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Frontier advances in molecular dynamics simulations for the design and optimization of oil-displacement polymers

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This comprehensive review paper delves into the application and recent advancements of molecular dynamics (MD) simulation techniques in the design and optimization of polymers for oil displacement. Initially, the paper outlines the pivotal role of polymers in oil displacement, particularly highlighting the challenges associated with their stability and rheological property optimization under high-temperature and high-salinity conditions. Subsequently, it meticulously introduces the theoretical foundation of MD simulations, the selection of simulation parameters, and the emerging trends in the integration of machine learning with MD simulations. The core viewpoint revolves around the utilization of MD simulation techniques in elucidating the mechanisms of polymer-enhanced oil recovery (PEOR), optimizing polymer properties, and designing novel polymers. This includes observing polymer–oil interactions at the atomic scale and predicting the impact of polymer wettability changes on recovery efficiency. The unique contribution of this paper lies in systematically summarizing the application achievements of MD simulation techniques in the field of oil displacement polymers and providing insights for future research directions, thereby advancing the application and development of MD simulations in EOR polymer design. Future research endeavors will concentrate on developing multiscale simulation methodologies, exploring high-performance computing technologies, integrating experimental and simulation data, and assessing the environmental impact of polymers to foster the development of environmentally friendly oil displacement technologies. This review offers fresh perspectives to both the academic and industrial communities, particularly emphasizing the practical application potential in oilfield development and environmental management. By presenting an integrated view, this review paper serves as a catalyst for fostering innovative approaches and strategies in the domain of oil recovery enhancement through polymer technology.

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1. Introduction

1.1 The crucial role of oil-displacement polymers

Enhanced Oil Recovery (EOR) technologies have been widely employed in the global petroleum industry, particularly as conventional oil extraction methods gradually become less effective. These technologies extend the lifecycle of oil fields and significantly improve recovery rates.[1] EOR projects are primarily concentrated in countries such as China, the United States, and Canada, where the application of EOR technologies has greatly increased the utilization rate of crude oil.[2–5] In recent years, with the increasing difficulty of oil resource extraction, chemical flooding techniques within EOR, especially polymer flooding for oil displacement, have gradually emerged as one of the core technologies in oil production.[6]

Polymer flooding technology for oil displacement enhances the viscosity of injected water, thereby reducing the oil–water mobility ratio and enabling more uniform water advancement. This, in turn, improves the efficiency of mobilizing remaining oil.[7,8] Numerous experiments have demonstrated that polymer flooding can increase recovery rates by 10% to 12%.[9,10] The industrial application of this technology in the Daqing Oilfield has provided valuable experience for other oilfields globally.[2,11] However, high-temperature and high-salinity environments pose significant challenges to the performance of polymer flooding. Under these extreme conditions, the stability and rheological properties of polymers are significantly reduced, thereby affecting recovery rates.[12]

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To address these challenges, the design of polymers tailored to specific environments has emerged as a crucial task, with the development of novel materials such as biopolymers and nanoparticle-enhanced polymers gradually becoming research hotspots. Biopolymers like xanthan gum have garnered significant attention due to their excellent salt and temperature tolerance.[13] Meanwhile, the combined use of polymers and nanoparticles has been proven to effectively enhance their stability and oil displacement efficiency.[14] Furthermore, research has shown that ASP (alkali–surfactant–polymer) flooding and high-concentration polymer flooding techniques can further improve recovery rates, with the former increasing recovery rates by 10.1% to 22.9%,[15–17] and the latter demonstrating outstanding economic and technical benefits. Simulation studies have indicated that, under these conditions, adjusting the molecular structure and rheological properties of polymers can significantly enhance their oil displacement efficiency.[2,15] Synthetic polymers and natural polymers exhibit different advantages in EOR applications. Synthetic polymers, such as partially hydrolyzed polyacrylamide (HPAM), are widely used in high-temperature and high-salinity environments, but their salt tolerance needs improvement.[18] Biobased polymers, on the other hand, are considered potential candidates for future polymer flooding due to their good environmental compatibility and renewability.[12,19] Additionally, experimental and simulation studies have shown that adjustments in chain length, degree of branching, and functional groups can further improve polymer performance under complex reservoir conditions.[7,20] These advancements have laid a solid foundation for the widespread application of polymer flooding technology globally and have pointed the way forward for the development of future EOR technologies.[6,16]

In industrial applications, polymer flooding technology not only possesses significant technical advantages but also has the potential to reduce the environmental impact of oilfield development. For instance, the utilization of biopolymers derived from natural sources contributes to mitigating environmental pollution and alleviating issues associated with biodegradation.[13,19] Additionally, the integration of nanotechnology and multi-component composite flooding techniques offers further options for enhancing recovery rates in the future.[21]

Polymer flooding, as the cornerstone technology of chemical flooding, has achieved remarkable results in enhancing oil recovery and will continue to play a pivotal role in future oilfield development.

1.2 Molecular dynamics simulation techniques and their potential in polymer optimization

In recent years, the emergence of Molecular Dynamics (MD) simulation technology in materials science has provided a powerful tool for polymer optimization (Fig. 1). MD simulations, by accurately describing intermolecular interactions, can predict the physical, chemical, and mechanical properties of polymer materials, significantly accelerating the design and optimization process of new materials.[22] Furthermore, MD simulations offer a cost-effective method to optimize polymer properties at the molecular level, reducing the need for expensive experimental testing. This is particularly valuable in the oil industry, where cost reduction is a critical factor. Additionally, MD simulations help address scaling challenges by enabling the prediction of polymer behaviour under a variety of field conditions, ensuring more efficient, economical, and scalable polymer flooding processes. Compared to traditional experimental methods, MD simulations offer direct insights into the microstructure and dynamic behaviour of polymers at the molecular scale, particularly demonstrating unique advantages in tackling complex multi-scale problems.[23]

In the field of polymer optimization, MD simulation technology has been extensively applied to the study of polymers' mechanical properties. Through MD simulations of polymer materials such as polystyrene under shear deformation and tensile conditions, researchers have discovered that polystyrene exhibits viscoelastic behaviour under small strains and viscoplastic behaviour under large deformations.[24] This investigation of stress responses at the molecular level provides a deeper understanding of the application of polymer materials in engineering fields.

MD simulations have also demonstrated a significant role in exploring the potential of polymers in Enhanced Oil Recovery (EOR) processes. EOR techniques commonly employ methods such as water flooding or chemical flooding to enhance the

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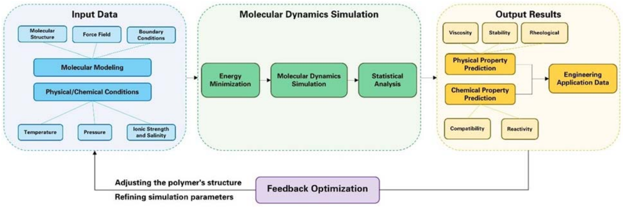


Fig. 1 Workflow of molecular dynamics simulations in polymer design and optimization.

recovery rate of oil reserves, where polymers function as viscosity enhancers, increasing the viscosity of water to optimize oil displacement efficiency. Research using molecular dynamics simulations to investigate nanocellulose as a viscosity enhancer for EOR has shown that nanocellulose can effectively increase the viscosity of water but has a limited effect on oil–water interfacial tension.[25] These findings provide guidance for the development of more efficient EOR polymer materials.

In summary, the rapid development and application of molecular dynamics (MD) simulation technology have significantly transformed the approach to polymer optimization and material design. It has not only demonstrated immense potential in predicting material performance but also facilitated more complex multiscale material research by enhancing computational efficiency. In the future, with further advancements in computational capabilities, MD simulations are poised to play an even more pivotal role in a broader range of materials science fields, particularly in the development of EOR and high-performance polymer composites.[22,26]

1.3 Objectives of this review

This paper aims to systematically review the latest advancements in the application of molecular dynamics (MD) simulation technology for the design and optimization of polymers used in oil displacement. By integrating existing literature, this paper will explore the unique advantages of MD simulations in addressing complex physicochemical challenges in the oil displacement process, particularly focusing on optimizing polymer stability and rheological properties in high-temperature and high-salinity environments. Additionally, this paper will summarize how MD simulation technology aids scientists in designing novel polymer materials to enhance oil recovery (EOR) and analyze the potential for future integration of this technology with other advanced methods, such as machine learning. The ultimate goal is to provide guidance for future research directions and to promote further application and development of MD simulation technology in the design of EOR polymers.

2. Theoretical foundations and methods of molecular dynamics simulation

2.1 Basic principles of molecular dynamics simulation

Molecular dynamics (MD) simulation is a computational tool grounded in physics and mathematics, utilized to investigate the dynamic behaviour of molecular systems under specific conditions. The core theories of MD simulation encompass potential energy functions, intermolecular interactions, and the selection of time steps, which collectively determine the accuracy and stability of the simulation results. The fundamental principles of MD are based on Newton's laws of motion, whereby the interactions between molecules and atoms are described to simulate the trajectories and dynamic evolution of the system.[27–29]

In MD simulations, the potential energy function or force field is crucial as it accurately describes the intermolecular interactions. Common potential energy functions include the Lennard-Jones potential and the Coulomb potential, primarily used to model van der Waals forces and electrostatic interactions.[30,31] Different force field models are optimized for various types of interactions during their construction, such as the specific interactions in protein–ligand binding and the dynamic behaviour of ions in solution.[26,29] In recent years, the application of enhanced sampling techniques in MD simulations, such as meta dynamics and variationally enhanced sampling, has provided effective means for more precise potential energy calculations and simulations over longer timescales.[27,32] These enhanced sampling techniques, by improving the accuracy of the potential energy function, have broadened the applicability of MD simulations in biological macromolecule systems and significantly enhanced their reliability in analyzing biological systems.[33,34]

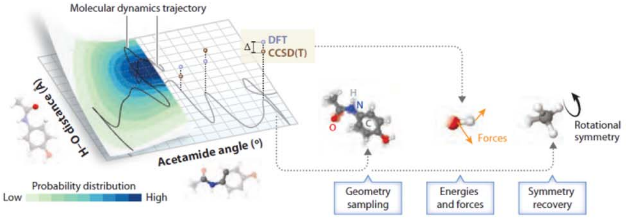
The model of intermolecular interactions between atoms represents another pivotal component of MD simulations. MD determines the trajectory of each atom by computing the forces and accelerations among them, thereby generating the temporal evolution information of the system. Typical interaction models encompass bonding forces, repulsive forces, and electrostatic forces, and the dynamic interplay of these forces provides theoretical support for studying the behaviour of biomolecules within cellular environments.[35,36] For instance, in protein folding simulations, precise calculations of intermolecular forces can uncover the dynamic relationships among different amino acid side chains.[31,37]

The choice of time step length plays a significant role in MD simulations. Excessively large time steps can lead to system instability or even simulation failure, while excessively small time steps significantly increase computational costs. Therefore, careful selection is required to balance computational accuracy and efficiency. Generally, typical MD simulation time steps range from 1 to 2 femtoseconds (fs), but shorter time steps may be chosen when more precise kinetic process simulations are needed.[38,39] Some modern optimization techniques, such as acceleration models based on graph neural networks and adaptive step size methods, allow for the use of slightly larger time steps while maintaining accuracy, enabling long-timescale simulations in complex molecular systems.[35,40]

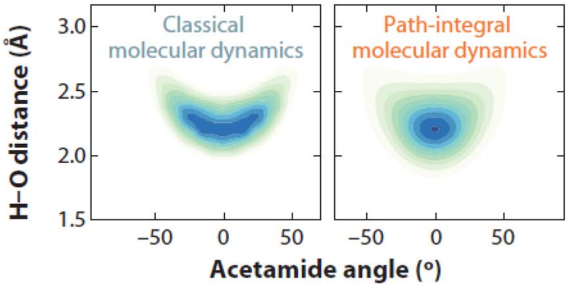
2.2 Selection of simulation parameters

To ensure the accuracy of simulation results, it is crucial to make reasonable choices for simulation parameters, such as temperature, pressure, and molecular models. This not only affects the consistency between simulations and experimental conditions but also relates to the predictive capability of system properties.[41,42]

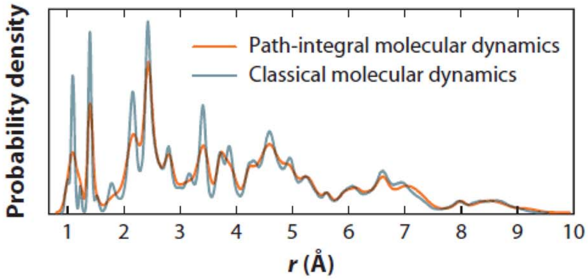
2.2.1 Choice of temperature and pressure. Temperature and pressure are two critical parameters for controlling the macroscopic state of a system, directly influencing its thermodynamic and kinetic behaviours. In molecular dynamics simulations, ensembles such as the constant temperature (NVT) or



(a) Molecular dynamics simulation (b) Constructing machine learning force fields



(c) Applications: free energy surfaces



(d) Interatomic distance distribution

Fig. 2 A workflow integrating machine learning-assisted force field modelling with molecular dynamics simulations. This figure illustrates the specific application of machine learning in constructing force field models and performing molecular dynamics simulations. The process involves sampling reference geometric configurations from molecular dynamics trajectories (a), computing high-level theoretical energies and forces for these configurations (b), and utilizing these data to train a machine learning model to predict potential energy surfaces (c). Ultimately, this model is employed to accelerate path-integral molecular dynamics simulations for studying the behaviour of polymers under extreme conditions (d). This process not only enhances the efficiency and accuracy of simulations but also expands the capability to investigate complex material systems.[51]

constant pressure (NPT) ensembles are commonly employed to control these conditions. Jung and Sugita introduced a group-based temperature and pressure evaluation method that maintains simulation accuracy while extending the time step length, effectively enhancing computational efficiency.[43] In simulations of high-pressure environments, it is essential to optimize force field parameters to accommodate different pressure conditions, as exemplified by Hata *et al.*, who successfully simulated structural changes in proteins under high pressure.[44] Additionally, Kim *et al.* proposed a new method for constant temperature and pressure simulations that avoids disturbing the internal molecular dynamics of the system by applying temperature and pressure control only to the molecules at the simulation box boundaries, thereby improving the reliability of the simulations.[45]

2.2.2 Selection of molecular models. Molecular models, or force fields, are central to determining intermolecular interactions. In recent years, the trend has been towards optimizing force fields based on quantum mechanical calculations. For instance, the ff19SB force field developed by Tian *et al.* significantly improved the prediction accuracy of dihedral angles in protein backbones, enabling molecular dynamics simulations to better capture sequence-specific behaviors.[41] Meanwhile, Naserifar *et al.* developed accurate long-range non-bonded interaction potentials based on density functional theory, demonstrating their superior performance in liquid water and biological systems.[46] In studies of gaseous systems, Saeteaw *et al.* employed molecular dynamics simulations to investigate the van der Waals parameters of different gases, highlighting the influence of gas molecule shape and polarity on thermodynamic properties.[47] Furthermore, a comparative study by Chen *et al.* on various carbon dioxide models revealed significant differences in the applicability of different force fields for predicting thermodynamic properties, suggesting that model selection should be tailored to specific applications.[48]

