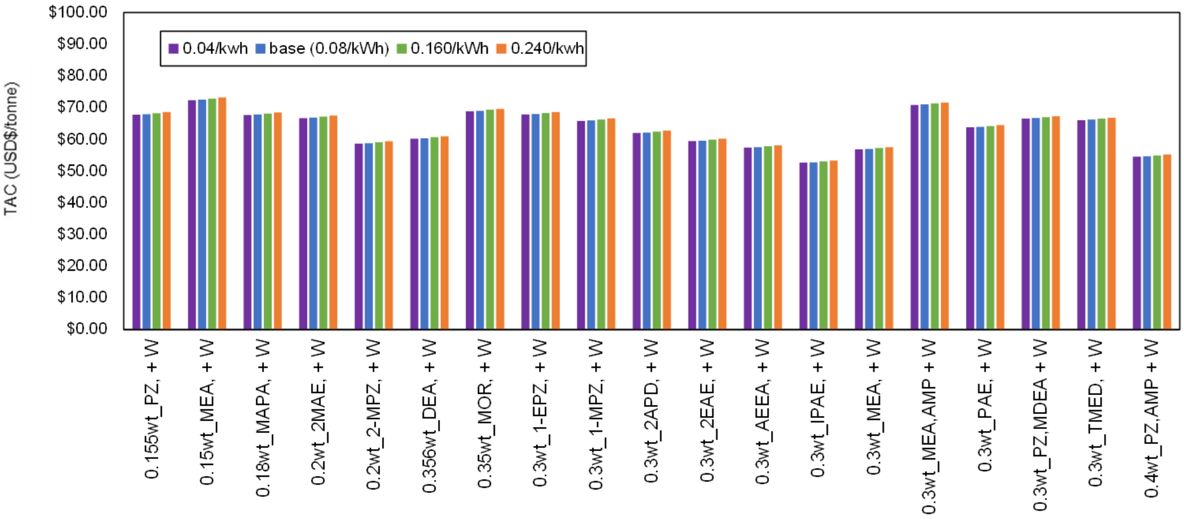


Figure 7.7 *Sensitivity analysis of the electricity cost using the CO_2SOLV Database.*

7.3 BEST PERFORMING PCC PROCESSES

An additional feature integrated in the decision tool to account for possible benefits in the process includes the **process modifications** mentioned in **Task 2**. **Table 7.1** summarizes the average percentages of benefits achieved by applying a specific configuration. The choice of these configurations is bounded by the data available in the literature. To account for the solvent-process interaction, different factors were obtained from different solvents as per their availability in the literature. As the decision tool encompasses more than 50 solvents, the performance of each solvent class is generalized from the data available of the representing solvent. For example, values obtained for MEA would be generalized over all primary amines, and so on. This would be the best approximation of the performance of a given process modification with different solvents because the properties of a solvent dictate the extent of the modification's effect. Other assumptions on calculating the benefits of process modifications are as follows:

- The change in the capital cost of a process modification compared to the conventional process is the same for all solvents.
- The change in the operating costs of a process modification compared to the conventional process is the same for the same class of solvents.
- The change in the operating costs of a process modification for solvents other than MEA is calculated from the average specific reboiler duties (obtained from **Figure 2.10**), in which the SRD is multiplied by a factor that is extracted from the MEA-modified process. For instance, for a MEA-based LVC-modified process, the ratio of the SRD to the OPEX is calculated and generalized over all LVC-modified processes, regardless

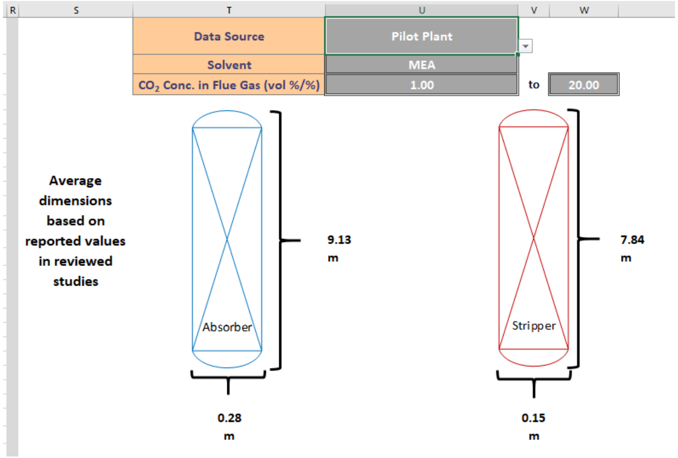
of the solvent. This will allow the calculation of OPEX changes with respect to the change of the SRD's of the solvents that have no monetary values reported.

The above assumptions would allow quantifying the CAPEX and OPEX of modified processes while accounting for the solvent-modification interaction. Yet, further optimization and evaluation would be needed to have more accurate results for a candidate solvent-modification pair, which is an expected consequence of using shortcut methods for screening. Noteworthy, amine blends are approximated with the values of MDEA/PZ and AMP/PZ, which is not the most accurate method, as blends would exhibit variant performances as per their constituents. Also, water-lean/free are not considered here, as no enough data is available. Check [202] for more information on that.

Table 7.1 *Summary of average percentage of benefit of different process configurations included in the decision tool. Reference value for each solvent is the performance of the conventional process of the same solvent. CAPEX (%) values were calculated from* [144,159]. *SRD (%) values are taken from* ***Figure 2.10****. The OPEX (%) values are calculated by multiplying the SRD (%) by a factor (OPEX:SRD) calculated from MEA cases for each modification* [122,144].

Process Modification		Lean Vapour Compression (LVC)	Rich Solvent Split (RSS)	Absorber Inter-Cooling (AIC)	Split Flow (SF)
CAPEX		-24.83%	4.45%	0.20%	0.78%
Primary amines (e.g., MEA)	SRD	18.40%	6.90%	7.00%	6.20%
	OPEX	5.88%	6.80%	5.36%	4.71%
Secondary amines (e.g., DEA)	SRD	11.90%	7.00%	2.80%	7.80%
	OPEX	4.09%	5.97%	2.14%	5.92%
Tertiary amines (e.g., MDEA)	SRD	16.80%	7.13%*	13.10%	6.00%***
	OPEX	5.77%	6.07%	10.02%	4.56%
Cyclic amines (e.g., PZ)	SRD	18.20%	4.80%	11.70%**	6.00%***
	OPEX	6.25%	4.09%	8.95%	4.56%
Blends (e.g., AMP/PZ)	SRD	11.60%	7.90%	12.40%	6.00%
	OPEX	3.99%	6.73%	9.49%	4.56%

Additionally, from the data in the "**Process Design**" tab in the **CO$_2$SOLV** database, an estimation was included for the dimensions of the absorber and stripper columns based on reported numbers from industrial projects, pilot plants, and process simulations. This estimation is rough and tends to give a general intuition rather than an accurate representation of the sizing of the columns. The user can choose from the drop-down menu a data source, solvent (can be extended to more components), and range of CO$_2$ concentration in the flue gas. The solvent pertains to "Component 1" column in the "**Process Design**" tab (includes blends, which can be tuned to ignore) and all other information are linked to the "**Process Design**" tab and hence, subjective to the entries in this tab. That said, the entries need to be similarly formatted in order to include more data points in this estimation. More properties/factors can be added using the same manner of calculating the existing three factors. This can be beneficial when including more data points to the "Process Design" tab.



