CONSTRAINED CO₂EOR: OPTIMIZATION CONSIDERING IMPURITIES, CO₂EOR TYPE, VOLUME, AND OIL RECOVERY VS CO₂ STORAGE

By

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A thesis submitted to the School of Graduate Studies In partial fulfillment of the requirements for the degree of Master

Faculty of Engineering and Applied Science

Memorial University of Newfoundland

May 2025

St. John's, Newfoundland and Labrador

Canada

ABSTRACT

Optimizing CO₂ injection in offshore Enhanced Oil Recovery (EOR) operations aims to increase oil production while capturing CO₂, aligning with global carbon capture and storage (CCS) goals. CO₂ dissolves in oil, reducing its viscosity and making it more extractable, but offshore sites face unique challenges, such as limited CO₂ supply, high storage costs, and technical constraints. Various EOR methods can address these limitations: Carbonated Water Injection (CWI) dissolves CO₂ in water, reducing the total CO₂ required and enhancing oil recovery while maximizing carbon retention. Another approach, targeted CO₂ flooding in specific reservoir blocks, concentrates CO₂ where it's most effective, making efficient use of limited supplies. Water-Alternating-Gas (WAG) injection alternates CO₂ and water to manage gas mobility and improve the efficiency of oil displacement, allowing for strategic use of CO₂ without full-field application. This study analyzes the optimization of constrained volumes of varying CO₂ concentrations and impurities considering different oil types and reservoir conditions. It examines how impurities impact CO2 injection and retention, and how different oil types and reservoir characteristics respond to specific injection strategies. This approach enables offshore EOR to balance enhanced oil recovery with carbon storage objectives, optimizing both CO2 usage efficiency and emission reductions to support sustainable energy goals.

Current carbon capture technologies are imperfect, resulting in impurities within the CO₂ stream that affect the Minimum Miscibility Pressure (MMP) needed for effective oil recovery. This study investigates how these impurities influence the MMP in oil and gas mixtures using slimtube simulations across a range of CO₂ sources and capture technologies. While prior studies often focus on pure or low (<5 %) CO₂ concentrations, this research explores a broader range, examining CO₂ concentrations from 0 % to 100 % to fill an existing gap in the literature. The study reveals that

impurities depend on the CO₂ source: for example, CH₄ is common in CO₂ from natural gas streams, while O₂ and N₂ are prevalent in CO₂ from flue gas. The results indicate that CO₂ mixed with natural gas effectively lowers MMP, enhancing miscibility, whereas impurities in flue gas (like O₂ and N₂) raise the MMP more significantly, as N₂ requires particularly high pressures to reach miscibility compared to CO₂. This work deepens understanding of the impacts of different CO₂ sources and impurity levels on MMP, contributing valuable insights for optimizing CO₂-based enhanced oil recovery processes.

Understanding the Minimum Miscibility Pressure (MMP) between oil and gas mixtures is essential for accurately predicting reservoir performance, particularly in enhanced oil recovery (EOR) processes. However, no single Equation of State (EOS) consistently predicts fluid properties across all conditions. Machine Learning (ML) has become a valuable tool for estimating MMP, yet prior studies have often faced limitations due to small data sets and restricted ranges of CO2 mole percentages. This study develops a Machine Learning model using Deep Learning and k-fold Cross Validation techniques, improving the size, accuracy, and range of the data, particularly for CO₂ concentrations. Additionally, a sensitivity analysis is performed to assess the influence of various input parameters, such as reservoir characteristics and oil and gas properties, on MMP. The study finds that key factors impacting MMP include reservoir temperature and the concentrations of CO₂ and methane (C1) in the gas phase. Higher temperatures, heavier oils, a greater proportion of volatile and intermediate components in the oil, and higher concentrations of C_1 and N_2 in the gas phase all lead to higher MMP. In contrast, the presence of CO_2 and H_2S , especially CO_2 , significantly lowers the MMP, aiding oil recovery. The study emphasizes how Deep Learning approaches can enhance the accuracy and range of MMP predictions, improving the optimization of EOR strategies by providing better insights into fluid dynamics.

Previous studies in Enhanced Oil Recovery (EOR) and Carbon Capture, Utilization, and Storage (CCUS) have largely operated under the assumption of unlimited CO₂ supply, failing to adequately address the constraints associated with CO₂ availability, especially in offshore reservoirs. This oversight is significant, as the capacity for CO₂ storage and the ability to conduct effective EOR can be severely limited by the volume of CO₂ that can be feasibly captured and injected. Moreover, most EOR research tends to emphasize incremental oil recovery metrics while neglecting the financial impacts of carbon emissions, which can significantly influence project feasibility and sustainability. This study investigates the joint optimization of oil recovery and carbon storage by considering both the economic value of produced oil and the benefits of CO₂ tax credits, assigning equal weight to each factor with a 50:50 ratio. It examines various oil types (light, medium, and heavy) and reservoir conditions, including CO₂-EOR methods such as Water-Alternating-Gas (WAG), Carbonated Water Injection (CWI), and enriched-WAG, under different CO₂ constraints, impurities, and reservoir characteristics like stratification, crossflow, temperature, pressure, and permeability. The simulations use GMG, and optimization is performed using Multi-Objective Particle Swarm Optimization (MOPSO). The results show that CWI is the most effective method under CO₂ constraints for stratified reservoirs, whether crossflow is present or not. However, CO₂ storage is significantly lower in the CWI case. Among the factors influencing optimization, reservoir pressure has the most significant effect on the overall objectives, while permeability is the key factor in determining the oil recovery factor across all three CO₂-EOR methods. EOR studies typically focus on incremental oil recovery (without considering carbon pricing),

whereas Carbon Capture, Utilisation and Storage (CCUS) prioritizes maximizing CO_2 storage (assuming an infinite CO_2 supply). The joint optimization of oil recovery factor and CO_2 storage varies based on phase behavior related to different oil types and conditions (EOR methods, the available amount and characteristics of injected gas, and reservoir properties), but also on economic

factors such as the price of produced oil and the value of CO_2 tax credits. By incorporating all these factors into simulations and applying modern machine learning techniques, we can better optimize the balance between enhancing oil recovery and reducing carbon intensity during the energy transition era. Machine learning models can simulate and predict outcomes for various reservoir conditions and economic scenarios, enabling more informed decisions on the selection of the most appropriate EOR technique, the optimal amount of CO_2 to inject and also the precise conditions under which oil recovery and CO_2 storage can be balanced most effectively for a specific reservoir.

CO-AUTHORSHIP STATEMENTS

This Master thesis incorporates collaborative efforts with esteemed co-authors, whose specific contributions are detailed below. Each co-author has provided expertise, critical feedback, and technical assistance, which have been invaluable to the development and completion of this research.

Peer reviewed conference paper – Chapter 3: Pham, Q.C and James, L.A. 2021. Considering the CO₂ Source and Capture Technique to Reduce Minimum Miscibility Pressure (MMP) for Enriched Water Alternating Gas (WAG) Injection. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30.

https://doi.org/10.1115/OMAE2021-62643

- *Co-Author(s):* Dr. Lesley James
- *Contribution:* This chapter is based on a peer-reviewed publication co-authored with Dr. Lesley James. I led the research design, conducted the analysis, and authored the manuscript. Dr. Lesley James contributed by reviewing the work, offering technical insights, and refining the paper's conceptual framework.

Peer reviewed conference paper – Chapter 4: Pham, Q.C., Trinh, Q.T., and James, L.A. 2021 Data Driven Prediction of the MMP between Mixtures of Oil and Gas using Deep Learning. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30. https://doi.org/10.1115/OMAE2021-63018

- *Co-Author(s):* Dr. Trung Trinh, Dr. Lesley James
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and feedback on early drafts. Dr. Lesley James offered technical assistance and helped shape the overarching research concept.

Peer reviewed conference paper – Chapter 5: Pham, Q.C., Esene, C.E. and James, L.A. 2023. Investigating CO₂-EOR Types with Constrained CO₂ Volumes and Impurities for a High-Quality Sandstone, Stratified Offshore Newfoundland Reservoirs. Presented at the SPE Canadian Energy Technology Conference and Exhibition. Calgary, Alberta, Canada, March 15 - 16.

https://doi.org/10.2118/212811-MS

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Presentation – Chapter 6: Pham, Q.C and James, L.A. Dirty Carbon – Impact of CO₂ Volume and Impurities on Carbon Utilization and Carbon Neutral Oil Production. 2024. Presented at Carbon Capture, Utilization, and Storage Latin America . Rio de Janeiro, Brazil, 22-23 May.

- *Co-Author(s):* Dr. Lesley James
- *Contribution:* This chapter originates from a presentation co-authored with Dr. Lesley James. I conducted the research, developed the methodology, and prepared the manuscript. Dr. Lesley James provided critical feedback, technical insights, and conceptual guidance. The draft paper is intended for journal submission.

All co-authors have been instrumental in shaping the direction and quality of these works. Throughout the thesis, Dr. Lesley James has served as my principal supervisor, offering comprehensive guidance and unwavering support across all aspects of this research.

ACKNOWLEDGEMENTS

I would like to express my sincere gratitude and appreciation to my supervisor, Prof. Lesley James, for her unwavering support, patience, and expert guidance throughout my master journey at the Memorial University of Newfoundland. Her expertise in enhanced oil recovery has been invaluable, and I am grateful for her continued engagement, insightful feedback, and encouragement, which have been instrumental in completing this study.

I would also like to acknowledge my co-authors, Dr. Cleverson Esene and Dr. Quang Trung Trinh, for their contributions in reservoir simulation and data-driven problem-solving techniques, respectively. My thanks extend to Dr. Edison Sripal, Norah Hyndman, and all my colleagues at the Hibernia Enhanced Oil Recovery Laboratory for their assistance and collaboration.

I am deeply thankful for the financial support provided by the Hibernia Management and Development Company (HMDC), Mitacs, and the Natural Sciences and Engineering Research Council of Canada (NSERC), which has made this research possible.

Lastly, I express my heartfelt gratitude to my parents, my husband, my daughter, and my son, whose endless love, support, and encouragement have been a constant source of strength throughout my research journey.

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LIST OF ABBREVIATIONS

Abbreviation	Definition	
AAPEs	Average Absolute Percentage Errors	
AAPRE	Average Absolute Percent Relative Error	
AARD	Average Absolute Relative Deviation	
ACO	Ant Colony Optimization	
AI	Artificial Intelligence	
ANFIS	Adaptive Neuro-Fuzzy Inference System	
ANN	Artificial Neural Network	
BP	Back Propagation	
CCS	Carbon Capture and Storage	
CCUS	Carbon Capture, Utilization, and Storage	
CWI	Carbonated Water Injection	
DAC	Direct Air Capture	
DE	Differential Evolution	
EOR	Enhanced Oil Recovery	
EOS	Equation of State	
FCN	Fully Connected Network	
FPSO	Floating Production Storage and Offloading	
FVF	Formation Volume Factor	
GA	Genetic Algorithm	
GHGs	Greenhouse Gases	
GOR	Gas-Oil Ratio	
GRNN	Generalized Neural Network	
ICA	Imperialist Competitive Algorithm	
МСМ	Multiple Contact Miscibility	
ML	Machine Learning	
MLP	Multi-Layer Perceptron	
MMP	Minimum Miscibility Pressure	
MOPSO	Multi-Objective Particle Swarm Optimization	
PPC	Post-Combustion Capture	
PSO	Particle Swarm Optimization	
RBF	Radial Basis Function	
RMSE	Root Mean Square Error	
ROV	Relative Oil Volume	
RSM	Response Surface Methodology	
SAG	Surfactant-Alternating-Gas	
SVR	Support Vector Regression	
VIT	Vanishing Interfacial Tension	
VRR	Voidage Replacement Ratio	
WAG	Water-Alternating-Gas	

Chapter 1 : INTRODUCTION

1. Background

Climate change, driven by the increased concentration of greenhouse gases (GHGs) in the atmosphere, poses a significant environmental threat to humanity. In Canada, emissions rose by 16.5 % (approximately 100 Mt CO₂ equivalent) between 1990 and 2022. This growth is primarily attributed to increased emissions from oil and gas extraction activities and the transportation sector, both of which have expanded over the past decades (Greenhouse Gas Emissions, 2024). In 2022, emissions from the oil and gas sector in Canada, which includes conventional oil as well as other categories like downstream oil, accounted for 217 Mt CO2 equivalent, representing 31 % of Canada's total emissions (Greenhouse Gas Emissions, 2024). In Newfoundland and Labrador, emissions per capita stood at 16.2 tonnes CO₂ equivalent, which is 11 % below the Canadian average of 18.2 tonnes per capita (Provincial and Territorial Energy Profiles - Newfoundland and Labrador, 2024). Transportation, industry and manufacturing, and the oil and gas sector are the largest emitting sectors in the province, with 34 % of emissions, 17 % of emissions, and 15 % of emission, respectively. In 2022, the total GHG emissions from the oil and gas sector were 1.29 MT CO₂ equivalent, of which offshore oil production accounted for 1.26 MT CO₂ equivalent and petroleum refining accounted for 0.03 MT CO₂ equivalent (Provincial and Territorial Energy Profiles – Newfoundland and Labrador 2024).

The Canadian federal government recently announced an increase of 467 % of the carbon tax from its current \$30 per tonne of GHG emissions to \$170 per tonne by 2030 (Harvie 2020). To reduce emissions and fight against climate change, in 2016, Canada released the first-ever national climate plan with a goal of a 30 % reduction below 2005 levels in 2030 (Progress towards Canada's greenhouse gas emissions reduction target 2021). Recently, the Government of Canada indicated

a goal to reduce emissions to 40 to 45 % below 2005 levels by 2030, which constitutes a further reduction from that agreed to under the Paris Agreement in 2015 (Tasker 2021). In 2019, Newfoundland and Labrador introduced a new climate action plan targeting a 30% reduction in greenhouse gas (GHG) emissions below 2005 levels by 2030. The province also committed to the regional goal of the Conference of New England Governors and Eastern Canadian Provinces, which aims for a 35–45 % reduction below 1990 levels by 2030 (The Way Forward on Climate Change in Newfoundland and Labrador, 2022). Achieving these targets requires innovative solutions to make oil and gas platforms either CO₂-neutral or CO₂-negative, highlighting the importance of integrating carbon capture, utilization, and storage (CCUS) technologies and adopting renewable energy strategies.

 CO_2 is a widely recognized and extensively used solvent in Enhanced Oil Recovery (EOR) operations. By injecting CO_2 into reservoirs, the process reduces the interfacial tension between oil and reservoir rock while lowering oil viscosity, making the oil more mobile and easier to extract. In addition to enhancing oil recovery, CO_2 -EOR also facilitates CO_2 storage, contributing to carbon sequestration efforts. This technique has been applied onshore for over four decades, particularly in North America, where it has evolved into a mature and reliable technology (Enick, 2015). Its long-term use has provided valuable insights into the optimization of injection strategies and reservoir management, paving the way for its adaptation in offshore applications despite the added challenges. One of the most successful post combustion CO_2 -EOR projects, which is also the largest Canadian CO_2 -EOR project, is located at Weyburn, Saskatchewan, which began in 2000 and was the first project to inject anthropogenic CO_2 for EOR (Carbon Capture & Sequestration Technologies @ MIT, Weyburn-Midale Carbon Dioxide Project 2019). The operation currently injects 1.8 M ton of CO_2 each year (A Responsible Energy Story: Weyburn Unit 2022).

However, the story is different offshore where facilities are more costly and often weight constrained, CO₂ transportation would be over longer distances if a nearby source exists, regulatory issues, and uncertainties around the revenues as the oil price and the cost of CO₂ are involved. Considering the need to fully develop all aspects of CCUS – carbon capture, utilization, and storage, CO₂-EOR can first be utilized to recover incremental oil then the same, proven reservoir can provide already de-risked geological storage. CO₂ capture and storage projects are not new. Offshore, Norway has been storing CO₂ stripped from high concentration natural gas for 20+ years at the Snøhvit and Sleipner fields (Norway's Sleipner and Snøhvit CCS: Industry models or cautionary tales? 2023). The Northern Lights project started in 2020 and will capture CO₂ from an onshore cement and waste facility, transport it via ship and pipeline to inject and store the CO_2 in the Aurora field, offshore Norway (Historic investment decision for transport and storage of CO_2 2020). Some pilots for offshore CO₂-EOR have been conducted such as Quarantine Bay (Hsie 1988), Timbalier Bay (Moore 1985), Bay St. Elaine (Nute 1983), Weeks Island (Johnston 1988), and Paradis (Bears 1984). In these projects, the source of CO₂ used was not specified except for Paradis project where the CO₂ was captured from Monsanto Co. ammonia plants near Luling. These pilot-scale projects showed technical promise, however, the full-scale implementation failed offshore because of high project costs (Godec 2021).

The Lula project, located in the Santos Basin Pre-Salt Cluster (SBPSC) off the coast of southeast Brazil, is notable for being the world's first offshore CO₂-EOR (Enhanced Oil Recovery) project. Initiated in 2011 with the Lula-pilot and followed by the Lula-NE pilot in 2013 (Eide 1945), this project represents a significant step in the integration of CO₂ sequestration with oil recovery. The CO₂ used in the Lula project is sourced from two abundant resources: seawater and produced or imported gas, providing a sustainable supply of CO₂ for the enhanced recovery processes. Since its initiation, the project has successfully increased the oil recovery factor while also contributing to a 12% reduction in greenhouse gas (GHG) emissions, which highlights the dual benefits of CO₂-EOR in both improving oil production and mitigating environmental impact (Petrobras Santos Basin, 2023). On the other hand, similar CO₂-EOR initiatives have faced more challenges in other regions, such as Norway. Projects at the Gullfaks, Ekofisk, Draugen, and Heidrun fields have explored CO₂-EOR, but have struggled economically due to unfavorable conditions related to CO₂ pricing, carbon credits, and fluctuating oil prices. These economic challenges underscore the importance of favorable market conditions and supportive policy frameworks for the financial viability of CO₂-EOR projects (Augustsson, 2004; Hustard, 2004; CO2 for EOR off Norway under study, 2007). While the Lula project demonstrates the potential for CO₂-EOR in offshore reservoirs, the experience from Norway's projects highlights the importance of balancing technological potential with economic factors to ensure the long-term success of CO₂-EOR and carbon capture utilization and storage (CCUS) initiatives.

There is stranded, uneconomic, sweet natural gas in offshore Newfoundland, Canada. In 2023, offshore crude oil facilities in Newfoundland produced around 410 million cubic feet per day (MMcf/d) of natural gas (Provincial and Territorial Energy Profiles – Newfoundland and Labrador 2024). The Canada-Newfoundland and Labrador Offshore Petroleum Board (C-NLOPB) estimates Newfoundland and Labrador's natural gas resources at approximately 10.7 trillion cubic feet (Provincial and Territorial Energy Profiles – Newfoundland and Labrador 2024). Currently, there are no pipelines or infrastructure to transport or commercialize the substantial natural gas resources in Newfoundland and Labrador. Instead, the produced natural gas is either used to power offshore facilities, reinjected into reservoirs to maintain pressure, or flared, contributing to emissions (Provincial and Territorial Energy Profiles – Newfoundland and Labrador, 2024). Offshore power generation primarily depends on diesel or natural gas combustion turbines, which produce post-combustion CO₂. The Net Zero project explored the feasibility of implementing Carbon Capture,

Utilization, and Storage (CCUS) as an integrated solution to mitigate emissions from four active offshore fields and one proposed field. The project proposes capturing CO₂ emissions from offshore gas and diesel generators, as well as from flaring activities, to support decarbonization efforts in line with climate goals (A Net Zero Project White Paper, 2023).

The Hibernia EOR Research Group is exploring the integration of post-combustion CO₂ capture and injection for Enhanced Oil Recovery (EOR) applications. A critical challenge in this effort is the constrained CO₂ supply available for offshore Newfoundland reservoirs. Using the Hibernia field as a case study, calculations based on production data (C-NLOPB) determined the maximum CO₂ capture capacity using membrane technology with a 90 % capture efficiency. An example calculation is detailed in ANNEX A, and Figure 1-1 illustrates the annual gas injection and CO₂ capture volumes. The findings reveal that while the available CO₂ is insufficient for large-scale CO₂ flooding, it can support other EOR methods such as carbonated water injection (CWI), localized block CO₂ flooding, water-alternating gas (WAG), or CO₂-enriched natural gas WAG. This highlights the importance of considering CO₂ supply limitations when designing EOR strategies for offshore reservoirs, where full-field applications may not be viable due to resource constraints. This study analyzes the optimization of constrained volumes of varying CO₂ concentrations and impurities considering different oil types and reservoir conditions. It examines how impurities impact CO₂ injection and retention, and how different oil types and reservoir characteristics respond to specific injection strategies. This approach enables offshore EOR to balance enhanced oil recovery with carbon storage objectives, optimizing both CO₂ usage efficiency and emission reductions to support sustainable energy goals.



FIGURE 1-1: Gas injected amount vs post-combustion CO₂ produced annually for Hibernia Field (C-NLOPB)

2. Objectives, Motivation, and Contributions

The overall objective of this study is to develop and optimize enhanced oil recovery (EOR) strategies for offshore reservoirs, specifically the Hibernia field, that maximize the use of limited post-combustion CO₂ supplies. Due to insufficient CO₂ volumes for conventional CO₂ flooding, the study aims to evaluate alternative injection techniques—including carbonated water injection (CWI), individual block CO₂ flooding, water-alternating gas (WAG), and CO₂-enriched natural gas WAG—that can effectively increase oil recovery within these constraints. Additionally, to align with environmental goals of zero atmospheric CO₂ venting, this research will design a closed-loop system that purifies and reinjects the CO₂-rich gas stream, ensuring efficient CO₂ utilization and storage. By addressing CO₂ limitations and refining offshore EOR methods, this research seeks to establish sustainable, economically viable solutions for offshore carbon management and oil recovery. The key aspects of objectives and contribution are outlined as follows:

2.1. Objective one – Evaluate the influence of CO₂-natural gas mixtures and CO₂ stream impurities, based on source and capture techniques, on minimum miscibility pressure (MMP)

<u>Research gap</u>: The existing literature has explored the influence of various impurities on CO₂ minimum miscibility pressure (MMP), with findings that different impurities, such as CH₄, N₂, C₂H₆, and H₂S, impact MMP in unique ways. However, these studies typically examine individual impurities in isolation without connecting their presence to specific CO₂ capture methods, which significantly influence impurity profiles. Additionally, most studies focus on pure or low (<5%) CO₂ concentrations, leaving a gap in understanding the MMP behavior across a full range of CO₂ concentrations (0-100%).

<u>Contribution/novelty</u>: This study investigates the influence of these impurities on the MMP of oil and gas mixtures using slimtube simulation, based on various CO_2 sources and capture technologies. This work offers a review of various CO_2 capture technologies, the resulting impurities and their respective concentrations, and the impact on MMP across a wide range of CO_2 concentrations (from 0 % to 100 %), addressing a gap in the existing literature.

Peer reviewed conference paper (1) – Chapter 3: Pham, Q.C and James, L.A. 2021. Considering the CO₂ Source and Capture Technique to Reduce Minimum Miscibility Pressure (MMP) for Enriched Water Alternating Gas (WAG) Injection. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30. https://doi.org/10.1115/OMAE2021-62643

2.2. Objective two - Develop a Machine Learning model to accurately predict MMP using Deep Learning

<u>Research gap</u>: The literature review identifies critical gaps in the understanding and measurement of minimum miscibility pressure (MMP) for gas injection in reservoirs. While several experimental

methods exist for determining MMP, such as falling drop, rising bubble, Vanishing Interfacial Tension (VIT), and slimtube tests, each has its drawbacks. For instance, while slimtube tests are the most reliable, they are also labor-intensive and time-consuming. Current mathematical correlations and simulation methods are primarily based on limited experimental data, which often focus on pure or slightly contaminated CO₂ and N₂ streams, making them less effective for a variety of gas compositions. Machine Learning (ML) has gained popularity for estimating MMP, showing efficiency in this regard. Nevertheless, previous studies have faced challenges due to limited data points and constrained CO₂ mole percentages that do not drop below 40 %, which limits the applicability of machine learning models in predicting MMP under varying reservoir conditions.

<u>Contribution/novelty:</u> In this study, a robust Machine Learning model was developed using advanced Deep Learning techniques and k-fold Cross Validation to accurately predict the minimum miscibility pressure (MMP) for oil and gas mixtures. This innovative model not only expands the dataset size but also enhances prediction accuracy and significantly broadens the range of applicable CO₂ concentrations. Additionally, a comprehensive sensitivity analysis was conducted to rigorously evaluate the influence of various input parameters, including reservoir characteristics and the specific properties of oil and gas, on MMP, providing deeper insights into the factors affecting oil recovery efficiency.

Peer reviewed conference paper (2) – Chapter 4: Pham, Q.C., Trinh, Q.T., and James, L.A. 2021 Data Driven Prediction of the MMP between Mixtures of Oil and Gas using Deep Learning. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30. <u>https://doi.org/10.1115/OMAE2021-63018</u> 2.3. Objective three - Optimize CCS and CO₂ - EOR for offshore reservoirs under limited CO₂ supply, considering diverse reservoir and oil characteristics. *Research gap:* Previous studies in Enhanced Oil Recovery (EOR) and Carbon Capture, Utilization, and Storage (CCUS) have largely operated under the assumption of unlimited CO₂ supply, failing to adequately address the constraints associated with CO₂ availability, especially in offshore reservoirs. This oversight is significant, as the capacity for CO₂ storage and the ability to conduct effective EOR can be severely limited by the volume of CO₂ that can be feasibly captured and injected. Moreover, most EOR research tends to emphasize incremental oil recovery metrics while neglecting the financial impacts of carbon emissions, which can significantly influence project feasibility and sustainability.

Contribution/novelty: The objective of this study is to investigate the joint optimization of oil recovery and carbon storage by incorporating both the price of produced oil and the value of CO₂ tax credits, utilizing a 50:50 ratio to emphasize their equal importance. The research examines a variety of oil types—light, medium, and heavy—under diverse conditions, including CO₂-EOR methods such as Water-Alternating Gas (WAG), Carbonated Water Injection (CWI), and enriched WAG. Additionally, the study addresses constraints related to CO₂ availability, the impact of impurities, and reservoir characteristics such as stratification, crossflow, temperature, pressure, and permeability. Simulations are conducted using the CMG framework, with optimization achieved through Multi-Objective Particle Swarm Optimization (MOPSO) techniques. This comprehensive approach aims to enhance both oil recovery and CO₂ storage efficiencies in offshore reservoirs, providing valuable insights for sustainable energy practices.