2.2.3 Optimization of specific conditions. For simulations involving complex environments or specific systems, further parameter adjustments are necessary. For example, in studying the dissociation process of methane hydrates, Li *et al.* demonstrated that temperature, pressure, and initial gas concentration significantly influence the dissociation kinetics.[49] Furthermore, Du *et al.* investigated the solubility of supercritical carbon dioxide in cosolvent systems and proposed a method for optimizing cosolvent selection based on a linear relationship between pressure and temperature.[50] In large-scale simulations, Kim *et al.* introduced an improved neighbour list algorithm, which reduced non-physical deformations and enhanced the accuracy of simulation results.[42]

2.3 Integration of machine learning with molecular dynamics simulation

In recent years, the integration of machine learning with molecular dynamics simulations has emerged as a significant direction in materials science research. This integration is primarily manifested in accelerating simulation processes, enhancing simulation accuracy, and expanding research areas that are beyond the reach of traditional molecular dynamics (Fig. 2). By applying machine learning models to molecular dynamics simulations, researchers have achieved remarkable technological breakthroughs in the analysis and prediction of complex systems.[51,52]

2.3.1 Force field optimization and construction. One of the pivotal applications of machine learning in molecular dynamics simulations is the construction of high-precision force field models. Traditional force fields rely on empirical parameters, whereas machine learning-based force field models can be trained using quantum mechanical calculations, enabling accurate predictions across multiple scales.[52] For instance,

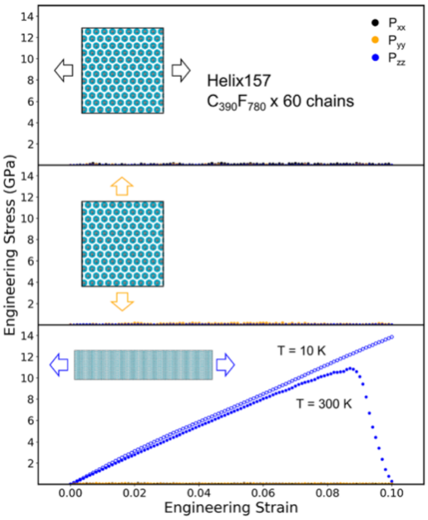


Fig. 3 Comparison of predicted and experimental thermal properties of polytetrafluoroethylene (PTFE) using machine learning-driven force fields. Calculated Young's modulus of $60C_{390}F_{780}$ with helix 157 using ML-FF-based MD simulations at a temperature range of 300 °C to 350 °C under standard atmospheric pressure.[52]

methods such as Gaussian processes and kernel functions have been employed to develop machine learning force fields suitable for complex polymers, which are capable of accurately capturing van der Waals forces and interactions between long-chain molecules.[52,53]

A notable example of enhancing thermal stability using machine learning-driven force fields can be found in fluoropolymer simulations, where first-principles-based machine learning molecular dynamics (ML-MD) models have been used to predict the melting point, thermal expansion coefficient, and Young's modulus of polytetrafluoroethylene (PTFE) with high accuracy. In a comparison with traditional empirical force fields, the ML-based model predicted the melting point of PTFE at 327.5 °C with an error margin of just 1.5%, compared to the experimental value of 329 °C. The thermal expansion coefficient predicted by the ML model was 3.2×10^{-5} K^{-1}, which was in excellent agreement with the experimental value of 3.1×10^{-5} K^{-1}, showing the ML-driven force field's potential to accurately simulate polymer thermal stability (Fig. 3).[52]

Similarly, machine learning-driven force field optimization has been applied to salt tolerance enhancement, particularly in water-soluble polymers used in extreme salinity environments. By employing Bayesian inference-based parameter optimization, the force field parameters were systematically refined to accurately describe polymer–water-ion interactions, leading to more reliable predictions of polymer conformational changes in saline solutions. For example, the model predicted a shift in the polymer's radius of gyration when exposed to 3 M NaCl solution, showing a reduction of 12%, which closely matched experimental observations. This approach has been demonstrated to improve the modelling accuracy of ionic effects on polymer behaviour, making it particularly useful for polymer flooding in high-salinity oil reservoirs (Fig. 4).[53]

Data sparsity is a significant challenge in force field optimization for polymer systems. Accurate machine learning models require large amounts of experimental and high-quality simulation data. However, due to the complexity of polymer systems, obtaining sufficient data is often difficult. Particularly for novel polymers or systems that have not yet been experimentally validated, the lack of adequate real-world data presents a significant obstacle to model training. To address data sparsity, the following approaches can be employed.

(1) Data augmentation: synthetic data generation or the use of data from similar systems can expand the training set. Techniques such as Synthetic Minority Over-sampling Technique (SMOTE) can effectively enhance the diversity of the dataset.

(2) Transfer learning: transfer learning allows knowledge learned from one domain to be applied to another, which reduces the need for large amounts of new data, particularly in cases where data is limited.

(3) Active learning: active learning is a machine learning technique where the model selects the most informative samples to label during the training process. This approach helps extract more valuable information from a limited training sample.

2.3.2 Data-driven simulation acceleration. Machine learning has demonstrated exceptional performance in

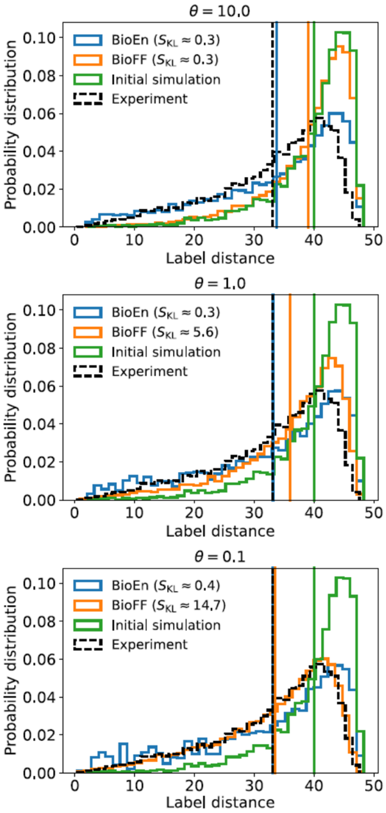


Fig. 4 Prediction of polymer conformational change in saline environments using machine learning-driven force fields. Distribution of the label distance used for refinement and its mean value (vertical lines) for the initial reference simulation ($\kappa_0 = 20$, green), the synthetic experimental data ($\kappa_{\text{exp}} = 10$, black dashed lines), BioEn (blue), and BioFF(orange). The confidence in the reference ensemble decreases top to bottom ($\theta = 10, 1, 0.1$).[53]

handling high-dimensional data from molecular dynamics simulations. Unsupervised learning algorithms can extract key structural features and perform clustering from complex simulation data, enabling efficient analysis of the microscopic motion behaviour of polymer nanocomposites.[54] Furthermore, supervised learning models, through training on time-series data, can effectively predict the dynamic behaviour of polymer systems, such as the evolution of energy distributions and dynamic changes in intermolecular forces.[55,56] For instance, using Recurrent Neural Networks (RNNs) and Long Short-Term Memory networks (LSTMs), researchers have predicted the energy change trajectories of polymer–solvent systems in solution, significantly improving the accuracy of short-time dynamic predictions.[55]

When using machine learning for data-driven simulation acceleration, generalization is a critical issue. Polymer systems exhibit high diversity, and the molecular structures and physical–chemical properties of different systems mean that a model trained on a specific system may not directly apply to others. If a model is trained solely on data from one system, it may suffer from overfitting, which reduces its performance on other systems. To improve generalization across different polymer systems, the following strategies can be implemented.

(1) Domain adaptation: domain adaptation, a technique in transfer learning, helps adjust models trained in one system to be applied to another, improving the model's ability to generalize.

(2) Cross-validation: cross-validation is an effective technique for assessing a model's generalization ability. By training and validating the model on different polymer systems, we can ensure that the model performs well across diverse environments.

(3) Multi-task learning: multi-task learning enables the model to learn relationships between different tasks, enhancing its generalization ability across multiple polymer systems. This is particularly useful when dealing with a variety of polymer types.

2.3.3 Self-assembly and structure analysis. In analysing the complex local structures of polymer systems, Machine Learning-assisted Local Structure Analyzer (ML-LSA) has proven to be an efficient tool. ML-LSA can automatically identify and classify ordered structures in liquid crystal polymers, and accurately characterize physical properties by extracting optimized parameters (Fig. 5).[57] Furthermore, the combination of coarse-grained molecular dynamics and machine learning enables researchers to rapidly generate long-time dynamical trajectories for large-scale polymers and stabilize simulations of the long-time evolution of complex systems through geometric machine learning methods.

2.3.4 Inverse design and optimization. The integration of machine learning with molecular dynamics simulations is also extensively utilized in the inverse design of polymer materials. By combining coarse-grained molecular dynamics with machine learning algorithms, researchers can establish the relationship between molecular structure and function from the perspective of monomer sequences, thereby accelerating the design of novel polymers.[58,59] For instance, multi-task machine learning models have successfully screened out various polymer membranes with ultra-high gas permeability, whose performance significantly surpasses the current upper limits of separation efficiency.[59] Furthermore, optimized force field models, leveraging Bayesian inference, can systematically address the error issues arising from parameter simplification in traditional simulations.[53]

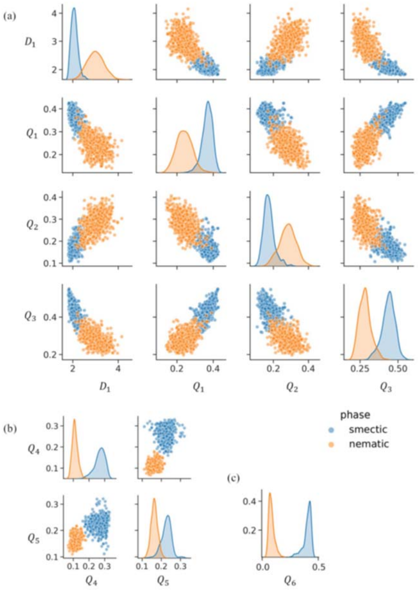


Fig. 5 Utilization of machine learning-enhanced local structure analyzer (ML-LSA) for insights into liquid crystal polymers. This figure demonstrates the application of the Machine Learning-assisted Local Structure Analyzer (ML-LSA) in analyzing liquid crystal polymer (LCP) systems. By comparing the classification results using different combinations of features: (a) $N = 4$ with four features, (b) $N = 8$ with two features, and (c) $N = 12$ with one feature, ML-LSA is capable of automatically identifying and classifying the ordered structures within liquid crystal polymers. The blue and yellow points in the figure represent particles in smectic-like and nematic-like trajectories, respectively. The results indicate that as the number of neighbouring particles N increases, the classification accuracy of ML-LSA significantly improves. Specifically, the best classification performance is achieved with a single feature Q6 when $N = 12$, yielding a consistency index X_c of 0.92, which demonstrates that this feature can effectively distinguish between the smectic-like and nematic-like structures in liquid crystal polymers. These findings underscore the potential of ML-LSA in automatically identifying and classifying ordered structures in complex molecular systems.[57]

Computational cost is a significant challenge in inverse design and optimization. When integrating machine learning with molecular dynamics simulations, especially when simulating large or complex polymer systems, the computational resource demands can be extremely high. Inverse design typically requires simulating large numbers of candidate materials to identify the optimal design, and each simulation can be computationally intensive, leading to long processing times. To address computational cost, the following approaches can be employed.

(1) High-performance computing (HPC): leveraging high-performance computing resources can significantly accelerate simulations. Parallel computing and distributed computing

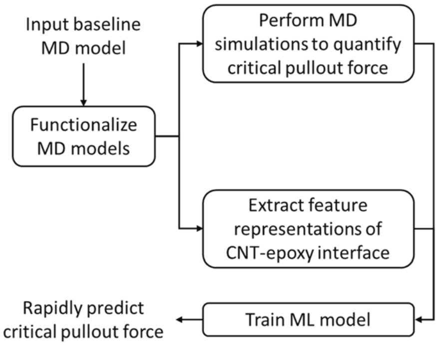


Fig. 6 Predictive capabilities of machine learning frameworks for shear strength at carbon nanotube-polymer interfaces. This figure illustrates a machine learning framework that predicts the shear strength of carbon nanotube-polymer interfaces based on molecular dynamics simulation data. This framework encompasses three primary steps: (1) functionalization of the molecular dynamics model, which involves creating covalent bonds on the surface of carbon nanotubes to simulate different chemical environments. (2) Execution of molecular dynamics simulations to quantify the critical pull-out force, *i.e.*, the force required to pull a carbon nanotube out of the polymer matrix. (3) Extraction of feature representations from the carbon nanotube-epoxy interface and training of a machine learning model to rapidly predict the critical pull-out force. This model is capable of handling the large variability associated with pull-out forces, providing a powerful tool for the design and optimization of nanocomposites. Through this approach, researchers can quickly predict and optimize the performance of carbon nanotube-polymer interfaces without the need for time-consuming molecular dynamics simulations.[61]

techniques can share the computational load, making large-scale simulations more feasible.

(2) Simulation algorithm optimization: by optimizing existing molecular dynamics simulation algorithms, unnecessary computations and iterations can be reduced. For example, coarse-grained models can be used to reduce the number of particles in the simulation, thereby lowering the computational burden.

(3) Machine learning-assisted simulation acceleration: machine learning models can assist in accelerating molecular dynamics simulations by predicting potential energy, thus reducing the need for repetitive simulations. Additionally, machine learning can be used to predict trends in simulation results, helping to eliminate unfeasible designs early and reduce unnecessary calculations.

2.3.5 Multi-objective optimization and modelling of complex systems. Machine learning has demonstrated immense potential in multi-objective optimization. For instance, by combining metaheuristic optimization with coarse-grained molecular dynamics, researchers have optimized the morphology of heterojunctions in organic photovoltaic devices, revealing the role of morphology optimization in enhancing photoelectric conversion efficiency.[60] Similarly, the use of machine learning models to predict shear strength has significantly simplified the optimization process for carbon nanotube-polymer interfaces, providing an important tool for the efficient design of future nanocomposites (Fig. 6).[61]

Despite significant progress made in material science through the integration of machine learning with molecular dynamics simulations, challenges remain. For instance, effectively integrating data across different scales, enhancing the generalization capability of models, and maintaining efficient prediction performance in non-equilibrium systems are issues that still need to be addressed in the future.[51,62] With the continuous optimization of deep learning algorithms and the enhancement of computational resources, this direction holds promise for playing an even more critical role in the study of complex material systems.