Data Source	Pilot Plant		
Solvent	MEA		
CO_2 Conc. in Flue Gas (vol %/%)	1.00	to	20.00

Figure 7.8 *Rough empirical estimation of columns' dimensions in the "Process Design Summary" in the CO_2SOLV database.*

7.4 Ranking of best performing PCC solvents and processes (Deliverable 3)

As more solvents are being proposed for the application of PCC, rapid screening of solvents becomes a necessity. We have developed a decision tool allowing high throughput screening of solvents inclusive of technical and economic indicators. With this screening tool, solvents can be fairly compared under the same operating conditions. Such methodology is valid given the context of this study, which allows the analysis of huge number of options and elucidate a small pool of promising solvents. Additionally, the decision tool has sufficient flexibility to conduct sensitivity analyses with respect to monetised and non-monetised variables.

Based on the collected data and their detailed analysis (see **Figures 6.3 to 6.8)**, no single amine was identified to have an absolute superior performance in terms of capital and operating costs. Most of the amines spanned between slightly better and poorer performance than MEA. As a result of the screening, it is recommended to perform more detailed optimised process simulations for the promising amines identified in **Task 6: PZ/AMP, IPAE, AEEA, 2-MPZ, 2EAE, 2APD, MAPA, and lean MEA/EG** (most promising lean solvent). This list includes solvents from a myriad of classes, namely primary, secondary, sterically hindered, and cyclic, as well as blends and diamines. The PZ/AMP formulation has been recently claimed as the updated benchmark for the PCC process [13,139], which also proved in this study to have a comparably better performance than MEA. As it is a blend of cyclic and sterically hindered amines, the PZ/AMP would exhibit both fast kinetics and high absorption capacity. To out-perform MEA, candidate solvents should react at least as fast as MEA and with elevated absorption capacities. IPAE, AEEA, 2APD, and MAPA are characterised with high capacities and comparable absorption rates to MEA. Yet, faster than MEA would also be desirable, as in the case of 2MPZ. Apart from the capacity and rates, 2EAE is highly resistant to corrosion and exhibits low regeneration energy, which has placed it in the top promising solvents to replace MEA.

Reaching to this list of promising solvents was accompanied by a collection of assumptions pertaining to technical and economic variables. These include fixing solvent losses, solvent cost, CO_2 inlet concentration, capture efficiency, utilities costs, among others. Such assumption would hinder the optimization of the cases, which is not intended at this stage of screening. As such, these variables need to be optimised for the promising solvents to ascertain any projected benefits. Another assumption that was made in this study is the equilibrium stage absorption model, which is fairly accurate. Yet, the choice of other models might prove more suitable with some solvents. This should be taken into consideration, especially when exploring emerging solvent classes, such as the water-lean/free solvents.

Sensitivity analyses with respect to the fixed variables can give an indication of the optimization pathway and what factors have significant effects on the economics and overall performance of a given solvent. Using the CO_2SOLV Database, several sensitivity analyses were performed. As the initial CO_2 inlet concentration decreased, the TAC increased for all solvents, and was the trend with increasing solvent cost. When the capture rate was varied, a minimum of TAC was observed at 95%, which aligns with the previous IEAGHG 2019/02 report. Considering the regional context, the change in the electricity cost did not show a significant change in the TAC for all solvents. Regional context can thus be further explored by looking into an interplay of multiple factors that are imposed by the geography and/or location of the capture plant.

In terms of process configurations, the most promising modifications include absorber inter-cooling, rich solvent split, stripper overhead compression, split flow, and lean vapour compression as per the reduction in the specific reboiler duty. Yet, a complete techno-economic analysis would be needed to modified processes to account for the possible off-set increase in the capital costs, especially with compression-based modifications. Details on each modification have been provided in **Task 2**, and a list of average benefits of LVC, RSS, AIC, and SF in terms of KPIs (used in the tool) was presented in **Table 7.1**. These process modifications were chosen as per the availability of data in the literature for different solvents. AIC, SF, and LVC have been experimentally trialled (AIC is sometimes considered as a default design rather than a modification).

As a valuable contribution to the literature, the compilation of solvent screening results, solvent properties, and pilot-scale solvent testing included in CO_2SOLV database allows the ease of accessibility for end-users to identify a quick ranking of promising solvents based on limited set of KPIs, along with identification of data gaps and needs. The database includes a wide array of PCC solvents, such as single aqueous amines, amine blends, water-free and water-lean hybrid solvents. A growing trend in solvent development and testing is focused on solvents with low total energy of regeneration. An additional outcome of this study is the detailed review on available works on solvent degradation, corrosion, process emission, and amine consumption. Pilot-plant testing campaigns established the dominance of oxidative degradation as a primary factor in amine losses and subsequent make-up. In terms of process emissions, studies are more focused on the formation of nitrosamine and aerosol emissions. The factors influencing each of these operational issues are directly linked to the type of amine solvents and process operating conditions. A careful selection of the utilized solvent and operating conditions can effectively minimize the negative outcomes of the aforementioned operational issues. Another alternative is the installation of solvent management strategies, which have also been included in this study. However, the inclusion of th information within the context of solvent selection, or process modelling, remains limited by the availability of information.

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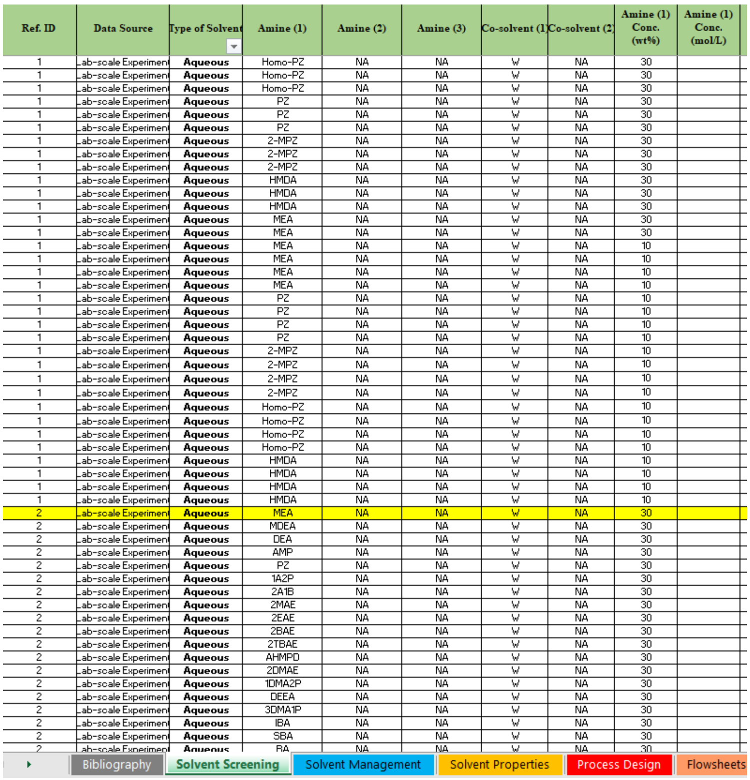
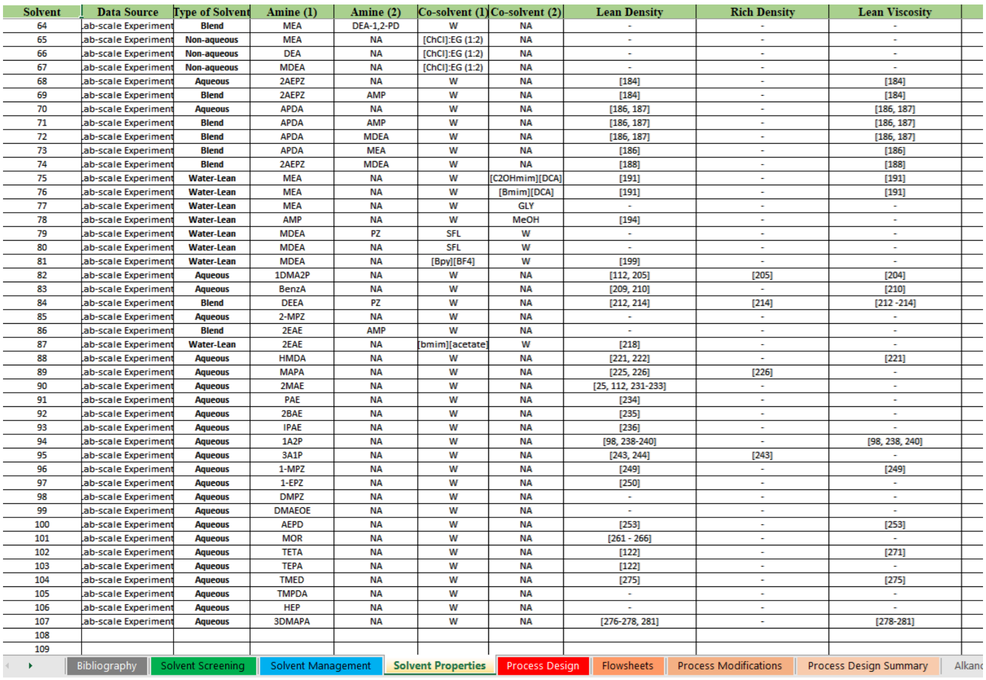
ANNEX I: SAMPLE SNAPSHOTS OF THE CO_2SOLV DATABASE



