

REVIEW



The Evolving Landscape of Oil and Gas Chemicals: Convergence of Artificial Intelligence and Chemical-Enhanced Oil Recovery in the Energy Transition Toward Sustainable Energy Systems and Net-Zero Emissions

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Abstract: Chemical-enhanced oil recovery (EOR) is a field of study that can gain significantly from artificial intelligence (AI), addressing uncertainties such as mobility control, interfacial tension reduction, wettability alteration, and emulsifications. The primary objective of this paper is to introduce an integrated framework for AI and chemical EOR for energy harvest operations. Central emphasis is placed on the energy transition, with the aim of expediting the development of cleaner energy harvesting systems and attaining the goal of net-zero emission. To do so, we present how the energy transition is changing the manufacturing of the chemicals for EOR application. For this, the uncertainty associated with materials' design and critical role of the simulators for transferring the laboratory experiences into full-field implementations is discussed. The concept of digitalization and its impact on energy companies are highlighted. The role of digital twin in simulators integration is discussed, emphasizing how increased data access can help design more tolerant chemicals for harsh reservoir environments using real-time data. Also, we discuss how the chemical suppliers, research institutes, startups, and field operators can benefit from self-learning and robotic laboratories for chemicals manufacturing. Moreover, this paper explores how including AI perspectives can improve our understanding of developing chemical formulations by blending hybrid capabilities. This approach contributes to making energy production more sustainable and aligning with the goal of zero emissions. A workflow is presented to demonstrate how the integration of AI and chemical EOR can be used for both hydrocarbon production and other energy transition operations, such as carbon capture, utilization and storage, hydrogen storage, and geothermal reservoirs. The outcome of this paper stands as a pioneering effort that uniquely addresses these challenges for both academia and the industry and can open many additional doors and identify topics requiring further investigations.

Keywords: artificial intelligence, chemical-enhanced oil recovery, surfactant, polymer, energy transition

1. Introduction

1.1. The background and motivation

Artificial intelligence (AI) is a field that is rapidly transforming modern life. Integrating AI into various industries is revolutionizing traditional practices that were operated manually, leading to a significant boost in the efficiency of outdated methodologies (Agrawal & Choudhary, 2016). The aviation, auto industry, and particularly the energy industry have witnessed a remarkable paradigm shift toward digitization. More specifically, the petroleum industry, with its complex and dynamic operations aimed at enhanced oil recovery (EOR), requires innovative solutions that AI can fulfill for these purposes (Cheraghi et al., 2021; Larestani et al., 2022; Kuzior et al., 2022).

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Due to the complex interactions of chemical EOR methods, which can involve chemical selection, phase behavior studies, dynamic and static investigation of materials with brine, crude oil, and rock, scaling them from core to pilot and pilot to field scales (Bigdeli & Delshad, 2023), the AI algorithms and data-driven techniques can be considered as valuable tools for parallel optimization and decision-making processes (Salimova et al., 2021; Sun et al., 2021). In recent years, there have been efforts where AI has been deployed for chemical EOR operations.

In this regard, recent investigations have tried to utilize the benefits of AI in chemical EOR studies. For example, Ahmadi and Pourmik (2016) employed support vector machines to estimate recovery factor (RF) and net present values (NPVs) for chemical flooding models. The parameters utilized for statistical analysis included surfactant slug size, surfactant concentrations, polymer drive size, salinity of polymer drive, polymer concentration in surfactant slug, and the vertical to horizontal permeability ratio.

Their original dataset comprised 202 data points. Among the various parameters, surfactant concentration was identified as the most influential factor on both RF and NPV.

Le Van and Chon (2016) utilized artificial neural network (ANN) to estimate the performance of alkali-surfactant-polymer (ASP) flooding, considering 13 parameters, including alkali concentration in AS slug, alkali concentration in the ASP slug, polymer concentration in the first polymer slug, polymer concentration in the ASP slug, polymer concentration in the second polymer slug, surfactant concentration in the AS slug, surfactant concentration in the ASP slug, first polymer slug size, AS slug size, ASP slug size, second polymer slug size, slug size of water pre-flush, and well distance. The ASP slug concentration and slug size were identified as the first and second most important parameters. The authors also provided some economic discussions in their analysis.

Ebaga-Ololo and Chon (2017) reported using ANN for predicting the performance of different injection stages of two polymer slugs during polymer flooding. They considered the following variables: polymer slug size 1, water drive, polymer slug 2, concentration of polymer slug size 1, concentration of polymer slug size 2, and injection rate. The results indicated that the size of polymer slug 1 and the injection rate were the most influential parameters.

In a related study, Sun and Ertekin (2020) employed ANN to optimize the NPV of polymer flooding. The input parameters include reservoir rock properties, initial conditions (saturation, pressure, and oil viscosity), polymer properties (viscosity, adsorption, salinity coefficient), relative permeability coefficients, slug size, pattern size, injection rate, and most notably, bottom hole pressure.

The same group of researchers (Sun et al., 2021) conducted a techno-chemical analysis for ASP using ANN. In their studies, additional parameters such as surfactant characterization parameters, molecular weight of surfactant, and adsorption of surfactant were also considered. Some additional parameters, including total acid number (TAN) and API gravity of crude oil, were also incorporated. In that work, the authors noted that project location, available chemical additives, and project times are some additional objective functions (rather than NPV) that can be considered.

Larestani et al. (2022) used ANN, decision tree, support vector machine, and gradient boosting for RF and NPV of surfactant-polymer flooding.

Applications of AI for predicting the performance of low salinity water in sandstone, including the use of linear regression, multilayer perceptron, support vector machine, and committee machine intelligent systems, were explored in a study by Tatar et al. (2021). Additionally, for carbonate samples, recent research has utilized ANN, support vector machines, and decision trees for similar predictions (Salimova et al., 2021).

Furthermore, various AI techniques, including linear regression, support vector machine, regression decision tree, and ANN, have been employed by Shakeel et al. (2023) to predict the viscosity of polymer solutions. As observed, the increasing complexity of chemical EOR methods necessitates correspondingly complex numerical models.

The primary motivation of this work is, to the best of our knowledge, to present the recent advances in chemical EOR technology with emphasis on the new horizons that AI is adding to the adoption of these methods. While some material properties and characterization have been the target of previous reviews (Sheng, 2013; Sheng, 2015; Sheng et al., 2015), and recent papers have addressed the field application (Bigdeli & Delshad, 2023), the combination of these methods with AI is lacking in the literature. Thus, this becomes the focus and motivation of this paper – to familiarize the reader with recent advancements in the chemical EOR field with the adaptation of AI techniques.