3. Molecular structure and performance requirements of oil-displacement polymers

3.1 Key performance requirements for oil-displacement polymers

3.1.1 Solubility. Good solubility of polymers is a fundamental requirement in oil displacement applications. Solubility directly influences the preparation efficiency and rheological properties of polymer solutions. Recent research has found that the dissolution behaviour of ultra-high molecular weight polymers, such as polyacrylamide and its derivatives, significantly affects their molecular weight distribution and solution characteristics. By utilizing Field-Flow Fractionation (FFF) technology, researchers are able to precisely analyze the molecular weight distribution of polymers and optimize their solubility to meet the requirements of specific reservoir conditions.[63,64]

3.1.2 Viscosity maintenance. Viscosity is one of the most important properties of oil displacement polymers, as it increases the viscosity of injected water, improving the mobility ratio of water to oil and subsequently enhancing oil recovery.[65–67] Oil displacement polymers typically behave as non-Newtonian fluids, and their viscosity is closely related to factors such as shear rate, temperature, and salinity. These polymers usually exhibit shear-thinning behaviour, meaning that their viscosity decreases with increasing shear rate.

The viscosity of polymer solutions is influenced by the conformation of the polymer chains, polymer concentration, solvent properties, and external conditions such as temperature and salinity. At low concentrations, polymer chains are more compact, resulting in lower viscosity. As concentration increases, the interactions between polymer chains strengthen, leading to a rise in viscosity. When the concentration exceeds the overlap concentration (C^*), polymer chains begin to form a network structure, and viscosity increases significantly.

The addition of salt can alter the viscosity of polymer solutions because salt ions shield the electrostatic interactions between polymer chains, reducing the expansion of the polymer and consequently lowering the viscosity. The mechanisms by which different cations affect the polymer vary.[68] Na^+ and Ca^{2+} can directly enter the first hydration shell of acrylic acid anions and interact with them, forming stable dipole pairs. In contrast, Mg^{2+}, due to its tightly bound hydration shell, can only interact with acrylic acid anions in the second hydration shell, resulting

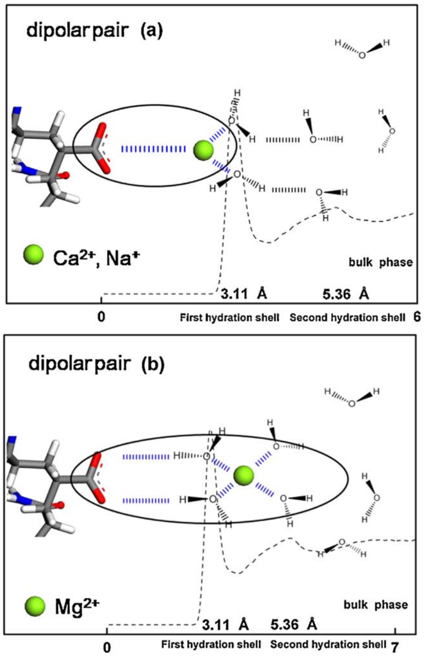


Fig. 7 Schemes of dipolar pair formed by cations and acrylic anion: (a) Na^+, Ca^{2+}, and (b) Mg^{2+}. This figure illustrates the dipole pair structures formed between different cations (Na^+, Ca^{2+}, and Mg^{2+}) and acrylic acid anions, revealing the microscopic mechanism by which salts affect the properties of polymer solutions. This further supports the view that interactions between cations and polymers lead to conformational changes such as the coiling and aggregation of polymer chains. These microscopic structural changes directly influence the viscosity of polymer solutions.[68]

in an unstable dipole pair. These differences in direct contact and hydration state explain why Ca^{2+} and Na^+ have a stronger effect on polymer solution properties, while Mg^{2+} has a weaker impact. Additionally, there are differences in the stability of the dipole pairs: Ca^{2+} forms stable "salt bridges" with multiple acrylic acid anions, significantly enhancing the coiling and aggregation of polymer chains, thereby reducing the viscosity of the solution. The dipole pairs formed by Na^+ are relatively weak and have a smaller impact on polymer chain aggregation (Fig. 7). High temperatures affect the rheological properties of the solution by increasing the mobility of the polymer chains, which can lead to polymer degradation and a subsequent decrease in stability.

3.1.3 Interfacial activity. The interfacial activity of polymers is a crucial characteristic in improving the stability of oil–water interfaces. Molecular dynamics simulation studies have shown that polyacrylamide and its modified polymers can significantly reduce interfacial tension at the oil–water interface, thereby enhancing oil displacement efficiency.[69] Furthermore, the incorporation of functional monomers, such as sulfonates or carboxylates, can bolster the interfacial properties of polymers, enabling them to operate effectively under high-salinity and high-hardness conditions.[70]

3.1.4 Stability under reservoir conditions. The high temperatures, high pressures, and high salinity in reservoir environments pose challenges to the stability of polymers. Recent research has focused on enhancing the heat resistance and salt tolerance of polymers through molecular structure optimization. For instance, acrylamide–acrylic acid copolymers containing sulfonate groups exhibit superior temperature resistance in reservoir conditions.[70] Additionally, methods for hydrolysis and crosslinking of partially hydrolyzed polyacrylamide (PHPAM) have significantly improved its solution viscosity, allowing it to maintain good rheological properties under extreme conditions.[20]

3.1.5 Optimization of molecular weight and molecular weight distribution. The molecular weight and its distribution of polymers have significant impacts on their performance. Studies have shown that high-molecular-weight polyacrylamide can provide high viscosity at lower concentrations, but simultaneously faces higher risks of retention and shear degradation.[63,64] By optimizing the molecular weight distribution, a balance can be achieved between viscosity and mechanical stability, thereby enhancing the overall performance of the polymers.

3.2 Design and application of different types of polymers

In Section 3.1, the key performance requirements of polymer flooding agents were reviewed, particularly their solubility, viscosity retention, interfacial activity, and stability in high-temperature and high-salinity environments. These performance requirements provide fundamental guidance for the design and application of polymers. In this section, the design strategies of different types of polymers were further explored, with a focus on the applications and developments of both conventional and novel polymers in complex environments.

3.2.1 Traditional polymer design and application. Partially hydrolyzed polyacrylamide (HPAM), as a core polymer in chemical enhanced oil recovery (EOR), has been a focus of research and practical application due to its lower cost and ease of field application. The design objectives of HPAM primarily aim to improve its performance in oil reservoirs by optimizing molecular weight, enhancing salt tolerance, and improving thermal stability.[3,71] However, HPAM's performance under high-temperature and high-salinity conditions is limited. For instance, under simulated conditions of a salt concentration of 10.1×10^4 mg L^{-1} and a temperature of 85 °C, the viscosity of HPAM solutions drops significantly, maintaining only 30% of its initial viscosity, and its oil recovery rate increases by only 10% (Fig. 8).[71]

To address this challenge, researchers have enhanced the performance of polymers through molecular structural modifications. Specifically, optimizing the molecular weight distribution of HPAM (hydrolytically polyacrylamide) has been found to improve its viscosity retention capacity. Utilizing field-flow fractionation techniques, studies have revealed that HPAM with a more concentrated molecular weight distribution can maintain 90% of its viscosity under a shear rate of 1 s^{-1}, significantly enhancing its field applicability.[64] Additionally, the introduction of hydrophobic groups to form hydrophobic associating polymers (HAPs) has proven to be an effective strategy. These polymers exhibit superior rheological properties

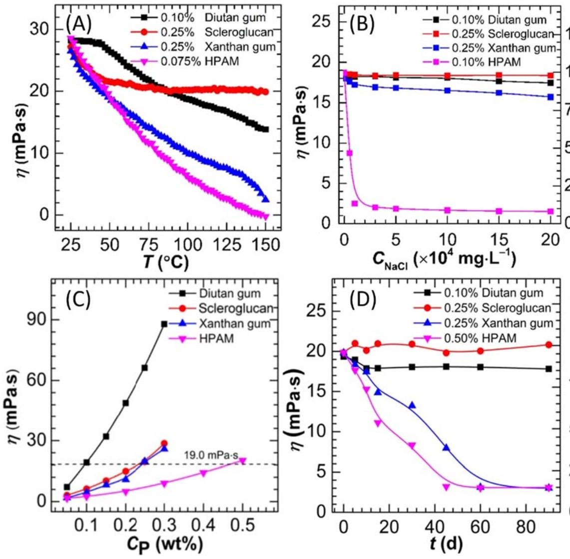


Fig. 8 The viscosity changes of different polymers under different influencing factors. (A) Temperature. (B) Salinity. (C) Polymer concentration. (D) Time.[71]

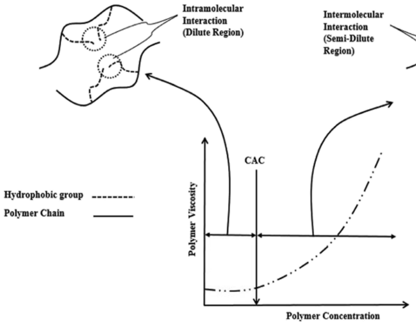


Fig. 9 Evolution of viscosity in hydrophobically associating polymers across the critical aggregation concentration threshold. This figure demonstrates the viscosity changes of hydrophobically associating polymers before and after reaching the critical aggregation concentration (CAC).[67]

and enhanced oil recovery efficiencies under high-salinity conditions.[67]

3.2.2 Novel polymer design and application. In recent years, novel polymers have emerged as research hotspots due to their molecular structural diversity and exceptional performance. Among them, the following design strategies and performance manifestations of novel polymers stand out prominently.

3.2.2.1 Hydrophobic associating polymers (HAPs). Hydrophobic associating polymers (HAPs) have improved their rheological properties and salt tolerance by introducing hydrophobic groups into their hydrophilic backbone (Fig. 9).[67] Experimental results demonstrate that, under high-salinity conditions (200 000 mg per L NaCl), the viscosity of HAPs solutions is enhanced by 40% compared to traditional HPAM. Furthermore, they maintain good viscoelasticity at a shear rate of 1000 s^{-1}.[8,72] These characteristics make them an ideal choice for high-temperature, high-salinity reservoir environments. Quan *et al.*[73] synthesized a hydrophobically associating polymer HPAAT containing sulfonate groups. This polymer is synthesized from acrylamide (AM), allyl polyethylene glycol (APEG), octadecyl dimethyl allyl ammonium chloride (DMAAC-18), and sodium styrene sulfonate (SSS) (Fig. 10). It exhibits excellent thickening and stability even under harsh reservoir conditions, making it particularly advantageous for its application in enhanced oil recovery (EOR). Hydrophobically associating polymers (HAPs) are created by incorporating hydrophobic monomers (such as alkyl or aromatic groups) into hydrophilic polymer chains (*e.g.*, polyacrylamide). These hydrophobic monomers facilitate intermolecular hydrophobic interactions between polymer chains, which become significantly enhanced when the polymer concentration exceeds the critical aggregation concentration (CAC), leading to an increase in the viscosity of the polymer solution. The hydrophobic association strengthens the interactions between polymer chains, forming larger polymer aggregates, which in turn improve the flowability and microscopic oil displacement efficiency of the polymer in the reservoir.

In addition, the negative charge of the sulfonate group enhances the compatibility of the polymer with the oil–water interface. By promoting the interaction between the hydrophilic part of the polymer and the water phase, as well as the association between the hydrophobic part and the oil phase, HAPs containing sulfonate groups can effectively promote adsorption

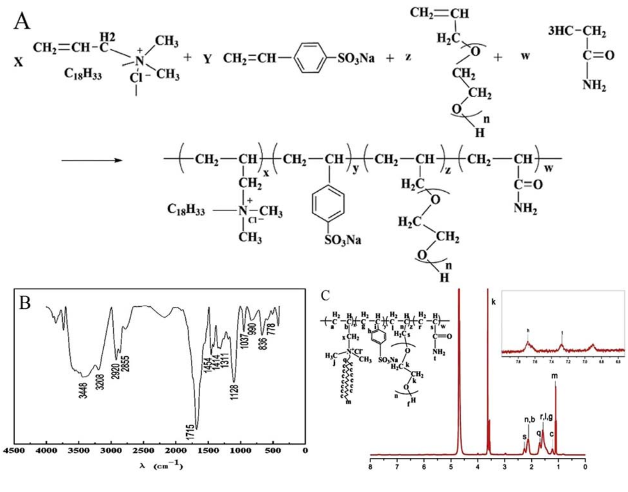


Fig. 10 (A) Molecular structure of HPAAT. (B) FTIR spectrum of HPAAT. (C) Nuclear magnetic resonance spectrum of HPAAT. The introduction of sulfonate groups further enhances the performance of HAPs. Sulfonate groups ($-SO_3H$), as highly polar functional groups, significantly increase the hydrophilicity of the polymer, resulting in better solubility in water. These sulfonate groups can coordinate with sodium, calcium, magnesium, and other ions in the solution, reducing the shielding effect of salts on the polymer chains, thereby improving the stability and solubility of the polymer in high-salinity environments. This chemical interaction allows sulfonate-modified HAPs to maintain excellent rheological performance even under extreme conditions such as high salinity and temperature, making them a more reliable material for oil recovery.[73]

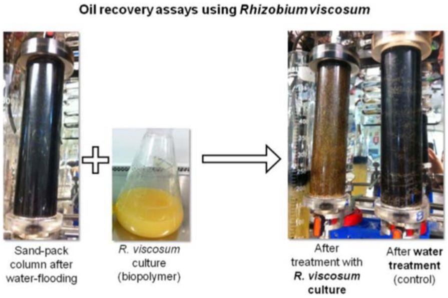


Fig. 11 Oil recovery assay results using *Rhizobium viscosum*.[74]

at the oil–water interface, improving the distribution of oil and water. This structure enables the polymer to distribute more effectively in complex reservoirs, optimizing the reservoir.

3.2.2.2 *Biobased polymers.* Biobased polymers, represented by xanthan gum (XG), diutan gum (DG), and rhizobium-derived polymers, have garnered attention due to their environmental friendliness and exceptional performance. In simulated reservoir experiments, xanthan gum exhibited a viscosity retention rate of up to 85% under high-salinity conditions (200 000 mg per L NaCl) and high temperatures (80 °C), significantly higher than the 30% retention rate of traditional HPAM. Furthermore, it enhanced oil recovery by 16%, compared to the 10% increase achieved by HPAM.[71,74] Additionally, rhizobium-derived polymers demonstrated superior viscosity retention capabilities, with an oil displacement efficiency of 25.7% (Fig. 11 and 12).[74] This is partly attributed to the shear thinning (pseudoplasticity) properties exhibited by this biopolymer, similar to xanthan gum. When injected into the reservoir, the viscosity of the polymer solution decreases under high shear rates, which enhances injectability. As the solution moves further from the injection point and the shear rate decreases, the viscosity recovers, thereby improving the efficiency of oil displacement and contributing to a higher oil recovery rate.