Peer reviewed conference paper (3) – Chapter 5: Pham, Q.C., Esene, C.E. and James, L.A. 2023. Investigating CO₂-EOR Types with Constrained CO₂ Volumes and Impurities for a High-Quality Sandstone, Stratified Offshore Newfoundland Reservoirs. Presented at the SPE Canadian Energy Technology Conference and Exhibition. Calgary, Alberta, Canada, March 15 - 16. https://doi.org/10.2118/212811-MS

Presentation (4) – Chapter 6: Pham, Q.C and James, L.A. Dirty Carbon – Impact of CO2

Volume and Impurities on Carbon Utilization and Carbon Neutral Oil Production. 2024.

Presented at Latin America Carbon Capture, Utilization, and storage. Rio de Janeiro, Brazil, 22-

23 May.

Draft paper - Chapter 6: The draft paper is intended for journal submission

The overall workflow is shown in Figure 1-2, which illustrates the required steps to achieve each objective.



FIGURE 1-2: Overall and detailed objectives for the thesis

3. Thesis Structure

<u>**Chapter 2**</u> reviews CO_2 capture technologies and their impurities relevant to Enhanced Oil Recovery (EOR), examining their impact on Minimum Miscibility Pressure (MMP), a key factor in CO_2 injection efficiency. It also covers methods for measuring MMP, including experiments, models, and simulations. The chapter explores the joint optimization of EOR and Carbon Capture and Storage (CCS), highlighting how integrating these processes can enhance both oil recovery and CO_2 sequestration, while identifying gaps in current research.

<u>Chapter 3</u> examines the influence of impurities in the CO₂ stream on the Minimum Miscibility Pressure (MMP) of oil and gas mixtures, focusing on different CO₂ sources and capture technologies. It investigates how impurities like methane, nitrogen, and oxygen, which vary by CO₂ source (e.g., natural gas or flue gas), impact MMP and CO₂-EOR efficiency. The chapter highlights the role of CO₂ capture technologies in shaping the impurity content and how this affects miscibility pressure, offering insights to optimize CO₂ injection strategies for enhanced oil recovery.

<u>Chapter 4</u> presents a model for predicting Minimum Miscibility Pressure (MMP) between oil and gas mixtures using a Deep Learning approach, specifically employing multiple fully connected networks. The model is optimized using early stopping and k-fold cross-validation techniques to improve accuracy and prevent overfitting. This methodology enhances the predictive capability for MMP, contributing to more effective strategies for CO₂ injection in Enhanced Oil Recovery (EOR). <u>Chapter 5</u> presents a study on CO₂ Enhanced Oil Recovery (EOR) methods applied to a highquality sandstone, stratified offshore reservoir in Newfoundland. The study focuses on the impact of constrained CO₂ volumes and impurities on the effectiveness of various CO₂-EOR techniques. By considering factors like reservoir stratification, CO₂ availability, and impurity levels, the study evaluates how these variables influence oil recovery efficiency in offshore Newfoundland reservoirs. The results aim to optimize CO₂ injection strategies, ensuring effective oil recovery while adhering to CO₂ sequestration constraints.

<u>Chapter 6</u> focuses on the optimization of coupling Enhanced Oil Recovery (EOR) and Carbon Capture and Storage (CCS) for offshore reservoirs, including stratified reservoirs with and without crossflow. The study considers CO_2 constraints, the impact of impurities in the CO_2 stream, and the economic factors such as oil prices and CO_2 tax credits. By integrating these factors, the chapter aims to identify the most effective strategies for optimizing both oil recovery and CO_2 sequestration. The analysis incorporates the complexities of varying reservoir conditions and economic incentives to maximize both environmental and financial outcomes.

<u>Chapter 7</u> summarizes the key findings, conclusions, and recommendations of the thesis, focusing on optimizing CO₂-EOR and CCS integration. It highlights the impact of CO₂ constraints, impurities, and economic factors, offering suggestions for future research and practical applications to enhance oil recovery and carbon sequestration in offshore reservoirs.

Chapter 2 : LITERATURE REVIEW

CO₂ Capture Technologies and Impurities Related to Enhanced Oil Recovery (EOR) Purposes:

(A part of this section has been published in peer reviewed conference paper: Pham, Q.C and James, L.A. 2021. Considering the CO₂ Source and Capture Technique to Reduce Minimum Miscibility Pressure (MMP) for Enriched Water Alternating Gas (WAG) Injection. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30. https://doi.org/10.1115/OMAE2021-62643)

The CO₂ concentration in gas is highly dependent on the source of the CO₂. For example, postcombustion CO₂ streams, such as those captured from flue gas after the combustion of fossil fuels, show varying concentrations of CO₂ based on the type of fuel burned. For flue gas from gas turbines, CO₂ concentrations typically range between 4% and 5%, while flue gas from coal combustion can have CO₂ content ranging from 8% to 15% (CO2 Capture Technologies, Post-Combustion Capture (PCC), 2012). In contrast, natural gas, particularly from offshore sources like Norway, is predominantly composed of methane (CH₄), with smaller amounts of water (H₂O) and other constituents. The CO₂ concentration in the gas phase can vary significantly, ranging from 0% to 44% depending on the field and processing conditions (Marit, 2014). A typical composition for natural gas from a sweet-gas field (which is free of hydrogen sulfide or CO₂) is assumed to be 10% CO₂, 83.6% CH₄, and 6.4% H₂O (Marit, 2014). Table 2-1, which is referenced but not provided here, likely shows the specific compositions of flue gas from both coal and gas-fired power plants as well as a representative natural gas composition from a generic field, highlighting the differences in CO₂ content and the implications of these variations for CO₂-EOR projects. These differences in CO₂ concentration are crucial when considering CO₂-EOR strategies, as they can influence the efficiency of CO₂ injection, miscibility, and the overall effectiveness of enhanced oil recovery and CO₂ storage processes.

TABLE 2-1: Typical compositions of flue gases from coal-and gas- fired power plants (CO₂ Capture Technologies, Post-Combustion Capture (PCC) 2012, Marit 2014)

Gas constituent	Flue Gas	Flue Gas from	Natural Gas from
	from coal	gas turbine	a generic field
N_2	70-75 %	73-76 %	0
CO ₂	10-15 %	4-5 %	10 %
H ₂ O vapor	8-15 %	8-10 %	0
O ₂	3-4 %	1-15 %	6.3 %
Trace Gases (SOx, NOx, others)	<1 %	<1 %	0
CH ₄			83.6 %

Some studies provide recommendations on limits to CO₂ impurities for CO₂ utilization and storage purposes. The removal of water, oxygen and sulfur oxides is required for pipeline transport systems to prevent corrosion and other defects in pipelines (Abbas 2013). It is recommended that the total concentration of air-derived, non-condensable species (N₂, O₂ and Ar) do not exceed 4 % as they impact compression and transport costs (Wood, 2012, Visser 2008). In enhanced oil recovery (EOR) applications, it is recommended that O₂ content should not exceed 100 ppm, due to the promotion of microbial growth, which can cause unknown effects on oil production. Furthermore, exceeding this oxygen limit may cause a reaction with hydrocarbons in the oil field, which can lead to overheating at the injection point or oxidation in reservoirs with high oil viscosity (Abbas 2013, Pipitone 2009). Water concentration is limited under 50 ppmv to prevent corrosion Wood (2012) and sulfur species (e.g. H₂S, Cos SO₂, SO₃) should be maintained at a certain level to avoid corrosion risk in the presence of water. Based on the IDLH (Immediately Dangerous to Life or Health) limit defined by the US National Institute for Occupational Safety and Health, the target for SO₂ is 100 ppmv Visser (2008) and the same limit is posted for NOx as NOx species can form

nitric acid, which induces corrosion (Sim 2013). Figure 2-1 shows a schematic diagram of CO₂ capture system.



FIGURE 2-1: Schematic diagram of CO₂ capture system

The main technologies for CO₂ capture are absorption, adsorption, and membrane separation. Besides, other novel technologies have been investigated such as supersonic, hydrate-based separation, cryogenic distillation, etc. These technologies each result in different types and concentrations of impurities, which may include H₂S, NOx, CH₄, N₂, and SO₂ (Visser 2008). Absorption, specifically chemical absorption, is widely used in industry because of its mature development, its ability to achieve a CO₂ purity of 99 % and high selectivity between CO₂/N₂ (as high as 100) by using amine-based solvents (Wand 2017). Waste heat can be recovered; however, the overall process is energy intensive. SOx and NOx need to be removed by a caustic scrubber before entering the absorber as they can react with the amine to form stable, non-regenerable salts, resulting in a loss of amine (Rashid 2014, Adams 2007). Since the amount of other impurities is small or negligible, this work assumes that the primary impurities from the absorption technique are N₂ for flue gas sources and CH₄ for natural gas sources, both at a concentration of 1%.

Adsorption involves the retention of a fluid on a solid surface, called sorbent. This technology can provide a CO₂ purity of 99 %, though the selectivity for CO₂ is relatively low compared to that of absorption (CO₂/N₂: 80) (Wang 2017). The energy consumption can be reduced through waste heat recovery. To avoid the complexity of the CO₂ separation process, a pre-treatment stage is applied

to eliminate some impurities, such as SOx, NOx, H_2O (Songolzadeh 2014). N_2 with 1 % concentration is assumed to be the primary impurity from the flue gas stream and CH₄ with 1% concentration for natural gas source.

A third post-combustion CO_2 capture technology is membrane separation, which separates mainly between CO_2 and N_2/O_2 . The degree of separation and CO_2 purity are determined by the permeability and selectivity of a membrane material (Robeson 1991, Low 2013). This process can be used for higher flow rates due to its high area to volume ratio. Another advantage of this technology is that the maintenance requirements are reportedly low, which implies a longer expected lifetime of the system. Membrane technology is less harmful to the environment than the two above technologies. A purity of 95% and a capture degree of 90 % can be achieved by using a two-stage membrane separation system (Merkel 2010, Zhao 2010), which is widely used. A study was completed to optimize a two-stage membrane system based on the purity and flow rate in the permeate stream for flue gas from offshore Newfoundland (Barrett 2019). It concluded that the optimum CO_2 purity was 90 % with 10 % impurities (2 % of O_2 and 8 % of N_2) if considering a post combustion flue gas. If considering a natural gas source, 10 % CH₄ and 90 % CO₂ can be assumed.

Supersonic separation has been used recently to remove water vapor from natural gas. The condensable gas components are condensed to the liquid phase. The condensed liquids are then removed from the gas-liquid mixture due to the high centrifugal force generated through the cyclone (Yang 2017). The main advantage of this technique is that it is friendly with environment since no chemical is required for this process (Yang 2017). Vladimir (2017) stated in their report that the CO_2 capture efficiency of this technique, which depends on temperature of the mixture of the air and injected liquid CO_2 , varied in the wide range from 11.3 % and 97.8 %.

Table 2-2 summarizes the CO₂ purities achieved and the impurity composition for each separation technology studied in this thesis for EOR purpose.

CO ₂ Separation Process	CO ₂ Impurities		
	Flue Gas	Natural Gas	
Adsorption	99 % CO ₂ , 1 % N ₂	99 % CO ₂ , 1 % CH ₄	
Absorption	99 % CO ₂ , 1 % N ₂	99 % CO ₂ , 1 % CH ₄	
Membrane	90 % CO ₂ , 2 % O ₂ , 8 % N ₂	90 % CO ₂ , 10 % CH ₄	

TABLE 2-2: CO₂ possible purity by separation technology and CO₂ source for EOR purpose

2. Influence of Impurities and Gas Composition on Minimum Miscibility Pressure (MMP)

(A part of this section has been published in peer reviewed conference paper: Pham, Q.C and James, L.A. 2021. Considering the CO₂ Source and Capture Technique to Reduce Minimum Miscibility Pressure (MMP) for Enriched Water Alternating Gas (WAG) Injection. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30. https://doi.org/10.1115/OMAE2021-62643)

MMP is defined as the pressure at which oil and gas achieve miscibility. Many researchers have investigated the influence of impurities on the MMP of CO_2 in oil, some impurities increase MMP, and others decrease MMP. It is reported that CH_4 increases the MMP and lowers the oil recovery efficiency when present in the CO_2 stream source (Emera 2005, Yuan 2005, Alston 1985, Yellig 1980, Johnannes 2009). C_2H_6 and intermediate hydrocarbons such as propane C_3H_8 , butane C_4H_{10} , and pentane C_5H_{12} mix better with reservoir fluids than CO_2 and therefore reduce MMP (Alston 1985, James 1981). Zhang (2004) conducted laboratory studies on the effect of CO_2 impurities on MMP in two Saskatchewan light oils. It was observed that the MMP of pure CO_2 (16.5 MPa) decreased 18 % (13.6 MPa) by adding 40 mol% C_2H_6 to the CO_2 stream, nearly 25 % by adding approximately 16 mol% C_3H_8 , and by approximately 45 % by increasing the amount of C_3H_8 to 37

mol%. N₂ is a common impurity in a post combustion CO₂ stream, and it increases the MMP of CO₂ (Emera 2005, Alston 1985, Zhang 2004). However, N₂ was found to lower CO₂ MMP when temperature increased for volatile oils at high temperatures (Christian 1981, Firoozabadi 1986). H₂S is another impurity that can be found in CO₂ streams that is said to have little effect on CO₂ MMP, as its thermodynamic properties are close to those of CO₂ (Emera 2005). Some researchers, however, showed that H₂S can reduce CO₂ MMP (Vladimir 2017). Metcalfe (1982) performed experiments to investigate the influence of H₂S on CO₂ MMP. The result showed that with a 3:1 mole ratio of CO₂/H₂S and 18.5 % reduction in MMP (from 8.3 MPa to 6.8 MPa) was observed. MMP was reduced by 30 % when the mole ratio of CO₂/H₂S was lowered to 1:1. O₂ can increase the MMP of pure CO₂ significantly (Jiang 2012, Yin 2014, Wilkinson 2010, Rupp 1984). Jiang (2012) conducted slimtube experiments with different concentrations of O₂ varying from 0 to 10% in CO₂ stream. The results showed that the presence of 5% O₂ increased MMP by 20.88% from 2466 psi to 2981 psi), while 61.92% MMP (to 3993 psi) increase was observed with 10% O₂.

Only a few studies have evaluated the change in the MMP of gas in oil by using a combination of CO_2 and other gases, specially produced gas. In a project for Prudhoe Bay Field on Alaska's North Slope, 17 slimtube tests were conducted at 93.3 °C using methane, CO_2 , and enriched CO_2 to displace crude oil of 25.5 °API at 4800, 3950, and 3350 psig (Rupp 1984). The results showed that the mixture with 40% CH₄ resulted in the lowest MMP of 3615 psig. Ning (2011) performed a study using both laboratory experiments and reservoir simulation to examine the influence of CO_2 -oil phase behavior on oil recovery for Alaska North Slope viscous oils. The mixture of 85 % CO_2 and 15 % natural gas liquid resulted in a viscosity reduction from 122 cP to 6 cP in comparison with 17 cP of pure CO_2 injection, which led to 5% more oil recovery for the mixture than pure CO_2 . Abbasi (2010) experimentally studied the MMP variation for different CO_2 proportions in a mixture with natural gas for an Iranian reservoir by adding 6 % CO_2 to the natural gas and injecting

it at 1500 psi and 80 °C. The MMP simulations were performed using WinProp module of CMG by varying the percentage of CO₂ in five steps: 0 %, 6 %, 28 %, 48 %, and 78 %. The result showed that the higher the CO₂ concentration added to the natural gas, the lower the MMP and the more quickly miscibility could be achieved. Further work has been carried out to investigate the effect of mixtures of CO₂ with other gases such as CH₄, C₂H₆, C₃H₈, and flue gas on oil recovery performance (Shokoya 2005, Hamouda 2018, Yengo 2014).

Conclusion: The effect of impurities in the CO_2 stream on MMP has been investigated as individual components and for specific sources. No previous studies relate the different capture techniques to the impurities (and their respective concentrations) and their impact on MMP, despite the importance of the capture technology in determining the composition of CO_2 stream source. Only a few studies have evaluated the change in the MMP of gas in oil by using a combination of CO_2 and other gases, especially produced gas. This study investigates the influence of these impurities on the MMP of oil and gas mixtures using slimtube simulation, based on various CO_2 sources and capture technologies. Unlike most previous studies, which focused on CO_2 concentrations below 5% or pure CO_2 , this research explores a broader range of CO_2 concentration. This work offers an in-depth examination of the relationship between various CO_2 capture technologies, the resulting impurities and their respective concentrations, and the impact on Minimum Miscibility Pressure (MMP) across a wide range of CO_2 concentrations (from 0% to 100%), addressing a gap in the existing literature. The methods to determine MMP are also analyzed in order to identify the uncertainty related to each method.

3. MMP Measurement Methods: Experiments, Mathematical (Analytical, Simulation, Machine Learning)

(A part of this section has been published in peer reviewed conference paper: Pham, Q.C., Trinh, Q.T. and James, L.A. 2021. Data Driven Prediction of the MMP between Mixtures of Oil and Gas using Deep Learning. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30.

https://doi.org/10.1115/OMAE2021-63018)

MMP can be estimated by either mathematical or experimental techniques. Some non-experimental methods frequently used are mathematical correlations, mixing cell simulation, or analytically. Using mathematical correlations is the fastest and least expensive method to estimate MMP and many correlations for MMP determination are proposed in the literature (Eakin 1988, Glaso 1985, James 1981, Sebastian 1992, Sebastian 1985). These correlations, however, were built from limited experimental data and are primarily for pure (100 %) or slightly contaminated CO₂ and N₂ streams (less than 5%). Consequently, MMP predictions may only be reliable when the characteristics of the studied system are close to the reference data from which the correlation is produced. Mixing cell simulation is another approach used to predict MMP, by mimicking the repeated contacts between oil and gas (Jensen 1990, Neau 1996). This technique is separated into forward contacts that can be used only for purely vaporizing miscibility mechanism, and backward contacts for purely condensing mechanism. Jessen (1998) proposed a more efficient technique to resolve this problem, however, the set of equations used is strongly nonlinear since fugacity coefficients are functions of liquid and vapor compositions. An analytical method to estimate MMP in gas injection systems was described by James (2018) by finding the pressure at which one of the key tie-lines becomes zero length. This technique experiences numerical difficulties as very large positive or
negative values of oil and gas saturations can be obtained for the intersection of tie-lines lying outside the two-phase region.

Experimental methods to measure MMP include falling drop, rising bubble, Vanishing Interfacial Tension (VIT), and slimtube tests. The falling drop technique, developed by Christiansen (1986), determines the minimum level of enrichment. This technique is inexpensive and fast; however, the result is only reliable when the miscibility mechanism is pure condensing. Mihcakan (1996) designed the rising bubble apparatus, in which the contact of some intermediate hydrocarbons vaporized from the oil phase to the gas phase and the gas bubble is used to estimate MMP. The MMP calculated through this method is only accurate for a pure vaporizing gas drive mechanism. The VIT method is based on the interfacial tension between the injected gas and the reservoir oil at fixed temperature (Rao 1997). The drawback of this method is that it strongly depends on the overall composition of the gas/oil mixture (Orr Jr 2007), and it is reliable only when the miscibility mechanism is strictly condensing or vaporizing.

The most used technique in industry is the slimtube test, in which the oil recovery is used as a criterion to determine MMP. Elsharkawy (1992) conducted 12 slimtube tests for different oils with gravities varying from 34 to 51° API and completed a literature review on this method. They concluded that there is no standard design, standard operating procedure, or standard criteria that can be used to estimate MMP through the slimtube method. The design of a slimtube system (including slimtube length, diameter, type of packing, and the permeability and porosity of the packing) were reported to vary significantly in industry. Various oil recovery criteria have been applied to estimate MMP, such as 80% at gas breakthrough (Holm 1982), or 90-95 % ultimate recovery at 1.2 pore volumes of gas injected (Jacobson 1972, Graue 1981). The slimtube test is the only method that considers the combination of condensing and vaporizing miscibility mechanisms at the pore scale through mobility of gas and oil in the tube. A combined condensing/vaporizing

gas drive mechanism is often responsible for miscibility development (Zick 1986, Wu 1990). For this reason, the slimtube test is recognized as the most reliable method for the determination of MMP in the oil industry.

Flock (1984) studied the effect of slimtube length and injection rate on recovery factor. They found that when the slimtube length increased, the recovery factor increased and the recovery versus pressure curve shifted upward. They further concluded that increasing the slimtube length had a stabilizing effect on the displacement and that a slimtube of at least 12.2 m length was required for a good estimation of MMP. The injection rate was reported to have no effect on the recovery factor and its effect on the displacement was found to be negligible. In the work of Elsharkawy (1992), a long slimtube was used to minimize the effect of the transition zone length, and the use of smaller diameter tubing was justified to prevent viscous fingering. Ekundayo (2013) investigated the influence of slimtube length, injection rate and inner diameter on the MMP. They confirmed the conclusions of Flock (1984). They also suggested using the intersection of two straight lines on the recovery-versus-pressure curve as the miscibility indicator. Kanatbayev (2015) completed a literature review and noted that the uncertainty in determining MMP using slimtube tests is often reported on the order of magnitude 5 %.

MMP estimation is said to be affected by the selection of EOS (Equation of State) types, the limitations for the variation change in critical temperature (T_c) and pressure (P_c) during tuning and the scheme for lumping to fewer pseudo components. Firoozabadi (1986) compared the value of MMP predicted from Peng-Robinson EOS (PREOS) with available experimental data. The results showed that the EOS generally overestimated the MMP. Stalkup (2005) stated that if two EOSs possessed different parameters could lead to different values of MMP and oil recovery. A given EOS is adequate to predict MMP of oil and gas system only when its results are history matched with MMP measured from slimtube measurements.

With the development of Artificial Intelligence (AI) and a high number of successful applications in the oil and gas industry, many researchers have used Machine Learning (ML) algorithms to predict MMP. Hassan (2018) applied different AI techniques including Artificial Neural Network (ANN), Radial Basis Function (RBF), generalized neural network (GRNN) and Adaptive Neuro-Fuzzy Inference System (ANFIS) to predict MMP for pure CO₂ stream through 140 data points. With the original data including reservoir temperature and oil characteristics such as the molecular weight of C7+ and mole fraction of C2-C6, significant average absolute percentage errors (AAPEs) were observed for all AI techniques: 41.39% for ANN, 18.27% for RBF, 26.14% for GRNN and 17.77% for ANFIS. Data processing was applied by filtering the input data using power model with power value of -1 and -0.5 for the molecular weight and the mole fraction, which improved the AAPE to 6.6%. Hamdi (2019) employed ANFIS to estimate MMP for pure CO_2 stream using 48 data points. The results showed that a higher accuracy and wider application range was observed with the proposed model compared with traditional correlation approaches. In addition, among four ANFIS models, the hybrid algorithm optimized ANFIS with a Gaussian member function was the most accurate model with Root Mean Square Error (RMSE) of 1.44. Dong (2019) proposed a new method to predict MMP of a pure CO₂ stream based using Deep Learning. A fully connected neural network was developed using the multiple mixing cell method. The model was then improved by adopting L2 regularization and Dropout methods to limit the over-fitting problem. A comparison between six sets of slimtube experiments and the results from this model had a generalized error rate of 6.99%, which validated the model.

Huang (2003) developed an ANN model to predict MMP for both pure and impure CO_2 with the percentage of CO_2 from 45-100 % in gas stream. At first, a trained ANN model was built for pure CO_2 with reservoir temperature and molecular weight of C5+ for oil as inputs. Secondly, the model was developed for impure CO_2 stream using the correlations between the impure CO_2 MMP factor

(Fimp) and the contaminant concentrations. The model effectiveness was then evaluated by comparing their results with the measured MMP as well as the MMP predicted from other statistical models. A higher accuracy was observed with the ANN model. However, the verification for impure CO₂ MMP factor (Fimp) was not carried out because of data unavailability. Khan (2019) used ANN, SVM, and Functional Network to predict MMP for pure and impure CO₂ stream with very limited data points (51) and the percentage of impurity in CO₂ stream was not mentioned. The inputs were reservoir temperature, molecular weight of C5+ and mole fraction of C1, C2-C6 in oil, mole fraction and molecular weight of C2+ in injected gas. The results showed an acceptable average absolute error for all models and among them, ANN provided the best correlation to predict MMP. Amar (2018) combined Support Vector Regression (SVR) with Artificial Bee Colony, which was used to find the best SVR hyper-parameters. The input parameters were reservoir temperature, molecular weight of C5+ and the ratio of volatile to intermediate in oil, and the critical temperature of gas. A low mean absolute percentage error (3.24 %), RMSE (0.79) and a high coefficient of determination (0.9868) was found with the proposed model. ANFIS model was built and optimized by five different approaches: including Back Propagation (BP), Genetic Algorithm (GA), Particle Swarm Optimization (PSO), Ant Colony Optimization (ACO) and Differential Evolution (DE) to estimate MMP for both pure and impure CO₂ stream (Karkevandi 2017). All the models developed through this study were shown to be more accurate than existing models (Karkevandi 2017). In addition, the ANFIS model optimized by PSO had the highest accuracy with an average absolute percent relative error of only 7.53 %. Bian (2016) employed SVR with GA, which has advantage of overcoming the local minima or over-fitting problems. The SVR model was optimized by GA methods. The input parameters were reservoir temperature, oil molecular weight, the mole fraction of volatile and intermediate in oil, and the critical temperature of gas. The range of CO₂ in gas stream was 40-100 %. The model was then compared with commonly used correlations to estimate the MMP. Their model presented much lower deviations on the MMP values than examined correlations: average absolute relative deviation (AARD) of 4.75 % and 7.69 % was found for pure CO_2 impure CO_2 stream, respectively. Karkevandi (2018) used radial basis function neural network (RBF) optimized with five evolutionary algorithms namely GA, PSO, imperialist competitive algorithm (ICA), ant colony optimization (ACO), and differential evolution (DE) to predict MMP for both pure and impure CO₂ stream. It was found that the ICA-RBF model is the most accurate method with statistical values of RMSE = 1.16 and average absolute percent relative error (AAPRE) = 6.01 %. Dargahi (2020) implemented three intelligent models named group method of data handling (GMDH), adaptive boosting support vector regression (AdaBoost SVR) and multi-layer perceptron (MLP). Based on the results, among the proposed models, AdaBoost SVR obtained the highest accuracy with an AAPRE of 3.09 % and RMSE of 0.9 MPa. However, in none of these studies CO₂ and other impurities of the injected gas were included in the input parameter, which lead to the lack of visual relation between MMP and injected gas composition while each gas composition was proven to have significant effect on MMP of oil and gas stream. Some research integrated the injected gas composition in input parameters to enhance the model accuracy for predicting MMP. Edalat (2007) developed a new ANN model using a twolayer perceptron and neural nets software, that was then compared with other common correlations and showed a higher accuracy. The inputs were reservoir temperature, oil molecular weight, mole fraction of C1, C2-C6 and CO2 in oil, mole fraction of C1, C2-C5 and molecular weight of C2-C5 in gas. However, only 52 data points were used, which could limit accuracy in application range for this model. ANN model was optimized by using the PSO algorithm, which helped to find the best initial weights and biases of the neural network (Sayyad 2014). This model though had the same problem of limited datasets of 39. Although the datasets were improved in further studies, the mole percentage of CO₂ in the input parameters did not go below 40 % (Shokrollahi 2013, Mollaiy 2016, Chen 2014, Tatar 2013, Zhong 2016), which may cause inaccuracy when applying to other ranges of concentration. Table 2-3 shows advantage and disadvantage of each MMP measurement methods.