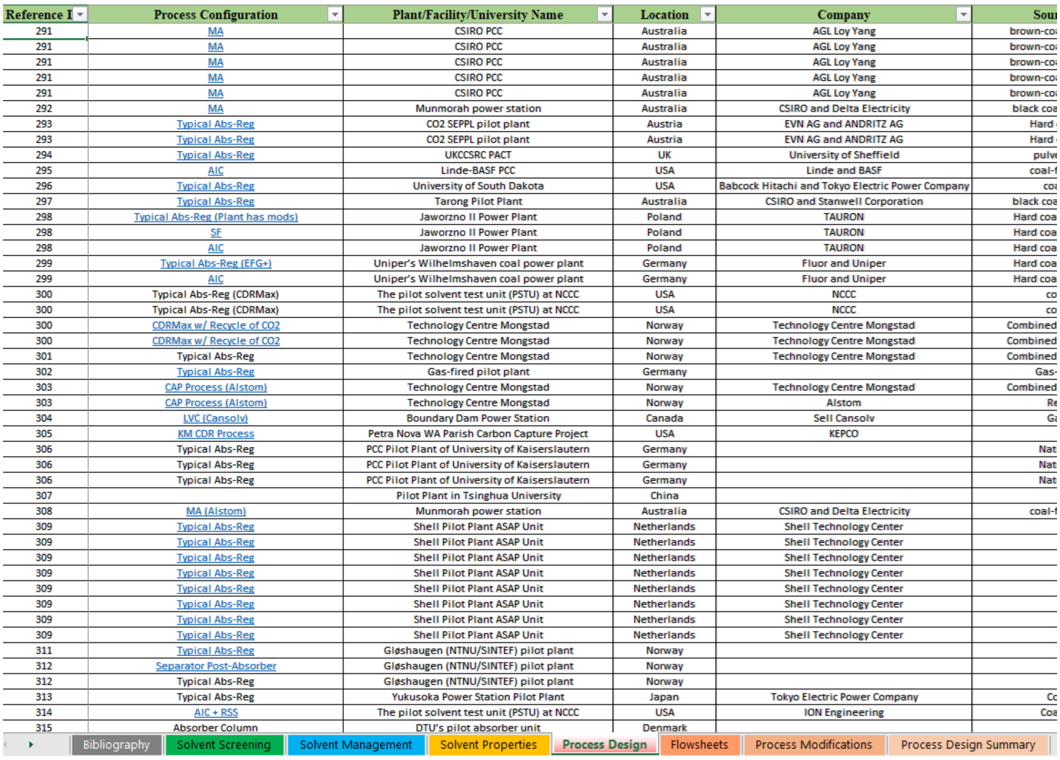
Ref. ID	Data Source	Type of Solvent	Amine (1)	Amine (2)	Amine (3)	Co-solvent (1)	Co-solvent (2)	Amine (1) Conc. (wt%)	Amine (1) Conc. (mol/L)
1	ab-scale Experimen	**Aqueous**	Homo-PZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	Homo-PZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	Homo-PZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	PZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	PZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	PZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	2-MPZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	2-MPZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	2-MPZ	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	HMDA	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	HMDA	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	HMDA	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	MEA	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	MEA	NA	NA	W	NA	30	
1	ab-scale Experimen	**Aqueous**	MEA	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	MEA	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	MEA	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	MEA	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	PZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	PZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	PZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	PZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	2-MPZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	2-MPZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	2-MPZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	2-MPZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	Homo-PZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	Homo-PZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	Homo-PZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	Homo-PZ	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	HMDA	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	HMDA	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	HMDA	NA	NA	W	NA	10	
1	ab-scale Experimen	**Aqueous**	HMDA	NA	NA	W	NA	10	
2	ab-scale Experimen	**Aqueous**	MEA	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	MDEA	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	DEA	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	AMP	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	PZ	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	1A2P	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	2A1B	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	2MAE	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	2EAE	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	2BAE	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	2TBAE	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	AHMPD	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	2DMAE	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	1DMA2P	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	DEEA	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	3DMA1P	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	IBA	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	SBA	NA	NA	W	NA	30	
2	ab-scale Experimen	**Aqueous**	BA	NA	NA	W	NA	30	

Figure A1. *Sample information for "Solvent Screening" tab in the CO_2SOLV database.*