This enhanced viscosity retention suggests that rhizobium-derived polymers could be scaled up for field applications, where maintaining polymer performance under extreme reservoir conditions is crucial. These superior rheological properties make it feasible for large-scale synthesis, as polymers with stable viscosity under harsh conditions are essential for efficient and economical oil recovery at the industrial level. Additionally, the *R. viscosum* CECT 908 biopolymer has demonstrated stability at high shear rates (up to 300 s^{-1}), high temperatures (up to 80 °C), and high salinities (up to 200 g per L of NaCl), making it particularly suitable for enhanced oil recovery (EOR) in mature, high-salinity reservoirs. Compared to xanthan gum, this biopolymer shows greater efficiency in oil displacement and is more resistant to mechanical degradation, which is crucial for scalable field applications. These findings underscore its potential for use in Microbial Enhanced Oil Recovery (MEOR), where the ability to maintain polymer stability and enhance oil recovery over long-term operations is essential for cost-effective and efficient field performance.[74]

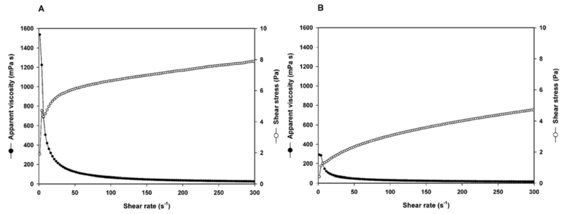


Fig. 12 Comparative rheological analysis of rhizobium-derived polymers *versus* xanthan gum. This figure illustrates the viscosity performance of rhizobium-derived polymer (*R. viscosum* CECT 908) and xanthan gum (XG) at various shear rates under conditions of 40 °C. The rhizobium-derived polymer exhibits higher viscosity than xanthan gum under identical conditions, indicating its greater potential in enhancing the viscosity of injected water, particularly in high-temperature, high-salinity reservoir environments.[74] (A) *Rhizobium viscosum* CECT 908 biopolymer (B) Xanthan gum.

Biobased polymers, particularly those synthesized from monoterpenes (*e.g.*, limonene, pinene), offer significant advantages in terms of environmental sustainability. Monoterpene-based polymers have demonstrated good biodegradability, which makes them promising candidates for use in enhanced oil recovery (EOR) applications. These polymers degrade gradually in the reservoir environment, primarily through microbial activity, thereby reducing their long-term environmental impact. Specifically, under anaerobic conditions typical of oil reservoirs, monoterpene polymers exhibit slow degradation, which helps minimize the accumulation of residual polymer in the subsurface. Furthermore, the lifecycle analysis of biopolymer production shows that biopolymers consume fewer fossil resources compared to conventional petroleum-based polymers and can degrade into non-toxic substances after use, contributing to the sustainable development of oilfields.[75]

3.2.2.3 *Nanoparticle-composite polymers.* Nanoparticle-composite polymers exhibit significant performance advantages in enhanced oil recovery (EOR), particularly in improving the rheological properties, shear stability, temperature and salt tolerance, and oil displacement efficiency of polymers. Studies have shown that nanoparticles can effectively enhance the viscosity and stability of polymer solutions, thereby improving the efficiency of oil recovery.[8,72]

Specifically, nanoparticles (such as SiO_2) strengthen the polymer network structure through hydrogen bonding and electrostatic interactions with polymer molecules (Fig. 13 and 14). This structure allows the polymer solution to maintain a high viscosity under high shear rates, thus improving the oil displacement efficiency (Fig. 15). For instance, the viscosity of the solution significantly increases when SiO_2 nanoparticles are incorporated into polyacrylamide (PAM), especially at low shear rates, where the solution exhibits better shear-thinning behaviour.

Moreover, nanoparticle-composite polymers demonstrate excellent temperature and salt tolerance. Research has found that SiO_2 nanoparticles can effectively enhance the stability of polymers in high-temperature and high-salinity environments. Under conditions of 60 °C, the addition of SiO_2 significantly reduces the viscosity loss of HPAM solutions. In high-salinity environments, the addition of nanoparticles helps mitigate

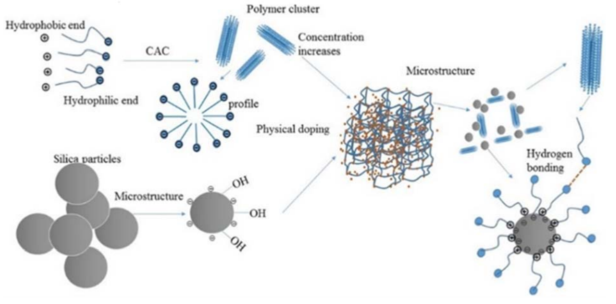


Fig. 13 Mechanism of increasing fluid viscosity by combining silica nanoparticles with amphiphilic polymers.[76]

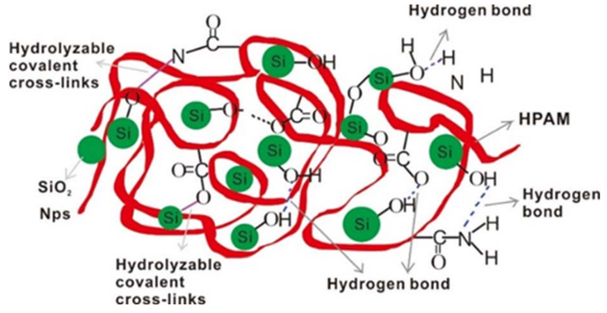


Fig. 14 Potential interactions between SiO_2 and HPAM.[77]

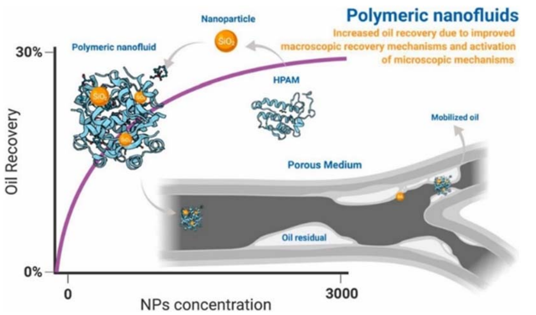


Fig. 15 Macro–micro theoretical mechanism of SiO_2 nanoparticles-polymer flooding system.[78]

polymer degradation, increases polymer rigidity, and thus improves the rheological properties of the solution and oil recovery efficiency.

In terms of oil displacement performance, nanoparticle-composite polymers can alter the wettability of reservoir rocks, transforming them from oil-wet to water-wet, thereby promoting oil displacement. For example, the addition of SiO_2 nanoparticles significantly reduces the interfacial tension between oil and water, further enhancing oil recovery rates.

3.2.2.4 Hyperbranched polymers. Hyperbranched polymers (HBPs) are a class of macromolecules with a three-dimensional dendritic structure. Due to their unique architecture, excellent properties, and easy synthesis methods, they have been widely applied in the field of enhanced oil recovery (EOR). Compared to traditional linear polymers, the molecular structure of hyperbranched polymers contains a greater number of terminal groups, which provide more functional groups. This characteristic makes them particularly attractive for applications in oilfield chemistry.

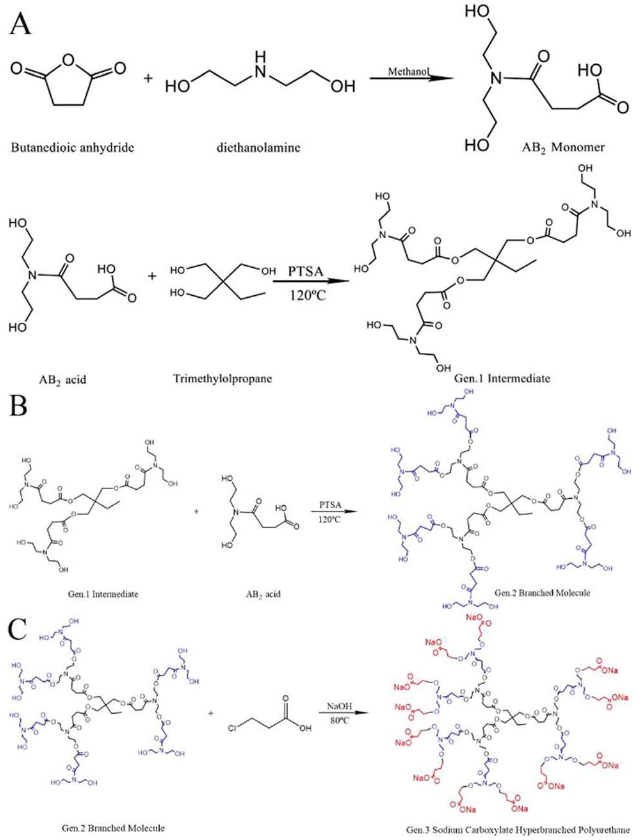


Fig. 16 (A) Synthesis of the AB2 monomer and Gen.1 intermediate. (B) Synthesis of Gen.2 hyperbranched polyurethane (HPAE). (C) Synthesis of HPAE with sodium carboxylate at the end of Gen.2 (*m*-HPAE).[81]

The synthesis of hyperbranched polymers typically involves the polycondensation reaction of ABx-type monomers, as discussed by Flory.[79,80] By precisely controlling the monomer ratio, hyperbranched polymers of different generations can be synthesized. The branched structure of these polymers can be further improved by modifying their functional groups. For example, esterification reactions can be employed to react polyhydroxy compounds with monomers containing acidic groups, leading to the formation of the final hyperbranched polymer.

In the application of enhanced oil recovery, hyperbranched polymers exhibit excellent interfacial activity, low critical micelle concentration (CMC), and good emulsification properties. Qiao *et al.*[81] synthesized a hyperbranched carboxylate-type polymer (*m*-HPAE), which had a CMC of 433.63 mg L^{-1}, a Krafft point of 5 °C, and reduced surface tension to 28 mN m^{-1} (Fig. 16). These properties make this polymer outstanding in reducing oil–water interfacial tension and improving oil drop migration efficiency (Fig. 17). Through further modifications, *m*-HPAE can be functionalized *via* its abundant terminal groups, enhancing its performance in oilfield applications. For

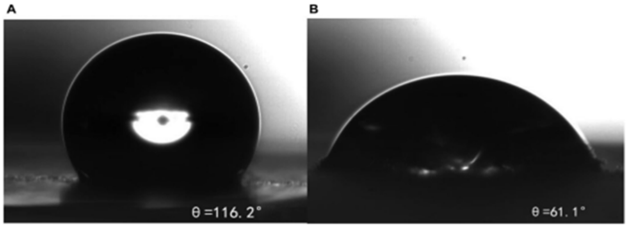


Fig. 17 Contact angle of hydrophobic formation of the rock sample (A) and rock sample after *m*-HPAE treatment (B). This figure demonstrates the interface improvement capability of *m*-HPAE.[81]

instance, when *m*-HPAE is used in combination with sodium dodecyl sulfate (LAS), the interfacial tension can be further reduced to 10^{-3} mN m^{-1}. Experimental results have shown that oil recovery using *m*-HPAE alone or in combination with LAS increased by 10.4% to 32.21% compared to water flooding, with the combination system showing more significant effects, especially in low-permeability reservoirs.

In synthesizing the aforementioned discussions, it is evident that traditional polymers, such as partially hydrolyzed polyacrylamide (HPAM), continue to occupy a central position within the realm of chemical enhanced oil recovery (EOR) due to their cost-effectiveness and versatility across a wide range of applications. Nevertheless, the evolving landscape of reservoir conditions, characterized by increasing complexity, and the heightened emphasis on environmental stewardship, have necessitated the emergence of novel polymer classes. Notably, hydrophobic association polymers, bio-based polymers, and nanocomposite polymers have exhibited substantial promise and adaptability, marking a significant advancement in the field.

3.2.3 Environmental trade-offs of using synthetic *versus* natural polymers in EOR. The selection of polymers for Enhanced Oil Recovery (EOR) involves a careful balance between performance, sustainability, and environmental impact. Both natural and synthetic polymers offer distinct advantages and drawbacks in terms of their environmental sustainability, which must be considered when choosing the most appropriate material for specific reservoir conditions (Table 1).[82]

Natural polymers, such as xanthan gum and rhizobium-derived polymers, are generally more environmentally friendly due to their biodegradability. They can degrade gradually in the reservoir environment through microbial activity, which helps to minimize long-term environmental pollution. Furthermore, the degradation products of natural polymers are typically non-toxic and do not impose additional burdens on ecosystems, making them highly compatible with the environment. In addition to their biodegradability, natural polymers often exhibit high biocompatibility, which reduces negative impacts on the surrounding ecological system.

However, despite these advantages, natural polymers have certain limitations. Their mechanical strength is often weaker compared to synthetic polymers, and their performance can be severely compromised in extreme reservoir conditions, such as high temperature and high salinity. Furthermore, the cost of production for natural polymers tends to be higher, and their sources are often limited, making large-scale application challenging and economically burdensome in some cases.

On the other hand, synthetic polymers such as partially hydrolyzed polyacrylamide (HPAM) offer superior mechanical properties, thermal stability, and salt tolerance, making them particularly effective in harsh reservoir environments. These polymers are also cost-effective and easy to produce on a large scale, which makes them widely used in EOR applications. However, the production of synthetic polymers typically requires significant amounts of energy and chemical raw materials, which contribute to environmental impact. Additionally, many synthetic polymers have poor biodegradability, which raises concerns about their potential long-term environmental persistence and the risks of residual polymers in oil fields.

Thus, while synthetic polymers offer better performance under extreme conditions, their environmental trade-offs, particularly in terms of biodegradability and production impact, cannot be overlooked. The decision to use natural or synthetic polymers in EOR must therefore be based on a careful evaluation of the polymer's performance characteristics and its environmental footprint. Striking a balance between the polymer's ability to enhance oil recovery and its sustainability is crucial, especially as environmental concerns continue to gain prominence in the oil and gas industry.

3.2.4 Green synthesis methods for oil-displacement polymers. The development of green synthesis methods for oil-displacement polymers has gained significant attention in recent years, as these methods align with global sustainability goals by reducing the environmental impact of polymer production. Various innovations in green synthesis have emerged, focusing on utilizing renewable resources, improving energy efficiency, and minimizing pollution, making them particularly relevant to the oil industry and aligned with global sustainable development goals.