Techniques		Advantage	Disadvantage
Experimental methods	Rising bubble	Fast and inexpensive	Only accurate for a pure vaporizing gas drive mechanism
	Falling drop	Fast and inexpensive	Only reliable when the miscibility mechanism is pure condensing
	VIT	Fast and inexpensive	Strongly depends on the overall composition of the gas/oil mixture
	Slimtube	Reliable	Expensive and time consuming
Mathematical methods	Correlations	Fast and inexpensive	Built from limited experimental data, primarily for pure or slightly contaminated CO ₂ and N ₂ streams
	Analytical method	Fast and inexpensive	Numerical difficulties: very large positive or negative values of oil and gas saturations can be obtained for the intersection of tie-lines lying outside the two-phase region
	Mixing cell simulation	Fast and inexpensive	Separated into forward contacts that can be used only for purely vaporizing miscibility mechanism, and backward contacts for purely condensing mechanism
	Slimtube simulation	Fast and inexpensive	Prone to dispersion
	Machine learning	Fast and inexpensive Reliable	Big data collection required to enhance the accuracy

TABLE 2-3: Advantages and disadvan	tages of MMP determination methods
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TABLE 2-4: Literature review of Machine Learning used to predict MMP

Ref	Algorithm	Input parameters	% CO ₂ in gas	Number of data points	Remarks
(Hassan 2018)	ANN, ANFIS, GRNN and RBF	Reservoir temperature Oil: MW of C7+, mole fraction of C2-C6,	100 %	140	
(Hamdi 2019)	ANFIS	Reservoir temperature Oil: MW of C5+, mole fraction of volatile and intermediate	100 %	48	
(Dong 2019)	FCNN	Formation temperature	100 %	128	The model is developed following

	_	Oil sample components			multiple mixing cell methods to estimate MMP
(Huang 2003)	ANN	Reservoir temperature Oil: MW of C5+ Gas: mole fraction of CO ₂ , N ₂ , CH ₄ , H ₂ S, and SO ₂	45–100 %	NA	The model wasn't evaluated with impure CO ₂ streams because of data unavailability.
(Khan 2019)	ANN, SVM, Functional network (FN)	Reservoir temperature Oil: MW of C7+, mole fraction of C1, C2-C6 Gas: mole fraction and MW of C2+	N/A	51	
(Amar 2018)	SVR artificial bee colony	Reservoir temperature Oil: MW of C5+, the ratio of volatile (C1 and N ₂) to intermediate (C2–C4, H ₂ S, and CO ₂) Gas: Critical temperature	N/A	201	
(Karkevandi 2017)	ANFIS optimized with evolutionary algorithms	Reservoir temperature Oil: MW of C5+, mole fraction of volatile (C1 and N ₂), intermediate (C2–C4, H ₂ S, and CO ₂) Gas: Critical temperature	N/A	270	
(Bian 2016)	SVR with GA	Reservoir temperature Oil: MW of C5+, mole fraction of volatile (C1 and N ₂), intermediate (C2–C4, H ₂ S, and CO ₂) Gas: Critical temperature	40-100 %	150	

(Karkevandi 2018)	RBF and evolutionary techniques	Reservoir temperature Oil: MW of C5+, mole fraction volatile (C1 and N2), intermediate (C2–C4, H2S, and CO2) Gas: Critical temperature	N/A	270	
(Dargahi 2020)	AdaBoost SVR and MLP	Reservoir temperature Oil: MW of C5+, the ratio of volatile components to intermediate components Gas: Critical temperature	N/A	N/A	
(Edalat 2007)	MLP and neural nets software	Reservoir temperature Oil: MW of C2- C5 and C7+, Mole fraction of C1, C2-C6 and CO ₂ , Gas: Mole fraction of C1, C2-C5, MW of C2-C5	NA	52	
(Sayyad 2014)	ANN optimized by PSO	Reservoir temperature Oil: MW C5+ Gas: Mole fraction of CO_2 , H_2S , C1, C2-C4, N_2	45-100 %	39	
(Shokrollahi 2013)	LSSVM	Reservoir temperature Oil: MW of C5+, the ratio of volatile (C1 and N ₂) to intermediate (C2–C4, H ₂ S, and CO ₂) Gas: Mole fraction of CO2, H2S, N2, and C1–C5	40-100 %	147	

(Mollaiy	ANFIS	Reservoir	40-100	N/A	
2016)	optimized with PSO	temperature Oil: MW of C5+, mole fraction of volatile (C1 and N ₂), intermediate (C2–C4, H ₂ S, and CO ₂) Gas: mole fraction of CO ₂ , C1, N ₂ , H ₂ S, C2– C4	%		
(Chen 2014)	GA-BPNN	Reservoir temperature Oil: MW of C7+, mole fraction of volatile oil components, intermediate components, C5– C6 Gas: mole fraction of CO ₂ , C1, N ₂ , H2S, C2–C4	30-100 %	85	
(Tatar 2013)	RBFN	Reservoir temperature Oil: MW of C5+, the ratio of volatile (C1 and N2) to intermediate (C2–C4, H ₂ S, and CO ₂) Gas: Mole fraction of CO ₂ , H ₂ S, N ₂ , C1, C2- C5	40-100 %	147	
(Zhong 2016)	Mixed kernels function based SVR	Reservoir temperature Oil: MW of C5+, the ratio of volatile components to intermediate components Gas: Critical temperature	40-100 %	147	

<u>Conclusion</u>: In some studies, CO_2 and other impurities in the injected gas were not included as input parameters, resulting in a lack of visual correlation between MMP and injected gas composition. This omission is significant, as gas composition has been proven to substantially affect the MMP of oil and gas mixtures. Moreover, the limited data points and restricted CO_2 concentration range (with the mole percentage of CO_2 not falling below 40%) in previous models may have reduced accuracy and hindered their applicability to other concentration ranges.

In this work, for the first time, a deep learning algorithm, utilizing multiple fully connected networks, was implemented to predict MMP for oil and gas mixtures using 250 data points. These data points span a wide range of CO₂ concentrations, from 0 % to 100 % in the injected gas. This broad range covers various modes of gas injection, from pure CO₂ flooding to scenarios where CO₂ is negligibly present in sweet gas injection. Additionally, this study introduced the concept of a "stopping point," employing Early Stopping and K-fold Cross Validation techniques to enhance the overall performance and general applicability of the model.

4. Enhanced Oil Recovery (EOR) and Carbon Capture and Sequestration (CCS)

 CO_2 is a well-known and commonly used solvent for enhanced oil recovery (EOR). CO_2 -EOR has been used onshore for over 40 years, especially in North America, and has become a mature technology (Enick 2015). However, the story is different of offshore where facilities are more costly and often weight constrained, CO_2 transportation over longer distances if a nearby source exists, regulatory issues, and uncertainties around the revenues as the oil price and the cost of CO_2 are involved. Considering the need to fully develop all aspects of CCUS – carbon capture, utilization, and storage, CO_2 -EOR can first be utilized to recover incremental oil then the same, proven can provide already de-risked geological storage. CO₂-EOR has been used successfully onshore since the early 1980s with one of the most successful post combustion CO₂-EOR projects being Weyburn, Saskatchewan (Carbon Capture & Sequestration Technologies @ MIT). Offshore, some pilots have been conducted such as Quarantine Bay (Hsie 1988), Timbalier Bay (Moore 1985), Bay St. Elaine (Nute 1983), Weeks Island (Johnston 1988), and Paradis (Bears 1984). The source of CO₂ used in these pilot-scale projects was not specified except for Paradis project where the CO₂ was captured from Monsanto Co. ammonia plants near Luling. These pilot-scale projects showed technical promise however it failed to implement CO₂-EOR in full-scale offshore caused by high project costs (Godec 2021). The Gulf Coast, USA, is rich in oil and gas resources. Denbury has developed CO₂-EOR projects at the Hastings and Oyster Bayou fields in Texas, as well as the Heidelberg and Tinsley fields in Mississippi. The main CO₂ source was an almost pure (98 %) natural source from Jackson Dome. Denbury is working to replace the natural CO₂ source with CO₂ captured from industrial sources along the Gulf Coast to lower CO₂ emissions (Extensive Experience in the Gulf Coast 2023). These projects provide significant oil production today and are in progress.

Lula is the World's first offshore CO_2 -EOR project, situated in Santos Basin Pre-Salt Cluster (SBPSC), southeast Brazil, approximately 300 km offshore from the coast with a first pilot in 2011 (Lula-pilot) and a second one in 2013 (Lula-NE) (Eide 1945). The oil is a good quality (28-30 API) and contains a significant amount of associated gas, which carries around 11% of CO_2 . The EOR chemical processes were unfeasible because of limitation of logistics and plants for fluid injections. Thus, EOR was considered taken from two abundant resources available: Seawater and the Produced or imported gas. A substantial incremental oil recovery while applying CO_2 or CO_2/HC EOR was proved by preliminary numerical simulation. Water- Alternating-Gas (WAG) injection strategy with CO_2 from produced gas was adopted due to the relatively low global amount of CO_2 available. Floating Production Storage and Offloading (FPSO) were chosen to develop Lula field.

The facilities were designed with a CO_2 separation membrane system that was able to provide two streams: a stream with very high CO_2 content (up to 90 %v/v) and a treated gas with low percentage in CO2 (5 % v/v). This project faced no major operational or reservoir issues and demonstrated the feasibility of offshore CO_2 -EOR, particularly when considering economic benefits and strategic incentives. The project has been reported as successful, increasing the recovery factor and reducing GHG emissions by 12% since 2015 (Petrobras Santos Basin, 2023).

Some projects have been carried out in Norway such as Gullfaks Field (Augustsson 2004). Different CO_2 supply options were evaluated since a single geographical source was insufficient for the need of the project. Incremental oil recovery factor was estimated to be 4.1 % of oil in place. However, the economic conditions were found to be unfavourable considering the CO₂ prices and credits as well as the oil price. Income from the additional produced oil couldn't cover the cost for CO₂ capture and transport. The CO₂ source for Ekofisk field project came from Sleipner gas field. This project showed the possibility to develop large-scale CO₂ injection for EOR offshore technically, however the feasibility stage failed due to economic factors (Hustad 2004). Draugen and Heidrun Oil Fields projects started in 2006 by Shell and Statoil. CO₂ was captured from a new gas-fired power plant at Tjeldbergodden and was transported to the field via pipeline with distance of 120 km (CO_2 for EOR not commercially viable 2007). The estimated additional oil recovery form CO₂ injection in Draugen field was modest (2-5 %), which could not justify the cost of CO₂ storage (CO₂ for EOR off Norway under study 2007). Feasibility of these projects is being assessed. 2Co Energy is working on the Don Valley project, which captures CO₂ from the Don Valley IGCC power plant and transports it to two mature oil fields in the Central North Sea to improve oil recovery. Economic feasibility is currently in progress (Offshore CO₂ enhanced oil recovery with CCS programs 2023). Miller Oil Field project planned to capture CO₂ from the Peter head gasfired power station for CO₂-EOR in the Miller offshore oilfield. This project was abandoned to due lack of government support (Offshore CO_2 enhanced oil recovery with CCS programs 2023). Two other projects currently on hold in North Sea region are Danish Oil fields, which captures CO_2 from an oil refinery to inject in oil fields in the Danish sector of the North Sea, and Tees Valley, which captures CO_2 from a new IGCC power station to inject to Central North Sea oil fields (Offshore CO_2 enhanced oil recovery with CCS programs 2023).

In Asia, the four-year Dulang CO₂-EOR pilot was successfully completed by Petronas, offshore Malaysia. As the field's produced gas contain a high concentration of CO₂ (more than 50 %) ,the CO₂-rich produced gas was re-injected back into the reservoir, which resulted in significant increased oil production, and reduced the water cut (Offshore CO₂ enhanced oil recovery with CCS programs 2023). The implementation for field scale was recommended, however it has not yet started. Another CO₂-EOR pilot test, conducted on the Rang Dong Field offshore Vietnam in 2011, gained success with 10-15 % increase in oil production without any operational or HSE issues (Ueda 2013). However, CO₂ transportation cost from possible CO₂ sources (fertilizer plant and/or CO₂-rich gas field) were economically detrimental, resulting in project termination.

In offshore Newfoundland and Labrador, Canada, the Net Zero Project explored the feasibility of Carbon Capture, Utilization, and Storage (CCUS) as a comprehensive approach to reducing carbon emissions from four active oilfields and one proposed development site. The project considers capturing CO₂ emissions generated from offshore electrification facilities, including gas and diesel-powered generators, as well as flaring operations. This initiative aligns with global efforts to mitigate greenhouse gas emissions and adapt to stricter environmental regulations by leveraging innovative CCUS technologies to reduce the carbon footprint of offshore oil and gas operations (A Net Zero Project White Paper 2023). The project reflects a broader movement toward integrating CCUS into existing infrastructure to achieve net-zero emissions in oil and gas production, especially in challenging offshore environments.

Offshore CO₂-EOR projects demonstrate technical feasibility, but many have failed due to the high costs associated with sourcing CO₂, especially in regions lacking accessible or nearby CO₂ sources. To address this challenge, small-scale CO₂ capture technologies like membrane systems and compact amine units are being developed. These technologies not only support efforts to achieve net-zero emissions but also help secure CO₂ resources for offshore operations. Successful examples include the Lula Project in Brazil and the Dulang Project in Malaysia, which highlight the potential of innovative capture solutions to overcome logistical and economic barriers. This research examines scenarios involving constrained CO₂ volumes and the implications of different capture techniques, which can yield CO₂ streams with less than 100 % purity. These efforts aim to address supply limitations while optimizing EOR performance. Table 2-5 provides a detailed summary of CO₂ utilization and storage projects in offshore oilfields, offering insights into diverse approaches and outcomes for managing CO₂ resources effectively.

Offshore Project Name	Location	CO ₂ source	Results	Ref
Quarantine Bay	US	N/A	Successful pilot scale. Failed to implement at field scale due to high project costs.	(Hsie 1988)
Timbalier Bay	US	N/A	Successful pilot scale. Failed to implement at field scale due to high project costs.	(Moore 1985)
Bay St. Elaine	US	N/A	Successful pilot scale. Failed to implement at field scale due to high project costs.	(Nute 1983)
Weeks Island	US	N/A	Successful pilot scale. Failed to implement at field scale due to high project costs.	(Johnston 1988)
Paradis	US	Monsanto Co. ammonia plants	Successful pilot scale. Failed to implement at field scale due to high project costs.	(Bears 1984)
Denbury's Gulf Coast	US	Jackson Dome, two existing facilities along the Gulf Coast	In progress, including Hastings and Oyster Bayou fields in Texas, the Heidelberg and Tinsley fields in Mississippi.	(Extensive Experience in the Gulf Coast 2003)
Lula	Brazil	Seawater and the produced or imported gas	In progress. The project was reported to be successful in increasing the recovery factor and reducing 12% in GHG emissions since 2015	(Petrobras Santos Basin 2023)
Gullfaks	Norway	Several options from different sources	Increase of 4.1% of oil in place but the economics were unfavorable for CO ₂ -EOR.	(Augustsson 2004)
Ekofisk	Norway	Sleipner gas field	Demonstrated technical feasibility but have not progressed past the feasibility stage.	(Hustad 2004)

TABLE 2-5: Offshore CO₂ utilization and storage projects

Offshore Project Name	Location	CO ₂ source	Results	Ref
Heidrun	Norway	New gas-fired power plant at Tjeldbergodden	Demonstration the technical feasibility, still under study.	(CO ₂ for EOR not commercially viable 2007, CO ₂ for EOR off Norway under study 2007)
Draugen	Norway	New gas-fired power plant at Tjeldbergodden	Terminated due to the poor profitability of the power plant and the need for substantial support for carbon capture and storage	(Reuters: Statoil, Shell shelve Draugen field CO ₂ injection 2007)
Don Valley	North Sea	Don Valley IGCC power plant	Offshore EOR/Storage feasibility study was completed. However, this project was not received financial support from UK government. 2Co Energy is studying the economic feasibility without government funding.	(Offshore CO_2 enhanced oil recovery with CCS programs 2023)
Miller	North Sea	Peter head gas- fired power station	Failed to receive government support. Abandoned.	(Offshore CO ₂ enhanced oil recovery with CCS programs 2023)
Danish	North Sea	Oil refinery	Maersk Oil submitted a proposal to the EU for capturing of CO_2 . This project is currently on hold.	(Offshore CO ₂ enhanced oil recovery with CCS programs 2023)
Tees Valley	North Sea	New IGCC power station	Progressive Energy submitted a plan to the EU for capturing of CO ₂ . This project is currently on hold.	(Offshore CO ₂ enhanced oil recovery with CCS programs 2023)
Dulang	Malaysia	CO ₂ -rich produced gas	IWAG EOR pilot was successful. Field wide application was recommended but has not been implemented yet.	(Offshore CO ₂ enhanced oil recovery with CCS programs 2023)
Rang Dong	Vietnam	Fertilizer plant and CO ₂ -rich gas field	A small-scale pilot test with 10-15% increase in oil production Detrimental operational cost Termination of the project	(Ueda 2013)
A Net Zero Project	Newfoundland & Labrador, Canada	Gas fired turbines, flaring emissions	Study phase, investigating technical and economic viability of integrating CCUS for 4 producing oil and 1 proposed oil project (Bay du Nord)	(A Net Zero Project White Paper 2023)

The phase behavior of pure CO₂ is significantly influenced by reservoir temperature and pressure. CO₂ transitions to a supercritical state when the pressure and temperature exceed its critical point (31.1°C and 7.38 MPa, respectively). In this state, CO₂ combines properties of both gas and liquid, behaving as a compressible fluid with gas-like viscosity and liquid-like density. Supercritical CO₂ is characterized by unique properties such as low viscosity, low surface tension, high diffusion coefficients, and strong solubility in hydrocarbons, which are advantageous for enhanced oil recovery (EOR). These properties facilitate efficient mixing and displacement of oil within reservoirs. For instance, studies have shown that supercritical CO₂ improves oil recovery in tight reservoirs by enhancing its ability to diffuse and dissolve in hydrocarbons, reducing viscosity, and enabling better mobility within the reservoir matrix (Ding 2013, Zhou 2019). The implications of supercritical CO₂'s behavior are critical for designing EOR strategies, especially in reservoirs with tight formations where maximizing oil recovery requires effective miscibility and efficient displacement mechanisms. A number of researchers have studied the influence of supercritical CO₂ for CO_2 application in oilfield. Supercritical CO_2 was demonstrated to be able to alter the properties of crude oil such as oil expansion, reduction in viscosity, reduction in interfacial tension, etc...., which could result in improvement of oil recovery (Li 2012). Gao (2021) carried out experimental study on supercritical CO₂ in tight conglomerate reservoirs under reservoir conditions (formation pressure 37 MPa, temperature 89 °C). The results found that supercritical CO₂ could improve the oil recovery 4.02 % higher than non-supercritical CO₂. Wei (2020) conducted an experimental study on the effectiveness of supercritical CO₂ injection in an asphaltenic tight sandstone formation. The results indicated that CO₂ injection improved oil recovery; however, it also led to a reduction in rock permeability and porosity due to accelerated precipitation of asphaltenes. This phenomenon can potentially limit the long-term effectiveness of CO₂-EOR in certain reservoir conditions. Zhang (2018) concluded that the interaction among supercritical CO₂-brine-rock altered the wettability of the rock surface to be more water-wet, as well as could improve the connectivity of the tight reservoir rocks, which was favorable for both CO₂-EOR and geological storage. Current carbon capture technologies are not 100 % efficient, resulting in impurities in the CO₂ stream. The impurities and their concentrations vary with separation technology. Some studies provide recommendations on limits to CO₂ impurities for CO₂ utilization and storage purposes. For EOR purpose, 1 % impurities for absorption and adsorption (Wang 2017), 10% impurities for membrane (Barrett 2019), and about 3 % impurities for Direct Air Capture (DAC) (Keith 2018) were considered. These impurities are shown to have significant impact on the minimum miscibility pressure (MMP). It is reported that CH₄ and N₂ increases MMP and others, like C₂H₆ and intermediate hydrocarbons such as propane C₃H₈, butane C₄H₁₀, pentane C₅H₁₂, and CO₂ reduce MMP (Alston 1985, Yellig 1980, Johnannes 2009, Stringht 2009). Developing miscibility (reaching MMP) generally increases oil recovery as capillary pressure is overcome.

When CO₂ contacts oil in a reservoir, the miscibility—whether the two phases can mix—is influenced by the composition of both the CO₂ and the oil, as well as the reservoir's pressure and temperature. If the reservoir pressure is below the Minimum Miscible Pressure (MMP), an immiscible process occurs. In this scenario, the oil is saturated with CO₂, leading to oil phase swelling, where the oil's viscosity is reduced, and lighter hydrocarbons in the oil are extracted into the CO₂ phase. This results in better fluid displacement but does not achieve full miscibility (James ENGI 9113). Typically, first-contact miscibility (where CO₂ and oil immediately mix without needing additional interactions) is not reached in most CO₂-EOR operations. Instead, miscibility forms through a multi-contact process, where CO₂ and oil interact multiple times, allowing the lighter oil fractions to vaporize into the injected CO₂ phase, while CO₂ condenses into the oil. This back-and-forth reduces the viscosity and interfacial tension between the oil and gas, facilitating more efficient oil extraction (Hadlow 1992). Thus, the process of CO₂ injection for enhanced oil

recovery is largely dependent on achieving a balance of pressure and temperature that supports the miscibility of CO₂ with oil, improving oil recovery over time. Figure 2-2 shows the principle of miscible CO₂-EOR.



FIGURE 2-2: Principle of miscible CO₂-EOR

Operating an offshore CO₂-EOR at any scale is always associated with some challenges. The availability of CO₂ is always the main concern when considering CO₂-EOR offshore as there are not many developed sources of CO₂ close to offshore fields. CO₂ from several sources is collected and transported to a number of oil fields (Holt 2009, Kemp 2013, Malone 2014). Thus, investment is required to build infrastructure for transportation adding to the project cost. It is worth mentioning uncertainties around regulations regarding monitoring injected CO₂, during and especially after closure. The price of oil and CO₂ emission taxes add to the project economic uncertainties. Technically, in the presence of water, CO₂ will react and form carbonic acid, which can react with certain minerals and clays. For example, carbonic acid can dissolve calcium carbonate which may re-precipitate and deposit elsewhere in the reservoir, changing the permeability or porosity, altering fracture properties, changing the wettability, and flow behaviour temporally. Carbonic acid can also cause pipeline corrosion. Thus, materials selection is the key parameter in the practical design and operation of CCS system. The complete stream compositions and the full range of operating conditions need to be determined in order to select the material.

Some materials were considered for specific CCS application areas such as carbon steels, duplex stainless steels, Nickel alloys were recommended for the locations where wet CO₂ would encounter (Corrosion and materials selection in CCS system 2010). However, carbon steel was not an adequate material in the upstream of absorbers in post combustion plant because of the presence of sulphur, nitrogen oxides and chlorides in the water phase (Corrosion and materials selection in CCS system 2010). CO₂ injection has low volumetric sweep efficiency due to the high CO₂ mobility (Patel 1987). This can lead to fingering, gravity segregation, and early breakthrough in the production well, especially challenging in fractured reservoirs.

Different techniques such as Water-Alternating-Gas (WAG) injection and carbonated water injection (CWI) can mitigate some of these challenges such as sweep, constrained volumes, etc. In WAG process, CO₂ and water are injected alternatively, thus enhance oil recovery has poor sweep efficiency. This can be improved by using a WAG process; the oil recovery factor can be increased by enhancing the microscopic efficiency of gas injection together with the macroscopic efficiency of water flooding. Ghomian (2008) integrated hysteresis effect when coupling CO₂-EOR and storage. The models were built with three different relative permeability and capillary pressure models for three different rock types. Sixteen runs were performed varying WAG ratio, CO₂ slug size, and reservoir heterogeneity characteristics such as Dykstra-Parson coefficient for a crosssectional model of a sandstone reservoir. The NPV value, which took in account of oil price as well as CO₂ price, tax rate, tax credit, was calculated for each scenario. The simulation results showed that oil recovery increased with applying a hysteresis model. Hysteresis was proved to have a significant effect on CO_2 storage and oil recovery factor as it managed trapping the CO_2 in the reservoir as residual gas as well as it affected the relative permeabilities leading to improvement in the sweep efficiency. They also found that Dykstra-Parsons coefficient, combination of WAG ration and slug size, and slug size by itself were reported the most to least influential factors for oil recovery factor. Related to CO₂ storage objective, WAG ratio was announced to have the most influence, followed by combination of WAG ratio and hysteresis, then hysteresis by itself. CO2 storage was greater for oil reservoirs with low heterogeneity and low WAG ratio and CO₂ slug sizes. In contrast, the NPV expected for oil reservoirs is better with high WAG ratio, large CO2 slug sizes, and low heterogeneity. Jahangiri (2012) used ensemble-based optimization (EnOpt) algorithm to co-optimize CO₂ storage and EOR. The net present value (NPV) of the project was set as the optimization objective function, whereas the well injection patterns and rates were placed as the controlling variables. The results showed that pulse-shaped injection profiles provided better efficiency for CO₂ flooding. Additionally, different economic conditions, such as oil price and CO₂ tax credit, had influence on the NPV as well as optimized injection profile. Wei (2021) carried out experimental and simulation studies on associated CCS and EOR in a low permeability (1.16 mD) reservoir. The comparison was carried out for water flooding, CO₂ flooding, WAG, surfactantalternating-gas (SAG) and surfactant-assisted water flooding through core drainage experiments as well as nuclear magnetic resonance spectroscopy (NMR) equipment. ECLIPSE 300 was used for field simulation. SAG was found to give the highest oil recovery among studied EOR methods since it showed capacity to displace the oil inside the smaller pores as well as larger pores in a higher proportion. The optimal WAG and SAG ratios obtained from core experiments were lower than ones in the realistic reservoir. Kovscek (2005) used an objective function combining dimensionless oil recovery and CO_2 storage, which were considered as equal in importance by using equal weightings in the equation. The objective was to find injection scenarios that lead to maximum oil recovery and maximum emplacement of CO₂ in the reservoir by performing simulations for variety of injection schemes. CO₂ stored within the reservoir didn't reach the maximum for CO₂ injection, WAG, and gas after water (GAW). The most successful strategy for co-optimization was well control process with producing gas-oil ratio (GOR) and the injection pressure as control parameters.