1.2. An overview of the study

This paper explores the synergy between chemical EOR and AI, showcasing recent experiences and introducing an integrated framework for energy harvest operations. Focusing on the carbon footprint of chemical EOR methods, the study addresses material uncertainties and highlights the recent advancements. Discussions include the role of numerical simulators, the transformative impact of digitalization, new horizons in energy transition for chemical EOR, the advantages of using intelligent techniques (such as machine learning and deep learning), and the potential benefits of self-learning and robotic laboratories. The integration of AI with chemical EOR is evaluated for sustainable energy production and zero-emission goals. The workflow illustrates how the combined power of AI and CEOR can be applied to various energy transition operations. This paper represents a pioneering effort addressing crucial challenges in academia and the industry.

1.3. Paper structure

This paper is divided into two parts. The first part encompasses the background and introduction, which includes an exploration of the role of AI in chemical EOR applications. A general overview of the study is presented, and the motivation behind this paper – to familiarize the reader with recent advancements in the chemical EOR processes through the adaptation of AI techniques – is highlighted.

In the second part, more in-depth analysis and details of the most up-to-date studies are introduced. This section stands out as one of the pioneering works discussing the synergy of chemical EOR and AI techniques. Topics covered include the carbon footprint of chemical EOR operations, the digitalization of mature fields, an intelligent EOR technique incorporating both machine learning and deep learning, as well as the roles of digital twin and robotic and self-learning laboratories.

2. The Related Research

The next section will present recent advancements that comprehensive analysis of how AI has affected the domains of chemical EOR.

2.1. Carbon footprint of chemical EOR

Energy transition is the main pathway for shifting global energy systems from fossil to clean fuels while preserving the environment. Global warming and energy crises necessitate a re-evaluation of obligatory carbon management within upstream sectors. Furthermore, the unequal distribution of fossil fuels and the added energy costs resulting from military conflicts in Europe serve as catalysts, speeding the energy transition in European nations and consequently, on a global scale. Several academics have lately proposed employing chemical EOR and CO₂ footprint control to address this problem (Braun et al., 2022; Dupuis et al., 2021; Dupuis & Philips, 2022; Ghosh et al., 2022; Farajzadeh et al., 2021; Farajzadeh et al., 2022; Mogollon et al., 2022). For instance, in the case of carbon capture, utilization and storage (CCUS), the impact of EOR and carbon storage in terms of oil RF for a given reserve is defined as follows:

$$RF = \left[x_1 \times \frac{\text{Oil Produced}}{\text{OOIP}} \right] + \left[x_2 \times \frac{\text{CO}_2 \text{ Injected} - (\text{CO}_2 \text{ Produced} + \text{CO}_2 \text{ Loss})}{\text{CO}_2 \text{ Theoretical Storage Capacity}} \right]$$

where in the above equation the term OOIP is originally oil in place, x_1 and x_2 are the weighting variables and range from 0 to 1 (sum of x_1 and $x_2 = 1$) based on the project's priority – whether it is an EOR or CCUS

application. Further details about the amount of CO₂ theoretical storage capacity can be found in Bello et al. (2023).

In pioneering research, Beck (2000) introduced an initial emissions forecasting approach for offshore oil and gas production. This methodology aids oil companies in predicting CO₂ and NO_x emissions from fields powered by fossil fuels. Skjerve et al. (2022) devised a high-quality emission forecasting tool, integrating subsurface and operational data. This tool establishes links between drainage and operational strategies, particularly concerning emissions tied to reservoir drainage, such as CO₂. These tools are primarily used to assess the impact of CO₂ taxation on decision-making. Angga et al. (2022) explored CO₂ tax effects on recovery processes in existing fields with waterflooding. A novel procedure can assess the composition of reinjected gas for CO₂-rich Brazilian fields. This procedure enhances production prediction, gas balance, and plant design by integrating reservoir and production system insights. The eCalc™ software, developed by Skjerve et al. (2022), functions as a tool to calculate energy demands and quantify greenhouse gas emissions linked to operations in oil and gas production and processing.

In the work of Farjzadeh et al. (2020), the authors conducted an exergy analysis to evaluate the exergetic efficiency of CO₂ storage through EOR and identified the conditions under which it proves exergetically effective. Additionally, they presented the exergy RF. Fast-tracking the integration of innovative energy sources such as geothermal energy and hydrogen as energy carriers into the energy grid, coupled with initiatives for methane emission management, direct air capture, the integration of wind farms, and the efficient utilization of surplus energy through hydropower, signifies a collaborative endeavor to reduce dependence on carbon-based fuels. However, to sustain the secure supply of global energy, it is necessary to re-evaluate traditional chemical EOR methods, until the complete energy transition takes place, to achieve decarbonization goals. The fabrication of chemicals with optimal performance and functionality is crucial, in this sense. The chemical EOR and AI are two valuable technologies that enable researchers to design novel chemicals, aiding in the consistent production from mature reservoirs during the ongoing energy transition.

3. Uncertainty of Material Development

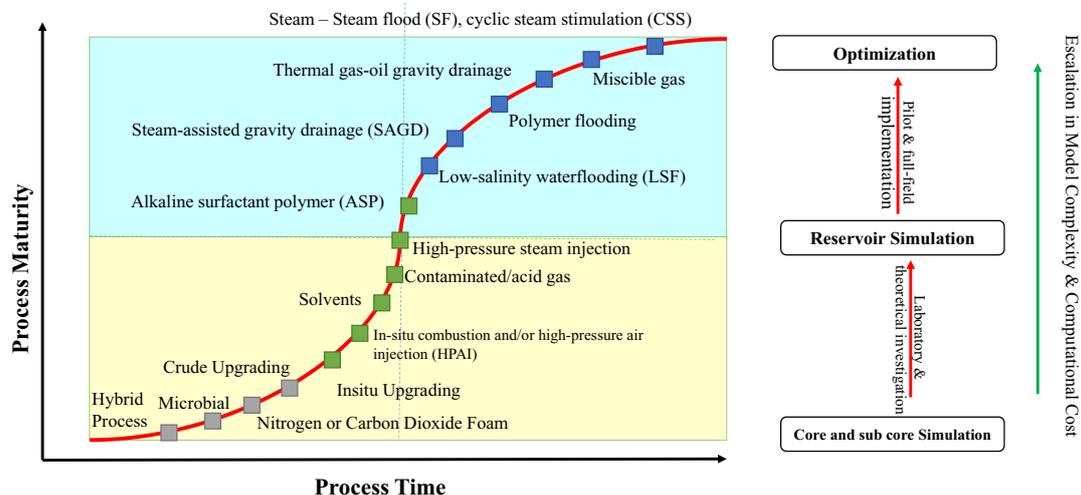
A primary challenge for developing chemicals for harsh reservoir conditions is the uncertainty associated with the fluid flow in porous media. High pressure, high salinity, high temperature, high capillary pressure, and complex fracture network are some examples that require detailed investigations before full-field commercial-scale implementations. The salinity of surfactant solution and/or shear rate selection for polymer flooding are some examples that need to be designed carefully with respect to the condition of a given reservoir (Bigdeli & Delshad, 2023). Static experimental uncertainties should also be verified under dynamic conditions, as fluids flow within the reservoir during the development of a given process for the field. The outcome of the laboratory experiments can greatly impact the economics of the EOR methods as candidates for a given reservoir. Depending on the field development plan, it is essential to understand the required method and how the uncertainty in the developed materials can impact the project, as shown in Figure 1.