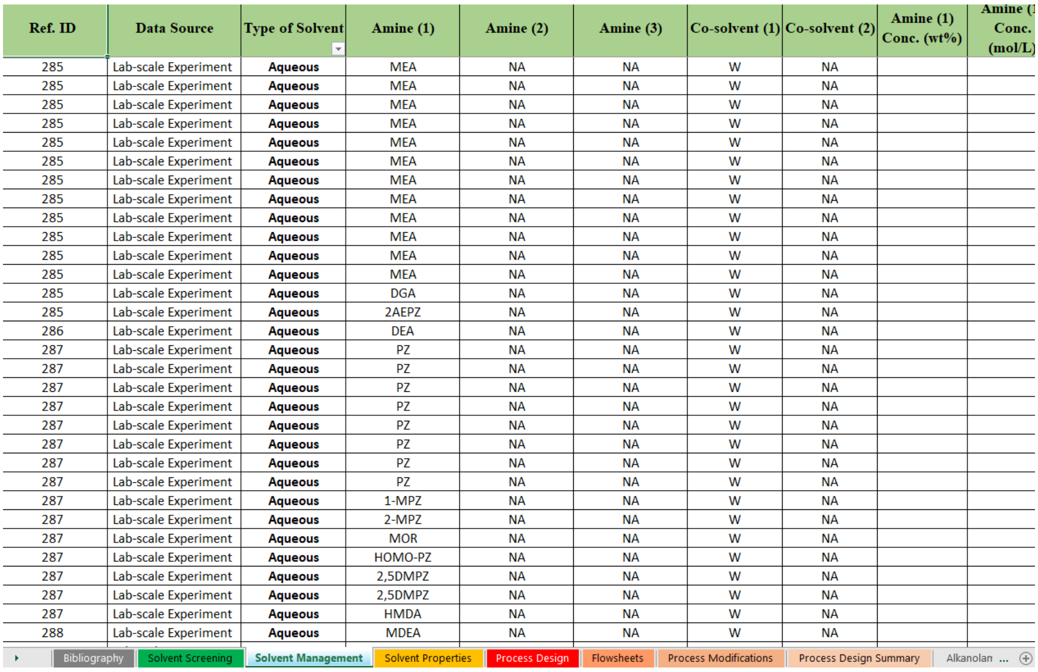
Solvent	Data Source	Type of Solvent	Amine (1)	Amine (2)	Co-solvent (1)	Co-solvent (2)	Lean Density	Rich Density	Lean Viscosity
64	ab-scale Experiment	**Blend**	MEA	DEA-1,2-PD	W	NA	-	-	-
65	ab-scale Experiment	**Non-aqueous**	MEA	NA	[ChCl]:EG (1:2)	NA	-	-	-
66	ab-scale Experiment	**Non-aqueous**	DEA	NA	[ChCl]:EG (1:2)	NA	-	-	-
67	ab-scale Experiment	**Non-aqueous**	MDEA	NA	[ChCl]:EG (1:2)	NA	-	-	-
68	ab-scale Experiment	**Aqueous**	2AEPZ	NA	W	NA	[184]	-	[184]
69	ab-scale Experiment	**Blend**	2AEPZ	AMP	W	NA	[184]	-	[184]
70	ab-scale Experiment	**Aqueous**	APDA	NA	W	NA	[186, 187]	-	[186, 187]
71	ab-scale Experiment	**Blend**	APDA	AMP	W	NA	[186, 187]	-	[186, 187]
72	ab-scale Experiment	**Blend**	APDA	MDEA	W	NA	[186, 187]	-	[186, 187]
73	ab-scale Experiment	**Blend**	APDA	MEA	W	NA	[186]	-	[186]
74	ab-scale Experiment	**Blend**	2AEPZ	MDEA	W	NA	[188]	-	[188]
75	ab-scale Experiment	**Water-Lean**	MEA	NA	W	[C2OHmim][DCA]	[191]	-	[191]
76	ab-scale Experiment	**Water-Lean**	MEA	NA	W	[Bmim][DCA]	[191]	-	[191]
77	ab-scale Experiment	**Water-Lean**	MEA	NA	W	GLY	-	-	-
78	ab-scale Experiment	**Water-Lean**	AMP	NA	W	MeOH	[194]	-	-
79	ab-scale Experiment	**Water-Lean**	MDEA	PZ	SFL	W	-	-	-
80	ab-scale Experiment	**Water-Lean**	MDEA	NA	SFL	W	-	-	-
81	ab-scale Experiment	**Water-Lean**	MDEA	NA	[Bpy][BF4]	W	[199]	-	-
82	ab-scale Experiment	**Aqueous**	1DMA2P	NA	W	NA	[112, 205]	[205]	[204]
83	ab-scale Experiment	**Aqueous**	BenzA	NA	W	NA	[209, 210]	-	[210]
84	ab-scale Experiment	**Blend**	DEEA	PZ	W	NA	[212, 214]	[214]	[212 -214]
85	ab-scale Experiment	**Aqueous**	2-MPZ	NA	W	NA	-	-	-
86	ab-scale Experiment	**Blend**	2EAE	AMP	W	NA	-	-	-
87	ab-scale Experiment	**Water-Lean**	2EAE	NA	[bmim][acetate]	W	[218]	-	-
88	ab-scale Experiment	**Aqueous**	HMDA	NA	W	NA	[221, 222]	-	[221]
89	ab-scale Experiment	**Aqueous**	MAPA	NA	W	NA	[225, 226]	[226]	-
90	ab-scale Experiment	**Aqueous**	2MAE	NA	W	NA	[25, 112, 231-233]	-	-
91	ab-scale Experiment	**Aqueous**	PAE	NA	W	NA	[234]	-	-
92	ab-scale Experiment	**Aqueous**	2BAE	NA	W	NA	[235]	-	-
93	ab-scale Experiment	**Aqueous**	IPAE	NA	W	NA	[236]	-	-
94	ab-scale Experiment	**Aqueous**	1A2P	NA	W	NA	[98, 238-240]	-	[98, 238, 240]
95	ab-scale Experiment	**Aqueous**	3A1P	NA	W	NA	[243, 244]	[243]	-
96	ab-scale Experiment	**Aqueous**	1-MPZ	NA	W	NA	[249]	-	[249]
97	ab-scale Experiment	**Aqueous**	1-EPZ	NA	W	NA	[250]	-	-
98	ab-scale Experiment	**Aqueous**	DMPZ	NA	W	NA	-	-	-
99	ab-scale Experiment	**Aqueous**	DMAEOE	NA	W	NA	-	-	-
100	ab-scale Experiment	**Aqueous**	AEPD	NA	W	NA	[253]	-	[253]
101	ab-scale Experiment	**Aqueous**	MOR	NA	W	NA	[261 - 266]	-	-
102	ab-scale Experiment	**Aqueous**	TETA	NA	W	NA	[122]	-	[271]
103	ab-scale Experiment	**Aqueous**	TEPA	NA	W	NA	[122]	-	-
104	ab-scale Experiment	**Aqueous**	TMED	NA	W	NA	[275]	-	[275]
105	ab-scale Experiment	**Aqueous**	TMPDA	NA	W	NA	-	-	-
106	ab-scale Experiment	**Aqueous**	HEP	NA	W	NA	-	-	-
107	ab-scale Experiment	**Aqueous**	3DMAPA	NA	W	NA	[276-278, 281]	-	[278-281]
108									
109									

Figure A2. *Sample information for "Solvent Properties" tab in the CO_2SOLV database.*