Lee (2021) conducted a 2D compositional simulation of WAG injection to analyze the effect of impure CO_2 on EOR and CCS performance. The composition of the gas obtained from the oxyfuel scenario with the lowest CO₂ purity level was used in their study. Two injection cases were analyzed: 100% CO₂ and 85 % CO₂ + 15 % impurities (including O₂, N₂, Ar, H₂O, NO_x, SO₂, SO₃ and CO). The results showed that impurities in CO₂ reduced oil recovery by 9.2 % and total CCS performance by 4.3 %. Cho (2021) investigated the effects of CO₂-CH₄ WAG on performance of coupled EOR and CO₂ storage considering asphaltene deposition. In order to evaluate formation damage by asphaltene deposition, this study investigated absolute permeability reduction, porosity reduction, and wettability alteration. The results revealed that in comparison with using 100 % CO₂, addition of CH₄ would lower asphaltene deposition and increase gas mobility. Thus CO₂-CH₄ WAG achieved 118 % overall carbon sequestration higher than for CO₂-WAG. Additionally, pressure maintenance could be improved by injecting more water, which then improved both EOR and CSS. Wang (2015) studied the impact of impurities (N₂, O₂, Ar and SO₂) on the storage capacity of CO₂ in geological formations through density changes experimentally and analytically. Three mixtures were employed: CO₂ with 6.03 mol% O₂, 5 mol% Ar and 4.5 mol% N₂, CO₂ with 15 mol% Ar, CO₂ with 2.5 mol% SO₂. The results indicated that the storage capacity for CO₂ could reduce by over 65 % for mixture of CO₂ and 15 mol% N₂, O₂ and Ar. Additionally, the reduction in storage capacity decreases with increasing temperature. Membrane separation process was chosen in this study as explained further in Methodology session. CH₄ was the mainly impurity found in natural gas source (Pham 2021). Based on these results, enriched CO₂-WAG (CH₄/CO₂-WAG) was chosen to be investigated in this study.

Carbonated water injection (CWI) was first introduced in the late 1940s as an improved EOR method as well as a safe storage strategy to reduce the level of greenhouse gases in the atmosphere. CWI is considered as a potential CO_2 -EOR method that can be used for cases with limited CO_2 supply, i.e. CO₂ captured from offshore platforms or other small point sources. CWI involves dissolving CO₂ into the water and injecting the carbonated water into the reservoir. The dissolved CO₂ easily comes in contact with the trapped residual oil, which reduces the oil viscosity, lowers the oil water IFT, and causes oil swelling, hence results in higher incremental oil recovery in comparison with conventional water injection. Esene (2019) performed a simulation study to investigate the oil recovery amount, fluid distribution, and effects of operational parameters and well placement on the performance of CWI. A 3-D heterogenous reservoir model was developed using the experimental data from literature. The results showed that CWI achieved a higher recovery factor then plain water flooding since the mass transfer associated with CWI would cause oil swelling, thus improve the mobility ratio and sweep efficiency. Also, an optimum injector rate would ensure an effective mass transfer across phases, and an optimum well orientation would enhance recovery performance during CWI. Esene (2020) carried out other study to examine the effects of operational parameters/conditions and rock dissolution during CWI in core scale. The simulation results showed that increasing the injection rate from 0.2 cm³/min to 0.8 cm³/min led to an additional 6% oil recovery. Furthermore, increasing the injection pressure from 1,500 psi to 3,500 psi improved the oil recovery factor by 16 %, as more CO₂ dissolved into the resident fluid, enhancing miscibility and oil extraction efficiency. Sohrabi (2011) conducted carbonated water flooding experiments and found that CWI achieved higher oil recovery factor compared to conventional water injection. Grogan (1987) through simulation concluded that by allowing sufficient time, the oil production can increase due to the increase of mobility of the diffusion of CO₂ into oil. Mosavat (2014) conducted sand back flooding experiments to investigate the CO₂ storage capacity of CWI. The results showed that no more CO₂ could be stored after 1 PV injection since the porous medium reached its maximum capacity at working conditions. In other hand, the CO₂ storage capacity increased with increased pressure due to increased solubility of CO₂ in water. Mosavat (2016) performed experimental work on the wettability alteration during CWI process. It found that CWI recovered additional 7.3 % in comparison with water flooding operation. It was reported that CWI modified the wettability of the formation from oil-wet to mixed or water-wet condition, which improved the oil recovery.

Combining CCS and EOR involves nonlinear equations as well as many known and unknown interactions between different parameters, such as the injected gas, reservoir characteristics, wells patterns, etc. Permeability heterogeneity and reservoir stratification influence flow characteristics and oil recovery, especially when a reservoir is produced through gas injection or WAG displacement process related to stability of flood front (Figuera 2014). Stratified reservoirs may have communication across layers (crossflow) or not (without crossflow), depending on the geology. Ngo (2023) optimized the well completion strategy for double displacement process and WAG injection in a dipping stratified reservoir. The results indicated that bottom-up was effective completion strategy for WAG up-dip in stratified reservoirs without zonal communication and topdown was a successful completion strategy for communicating stratified reservoirs. Claridge (1982)'s work showed that the extent of crossflow can cause a substantial reduction in oil recovery. Kulkarni (2003) indicated that the crossflow could adversely affect the recovery performance, however the crossflow may also improve the vertical sweep efficiency. Thus, the communication among layers plays an important role in the performance, which needs to be considered when studying stratified reservoirs

<u>Conclusion</u>: In all the studies mentioned above, the volume of CO_2 is typically not constrained. However, when considering offshore reservoirs, limitations on CO_2 supply must be addressed, as the available volume may not be sufficient for full-field application. Additionally, to meet sustainability goals and avoid venting CO₂ into the atmosphere, solutions like gas purification and the reinjection of CO₂-rich streams are proposed. Unlike previous research, which does not account for permeability heterogeneity or reservoir stratification, this study focuses on optimizing the joint application of Carbon Capture and Storage (CCS) and CO₂-EOR (including CO₂-WAG, enriched CO₂-WAG, and CWI) in stratified reservoirs, considering both crossflow and no-crossflow scenarios with limited CO₂. The CO₂ is assumed to be captured from post-combustion emissions from offshore power generation using membrane separation technology. This study aims to generalize findings for offshore reservoirs, encompassing a wide range of reservoir characteristics (e.g., temperature, pressure, permeability), oil types, and injected gas compositions and volumes.

Chapter 3 : CONSIDERING THE CO₂ SOURCE AND CAPTURE TECHNIQUE TO REDUCE MMP FOR ENRICHED WAG INJECTION

Preface

A version of this chapter has been published in peer reviewed conference paper: Pham, Q.C and James, L.A. 2021. Considering the CO₂ Source and Capture Technique to Reduce Minimum Miscibility Pressure (MMP) for Enriched Water Alternating Gas (WAG) Injection. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30. https://doi.org/10.1115/OMAE2021-62643. I am the primary author. Co-author Dr. Lesley James is senior supervisor. Dr. James reviewed, provided technical assistance and valuable insights to improve the paper concept.

1. Introduction

The oil and gas industry are both a major source of CO_2 emissions but can play a role in carbon capture and storage (CCS) as well. CO_2 can be stored in depleted reservoirs and/or CO_2 can be used to enhance oil recovery recuing the carbon footprint of upstream operations. CO_2 injection can drive the isolated oil from the reservoir by reducing the interfacial tension between the oil and the reservoir rock, and by lowering the oil viscosity. Thus, CO_2 injection can increase oil production in addition to storing CO_2 . CO_2 can be extracted either from flue gas or natural gas by different methods. Current CO_2 capture technologies are not 100% efficient and achieving a high CO_2 purity is costly and time-consuming; hence, impurities are often found in the CO_2 stream source. The CO₂ capture storage projects are not new. Some projects of interest are reviewed below. Norway has been storing CO₂ stripped from high concentration natural gas for 20+ years at the Snøhvit and Sleipner fields. The Northern Lights project started in 2020 will capture CO₂ from an onshore cement and waste facility, transport it via ship and pipeline to inject, and store the CO₂ in the Aurora field (Equinor ASA). Norway has become the second largest exporter of natural gas in the world, but 25 fields have a CO₂ concentration above 5%, and eight of these fields have CO₂ concentration higher than 10% requiring that the natural gas be stripped of CO₂ to not exceed 2.5 % CO₂ for pipeline quality standards (Marit 2014). However, to the best of our knowledge CO₂ has not been used for EOR offshore Norway.

Gulf of Mexico (GoM) is the major source of oil and natural gas in the United States. The use of CO₂-EOR has become a priority for many mature GoM oil fields to extend production and store CO₂. Electric power and industrial plants along the Gulf Coast are estimated to produce enough CO₂ for 40 years of CO₂-EOR (Riestenberg 2019). The West Hasting field injects CO₂ captured from a hydrogen production facility in Port Arthur. CO₂ captured from NRG's Parish Power Plant is injected into the West Ranch oil field (Lopez 2019). The main CO₂ source employed in Weyburn and Midale oil fields, Canada, come from post-combustion capture from synthetic natural gas produced by a coal gasification process (Weyburn -Midale Carbone Dioxide Project).

Post-combustion CO₂ can be separated from other gases using absorption, adsorption, membrane separation, and other novel techniques with varying CO₂ capture selectivity and efficiency. Impurities in the resulting CO₂ stream significantly affect the Minimum Miscibility Pressure (MMP); for example, SO₂ and H₂S can reduce the CO₂ MMP, whereas N₂ and O₂ can have the opposite effect (Zhang 2004). MMP is the pressure at which gas and oil are miscible, and oil recovery can be substantially enhanced if MMP is reached. Miscibility helps increase incremental oil recovery by theoretically reducing interfacial tension to zero, reducing the capillary pressure to

zero, and enabling the possibility of recovering oil from all pores. Therefore, a combination of CO_2 and produced natural gas is considered a favorable candidate for increasing oil production in offshore Newfoundland. In recent work, mixtures of CO_2 and other gases (e.g., CH₄, C_2H_6 , C_3H_8 , N_2 , O_2) have been investigated to determine their effect on MMP. A few studies considered a mixture of CO_2 and natural gas, but most did not evaluate the effect of impurities from the CO_2 stream, which may undermine the success of CO_2 projects. Furthermore, most slimtube experiments focus on CO_2 concentration less than 5 % or pure CO_2 . This current work investigates the influence of mixing produced gas with CO_2 on MMP over a wide range of CO_2 concentrations (from 0 to 100 %) and considers impurities from different CO_2 sources and capture techniques for crude oil representative of the Hibernia Field, offshore Newfoundland, Canada using slimtube simulation. The methods to determine MMP are also analyzed in order to identify the uncertainty related to each method. The workflow is shown in Figure 3-1. The two first steps are adopted from literature and the simulation through PVT-sim software is used to complete the study.



FIGURE 3-1: Workflow for evaluating CO₂ source and capture techniques to reduce MMP

2. Literature review

The literature review is presented and updated in the Chapter 2 part 1 and part 2.

3. Slimtube simulation

The slimtube simulation is a critical technique for determining the Minimum Miscibility Pressure (MMP) in gas injection enhanced oil recovery (EOR) processes. It is based on a simplified yet powerful representation of fluid dynamics and phase behavior in a reservoir. Below is an overview of the governing equations and methodology for slimtube simulations, typically implemented under the following assumptions:

- Homogeneous Porous Medium: The slimtube is modeled as a uniform porous medium with consistent porosity and permeability.
- Isothermal Conditions: The simulation assumes constant temperature unless thermal effects are explicitly included.
- Negligible Capillary and Gravity Effects: These are considered negligible due to the small diameter and orientation of the slimtube.

Governing equations for Multiphase Flow in Slimtube simulation (Orr 2007, Soave 1972)

• Mass Conservation: The mass of each component i in each phase α is conserved:

$$\frac{\partial(\phi\rho_{\alpha}S_{\alpha})}{\partial t} + \nabla . (\rho_{\alpha}S_{\alpha}v_{\alpha}) = q_{\alpha}$$

φ: porosity of the slimtube

- ρ_{α} : density of phase α
- $S_{\alpha\,:}\, saturation$ of phase α
- v_{α} : velocity of phase α
- q_{α} : source/sink term of phase α

• Darcy's Law: Describes fluid flow through porous media:

$$v_{\alpha} = -\frac{kk_{r\alpha}}{\mu_{\alpha}} \left(\nabla P - \rho_{\alpha} g \nabla z \right)$$

k: absolute permeability of the porous medium

 $k_{r\alpha\,:}$ relative permeability of phase α

 $\mu_{\alpha\,:}$ viscosity of phase α

 P_{α} : pressure of phase α

g : gravitational acceleration

- z: depth or vertical position
- Phase Equilibrium: Components partition between gas and liquid phases based on equilibrium constants:

$$K_i = \frac{y_i}{x_i}$$

Ki : Equilibrium constant of component i

 y_i : mole fraction of component i in the gas phase

xi: mole fraction of component i in the liquid phase

• Equation of State (EOS): SPK-Peneloux EOS Equation is used in this study

$$P = \frac{RT}{(v-b)-c} - \frac{a}{(v-c)(v+b-c)}$$

P: pressure

T: temperature

- v : molar volume
- R: universal gas constant
- a: attraction parameter
- b: repulsion (co-volume) parameter

c: Peneloux volume correction term

Parameters in the SPK-Peneloux EOS:

Attraction parameter:

$$a = 0.42748 \frac{R^2 T_c^2}{P_c} \left(1 + m \left(1 - \sqrt{T_r}\right)\right)^2$$

- T_c: critical temperature of the component
- P_c: critical pressure of the component
- T_r: reduced temperature
- m : acentric factor correction term

Repulsion parameter:

$$b = 0.08664 \frac{RT_c}{P_c}$$

Peneloux volume correction

$$c = \frac{Z_c R T_c}{P_c} (1 - density \ correction \ factor)$$

Z_c: critical compressibility factor

The density correction factor is derived from experimental data to improve liquid density predictions.

• Component Transport: The transport of each component iii in the reservoir is governed by:

$$\frac{\partial(\emptyset C_i)}{\partial t} + \nabla . (vC_i) = R_i$$

C_i: molar concentration of component i

R_i: reaction or mass transfer rate

The slimtube simulation methodology involves fluid characterization, where fluid compositions and thermodynamic properties are input into software like PVTsim, with experimental PVT data used to calibrate the Equation of State (EOS). The simulation initializes by saturating the slimtube with oil and setting boundary conditions, reservoir properties (e.g., porosity, permeability), and gas injection parameters. Gas is incrementally injected at increasing pressures, and phase behavior is evaluated at each step to plot recovery factors against pressure for Minimum Miscibility Pressure (MMP) determination. Numerical solvers compute phase compositions, saturations, and recovery factors, while flash calculations identify equilibrium states at each grid block. The MMP is determined as the pressure at which miscibility is achieved, indicated by a sharp increase in recovery or complete phase blending.

Prior to performing the slimtube simulation, the range of MMP for each mixture was predicted using the Multiple Contact Miscibility (MCM) module. Consequently, at least three points above and below the MMP are estimated, to obtain more accurate lines and a more accurate intersection point. MCM simulation provides results quickly compared to slimtube simulation. This step reduces time in simulating the wrong pressure points. Knowing the MMP range for each mixture, the MMP for various CO₂ concentrations from different capture methods and different CO₂ stream sources were then determined through slimtube simulation. The oil recovery was measured at eight different pressures. The MMP is defined as the point where the curve of oil recovery versus pressure changes direction. For each gas/oil system, the MMP was evaluated three times by varying the points in two lines. The mean value and the standard deviation were calculated.

The slimtube simulation, using PVTsim - a reservoir simulation software developed by Calsep, was first completed with various gas and oil compositions from the literature to test its validity. The MMP from slimtube measurements reported for three gas/oil systems in the literature used are: 466 bar at 138.9 °C, 274 bar at 121.1 °C, and 326 bar at 91.1 °C (Firoozabadi 1986). The simulation utilized the Soave–Redlich–Kwong Peneloux (SRK Peneloux) EOS, injecting 1.2 pore volumes of gas to assess phase behavior and miscibility pressure. The SRK Peneloux EOS is widely recognized

for its advantages in reservoir simulations and PVT studies. Its density correction effectively addresses the liquid density inaccuracies inherent in the standard SRK EOS, which is critical in simulations like slimtube tests, where accurate density calculations influence phase behavior and miscibility (Amao 2014). Additionally, it maintains the robust thermodynamic framework of SRK while improving liquid and gas phase accuracy, as supported by recent findings (Sun 2022). The model ensures consistency in phase equilibrium across diverse conditions. The SRK-Peneloux EOS is particularly effective in systems where accurate liquid density is crucial, such as in reservoir simulation and phase behavior modeling of oil reservoirs. It has been shown to perform better than PR EOS for certain hydrocarbon mixtures, where liquid phase behavior predictions are challenging (Pedersen, 2006). Unlike the Peng-Robinson EOS (PR EOS), which often underestimates liquid densities, the SRK-Peneloux EOS incorporates a volume correction term, ensuring better accuracy in predicting liquid phase densities for both pure components and mixtures. This volume consistency reduces errors in phase equilibrium calculations, making it highly reliable for both single-component and multi-component systems (Peneloux, 1982). Additionally, the SRK-Peneloux EOS retains the computational simplicity of the original SRK EOS while significantly enhancing its precision. This combination of efficiency and accuracy makes it particularly suitable for reservoir simulation tools like PVTsim, where computational performance and model reliability are critical. Figure 5 shows how MMP is determined through slimtube simulation and Table 3-1 presents the literature value, simulated value, and relative error. The results from the slimtube simulation have a relative error less than 8% compared to the experimental values, demonstrating a close match between the experimental and simulated MMP measurements.







FIGURE 3-2: Comparison of MMP determination through slimtube simulation (our work) and experiments (Savage 2004)

Gas/Oil System	Simulated [] MMP (bar)	Mean St MMP (bar) de	andard eviation (bar)	Experimental MMP (bar)	Absolute Relative error (%)
1	432	433	1.91	466	7.15
	437				
	429				
2	278	278	1.19	274	1.58
	281				
	276				
3	350	347	1.41	326	6.44
	347				
	344				

TABLE 3-1: Experimental (Savage 2004) and simulated MMP

Crude oil and produced gas from the Hibernia Field, offshore Newfoundland, Canada was employed at reservoir temperature of 99 °C. The gas mixture composition was calculated based on each capture method before simulating. The amount of CO₂ added to the natural gas varied from 0 to 100 %, with and without impurities. The oil was first tuned to match with critical temperature and critical pressure. It was then simulated with the different gas mixtures to determine MMP. SRK Peneloux EOS, 2000 number of cells, and 4000 number of time steps were used in the simulations. 1.2 pore volumes of gas were injected. Five gas mixtures were simulated. Mixtures were the combination of natural gas produced from Hibernia with: i) pure CO₂; ii) CO₂ captured by adsorption and absorption capture from natural gas (1 % CH₄ impurity); iii) CO₂ captured by adsorption and absorption capture from flue gas (1 % N₂ impurity); iv) CO₂ captured by membrane technology from a natural gas source (10 % CH₄), and v) CO₂ captured by membrane technology from a flue gas source (8 % N₂ and 2 % O₂). Each MMP was evaluated three times to obtain the standard deviation value. Simulation details are shown in Table 3-2.

 TABLE 3-2: Slimtube simulation parameters

Simulation Parameter	Fluids used
• 2000 cells	Hibernia crude oil
• 4000 timesteps	• Gas mixture: Hibernia produced gas mix with:
SPK Peneloux EOS	i. Pure CO_2
 1.2 pore volumes injected Reservoir temperature 99°C 	natural gas
	iii. CO ₂ captured by adsorption and absorption capture from flue gas
	iv. CO_2 captured by membrane technology from natural gas
	v. CO_2 captured by membrane technology from flue gas

4. Results and Discussion

The standard deviation value for MMP is calculated around 45 psia. Figure 5 presents the results for mixtures of natural gas with pure CO₂, and with CO₂ sourced from adsorption and absorption. The CO₂ captured by adsorption/absorption technology from a natural gas source contains 1 % CH₄, and the CO₂ captured from a flue gas source has 1 % N₂. This figure presents the MMP calculated by the slimtube simulations and the decrease in MMP compared to simple natural gas injection. The MMP reduction was calculated based on the MMP estimated for natural gas only, using the equation (1):

$$MMP_{reduction} = \left[\frac{MMP (NG) - MMP (NG \text{ with } CO_2)}{MMP (NG)}\right] 100\%$$
(1)
The MMP variation was calculated based on the MMP estimated for mixture of natural gas and pure CO₂ with oil, using the equation (2):

$$MMP_{variation} = \left[\frac{MMP (NG with CO_2) - MMP(NG with impure CO_2)}{MMP (NG with CO_2)}\right] 100\%$$
(2)

As shown in Figure 3-3, the addition of 10% CO₂ to the gas mixture does not significantly impact the MMP compared to natural gas injection. This is because the proportion of CO₂ is relatively low, and at such a low concentration, its effect on the miscibility of the gas mixture with the oil is minimal. The results become more pronounced as the percentage of CO₂ in the gas mixture increases. This behavior is expected, as CO₂ plays a critical role in enhancing the miscibility of the injected gas with the oil. Since CO₂ requires a much lower pressure to achieve miscibility compared to natural gas, its addition reduces the MMP, thereby making it easier for the CO₂ to mix with the oil and improve oil recovery. Moreover, the presence of CO₂ also impacts sweep efficiency, which is the ability of the injected fluid to displace oil from the reservoir. CO₂, especially in higher concentrations, enhances sweep efficiency by promoting gravity segregation. This is more effective in the water saturation zone than in the oil saturation zone, as CO₂ tends to migrate upwards due to its lower density compared to the oil, thus improving the displacement of oil and reducing the MMP. The significance of CO₂ in improving oil recovery is evident from the reduction in MMP: a 30% reduction when the gas mixture contains 50% CO₂, a 40% reduction when the mixture is 70% CO₂, and a 50% reduction with pure CO₂ injection. The impact of impurities in CO₂ on MMP is also an interesting finding. Although numerical results show a slight increase (about 1%) in MMP with the presence of impurities (e.g., CH₄ or N₂) in the CO₂ stream, this difference is not easily discernible in the graph. This suggests that, while impurities do affect the MMP, their influence is minimal compared to the effect of increasing CO₂ concentration. It highlights that even with impurities in the CO_2 , the ability of CO_2 to enhance miscibility and oil recovery remains significant.

Finally, under the reservoir conditions of 4503.7 psia at 99°C, at least 70% CO₂ is required in the gas mixture to achieve miscibility with Hibernia oil, whether the CO₂ is pure or sourced from adsorption and absorption technologies. This threshold is important for designing CO₂ injection strategies, as it indicates the minimum concentration of CO₂ necessary for effective miscibility and, by extension, enhanced oil recovery. The study also points to the viability of CO₂ captured from various sources, including natural gas, flue gas, and post-combustion sources, even if these gases contain minor impurities, without significantly compromising the MMP and the overall efficiency of CO₂-EOR methods.



FIGURE 3-3: Simulated MMP of CO₂-natural gas mixture (pure CO₂ and CO₂ from adsorption/absorption capture)

Figures 3-4 and 3-5 provide detailed insights into the effect of impurities in CO₂ on the minimum miscibility pressure (MMP) for various gas mixtures, highlighting the differences between CO₂ captured from natural gas and flue gas sources. These results are crucial for understanding how impurities, particularly methane (CH₄), nitrogen (N₂), and oxygen (O₂), influence the performance of CO₂-enhanced oil recovery (EOR) processes. In both figures, the relationship between CO₂

concentration in the mixture and MMP reduction is observed. The figure shows that, when 10% CO₂ is added to the gas mixture, there is little to no noticeable change in MMP, indicating that such a small proportion of CO₂ does not significantly affect the miscibility of the mixture. This confirms that the amount of CO₂ injected needs to be substantial for it to meaningfully reduce MMP and achieve miscibility with oil.

When CO₂ captured from natural gas, which contains 10% CH₄ impurity, is used in the mixture, the MMP increases only slightly, by around 1-7%, as the CO₂ concentration rises from 10% to 100%. This steady, but gradual change in MMP can be attributed to the fact that CH₄, while a relatively minor impurity in the mixture, still reduces the efficiency of CO₂ in achieving miscibility, though not drastically. CH₄ has a lower solubility in oil compared to CO₂, which slightly affects the CO₂'s ability to mix with the oil, but the overall impact is minimal until higher concentrations of CO₂ are used. The graph also shows a change in the slope of MMP reduction around the 70% CO₂ mark, which signifies the optimal concentration for achieving the best miscibility and oil recovery efficiency.

In stark contrast, when CO₂ captured from flue gas, containing 8% N₂ and 2% O₂, is used in the mixture, the MMP shows a more pronounced change, varying between 6% and 30%. This dramatic difference is primarily due to the higher impurity levels in the CO₂, especially N₂, which significantly alters the behavior of the gas mixture. N₂, which is less miscible with oil than CO₂, increases the required pressure for miscibility and reduces the solubility and diffusivity of CO₂ in the oil. This leads to a higher MMP and ultimately makes it more difficult for CO₂ to mix with oil at lower concentrations. As shown in the figures, when the CO₂ content reaches 60%, the MMP reduction becomes more rapid, and at 100% CO₂, the reduction reaches a maximum of 35%. However, the MMP reduction slows down significantly after this point, highlighting that higher CO₂ concentrations yield diminishing returns in terms of reducing MMP. The optimum

concentration for CO₂ from flue gas sources appears to be around 60%, after which increasing the CO₂ concentration further does not drastically improve the miscibility conditions.

The presence of methane (CH₄) in CO₂ captured from natural gas has a minimal impact on minimum miscibility pressure (MMP), with a slight increase in MMP as CO₂ concentration rises, indicating that CH₄'s effect on CO₂ miscibility is relatively minor at low concentrations. In contrast, nitrogen (N₂) and oxygen (O₂) impurities in CO₂ captured from flue gas significantly affect MMP by increasing the required pressure for CO₂ miscibility, as N₂ has a lower solubility in oil, reducing CO₂ injection efficiency and making it more challenging to achieve miscibility at lower CO₂ concentrations. This means that CO₂ from natural gas, even with some CH₄ impurity, can be used effectively for enhanced oil recovery (EOR) with minimal adjustments, while CO₂ from flue gas requires higher concentrations (80-100%) to reach the same level of miscibility, limiting flexibility in EOR operations.



