

Investigating Deep Eutectic Solvents (DESS) for Carbon Capture in the Oil and Gas Sector Through Process Simulation

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Abstract

Rising carbon dioxide (CO₂) emissions, especially from oil and gas operations, have sparked a critical need for better carbon capture methods in today's industrial landscape. Traditional monoethanolamine (MEA) systems, despite their widespread use, face mounting environmental concerns that point to the necessity of greener alternatives. This study investigates Deep Eutectic Solvents (DESS), with a focus on Reline - a unique blend of choline chloride and urea - as a potentially sustainable alternative. Industrial-scale simulations using DWSIM software indicated Reline's better CO₂ absorption capabilities, which result from its optimized solubility and flow properties as compared to standard MEA systems. Environmental impact analysis using OpenLCA revealed that employing DESS resulted in dramatically decreased ecological consequences, notably in terms of toxicity and total environmental footprint. The findings establish DESS as a practical, scalable approach to industrial carbon capture that is consistent with global climate commitments under the Paris Agreement, while also closing the gap between theoretical DES applications and the practical demands of emission reduction in energy-intensive industries.

1. Introduction

The Paris Agreement, adopted in 2015, represents a pivotal global commitment to mitigate climate change by limiting the rise in global temperatures to no more than 1.5°C above pre-industrial levels [1]. This agreement underscores the urgent need for reducing anthropogenic greenhouse gas (GHG) emissions, which pose severe risks to environmental and societal stability. The oil and gas industry, a significant contributor to global emissions, accounted for approximately 15% of total global energy emissions in 2022, equivalent to 5.1 billion tonnes of GHG emissions [2]. In Malaysia, the fossil fuel sector is responsible for nearly 80% of the country's GHG emissions, further emphasising the need for effective carbon reduction strategies [3].

Carbon Capture and Storage (CCS) technology has gained traction as a promising solution to address CO₂ emissions from industrial sources. CCS involves capturing carbon dioxide from flue gases or industrial emissions and sequestering it in geological formations, thus preventing its release into the atmosphere [4]. Among the available techniques, chemical absorption, particularly using monoethanolamine (MEA), is widely applied for post-combustion CO₂ capture due to its efficiency [5]. However, MEA has notable drawbacks, including high energy consumption, corrosivity, and adverse environmental effects, highlighting the need for greener alternatives [6].

Deep Eutectic Solvents (DESS) have emerged as potential eco-friendly substitutes for conventional chemical solvents like MEA. DESS are tunable solvents with low toxicity, high thermal stability, and biodegradability, making them suitable for sustainable carbon capture applications [7]. This study focuses on Reline, a DES composed of choline chloride and urea, and its performance compared to 35 wt% MEA in CO₂ capture simulations. The study evaluates their effectiveness and environmental impact under conditions mimicking industrial settings, including specific gas compositions, flow rates, and operating parameters.

By analysing DESS' capabilities and their potential to reduce CO₂ emissions, this research contributes to global climate change mitigation efforts. It aligns with international goals, such as the Paris Agreement, and provides insights for the oil and gas sector to adopt sustainable practices. Moreover, the findings from these simulations can serve as training models for engineers and operators, promoting knowledge transfer and supporting the broader implementation of CCS technologies [8].

2. Methodology

The methodology chart outlines the process flow and the procedures involved in this study. It serves as a theoretical framework, guiding the research. Figure 1 shows the flowchart summarising the methodology of the two processes, which are the simulation of CO₂ removal using DWSIM and life cycle assessment (LCA) using OpenLCA.

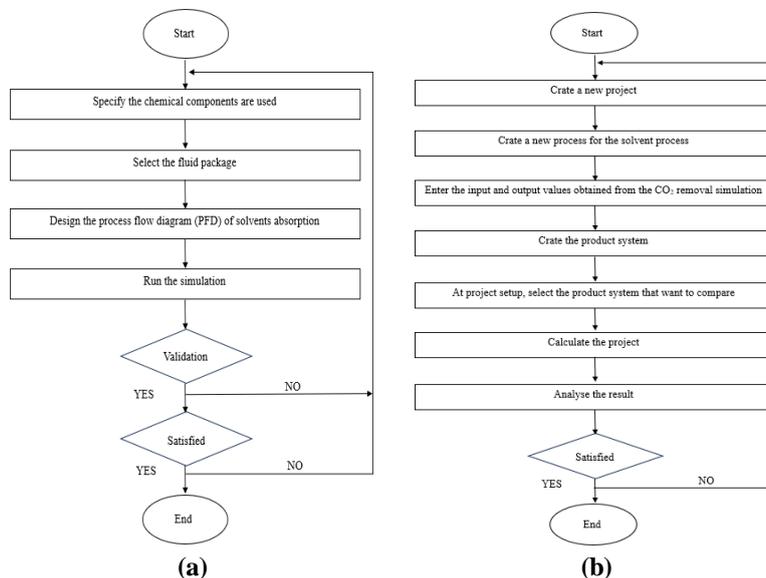


Fig. 1 Methodology flowchart of (a) simulation of CO₂ removal using DWSIM; (b) life cycle assessment (LCA) using a OpenLCA