Table 1 Typical advantages and drawbacks of natural and synthetic polymers[82]

Polymers	Advantages	Drawbacks
Natural polymers	(1) High biocompatibility inmost cases (2) Suitable biodegradability (3) Non-toxic degradation products	(1) Relatively weak mechanical properties (2) Restricted sources (3) High production costs
Synthetic polymers	(1) Low cost (2) Easy to produce massively (3) Adjustable mechanical properties	(1) Lack of biological cues (2) Relatively poor biodegradability in most cases

3.2.4.1 Biobased and biodegradable polymers development. One of the most promising developments is the production of biobased and biodegradable polymers, such as polylactic acid (PLA). PLA, which is derived from renewable resources like corn starch, reduces reliance on fossil fuels.[83] The synthesis of PLA is designed with green chemistry principles in mind, such as using enzyme-catalyzed polymerization techniques, which lower energy consumption and minimize by-product formation.[84] Similarly, plant oil-based polycarbonates, synthesized through the copolymerization of epoxy plant oils (*e.g.*, soybean oil, linseed oil) with CO_2, not only utilize CO_2 as a resource but also enhance the polymer's biodegradability. These materials can degrade naturally after use, reducing environmental residues and supporting the circular economy.[85]

3.2.4.2 Innovations in green synthesis technologies. In addition to biobased polymers, green synthesis technologies have seen innovations that improve the environmental sustainability of polymer production processes. Solvent-free polymerization is one such innovation, which eliminates volatile organic solvents like *N*,*N*-dimethylformamide (DMF), thereby reducing the emission of toxic substances during production. This method also decreases energy consumption, making it more eco-friendly.[84,86] Another noteworthy approach is mechanochemical synthesis, where mechanical force, such as ball milling, is used to initiate polymerization reactions. This avoids the need for high temperature and pressure, significantly reducing energy consumption.[87,88] Photopolymerization technologies also allow for polymerization at ambient temperatures, using light initiators to carry out reactions efficiently without solvents, thereby reducing VOC emissions.[84]

3.2.4.3 Circular economy and resource-efficient utilization. Furthermore, the resource-efficient utilization of CO_2 has led to the synthesis of carbonates and polycarbonates from CO_2, helping to mitigate greenhouse gas emissions and substitute petroleum-based raw materials. Zinc- or copper-catalyzed systems have been used to achieve high-efficiency copolymerization of CO_2 with epoxides under mild conditions. This process aligns with the circular economy model, effectively turning waste CO_2 into valuable products while reducing environmental impact.[89]

3.3 Causal analysis of polymer molecular structure and macroscopic properties

The intricate molecular architecture of polymers, characterized by variables like chain length and the presence of specific functional groups, profoundly impacts their macroscopic characteristics and the efficacy of oil displacement processes. Extensive and recent research endeavours have unequivocally shown that through meticulous adjustments to the polymer's molecular structure, remarkable improvements can be realized in terms of viscosity augmentation, salt resistance, and the injectability profile within the reservoir.

3.3.1 Impact of polymer chain length

3.3.1.1 Effect of molecular chain length on viscosity enhancement and injectivity. Viscosity enhancement is a key indicator for evaluating the efficiency of polymer flooding, as it directly affects the effectiveness and injectivity of the process. The molecular structure of the polymer, particularly its chain length and intermolecular interactions, determines its rheological properties. In polymer flooding, longer molecular chains generally provide stronger intermolecular forces, thereby enhancing the viscosity of the solution.

The study by Li *et al.*[90] demonstrated that a polymer with 18 ethoxy (EO) units exhibited significant viscosity enhancement. At a concentration of 1500 mg L^{-1}, the viscosity of this polymer was 113.1 mPa s, approximately 2.5 times higher than that of conventional polymers. This significant viscosity enhancement results from the longer molecular chains forming stronger aggregates through intermolecular hydrogen bonding and hydrophobic interactions, which lead to a denser three-dimensional network in the aqueous solution. The increase in EO chain length strengthens the interactions between molecular chains, promoting tighter molecular associations and enhancing the viscosity and stability of the solution. The growth of molecular chains significantly impacts the polymer's structure and dynamic properties. Additionally, Corredor *et al.*[91] explored the combination of nanoparticles with HPAM and found that increasing molecular chain length and rigidity significantly enhanced both the viscosity and interfacial properties of the solution, particularly under high salinity conditions. However, although an increase in molecular chain length can enhance viscosity, it may also affect the injectivity of the polymer in the reservoir. During reservoir injection, longer molecular chains can reduce the polymer's permeability, thereby affecting its injection efficiency. The molecular chain length determines the permeability and distribution characteristics of the polymer during the injection process. The adaptive polymer (SAP) proposed by Zhang *et al.*[92] demonstrated that shorter but more efficient molecular chains not only achieved good injectivity but also avoided the reservoir plugging issues caused by high molecular weight polymers.

3.3.1.2 Design of molecular chains in high-temperature and high-salinity environments. In high-salinity environments, the molecular chain length significantly affects the salt tolerance and degradation resistance of polymers. Polymers with longer molecular chains are generally more prone to degradation, especially under high-salinity conditions. Åsen's research[93] found that high molecular weight HPAM polymers in high-salinity environments are prone to shear degradation, resulting in a loss of viscosity. However, molecular structure modifications, such as using ATBS copolymer monomers, can significantly improve their salt tolerance. In contrast, biopolymers like guar gum exhibit higher stability and degradation resistance in divalent salt (*e.g.*, $CaCl_2$) environments.[94] Furthermore, in the study by Li *et al.*,[90] the PAAP-18 polymer maintained a viscosity of 34.6 mPa s at a salinity of 20 000 mg L^{-1} (at 50 °C and a polymer concentration of 1500 mg L^{-1}), whereas the viscosity of the conventional polymer P1 decreased to 19.4 mPa s. This remarkable salt tolerance is primarily attributed to the unique amphiphilic molecular structure of PAAP-18 and the specific interactions among its components under high salinity conditions. The hydrophilic ethoxy (EO) units in the molecule enhance the polymer's dispersibility in high salinity solutions, while the hydrophobic

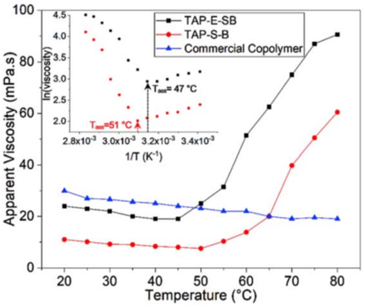


Fig. 18 Viscosity retention of acrylamide-based polymers under high temperature and high salinity conditions. This figure shows the temperature-dependent viscosity behaviour of different acrylamide-based polymers (including TAP-E-SB, TAP-S-B, and commercial AM-based copolymers) at a concentration of 2000 ppm in a 5% KCl aqueous solution.[95]

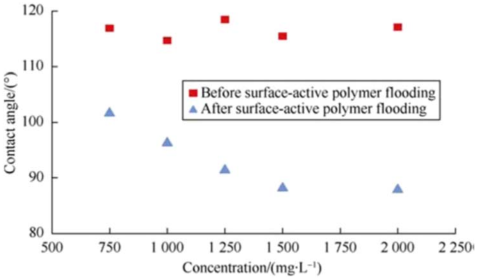


Fig. 19 Change in rock contact angle before and after treatment with surfactant polymers.[96]

segments promote the formation of a stable network structure. Under high salinity conditions, metal cations in the solution (such as Na^+ and Ca^{2+}) induce charge shielding effects, reducing the electrostatic repulsion between polymer chains and allowing them to aggregate more closely. This aggregation enhances the polymer's rheological properties and maintains its viscosity. Additionally, the enhanced hydrophobic interactions between alkyl or aromatic groups further stabilize the polymer's network structure and prevent chain dissociation.

Some reservoir conditions, where the environment is both highly saline and at very high temperatures, make the design of molecular chain length and structure particularly crucial. The acrylamide-based polymers (TAP-E-SB and TAP-S-B) synthesized by Tamsilian *et al.*[95] exhibited excellent viscosity retention under high-temperature (up to 80 °C) and high-salinity conditions, with TAP-E-SB showing a significant viscosity increase at high temperatures, indicating good thermal stability and potential for enhanced oil recovery applications (Fig. 18). In contrast, traditional AM-based copolymers showed a tendency for viscosity decrease under high-temperature conditions, indicating poor thermal stability.

3.3.1.3 *Optimization of molecular chain length and enhancement of interfacial properties.* The effect of molecular chain length on interfacial properties is reflected in wettability and interfacial tension regulation. Qiannan *et al.*[96] experimentally demonstrated that surfactant polymers, with larger molecular coil sizes and enhanced interfacial tension regulation capabilities, significantly improve reservoir wettability, causing the rock surface to transition from oil-wet to water-wet. This improvement in wettability aids in reducing oil–water interfacial tension and enhances the dispersion of oil droplets in the water phase, thereby increasing oil recovery efficiency (Fig. 19). Furthermore, the ability of surfactant polymers to significantly alter the wettability of reservoir rocks has important implications for their scalability in field applications. As shown in the experimental results, these polymers maintain their effectiveness at various concentrations, suggesting that they can be synthesized at large scales for field use without significant loss of performance. This characteristic makes surfactant polymers particularly promising for enhanced oil recovery (EOR) in mature oilfields, where maintaining stable wettability and improving oil recovery efficiency are critical for the success of large-scale operations. Additionally, Majeed *et al.*[97] proposed sulfonated polymers that enhance solution viscosity and reduce liquid drainage, thereby improving foam stability and interfacial tension control capabilities. What's more, the PAAP-18 polymer synthesized by Li *et al.*[90] with 18 ethoxy (EO) units can significantly reduce the interfacial tension (IFT) between oil and water, primarily due to its unique molecular structure and interfacial properties. PAAP-18 is an amphiphilic polymer, containing hydrophilic polyethylene glycol (PEG) segments and hydrophobic alkyl or aromatic groups in its molecular chain. This amphiphilic nature allows the polymer to align directionally at the oil–water interface, forming a stable adsorption layer that reduces interfacial tension. The presence of EO units enhances the polymer's hydrophilicity and flexibility, enabling PAAP-18 to adsorb more uniformly on the interface and adapt to interfacial deformations. Additionally, the intermolecular forces between PAAP-18 chains, such as hydrogen bonds and van der Waals forces, further strengthen its adsorption capacity and stability at the interface. Experimental results indicate that at a concentration of 1500 mg L^{-1}, PAAP-18 can reduce the oil–water IFT from 44.4 mN m^{-1} to 13.0 mN m^{-1}, whereas the conventional polymer P1 can only reduce it to 30.6 mN m^{-1}. This demonstrates that PAAP-18 has superior interfacial activity and adsorption ability, which enable it to more effectively reduce interfacial tension and thereby significantly enhance heavy oil recovery efficiency.

3.3.2 **Effect of polymer functional groups on EOR performance.** Functional groups within polymer molecules play a pivotal role in determining their rheological properties, adsorption characteristics, and interfacial activity, thereby directly impacting their application effectiveness under reservoir conditions. In recent years, researchers have significantly enhanced the salt tolerance, thermal stability, and oil displacement efficiency of polymers by adjusting and optimizing the functional group structure, marking significant advancements in this field.

3.3.2.1 *The role of hydrophilic functional groups.* Hydrophilic functional groups, such as carboxyl and sulfonate groups, play a significant role in improving viscosity retention and enhancing oil recovery by enhancing polymer solubility and salt

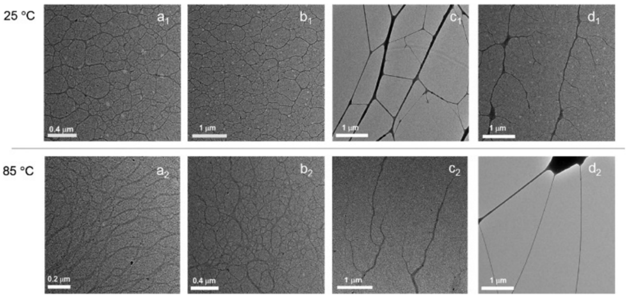


Fig. 20 TEM micrographs for diutan gum (a1 and a2), scleroglucan (b1 and b2), xanthan gum (c1 and c2), and HPAM (d1 and d2) at 25 and 85 °C ($C_p = 0.05$ wt%, no salt). Diutan gum, scleroglucan, and Xanthan gum were biopolymers produced through fermentation by the bacteria *Sphingomonas*, the plant pathogenic fungus *Sclerotium*, and the bacteria *Xanthomonas*, respectively.[71]

tolerance. For instance, Aguiar *et al.*[98] demonstrated that polymers containing sulfonate groups can significantly enhance solution stability under high-salinity conditions while improving rheological properties. Additionally, biopolymers such as xanthan gum, due to the carboxyl and hydroxyl groups in their molecules, exhibit excellent salt tolerance and thermal stability, particularly under high-salinity and high-temperature environments (Fig. 20).[70,99] These hydrophilic groups, through ionic interactions and intermolecular electrostatic repulsion, reduce the risk of molecular entanglement and degradation, providing effective solutions for complex reservoir conditions.

3.3.2.2 *The contribution of hydrophobic functional groups.* Hydrophobic functional groups within polymers contribute to enhancing both the viscoelasticity of solutions and the microscopic displacement efficiency by forming intermolecular hydrophobic association networks.[8,67] For instance, oil-affinity-modified polymers, under high-temperature and high-salinity conditions, form viscous networks through the self-assembly effect of hydrophobic groups, significantly improving the fluid mobility control within reservoirs. Studies have shown that the synergistic action of nanoparticles with hydrophobic groups can further elevate the viscosity and shear stability of polymers, thereby reducing adsorption losses and enhancing oil recovery efficiency.[8,72] Additionally, hydrophobic segments within thermosensitive polymers spontaneously form structured networks under high-temperature conditions, further augmenting their oil displacement performance.[98]

3.3.2.3 *Enhancement of interfacial behaviour by surface-active functional groups.* Surface-active functional groups, such as amide, long-chain alkyl, and sulfonate groups, play pivotal roles in reducing interfacial tension, altering rock wettability, and forming stable emulsions. For instance, experiments conducted by Qiannan *et al.*[96] demonstrated that surface-active polymers can effectively drive residual oil out of pores by reducing interfacial tension to as low as 10^{-2} mN m^{-1} and simultaneously transforming the rock surface from oil-wet to water-wet. These surface-active groups also significantly enhance the emulsification capacity of oil under non-ultra-low interfacial tension conditions, further expanding the microscopic contact area for oil displacement (Fig. 21).