Reference I	Process Configuration	Plant/Facility/University Name	Location	Company	Sou
291	MA	CSIRO PCC	Australia	AGL Loy Yang	brown-coa
291	MA	CSIRO PCC	Australia	AGL Loy Yang	brown-coa
291	MA	CSIRO PCC	Australia	AGL Loy Yang	brown-coa
291	MA	CSIRO PCC	Australia	AGL Loy Yang	brown-coa
291	MA	CSIRO PCC	Australia	AGL Loy Yang	brown-coa
292	MA	Munmorah power station	Australia	CSIRO and Delta Electricity	black coa
293	Typical Abs-Reg	CO2 SEPPL pilot plant	Austria	EVN AG and ANDRITZ AG	Hard
293	Typical Abs-Reg	CO2 SEPPL pilot plant	Austria	EVN AG and ANDRITZ AG	Hard
294	Typical Abs-Reg	UKCCSRC PACT	UK	University of Sheffield	pulve
295	AIC	Linde-BASF PCC	USA	Linde and BASF	coal-f
296	Typical Abs-Reg	University of South Dakota	USA	Babcock Hitachi and Tokyo Electric Power Company	coa
297	Typical Abs-Reg	Tarong Pilot Plant	Australia	CSIRO and Stanwell Corporation	black coa
298	Typical Abs-Reg (Plant has mods)	Jaworzno II Power Plant	Poland	TAURON	Hard coa
298	SF	Jaworzno II Power Plant	Poland	TAURON	Hard coa
298	AIC	Jaworzno II Power Plant	Poland	TAURON	Hard coa
299	Typical Abs-Reg (EFG+)	Uniper's Wilhelmshaven coal power plant	Germany	Fluor and Uniper	Hard coa
299	AIC	Uniper's Wilhelmshaven coal power plant	Germany	Fluor and Uniper	Hard coa
300	Typical Abs-Reg (CDRMax)	The pilot solvent test unit (PSTU) at NCCC	USA	NCCC	co
300	Typical Abs-Reg (CDRMax)	The pilot solvent test unit (PSTU) at NCCC	USA	NCCC	co
300	CDRMax w/ Recycle of CO2	Technology Centre Mongstad	Norway	Technology Centre Mongstad	Combined
300	CDRMax w/ Recycle of CO2	Technology Centre Mongstad	Norway	Technology Centre Mongstad	Combined
301	Typical Abs-Reg	Technology Centre Mongstad	Norway	Technology Centre Mongstad	Combined
302	Typical Abs-Reg	Gas-fired pilot plant	Germany		Gas-
303	CAP Process (Alstom)	Technology Centre Mongstad	Norway	Technology Centre Mongstad	Combined
303	CAP Process (Alstom)	Technology Centre Mongstad	Norway	Alstom	Re
304	LVC (Cansolv)	Boundary Dam Power Station	Canada	Sell Cansolv	Ga
305	KM CDR Process	Petra Nova WA Parish Carbon Capture Project	USA	KEPCO	
306	Typical Abs-Reg	PCC Pilot Plant of University of Kaiserslautern	Germany		Nat
306	Typical Abs-Reg	PCC Pilot Plant of University of Kaiserslautern	Germany		Nat
306	Typical Abs-Reg	PCC Pilot Plant of University of Kaiserslautern	Germany		Nat
307		Pilot Plant in Tsinghua University	China		
308	MA (Alstom)	Munmorah power station	Australia	CSIRO and Delta Electricity	coal-f
309	Typical Abs-Reg	Shell Pilot Plant ASAP Unit	Netherlands	Shell Technology Center	
309	Typical Abs-Reg	Shell Pilot Plant ASAP Unit	Netherlands	Shell Technology Center	
309	Typical Abs-Reg	Shell Pilot Plant ASAP Unit	Netherlands	Shell Technology Center	
309	Typical Abs-Reg	Shell Pilot Plant ASAP Unit	Netherlands	Shell Technology Center	
309	Typical Abs-Reg	Shell Pilot Plant ASAP Unit	Netherlands	Shell Technology Center	
309	Typical Abs-Reg	Shell Pilot Plant ASAP Unit	Netherlands	Shell Technology Center	
309	Typical Abs-Reg	Shell Pilot Plant ASAP Unit	Netherlands	Shell Technology Center	
309	Typical Abs-Reg	Shell Pilot Plant ASAP Unit	Netherlands	Shell Technology Center	
311	Typical Abs-Reg	Gløshaugen (NTNU/SINTEF) pilot plant	Norway		
312	Separator Post-Absorber	Gløshaugen (NTNU/SINTEF) pilot plant	Norway		
312	Typical Abs-Reg	Gløshaugen (NTNU/SINTEF) pilot plant	Norway		
313	Typical Abs-Reg	Yukusoka Power Station Pilot Plant	Japan	Tokyo Electric Power Company	Co
314	AIC + RSS	The pilot solvent test unit (PSTU) at NCCC	USA	ION Engineering	Coa
315	Absorber Column	DTU's pilot absorber unit	Denmark		

Figure A3. *Sample Information for "Process Design" tab in the CO_2SOLV.*



Ref. ID	Data Source	Type of Solvent	Amine (1)	Amine (2)	Amine (3)	Co-solvent (1)	Co-solvent (2)	Amine (1) Conc. (wt%)	Amine (Conc. (mol/L)
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	MEA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	DGA	NA	NA	W	NA		
285	Lab-scale Experiment	**Aqueous**	2AEPZ	NA	NA	W	NA		
286	Lab-scale Experiment	**Aqueous**	DEA	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	1-MPZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	2-MPZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	MOR	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	HOMO-PZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	2,5DMPZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	2,5DMPZ	NA	NA	W	NA		
287	Lab-scale Experiment	**Aqueous**	HMDA	NA	NA	W	NA		
288	Lab-scale Experiment	**Aqueous**	MDEA	NA	NA	W	NA		

Figure A4. *Sample Information for "Solvent Management" tab in terms of degradation in the CO_2SOLV database .*

ANNEX II: LIST OF PCC SOLVENTS INCLUDED IN THE CRITICAL COMPARISON

1A2P[20%] + H_2O
1A2P[30%] + H_2O
1A2P[40%] + H_2O
1A2P[50%] + H_2O
1DMA2P[30%] + H_2O
1-EPZ[30%] + H_2O
1-MPZ[10%] + H_2O
1-MPZ[30%] + H_2O
1-MPZ[40%] + H_2O
2AEPZ + H_2O
2APD[30%] + H_2O
2BAE[15%] + H_2O
2BAE[30%] + H_2O
2EAE[15%] + H_2O
2EAE[30%] + H_2O
2MAE[20%] + H_2O
2MAE[30%] + H_2O
2-MPZ[10%] + H_2O
2-MPZ[30%] + H_2O
2-MPZ[80%] + H_2O
3A1P[15%] + H_2O
3A1P[20%] + H_2O
3A1P[30%] + H_2O
3A1P[37.5%] + H_2O
AEEA[30%] + H_2O
AEEA+MDEA + H_2O
AEPD + H_2O
AMP + 1P
AMP + 3DMAPN
AMP + DEG
AMP + DMSO
AMP + EG
AMP + NMP
AMP + NMP+ H_2O
AMP + TEG
AMP + TEGDME
AMP + H_2O +MeOH
AMP[10%]+MDEA[40%] + H_2O
AMP[10%]+PZ[20%] + H_2O
AMP[13%]+MDEA[18%] + H_2O
AMP[15%]+PZ[15%] + H_2O
AMP[16.5%] + SFL+ H_2O
AMP[20%]+PZ[10%] + H_2O
AMP[30%] + H_2O
AMP[30%] + SFL+ H_2O
AMP[42.5%] + H_2O
APDA + H_2O
APDA+AMP + H_2O
APDA+MDEA + H_2O

APDA+MEA + H_2O
BenzA + H_2O
DEA + [ChCl]:EG [1:2]
DEA + MeOH+ H_2O
DEA + NMP
DEA + PEG400+ H_2O
DEA + SFL
DEA[10%]+MDEA[40%] + H_2O
DEA[10%]+PZ[20%] + H_2O
DEA[15%]+PZ[25%] + H_2O
DEA[20%]+PZ[10%] + H_2O
DEA[25%]+AMP[25%] + H_2O
DEA[30%] + H_2O
DEA[30%] + PEG200
DEA[40%]+AMP[10%] + H_2O
DEA[40%]+MDEA[10%] + H_2O
DEA[50%] + H_2O
DEEA+PZ + H_2O
DETA[17.1%] + H_2O
DETA[20%] + SFL[20%]+ H_2O
DETA[20%] + SFL[30%]+ H_2O
DETA[20%] + SFL[40%]+ H_2O
DETA[20%] + SFL[50%]+ H_2O
DETA[20%] + H_2O
DETA[30%] + H_2O
DETA+PZ + H_2O
DGA[30%] + PEG200
DMAEOE + H_2O
DMPZ[30%] + H_2O
HEP + H_2O
HEP[30%] + H_2O
HMDA [10%] + H_2O
HMDA [30%] + H_2O
IPAE[15%] + H_2O
IPAE[30%] + H_2O
MAPA[15%]+DEEA[30%] + H_2O
MAPA[17.5%] + H_2O
MAPA[17.5%]+1-[2HE]PP[40%] + H_2O
MAPA[17.5%]+DEA-1,2-PD[45%] + H_2O
MAPA[19.5%]+DEEA[63.5%] + H_2O
MAPA[20%]+DEEA[35%] + H_2O
MAPA[40%]+DEEA[11%] + H_2O
MAPA[9%] + H_2O
MAPA[9%]+DEEA[62%] + H_2O
MDEA + [Bpy][BF4]+ H_2O
MDEA + [ChCl]:EG [1:2]
MDEA + TEGMME
MDEA[10%]+PZ[20%] + H_2O
MDEA[15%]+PZ[15%] + H_2O