Figure 1 shows the maturity of the process versus the development schedule (Babadagli, 2022).

For gas injection EOR techniques, including miscible gas injection (such as CO₂ injection), steam-assisted gravity drainage (considering steam quality), and cyclic steam stimulation, uncertainties arise from the study of phase behavior associated with the injection gas composition. Determining the minimum miscibility pressure conditions or assessing the impact of impurities, such as nitrogen oxides or sulfur oxides, on the phase envelope, significantly affects the overall performance of injection fluids. These are some examples of challenges in this field.

For thermal EOR techniques, such as in-situ combustion, solvent injection, high-pressure air, and steam injection (cyclic or gravity drainage), the process involves using heat to alter the undesirable conditions of the reservoir and fluids. This process involves reducing the viscosity of the oil, upgrading crude oil with nanoparticles, especially for heavy oils, and understanding their interactions. These are examples of uncertainties associated with thermal EOR, where AI can be utilized. Enthalpy, equation of states, phase equilibrium due to the vapor-liquid interaction, and crude oil detachment from the surface of the rock (especially

Figure 1
The maturity versus time for different EOR processes and the transformation from the lab to the full-field deployment is fulfilled by reservoir simulators



for Carbonate reservoirs) are some of the parameters that can be altered due to the thermal flux at the reservoir. The combination of all these parameters contributes to the final recovery, and the selection of associated materials, such as nanomaterials and surfactants for hybrid EOR techniques, can be accelerated when AI techniques are employed and proper databanks from previous experiments are available.

For other EOR techniques, such as low salinity water, microbial, electrical heating, or ultrasonic methods, the process of condition selection presents various uncertainties. These include determining the type of salts, pH levels, frequency, power requirements, injection rates and sequences, phase behavior considerations, as well as methodology screening. Additionally, upscaling from micro to macro scales poses challenges that AI can be useful to resolve them.

The most important consideration for transferring a newly developed chemical EOR mixture, such as a customized formulation comprising several surfactants (in-house synthesized or commercial), co-solvents, nanoparticles, and alkalis, from laboratory and theoretical investigations to either a pilot or full-field implementation is to have a reservoir simulator with capabilities for the specific EOR process, in addition to an economic model (Bigdeli & Delshad, 2023). Reservoir simulation studies can improve the practical knowledge of developed research-based materials and show their weakness/readiness at both pilot and field scales. Another useful metric for evaluating the developed material is the technical readiness level, which has been utilized in the oil and manufacturing industries (Robertson et al., 2019; Rushby et al., 2013). The upscaling of chemical EOR technologies is also a crucial aspect of their application. According to Veedu et al. (2010), as chemical EOR processes are scaled up, the number of linked variables increases dramatically. For instance, several parameters must be upscaled from lab measurements to field scale including salinity gradient, surfactant dilution, dispersion, adsorption, critical micelle concentration, and capillary desaturation curves. A recent review paper on the capillary desaturation curves for both sandstone and carbonate rocks can be found in Siyal et al. (2023). In the case of co-solvent, additional research is required regarding co-solvent partitioning and its impact on microemulsion viscosity (Dwarakanath et al., 2008). Designing new chemicals and formulations and simulation studies from sequential into parallel implementation can reduce the time required to advance from screening analysis to full-field implementation from 8 to 4 years (Rotondi et al., 2015).

The complexity of the modeling workflow is further increasing due to the large number of multi-mechanisms and multi-component processes associated with chemical EOR, as shown, for instance, in Figure 2. To compare the performance of various implemented

chemical EOR methods, a water flood can serve as the base case for efficiency evaluation (Al-Mjeni et al., 2010).

When employing hybrid EOR techniques, such as chemical huff and puff (Farog et al., 2016) or low salinity surfactant flooding (Gbadamosi et al., 2022), the interaction of the mechanisms for each process becomes significantly more intricate. Therefore, the developed numerical model should be mechanistic.

However, there is uncertainty regarding the sequence in which these processes occur. For instance, although several mechanisms for low salinity water flooding have been proposed, it remains unclear which one occurs first, or which combinations occur simultaneously (Bigdeli et al., 2023). Secondly, after selecting the appropriate EOR method, it is unclear how to transition between upscaling and downscaling at various levels while addressing multiple mechanisms. To transfer laboratory measurements into simulators for ASP flooding, Moreno et al. (2018) have made some recommendations. The findings of Kazemi Nia Korrani and Jerauld's (2022) study indicated that the upscaling of low salinity water flooding might not accurately reflect the benefits of the core scale. Moreover, the experiences reported by Sarma et al. (2022), Torrealba et al. (2019), Najafabadi and Chawathe (2016), Babaei and King (2013), Dair et al. (2020), Talabi et al. (2019a), Talabi et al. (2019b) and Moreno et al. (2021), Moreno et al. (2019a), Moreno et al. (2019b), Moreno et al. (2015), Moreno et al. (2014), Moreno et al. (2013), and Moreno and Flew (2011) are useful for practical upscaling and downscaling practices. This information is essential for chemical suppliers and field operators as they are facing more risks compared to the lab researchers (Bigdeli & Delshad, 2023).

4. Old Versus New Chemical EOR Classification

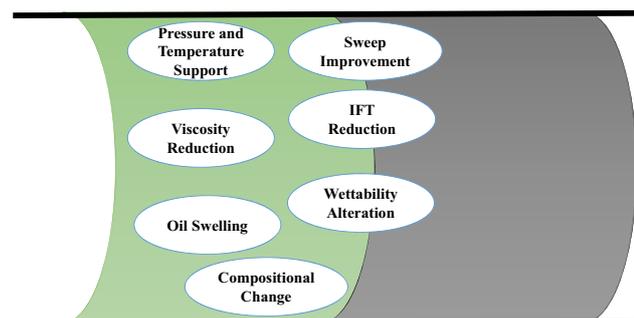
It is necessary to review the classifications of chemical EOR before exploring how AI can enhance the accuracy of current knowledge. Despite the impact of climate change and global warming on industries, it is imperative to ensure the world's energy supply continues to drive the oil and gas upstream sector to explore new frontiers. These include deep offshore reservoirs, heavy oil reservoirs, and matured water-flooded fields, all in pursuit of increased oil extraction.