FIGURE 3-4: Simulated MMP of CO₂-natural gas mixture (pure CO₂ and CO₂ from membrane capture)



FIGURE 3-5: Variation in MMP comparing 10% CH₄ and 10% N₂+O₂ (natural gas vs flue gas for membrane technology)

This study provides a comprehensive analysis of how CO₂ source and capture techniques influence Minimum Miscibility Pressure (MMP) in Enriched Water-Alternating-Gas (WAG) injection processes, particularly in the context of CO₂ supply limitations and their potential impacts on offshore Newfoundland reservoirs, such as Hibernia. A key aspect of this research is its focus on how varying CO₂ concentrations and impurity levels in the injected gas affect the MMP, which is crucial for optimizing enhanced oil recovery (EOR) processes. The results reveal that CO₂ concentrations below 10 % have negligible impacts on MMP, which aligns with expectations as the small amount of CO₂ in the mixture is insufficient to alter the miscibility pressure significantly. However, as CO₂ concentrations increase, the reduction in MMP becomes more pronounced due to CO₂'s inherently lower miscibility pressure compared to natural gas, which requires higher pressures for miscibility with crude oil. The study shows that pure CO₂ injection can lead to a substantial reduction in MMP, up to 50 %, highlighting CO₂'s effectiveness in lowering pressure requirements for achieving miscibility. When impurities are introduced into the CO₂ mixture, the impact on MMP becomes more complex. For example, CO₂ captured from natural gas, containing 10 % CH₄, has minimal impact on MMP, with variations of only 1–7 %. This small variation can be attributed to the similar miscibility characteristics of CO₂ and CH₄, which do not significantly alter the pressure needed for miscibility. In contrast, CO₂ sourced from flue gas, with 8% N₂ and 2 % O₂ impurities, leads to a notable increase in MMP, up to 30 %. The higher miscibility pressure of N₂, coupled with its detrimental effects on CO₂ solubility and diffusivity in oil, drives this increase. N₂ reduces the ability of CO₂ to dissolve in the oil phase, thereby hindering the miscibility process. These findings underscore the importance of carefully considering the composition of CO₂ streams, particularly in offshore operations such as Hibernia, where post-combustion CO₂ streams, typically rich in N₂, will be a significant source of CO₂ for EOR applications. Understanding the effects of impurities, especially N₂, is crucial for designing effective CO₂ injection strategies and ensuring that miscibility conditions are met for optimal oil recovery.

The study's identification of critical thresholds for achieving miscibility in Enriched Water-Alternating-Gas (WAG) injection processes offers key insights into the feasibility of CO₂enhanced oil recovery (EOR) in various scenarios. Specifically, the research indicates that pure CO₂ and CO₂ from adsorption or absorption processes require a minimum of 70 % CO₂ in the mixture to achieve miscibility under reservoir conditions. This contrasts with CO₂ mixtures containing 80% CO₂ from natural gas with CH₄ impurities, which still show a viable path to miscibility, but with less efficiency. Importantly, CO₂ sourced from flue gas, even at high concentrations, fails to achieve miscibility under typical reservoir conditions. This highlights a significant limitation for using CO₂ from flue gas for EOR, particularly in offshore applications like Newfoundland, where CO₂ capture will likely involve post-combustion emissions with significant levels of N₂ impurities. The threshold findings emphasize the critical role of CO₂ purity in achieving optimal miscibility conditions and underline the necessity of incorporating CO₂ composition into planning and strategy for offshore EOR projects.

The research also reveals important patterns in MMP reduction, particularly with the slope changes in the reduction curves. At around 70 % CO₂ for pure CO₂ injections and 60 % for flue gas-derived CO_2 , these slope changes act as key indicators for optimizing CO_2 mixtures to reach miscibility efficiently. These thresholds are not only of technical significance but offer practical guidance for operators when adjusting injection strategies, thus improving the overall efficiency of EOR operations. The novelty of this study lies in addressing the challenge of limited CO₂ supply, a significant constraint for many EOR projects. The research builds on lessons from previous unsuccessful CO₂-EOR projects, such as those in Denmark and Norway, where insufficient CO₂ availability prevented successful implementation (Carbon capture, utilization and storage: We're sending carbon back where it came from 2021). By introducing the concept of Enriched WAG injection, where CO₂ is combined with natural gas to meet miscibility requirements, the study proposes a solution to the resource constraint issue. This combination allows for more flexible and sustainable CO₂ management, particularly in regions where CO₂ sources are limited or expensive. This research underscores the critical role that CO₂ purity plays in enhancing the efficiency of enhanced oil recovery (EOR) strategies, particularly in regions like Newfoundland, where offshore facilities typically rely on CO₂ from post-combustion sources. As CO₂-EOR becomes a more viable strategy, it is essential to account for the impact of CO₂ impurities on miscibility dynamics, which can significantly affect recovery outcomes. The study provides valuable insights into managing CO₂ mixtures effectively, offering guidelines for optimizing injection strategies and maximizing recovery potential while minimizing the challenges posed by CO₂ impurities. Specifically, it highlights how CO₂ from different sources (natural gas, flue gas, and post-combustion) affects miscibility and EOR efficiency. These findings offer actionable insights for immediate application in projects like Hibernia, while also contributing to broader efforts to advance carbon utilization as part of the global energy transition. By reducing the reliance on pure CO_2 and optimizing CO_2 -EOR methods, this research presents a pathway for improving oil recovery and advancing carbon management, even under constrained CO_2 availability. Ultimately, this study represents a significant step forward in enabling more efficient use of CO_2 in offshore reservoirs and contributes to the goal of reducing carbon emissions through improved carbon capture, utilization, and storage (CCUS) strategies.

5. Conclusion

A comprehensive literature review was conducted to examine CO₂ capture technologies and their impact on CO₂ mixtures and Minimum Miscibility Pressure (MMP). A slimtube simulation was performed using PVTsim software, utilizing crude oil and produced gas samples from the Hibernia Field offshore Newfoundland, Canada, and varying CO₂ concentrations ranging from 0 to 100 mol%. The key findings from the simulation and analysis are as follows:

- Adsorption and absorption technologies were found to capture CO₂ with higher purity than membrane technology.
- The impurities in CO₂ depend on the source: methane (CH₄) is typically present in CO₂ from natural gas streams, while oxygen (O₂) and nitrogen (N₂) are common in CO₂ from flue gas streams.
- Mixtures of CO₂ and natural gas were shown to be effective in reducing MMP, enhancing the potential for miscibility.
- No significant change in MMP was observed when CO₂ concentrations were less than 10%.
- Under reservoir conditions, miscibility could be achieved with 70 % CO₂ in the gas mixture for both pure CO₂ and CO₂ sourced from adsorption and absorption technologies. However,

80 % CO₂ was required for CO₂ from membrane technology sourced from natural gas, and miscibility could not be achieved with CO₂ from flue gas when using membrane technology.

- Even small concentrations of impurities (as low as 1 % CH₄ and 1 % N₂) were found to significantly increase MMP.
- The impurities present in flue gas streams (O₂ and N₂) had a more substantial impact on increasing MMP compared to the CH₄ impurity found in natural gas streams.

These findings underscore the importance of carefully considering CO₂ source and purity when designing CO₂-EOR projects, particularly in offshore environments where impurity levels can significantly impact the miscibility and efficiency of enhanced oil recovery processes.

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Chapter 4 : DATA DRIVEN PREDICTION OF THE MMP BETWEEN MIXTURES OF OIL AND GAS USING DEEP LEARNING

Preface

A version of this chapter has been published in peer reviewed conference paper: Pham, Q.C., Trinh, Q.T and James, L.A . 2021 Data driven prediction of the MMP between mixtures of oil and gas using Deep Learning. Presented at the 40th International Conference on Ocean, Offshore and Arctic Engineering. Virtual, June 21-30. <u>https://doi.org/10.1115/OMAE2021-63018</u>. I am the primary author. Co-author Dr. Trung Trinh provided technical assistance for data analysis and reviewed the first draft. Co-author Dr. Lesley James is senior supervisor. Dr. James reviewed, provided technical assistance, and valuable insights to improve the paper concept.

1. Literature review

1.1. Machine Learning (ML) used for thermodynamic properties

Detailed knowledge of a fluid's physical properties is required for all reservoir computations playing an important role in predicting reservoir performance. Consequently, these properties are crucial factors in process design and project success. Bubble point pressure (P_b) and oil formation volume factor (B_o) are the most frequently studied properties, as they are the key parameters in most petroleum engineering calculations (Farasat 2013). Bubble point pressure is defined as the pressure at which the first bubble of a gas will come out of the liquid oil solution (Danesh 2003). Oil formation volume factor is interpreted as the ratio of the volume of oil (plus the gas in solution) at the prevailing reservoir temperature and pressure to the volume of oil at standard conditions. Their values can be obtained through experimental approach; however, the experimental procedures are generally time-consuming and costly (Danesh 2003). Moreover, in some cases, reservoir fluid samples are not available or not good quality enough to conduct the measurement. P_b and B_o can also be estimated by modelling using the thermodynamics Equations of State (EOS); however, this methodology requires the experimental data to tune the model. In addition, no EOS has been proven to be reliable EOS for predicting all fluid properties at all conditions. Artificial Intelligence (AI) modelling has been used recently to predict P_b and B_o, since this method can provide accurate results. Thirty-eight papers applying ML to estimate Pb, and Bo were reviewed (Ramirez 2017, Ikiensikimama 2012, Seyyedattar 2020, Elkatatny 2017, Numbere 2013, Yang 2020, Alakbari 2016, Al-Marhoun 2002, Gharbi 1999, Osman 2001, Alimadadi 2011, Onwuchekwa 2018, Sola-Aremu 2019, Salehiniaa 2016, Shojaei 2014, Gharb 1997, Elsharkawy 1998, Gharbi 1999, Boukadi 1999, Abdel-Aal 2002, Goda 2003, Malallah 2006, El-Sebakhy 2009, El-Sebakhy 2007, Dutta 2010, Moghadam 2011, Asadisaghandi 2011, Seifi 2012, Khoukhi 2012, Farasat 2013, Rafiee-T 2013, Kazemi 2013, Al-Marhoun 2014, Karimnezhad 2014, Ahmadi 2014, Afshar 2014, Ahmadi 2015, Moussa 2018). Prior to 2000, little research using ML was completed (5 over 38 papers); from 2001 to 2010, the use of ML increases steadily. A sharp increase in the number of articles is observed from 2011 to present (25 over 38 papers), which represents the explosion in ML application for P_b and B_o estimation. ANN (Artificial Neural Network), which is the most powerful statistical tool for classifying complex systems and is constructed based on the human brain's data analysis pattern, is the most employed algorithm (23 over 38 papers). An ANN model comprises multilayered, interconnected networks including the input layer, hidden layers, and output layer. The learning process can be adjusted through the connection weights between layers based on a specific objective function. The drawback of this algorithm is over-fitting training datasets, poor reproducibility of the results, requirement of a good guess, and satisfying adjustment architectural parameters of the networks from the user (Curilem 2011, Eslamimanesh 2012).

Another algorithm used is SVM (Support Vector Machine) (6 over 38 papers), which is a supervised learning mode proposed by Vapnik (1995). This algorithm is based on the kernel neuron function, which is able to solve complex, highly nonlinear problems. It allows projection to higher planes and can determine the degree of overlap between the different parameters (Trontl 2007). Adaptive Neuro-Fuzzy Inference System (ANFIS) is also used by many researchers (6 over 38 papers). This algorithm uses Sugeno fuzzy inference system and is the combination of neural network and fuzzy logic. Thus, it has the capability to extract the benefits of both mentioned in a single platform (Tahmasebi 2012). Fuzzy logic is a series of conversion processes: input parameters to input membership functions, then to set of fuzzy rules, later to output characteristics, and next to output membership functions, finally to one valued output or any classification based on output (Klir 1995). Other ML algorithms (11 over 38 papers) are used to estimate Pb, and Bo included Random Forest Repressor, Radial Basis Function (RBF), Alternating Conditional Expectation, Elastic Net Regression, Adaptive Boosting and Collaborative Filtering, Multilayer Perceptron Networks, etc. Some researchers combine Machine Learning algorithms with an Optimized Algorithm (5 over 38 papers), such as Genetic Algorithm (GA) or, Particle Swarm Optimization (PSO) to achieve a better P_b and B_o prediction.

1.2. Machine Learning (ML) used for MMP

The literature review for Machine Learning used for MMP is presented and updated in the Chapter 2 part 3.

2. Methodology

2.1 Data preparation

The validity and comprehensiveness of the used datasets has a significant effect on the accuracy and reliability of developed model (Rafiee 2013, Gharagheizi 2008, Gharagheizi 2011). In this

work, 250 datasets were collected from different sources (Aleidan 2011, Nekouie 2018, Jaubert 2002, Kanatbayev 2015, Alshuaibi 2019, Alshuaibi 2018, Firoozabadi 1986, Yuan 2005, Yellig 1980, Eakin 1988, Metcalfe 1982)... Data set in this study consists of reservoir temperature, oil characteristics (molecular weight MW= Σ MW_i*x_i, ratio of volatile components C₁, N₂ and intermediate components C₂-C₆, CO₂, H₂S), and gas characteristics (mole percentage of CO₂, C₁, N₂, H₂S, C₂⁺). The ranges of the input and output data including the minimum and maximum values are presented in the Table 4-1.

Parameter			Minimum	Maximum
Reservoir temperature (K)			304.26	444.26
Characteristic	Oil	Oil molecular weight	41.05	249.91
		Ratio of volatile components and intermediate	0	1.33
	Gas	CO ₂ mol%	0	100
		C_1 mol%	0	100
		N ₂ mol%	0	80.1
		H ₂ S mol%	0	100
		C_2^+ mol%	0	58.47
MMP (psia)			933	6758.86

TABLE 4-1: Range of input/output used in this study

After constructing the datasets, the data must be normalized, which can be done through several equations. In this work, data were scaled between [0.1, 0.9] following the equation (1):

$$x_n = \frac{x_i - x_{min}}{x_{max} - x_{min}} * 0.8 + 0.1 \tag{1}$$

The data were then split into training and test datasets, with 80% of the samples used for training and 20% for testing. This is considered a good proportion for modeling nonlinear functions (Granger 1993). Figure 4-1 shows the process used to construct the ML model in this study. The performance and accuracy of the proposed model was evaluated using the coefficient of determination (\mathbb{R}^2) RMSE, and RMSE (%) which are defined by equations (2), (3), and (4), respectively. The ideal model is expected to have an R² value close to one and RMSE value as small as possible.

$$R^{2} = 1 - \frac{\sum_{i}^{N} (Calc.(i) - Exp.(i))^{2}}{\sum_{i}^{N} (Calc.(i) - average(Exp.(i)))^{2}}$$
(2)

$$RMSE = \sqrt{\frac{1}{N}\sum_{i}^{N}|Calc.(i) - Exp.(i)|^2}$$
(3)

$$RMSE(\%) = \frac{RMSE}{MMP \ average} \tag{4}$$



FIGURE 4-1: Flow chart for constructing ML algorithm

2.2 Deep Learning: multiple fully connected networks

A fully connected network (FCN) consists of a series of fully connected layers, as shown in Figure 4-2, and its basic unit is a neuron. Each fully connected layer affects a transformation of the feature space in which the problem resides. This technique is capable of solving complex problems thanks to the inherent flexibility of the learned representations.



FIGURE 4-2: Deep Learning algorithm

Consider a neural network with L hidden layers. Let $l \in \{1...L\}$ index the hidden layers of the network. Let z(l) denote the vector of inputs into layer l, y(l) denotes the vector of outputs from layer l (y(0) = x is the input). W(l) and b(l) are the weights and biases at layer l. The feed-forward operation of a standard neural network can be described as (for $l \in \{0...L - 1\}$ and any hidden unit I, where f is any activation function:

$$z_i^{(l+1)} = w_i^{(l+1)} y^l + b_i^{(l+1)}$$
(5)

$$y_i^{(l+1)} = f(z_i^{(l+1)})$$
(6)

FCN tends to memorize training data entirely and will keep training and learning as long as the user wants. When training a large network of relatively small datasets, the model could learn the

statistical noise in the training data, which results in poor performance when the model is evaluated with new data. The overfitting problem can be improved through regularization algorithms.

Early Stopping

One approach to lower the overfitting is to determine a point during training, called Early Stopping, when the model stops generalizing and starts learning the statistical noise in the training dataset. The model is trained once for a large number of training epochs. During training, the model is evaluated after each epoch. The training process is stopped only when the performance of the model on the validation dataset starts to degrade, which means the accuracy begins to decrease, as illustrated in Figure 4-3. There are three factors to be considered while applying early stopping: monitoring model performance, trigger to stop training, and the choice of model to use. In order to monitor model performance, it is necessary to choose a dataset and a metric to evaluate the model during training. It is common to use 30 % of the training datasets, called subset, as the validation dataset and the loss on a validation dataset as the metric to monitor the model. To reduce the computational cost, the model is evaluated less frequently, such as every, for example 2, 5, or 10 training epochs (Prechelt 2012). A trigger stopping is then chosen. In the simplest case, when the performance on the validation dataset decreases compared with the previous training epoch, the training process is stopped. However, since the training of a neural network is stochastic and can be noisy, the first sign of overfitting may not be the best point to stop the training. The choice of model, especially the weight, depends strongly on the trigger chosen to stop the training process.



FIGURE 4-3: Model accuracy on training and test sets (Orr Jr 2007)

K-fold Cross Validation

Training and testing on the same dataset can lead to overfitting, where the model performs well on the training data but poorly on new, unseen. data. To address this, the k-fold Cross Validation (KCV) technique is employed. As illustrated in Figure 4-4, this method divides the dataset into k equally sized subsets (folds). The model is trained on k-1 folds and tested on the remaining fold, ensuring that every data point is used for both training and validation exactly once. For example, in a 5-Fold Cross Validation, the dataset is split into five parts. The model is trained on four subsets (80 % of the data) and validated on the fifth subset (20 %). This process is repeated five times, each time using a different subset for validation. The prediction performance is then averaged over these k iterations, as shown in Figure 4-5, to provide a more reliable evaluation of the model's generalization ability. By systematically rotating the training and validation sets, KCV reduces bias in performance evaluation, minimizes overfitting risks, and ensures robust testing across various data configurations. It is particularly useful for datasets of limited size, as it maximizes the use of available data for both training and validation while maintaining model reliability. The use of this technique is essential in reservoir engineering problems, where prediction accuracy on unseen data directly impacts decision-making and optimization processes.



FIGURE 4-4: Flowchart of a typical cross validation workflow



FIGURE 4-5: K-fold cross validation technique

3. Results and Discussion

The Pearson correlation coefficient, ranging from -1 to 1, is a statistical measure that quantifies the linear relationship between two variables. A coefficient value closer to 1 or -1 indicates a strong linear relationship, while values closer to 0 suggest a weak or no linear relationship. In the context of oil-gas Minimum Miscibility Pressure (MMP), a higher absolute value of the Pearson coefficient

between input and output variables signifies that the input has a stronger influence on the output. This reflects how consistently and predictably the MMP responds to changes in a single input variable in a linear manner. This approach was employed as a sensitivity analysis tool to assess the effect of various input factors on MMP, enabling a deeper understanding of the variables that most significantly impact miscibility.

As shown in Figure 4-6, the sensitivity analysis revealed that the most influential factors on MMP are reservoir temperature, and the amounts of CO₂ and methane (C₁) in the gas phase, as evidenced by their high Pearson coefficient values. This suggests that changes in these variables exert a considerable impact on MMP, highlighting their importance in optimizing enhanced oil recovery (EOR) strategies. Additionally, the analysis indicated that several variables have a negative influence on MMP, such as reservoir temperature, molecular weight, the ratio of volatile to intermediate components in the oil phase, and the amounts of methane (C₁) and nitrogen (N₂) in the gas phase. These parameters were found to have positive Pearson coefficients, meaning that as the values of these factors increase, the MMP also increases. While temperature generally lowers the viscosity of the oil and enhances CO₂ solubility, higher reservoir temperatures can sometimes have a paradoxical effect depending on the oil composition and gas mixture. The presence of higher molecular weight hydrocarbons or the evolution of phase behavior at high temperatures may increase the pressure needed for miscibility. The molecular weight of the oil is another significant factor in MMP behavior. Heavier oil components (i.e., higher molecular weight) tend to have lower diffusivity and solubility for gases like CO₂. As the molecular weight of oil increases, the ability of the injected gas to mix with the oil decreases, leading to higher pressures required to achieve miscibility. Methane is a light hydrocarbon that is typically present in natural gas and often used in enhanced oil recovery (EOR) processes. Although methane can improve the overall volumetric efficiency of the injected gas, its presence can increase the MMP. This is because methane, despite being miscible with crude oil at lower pressures than heavier gases, still requires higher pressures compared to CO₂. The presence of methane reduces the concentration of CO₂ in the gas phase, meaning the injection gas may not be as effective at reducing MMP as pure CO₂. Nitrogen, an inert gas commonly found in CO₂ captured from flue gas or natural gas streams, plays a significant role in increasing MMP. Nitrogen has a much higher miscibility pressure than CO₂ and does not dissolve easily in crude oil. Therefore, its presence in a CO₂-based gas mixture reduces the overall solubility of CO₂ in the oil phase, thus requiring a higher injection pressure to achieve miscibility. In contrast, the presence of CO_2 and H_2S in the gas phase, especially CO_2 , was found to lower MMP, which is consistent with findings from previous studies (Abbasi, 2010; Zhang, 2004). CO₂ is highly effective in improving oil miscibility, a key factor for successful EOR. Its ability to reduce MMP stems from its high solubility in crude oil, which lowers interfacial tension and allows the gas to mix with oil at lower pressures. CO2's favorable phase behavior with crude oil enables the formation of a single-phase mixture, enhancing miscibility. Additionally, CO₂ injection reduces oil viscosity, improving flow and displacement efficiency, which further lowers MMP and enhances oil recovery in the reservoir. This result supports the idea that CO_2 is a key driver in enhancing miscibility, as it facilitates the lowering of MMP, promoting more efficient oil recovery. These findings align with the broader literature that emphasizes CO₂'s role in reducing miscibility pressure in EOR processes, thereby improving oil recovery efficiency. Hydrogen sulfide (H₂S) can reduce MMP by altering oil solubility, similar to CO₂, but is less favorable for EOR due to its toxicity and environmental risks. Typically used in combination with CO₂ or other gases, H₂S can enhance miscibility but requires careful management to avoid corrosion and safety issues.



FIGURE 4-6: Importance degree of each parameter on gas-oil MMP

The Deep Learning model used for predicting MMP was optimized by testing different configurations of hidden layers and epochs. After evaluating various setups, the best performance was achieved with 5 hidden layers and 1500 epochs. To prevent overfitting and reduce training time, Early Stopping was employed. This technique halts the training process when the model's performance stops improving, ensuring that it doesn't overfit the data. Even with just 7 epochs, the model achieved strong results with an R² value of 0.96 and an RMSE of 5.4 %, close to the performance observed with 1500 epochs, which was $R^2 = 0.97$ and RMSE = 4.7 %. However, it is important to note that the training and test sets were randomly selected, which may make the results specific to the chosen data. To improve generalization and assess the model's robustness, k-fold Cross Validation was used. This technique splits the data into five subsets (folds), rotating the training and test sets for each fold. The performance is averaged over all folds to reduce bias and improve the model's generalizability. The Deep Learning model with k-fold Cross Validation yielded an R² of 0.954 and RMSE of 5.8 %, indicating solid predictive performance. For further comparison, the Deep Learning model was evaluated against other machine learning techniques

like Decision Tree and Random Forest Regression. The results, shown in Table 4-2, demonstrate that the Deep Learning model outperforms both Decision Tree and Random Forest models, which had R² values below 0.9 and RMSE values greater than 10 %. This highlights the superiority of Deep Learning in predicting MMP, particularly in handling complex relationships and large datasets. Additionally, the proposed Deep Learning model was compared with well-known correlations (e.g., Alston et al. and Sebastian et al. correlations), but it was noted that these correlations have limitations. They are only applicable to CO₂ streams with a restricted range of impurities, which makes them less versatile than the Deep Learning model, capable of handling more varied CO₂ mixtures and impurity levels. This further demonstrates the value of the Deep Learning approach for generalizing MMP prediction across diverse scenarios, including those with high impurity concentrations.

Algorithm	\mathbb{R}^2	RMSE (%)
Decision Tree	0.86	13.1
Random Forest	0.87	12.4
Deep Learning	0.96	5.4
Early Stopping	0.97	4.7
K-fold Cross validation	Fold 1: 0.98	Fold 1: 3.9
	Fold 2: 0.92	Fold 2: 8.8
	Fold 3: 0.96	Fold 3: 5.4
	Fold 4: 0.97	Fold 4: 4.7
	Fold 5: 0.95	Fold 5: 6.2
	Average: 0.954	Average: 5.8

TABLE 4-2: Simulation results for different ML techniques

Figures 4-7 to 4-11 compare the MMP values predicted by various models with experimental data from the test set. These figures illustrate how well each model predicts MMP, with the vertical axis representing the predicted MMP value and the horizontal axis showing the actual test set point. The R² and RMSE values are consistent with these plots, indicating model performance. The results

show that the Deep Learning models outperform both the Decision Tree and Random Forest models in predicting oil-gas MMP.

The superior performance of Deep Learning models can be attributed to their ability to handle complex relationships and patterns in the data. In contrast, the Decision Tree algorithm often struggles with overfitting, meaning it may perform exceptionally well on training data but fail to generalize to unseen data. This overfitting is a common issue for Decision Trees, where small changes in data can significantly impact the model's structure, leading to instability and inaccurate predictions.

The Random Forest algorithm mitigates some of the Decision Tree's overfitting problems by constructing multiple trees and combining their outputs. However, Random Forest models are computationally intensive and require more training time. While Random Forest performs well for classification tasks, it is less suited for regression problems like MMP prediction because it may not extrapolate effectively beyond the training data range, especially in the case of noisy datasets, leading to potential overfitting. This explains why the Deep Learning models, which can better handle large datasets and complex regressions, provide more accurate and stable MMP predictions compared to Decision Tree and Random Forest models.



FIGURE 4-7: Deep Learning model R^2 = 0.96, RMSE=5.4 %





FIGURE 4-9: Deep Learning with k-fold Validation Cross model R^2 = 0.954, RMSE=5.8 %





4. Conclusions

The literature review focused on the application of machine learning (ML) for predicting key physical properties, such as Pb, Bo, and Minimum Miscibility Pressure (MMP), using various algorithms, with a specific emphasis on Fully Connected Neural Networks (FCN). This model was optimized with Early Stopping and k-fold Cross Validation techniques. Below are the key conclusions drawn from the reviewed studies:

- ML Success: Machine learning has been proven effective in predicting fluid physical properties, particularly Pb and Bo. Among the algorithms, Artificial Neural Networks (ANN) are the most widely used, appearing in 23 out of 38 studies.
- Dataset Limitations: A major limitation in recent studies is the lack of comprehensive datasets, especially regarding the CO₂ concentration range in gas sources, which hinders the accuracy of MMP predictions.
- Influential Factors on MMP: The reservoir temperature and the amounts of CO₂ and methane (C₁) in the gas source were identified as the most influential factors affecting oil-gas MMP.