MDEA[20%] + SFL+ H_2O
MDEA[20%]+PZ[10%] + H_2O
MDEA[30%] + H_2O
MDEA[30%] + PEG200
MDEA[40%] + MeOH+ H_2O
MDEA[40%] + TEGMME+ H_2O
MDEA[50%] + H_2O
MDEA+PZ + SFL+ H_2O
MEA + [ChCl]:EG [1:2]
MEA + ACE
MEA + DEGDME
MEA + EG+ H_2O
MEA + FA
MEA + MeOH
MEA + PEG400+ H_2O
MEA + THFA+ H_2O
MEA + H_2O *+[Bmim][DCA]*
MEA + H_2O *+[C2OHmim][DCA]*
MEA + H_2O +GLY
MEA[10%] + THFA
MEA[10%]+AMP[40%] + H_2O
MEA[10%]+MDEA[40%] + H_2O
MEA[10%]+PZ[20%] + H_2O
MEA[12%]+1-[2HE]PP[39%] + H_2O
MEA[15%] + H_2O
MEA[15%]+PZ[15%] + H_2O
MEA[20%]+PZ[10%] + H_2O
MEA[25%]+MDEA[25%] + H_2O
MEA[30%] + 2ME
MEA[30%] + CC5
MEA[30%] + EG
MEA[30%] + NMP
MEA[30%] + H_2O
MEA[30%]+MDEA[12.5%] + H_2O
MEA[35%] + SFL
MEA[40%] + 2ME
MEA[40%]+AMP[10%] + H_2O
MEA[40%]+MDEA[10%] + H_2O
MEA[45%] + H_2O
MEA[60%] + H_2O
MOR[35%] + H_2O
MOR[45%] + H_2O
PAE[30%] + H_2O
PZ[15%] + H_2O
PZ[30%] + H_2O
TEA[30%] + H_2O
TMED[30%] + H_2O
TMPDA[30%] + H_2O

With transport properties (52% of the systems)
Compositions are weight-based.
“Typical” amines
Water-lean/water-free solvents

ANNEX III: PROCESS SIMULATION – MATHEMATICAL MODEL

Previous works have demonstrated that molecular modelling combined with macroscopic thermodynamics is a useful tool to screen solvents based on their cyclic capacity and heat of regeneration [9,17,18]. Although a priori desirable, rigorous process modelling might not be recommended during screening to evaluating how these solvents perform in terms of process-based metrics and cost; only the most promising ones should be rigorously evaluated. To provide decision makers with a systemic tool for solvent screening, we used a shortcut method for examination of CAPEX performance in addition to OPEX performance obtained using a simplified approach with the available data collected in the database.

Here, an equilibrium based model was used to study the absorption of CO_2 in amines. **Figure A5** shows a schematic representation of the system evaluated.

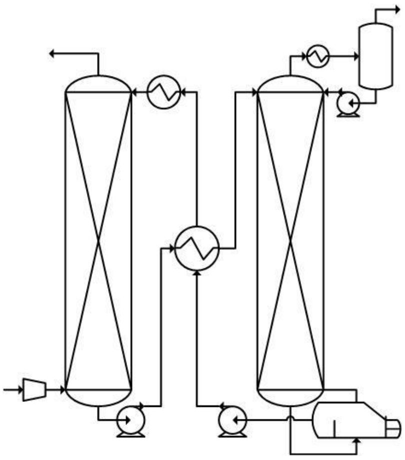


Figure A5. *Schematic diagram of the simulated model, showing the blower, absorber column, pumps, rich/lean heat exchanger, cooler, and solvent regeneration process (stripper, reboiler and condenser).*

The model comprises lower, absorption column, rich and lean solvent pumps, rich/lean heat exchanger, cooler, stripper, reboiler, condenser. Each of these sub-models incorporates standard cost equations based on the design equations, with the key equations presented here.

To calculate mass and energy balances, a global shortcut method was implemented. For mass balances (global and by component):

$$F^{IN} = G^{IN} + L^{IN} = G^{OUT} + L^{OUT} = F^{OUT} \tag{A1}$$

$$F^{IN} z_i^{IN} = G^{IN} y_i^{IN} + L^{IN} x_i^{IN} = G^{OUT} y_i^{OUT} + L^{OUT} x_i^{OUT} \tag{A2}$$

$$F^{IN} z_i^{IN} - n_i^{abs} = F^{OUT} z_i^{OUT} \tag{A3}$$

where G^{IN}, G^{OUT}, L^{IN} and L^{OUT} symbolise the flowrate of gas into, gas out, liquid into and liquid out of a specific unit, respectively; $y_i^{IN}, y_i^{out}, x_i^{IN}$ and x_i^{OUT} denote the molar fraction of component i in inlet gas stream, outlet gas stream, inlet liquid stream and outlet liquid stream.

Therefore, for phase equilibria, the following relationship can be derived to solve the compositions of both L-V phases:

$$\sum_i \frac{z_i(K_i-1)}{1+\frac{G}{F}(K_i-1)} = 0 \qquad \text{(A4)}$$

With K_i the equilibrium distribution coefficient between gas and liquid phase. It can be obtained whether by from the solubility data and equilibrium diagrams in the CO2_SOLV database, or by assuming Raoult's law ($K_i = p_i^{sat(T)}/p$) if no data was available.

The energy balance is as follows [338]:

$$\sum\ G_i^{IN}\widehat{C_{p,G}}(T^{IN}-T^R) + \sum\ L_i^{IN}\widehat{C_{p,L}}(T^{IN}-T^R) + Q = \sum\ G_i^{OUT}\widehat{C_{p,G}}(T^{OUT}-T^R) + \sum\ L_i^{OUT}\widehat{C_{p,L}}(T^{OUT}-T^R) \qquad \text{(A5)}$$

where $\widehat{C_p}$ is the average heat capacity, and ΔT is the temperature difference and the inlet and the outlet. (No phase change was assumed).

For heat exchangers, $Q = UA_{HEX}\Delta T_{LM}$ (A6)

where A_{HEX} is the heat transfer area, Q is the heat rate, ΔT_{LM} is the logarithmic mean temperature difference of the two streams exchanging heat, and U is the overall heat transfer coefficient which is the reciprocal of the sum of the heat transfer resistances in the fluids and heat exchanger wall. Then, the overall heat transfer coefficient for a tube is estimated using:

$$\frac{1}{U} = \frac{1}{h_i} + \frac{e_t}{k_{wall}} + \frac{1}{h_o} + \frac{2}{h_d} \qquad \text{(A7)}$$

where h_i, h_o and h_d the heat transfer coefficient of the fluid inside the tube, the heat transfer coefficient of the fluid outside the tubes (in the shell) and the heat transfer coefficient of the dirt, respectively. e_t is the thickness of the tube, and k_{wall} is the thermal conductivity of the heat exchanger wall. The heat transfer coefficient depends on the physical properties, e.g., density, viscosity, heat capacity, thermal conductivity, etc., and is estimated via correlations of the Nusselt number [339]:
Then, the technical performance of the process is estimated by non-monetised indicators namely %capture, specific energy consumption, and cyclic capacity, defined as:

$$cyclic\ Capacity, \Delta\alpha_{CO_2} = q_s\left(x_{CO_2}\big|_{ads} - x_{CO_2}\big|_{evac}\right) \qquad \text{(A8)}$$

$$\%capture_{CO_2} = \frac{G_{in}y_{CO_{2-in}} - G_{out}y_{CO_{2-out}}}{G_{in}y_{CO_{2-in}}} \qquad \text{(A9)}$$

$$Specific\ Energy\ Consumption = \frac{Q_{des}+Q_{sens}+\cancel{Q_{vap}}}{WC_{CO_2}} = \Delta H_{CO2} + \frac{\rho Cp\Delta T}{(\alpha_{rich}-\alpha_{lean})C_{amine}} \qquad \text{(A10)}$$

Heat of vaporisation is neglected since the model assumes the reboiler will work below the boiling point of the aqueous system, and no additional energy should to overcome evaporation, while at the same time avoids losses due to volatility and reduces degradation potentiality.