To achieve this, the price of oil plays a major role in either expediting or postponing the advancement of chemical materials. Chemical EOR methods tend to be costlier compared to other techniques such as water flooding for boosting oil production. The higher cost is attributed not only to the development of the chemicals themselves but also to the need for injection and subsequent separation facilities for these chemicals from the produced fluids (Bigdeli & Delshad, 2023). As an example, as mentioned by Fink (2015), chemicals like surfactants, polymers, inhibitors, and nanomaterials have over 20 applications related to oil and gas fields. These applications include functions such as drilling mud, corrosion inhibition, scale inhibition, clay stabilization, bacterial control, filter cake removal, cement additives, gas hydrate control, fracturing fluids, water shutoff, demulsifiers, defoamers among others.

Although there has been a huge amount of effort to introduce and improve the quality of the developed chemical, the conventional approach to assessing chemical EOR methods is outdated. Surfactant phase behavior, core flooding, analysis of chemical adsorption and retention, the residual resistance factor of polymers, filtration ratio of polymers, and polymer stability are some of the standard experiments (Dean et al., 2022). By reviewing and updating these tests, reservoir engineers and field engineers can update the reservoir simulator models to forecast the final performance of chemicals at

Figure 2

Multi-mechanisms are presented for modeling chemical EOR



both pilot and full-field scales. This is even more crucial when hybrid chemical EOR methods are under investigation.

Raffa (2021) recently introduced a new classification of chemical EOR in comparison with traditional classification. Hybrid methods, a combination of ASP, surfactant–polymer (SP), and alkaline–polymer (AP) with nanoparticles, surfactants with ultra-low interfacial tension (IFT), surfactants, and polymers that tolerate high pressure and high temperature, low salinity, smart and engineered water flooding are some new improvements. In this regard, Bigdeli and Delshad (2023) reported a comprehensive review paper on the practical applications of chemical EOR methods and the current experiences of chemical EOR operations can be transferred from laboratory to full-field operations.

The mineralogy of reservoir rocks, composition of injected brine and crude oil properties, such as TAN, and equivalent alkane carbon number (EACN), reservoir temperature, and geochemical interactions of fluid with reservoir rock minerals, the price of chemicals, and their availability and quality are a few factors that must be considered. The increased surface activity particularly in carbonate reservoirs, chemical reactions, cation exchange, and mineral dissolution necessitate coupled reactive transport models such as PH REDox EQUilibrium in C language (PHREEQC) (Kazemi Nia Korrani, 2014) and chemical flood reservoir simulators.

As an example, Delforce et al. (2022) presented two new methods to calculate the EACN with neural network and graph machines. The information from COSMOtherm, a tool for the quantitative calculation of solvation mixture thermodynamics based on quantum chemistry, was employed by neural networks while the graph machines combined simplified molecular input line entry specification tools. These studies demonstrate that there are new methods to select the appropriate experimental conditions in addition to conventional test tube evaluation of surfactant phase behavior.

The new EOR classification facilitates a better understanding of the required methods, resulting in the precise selection and application of new materials. Hybrid capabilities can boost innovative approaches for complex reservoirs, depending on tailored experimental conditions. Accurate modeling is essential, and the transferability of these new methods to full-field operations can be questioned.

Complexity and cost, along with limited practical experience, especially for full-field operations, are challenges. Dependency on technology, such as ANNs and deep learning, as well as simulators that can handle all required chemical EOR methods, including microemulsion flooding and their complex thermodynamic interactions, poses potential issues. Consideration of multiple factors, such as reservoir rock mineralogy, brine properties, crude oil characteristics, quality, and affordability of chemicals, and the facilities for their injection processes at the surface are some of the advantages and disadvantages of old versus new chemical EOR classifications.

5. Digitalization of Mature Oil Fields

Manual production methods in mature petroleum fields are outdated, and digitization should be employed for such fields. The pace of digitalization and the use of automated systems are rapidly increasing in other industries that have embraced real-time data-driven solutions and the Internet of Things (IoT), including healthcare, finance, and transportation services such as airlines. Although the idea of digitization, such as supervisory control and data acquisition, was first proposed in the 1970s (Anton et al., 2017), most of the oil and gas operators still saw it primarily as an Information Technology (IT)-based tool (Carvajal et al., 2017). Managers, engineers, operators, and IT specialists all need to have a thorough understanding of digitalization when it comes to the

upstream sector, and this connection is established through data. The performance of monitoring and measurement methods in digital oil fields is dependent on complex algorithms that integrate surface and subsurface equipment. Reservoir pressure, temperature, and water/oil/gas production rates are the major characteristics that these algorithms are attempting to determine, and the accuracy and rapid evaluation of these parameters is crucial for making real-time decisions to manage risks. In chemical EOR projects, the complexity escalates due to the multitude of parameters that require evaluation, particularly considering the properties of chemical materials such as surfactants and polymers, or their blends with co-surfactants and alkali agents (Henthorne et al., 2011). Properties such as injected fluid and reservoir pH values, divalent ions in the injected fluids and initial reservoir brine composition, conductivity, fluid viscosity, density, and their mixture are only a few examples (Henthorne et al., 2014).

In addition, for a chemical EOR project to achieve success, mobile communication is essential across a variety of domains. This includes sensor data, such as temperature, pressure, and in-situ saturation of injected fluids in chemical tracer tests, accurate computational modeling, and handling and transferring vast volumes of data (big data). Furthermore, the real-time data acquired from sensors assessing fluid properties at wells, pipes, and processing equipment can also be used by advanced computational techniques such as machine learning and deep learning. Cloud computing can speed up the digitization of oil fields. In the case of complex fractured reservoirs, experts from around the world can access the reservoir model for precise investigations using a cloud-based system. Digitalization enables managers and major oil and gas companies to grant remote access to a broader range of experts. A cloud-based system enables the modeling of offshore reservoirs, allowing production engineers from the platform to connect with reservoir engineers in remote offices, efficiently delivering information and modeling results. Due to the difficulty of accessing the subsea floor, if the fluid sampling is inaccurate, the predicted characteristics from the numerical models may lead to inaccurate calculations of oil and gas volumes, leading to unreliable capital expenditures (CAPEX), operational expenditures (OPEX), and NPV estimates.