Figure 1 shows the methodology for the simulation of CO₂ removal using DWSIM (a). The process begins with specifying the chemical components used in the CO₂ removal system. These include Reline or MEA as the solvent, alongside gases such as CO₂, N₂, and H₂O. The next step is selecting the appropriate fluid package, such as Peng-Robinson or UNIQUAC, to ensure accurate thermodynamic modelling during the simulation. Once the components and fluid package are defined, the process flow diagram (PFD) is designed. This diagram includes key stages, such as CO₂ absorption in the absorber and solvent regeneration in the regenerator. After the PFD is built, the simulation is run, and the results are validated to ensure accuracy. If the results do not meet the required criteria, adjustments are made, and the simulation is re-run until the outcomes are satisfactory.

After simulating CO₂ removal, the next method is to see the environmental impact produced by the solvent when doing the CO₂ removal process through life cycle assessment (LCA). It can be seen in Figure 1 that shows the summary of the process of life cycle assessment (LCA) using an OpenLCA (b). The process starts with creating a new project in OpenLCA to evaluate the environmental impacts of the solvent systems, such as Reline and MEA. A separate process was developed for each solvent system, where the input and output data obtained from the DWSIM simulation were used. This data included material flows, energy usage, and other relevant parameters necessary for conducting an environmental evaluation. These processes were carefully designed to reflect the operational aspects of the CO₂ removal system accurately.

Once the individual processes were set up, product systems were created for both solvents to establish the boundaries and scope of the life cycle assessment. During the project setup, these product systems were selected for comparison, and the environmental analysis was conducted. Metrics such as global warming potential (GWP) and toxicity were calculated to quantify the environmental impacts of each solvent. The results were then reviewed and analysed to determine the overall performance of the solvents. If the findings did not meet the

research objectives or inconsistencies were observed, the processes were refined, and the analysis was repeated to ensure accuracy and reliability.

2.1 Simulation Setup

Simulating the process of carbon dioxide (CO₂) removal using DWSIM software. The gas mixture used in the simulation consisted of 71.3% nitrogen (N₂), 13.0% oxygen (O₂), 11.0% water vapor (H₂O), and 3.1% carbon dioxide (CO₂), representing a typical flue gas composition.

Key operating parameters for the simulation included a gas inlet flow rate of 959,820 kilograms per hour (kg/h) and a solvent flow rate of 95,000 cubic meters per hour (m³/h). The gas mixture entered the system at a pressure of 1.0279 bar and a temperature of 150°C, while the solvent was introduced at a higher pressure of 18 bar and a temperature of 25°C to enhance its CO₂ absorption efficiency.

Two types of solvents were used in the study. The first was Reline, a deep eutectic solvent (DES) composed of choline chloride and urea in a 1:2 molar ratio. The second was amine solvent represented by monoethanolamine (MEA), a conventional chemical solvent commonly used in carbon capture processes, prepared at a 35% weight concentration for comparison purposes.

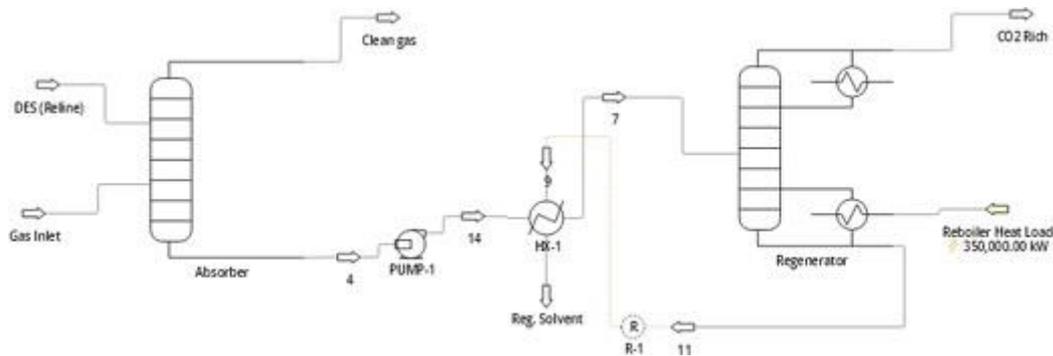


Fig. 2 The process flow diagram (PFD)

Figure 2 shows the process flow diagrams (PFDs) that were constructed to illustrate the absorption system. These diagrams depict key stages such as the absorber, where CO₂ is captured, and the regenerator, where CO₂ is released and the solvent is recovered for reuse. This setup allowed for a detailed evaluation of the performance of Reline compared to MEA in industrial-scale CO₂ capture applications.