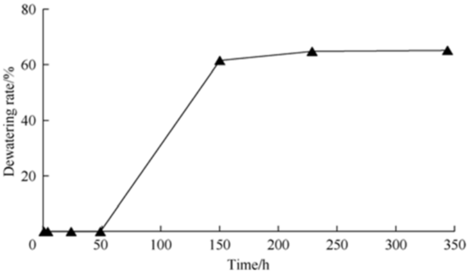


Fig. 21 Stability analysis of surfactant–polymer emulsions: insights into structural integrity. This figure illustrates the dehydration rate of emulsions generated by surface-active polymers over time, reflecting their emulsification capacity under non-ultra-low interfacial tension conditions. The higher the stability of the emulsions, the more effectively the surface-active polymers can stably disperse oil droplets in water, thereby enhancing oil washout efficiency. This emulsification effect is crucial for improving oil recovery in high-water-cut mature reservoirs.[96]

3.3.2.4 *Adaptability of special functional groups to extreme environments.* In high-temperature, high-salinity reservoirs, the incorporation of special functional groups is crucial for the optimal design of polymers. For instance, research by Liang *et al.*[71] has shown that alginate and schizophyllan, which contain polysaccharide-based functional groups, maintain stable viscosity under high-temperature conditions, serving as effective alternatives to traditional polyacrylamide (HPAM). Furthermore, Couto *et al.*[74] reported on a biopolymer produced by *Rhizobium viscosum*, whose natural functional group structure grants it high viscosity stability, maintaining efficient oil displacement performance even under conditions of 80 °C and 200 g per L NaCl. These natural functional groups not only reduce the risk of shear degradation of polymer molecules but also significantly enhance rheological properties and adsorption stability.

3.3.2.5 *Environmental potential of functional groups in green polymers.* Green polymers are increasingly gaining attention due to their natural functional group structures and environmentally friendly characteristics. For example, the hydroxyl and carboxyl groups in xanthan gum exhibit superior rheological properties under high-salinity conditions, far surpassing traditional synthetic polymers.[99] Furthermore, the branched polymers prepared by combining chitosan and polyamidoamine (PAMAM) dendrimers exhibit significantly enhanced fluidity and oil displacement capability in porous media, thanks to their special functional groups. The optimization of these functional groups not only improves the oil displacement ability of the polymers but also demonstrates excellent biodegradability, providing a new direction for environmentally friendly Enhanced Oil Recovery (EOR) technologies.

As the challenges posed by extreme reservoir environments continue to escalate, the design of polymer functional groups will increasingly trend towards intelligence and multifunctionality. By integrating nanotechnology, smart responsive moieties (such as thermosensitive and pH-sensitive groups) along with green chemistry approaches, the performance and environmental adaptability of polymers will be further enhanced. These research endeavours provide novel insights and technical support for the efficient recovery of hydrocarbons from complex reservoirs in the future.

4. Application of molecular dynamics simulation in the design and optimization of oil-displacement polymers

4.1 Molecular-level analysis of polymer-driven oil recovery mechanisms

A profound understanding of the interactions between polymers and oil is crucial for optimizing polymer-flooding oil recovery techniques. The advancement of molecular dynamics simulation technology has provided a powerful tool for research in this field, enabling researchers to observe these interactions at the atomic scale and uncover how they influence oil droplet displacement and oil recovery efficiency.

4.1.1 Oil displacement mechanisms of viscoelastic polymers in nanopores. At the molecular level, the oil displacement efficiency of viscoelastic polymers in nanopores is closely related to their unique rheological properties. Through molecular dynamics simulations, researchers can observe in detail the interactions between polymer chains and oil droplets, including the encapsulation and stretching of oil droplets by polymer chains, which result in displacement (Fig. 22). Studies by Fan *et al.* have shown that the interactions between polymers and oil droplets provide additional drag forces, which are crucial for enhancing oil displacement efficiency. Specifically, longer polymer chains (*e.g.*, $N = 250$) are more effective than shorter chains (*e.g.*, $N = 100$) in pulling oil droplets out of dead-end pores, with a significant reduction in the required injected pore volume (PV). For instance, polymers with $N = 150$ require 1.87 PV to fully displace oil droplets, while those with $N = 250$ only need 0.85 PV, indicating that longer polymer chains improve oil displacement efficiency while reducing the amount of polymer required (Fig. 23).[100]

4.1.2 Molecular-level analysis of interactions between polymers and oil. Further molecular dynamics simulations were conducted to investigate polymers of varying chain lengths, assessing their oil displacement capabilities and revealing the interactions between polymers and oil. These research findings indicate that the interaction between polymer chains and oil droplets can provide an additional pulling effect, which is crucial for enhancing oil droplet displacement efficiency. In particular, polymers with longer chains exhibit stronger elastic properties, amplifying the aforementioned pulling effect and thus improving oil droplet displacement efficiency. Wang's research in 2008 explored the interaction mechanism between active polymers and crude oil, and provided calculations of the adsorption energy of active polymers on rock surfaces. These calculations reveal that the adsorption energy of active polymers on rock surfaces is much greater than that of heavy crude oil from isolated oilfields on rock surfaces, suggesting that active polymers can desorb crude oil from rock surfaces, making it mobile oil.[101]

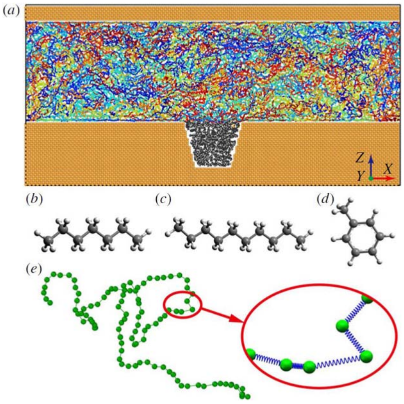


Fig. 22 (a) Snapshot of the initial structure for MD simulations. The yellow part represents the wall of the pore; the grey part is the oil droplet trapped in the dead end; the colourful chains confined between the walls are polymer molecules. The molecular structures of (b) heptane, (c) decane and (d) toluene are also illustrated. (e) The detail of a representative polymer molecule. Inset illustrates the bead-spring model of the polymer chain.[100]

4.2 Application of molecular dynamics simulation in polymer performance optimization

In Section 4.1, the molecular-level mechanisms underlying the interactions between polymers and oil were analyzed, highlighting the critical role of these interactions in enhancing oil displacement efficiency. The subsequent Section 4.2 will focus on how molecular dynamics simulations can be utilized to optimize the rheological properties of polymers, further improving their performance in enhanced oil recovery processes.

4.2.1 Simulation studies of rheological properties and viscosity changes in polymer solutions. Molecular dynamics simulation technology has played a pivotal role in exploring the rheological properties and viscosity changes of polymer solutions, particularly in the design and optimization of oil-displacement polymers. This technology enables us to observe the behaviour of polymer chains and the detailed processes of their interactions with fluids at the atomic level, thus providing a microscopic explanation for the macroscopic rheological characteristics of polymer solutions.

Li *et al.* conducted molecular dynamics simulations to investigate the influence of hydrated montmorillonite on the viscosity of polyacrylamide (PAM) under confined shear conditions. Their research revealed that, as the temperature increased from 298 K to 343 K, the viscosity of PAM exhibited a decreasing trend. This may be attributed to the weakening of interactions between polymer chains due to the temperature rise, which subsequently affected the overall viscosity of the solution. Furthermore, the study also found that, at high shear rates, the viscosity reduction of PAM was more pronounced. This could be related to the adjustment of polymer chain conformations by shear forces, leading to a more ordered

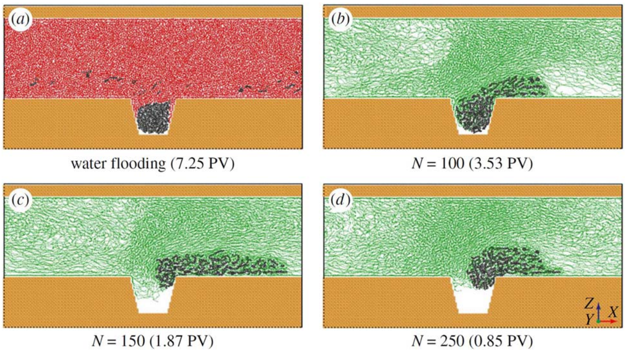


Fig. 23 Displacing behaviours of trapped oil by different flooding agents, namely (a) water and (b–d) polymers with varying chain lengths. This figure illustrates the displacement behaviour of oil droplets using different oil displacement agents. Specifically, (a) depicts the oil displacement effect of water flooding, while (b) to (d) show the displacement effects of polymers with varying chain lengths on oil droplets, respectively. The experimental results indicate that longer polymer chains (*e.g.*, $N = 250$) are more effective than shorter chains (*e.g.*, $N = 100$) in pulling oil droplets out of dead-end pores, with a significant reduction in the required injected pore volume (PV). To elaborate, polymers with $N = 150$ require 1.87 PV to fully displace oil droplets, whereas those with $N = 250$ only need 0.85 PV, demonstrating that longer polymer chains enhance oil displacement efficiency while reducing the amount of polymer required. These findings support the theory that viscoelastic polymers improve oil displacement efficiency in nanopores through their unique rheological properties, particularly in enhancing oil droplet displacement efficiency.[100]

arrangement of polymer chains and thus reducing the viscosity of the solution.[102]

Chen *et al.* employed molecular dynamics simulations to explore the solution models of hydroxypropyl polyacrylamide (HPAM) and polyacrylamide (PAM) at varying NaCl concentrations, revealing the impact of salt concentration on the rheological properties of polymer solutions. The research findings indicated that, as the NaCl concentration increased, the viscosity of HPAM solutions decreased significantly. This may be attributed to the compression of the electrical double layer between carboxylate groups on HPAM molecules by the addition of NaCl, which reduced the repulsive interactions between molecules, leading to a greater tendency for polymer chains to aggregate and consequently lowering the solution's viscosity. In contrast, the viscosity changes of PAM solutions were not pronounced, possibly due to the lack of ionic groups on PAM molecules, rendering them insensitive to variations in salt concentration.[103]

These molecular-scale simulation results not only deepen our understanding of the rheological behaviour of polymer solutions but also provide crucial guidance for designing polymers with specific rheological properties. By adjusting the chemical structure of the polymers and external conditions (such as temperature, shear rate, and salt concentration), the rheological properties of the polymers can be optimized to meet specific requirements for oil displacement applications.

4.2.2 Simulation applications for wettability alteration and enhanced oil recovery. In the field of oil displacement, the alteration of polymer wettability plays a pivotal role in enhancing oil recovery from reservoirs. Molecular dynamics simulation technology has played a crucial role in unveiling the interactions between polymers and reservoir rocks, predicting wettability changes, and assessing oil displacement efficiency. In recent years, research in this field has made significant progress, particularly in understanding how polymers enhance recovery rates by altering wettability.

4.2.2.1 Molecular mechanisms underlying the alteration of polymer wettability. Ahsani *et al.* investigated the influence of hydrolyzed polyacrylamide (HPAM) on the wettability of carbonate surfaces. Through a combination of molecular dynamics simulations and experimental approaches, they discovered that the adsorption of HPAM significantly reduces the water contact angle, thereby transforming the oil reservoir rock surface from a strongly oil-wet state to a moderately oil-wet state. This transition is crucial for enhancing water mobility and oil displacement efficiency. Specifically, after HPAM adsorption, the water contact angle decreases to approximately 130° and 140° at ambient and reservoir temperatures, respectively, which aligns well with the experimental results, validating the accuracy of the simulation findings.[104]

Yuan *et al.* focused their research on the interaction between polyvinylpyrrolidone (PVP) and the surfactant AOT. Through dissipative particle dynamics (DPD) simulations, the researchers observed that the addition of AOT induced changes in the dihedral angle distribution of PVP chains, indicating the occurrence of interactions between the polymer and the surfactant. The impact of this interaction on wettability provides a theoretical basis for designing polymers with specific wettability alteration functionalities.[105]

4.2.2.2 Effectiveness of simulation applications in enhancing oil recovery. Molecular dynamics simulations not only aid in understanding the molecular mechanisms underlying wettability changes but also enable the prediction of oil recovery enhancements during polymer flooding processes. Ahsani *et al.* combined simulation and experimental methods to verify the effectiveness of HPAM in altering the wettability of carbonate surfaces at different temperatures. They found that as temperature increases, the adsorption tendency of HPAM on carbonate surfaces intensifies, potentially due to ion exchange and thermal decarboxylation phenomena. This discovery offers new directions for further molecular dynamics research, particularly in the application of different polymers as wettability modifiers through Enhanced Oil Recovery (EOR) processes.[104]

In summary, molecular dynamics simulation technology has played a pivotal role in research on polymer wettability alteration and oil recovery enhancement. By combining simulation and experimental methods, researchers can gain deeper insights into the interactions between polymers and reservoir rocks, as well as predict wettability changes and oil recovery enhancements during polymer flooding processes.

4.3 Application of molecular dynamics simulation in polymer design and solution characterization

4.3.1 Molecular design: simulation studies of novel polymers. Molecular dynamics (MD) simulation, as a powerful computational tool, has increasingly played a crucial role in the design and performance optimization of novel polymers. Especially in the research of special polymers such as fluorocarbon-modified polyacrylamide (FPAM), MD simulation can provide insights at the molecular level, assisting scientists in understanding the behaviour and properties of polymers under different environmental conditions.

4.3.1.1 Performance optimization of fluorocarbon-modified polyacrylamide. Fluorocarbon-modified polyacrylamide (FPAM), due to its unique hydrophobic properties, holds broad application prospects as an oil-displacement agent in oilfield chemistry. Research indicates that the introduction of fluorocarbon units into the polyacrylamide chain can significantly enhance the stability and efficiency of the polymer in high-salt and high-temperature environments. MD simulation technology is capable of simulating the self-assembly behaviour and intermolecular interactions of these polymers under different conditions, thereby providing theoretical guidance for experimental design.

For instance, Ni *et al.* investigated the hydrophobic association properties of aqueous solutions of fluorocarbon-modified polyacrylamide using Dissipative Particle Dynamics (DPD) simulations. The simulation results revealed that, as the length of the fluorocarbon chain increased, the hydrophobic interactions between polymer chains intensified, leading to enhanced solution association. Notably, P(AM-AANa-12F) exhibited lower hydrophobic association in pure water compared to saline solutions, and demonstrated a stronger positive salinity sensitivity. At a concentration of 0.05 mol/mol, the root mean square (RMS) end-to-end distance of P(AM-AANa-12F) was longer in pure water than in saline solutions, indicating that the stronger hydrophobic association was influenced by salinity. These findings provide important molecular-level insights for the design of salt-tolerant and high-temperature-resistant oil-displacement polymers (Fig. 24).[106]

4.3.1.2 Enhancing the salt tolerance of polyacrylamide. Salt tolerance is a crucial performance indicator for polyacrylamide in oilfield applications. Yao *et al.* modified polyacrylamide by incorporating three functional monomers and employed molecular dynamics (MD) simulations to investigate the impact of these modifications on the polymer's salt tolerance. The simulation results revealed that the modified polyacrylamide (HM-HPAM) exhibited stronger salt tolerance compared to the unmodified polyacrylamide, with the salt tolerance increasing as the steric hindrance of the monomers increased. For instance, the intrinsic viscosity ($[\eta]$) of HM-HPAM1 was 5.2 dl g^{-1} at a NaCl concentration of 0 mol kg^{-1}, decreasing to 4.1 dl g^{-1} at a NaCl concentration of 0.28 mol kg^{-1}. This discovery holds significant implications for the design and optimization of polymers suitable for high-salinity environments.[107]

Furthermore, in this study, Yao *et al.* also investigated the dynamic properties of the modified polyacrylamide under different ionic strengths through MD simulations, encompassing the radius of gyration (R_g), hydrodynamic radius (RH), and intrinsic viscosity ($[\eta]$). The study found that as the NaCl concentration increased, the R_g of HM-HPAM decreased from 4.5 nm at 0 mol kg^{-1} to 3.2 nm at 0.28 mol kg^{-1}, with corresponding decreases in RH and $[\eta]$. In contrast, the changes in HM-PAM were insignificant. These results indicate that the introduction of monomers with steric hindrance can reduce the coiling of molecular chains, thereby enhancing the salt tolerance of the polymer.[107]

4.3.2 Solution characterization: simulation of self-assembly behaviour of polyacrylamide and surfactants. In recent years, molecular dynamics simulations have achieved remarkable progress in studying the self-assembly behaviour of polyacrylamide (PAM) and surfactants in aqueous solutions, as well as their impact on the properties of polymer solutions. These studies have enabled researchers to observe and analyze these self-assembly processes in detail, not only enhancing our understanding of the interactions between polymers and surfactants, but also providing a theoretical foundation for designing and optimizing polymers used in oil displacement.