A digital twin is another advanced technology in which a digital representation is employed to mimic real-world systems. It should be underlined that the successful deployment of digital twin is highly dependent on integration processes, the implementation of AI, machine learning, and deep learning. The coupling of FieldTwin™ and SLB Olga software is an example of using digital twin capabilities for flow assurance in subsea field studies (SLB, 2021). More precisely, digital twin and production system models are coupled through machine learning augmentation tools, and then the digital twin can be applied to monitoring, optimizations, and abnormal situation detection (i.e., what-if scenarios) (SLB, 2024). This capability empowers production engineers to achieve a higher level of precision and effectiveness in monitoring extensive fields, particularly when dealing with tasks such as chemical injection into mature oil reservoirs. Data analysis (pattern recognition, statistical analysis, and machine learning), cloud computing operations, and other technologies considerably expand the complexity of the digital twin when combined with the existing simulators (SLB, 2023). Although these activities increase the cost of computation and the effort required to develop software and train model and engineers, they will provide ample information about remote locations, such as deep-water reservoirs. As a result, chemical suppliers will have access to more realistic tools and data for performance evaluation of their products. When applied to the

material design and fabrication of a specific reservoir, the data provided by this set of tools can be incredibly useful.

The required level and sophistication of processing equipment and the deployed chemicals are the main questions that should be answered in the process of digitalization. As an example, according to Fadili et al. (2009), to establish an automated chemical EOR system, the project should be designed such that injection and production schedules are continually adapted in response to variations of chemical concentrations due to surfactant retention or polymer adsorption in the reservoir. This dynamic approach is essential for achieving the highest possible productivity. In ASP flooding, an early water breakthrough indicates insufficient ASP injection concentration and poor oil sweep efficiency. This concentration level can be precisely monitored by AI. Another advantage of using AI in the petroleum industry is computer vision, a field of AI to capture and extract information from images and videos, for remote production tracking, pipeline inspection, drilling plans for geologically complex areas, and digital rock physics for core and subcore scale analysis (Balcewicz et al., 2021; Schäfer et al., 2023). The adoption of digitization by the upstream sector is not a good-to-have option but a must-have choice for field operators.

For controlling processes, as noted by Fadili et al. (2009), the AI algorithm should be designed to monitor the transportation of chemicals in the reservoir (fluid flow) through observation wells to generate data. The behavior of production wells should be monitored in terms of water cuts, GOR levels, breakthroughs of chemicals, and, ultimately, the economics of projects, including the price of chemicals (both manufacture and deliverability to the injection point), capacity of surface facilities, and maintenance costs. These factors can be assigned as the objectives of the AI algorithms that control the digitization of mature oil fields.

In such a scenario, the previous experience and information on the characteristics of the reservoir condition through well logs and well tests become additional advantages for the AI algorithm, ensuring that production meets the targets of the field development plans. For more practical information on this topic, readers can refer to the recent paper by Bigdeli and Delshad (2023).

6. Energy Transition

The governmental commitments to a net-zero future are the key driving factor for a low-carbon economy. The energy sector can benefit from adopting AI in a few ways, including better predictions, improved demand forecasts, asset management,

automation capabilities, and cost savings for stakeholders. Besides digitalization, the energy transition is also accelerating the ongoing paradigm shift in geo-energy sciences. This shift is evident in the growing sophistication of data-driven tools. Consequently, it is essential for the proper assessment of developed chemicals and their impact on the digitalization of petroleum fields.

Figure 3 shows paradigm shifts in scientific discoveries (Agrawal & Choudhary, 2016).

As shown in Figure 3, the fourth paradigm of scientific discovery is one in which AI and machine learning play a significant role. This classification is general in nature and not specifically focused on petroleum engineering. As computational power and modeling tools improve, data-driven science is enabling researchers to detect patterns and anomalies in the data with a considerably greater volume of information. This becomes particularly important for applications in energy transition when determining chemical formulations of surfactants and polymers, as well as their blending with alkaline co-solvents and nanoparticles. These characteristics are often challenging to ascertain through experimental investigation across various ranges of pressure and temperature. The power of AI and machine learning can detect optimal conditions that may not be easily discerned through human investigation. In a narrower context, leaders in the chemical industries are employing AI to achieve business growth and sustainability, especially considering the COVID-19 pandemic, geopolitical challenges, and fluctuating fuel prices, which have an impact on supply chain restrictions, the cost of materials, and the dependability of chemical suppliers. Demand estimation, tracking raw materials to their sources, real-time order tracking, delivering and automation at warehouses and ports for sorting and safety, and supply network optimization are a few examples of how AI may help chemical suppliers. Cybersecurity concerns are one of the negative aspects of digitization considering energy transition. Networking and customer satisfaction are two other problems that digitization may encounter as obstacles. Cybersecurity may also receive attention in the chemical supply industry, from R&D division to customer services and support.

As the subsurface characterization becomes more complex (fractures, faults, shale layers, etc.), the process of successfully implementing a chemical EOR project becomes more challenging. This is primarily due to the limited access to real-time data for a full reservoir characterization. AI can detect bottlenecks and obstacles more efficiently in maintenance chemical EOR applications for energy transition purposes. In such a situation, having access to prior

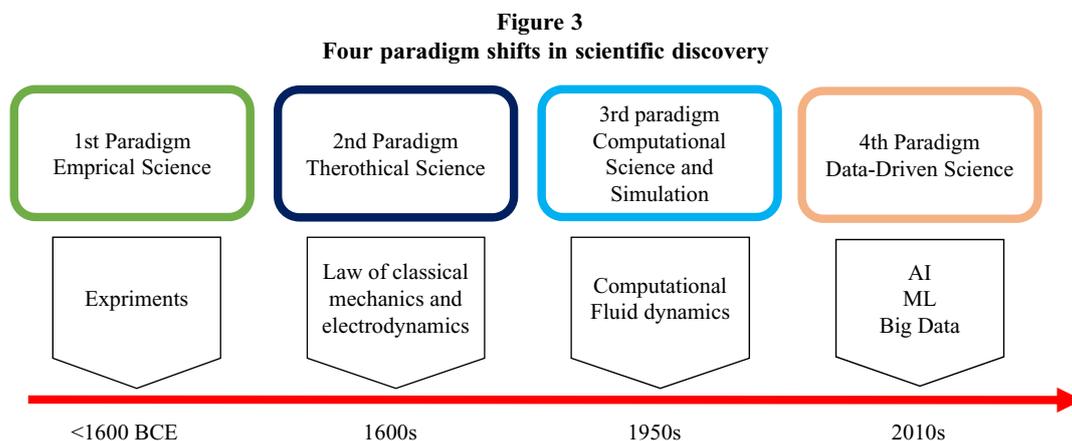
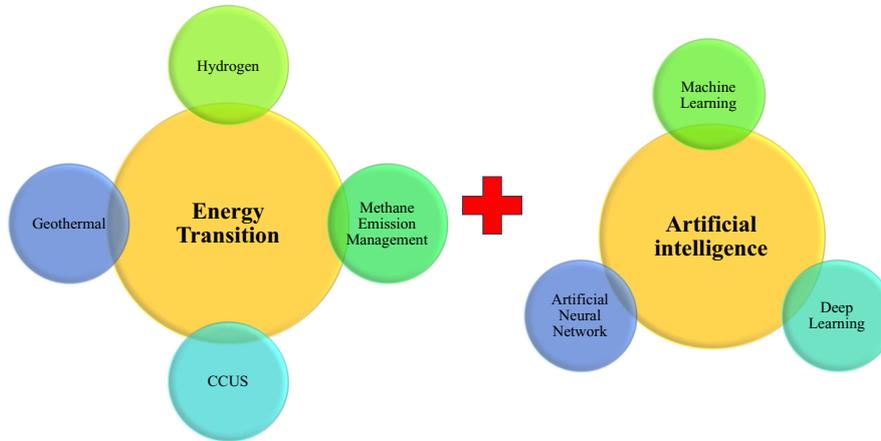