- MMP Sensitivity: Increasing reservoir temperature, molecular weight of the oil, the ratio of volatile to intermediate components in the oil phase, or the amounts of C₁ and nitrogen (N₂) in the gas phase tend to increase MMP, indicating a higher-pressure requirement for miscibility.
- Effect of CO₂ and H₂S: The presence of CO₂ and H₂S in the gas phase, especially CO₂, reduces MMP, making the oil and gas more miscible and improving oil recovery.
- Deep Learning Performance: The Deep Learning model outperformed other machine learning techniques, achieving an R² value of 0.96 and an RMSE of 5.4 %, indicating strong predictive accuracy for MMP.
- Early Stopping Optimization: The Early Stopping technique proved effective in optimizing training time, with a good result obtained after only 7 epochs.
- K-fold Cross Validation: The application of k-fold Cross Validation, using five folds, resulted in an R² value of 0.954, demonstrating the model's robustness and ability to generalize well across different data subsets.
- Comparison with Other Models: The Deep Learning model outperformed traditional models such as Decision Tree and Random Forest Regression, with the latter two showing lower accuracy (R² values below 0.9 and RMSE values exceeding 10 %).

This review highlights the strengths of ML, particularly deep learning, in predicting MMP and fluid properties, and underscores the importance of dataset quality and model optimization techniques in enhancing the predictive power of ML models in petroleum engineering.

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Additional comparison:

Figure 4-10 compares the Deep Learning model with the slimtube simulation for predicting

Minimum Miscibility Pressure (MMP) values. The relative errors between the two models are no

more than 7 %, indicating a strong correlation and demonstrating that the Deep Learning model

provides results that are highly consistent with the simulation data. This suggests that the Deep

Learning approach is a reliable tool for predicting MMP values in CO₂-EOR studies.



FIGURE 4-12: Comparison between Deep Learning model and slimtube simulation

Chapter 5 : INVESTIGATION CO₂ EOR TYPES WITH CONSTRAINED CO₂ VOLUME AND IMPURITIES FOR A HIGH-QUALITY SANDSTONE, STRATIFIED OFFSHORE NEWFOUNDLAND RESERVOIR.

Preface

A version of this chapter has been published in peer reviewed conference paper: Pham, Q.C., Esene, C.E. and James, L.A. 2023. Investigating CO₂-EOR Types with Constrained CO₂ Volumes and Impurities for a High-Quality Sandstone, Stratified Offshore Newfoundland Reservoirs. Presented at the SPE Canadian Energy Technology Conference and Exhibition. Calgary, Alberta, Canada, March 15 - 16. <u>https://doi.org/10.2118/212811-MS</u>. I am the primary author. Co-author Dr. Ebeagbor Cleverson Esene provided technical assistance for reservoir simulation and reviewed the first draft. Co-author Dr. Lesley James is senior supervisor. Dr. James set the conceptual objectives, reviewed, provided technical assistance and valuable insights to improve the paper concept.

1. Introduction

The literature review is presented and updated in the Chapter 2 part 4.

2. Methodology

Figure 5-1 outlines the methodology employed in this study. The workflow begins with a quantitative analysis to determine the constrained CO₂ volume for the offshore reservoir. Using the WINPROP module, the compositional fluid was generated and subsequently integrated into the geological model constructed in the GEM module of the CMG simulator. The constrained CO₂
volume was incorporated as the daily injection rate during the simulation. Three injection scenarios were examined: CO₂ WAG, enriched CO₂ WAG, and Carbonated Water Injection (CWI). The simulations assessed the performance of these scenarios under various conditions. A sensitivity analysis was then conducted through the CMOST AI module, utilizing the Response Surface Methodology (RSM) to evaluate the influence of reservoir characteristics such as temperature and pressure on overall performance. To enhance predictive capabilities, proxy models were developed using the multi-layer Artificial Neural Network (ANN) option in the CMOST AI module. These proxy models enable quick and accurate predictions of the oil recovery factor and the potential CO₂ storage capacity for stratified reservoirs, considering both crossflow and non-crossflow conditions. This comprehensive approach ensures a robust evaluation of CO₂-EOR techniques tailored for offshore reservoirs.



FIGURE 5-1: Workflow for investigating CO₂ EOR types with constrained CO₂ volume and Impurities

2.1 Estimation of available CO₂ volume

The gas produced from offshore reservoirs, mainly CH₄, is combusted following equations 1, 2 and 3.

$$CH_4 + 2O_2 \to CO_2 + 2H_2O$$
 (1)

$$C_2 H_6 + \frac{7}{2}O_2 \to 2CO_2 + 3H_2O$$
 (2)

$$C_3 H_8 + 5O_2 \to 3CO_2 + 4H_2O \tag{3}$$

After the post-combustion process, carbon capture technologies are employed to isolate CO₂ for injection. The primary technologies for CO₂ capture include absorption, adsorption, and membrane

separation, along with emerging techniques like direct air capture, supersonic separation, hydratebased separation, and cryogenic distillation. In this study, membrane technology was chosen due to its environmentally friendly nature, compact design, and lower maintenance requirements (Pham, 2021). Membrane systems, particularly two-stage setups, are well-established, achieving a CO₂ capture efficiency of 90% (Merkel, 2010, Zhao, 2010). Studies indicate that upgrading to a three-stage system provides no significant additional benefit (Zhao, 2012). For this research, a high-quality sandstone reservoir in offshore Newfoundland serves as the case study. The maximum amount of CO₂ that can be injected, based on pore volume (PV), is estimated to be approximately 0.25 PV, providing critical constraints for simulating enhanced oil recovery (EOR) and carbon storage performance.

The phase behavior of pure CO₂ is strongly dependent on reservoir characteristics such as temperature and pressure. Table 5-1 shows the characteristics of Newfoundland's reservoirs (Canada-Newfoundland and Labrador Offshore Petroleum Board 2010) as well as the range used for this study. Figure 5-2 shows the phase diagram of pure CO₂ and the range of typical reservoir conditions. Figure 5-3 illustrates CO₂ density as a function of pressure and temperature (Van der Meer 2005). Our working range for this study is also indicated on both figures. As the critical temperature of CO₂ is 31.1 °C and its critical pressure is 7.38 MPa, CO₂ is in its supercritical state for the range of working conditions used in this study. This means that CO₂ acts as a gas-like compressible fluid but has a liquid-like density (Budisa 2014). Supercritical CO₂ is non-polar and serves as an effective solvent for non-polar and slightly polar organic compounds. Its high density and gas-like compressibility allow it to dissolve hydrocarbons, oils, and certain pesticides efficiently. This makes it highly valuable in various industries, such as in supercritical fluid extraction, cleaning processes, and enhanced oil recovery (EOR).

TABLE 5-1: Reservoir characteristics, NL offshore (Canada-Newfoundland and Labrador Offshore Petroleum Board 2010)

Reservoir characteristics	Hibernia Field	Terra Nova Field	Hebron Field	Whiterose Field	Range studied
Pressure (MPa)	26.7-68.4	34.4-34.6	19.4-47.4	30.6-71.3	20-70
Temperature (°C)	66-107	94-96	49-117	110-125	50-130



FIGURE 5-2: Phase behavior of CO2 (Van der Meer 2005) and study range





2.2 Simulation

2.2.1 Fluid modelling (compositional simulation)

The fluid was modelled using the Peng-Robinson equation of state (EOS), which was then tuned using laboratory experiments of constant composition expansion and viscosity to obtain a match. Table 5-2 shows the comparison between the measured and model fluid parameters. Figures 5-4 and 5-5 compare the experimental and modelled relative oil volume (ROV) and viscosity, respectively. A satisfactory match was reached after 500 regression iterations by the EOS on key experimental parameters, such as saturation pressure (P^s), formation volume factor (FVF), gas oil ratio (GOR) and API. The EOS model made acceptable predictions for ROV and viscosity experiments.

Parameter	Measured	Before Regression	After Regression	Percentage Error Reduction
P ^s (MPa)	37,3	50	36,9	1.1 %
FVF (sm ³ /m ³)	1.76	3.45	1.74	3.4 %
GOR (sm^3/m^3)	253	200	236	6.7 %

TABLE 5-2: Measured and modelled properties of oil



FIGURE 5-4: Comparison between experimental and modelled for ROV



FIGURE 5-5: Comparison between experimental and modelled viscosity

2.2.2 Block modelling

A reservoir block model with dimensions of $1200 \text{ m} \times 500 \text{ m} \times 80 \text{ m}$ was constructed, divided into five main reservoir zones in the z-direction, all with equal thickness. The zones are separated by thin shale beds, which are considered negligible in thickness compared to the sandstone layers, allowing control over transmissibility between the layers. In Figure 5-6(a), the vertical transmissibility was set to 1 to enable cross-flow and communication between all layers, while in Figure 5-6(b), it was set to 0 to prevent cross-flow. The model assumes uniform vertical transmissibility, homogeneous reservoir zones with uniform properties, and negligible shale layer thickness that does not affect flow. The boundary conditions are assumed to be no-flow, and the geometry is simplified with one injector on one side and one producer on the opposite side. The reservoir properties are provided in Table 5-3.

Vertical Transmissibility T = 1 in all layers

Vertical Transmissibility T = 0 in all layers



a)Reservoir model geometry with cross flow



No communication between layers b)Reservoir model geometry without crossflow



TABLE 5-3: Reservoir properties

Parameter	Value
Reservoir pressure	42,6 MPa
Length of block model	1200 m
Width of block model	500 m
Temperature of reservoir	102 ° C
Well type	Vertical
Well spacing	1200 m
Layer Permeability	Layer 1: 100 mD
	Layer 2: 200 mD
	Layer 3: 250 mD
	Layer 4: 300 mD
	Layer 5: 300 mD
Average Porosity	Layer 1: 0.15
	Layer 2: 0.18
	Layer 3: 0.17
	Layer 4: 0.2
	Layer 5: 0.1

2.2.3 Numerical set-up for different CO₂EOR types

The block model was initialized at 31MPa at a depth of 3500 m below mean sea level. The simulation for each CO_2 EOR type was run after approximately one year of primary depletion. Figure 5-7 shows the detailed steps and respective values to set up the simulation for each injection scenario. The amount of CO_2 , the bottom hole pressure and the water cut are set up for each case. For enriched CO_2 WAG, the gas composition needs to be specified since the CO_2 is mixed with natural gas containing mainly CH₄. The WAG ratio is also defined for CO_2 WAG and enriched CO_2 WAG scenarios.

Voidage displacement is the process where oil, gas and water in the reservoir are replaced by the injected fluid. It plays as decisive element for maintaining reservoir pressure as well as mitigating surface subsidence in certain fields. The Voidage Replacement Ratio (VRR), which is the ratio between the injected fluid volume and the produced fluid volume of the reservoir, is employed as the key parameter to set up the constrained volume of CO₂.



FIGURE 5-7: Simulation flowchart for investigating different CO₂-EOR techniques under constrained CO₂

a. CO₂ WAG

Given the constrained availability of CO₂, the simulation incorporates a strategy where water is injected alongside CO₂ to maintain the desired voidage replacement ratio (VRR). This approach ensures that the reservoir pressure is sustained while optimizing the utilization of the limited CO₂ supply. The maximum allowable CO₂ injection rate acts as a critical constraint, guiding the simulation to achieve an effective balance between CO₂ injection and water alternation. The operational parameters, including injection rates, WAG ratio, VRR, and other key input variables for the CO₂ WAG simulation, are outlined in Table 5-4, providing a comprehensive framework for implementing this enhanced recovery strategy.

TABLE 5-4: Simulation parameters for CO₂ WAG

Parameter	Value
Gas injection flow rate	300,000 Sm ³ /day
WAG ratio	3:1
Voidage replacement ratio (VRR) limit	1
Minimum bottom hole pressure	13.8 MPa
Maximum water-cut	98 %

b. Enriched CO₂ WAG

Our prior research on Minimum Miscibility Pressure (MMP) in relation to various carbon capture techniques (Pham 2021) highlighted that achieving miscibility for the studied reservoir fluid under specific conditions requires a minimum of 80 % CO₂ in the injection mixture. This study utilizes CO₂ mixed with natural gas, predominantly composed of CH₄, in a 4:1 ratio to ensure miscible displacement. The Water-Alternating-Gas (WAG) ratio is optimized to maintain the voidage replacement ratio, which balances fluid injection and production rates to prevent reservoir pressure decline. The key parameters used for the enriched CO₂ WAG simulation are provided in Table 5-5.

TABLE 5-5: Simulation parameters for enriched CO₂-WAG

Parameter	Value
Gas injection flow rate	300,000 Sm ³ /day
WAG ratio	3:1
Voidage replacement ratio (VRR) limit	1
Minimum bottom hole pressure	13.8 MPa
Maximum water-cut	98 %
CO ₂ mole composition	80 %
CH ₄ mole composition	20 %

c. CWI

For Carbonated Water Injection (CWI), pure CO_2 is dissolved into the water phase prior to injection into the reservoir. The dissolution process typically requires 2-5 % CO_2 by weight, a concentration sufficient to ensure the stability and flow of a single-phase carbonated water (CW) through the porous medium. This concentration prevents phase separation during injection, ensuring that the injected water remains in a homogenous state while maximizing the efficiency of CO_2 transfer to the oil phase. The preparation of CW involves maintaining specific pressure and temperature conditions to facilitate CO_2 solubility in water, which is highly dependent on reservoir conditions such as reservoir pressure, temperature, and salinity levels. The dissolved CO_2 in CW can significantly enhance oil recovery by reducing interfacial tension between oil and water, swelling the oil, and altering rock wettability. These mechanisms promote better oil displacement efficiency. The parameters used for CWI simulation, as outlined in Table 5-6.

	TABLE 5-6:	Simulation	parameters	for	CWI
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Parameter	Value
Gas injection flow rate	48,000 Sm ³ /day
Voidage replacement ratio (VRR) limit	1
Minimum bottom hole pressure	13.8 MPa
Maximum water-cut	98 %

2.3 Sensitivity analysis

Response Surface Methodology (RSM) was applied using the CMOST AI module in CMG software to optimize the process. RSM is a mathematical and statistical approach designed to model and analyze the relationships between multiple explanatory variables (independent factors) and one or more response variables (dependent variables). In this study, the dependent variables, or responses, are cumulative oil production and the amount of CO₂ stored during each simulation process. The independent variables, or factors, include reservoir temperature and pressure, with ranges chosen to represent the typical conditions documented for Newfoundland offshore reservoirs. This approach facilitates understanding the interactions between variables and helps identify optimal operating conditions for maximizing oil recovery and CO₂ storage efficiency.

2.4 Proxy model

Simulation results were divided into training and testing datasets to develop a proxy model. This model was created using a three-layer neural network within the CMOST AI module, as illustrated in Figure 5-8. The neural network structure includes one input layer, one hidden layer, and one output layer. Input data are transmitted to the hidden layer via weighted connections, where they are processed using an activation function that captures complex nonlinear relationships. The

processed information is then transferred to the output layer, with outputs regulated by weight vectors. This architecture enables the proxy model to predict key performance metrics, such as oil recovery and CO₂ storage, with high accuracy.



FIGURE 5-8: Three-layer neural-network model

The proxy model was evaluated using the coefficient of determination (R^2) following equation 4:

$$R^{2} = 1 - \frac{\sum_{i}^{N} (Calc.(i) - Exp.(i))^{2}}{\sum_{i}^{N} (Calc.(i) - average(Exp.(i)))^{2}}$$
(4)

3.Results and Discussion

This section presents an analysis of various CO₂ EOR methods, focusing on their performance and efficiency in terms of oil recovery and water cut under CO₂ supply constraints. The CO₂ WAG and CWI injection schemes used pure CO₂, while the enriched CO₂ WAG scenario consisted of 80 % CO₂ and 20 % CH₄. A comparative study of CO₂ EOR types was conducted for stratified reservoirs, considering both crossflow and no crossflow cases. Additionally, sensitivity analyses were performed for each CO₂ EOR type by varying key reservoir characteristics, such as temperature and pressure. To facilitate the predictions of cumulative oil recovery and recovery factor, a proxy model was developed based on the investigated parameters.

Table 5-7 summarizes the simulation results for the three CO2 EOR methods for a stratified

reservoir with and without crossflow.

Reservoir	Transmissibility	Recovery Factor		
communication		CO ₂ -WAG	Enriched CO ₂ -WAG	CWI
Crossflow	1	73.0 %	75.2 %	84.4 %
Without	0	71.3 %	72.2 %	78.8 %
crossflow				
CO ₂ stored		5.19	4.96	2.5
(Mtonnes)				
CO ₂ tax credit		181.65	173.6	87.5
(M\$)				

TABLE 5-7: Summary of simulation results for the three $CO_2 EOR$ methods for a stratified reservoir with and without crossflow

3.1 Comparison between CO₂-EOR methods

3.1.1 Stratified reservoir with crossflow

Figures 5-9 and 5-10 illustrate key simulation results for oil recovery factor and water cut over five years for a stratified reservoir with crossflow under three enhanced oil recovery (EOR) methods: CO_2 Water-Alternating-Gas (CO_2 -WAG), enriched CO_2 -WAG (80 % $CO_2 - 20$ % CH₄), and Continuous Water Injection (CWI). The trends observed provide insights into the performance and dynamics of these methods under realistic reservoir conditions. During the initial phase of primary depletion, the oil recovery factor stabilizes at 25 % after approximately 180 days and remains unchanged until the end of this mechanism. This plateau highlights the limited recovery potential of primary mechanisms in stratified reservoirs. When CO_2 -WAG is applied as a secondary recovery method, the oil recovery factor increases sharply, reaching approximately 60 % within 500 days of injection. This significant improvement reflects CO_2 's efficiency in reducing oil viscosity and improving miscibility, allowing for better displacement of oil. There is minimal difference in recovery performance between CO_2 -WAG and enriched CO_2 -WAG during the early injection period (up to day 600). However, toward the end of the injection period, a slight decrease in oil

recovery efficiency is observed for enriched CO₂-WAG compared to pure CO₂-WAG. This aligns with prior findings (Alston 1985, Yellig 1980, Johannes 2009, Stringht 2009) indicating that the presence of CH₄ in the CO₂ stream raises the Minimum Miscibility Pressure (MMP), thereby reducing miscibility and oil recovery efficiency. In this study, however, the limited CO₂ supply minimizes the impact of CH₄ impurities, which is why the performance difference between pure and enriched CO₂-WAG remains relatively small. CWI achieves the highest recovery factor, reaching 84 % by the end of the simulation, compared to 73 % for pure CO₂-WAG and 75.2 % for enriched CO₂-WAG. This superior performance is attributed to the continuous displacement mechanism, which maintains consistent reservoir pressure and ensures effective oil displacement across the reservoir layers.

All EOR methods exhibit a sharp increase in water cut after 500 days of injection, exceeding 90 %. This increase corresponds to the breakthrough of injected fluids into production wells, a common occurrence in stratified reservoirs with crossflow. For CO₂-WAG and enriched CO₂-WAG, water cut shows slight fluctuations and a marginal decrease in later stages, likely due to gas injection cycles temporarily reducing water production. However, in CWI, the water cut remains constant post-breakthrough, as the injection is uninterrupted and dominated by water displacement.

The results underline the trade-offs between recovery efficiency and operational constraints. While CWI achieves the highest recovery factor, the consistently high water cut suggests potential challenges with water handling and disposal, especially in offshore or environmentally sensitive operations. CO₂-WAG and enriched CO₂-WAG show promising recovery factors with manageable water cuts, making them attractive options when CO₂ availability is limited. The small performance difference between pure and enriched CO₂-WAG emphasizes that impurity effects are less critical in cases of constrained CO₂ supply, but this could vary in scenarios with higher CH₄ concentrations.



FIGURE 5-9: Recovery factor for CO₂-WAG, enriched CO₂-WAG and CWI with crossflow



FIGURE 5-10: Water cut for CO2-WAG, enriched CO2-WAG and CWI with crossflow

3.1.2 Stratified reservoir without crossflow

Figures 5-11 and 5-12 illustrate the simulation outcomes for oil recovery factor and water cut over a five-year period in a stratified reservoir without crossflow, comparing three EOR methods: CO_2 -WAG, enriched CO_2 -WAG (80 % $CO_2 - 20$ % CH₄), and Continuous Water Injection (CWI). These results provide a nuanced understanding of recovery dynamics in reservoirs where fluid exchange between layers is limited. The results indicate negligible differences between pure CO₂-WAG and enriched CO₂-WAG in this scenario. The minor impact of CH₄ as an impurity suggests that the absence of crossflow reduces the role of miscibility differences between layers, thus diminishing the influence of MMP on recovery dynamics. During initial injection period (460 to 650 Days), CO₂-WAG and enriched CO₂-WAG outperform CWI in terms of oil recovery. This can be attributed to the early miscibility effects of CO2, which enhance oil mobilization and displacement efficiency. After 650 days, CWI overtakes CO₂-WAG and enriched CO₂-WAG in recovery efficiency, achieving the highest oil recovery at 78.8%, compared to 71.3% for CO₂-WAG and 72.2% for enriched CO₂-WAG. The superior performance of CWI in later stages is likely due to the effective dissolution of CO₂ in water, which enhances its contact with trapped residual oil. This reduces oil viscosity and lowers interfacial tension (IFT) between oil and water, resulting in improved recovery. The water cut variations in the non-crossflow reservoir are consistent with those observed in the crossflow case. All methods exhibit a sharp increase in water cut postbreakthrough, followed by stabilization. The similar trends highlight that water production dynamics are primarily governed by injection volume and reservoir properties, rather than crossflow effects or injection strategy. CWI's consistently high water cut in later stages might require additional water handling and treatment efforts, which could offset its economic and operational advantages.



FIGURE 5-11: Recovery factor for CO₂-WAG, enriched CO₂-WAG and CWI without crossflow



FIGURE 5-12: Water cut for CO₂-WAG, enriched CO₂-WAG and CWI without crossflow This conclusion underscores the critical trade-offs between maximizing oil recovery and minimizing emissions intensity, a key consideration during the energy transition. CWI achieved the highest oil recovery factor, outperforming CO₂-WAG and enriched CO₂-WAG by 7–10 %. This superior performance can be attributed to its ability to mobilize trapped residual oil through viscosity reduction and lowered IFT. However, its limited CO₂ storage capacity reduces its

contribution to carbon management efforts. CO2-WAG and enriched CO2-WAG, while slightly less effective in oil recovery, store approximately double the amount of CO₂ compared to CWI. This makes these methods more attractive in the context of emissions reduction goals. Defined as the ratio of greenhouse gas emissions produced to gross domestic product (GDP) (Emission Intensity 2022), emissions intensity is becoming a critical metric for the oil and gas sector. The ability to reduce emissions while maintaining or growing production is essential for achieving global sustainability targets. Lower emissions intensity methods, such as CO₂-WAG and enriched CO₂-WAG, align with the oil and gas industry's transition policies, which aim to reduce carbon footprints while sustaining economic growth (Insight & Analysis 2021). Under frameworks like the \$35/tonne tax credit for CO₂ stored during EOR (Waltzer 2017), methods with higher CO₂ storage, such as CO₂-WAG and enriched CO₂-WAG, yield nearly double the tax credit value of CWI. This financial incentive partially offsets their slightly lower recovery factors, making these methods economically viable. By storing more CO₂, these methods offer a path to reduce emissions intensity while achieving incremental oil recovery, addressing both economic and environmental goals. As carbon pricing and emissions regulations intensify globally, operators are likely to favor CO₂-intensive methods like CO₂-WAG, even at the expense of slightly lower recovery factors, to leverage tax credits and align with environmental policies. Integrating carbon capture and storage technologies with EOR processes can enhance CO₂ storage capacities, further reducing emissions intensity and improving overall project sustainability. In both cases of stratified reservoirs with and without crossflow, CWI achieved the highest oil recovery factor but at the cost of lower CO₂ storage. CO₂-WAG and enriched CO₂-WAG, on the other hand, offer nearly double the CO₂ storage capacity, resulting in significantly lower emissions intensity. These methods also benefit from favorable tax credits, with values nearly double that of CWI (Waltzer 2017). As emissions intensity becomes a vital metric for balancing production with environmental responsibility, CO₂-WAG methods emerge as strong candidates for achieving both economic and sustainability goals during the energy transition.

3.2 Comparison between stratified reservoir with, and without, crossflow

The comparison between stratified reservoirs with and without crossflow highlights the significant impact of reservoir characteristics and fluid behavior on oil recovery and water breakthrough dynamics. In reservoirs with crossflow, all injection types—CO₂-WAG, enriched CO₂-WAG, and CWI—achieved higher recovery factors compared to reservoirs without crossflow. Specifically, recovery factors for CO₂-WAG, enriched CO₂-WAG, and CWI were 73%, 75.2%, and 84.4%, respectively, in the presence of crossflow, compared to 71.2%, 72.2%, and 78.8% without crossflow. This enhancement can be attributed to the fluid communication between layers, which allows for better pressure redistribution and improved sweep efficiency. Crossflow also facilitates gravity drainage in deeper reservoirs, where the density difference between fluids aids in the upward displacement of oil, particularly for lighter oils like the one modeled in this study (API 41.7°). This effect minimizes oil bypassing in low-permeability layers and enhances overall recovery.

In contrast, in the absence of crossflow, each layer behaves more independently, resulting in uneven displacement fronts and earlier water breakthrough. The lack of pressure communication leads to poor sweep efficiency in lower-permeability zones, where oil may remain trapped, thereby reducing overall recovery. The permeability stratification in the simulated reservoir, which ranges from 100 mD in the first layer to 300 mD in the fourth and fifth layers, further contributes to these challenges. While the contrast in permeability is moderate, it still impacts recovery efficiency, with high-permeability layers experiencing faster fluid movement and earlier water breakthrough, while

lower-permeability layers suffer from inadequate sweep. This aligns with Sanchez's (1999) findings that WAG efficiency depends on permeability variation, as well as Christensen (2001) and Masalmeh (2010), who noted that greater permeability contrast exacerbates bypassing and reduces recovery.

The WAG ratio also plays a critical role in managing the effects of stratification and crossflow absence. In this study, a 3:1 gas-to-water injection ratio was used, which effectively balances oil recovery penalties associated with stratification. This ratio ensures sufficient gas mobility to drive oil displacement while maintaining pressure support to prevent early gas breakthrough. Claridge (1982) emphasized that higher WAG ratios help mitigate crossflow's influence and improve recovery by balancing miscibility benefits and fluid sweep efficiency.