4.3.2.1 Self-assembly of polyacrylamide and SDS. Wang *et al.* employed coarse-grained molecular dynamics simulations to investigate the self-assembly behaviour of polyacrylamide (PAM) and sodium dodecyl sulfate (SDS) in aqueous solutions. Their findings revealed that in the absence of SDS, PAM spontaneously curls to form aggregates. However, the addition of SDS causes PAM to stretch and ultimately forms the widely accepted "necklace" structure, where PAM is located at the interface between the hydrophobic and hydrophilic regions of the SDS micelles. Specifically, the radius of gyration (R_g) of PAM

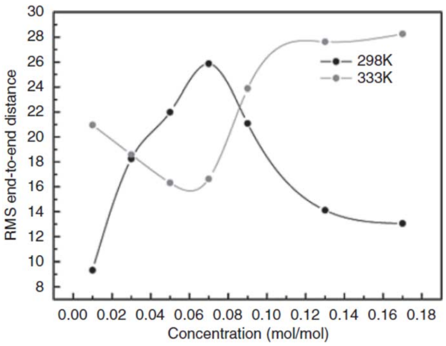


Fig. 24 The RMS end-to-end distance of P(AM-AANa-12F) in salt solution at different concentrations under different temperature. This figure illustrates the impact of temperature on the root mean square (RMS) end-to-end distance of P(AM-AANa-12F) in saline solutions at various concentrations. The results indicate that, at 333 K, as the concentration increases, the RMS end-to-end distance of P(AM-AANa-12F) initially decreases and then increases. At higher temperatures, the thermal motion of the hydrophobic groups on the macromolecular chains intensifies, weakening the ice-like structure of surrounding water molecules and causing the macromolecular chains to contract. As the concentration rises, the polymer chains begin to form physical networks, which expand at higher temperatures, leading to an increase in the RMS end-to-end distance. When the concentration continues to increase, the associative behaviour of the polymers reaches a relative equilibrium, and the RMS end-to-end distance remains unchanged. These findings further corroborate the stability and efficiency of fluorocarbon-modified polyacrylamide in high-salinity, high-temperature environments, providing crucial molecular-level insights for the design of oil-displacement polymers suitable for high-temperature, high-salinity reservoirs.[106]

in the absence of SDS is 8.0 Å, while in the presence of SDS, R_g increases to 16.6 Å, indicating the stretching of PAM. This process primarily consists of three stages: firstly, PAM rapidly adsorbs SDS monomers, causing R_g to decrease rapidly from 8.0 Å to 11.7 Å. Secondly, as more SDS adsorbs, PAM gradually stretches, leading to an increase in R_g and finally, a stable "necklace" structure is formed. These discoveries highlight the primary role of hydrophobic interactions in the self-assembly of PAM and SDS, which is consistent with experimental results and other simulation studies.[108]

4.3.2.2 Interaction between neutral polymers and ionic surfactants. Yuan *et al.* utilized Dissipative Particle Dynamics (DPD) simulation methodology to investigate the interaction between neutral polymers and ionic surfactants in aqueous solutions. Their observations revealed a transition process in the polymers as the surfactant concentration increased: from a freely extended state to the formation of dispersed rod-like structures, subsequently evolving into a pearl-necklace-like micelles structure, and ultimately distributing within hexagonal and lamellar phases. Specifically, as the surfactant volume fraction increased from 0.01 to 0.05, the end-to-end distance of the polymers initially decreased and then increased, indicating a transformation from a freely extended state to a compressed rod-like structure, and ultimately the formation of the pearl-necklace micelles structure. This research provides intuitive molecular-level evidence for understanding the aggregation morphology of polymers in surfactant solutions.[109]

4.4 Application of molecular dynamics simulation in the study of polymer–surfactant interactions

4.4.1 Simulation studies of properties of polymer–surfactant solutions. Molecular dynamics simulation technology plays a pivotal role in exploring the characteristics of polymer–surfactant solutions, particularly in understanding how polymers and surfactants synergistically stabilize complex fluid systems such as CO_2 foams. In recent years, research in this field has made significant advancements, especially in elucidating the interaction mechanisms between polymers and surfactants at the molecular level.

4.4.1.1 Molecular simulation of CO_2 foam stabilization by HPAM and ionic surfactants. Jia *et al.* conducted molecular dynamics simulations to investigate the interaction between hydrolyzed polyacrylamide (HPAM) and ionic surfactants (SDS and CTAB) at the interface between CO_2 and the aqueous phase. Their findings revealed that CTAB exhibited a stronger ability to reduce the interfacial tension (IFT) between CO_2 and water compared to SDS. Specifically, the IFT at the CTAB-treated interface decreased to approximately 10.766 mN m^{-1}, while that at the SDS-treated interface was around 11.857 mN m^{-1}, both significantly lower than the IFT between pure CO_2 and the aqueous phase (32.457 mN m^{-1}). Furthermore, the interfacial film formed by CTAB possessed a larger interfacial width (2.281 nm) and higher interfacial coverage, thereby more effectively reducing the energy per unit area at the interface. Competitive adsorption occurred between HPAM and the counterion Br on the CTAB interfacial film, whereas salt bridge structures formed between HPAM and Na^+ near the SDS interface. These structural changes directly influenced the interfacial tension and foam stability.[110]

4.4.1.2 Simulation study on solution properties of polymer surfactant KL-6. Wu *et al.* conducted a study on the solution properties of the polymer surfactant KL-6 using dissipative particle dynamics (DPD) simulations. Their findings revealed that the critical association concentration (CAC) of KL-6 was 0.6 g L^{-1}. Above this concentration, the viscosity of KL-6 solutions was significantly higher than that of HPAM solutions. Specifically, the viscosity of KL-6 solutions at 0.6 g L^{-1} was approximately twice that of HPAM solutions. Furthermore, at the same concentration, the surface tension of KL-6 solutions was 46% lower and the interfacial tension value was reduced by 37% compared to HPAM solutions, indicating that KL-6 polymer solutions exhibited higher surface activity. In saline solutions, KL-6 molecules formed a three-dimensional network structure, significantly enhancing its salt tolerance. This characteristic is particularly important in applications aimed at improving oil recovery.[111]

4.4.2 Multiscale simulation of aggregate structures of polymers and surfactants. In the field of oil displacement, polymer–surfactant complexes have been extensively studied due to their excellent rheological modification and interfacial activity. Multiscale simulation methods, encompassing quantum chemistry, molecular dynamics simulations, and coarse-grained force field simulations, provide the ability to explain experimental phenomena, summarize patterns from the molecular level, and offer theoretical insights for binary composite oil displacement experiments. These methods have emerged as pivotal tools in revealing the aggregated structures and interaction mechanisms of these complex systems. Not only do they offer deep insights at the microscopic level, but they also enable the prediction and optimization of oil displacement efficiency for polymer–surfactant complexes.

4.4.2.1 Aggregate structures of temperature- and salt-tolerant surfactants with polyacrylamide (PAM). The aggregate structures of temperature- and salt-tolerant surfactants with polyacrylamide (PAM) are crucial for enhancing oil displacement efficiency. Yuan *et al.* employed the dissipative particle dynamics (DPD) method to investigate the interactions between partially hydrolyzed polyacrylamide (HPAM) and ionic surfactants. Their findings revealed that as the surfactant concentration increases, the aggregate structures of the polymer and surfactants sequentially transition from a "bottle-brush" configuration to a "bead-on-string" structure, and further to a hexagonal phase and an inverse hexagonal phase at higher concentrations. These structural transformations directly influence the rheological properties and interfacial stability of the oil displacement system.[112]

Wu *et al.* have reviewed the applications of dissipative particle dynamics (DPD) and coarse-grained molecular dynamics (CG-MD) in studying the interactions between polymers and surfactants, highlighting that these simulation techniques can unveil the underlying patterns governing the structural morphologies of polymer/surfactant aggregates.[113] As an illustrative example, Wang *et al.* employed the CG-MD method to investigate the self-assembly behaviour of polyacrylamide (PAM) and sodium dodecyl sulfate (SDS) in solution. Their findings revealed that the self-assembly process of PAM and SDS progresses through three distinct stages: the rapid coiling of PAM chains, the adsorption of SDS molecules onto the polymer backbone, and ultimately the formation of a "bead-on-string necklace" structure.[108]

4.4.2.2 Applications of multiscale simulation methods. Multiscale simulation methods have offered a comprehensive understanding of the aggregated structures formed by temperature- and salt-tolerant surfactants with polyacrylamide, spanning from individual molecules to multimolecular assemblies. For instance, Yuan *et al.* conducted research utilizing full-atom molecular dynamics (MD) to investigate the aggregated structures of surfactants and polymers, and subsequently developed coarse-grained (CG) model force fields. By comparing structural information obtained from both full-atom and CG models, they refined the parameters of the CG force fields. These research systems could reach dimensions of several tens of nanometers, offering a larger scope in terms of both temporal and spatial scales compared to full-atom MD studies. Furthermore, they enabled the investigation of aggregation kinetics over a broader range of time scales.[112]

4.5 Application of molecular dynamics simulation in the development of novel polymer-based oil recovery agents

4.5.1 Performance evaluation of novel injectants. In the field of Enhanced Oil Recovery (EOR), the development of novel injectants is pivotal for achieving efficient oil displacement. Molecular dynamics simulation, as a powerful tool, offers an in-depth molecular-level understanding for the performance evaluation of these novel injectants. In recent years, novel injectants such as modified papaya gum and silane-polyacrylate composites have garnered attention due to their unique properties.

4.5.1.1 Performance of modified papaya gum as a novel injectant. El-Hoshoudy *et al.* investigated the application of modified papaya gum (PGG) as a novel injectant in subsurface oil reservoirs through experimental and Monte Carlo simulation studies. They discovered that PGG exhibited significantly higher viscosity above the critical association concentration (0.6 g L^{-1}). Specifically, the viscosity of PGG solutions at 0.6 g L^{-1} was more than 1.5 times that of natural guar gum (GG), indicating that PGG holds greater potential for enhanced oil recovery (EOR). In Monte Carlo simulations, PGG membranes exhibited higher stability and more negative electrostatic energies when interacting with SiO_2^- quartz crystals compared to GG membranes, further confirming the superior performance of PGG under reservoir conditions.[114]

4.5.1.2 Properties of silane polyacrylate composite materials. In a separate study, El-Hoshoudy *et al.* explored the synthesis, evaluation, and application of silane-polyacrylate composites as candidate materials for EOR. Through molecular dynamics simulations, they found that the introduction of silane coupling agents significantly enhanced the mechanical properties of the composites. Specifically, the bulk modulus of the silane-polyacrylate composites increased by approximately 40%, the elastic modulus by about 50%, Young's modulus by nearly 60%, and the shear modulus by roughly 70%. Meanwhile, the Poisson's ratio decreased by approximately 20%. These enhanced mechanical properties enabled the composites to exhibit better stability and effectiveness under high-shear, high-salt, and high-temperature reservoir conditions.[115]

The aforementioned studies clearly demonstrate the potential of novel injectants in enhancing oil recovery (EOR) and the application value of molecular dynamics simulations in assessing the performance of these novel materials.

4.5.2 Synthesis and molecular dynamics simulation of amphiphilic low-molecular-weight polymer viscosity reducers. In recent years, research on amphiphilic low-molecular-weight polymers as oil-displacement agents has witnessed remarkable advancements. These polymers, owing to their unique molecular architectures and surface activities, exhibit tremendous potential in reducing crude oil viscosity and enhancing oil recovery rates from reservoirs. The application of molecular dynamics simulation techniques in this domain not only facilitates the elucidation of the synthetic feasibility of polymeric viscosity reducers but also deepens our understanding of their viscosity-reducing mechanisms, thereby providing robust theoretical support for the development of novel polymeric oil-displacement agents.