Figure 4
Diverse energy transition domains influenced by various AI technologies



information and experiences is essential for raising the success rate. However, it should be emphasized that chemical EOR methods have less full-field experience than EOR techniques like water flooding and thermal EOR techniques (Cheraghi et al., 2021). Major oil and gas companies are transferring themselves into energy companies, such as BP, Chevron, Baker Hughes, SLB, and Total Energies, which can leverage digitalization, particularly AI and ML, for pattern recognition and anomaly detection in the large datasets they acquire. Seasonal energy demand, forecast weather conditions, infrastructure maintenance, and energy price fluctuation are some examples of how AI can expedite the energy transition, in addition to the development of chemical formulations (Cheraghi et al., 2021; Kuzior et al., 2022; Ugoyah & Igbine, (2021)).

AI can accelerate multiple complicated activities simultaneously with the use of other technologies like the IoT, sensors, and distributed ledger technology (blockchain) (Kuzior et al., 2022). For instance, SLB's (2024) ultra-high pressure and high-temperature sensors enable operators to work at temperatures of 250 °C and pressures of up to 35000 psi. These technologies are essential to produce materials in deeper and hotter reservoirs because they can provide laboratory technicians with real-time data to develop chemicals that are more appropriate for such harsh conditions.

In the upstream sector, the consequences of the energy transition can be observed in four main areas where reservoir engineering and chemical EOR technologies can be beneficial: carbon capture, storage, and utilization; geothermal reservoir; hydrogen production; and methane emission management. As can be seen from Figure 4, the energy transition and its domains are heavily influenced by AI.

7. Intelligent EOR

Due to the energy crisis of the 1970s, EOR studies have become a firmly established field of science and application within the upstream sector (Drumond Filho, 2017). Researchers and managers are attempting to leverage and combine the benefits of various chemical EOR methodologies through hybrid approaches. In comparison to other EOR methods, such as thermal and gas injection, less scholarly focus has been given to the use of AI and ML in chemical EOR technologies. According to Cheraghi et al. (2021), there are fewer publicly available data and field examples to confirm this. In general, the application of data-driven

modeling covers multiple disciplines, including subsurface characterization and petrophysics, drilling, production, reservoir studies and EOR, reservoir management, facility, and pipeline remediation (Balaji et al., 2018). In addition to geology, petrophysics, and reservoir data, the chemical EOR data required for AI include chemical concentrations, adsorption, dilution, partitioning (for alkaline and surfactant), relative permeability, residual oil reduction, flood mechanisms, duration of pre-flush, post-flush, slug size, and injection fluid composition. For further reading, readers can refer to Han et al. (2022), Al-Murayri et al. (2019), and Khanifar et al. (2019).

To illustrate how AI can be used for EOR methods, some examples are provided here. Intelligent petroleum engineering was the subject of the work reported by Mirza et al. (2022). In that work, it was argued that machine learning and data-driven modeling are two essential tools to transition the petroleum industries into digitalization. Intelligence geoscience, intelligent reservoir engineering, intelligent production engineering, and intelligent drilling engineering are the domains that are covered by authors. Large data volumes, various data formats, inconsistent and unreliable data sources, and a quick rate of data flux are issues with machine learning adoption in the petroleum industry. The petroleum industry is not able to effectively utilize machine learning technology as quickly as other engineering disciplines due to reservoir model uncertainty, the preparation of raw data, and data processing time delays. The authors argued that one approach to resolving this issue is to use a hybrid model to give additional insight into the necessary model and be based on physical principles when a pure data-driven solution cannot be applied in this field.

ANN has also been applied to waterflooding of heterogeneous models. ANN, adaptive neuro-fuzzy inference system, and support vector machine were used to determine the accuracy of the model and the RF was reported as a function of Dykstra-Parsons permeability variation coefficient, mobility ratio, permeability anisotropy ratio, water cut, wettability indicator, and oil/water density ratio (Kalam et al., 2022).

More examples of using AI for the implementation of EOR methods can be found in Huang and Chen (2021) for steam-assisted gravity drainage, in Nasr et al. (2021) for silica nanofluids, in Larestani et al. (2022) for surfactant-polymer flooding, and in Dang et al. (2020) for low salinity surfactant flooding. These examples show that ML, particularly ANN, can

be employed for the optimization of chemical EOR, even when dealing with a large number of associated variables.

Selecting an EOR strategy for a particular field is another application of ML. In this regard, different authors demonstrated how ML can be used for this purpose (Ahmadi & Bahadori, 2016; Alvarado et al., 2002; Cheraghi et al., 2021; Dang et al., 2020; Giro et al., 2019; Huang & Chen, 2021; Huerta & Meza, 2022; Kalam et al., 2022; Larestani et al., 2022; Nasr et al., 2021; Suzanne et al., 2022; Tarrahi et al., 2015; Thomas et al., 2023).

These examples demonstrate that AI can serve as a powerful tool for selecting various EOR methods, including chemicals that are in development, tailored to a specific reservoir pressure, temperature, and water salinity.