2.2 Life Cycle Assessment (LCA)

The life cycle assessment (LCA) in this study was conducted using OpenLCA software to evaluate the environmental impacts of the solvents. The analysis covered the entire lifecycle of the solvents, starting from their production through to their disposal. This comprehensive approach provided a detailed environmental profile for each solvent, ensuring that all significant environmental aspects were accounted for.

Several key metrics were analysed during the assessment. The Global Warming Potential (GWP) was calculated in terms of kilograms of CO₂-equivalents, providing insights into the contribution of each solvent system to climate change. Additionally, toxicity indicators were assessed, which included freshwater, marine, and terrestrial ecotoxicity. These metrics offered a deeper understanding of the potential harm each solvent could cause to different ecosystems. This holistic evaluation allowed for a thorough comparison of the solvents' environmental performance, aiding in identifying the more sustainable option for CO₂ removal.

3. Result and Discussion

This study evaluated the effectiveness between Reline and MEA solvent in capturing CO₂ and the environmental impact of this when doing the CO₂ removal process.

3.1 Simulation Results of Carbon Dioxide Removal

The investigation focused on the difference between the mass flow rate and molar flow rate of CO₂ captured by each solvent under the same conditions. This method offers a clear indication of their efficiency in CO₂ capture and highlights the operational differences between the two solvents.

3.1.1 Carbon Dioxide Removal Using Deep Eutectic Solvents (DES)

Simulations show the effectiveness of Reline (a 1:2 molar ratio mixture of choline chloride and urea) as a CO₂ absorber, leading to a molar flow of 204.556 kmol/h on the clean gas, in contrast to 1082.79 kmol/h on the

gas inlet. Likewise, for the mass flow at the clean gas outlet, which shows 9002.4 kg/h, compared to the gas inlet, which is 47653.1 kg/h. This means that 878.234 kmol/h molar flow and 38650.7 kg/h mass flow of CO₂ have been absorbed to enter the generator. From the molar and mass flow of CO₂ captured, it can know the percentage of the CO₂ captured by Reline is 81.12%.

3.1.2 Carbon Dioxide Removal Using Amine Solvent

In comparison, the MEA exhibits a CO₂ absorption efficiency with a molar flow and mass of CO₂ captured in the clean gas of 173.889 kmol/h and 7652.75 kg/h, while in the inlet gas the molar flow of CO₂ captured is 1082.79 kmol/h and for mass flow 47653.1 kg/h. It produces as much as 908.901 kmol/h molar flow and 40000.35 kg/h mass flow of captured CO₂ entering the regeneration. That means the CO₂ capture percentage is 83.94%.

3.1.3 Comparison of Solvent Efficiency

Figure 2 shows a bar graph and a visual analysis of the percentages of carbon dioxide (CO₂) captured by different types of solvents. The y-axis shows the percentage of CO₂ captured, while the x-axis identifies the types of solvents. The bar graph depicts the percentage of CO₂ captured, which is calculated using data from molar flow and mass flow measurements at the gas input and clean gas.