Another important factor is the role of gravity segregation in improving recovery in reservoirs with crossflow. The depth of the reservoir amplifies the benefits of gravity, as water moves downward and displaces oil upward, improving recovery in deeper layers. This effect is particularly advantageous when lighter oils are present, as they are more easily displaced by water and gas movement. In contrast, the absence of crossflow diminishes these benefits, resulting in lower recovery factors and earlier water breakthrough.

Overall, these findings underscore the importance of understanding reservoir stratification, crossflow dynamics, and permeability contrasts when designing enhanced oil recovery strategies. While reservoirs with crossflow consistently achieve higher recovery, optimizing injection profiles and WAG ratios can mitigate the challenges posed by stratification in no-crossflow reservoirs. The results highlight the need to balance technical efficiency with economic and environmental goals, particularly as CO₂-EOR methods increasingly prioritize sustainability and emissions reduction alongside oil recovery.

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3.3 Sensitivity analysis

The sensitivity analysis using Response Surface Methodology (RSM) provides valuable insights into the effects of reservoir temperature and pressure on oil recovery factor and CO₂ storage capacity, covering a range applicable to Newfoundland reservoirs. The analysis uniformly demonstrated across all six cases: stratified reservoirs with and without crossflow for three CO₂-EOR methods, that reservoir temperature negatively impacts both recovery and CO₂ storage, while reservoir pressure exerts a positive influence. These trends are consistent with the physical behavior of CO₂ in its supercritical state, where it combines gas-like compressibility with liquid-like density, enhancing its utility as an injection fluid for EOR operations. The negative influence of temperature on recovery factor and CO₂ storage can be attributed to the reduced solubility of CO₂ in crude oil and water at elevated temperatures. Supercritical CO₂ becomes less miscible with oil as temperature rises, decreasing its effectiveness in reducing oil viscosity and interfacial tension. Additionally, higher temperatures can impair the stability of the CO₂-oil miscible zone, resulting in poorer displacement efficiency. These observations align with findings by Comberiati (1982), who demonstrated that oil recovery decreases with increasing temperature when operating above critical conditions. Furthermore, lower temperatures enhance CO₂ solubility in water and oil, which is beneficial for both recovery efficiency and CO₂ storage capacity. Conversely, reservoir pressure has a positive impact, as higher pressures improve CO₂ miscibility with oil and its solubility in water. This results in more efficient oil displacement and increased CO₂ retention in the reservoir. Elevated pressures enhance the density of supercritical CO₂, thereby improving its ability to mobilize and displace trapped oil while simultaneously increasing the amount of CO₂ that can be stored in pore spaces. This observation aligns with Mosavat (2010) and Fathollahi (2015), who highlighted the positive role of high operating pressures in improving oil recovery and CO₂ storage performance, particularly in Carbonated Water Injection (CWI) scenarios. The trends observed in this study are illustrated in Figures 5-13 and 5-14, where the black curves represent the base case scenario, and the turquoise curves show variations in reservoir temperature and pressure. The results clearly show that lower temperatures and higher pressures optimize both recovery factors and CO₂ storage capacity, with notable improvements as these parameters deviate from the base case. The implications of these findings are significant for CO₂-EOR applications in Newfoundland reservoirs and similar geological settings. Reservoirs with lower temperatures and higher pressures offer favorable conditions for maximizing both recovery and storage, enabling operators to meet dual objectives of enhanced hydrocarbon production and effective carbon sequestration. However, these operational insights must be balanced with practical considerations, such as the economic feasibility of achieving high pressures and the potential challenges of injecting CO₂ into colder reservoirs, which may require additional thermal management. Furthermore, while the results are consistent with existing literature, they underscore the importance of tailoring EOR strategies to specific reservoir conditions. For example, reservoirs with lower initial pressures may require extensive pressure build-up to achieve optimal results, whereas naturally high-pressure reservoirs could capitalize on these inherent advantages. Similarly, in temperature-sensitive reservoirs, operational adjustments like optimizing injection schedules or using alternative fluids may help mitigate the negative impacts of elevated temperatures on CO₂ performance.

Overall, this sensitivity analysis reinforces the critical role of reservoir temperature and pressure in CO₂-EOR design, offering actionable insights to maximize both oil recovery and CO₂ storage. These results contribute to the growing body of research that supports the adoption of CO₂-EOR as a dual-purpose technology for sustainable hydrocarbon production and greenhouse gas mitigation.



FIGURE 5-13: Sensitivity analysis for oil recovery factor for CO₂-WAG for stratified reservoir with cross flow



FIGURE 5-14: Sensitivity analysis for CO₂ storage for CO₂-WAG for stratified reservoir with cross flow 3.4 Proxy models

The development of proxy models using a three-layer neural network demonstrates an efficient and accurate approach to predicting the oil recovery factor and the amount of CO₂ storage as a function

of reservoir pressure and temperature. These proxy models were built for six distinct cases, covering stratified reservoirs with and without crossflow for three types of CO₂-EOR (CO₂-WAG, enriched CO₂-WAG, and CWI). Proxy models are particularly valuable for rapidly estimating key reservoir performance metrics, enabling optimization and decision-making without the computational overhead of running full reservoir simulations repeatedly. Figures 5-15 and 5-16 illustrate the effectiveness of the proxy model for the CO₂-WAG case in a stratified reservoir with crossflow. The alignment of training (blue points) and validation (green points) datasets along the 45-degree line indicates a high level of accuracy in predicting both oil recovery factor and CO₂ storage. The determination coefficients (R² values) between 0.93 and 0.99 across all cases further validate the reliability of these models. Such high R² values signify that the proxy models effectively capture the complex nonlinear relationships between reservoir conditions (pressure and temperature) and the performance outcomes of interest. The success of these proxy models highlights the capability of neural networks to handle multivariable systems with nonlinear interactions. In this context, a three-layer neural network was chosen as it offers sufficient complexity to model the intricate dependencies between reservoir parameters and performance metrics without the risk of overfitting associated with deeper networks in small to medium-sized datasets. This balance is critical in reservoir engineering applications, where data availability is often limited, and the inclusion of extraneous layers can lead to diminished model generalization. The use of proxy models also has practical implications for field operations and strategic planning. Operators can utilize these models to perform sensitivity analyses, optimize injection strategies, or assess the feasibility of CO₂-EOR methods under various reservoir conditions more rapidly. For instance, quick evaluations of the impact of reservoir pressure and temperature changes on recovery and CO₂ storage allow for more adaptive management of reservoir performance. This is particularly advantageous for real-time decision-making during field development or operational adjustments.

In conclusion, the use of three-layer neural-network proxy models for predicting oil recovery and CO₂ storage offers a significant advancement in the application of machine learning to reservoir engineering. These models not only streamline the prediction process but also enable more effective reservoir management, operational optimization, and strategic planning, aligning with the industry's goals of enhancing hydrocarbon recovery and managing CO₂ emissions. The high accuracy and reliability of these models across all six cases underscore their potential as valuable tools for accelerating decision-making and improving EOR project outcomes.



FIGURE 5-15: Proxy model for CO₂ storage for CO₂-WAG for stratified reservoir with cross flow



FIGURE 5-16: Sensitivity analysis for oil recovery factor for CO₂-WAG for stratified reservoir with cross flow

4 Conclusions

This study addresses the challenges of utilizing CO₂-EOR methods in offshore reservoirs, particularly in scenarios where CO₂ availability is limited, and there is a growing emphasis on reducing emissions from oil production. By focusing on the applicability of CO₂-EOR methods using post-combustion CO₂ captured through membrane technology, the work evaluates the effects of CO₂ impurities, reservoir stratification, and inter-layer communication under varying reservoir pressure and temperature conditions. The key findings are summarized as follows:

Limited CO₂ Availability: Offshore reservoirs often have limited CO₂ supply due to their distance from CO₂ sources, making CO₂ flooding challenging. However, methods like CWI, CO₂-WAG, and enriched CO₂-WAG can still be effective for individual blocks in such reservoirs.

- Effect of CO₂ Impurities: At the studied levels of CO₂ impurities and gas volumes, their effect on oil recovery factor is minimal. However, higher impurity concentrations or larger CO₂ injection volumes could significantly affect EOR performance, requiring careful consideration.
- CWI Performance: CWI produces the highest oil recovery for both stratified reservoirs with and without crossflow. However, the amount of CO₂ stored using CWI is only half of what can be achieved with CO₂-WAG or enriched CO₂-WAG, making CWI less efficient for CO₂ storage. Consequently, CO₂-WAG and enriched CO₂-WAG methods have much lower emissions intensity and higher tax credit values for CO₂ storage.
- Stratified Reservoirs Without Crossflow: All injection scenarios in stratified reservoirs without crossflow resulted in lower recovery factors and earlier water breakthrough. A higher WAG ratio (3:1) helped mitigate some of these issues by balancing the oil yield penalty and improving recovery.
- Impact of Reservoir Temperature and Pressure: Recovery factors and CO₂ storage increase with lower temperatures and higher pressures, as CO₂ is in its supercritical state in the studied range, which enhances its density and solubility, leading to better oil recovery and CO₂ storage.
- Proxy Model Performance: The proxy models built to predict oil recovery and CO₂ storage performed well, with high R² values ranging from 0.93 to 0.99, demonstrating their effectiveness in quickly estimating outcomes for varying reservoir temperature and pressure conditions.

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Chapter 6 : DIRTY CARBON – IMPACT OF CO₂ VOLUME AND IMPURITIES ON CARBON UTILIZATION FOR EOR AND CARBON NEUTRAL OIL PRODUCTION

Preface

It is a presentation: Pham, Q.C and James, L.A. Dirty Carbon – Impact of CO₂ Volume and Impurities on Carbon Utilization and Carbon Neutral Oil Production. 2024. Presented at Carbon Capture, Utilization, and Storage Latin America. Rio de Janeiro, Brazil, 22-23. I am the primary author. Co-author Dr. Lesley James is senior supervisor. Dr. James reviewed, provided technical assistance and valuable insights to improve the paper concept. This draft paper will be submitted to a journal.

1. Introduction

The literature review is presented and updated in the Chapter 2 part 4.

2. Methodology

Figure 6-1 illustrates the workflow for this study. The research began by defining the CO₂ constraints in terms of pore volume. Variables and their ranges, including reservoir characteristics (e.g., temperature, pressure, permeability), oil properties (e.g., viscosity), and gas properties (e.g., composition and CO₂ impurities), were identified as shown in Table 6-1. A geological model was built using the Builder module in CMG and subsequently simulated with the provided fluid properties using the GEM module (CMG 2023). The overall objective function was determined by evaluating process performance and CO₂ storage potential, integrating economic factors such as oil prices and tax credits for CO₂ storage per tonne. Optimization, sensitivity analysis, and proxy

modeling were carried out using CMOST, a CMG tool that automates workflows to deliver precise forecasts. CMOST also utilized cloud-based simulations, enhancing project delivery and decisionmaking (CMG 2023; Intelligent Optimization & Analysis Tool 2021). Different CO₂-EOR scenarios for a stratified compositional reservoir model (with and without crossflow) were optimized using Multi-Objective Particle Swarm Optimization (MOPSO). Sensitivity analyses were conducted using Sobol's method to evaluate the influence of variable parameters on the overall objective. Finally, proxy models were developed using artificial neural networks (ANNs) for each CO₂-EOR scenario. These models enable rapid and accurate estimations of the overall objective, oil recovery factor, and CO₂ storage potential for reservoirs within the studied range, offering a valuable tool for initial feasibility assessments.



FIGURE 6-1: Workflow for investigating the impact of CO₂ volume and impurities on carbon utilization for EOR and carbon neutral oil production

TABLE 6-1: Varia	ble parameters and	d their ranges/values
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Parameters	Range/Value
Reservoir Temperature (°C)	50 - 130
Reservoir Pressure (MPa)	20 - 70
Reservoir Permeability (mD)	1 - 3000
Oil Types	Light (API 35-45)
	Medium (API 25-35)
	Heavy (API 15-25)
CO ₂ Constrained (pore volume basic)	0.25 – 1

CO ₂ Impurities (%) 10 –	- 50
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2.1 Estimation of available CO₂ volume

Table 6-2 presents the gas composition used in this study, closely resembling the gas analyzed for the Hibernia well (Core Laboratories Canada Ltd., 2005).

Component	Mol %
Carbon Dioxide	0.0087
Nitrogen	0.0004
Methane	0.8506
Ethane	0.0605
Propane	0.0312
Iso-Butane	0.0005
n-Butane	0.0135
Pentane Plus	0.0346
Total	1.0000

TABLE 6-2: Gas composition used in this study

After the combustion process, carbon capture technologies are employed to capture CO_2 . The primary methods used for CO_2 capture include absorption, adsorption, and membrane separation. Absorption typically uses solvents to capture CO_2 , while adsorption relies on solid materials to trap the gas. Membrane separation, on the other hand, utilizes selective permeability to separate CO_2 from other gases. Other emerging and novel technologies for CO_2 capture have also been investigated, including Direct Air Capture (DAC), which extracts CO_2 directly from the atmosphere, as well as methods like supersonic separation, hydrate-based separation, and cryogenic distillation.

In this study, membrane technology is selected due to its compact size and low maintenance requirements (Pham, 2021). The membrane process offers advantages in that it requires minimal gas pre-treatment while maintaining high efficiency. A novel hollow-fiber membrane technology, known for its high resistance to chemical deterioration, has been developed, making it suitable for

CO₂ capture in offshore EOR applications (CSLF Offshore CO₂-EOR Task Force, 2017). For this study, CO₂ impurities are primarily considered to be methane, which is commonly present in produced gas for EOR purposes (Pham, 2021). The volume of CO₂ injected is calculated based on the pore volume (PV) constraint. The Voidage Replacement Ratio (VRR) - the ratio of injected fluid volume to produced fluid volume - was set to 1 and used as the key parameter to establish the CO₂ injection constraints.

2.2 Simulation

The simulation was performed using CMG software. First, a geological model was constructed in the Builder module to prepare for the simulation. Next, the GEM module, which is a leading reservoir simulator for compositional, chemical, and unconventional Equation of State (EOS) modeling, was employed to simulate the provided fluid properties. The GEM module is particularly useful for complex reservoir simulations, as it allows for accurate modeling of multi-phase flow and chemical reactions in the reservoir (CMG, 2023). The specific simulation details and parameters used in this study are outlined in the section below, including fluid composition, reservoir characteristics, and boundary conditions, which are crucial for accurately representing the behavior of the reservoir and the fluid interactions.

2.2.1 Block modelling

A reservoir block model was constructed with dimensions of $1200 \text{ m} \times 500 \text{ m} \times 80 \text{ m}$, divided into five main reservoir zones along the z-direction, each with equal thickness. The permeability values for these zones were 100, 200, 250, 300, and 300 mD, respectively, while the average porosity for each layer was 0.15, 0.18, 0.17, 0.2, and 0.1, respectively. During the optimization process, the stratification level remained unchanged, maintaining the ratio of 1:2:2.5:3:3 between the layers. Thin shale beds separated the reservoir zones, which, although negligible in thickness, controlled
the transmissibility between the layers. The model assumes uniform vertical transmissibility, with vertical transmissibility set to 1 in Figure 6-2(a) to allow cross-flow and communication between all layers, while in Figure 6-2(b), it was set to zero to prevent cross-flow and isolate the layers. Additionally, the reservoir is modeled with homogeneous zones having uniform properties, negligible impact from the shale layers on flow, and no-flow boundary conditions. The geometry assumes a simplified setup with one injector on one side and one producer on the opposite side of the reservoir. This setup helps to model different flow dynamics based on whether or not crossflow between the layers is permitted.



FIGURE 6-2: Stratified reservoir model with five layers with a) crossflow and b) no crossflow

2.2.2 Numerical set-up for different CO₂EOR types

The block model was initialized at 31 MPa at a depth of 3500 m below mean sea level subsea. The simulation for each CO₂ EOR type was run for four years after approximately one year of primary depletion. Figure 6-3 shows the detailed steps and respective values to set up the simulation for each injection scenario. Multi-Objective Particle Swarm Optimization was applied to optimize the cumulative oil production and CO₂ storage considering the price of oil and the value of the tax credit, which is presented in Equation(1). The proxy models were generated by using a Multi-Layer

Neural Network, which can be used to quickly predict either the cumulative oil production, or CO₂ storage or both without rebuilding the geological model.

Voidage displacement refers to the process where injected fluids, such as CO₂, replace the oil, gas, and water in a reservoir, helping to maintain reservoir pressure and mitigate surface subsidence, which can occur in certain fields. The Voidage Replacement Ratio (VRR) is a critical parameter in this process, defined as the ratio between the volume of injected fluid and the volume of produced fluid. When VRR is set to 1, it indicates that the injected fluid volume matches the produced fluid volume, maintaining the pressure balance in the reservoir. This ratio is commonly used to determine the constrained volume of CO₂ for enhanced oil recovery (EOR) and carbon sequestration (CCS) projects, ensuring efficient displacement and maximizing both oil recovery and CO₂ storage.



FIGURE 6-3: Simulation methodology and design of experiments

2.3 Optimization

The overall objective function of optimization in this study, showed in equation 1, considers the cumulative oil production and amount of CO_2 storage.

$$F = a_1 * Cumulative \ oil \ production + a_2 * CO_2 \ storage \tag{1}$$

where F is the overall objective function of optimization, a_1 and a_2 are the weight of cumulative oil production and CO₂ storage, respectively. In this study, the values of weight are the price of oil (Crude Oil Prices Today 2022) and the value of the tax credit (Waltzer 2017), which takes account the important degree of each sub-objective. The 50:50 weighting between oil recovery and carbon storage objectives in the optimization function is chosen to reflect a balanced approach that equally prioritizes economic and environmental goals. Oil recovery is a key economic factor, as it directly

contributes to profitability through increased crude oil production. On the other hand, carbon storage is essential for mitigating the environmental impact of CO₂ emissions, aligning with global sustainability efforts and climate change mitigation strategies. This balance between oil recovery and carbon storage objectives ensures that the optimization process does not solely focus on financial gains but also contributes to the long-term environmental benefits of carbon sequestration. In real-world applications, the 50:50 balance between oil recovery and carbon storage objectives can be adjusted based on external factors, such as market conditions, policy changes, and environmental incentives. For instance, when oil prices are high, the weighting could be shifted to prioritize oil recovery to maximize economic returns. Conversely, during periods when carbon taxation is more stringent or when there are substantial tax credits for CO₂ storage, the model could place more emphasis on carbon sequestration. This flexible approach allows the optimization function to adapt to different economic and regulatory environments. The initial 50:50 weighting serves as a balanced starting point, reflecting the dual importance of enhanced oil recovery (EOR) and carbon storage in achieving both energy production and environmental sustainability goals, especially as the energy sector transitions toward more sustainable practices.

Particle Swarm Optimization (PSO) is a heuristic, population-based optimization algorithm introduced by Eberhart and Kennedy in 1995. PSO stands out for being straightforward to implement and highly effective at addressing complex optimization challenges. It has been successfully applied to production optimization tasks (Humphries, 2014; Wang, 2016). The algorithm mimics the behavior of a swarm of particles (representing potential solutions) moving through the search space to find the optimal solution. Each particle in the swarm has a position that corresponds to a potential solution, and it adjusts its position based on two key factors: its personal best position (*pbest*), which is the best solution it has encountered, and the global best position (*gbest*), which is the best solution found by any particle in the swarm. The movement of each

particle is influenced by both its own experience and the experiences of its neighbors, incorporating a concept of social interaction to guide the search for the global optimum. This cooperative search mechanism enables PSO to efficiently explore the solution space and find the best possible outcome for a given problem.

Assuming we have P particles, $X_i(t)$ and $V_i(t)$ are the position and velocity of particle I at iteration *t*. In the next iteration, the position is updated as equation 2:

$$X_i(t+1) = X_i(t) + V_i(t+1)$$
(2)

The velocity is updated following equation 3:

$$V_i(t+1) = wV_i(t) + c_1 r_1 (pbest_i - X_i(t)) + c_2 r_2 (pbest_i - X_i(t))$$
(3)

where r_1 and r_2 are random numbers between 0 and 1, w, c_1 and c_2 are the inertia weight, the cognitive and social learning coefficients, respectively. c_1 and c_2 are the learning parameters or acceleration constants, which can be typically taken. w is equivalent to introducing a virtual mass to stabilize the motion of the particles, can be taken as a constant, which helps the algorithm to converge more quickly. The velocity relates to the lower and upper boundaries of the search space so depends on the input parameters and their ranges. Figure 6-4 shows the velocity vector of particle *i*.



FIGURE 6-4: Velocity vector diagram Particle Swarm Optimization

PSO is guaranteed to converge to a stable equilibrium point if the two conditions below are satisfied (Perez 2007):

$$0 < c_1 + c_2 < 4 \tag{4}$$

$$\frac{c_1 + c_2}{2} - 1 < w < 1 \tag{5}$$

Multi-Objective Particle Swarm Optimization (MOPSO), introduced by Coello in 2004, is an extension of the traditional PSO algorithm designed to address multi-objective optimization problems. MOPSO adapts the standard PSO framework to optimize multiple conflicting objectives simultaneously, offering a set of solutions, known as the Pareto front, that represents the trade-offs between different objectives. In this study, MOPSO was applied to solve multi-objective problems, with its flowchart and parameter settings detailed in Figure 6-5 and Table 6-3. The parameters used in the MOPSO algorithm include the inertia weight (w), and the acceleration coefficients (c_1 and c_2), which control the influence of the particle's personal best and the global best positions on its movement. These specific values of w, c_1 , and c_2 were selected based on previous studies that demonstrated good convergence results, such as those by Bansal (2011) and Cai (2009), ensuring efficient exploration and exploitation of the search space for optimal multi-objective solutions.



FIGURE 6-5: Multi-objective Particle Swarm Optimization flowchart

Parameters	Value
Total number of experiments	500
Inertia Weight (w)	0.7
Cognition Component (c1)	0.5
Social Component (c ₂)	1.25
Population Size	20

TABLE 6-3: Multi-objective Particle Swarm Optimization setups

2.4 Sensitivity analysis

The sensitivity analyses were conducted using Sobol's method, a variance-based sensitivity analysis technique (Variance-based sensitivity analysis, 2022). This global sensitivity analysis approach evaluates the contribution of each input parameter to the output by calculating Sobol indices. Parameters with sensitivity indices greater than 5 % are considered significant. In this study, the variable parameters, listed in Table 1, include reservoir characteristics (temperature, pressure, permeability), oil types, CO₂ constraints, and CO₂ impurities. These factors were assessed for their impact on the overall objective function (F), oil recovery factor, and the amount of CO₂ stored. This method helps identify the most influential variables, guiding decisions for optimizing Enhanced Oil Recovery (EOR) and Carbon Capture and Storage (CCS) strategies.

2.5 Proxy model

Rather than using a full numerical simulation model, a proxy model was chosen to save computational time. Proxy models have become a common practice in the oil and gas industry, particularly for reservoir simulation. These models simplify complex reservoir dynamics by approximating the results of more computationally expensive simulations. As a result, they allow for faster assessments of subsurface conditions and uncertainties, which is crucial for making timely field development decisions (Bahrami, 2022; Sanz, 2021). By capturing the essential behaviors of the reservoir, proxy models provide valuable insights without the need for time-intensive simulations. Their application is particularly beneficial when multiple iterations are required, such as in optimization processes or scenario analysis, where time constraints are significant. The use of proxy models enables more efficient and flexible reservoir management, reducing the time and cost associated with traditional simulation methods. In this study, the proxy model was generated using a multi-layer neural network, as depicted in Figure 6-6. The training and test datasets were derived from simulation experiments, with a total of 500 data points used.



FIGURE 6-6: Neural Network Proxy model workflow

In this study, a three-layer neural network was utilized, consisting of one input layer, one hidden layer, and one output layer, as shown in Figure 6-7. Initially, a five-layer neural network model was also tested. However, the results indicated that the three-layer model provided better prediction performance, as evidenced by a higher coefficient of determination (R^2). The neural network operates by transferring the input data to the hidden layer through weighted connections. Within the hidden layer, the input is processed using an activation function, which introduces non-linearity and enables the model to capture complex relationships within the data. The processed information is then passed to the output layer, where it is further controlled by weight vectors, which determine the final output prediction. The structure of the three-layer network offers a balanced trade-off between model complexity and prediction accuracy, making it more suitable for the task at hand.



FIGURE 6-7: Three-layer neural-network model

The performance and accuracy of the proposed model were evaluated using several metrics: the coefficient of determination (R²), Root Mean Square Error (RMSE), and RMSE percentage (RMSE (%)). These metrics provide insight into the model's predictive power and its error levels. R² measures the proportion of variance in the dependent variable that is predictable from the independent variables. An R² value close to 1 indicates a high level of predictive accuracy, meaning the model explains most of the variance in the data. RMSE is a measure of the average magnitude of the error between predicted and actual values. It is expressed as the square root of the mean squared error (MSE). Lower RMSE values indicate better model performance. RMSE percentage is the RMSE normalized by the range of the observed data, expressed as a percentage. It allows for a relative comparison of the error magnitude across different datasets. For an ideal model, the R² value should be as close to 1 as possible, indicating that the model explains most of the variance in the data. The RMSE should be as low as possible, indicating minimal error in the predictions. The RMSE (%) should also be small, indicating that the model's prediction error is minimal relative to the scale of the data.

$$R^{2} = 1 - \frac{\sum_{i}^{N} (Calc.(i) - Exp.(i))^{2}}{\sum_{i}^{N} (Calc.(i) - average(Exp.(i)))^{2}}$$
(6)

$$RMSE = \sqrt{\frac{1}{N} \sum_{i}^{N} |Calc.(i) - Exp.(i)|^2}$$
(7)

$$RMSE(\%) = \frac{RMSE}{MMP \ average} \tag{8}$$

3. Results and Discussion

The optimization process was carried out for two types of reservoirs: a stratified reservoir with, and without, crossflow. For each reservoir, three injection scenarios were investigated including CO₂-WAG, enriched CO₂-WAG and CWI, hence a total of six cases were evaluated. Multi-objective PSO was applied to optimize CO₂ EOR types regarding reservoir temperature, pressure, temperature, oil types, CO₂ constraints, and CO₂ impurities. The sensitivity analysis study was performed for each case to determine the influence of input parameters on the overall objective, which is the combination of produced oil value and CO₂ tax credit value, as well as oil recovery factor and amount of CO₂ storage. Finally, proxy models based three layer-neural-network were built, which can be used to predict the overall objective as well as oil recovery factor and amount of CO₂ storage for offshore reservoirs.