Microfluidic devices can hasten the development of novel chemicals that are identified by AI for EOR applications. These devices have several advantages over traditional equipment. First, they require a small sample volume, the experiments are faster and less expensive. Furthermore, these techniques have proven to be resilient in withstanding the harsh reservoir conditions of high pressure, salinity, and temperature. Additionally, their pores can be designed with varying degrees of precision and resolution. Additionally, this sort of equipment is operator-independent and popular to use. Microfluidic devices can be used for testing oil recovery from conventional reservoirs and heavy oil in addition to carbon capture and storage. Polymer, surfactant, foam stability, thief zone detection, fracturing fluid properties, water/oil separation, and inhibitor performance analysis are examples of microfluid testing related to chemical EOR. For different applications of microfluidics in chemical EOR operations, readers are referred to Kenzhekanov et al. (2022), Valavanides et al. (2022), Vazquez et al. (2022), Yu et al. (2021a), Yu et al. (2021b), Wang et al. (2020), Liang et al. (2020), Ren et al. (2020), Du et al. (2019), Yuan et al. (2019), Quaglio et al. (2019), Al Shehhi et al. (2017), Xu et al. (2017), Bazazi et al. (2017), and Moiré et al. (2016).

8. Robotic and Self-Learning Labs

The use of robotics in petroleum engineering is not a novel idea; drones, automated rigs, production monitoring, and other similar applications have all made use of this technology. A comprehensive review of the robotic applications for onshore and offshore sites can be found in Shukla and Karki (2016a) and Shukla and Karki (2016b), respectively. The robotics application in the experimental and screening stages of designing chemical processes, however, is novel.

A robotic arm and high-throughput formulator are two specific examples of robotic equipment that can be used for designing chemicals at the laboratory scale (Jacobs, 2022). A robotic arm and a high-throughput formulator are especially useful for investigating the phase behavior of microemulsions and surfactants. This is because they can maintain more stable conditions, which are necessary for visualizing the generated emulsion phases. The chemical formulation design is not limited to EOR or IOR applications, but it can be used for well construction (drilling fluids, muds, and cement additives), well completion (acidizing and fracture fluids), midstream (water treatment, H₂S removal, corrosion inhibitors), and flow assurance. Depending on the required level of accuracy, the robotic arm and high-throughput formulator can increase the quality of manufactured chemicals.

An example of advanced robotic technology and automated workflows for waterflood core testing is reported by BP (Griffiths

et al., 2015) where the key elements of the automated workflow include (1) sample preparation robots, (2) automated robotic coreflood, and (3) effluent analysis laboratory. For each step, measurements and timelines are provided.

The integration of advanced laboratory workflow, combining AI technology with a coreflood simulator for special core analysis services (SCAL), was the focus of the study presented in Mathew et al. (2021). In this work, a framework was developed for the determination of the capillary pressure and relative permeability based on mathematical models. The advantage is to generate multiple capillary pressure and relative permeability curves. It should be noted that the framework was only developed for steady-state drainage experiments. A combination of machine learning and micro-CT images to determine the residual oil in carbonate reservoirs can be found in Rizk et al. (2022) where CPU-solver uses the lattice Boltzmann method on carbonate rock digital images, and the AI-based workflow estimates the residual oil saturation.

As machine learning and AI grow in several fields of study, self-learning laboratories are among the most cutting-edge and effective solutions for resource, time, and material optimizations. Although chemical engineering applications make up most self-learning laboratories, their benefits are still useful for energy transition goals. To discover and optimize the physical/chemical processes, closed-loop automated experiments are followed by an iterative decision-making algorithm. In such cases, machine learning and AI become crucial tools for assistance (Bennett & Abolhasani, 2022).

As shown in Figure 5, the process flow of a closed-loop self-learning laboratory may be divided into experiments, processing, model building, and prediction.

The benefit of adopting self-learning laboratories is that they can handle different time-scale operations and the optimization of enormous datasets (Abolhasani & Kumacheva, 2023; Hippalgaonkar et al., 2023). When the chemical EOR operations are utilizing self-learning laboratories – that collaborating with robotic arms and high-throughput formulators – the accuracy of the developed materials can improve significantly. The availability of data for both chemical EOR operations and specific conditions of designing materials is the sole problem that could serve as a barrier to the continued deployment of such an automated system. The role of materials science should be clarified to recognize how chemical quality can be improved for chemical EOR operations. More information about the roadmap to implement, current status, and limitation and future opportunities of self-learning laboratories for both chemical and materials science is reported in Bennett and Abolhasani (2022).

Figure 6 shows how chemical EOR operations and AI can be integrated. AI may be utilized as an interface between the manufacturing unit and the petroleum production system. In this case, the AI can monitor the field's response in terms of the amount of oil, gas, water, and chemical output, and based on that information, it can determine whether the desired goal has been achieved. The AI can instruct material sciences manufacturing facilities to update or reexamine the developing materials using their knowledge of physics, chemistry, engineering, and mathematics, depending on how well the designed materials are performed in the field. Once the chemicals are optimized, the AI can then inject them into the field. The digitalization of the field is crucial in such a process, according to what has been discussed earlier in the digitalization sections. It should be emphasized that the integrated workflow is not only applicable to hydrocarbon production but may also be used for energy transition operations such as carbon capture and storage, hydrogen storage, geothermal reservoir development, or operations involving methane emission monitoring and reduction. The presented workflow is useful for each scenario.

Figure 5
Process flow of a closed-loop self-learning laboratory

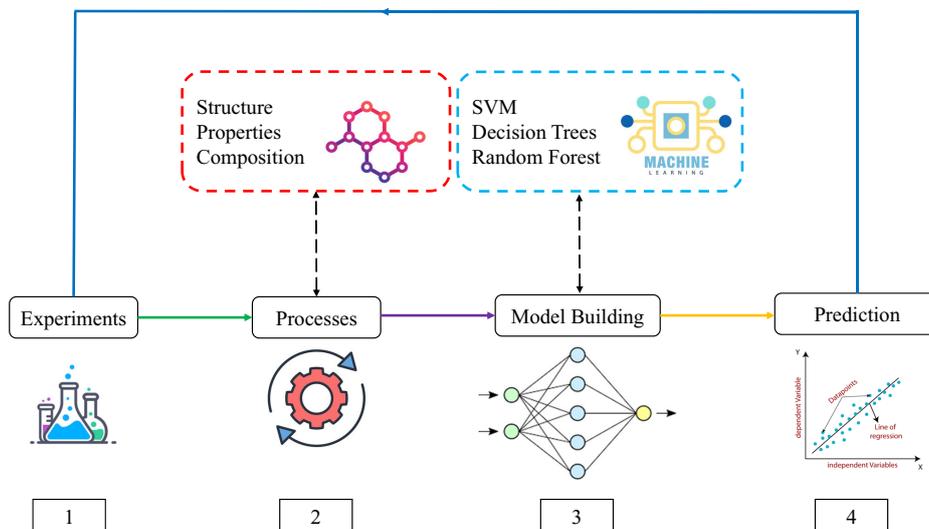
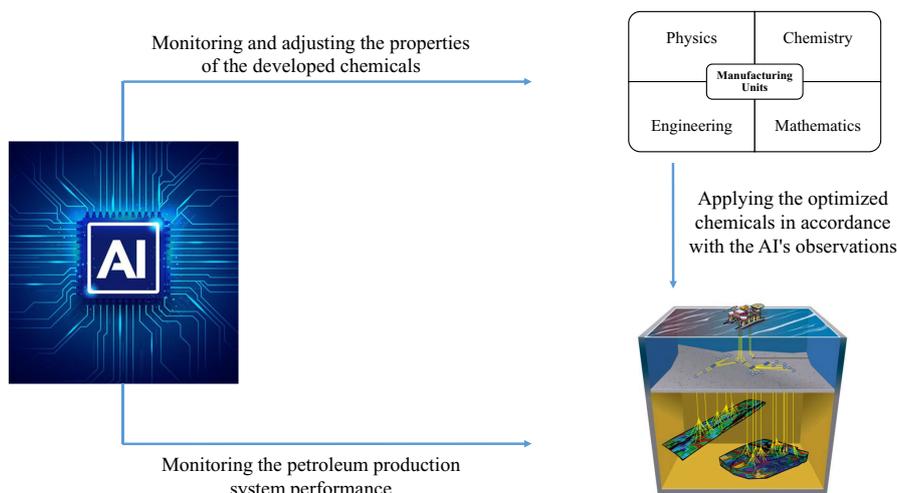