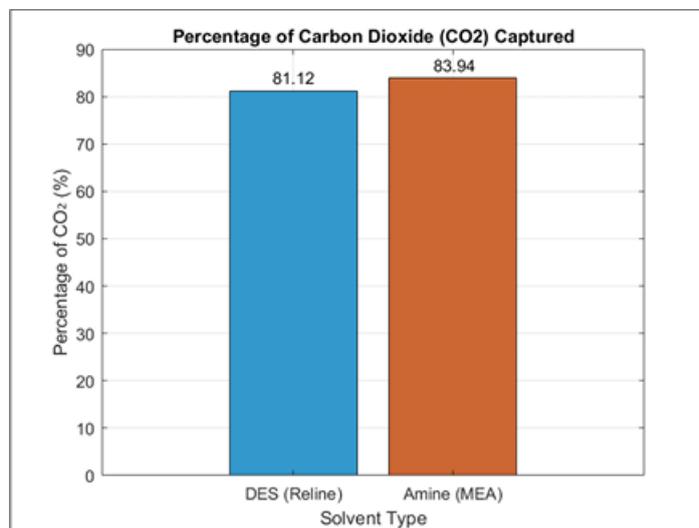


Fig. 3 The percentage of CO₂ captured by different solvents

This percentage shows that amine (MEA) is the most efficient solvent, with an 83.94% capture rate, followed by DES (Reline) at 81.12%. This comparison highlights that MEA exhibits higher CO₂ capture efficiency than Reline (DES), underscoring its superior performance under the simulated conditions. The stronger chemical reactivity of MEA with CO₂ enables the formation of carbamate compounds during the absorption process, which significantly enhances its ability to capture CO₂. In contrast, the slightly lower efficiency of Reline suggests its limited capacity to absorb CO₂ as effectively as MEA within the parameters of this study.

3.2 Environmental Impact Analysis

The environmental impact of using Reline and MEA was assessed using OpenLCA. Key indicators such as global warming potential (GWP) and toxicity levels were compared.

3.2.1 Global Warming Potential (GWP)

The Global Warming Potential (GWP) of a substance, measured in kilograms of CO₂ equivalent (kg CO₂ eq), quantifies its contribution to climate change. This study compared the GWP of two types of solvents: deep eutectic solvent (DES) and monoethanolamine (MEA). The comparison was summarized in Table 1.

The analysis revealed that both processes demonstrated similar environmental impacts in terms of GWP, with the DES process having a slightly higher carbon footprint (1.23292 kg CO₂ eq) compared to the MEA process (1.19132 kg CO₂ eq). While the difference is minor, it indicates that the production and application of DES emit marginally more greenhouse gases than MEA. This finding underscores the need for improvements in DES production techniques to reduce its carbon footprint and enhance its environmental sustainability, making it a more viable alternative for CO₂ removal.

Table 1: Global warming potential of the process of the different types of solvents

Process by the solvent	Global Warming Potential of CO ₂ (kg CO ₂ eq)
DES process	1.23292
MEA process	1.19132

3.2.2 Toxicity Analysis

The toxicity effects of two solvent processes, deep eutectic solvents (DES) and monoethanolamine (MEA), were evaluated across three environmental compartments: freshwater, marine and terrestrial ecosystems. The analysis was carried out using the kilogram of 1,4-dichlorobenzene (kg 1,4-DCB) as a standard unit to measure potential ecotoxicity. The results show a significant difference in the environmental impact of the two processes. This can be seen in Table 2, which shows the toxicity of the process for different solvents.

For freshwater ecosystems, the DES process exhibits almost negligible ecotoxicity (0.00951 kg 1,4-DCB), while the MEA process has a higher effect of 83.1832 kg 1,4-DCB. Similarly, for the marine ecosystem, the DES process showed negligible ecotoxicity (0.00172 kg 1,4-DCB) compared to the MEA process, which produced 16.14461 kg 1,4-DCB. This trend is more significant for terrestrial ecosystems, where the DES process has 63.06704 kg 1,4-DCB, while the MEA process reaches 455124 kg 1,4-DCB. These results clearly show that the DES process is much more environmentally friendly, with lower toxicity in all three ecosystems. The significant difference in ecotoxicity is due to the chemical stability of DES and the reduced production of harmful byproducts, while the degradation of MEA produces toxic intermediates that significantly impact the ecosystem.

These findings underscore the environmental benefits of adopting DES over MEA, especially for applications requiring minimal ecological impact. The results highlight the need to focus on the development of sustainable solvents such as DES to reduce ecological hazards and improve overall environmental sustainability.

Table 2: The toxicity of the process of the different solvents

Process by the solvent	Freshwater ecotoxicity (kg 1,4-DCB)	Marine ecotoxicity (kg 1,4-DCB)	Terrestrial ecotoxicity (kg 1,4-DCB)
DES process	0.00951	0.00172	63.06704
MEA process	83.1832	16.14461	455124

4. Conclusion

This research has provided valuable insights into the comparative performance and environmental impact of Deep Eutectic Solvent (DES), specifically Reline, and Monoethanolamine (MEA) in CO₂ capture applications for the oil and gas industry. Through comprehensive simulation studies and life cycle assessment, this study has revealed important findings regarding the efficiency and environmental sustainability of these two solvents.

The simulation results demonstrated that while MEA achieved a higher CO₂ capture efficiency, its significant environmental impacts raise concerns about its long-term sustainability. Conversely, DES (Reline) emerges as a promising alternative that offers substantially reduced environmental impact while maintaining relatively competitive capture efficiency. This critical trade-off between capture efficiency and environmental impact highlights the potential for DESs to support sustainable carbon capture practices, aligning with global climate commitments.

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