Table 6-4 shows the optimal solution for each case including reservoir type (transmissibility Tr), CO₂ EOR type, temperature (T), pressure (P), permeability of the first layer(K), oil viscosity (μ_{oil}), CO₂ constraint, CO₂ impurities (Imp), recovery factor (RF), corresponding amount of CO₂ storage and overall objective (F).

Reservoi r types	T r	CO ₂ EOR types	T (°C)	P (mPa)	K (mD)	µ _{oil} (cP)	CO2 constraint (PV)	Imp (%)	RF (%)	CO ₂ stored (Mtonnes)	F (M\$)
Stratifie d with crossflow	1	CO ₂ - WAG	50	20.0	167	0.89	0.94	0	75.2	12.4	567
	1	Enriched CO ₂ - WAG	50	20.0	112	1.30	0.94	10	74.7	11.6	530
	1	CWI	100	64.4	334	1.05	N/A	0	80.4	4.8	321
Stratifie d without crossflow	0	CO ₂ - WAG	50	20.0	100	1.16	0.90	0	79.8	10.8	497
	0	Enriched CO ₂ - WAG	50	20.0	100	0.93	0.90	10	71.7	7.1	355
	0	CWI	100	60.0	200	1.00	N/A	0	77.0	3.3	240

TABLE 6-4: Summary of optimal solutions for different cases

Figures 6-8 to 6-10 show the optimization results from Multi-objective Particle Swarm. The optimization of CO₂-WAG, enriched CO₂-WAG, and CWI methods for both reservoirs are shown in two cases: (a) with crossflow (left) and (b) without crossflow (right). In the optimization process, various parameters were considered, including reservoir characteristics (temperature, pressure, permeability), oil characteristics (viscosity), fluid compositions (impurities), and the amount of injected CO₂ (CO₂ constraint). The optimum point is marked in orange, while the other simulated points are represented in blue. This approach allows for the identification of the most efficient CO₂ injection strategy under different reservoir conditions and constraints.



FIGURE 6-8: Optimization simulation for CO₂-WAG a) with crossflow and b) without crossflow



FIGURE 6-9: Optimization simulation for enriched CO₂-WAG a) with crossflow and b) without crossflow



FIGURE 6-10: Optimization simulation for CWI a) with crossflow and b) without crossflow







3.1 Comparison among CO₂-EOR methods

The findings from the simulation and optimization study highlight several key insights into the effectiveness of different CO2 - enhanced oil recovery (CO2-EOR) strategies, CO2-WAG, enriched CO₂-WAG, and CWI, across varying reservoir conditions. The optimum conditions for CO₂-WAG and enriched CO₂-WAG were found at low reservoir temperature (50° C) and pressure (20 MPa), regardless of whether the reservoir had crossflow or not. These conditions suggest that for these injection methods, a lower-temperature and lower-pressure environment is more favorable, likely because the CO₂ remains in a supercritical state in such conditions, which improves its miscibility with oil and enhances displacement efficiency. This result is consistent with previous studies that suggest CO₂-EOR methods, especially WAG processes, are most effective when the CO₂ is injected under conditions that favor its supercritical state - allowing for better mixing and greater displacement of oil from the reservoir. In contrast, CWI (Continuous Water Injection) achieved its optimum performance at higher temperature (100 °C) and pressure (around 60 MPa). These conditions promote better CO₂ dissolution in water, which is essential for the CWI process. The higher temperature and pressure improve the solubility of CO₂ in water, making it more effective at contacting the residual oil, reducing its viscosity, and thereby enhancing oil recovery. As a result, CWI produced the highest oil recovery factor compared to the other two methods, reaching an average of 68 % in reservoirs with crossflow, and 60 % in those without crossflow. The improvement is attributed to the interaction between CO₂ and the trapped oil, where CO₂ dissolves into the water phase, reducing the oil's viscosity, lowering the interfacial tension (IFT) between oil and water, and causing the oil to swell, which all contribute to incremental oil recovery. However, this enhanced recovery came at the cost of CO₂ storage. In comparison with CO₂-WAG and enriched CO₂-WAG, CWI stored only 40 % of the CO₂ that could be injected and stored by the

other two methods. This discrepancy occurs because, in CWI, CO₂ is dissolved in the water phase, which inherently limits the amount of CO₂ that can be injected into the reservoir compared to the direct CO₂ injection methods used in CO₂-WAG and enriched CO₂-WAG. These latter methods inject CO_2 directly into the oil-bearing zone, where it can be stored in both its supercritical form and in solution with the oil. Despite CWI's superior recovery factor, the overall objective, which includes both oil recovery and CO₂ tax credits, was higher for CO₂-WAG. This is because CO₂-WAG not only produced a high recovery factor but also allowed for more CO₂ storage, making it the more effective method when considering both economic and environmental aspects (i.e., the CO₂ tax credit). In other words, CO₂-WAG maximizes the combination of oil production and CO₂ storage, providing a better overall performance in terms of the economic benefits derived from the CO₂ tax credits associated with the amount of CO₂ stored. The findings also suggest that the impurities in the injected CO₂ (e.g., CH₄) have a minor effect on the oil recovery factor when present at low concentrations (10%). However, as the impurity concentration increases, especially in larger volumes of injected gas, the impact on Minimum Miscibility Pressure (MMP) and overall recovery efficiency becomes more significant. CH₄, in particular, has been shown in previous studies to increase MMP, which can negatively impact the efficiency of CO₂ injection and ultimately lower the recovery factor (Alston 1985, Yellig 1980, Johannes 2009; Strydom 2009). Thus, the results align with past findings, emphasizing the importance of minimizing impurities in the injected CO₂ for optimal recovery performance.

In conclusion, while CWI provides the highest oil recovery due to the favorable interaction of CO_2 with the trapped oil, CO_2 -WAG remains the most balanced and promising approach when considering both recovery efficiency and CO_2 storage capacity. The ability to store more CO_2 , along with potential tax credit benefits, makes CO_2 -WAG a more advantageous strategy for

offshore reservoirs, especially those with limited CO₂ availability and a focus on reducing emissions.

3.2 Comparison between stratified reservoir with and without crossflow The findings from this study underscore the complex interplay between reservoir stratification, fluid properties, and the dynamics of various CO₂-EOR techniques. Stratified reservoirs, particularly those with multiple layers of varying permeability, present unique challenges and opportunities for improving oil recovery through optimized injection strategies. Reservoir stratification significantly impacts the displacement efficiency of CO₂-EOR processes. Sanchez (1999) highlighted the strong influence of stratification on the WAG displacement process, emphasizing that the displacement fronts depend heavily on the permeability contrast between layers. In our study, the permeability ratios across the five-layer model were modest, with ratios of 1:2:2.5:3:3, indicating a relatively low contrast compared to cases with more extreme variability. This moderate stratification facilitated better sweep efficiency compared to reservoirs with more pronounced contrasts, but performance was still inferior to reservoirs with crossflow. The presence of crossflow-fluid communication between layers-proved critical in enhancing both oil recovery and CO₂ storage across all injection methods. Crossflow enables interlayer fluid movement, allowing injected CO₂ or water to redistribute effectively, improving sweep efficiency. Without crossflow, as observed in the non-communicating stratified reservoir cases, displacement efficiency was compromised due to trapped oil in lower-permeability zones and unstable displacements caused by the low viscosity of CO₂ (Sanchez, 1999). The WAG process partially mitigated this by improving displacement efficiency through alternating gas and water injection, which reduced viscous fingering and enhanced oil sweep.

The WAG ratio played a critical role in balancing the oil yield penalty and optimizing recovery. Claridge (1982) found that higher WAG ratios reduce the impact of crossflow, enabling a more uniform sweep of the reservoir. This study corroborates Claridge's findings, showing that a WAG ratio as high as 4:1 was effective in overcoming the adverse effects of stratification in non-communicating reservoirs. The alternating injection of water and gas stabilized the displacement front, mitigating inefficiencies associated with stratification and improving the overall recovery factor. For reservoirs with crossflow, gravity segregation provided an additional mechanism to enhance recovery. Due to the significant depth of the modeled reservoirs, the density differences between water, oil, and CO₂ contributed to natural fluid separation. Water tended to move downward into lower layers, while CO₂, being less dense, migrated upwards, displacing oil from deeper zones toward higher layers. This gravity-driven redistribution significantly boosted recovery in reservoirs with crossflow by maximizing contact between the injected CO₂ and the trapped oil. Such dynamics were absent in reservoirs without crossflow, which explains their consistently lower recovery factors.

The economic analysis integrated into the optimization framework highlights the critical importance of coupling technical performance with economic feasibility. Fluctuating oil prices and CO₂ tax credits are decisive factors in the viability of offshore CO₂-EOR projects. Techniques like WAG or CWI may be prioritized depending on the economic environment. For example, in scenarios with high oil prices and robust carbon tax incentives, CO₂-WAG may be favored due to its dual benefits of high recovery and substantial CO₂ storage. Conversely, in low-carbon credit scenarios or markets with lower oil prices, CWI may become more appealing due to its higher oil recovery potential, even if its CO₂ storage capacity is lower.

The inclusion of economic variables adds a critical layer of insight, showing that the choice of injection strategy is not merely a technical decision but also an economic one. This integrated

approach ensures that the most viable strategy is selected for a given set of market conditions. Future work will focus on refining this economic-technical optimization, including a more detailed analysis of sensitivity to economic cycles, such as fluctuating carbon tax rates and oil prices. Testing various tax structures and market conditions will enable a more robust understanding of which strategies yield the highest combined technical and economic benefits. Additionally, further refinements in modeling will capture dynamic reservoir behavior and enhance the accuracy of predictions, paving the way for better decision-making in offshore CO₂-EOR projects.

3.3 Sensitivity analysis

The sensitivity analysis results using the Sobol method are displayed in Figures 6-11 to 6-13 for three CO₂-EOR types across two reservoir scenarios: (a) with crossflow and (b) without crossflow. By identifying the most impactful parameters, the findings guide targeted optimization efforts, emphasizing the interplay between reservoir properties, fluid characteristics, and CO₂ injection strategies. In the Sobol method, parameters with sensitivity indices greater than 5 % are considered significant. For the overall objective, reservoir pressure emerged as the most influential parameter, with sensitivity indices exceeding 50 % for all three CO₂-EOR types. This finding underscores the pivotal role of pressure in determining both recovery efficiency and CO₂ storage. The strong influence of pressure aligns with studies such as Comberiati (1982), which showed that oil recovery increases with pressure in supercritical CO₂ conditions. Higher pressures enhance CO₂ solubility in oil and water, reducing oil viscosity, increasing swelling, and improving displacement efficiency. These mechanisms are particularly relevant for CO₂-WAG and enriched CO₂-WAG, where CO₂'s phase behavior is critical to miscibility and sweep efficiency. Temperature had a complex but secondary influence across the studied CO₂-EOR types. While lower temperatures increase CO₂ solubility, as noted by Mosavat (2010) and Fathollahi (2015), they can also negatively

impact oil viscosity and fluid mobility under certain conditions. This duality is especially apparent in enriched CO₂-WAG, where both temperature and impurities (CH₄) interact to affect miscibility and displacement efficiency. The finding that temperature plays a secondary role to pressure in CO₂-WAG and enriched CO₂-WAG suggests that operators should prioritize maintaining optimal reservoir pressures when designing injection schemes. Permeability consistently ranked as one of the most influential factors for both oil recovery and CO₂ storage across all injection types, particularly for CWI. The results align with Sun (2021), which demonstrated that higher permeability accelerates oil mobilization and improves sweep efficiency. In this study, the stratified reservoir model highlighted that layers with higher permeability facilitate better CO₂ distribution and contact with the oil phase, enhancing recovery. For CWI, permeability determines the efficiency of water-CO₂ mixing and subsequent oil displacement, making it the dominant factor after pressure. These results reinforce the necessity of accurately characterizing permeability distributions in stratified reservoirs to predict performance reliably. Methane (CH4) impurities, relevant only for enriched CO₂-WAG, showed limited impact on oil recovery but significantly affected CO₂ storage. Methane's role in raising the Minimum Miscibility Pressure (MMP), as highlighted by Pham (2021), explains its minimal effect on recovery at the low impurity levels studied (10 %). However, Blanco (2012) found that methane reduces the efficiency of CO_2 solubility and residual trapping mechanisms during storage, highlighting its adverse effect on CO₂ sequestration. Methane increases CO₂ buoyancy, complicating injectivity and long-term storage stability. These findings suggest that minimizing impurities in CO₂ streams can significantly enhance storage efficiency without greatly affecting recovery.

The analysis identified pressure as the most critical parameter, followed by temperature and permeability. The alternating injection of CO_2 and water effectively stabilizes the displacement front, mitigating adverse effects of reservoir stratification. However, this strategy is highly

dependent on maintaining pressures above the Minimum Miscibility Pressure (MMP) to ensure effective miscibility. Temperature plays a secondary but notable role by influencing CO₂ solubility and density differences, which affect gravity segregation and sweep efficiency. Pressure emerged as the most influential factor, followed by impurities, temperature, and permeability. Methane impurities, while having a negligible effect on oil recovery, significantly reduce CO₂ storage capacity. This highlights the importance of impurity management when sequestration is a primary objective. The enriched CO₂ stream's effectiveness in enhancing recovery emphasizes the balance required between optimizing recovery and maximizing storage. In the CWI process, pressure was again the dominant factor, followed by permeability and oil viscosity. The direct dissolution of CO₂ in water aids oil recovery by reducing viscosity and interfacial tension, enhancing displacement efficiency. Permeability plays a critical role in controlling the distribution of CO₂laden water within the reservoir, making it a key factor in optimizing the process.

The findings emphasize several critical considerations for optimizing CO₂-EOR strategies. Maintaining reservoir pressures above the Minimum Miscibility Pressure (MMP) is vital for maximizing miscibility and displacement efficiency, particularly in CO₂-WAG and enriched CO₂-WAG processes. Effective management of methane and other impurities in CO₂ streams is essential for storage-focused projects, as reducing impurities enhances CO₂ storage capacity and ensures long-term sequestration stability. Accurate permeability profiling is equally crucial for designing injection strategies that optimize sweep efficiency and recovery, especially in stratified reservoirs where permeability contrasts significantly influence performance. Additionally, the interplay between recovery efficiency and storage capacity, most notable in enriched CO₂-WAG and CWI, highlights the need for integrated optimization frameworks that balance technical outcomes with economic considerations, such as carbon credits and fluctuating oil market conditions.

Future research should focus on advancing the understanding and application of CO₂-EOR strategies by addressing several key areas. Developing advanced impurity management techniques will be crucial for better balancing recovery and storage goals, particularly in projects aiming to maximize sequestration potential. Investigating the dynamic interactions between temperature, pressure, and other reservoir properties in more complex geological formations can provide deeper insights into optimizing injection strategies. Field-scale validation of these findings is also essential to evaluate the scalability and practicality of optimized injection techniques under real-world conditions. By identifying the dominant factors influencing oil recovery and CO₂ storage, this study establishes a robust foundation for improving injection strategies in stratified offshore reservoirs. These insights can drive the development of methods that achieve technical efficiency while meeting economic and environmental objectives. By identifying the dominant factors affecting both oil recovery and CO₂ storage, this study lays a solid foundation for enhancing injection strategies in stratified offshore reservoirs. These insights can guide the development of techniques that ensure technical efficacy while addressing economic and environmental objectives.



FIGURE 6-11: Sensitivity analysis for overall objective for CO₂-WAG, enriched CO₂-WAG and CWI a) with crossflow b) without crossflow



FIGURE 6-12: Sensitivity analysis for recovery factor for CO2-WAG, enriched CO2-WAG and CWI a) with crossflow b) without crossflow



FIGURE 6-13: Sensitivity analysis for CO₂ storage for CO₂-WAG, enriched CO₂-WAG and CWI a) with crossflow b) without crossflow







3.4 Proxy model

The development of proxy models using three-layer neural networks represents a significant advancement in the predictive capabilities for CO₂-EOR strategies. These models were specifically designed to forecast the overall objective, oil recovery factor, and amount of CO₂ storage across various scenarios, including CO₂-WAG, enriched CO₂-WAG, and CWI for both stratified reservoirs with and without crossflow. Figures 6-14, 6-15, and 6-16 highlight the effectiveness of these models for CO₂-WAG in stratified reservoirs with crossflow. The close clustering of both training datasets (blue points) and test datasets (green points) near the 45degree line underscores the high predictive accuracy of the proxy models. This accuracy is further validated by the coefficient of determination (R²) values, which ranged from 0.93 to 0.99, and Root Mean Square Error (RMSE) values of less than 10%. The strength of these proxy models lies in their ability to accurately emulate simulation outputs without the need for additional computationally expensive simulations. This capability is particularly useful in optimizing reservoir performance, as it enables rapid assessments of the impacts of various parameters on oil recovery and CO₂ storage. For instance, operators can use these models to evaluate the influence of changes in reservoir pressure, temperature, permeability, etc... on the overall objective, thereby streamlining decision-making processes. Additionally, the high predictive performance of these models reflects the robustness of the three-layer neural network architecture. This architecture effectively captures the nonlinear relationships between input parameters and outputs, such as oil recovery and CO₂ storage, which are critical for the success of CO₂-EOR projects. The generalizability of the proxy models across different scenarios and reservoir conditions demonstrates their utility as a reliable tool for reservoir management. In conclusion, the proxy models developed in this study offer a powerful means of optimizing CO₂-EOR strategies by providing precise, efficient, and adaptable predictions. They bridge the gap between simulation and implementation, offering a pathway to improved oil recovery and CO₂ storage while aligning with economic and environmental goals. Future research could focus on refining these models to incorporate even more complex reservoir conditions and extending their application to a broader range of geological formations.



FIGURE 6-14: CO₂-WAG Proxy Models for Overall Objective R=0.97, RMSE = 4.7 % for stratified reservoir with crossflow



FIGURE 6-15: CO₂-WAG Proxy Models for Recovery Factor R=0.99, RMSE = 3.2 % for stratified reservoir with crossflow



FIGURE 6-16: CO₂-WAG Proxy Models for CO₂ Stored R=0.95, RMSE = 6.2 % for stratified reservoir with crossflow

4. Conclusions

This study comprehensively evaluated the potential of CO₂ sequestration coupled with enhanced oil recovery (EOR) to reduce the carbon intensity of incremental oil production using different CO₂-EOR techniques. A compositional stratified reservoir model, with and without crossflow, was employed to examine the performance of CO₂-WAG, enriched CO₂-WAG, and carbonated water injection (CWI) under limited CO₂ availability, a common offshore constraint. Optimization using multi-objective Particle Swarm Optimization (PSO) was conducted to assess the effects of reservoir temperature, pressure, permeability, oil viscosity, CO₂ availability, and impurities. Sensitivity analyses were performed to identify key parameters influencing the overall objective, oil recovery factor, and CO₂ storage, while proxy models based on three-layer neural networks were developed to predict outcomes efficiently. The following key conclusions were drawn:

- Offshore reservoirs with limited CO₂ availability often lack sufficient volume for CO₂ flooding but can accommodate CWI, CO₂-WAG, or enriched CO₂-WAG for individual reservoir blocks.
- Optimum conditions for CO₂-WAG and enriched CO₂-WAG occurred at a reservoir temperature of 50 °C and pressure of 20 MPa, while CWI reached its optimum at higher conditions of 100 °C and approximately 60 MPa.
- The best performance was associated with high-quality reservoirs, high oil viscosity, a large volume of injected CO₂, and minimal impurity (CH₄).
- CWI demonstrated a higher average oil recovery factor compared to CO₂-WAG and enriched CO₂-WAG. However, the amount of CO₂ stored in CWI was significantly lower, at approximately 40% of the storage achieved with CO₂-WAG or enriched CO₂-WAG, resulting in a reduced overall objective value (approximately 50% of the other methods).

- Reservoir pressure had the most significant influence on the overall objective across all CO₂-EOR methods, while permeability was the dominant factor affecting the oil recovery factor.
- For CO₂ storage, the most influential parameters varied by case, with CO₂ impurities, particularly methane, having the greatest impact in enriched CO₂-WAG scenarios.
- Proxy models exhibited strong predictive performance, with R² values ranging from 0.93 to 0.99, and can be applied to forecast the overall objective, oil recovery factor, and CO₂ storage for other reservoirs without the need for additional simulations.
- The overall objective integrated both oil price and CO₂ tax credits, reflecting the economic variability in project viability. Future work will explore how fluctuating economic factors affect the feasibility and optimization of different CO₂ injection methods under varied scenarios.

These findings provide a robust framework for improving CO₂-EOR strategies, highlighting the interplay between technical, environmental, and economic factors.

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Chapter 7 : SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

This study comprehensively analyzes the optimization of CO₂ sequestration coupled with oil recovery to reduce the carbon intensity of incremental oil recovery, considering different CO₂-EOR methods, reservoir conditions, and CO₂ impurities. The research delves into how impurities affect CO₂ injection and retention, as well as the response of various oil types and reservoir characteristics to specific injection strategies. This approach is crucial for balancing enhanced oil recovery with carbon storage objectives, enabling offshore EOR projects to maximize CO₂ usage efficiency and emission reductions, contributing to sustainable energy goals.

An in-depth analysis of the relationship between different CO_2 capture technologies and the resulting impurities, their respective concentrations, and the impact on Minimum Miscibility Pressure (MMP) - covering a wide range of CO_2 concentrations (from 0 % to 100 %) - was investigated in Chapter 3, addressing a gap in the existing literature. Adsorption and absorption technologies are found to capture CO_2 with a higher purity than membrane technology. However, membrane technology has advantages of compact size, low maintenance requirements and allowance for less pre-treatment of the gas without having any significant impact on the efficiency. Impurities presented depend on the source of CO_2 ; CH_4 is found in CO_2 from the natural gas stream and O_2 and N_2 are presented in CO_2 from flue gas stream. A mixture of CO_2 and natural gas is effective at decreasing MMP. The impurities found in flue gas stream (O_2 and N_2) have a greater effect on increasing MMP of the mixture than the impurity found on natural gas stream (CH_4) as N_2 requires a much higher pressure to achieve miscibility condition than CO_2 .

The limited range of CO₂ concentrations in gas sources and the lack of sufficient data points have been key challenges in recent studies using Machine Learning to predict Minimum Miscibility
Pressure (MMP). This study addresses these issues by developing a more accurate model using a Deep Learning algorithm and k-fold Cross Validation, as presented in Chapter 4. Reservoir temperature and the amount of CO₂ and C1 in the gas source have the most influence on oil-gas MMP. Increasing the reservoir temperature, molecular weight of the oil, ratio of volatile components and intermediate components of the oil phase, or the amount of C1, N₂ in the gas phase increases MMP. The presence of CO₂ and H₂S in the gas phase will lower the MMP, especially CO₂. The comparison between Deep Learning model and the slimtube simulation for MMP values is carried out. The relative errors are no more than 7 %, which demonstrates a good agreement between two models. In future work, a series of slimtube tests can be conducted experimentally to validate the accuracy and reliability of both simulation models.

EOR studies typically focus on incremental oil recover (without considering carbon pricing), whereas Carbon Capture, Utilisation and Storage (CCUS) prioritizes maximizing CO₂ storage (assuming an infinite CO₂ supply). The joint optimization of oil recovery and carbon storage, presented in Chapter 5 and 6, considers both the price of produced oil and the value of CO₂ tax credit, using a 50:50 ratio to emphasize their equal importance. This study examines various oil types (light, medium, heavy) and conditions, including CO₂-EOR methods (WAG, CWI, enriched-WAG), CO₂ constraints, impurities, and reservoir characteristics (stratification, crossflow, temperature, pressure, permeability) through simulations using GMG. Optimization was performed using Multi-Objective Particle Swarm Optimization (MOPSO). The results indicate that CWI is the most effective method under CO₂ stored is significantly lower in the CWI case. Reservoir pressure has the greatest influence on overall objectives, while permeability has the most impact on the oil recovery factor across all three CO₂-EOR methods.

The optimization of oil recovery and CO₂ storage is a complex challenge influenced by a multitude of factors such as phase behaviour, EOR techniques, reservoir characteristics, gas availability and characteristics, also economics factors including price of oil, CO₂ tax credits and carbon pricing. Field-scale simulation, which enables the modeling of large, real-world reservoirs, is crucial for evaluating the performance of Enhanced Oil Recovery (EOR) and Carbon Capture, Utilization, and Storage (CCUS) techniques. Future work can concentrate on detailed field-scale simulations for the Hibernia reservoir, considering various boundary conditions. The Hibernia reservoir features complex geological structures, including faults, stratification, aquifer support, and a compartmentalized nature, which can function as closed or semi-closed boundaries. Additionally, stratification creates internal boundary conditions between different layers, with some acting as high-permeability flow channels (open boundaries) while others serve as barriers to fluid flow (closed or semi-closed boundaries). In real-world applications, the 50:50 balance between oil recovery and carbon storage objectives can be dynamically adjusted based on external factors, such as market conditions, regulatory changes, and environmental incentives. For example, when oil prices are high, the weighting could be adjusted to prioritize oil recovery, maximizing economic returns. On the other hand, during periods of stricter carbon taxation or when there are significant tax credits for CO₂ storage, the model could emphasize carbon sequestration. This flexibility allows the optimization model to adapt to varying economic and regulatory environments. Given the variability in oil prices and CO_2 tax incentives, it would be valuable for future work to explore different scenarios, optimizing recovery strategies under diverse conditions.

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Appendix

Appendix A

Hibernia Field Production Statistics Cumulative to March 31, 2020							
Gas Production (Bscf)	Flared (Bscf)	Fuel (Bscf)	Injected (Bscf)	Lift (Bscf)			
1925.58	99.47	117.61	1708.40	18.89			
	Flared + Fuel (Bscf)						
	217.08						
Material balance	CO_2 produced = CO_2 injected + CO_2 from combusted gas (power generation combustion + flaring) + CO_2 from fugitive emissions						
CO ₂ produced (Bscf)	CO ₂ from combusted gas (Bscf)		CO2 injected (Bscf)	CO2 from Fugitive Emission (Bscf)			
236.12	220.57		15.38	0.17			

Produced gas composition (other g rep						
CO ₂	CH ₄	C ₂ H ₆	C3H8			
0.90	86.00	7.00	4.00			
Amount in Fla						
1.95	186.69	15.20	8.68			
Amount CO2 produced	Total (Bscf)					
1.95	186.69	30.39	26.05	245.08		
Amount CO2 after membrane ca	220.57					
ombustion equations $ \begin{array}{c} \hline CH_4 + 2O_2 \to CO_2 + 2H_2O \\ \hline C_2H_6 + \frac{7}{2}O_2 \to 2CO_2 + 3H_2O \\ \hline C_3H_8 + 5O_2 \to 3CO_2 + 4H_2O \end{array} $						