The work in the blower is computed as follows:

$$W_{comp} = \frac{1}{\eta_b}u_0 WC_{CO_2}\frac{\gamma}{\gamma-1}\left[\left(\frac{\underline{P}|_{out}}{\underline{P}_{fin}}\right)^{\frac{(\gamma-1)}{\gamma}} - 1\right] \qquad \text{(A11)}$$

where $\underline{P}_f$ and$\underline{P}_{atm}$ are the dimensionless flue gas pressure and atmospheric pressure respectively; η_b and η_v are blower and vacuum efficiencies respectively; and γ is the adiabatic constant.

The absorption and stripper columns were represented as rate-based packed columns: a reaction model based on two-film theory for fast reaction and a gas-liquid contactor model based on the mass and energy balances [340]. The absorber has been modelled as an adiabatic column. The overall mass transfer coefficient, K_G, can be written as:

$$K_G = \left(\frac{1}{k_G} + \frac{H_{CO2}}{k_L E}\right)^{-1} \tag{A12}$$

With H_{CO2} being the Henry's constant. K_G is the overall mass transfer coefficient incorporating gas and liquid side transfer resistances, and E is the enhancement factor. In those cases when the Henry's law constant of a solute in a blend solvent is not available, it can be estimated from the Henry's law constants of the solute in each of the pure solvents [341]. The Henry's coefficient of reactive solvents was estimated using the so-called N_2O analogy, where dinitrogen monoxide (N_2O) is used as a non-reactive gas to estimate the properties of the gases in liquids such as diffusivity and solubility [36].
The mass transfer coefficients, k_G and k_L were estimated using the Onda's correlations for randomly packed columns [342]:

$$k_G = 5.23\left(\frac{\rho_G . v_G}{\mu_G . a_p}\right)^{0.7}\left(\frac{\mu_G}{\rho_G . D_{CO2,G}}\right)^{\frac{1}{3}}\frac{a_p D_{CO2,G}}{RT\left(a_p d_p\right)^2} = 5.23\frac{Re_G^{0.7} Sc_G^{1/3} a_p D_{CO2,G}}{RT\left(a_p d_p\right)^2} \tag{A13}$$

$$k_L = 0.0051\frac{Re_L'^{\frac{2}{3}}\left(a_p d_p\right)^{0.4}}{Sc_L^{0.5}}\left(\frac{\rho_L}{\mu_L . g}\right)^{-\frac{1}{3}} \tag{A14}$$

where Sc_L is the Schmidt number for the liquid phase, and Re_L' is the Reynolds number using the wet interfacial area (a') calculated as a correction of the packing specific area (a_p) using Onda's correlation:

$$a' = a_p\left(1 - exp\left(-1.45\left(\frac{\sigma_c}{\sigma}\right)^{0.75} Re_L^{0.1} Fr_L^{-0.05} We_L^{0.2}\right)\right) \tag{A15}$$

where σ is the surface tension of the liquid and σ_c is the critical surface tension of the packing. Fr_L and We_L are the Froude and the Weber dimensionless numbers for the liquid phase, respectively.

The enhancement factor needs to be considered for the mass transfer which is enhanced by chemical reaction. The enhancement factor E is the ratio between the chemical and the physical absorption flux at the same driving force. It is given as a function of the Hatta number (Ha). The enhancement factor may be considered a correction to the liquid side mass transfer coefficient due to the chemical reaction occurring in the concentration boundary layer [343]:

$$E = \frac{\sqrt{D_L k_2 C_{AM,L}}}{k_L} \tag{A16}$$

where k_2 is the apparent reaction rate constant, obtained from the literature (see references in the database) for specific case studies with available information. $C_{AM,L}$ is the amine molar concentration, and D_L is the diffusivity of the amine in liquid. The diffusion of CO_2 in amine solutions is obtained from N_2O analogy.

This approach reduces the numerical complexity of the absorption model in order to permit the rapid evaluation of the performance of a sorbent, but still capturing the influence of the reaction kinetics, the mass transfer across the gas–liquid interface, the thermodynamic equilibrium and the hydrodynamics of the packing.

The equipment design is based on the data collected in the database (see **Figure A6**). No commercial solvents have been included in the screening analysis.

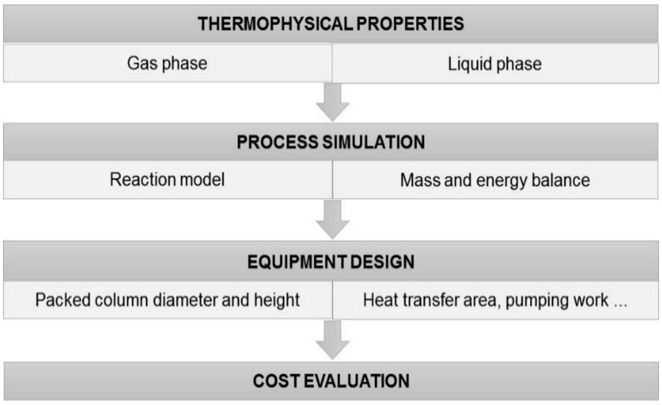


Figure A6. *Schematic procedure for absorption system sizing and costing*

The two most important parameters for the columns sizing are the column diameter and the column height. The column diameter is function of the liquid and gas flow rates and densities. The two main parameters in determining the column diameter are the flooding limitation and the pressure drop of packed height.

Moreover, the height of the column is calculated based on the mass transfer flux and the amount of CO_2 absorbed, and the overall mass transfer coefficient are from [344]:

$$z = \frac{G}{A.a'.P}\int_{y_{CO2}^{OUT}}^{y_{CO2}^{IN}} \frac{dy_{CO2,G}}{y_{CO2,G}.\left(1-y_{CO2,G}\right)^2} = \frac{G}{K_G.a'(y_{CO2,G}-y_{CO2}\,*)_{LM}} \frac{y_{CO2,IN}-y_{CO2,OUT}}{\left(1-y_{CO2,G}\right)_{LM}^{*}} = H_{OG}N_{OG} \quad \text{(A17)}$$

Additional assumptions include:

- Possible benefits regarding the use of modifications in the process were included, using the factors presented in table 7.1 for both CAPEX and OPEX.
- A system capacity (also called flooding factor) of 0.75 was used to account for possible foaming formation inside the packed columns.
-

The database provides all required/available thermo-physical properties of the flue gas under the studied conditions. The accuracies of calculated thermo-physical properties vary with the type of properties and the models used. To identify the property impacts within the possible deviation range of the property models, the sensitivity studies were conducted to evaluate the deviation range at ±20%

Economic (Costing) model

The total capture cost of CO_2 comprises the total capital cost (CAPEX) and operating and maintenance cost (O&M or OPEX) (see Table A1). The same approach used in AlHajaj et al. [326] is implemented here for estimating the cost of the equipment. The method,although relatively simple considering fewer elements contributing to the total capital cost, can eliminateaccumulated errors with estimations of a wide range of elements used in different processes (e.g., process pipelines, land, yard improvements, electrical) [326]. The purchased cost of the equipment were estimated using the cost correlations outlined in Couper and co-workers.