4.5.2.1 Synthetic feasibility and viscosity reduction mechanism. The synthesis of amphiphilic low-molecular-weight polymers typically involves copolymerization reactions of multiple monomers. For instance, Ma *et al.* synthesized an amphiphilic low-molecular-weight polymeric viscosity reducer composed of acrylamide (AM), acrylic acid (AA), 2-acrylamido-2-methylpropanesulfonic acid (AMPS), and butylstyrene (PB) through an emulsion copolymerization method. The synthetic feasibility and viscosity reduction mechanism of this polymer were analyzed using molecular dynamics simulations *via* the Materials Studio software. Simulation results indicated that the addition of the polymer altered the potential energy, non-potential energy, density, and hydrogen bonding distribution of the crude oil, effectively reducing its viscosity. Upon adding the viscosity reducer, the potential energy of heavy oil significantly increased, potentially due to the adsorption of asphaltene and resin molecules onto the viscosity reducer, forming numerous branched structures and leading to a steric hindrance effect. Concurrently, the strong polar groups (–COO– and $–SO_3–$) in AA and AMPS gradually dissociated the network structure of heavy oil from the inside out, promoting a reduction in its viscosity by approximately 86.14%. Structurally, the benzene rings in PB were able to intercalate into the layered structure of asphaltene, weakening the network structure of heavy oil. This structural design was inspired by previous research, which demonstrated that amphiphilic copolymers containing AM and *n*-butylstyrene could effectively adsorb emulsified oil droplets in heavy oil wastewater (Fig. 25).[116]

4.5.2.2 Application of molecular dynamics simulations in the advancement of amphiphilic low-molecular-weight polymer viscosity reducers. Molecular dynamics simulations have played a crucial role in the research and development of amphiphilic low-molecular-weight polymers as viscosity reducers. Through

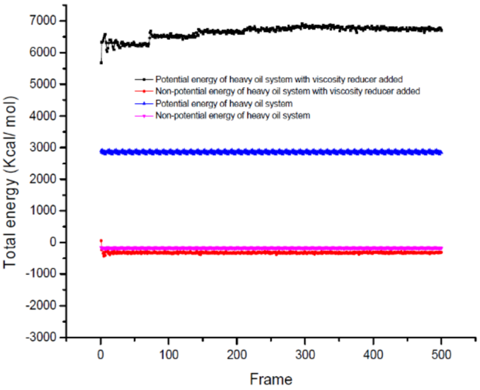


Fig. 25 Investigation of the effects of polymer viscosity reducers on the potential and non-potential energy profiles of heavy oil. This figure illustrates the impact of the viscosity reducer on the potential and non-potential energy of heavy oil after its addition. As depicted in the figure, compared to heavy oil without the viscosity reducer, the potential energy of heavy oil significantly increases upon the addition of the viscosity reducer. This phenomenon is primarily attributed to the adsorption of asphaltene and resin molecules onto the viscosity reducer, leading to the formation of numerous branched structures and, consequently, a steric hindrance effect. Simultaneously, the strong polar groups (–COO– and $-SO_3-$) within the viscosity reducer gradually disintegrate the network structure of heavy oil from the inside out, facilitating a reduction in its viscosity. Experimental results indicate that with an increase in the concentration of the viscosity reducer, the viscosity of heavy oil decreases by approximately 86.14%, confirming the effectiveness of this amphiphilic low-molecular-weight polymeric viscosity reducer in lowering the viscosity of heavy oil.[116]

these simulations, researchers are able to predict the interactions between polymers and crude oil, thereby facilitating the optimization of polymer structural designs. For instance, Tesha conducted a study on the compatibility of polysulfone and polystyrene-*co*-maleic anhydride polymer blends, utilizing molecular dynamics simulations to provide simulated data on the performance of these blends. This data is indispensable for gaining insights into the interactions and compatibility between polymers. The favorable interactions between the two polymers were confirmed through Differential Scanning Calorimetry (DSC) analysis, evidenced by the observed shift in the glass transition temperature (T_g).[117]

In practical scenarios, molecular dynamics simulations offer researchers the unique opportunity to observe the interactions between polymer viscosity reducers and crude oil. This includes the adsorption of asphaltene and resin molecules onto the viscosity reducers, as well as the resultant steric hindrance effects. The combination of these simulation results with experimental data provides a scientific basis for the molecular design and performance optimization of viscosity reducers.

5. Future trends and prospects for oil-displacement polymer design

5.1 Design and potential applications of novel intelligent polymers

5.1.1 Smart responsive polymers. In the future, intelligent responsive polymers will emphasize the precise regulation of their molecular structures to ensure sensitive responsiveness to fluctuations in reservoir conditions. Specifically, researchers may endeavour to create polymers that undergo phase transitions at designated temperatures or pH values, allowing them to seamlessly adapt to the temperature gradients and chemical property variations prevalent within oil reservoirs. By harnessing the power of molecular dynamics simulations, researchers can accurately predict the behavioural shifts of polymers in response to diverse external stimuli, including temperature, pH, and salinity. This predictive capability facilitates the design of intelligent polymers that are capable of responding dynamically to these changes. Furthermore, the research trajectory for intelligent polymers may encompass several promising avenues:

(1) Self-repairing polymers: the pursuit of polymers that possess the capability to self-heal and restore their performance within microfractures, thereby significantly prolonging their operational lifespan within oil reservoirs.

(2) Environmentally responsive polymers: the design and synthesis of polymers that are engineered to release active agents under precise environmental cues, ultimately enhancing oil recovery efficiency.

(3) Nanocomposite materials: the fusion of nanotechnology with intelligent polymers to bolster their robustness and stability under the challenging conditions prevalent in oil reservoirs.

Future endeavours in research should delve deeper into leveraging molecular dynamics simulations to fine-tune the performance characteristics of these intelligent polymers, ensuring they exhibit optimal responsiveness under the diverse conditions encountered within oil reservoirs.

5.1.2 Degradable and environmentally friendly polymers. Future research endeavours will focus intently on the creation of fully biodegradable polymers, which, upon fulfilling their oil displacement roles, can seamlessly degrade in the natural environment, thereby substantially reducing environmental contamination. Molecular dynamics simulations emerge as a powerful tool to illuminate the degradation mechanisms of these polymers within their natural habitats, and to elucidate their intricate interactions with various environmental factors, including microorganisms, temperature, and humidity. Potential research avenues in this domain may include:

(1) Biobased monomer polymerization: new biobased polymers are being developed by harnessing monomers derived from biomass, including lactic acid and polyhydroxyalkanoates (PHA), which serve as the foundational building blocks.

(2) Biodegradability evaluation: a rigorous assessment of the biodegradability of polymers within reservoir settings is conducted to ascertain their eco-friendliness once they have fulfilled their oil displacement roles.

(3) Minimizing ecological footprint: life cycle assessment (LCA) serves as a pivotal tool to refine polymer design, aiming to reduce their environmental impact throughout their entire existence from cradle to grave.

Future research endeavours should focus on pioneering novel biobased monomers and leveraging molecular dynamics simulations to foresee and tailor the degradation pathways and rates of these polymers, thereby guaranteeing their secure degradation post-oil displacement and mitigating their ecological footprint.

5.2 Future development of the integration of machine learning and molecular dynamics simulation

5.2.1 Integration of machine learning and molecular dynamics simulation. The fusion of machine learning with molecular dynamics simulations has opened up a fresh vantage point for the design of polymers. Leveraging machine learning algorithms to dissect the extensive datasets stemming from molecular dynamics simulations allows for the swift identification of pivotal factors that govern polymer performance. Furthermore, this methodology enables the prediction of polymer behaviour under diverse conditions. Future research should delve into the potential of this integrated framework to refine polymer design, thereby augmenting their efficacy and stability within intricate reservoir settings.

5.2.2 Enhanced sampling and predictive models. By merging machine learning-augmented sampling methodologies, the versatility of molecular dynamics simulations is expanded, empowering them to grapple with intricate systems and elongated timescales. This fusion significantly bolsters the precision of predictions regarding polymer behaviour, notably in anticipating the enduring stability and proficiency of polymers within reservoir environments.

5.2.3 Integration of experimental data and simulation results. Machine learning models are capable of leveraging the data generated through molecular dynamics simulations to forecast material attributes, encompassing rheological behaviours and compatibility. This data-centric methodology significantly speeds up the identification of new materials and finetunes the synthesis and utilization processes of polymers, thereby enhancing their efficiency and ecological sustainability.

5.2.4 Environmental impact assessment and sustainable development strategies. By creating automated simulation and analysis platforms that seamlessly integrate machine learning algorithms with molecular dynamics simulations, we can achieve a substantial increase in research productivity. These platforms facilitate the automatic execution of simulations, the thorough analysis of outcomes, and the prompt provision of real-time feedback, ultimately expediting the design and refinement phases of polymer materials.

5.2.5 Leveraging emerging machine learning techniques to enhance the scalability and efficiency of polymer design models. In the context of polymer design for oil displacement, emerging techniques such as federated learning, transfer learning, and active learning play a crucial role in enhancing the scalability and efficiency of machine learning models.

Federated learning is a distributed learning method that allows multiple participants to train models locally without sharing data. This approach is particularly valuable in polymer research, where data is often highly decentralized and involves multiple experimental and commercial institutions. Through federated learning, participants can share model updates instead of data, ensuring data privacy while improving the generalization ability of the models. This also enables the integration of diverse data from various sources, thus enhancing the adaptability of polymer design models across different experimental conditions.

Transfer learning allows models trained on one set of polymer systems to be applied to others, reducing the dependency on large amounts of new data. This technique is particularly useful for generalizing across diverse polymer types and systems, which is a common challenge in polymer design.

Active learning improves model efficiency by selecting the most informative data points for training, allowing models to perform well even with smaller datasets. This is particularly beneficial in polymer research, where data collection can be resource-intensive. By focusing on the most relevant data, active learning helps optimize the training process and reduces the need for large-scale data collection.

Additionally, meta-learning and self-supervised learning are emerging techniques that show great potential in polymer design. Meta-learning enables polymer design models to quickly adapt and make effective predictions when confronted with new types of polymers. Self-supervised learning, on the other hand, reduces the reliance on costly labelled data by training models using unlabelled data, which is especially useful in addressing the data scarcity issue in polymer design.

5.3 Industry applications and sustainability considerations

In addition to theoretical advancements, future research must focus on the practical application of these new polymers in real-world oilfield operations. Specifically, research should explore how biodegradable polymers can be used in microbial enhanced oil recovery (MEOR) systems to improve sustainability by reducing the environmental impact of chemical injection. Additionally, environmental life-cycle assessments (LCA) should be conducted to evaluate the long-term effects of polymer use in oil recovery processes, particularly in terms of biodegradation and toxicity. Future studies could explore the development of eco-friendly synthesis methods, such as green chemistry approaches for producing biodegradable polymers and the incorporation of renewable resources into polymer design to meet growing sustainability requirements.

5.4 Unresolved challenges and future research directions

5.4.1 Multiscale modelling from molecular to macroscopic scales. In future endeavours, it is imperative to devise multiscale simulation methodologies that bridge the gap from the molecular level to the macroscopic realm, enabling a thorough comprehension of the flow characteristics and interaction mechanisms of polymers within oil reservoirs. This endeavour must incorporate molecular dynamics simulations to elucidate fluid behaviour in nanoporous media, along with an exploration of how these microscopic behaviours propagate and influence macroscopic reservoir dynamics.

5.4.2 Advancements in high-performance computing and simulation technologies. To tackle the challenges posed by increasingly complex reservoir conditions and larger-scale systems, it is essential to advance computational techniques and simulation methodologies that offer superior performance. This involves refining and enhancing molecular dynamics simulation algorithms, as well as developing innovative machine learning models specifically designed to handle and interpret simulation data, ultimately leading to improvements in both the accuracy and efficiency of the simulations.

5.4.3 Integration of experimental data with simulation results. By integrating experimental data with the outcomes of molecular dynamics simulations, it is possible to significantly augment the predictive prowess and reliability of the models in use. Hence, future research endeavours should focus on identifying effective strategies to seamlessly integrate experimental and simulation data, with the ultimate goal of achieving higher fidelity in reservoir simulations and more precise predictions of polymer performance.

5.4.4 Environmental impact assessment and sustainable development strategies. Molecular dynamics simulations serve as a powerful tool to evaluate the environmental footprint of polymers, particularly focusing on their degradation characteristics and biocompatibility. By integrating machine learning techniques with these simulations, we can forecast the environmental behaviour of polymers with greater precision, thereby furnishing a robust scientific foundation for the innovation of environmentally benign oil displacement technologies. By pursuing these research avenues, we can harness the combined strengths of machine learning and molecular dynamics simulations more effectively, propelling the advancement of oil displacement polymer design and tackling real-world reservoir challenges.

6. Conclusions

This comprehensive review paper delves into the pivotal advancements of molecular dynamics (MD) simulation technology in the realm of designing and optimizing polymers tailored for oil displacement applications. The paper starts by revisiting the crucial role that polymers play in oil displacement processes, highlighting the significant challenges posed by maintaining stability and optimizing rheological properties under harsh conditions, such as high temperatures and high salinity environments. Following this overview, the paper delves deeper into the theoretical backbone and methodologies of molecular dynamics simulations, meticulously explaining their fundamental principles, the intricacies involved in selecting appropriate simulation parameters, and the burgeoning trends in combining machine learning with molecular dynamics simulations that have emerged in recent times.

The central thesis of this paper focuses on the application of molecular dynamics (MD) simulation technology in dissecting the molecular-level mechanisms underlying polymer-based oil displacement, refining polymer performance, and devising novel polymers. Leveraging MD simulations, researchers gain unprecedented insights into the atomic-scale interactions between polymers and oil, unveiling the displacement mechanisms of viscoelastic polymers within nanopores and elucidating the influence of interactions between polymer chains and oil droplets on displacement efficiency. Moreover, MD simulations have proven invaluable in probing the rheological properties and viscosity dynamics of polymer solutions, anticipating the ramifications of altered polymer wettability on recovery rates, and steering the design and performance optimization of innovative polymers. The distinctive contribution and novelty of this paper reside in its systematic compilation of the application outcomes of MD simulation technology within the realm of polymers for oil displacement, particularly emphasizing research on optimizing polymer stability and rheological properties under challenging reservoir conditions. By amalgamating existing literature, this paper not only addresses some of the research voids in MD simulation for enhanced oil recovery (EOR) polymer design but also offers a roadmap for future research endeavours, thereby fostering the advanced application and evolution of MD simulation technology in EOR polymer design.

Future research trajectories in this domain will prioritize the development of multiscale simulation methodologies, aiming to achieve a comprehensive understanding of the flow dynamics and interaction mechanisms of polymers within oil reservoir environments. A pivotal focus will be on advancing high-performance computing (HPC) technologies and refining simulation methodologies to address the complexity of these systems. Moreover, there is a pressing need to integrate experimental datasets with simulation results, thereby enhancing the predictive accuracy and reliability of the models employed. Simultaneously, rigorous assessments of the environmental footprint of polymers and the pursuit of environmentally friendly oil displacement technologies will be critical areas of emphasis. These research endeavours are poised to significantly propel the utilization of molecular dynamics (MD) simulations in practical oilfield development scenarios, particularly in the realms of enhancing oil recovery efficiencies and minimizing adverse environmental impacts.

The research outcomes presented herein contribute not only novel insights to the academic discourse but also present significant potential for practical applications within the industrial sphere, specifically in the areas of oilfield development and environmental stewardship. These findings enable us to leverage molecular dynamics (MD) simulation technology more effectively, thereby facilitating advancements in the design of oil-displacement polymers and addressing intricate reservoir challenges faced in practical scenarios.

Data availability

No primary research results, software or code have been included and no new data were generated or analysed as part of this review.

Author contributions

Conceptualization: Z. H., W. J., X. W., B. H., L. Z.; methodology: W. J., J. G., C. N., E. Y., B. H., C. D.; investigation: W. J., L. S., J. S., X. S., S. W., J. Z., L. Z., J. W., Y. W., G. Q., X. H., J. L., Y. M., S. Y., Y. W., X. Y., D. L., J. J., X. F., X. S., H. S.; project administration: S. L., Z. H., X. W.; supervision: S. L.,

Z. H., X. W.; writing—original draft: W. J., J. G.; writing—review & editing: Z. H., X. W., E. Y., B. H.

Conflicts of interest

There are no conflicts to declare.

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