Figure 6
AI integration in chemical EOR formulation development and operations



9. Discussion on Gap and Future Research

The application of AI in chemical EOR represents a promising avenue for advancing the efficiency and sustainability of oil extraction processes. However, several critical gaps and challenges exist, shaping the direction of future research in this domain.

One notable challenge is the limited field experiences and datasets available for chemical EOR compared to other established techniques like thermal or gas injection. This scarcity of real-world data hinders the ability to effectively tune AI models for optimal performance. Future research should prioritize expanding field trials and collaborations to gather more extensive datasets, enabling the development of robust and accurate AI models tailored specifically to chemical EOR.

Environmental considerations, particularly the carbon footprint of chemical manufacturing, emerge as another crucial aspect.

Although there are limited publications addressing this concern, future development in AI-assisted EOR must integrate carbon emissions considerations as a potential restriction. Aligning AI strategies with sustainability goals and conducting comprehensive environmental impact assessments are essential for shaping the future landscape of chemical EOR applications.

Furthermore, the absence of standardized protocols for selecting AI techniques in chemical EOR poses a significant challenge. Most studies focus on reporting RFs and NPV, neglecting the diversity of available AI techniques. To address this gap, future research should focus on developing guidelines that provide a systematic approach for selecting the most appropriate AI technique based on the specific requirements of each method.

The integration of AI education into the training of the new generation of students is critical. Beyond traditional reservoir engineering courses, students should be equipped with knowledge

in AI, machine learning, and deep learning to bridge the gap between theoretical knowledge and practical application. This additional educational requirement poses challenges in finding experienced users who can effectively apply accurately trained models in real-world scenarios.

The uncertainty associated with material development, especially for hybrid EOR methods, adds complexity to the problem. New guidelines, screen tables, and workflows need to be developed to accommodate these evolving challenges and facilitate the integration of novel materials into chemical EOR strategies.

The traditional classification of chemical EOR is considered outdated, urging the need for new guidelines, screen tables, and workflows that align with the development of new materials. The classification should be updated to reflect the evolving landscape of chemical EOR technologies.

The digitalization of mature fields requires substantial investment and technological updates. Cloud computing, digital twin technology, and advanced simulators operating at the field scale are essential for enhancing the precision of modeling and upscaling. The pace of digitization is closely tied to oil prices and the final cost of developed chemicals. Furthermore, the energy transition can be supported by producing oil with chemicals that have a lower carbon footprint, emphasizing the need for sustainability in oil extraction processes.

Intelligent EOR, a field focusing on data-driven techniques, must be recognized as a distinct area of study by both industry and universities. This recognition is crucial for fostering the development of a new generation of studies that outperform traditional EOR techniques relying solely on laboratory investigations and physics-based models.

Robotic and self-learning labs emerge as powerful tools for field operators, managers, engineers, and researchers to investigate new chemicals with higher precision. These technologies can significantly enhance the understanding and application of chemicals in EOR processes, contributing to more efficient and effective oil recovery strategies.

Real-time data and sensor-derived information are identified as additional fields that can accelerate the adoption of AI in chemical EOR operations. Integrating these technologies will enhance monitoring, control, and decision-making processes, making chemical EOR more adaptive and responsive to dynamic reservoir conditions. Future research should focus on developing advanced real-time monitoring systems and optimizing sensor-derived information for improved AI-driven decision support in chemical EOR operations.

10. Conclusions

This work addressed how the energy transition is affecting existing knowledge, limits, and practices of energy harvesting with a focus on the integration of AI and chemical EOR operations.

The following conclusions and recommendations are presented as the final insights of the paper:

- The carbon footprint of chemical EOR methods should be carefully considered as it can act as a barrier or constraint to the development and injection of complex chemical mixtures, such as blends of surfactant(s), co-solvent(s), and polymer.
- The uncertainty associated with the performance of the chemicals in harsh reservoir conditions needs to be clarified. Numerical reservoir simulators play a crucial role in scaling up laboratory investigations into pilot and full-field applications.

- Mathematical modeling of the multiple mechanisms and components involved in hybrid EOR methods, as well as the sequence of their occurrence, should be made clearer. Traditional classifications of chemical EOR methods should be updated to incorporate considerations related to energy transitions and achieving net-zero emissions.
- Digital twin technology, AI, machine learning, cloud computing, and the IoT are examples of digitalization in the petroleum field. The importance of real-time data and sensor-derived information is essential in this context.
- Areas such as underground hydrogen storage, geothermal reservoir engineering, CCUS, and methane emissions mitigation are critical aspects of the energy transition. These areas can benefit from the application of AI technologies, while chemical EOR enables continuous production from mature reservoirs. This concept can be termed as “Intelligent EOR,” involving the integration of data-driven techniques with the traditional science of EOR to advance our current knowledge.
- The utilization of robotic and self-learning labs, for the development of chemical formulations comprising surfactants, polymers, nanomaterials, and alkaline substances blended with reservoir simulators, can usher in a new era of investigations. These investigations can greatly assess the performance of chemical suppliers and field operations.

Conflicts of Interest

The authors declare that they have no conflicts of interest to this work.

Data Availability Statement

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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