In this way, we have developed a modelling framework which allows us to relate sorbent properties with process cost. For example, the installed cost of an absorption column is given by [345]:

$$C_{abs} = 1.218[\, f_1 C_b + V_p C_p + C_{p1}] C_I \tag{A25}$$

where f_1 refers to the material of construction and is assigned a value of 2.1 for SS316 and C_b is a function of the weight of the shell, given by:

$$Cb = 1.218 exp[6.629 + 0.1826(lnW) + 0.02297(lnW)^2] \tag{A26}$$

where W the weight of the shell. In this work, a thickness of 2 mm was assumed. The product V_pC_p corresponds to the cost of column internals where V_p is the volume of packing required and C_P is the specific cost of the packing used. V_p is directly calculated via the column sizing equations and C_p is assigned a value of USD$110/ft^3, representative of the packing used in this study. Finally, C_{p1} is given by:

$$C_{p1} = 300 D^{0.7396} Z_T^{0.7068} \tag{A27}$$

where D and Z are the column diameter and tan-to-tan height, respectively.
In the case of heat exchangers,

$$C_{HX} = 1.218(f_d f_m f_p C_b) C_I \tag{A28}$$

where f_d, f_m, and f_p are functions of the heat exchanger type, material of construction and pressure range, respectively. C_b is an explicit function of the heat transfer area, A, and is given by:

$$C_b = exp[8.821 - 0.30863(\ln A) + 0.0681(\ln A)^2] \tag{A29}$$

C_I is a cost multiplier to account for the cost of installation and is assigned the value 2.1 and 1.9 for stainless steel absorption columns and heat exchangers, respectively. More details on these equations and their derivation can be found in the work of Couper [346].

Thus, it is possible to make a direct connection with solvent thermophysical or kinetic properties and system cost. Finally, this dictates the installed cost of the absorber and thus the TAC of the entire system.

Table A1 *Instrument cost and costing factor for equipment considered in this study* [346].

	Instrumentation cost (USD$) [a]	PC_f
Blower	2,500	1.3
Pumps	2,500	1.5
Absorption/Stripper column	44,250	2.1
Reboiler	10,500	1.9
Condenser	9,750	1.9
Cooler	9,750	1.7
Heat exchanger	9,750	1.9

[a] *Instrumentation costs presented are estimated in 2004.*

The total capital cost of the capture plant can be estimated using the sequential approach of Chauvel et al. as highlighted in Table A2 [346–348]. Since the purchased cost and instrumentation cost of equipment were calculated based on cost estimates reported at a different time, the average Chemical Engineering Process Cost Index (CEPCI) was used to obtain their corresponding costs values dated to 2020.

$$\frac{Cost_{2020}}{Cost_{base\ year}} = \frac{CEPCI_{2020}}{CEPCI_{base\ year}} \qquad \text{(A18)}$$

It is mentioned that although a scaling-up strategy can be used to obtain the capital cost, the scaling factor usually depend on the type of process. For instance, Kuramochi et al. [349] used a scaling factor of 0.67 for the cement sector but individual scaling factors for each process within the iron and steel production, from 0.7 to 1.

The currency often used to estimating cost equipment is in US dollars, hence, an exchange rate of 0.82euro/US$ was used for the conversion, according to the market value in February 2021. The cost estimating accuracy shall normally be ±35% [350]. A material factor for the geographical context of the plant is not included, since the comparison is based on a same process for the different solvents studied, and reported values in figures from sections 6 and 7 present normalised values of the cost and other parameters with respect to MEA 30%wt.

Table A2. *Elements in calculating total plant cost (TPC) and total capital requirement (TCR)*

Elements	**Value**
Purchased equipment cost (E)	$E_i, \forall i = 1, \dots, n$
Instrument cost (I)	$I_i, \forall i = 1, \dots, n$
Direct equipment cost (DEC)	$\sum_i^n PC_{f,i}E_i + \sum_i^n IC_{f,i}I_i$
Indirect equipment cost (IEC), contingency	*31% × DEC*
Inside Battery Limit Investment (ISBL)	*DEC + IEC*
Off sites (OS)	*31% × ISBL*
Process unit investment (PUI)	*ISBL + OS*
Engineering (Eng)	*12% × PUI*
Paid-up royalties (PUR)	*7% × ISBL*
Facility capital cost (FCC)	*PUI + Eng. + PUR*
Interest during construction	*Interest rate × FCC*
Start-up cost	*1 month of Total operating cost*
Total capital cost (CAPEX)	*FCC + Interest + Start-up cost*
Working capital (WC)	*1 month of Total operating cost*

The CAPEX is annualised using the capital recovery factor (CRF).

$$CRF = \frac{i(1+i)^n}{(1+i)^n - 1} \qquad \text{(A24)}$$

The annual operating expenditure was estimated as the sum of the cost of the utilities, the solvent make-up, the labour cost and the maintenance. To annualise the capital cost, a **discount rate** of **10%** and an annuity period of **25 years** have been assumed.

Table A3 presents the main elements of the operating and maintenance cost. The variable cost comprises utilities consumption (mainly electricity and cooling water) and adsorbent replacement cost. It is noteworthy to say that steam is only required in adsorption-based capture technology if the post-combustion feed gas stream is at a lower temperature than the required adsorption temperature. The fixed component of the operating and maintenance cost consists of the cost for labour, maintenance, insurance, and overheads [348].

Table A3. *Elements for operating cost (OPEX) estimation.*

Elements	Value
Electricity	USD$0.08/kWh
Cooling water	USD$0.25/m^3
Steam	USD$4.1/GJ for coal and USD$7.5/GJ for natural gas [321]
Amine	$ 7 /kg
Utilities (U)	Electricity + Cooling water + steam
Absorbent replacement cost (ARC)	Absorber packing cost / Replacement rate
Variable cost (VC)	U + ARC
Maintenance (M)	4% × PUI
Taxes and insurance (T&I)	2% × PUI
Overhead (OH)	1% × PUI
Financial working capital (FWC)	9% × WC
Fixed operating and maintenance (FOM)	L + M + T&I + OH + FWC

[a] *A labour unit of USD$34.50/hour is used and the total labour cost includes 10% for supervision.*

The total annualised cost per tonne of CO_2 is then calculated as shown in equation A21. The cost of CO_2 captured is presented in the report unless the text mentioned something different. This is due in order to avoid include additional factors for specific industries/power plants, flue gas conditions, etc. Each plant will have a specific emissions indicator and cost indicator before including PCC, that should be integrated with the ones obtained for the PCC process and for each solvent studied. We encourage, that, as possible, use the metric "CO_2 avoided" (especially when reporting emissions metrics), since it includes the additional costs and emissions due to the installation of the capture plant.

$$\frac{CAPEX}{ton}(€tonne) = \frac{CAPEX\ (€)\times CRF}{CF\times\frac{tonne\ of\ CO_2\ captured}{yr}} \tag{A19}$$

$$\frac{OPEX}{ton}(€/tonne) = \frac{FOM}{tonne} + \frac{VC}{tonne} \tag{A20}$$

Therefore, the levelised cost per tonne avoided is calculated as:

$$\frac{TAC}{ton}(€/tonne) = \frac{CAPEX}{tonne} + \frac{OPEX}{tonne} \tag{A21}$$

where CAPEX, FOM, VC, OPEX, and TAC are the total capital cost, fixed operating and maintenance cost, variable cost, operating cost, and total annualised cost respectively in

Euros, CF is the cost factor which depends on the regional context (country, government incentives, etc).

The costs of compression of the CO_2 for transport and storage have not been included in this work. A previous study shows that the cost of CO_2 compression and dehydration is on the order of \$20–25 per t_{CO2} [327].

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