Application of Molecular Simulation Technology in Improving Oil Recovery

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Abstract. With the continuous development of oil exploitation, the research on the oil industry has gradually shifted from macro to micro. Molecular simulation technology has attracted wide attention due to its advantages of saving costs, shortening the experimental period, and realizing the limit simulation conditions that are almost impossible under physical experimental conditions. Petroleum workers use molecular model to study the effects of different properties on adsorption and desorption. The results show that the adsorption capacity of CH₄ increases with the increase of pore size and pressure, and decreases with the increase of temperature and water content. The interaction between clay minerals and CO₂ was discussed, and various reactions formed after CO₂ was inserted into clay minerals were discussed. Exploring the adsorption and aggregation behavior of surfactants on the interface and analyzing the influence of various properties of surfactants on oil displacement effect are helpful to optimize surfactants and improve oil displacement efficiency. Scientific research on microscopic seepage of polymer flooding has been carried out, and a large number of studies have been carried out on light hydrocarbon diffusion, polymer viscoelasticity and diffusion properties of small molecules in pores, which makes the evaluation of oil displacement effect more accurate. The application of molecular simulation technology in the above studies has obtained the properties that cannot be extracted from many macro experiments, which provides an effective method for the study of theoretical mechanism and better guides the actual production.

1. Introduction
Molecular simulation technology has been widely used in physics, chemistry, life science and other fields due to its precise predictability. Molecular simulation method can accurately simulate physical and chemical phenomena that cannot be simulated by modern experimental testing methods. It is a powerful tool for understanding complex material structures, studying chemical reaction paths, reaction mechanisms and other key issues, and has become an important bridge between theoretical science and experimental science. Molecular simulation technology has shown great potential in explaining the atomic and molecular properties of complex phenomena in the study of oil and gas reservoirs, which is a method to characterize the properties of oil and gas reservoirs from the micro perspective. In this paper, the molecular simulation theory is briefly introduced. Secondly, the
application of this method in enhanced oil recovery is systematically reviewed. Finally, the practical challenges and new research directions of molecular simulation are analyzed.

2. Overview of Molecular Simulation

Molecular simulation technology is based on the molecular model. This method does not involve the treatment of electronic problems. It has relatively small amount of calculation and fast speed, and is suitable for macromolecular systems. According to the different research objects and basic theories, it can be divided into Monte Carlo (MC) method and Molecular Dynamics (MD) method.

2.1. Monte Carlo (MC) method

The Monte Carlo method was established by Metropolis[1]in 1953. This method is a non-quantum calculation method. Based on probability theory and mathematical statistics theory, the actual problem is converted into a probability problem, and the solution of the problem is obtained through a large number of repeated experiments. This method is conceptually easy to understand and easy to operate because it only allows atoms to jump randomly and selects the lowest energy state. It can balance any degree of freedom, suitable for multi-dimensional and complex systems. However, since the particle displacement in Monte Carlo simulation is an artificial motion process, it cannot represent the real particle trajectory, and generally can only calculate the static properties of the system.

2.2. Molecular Dynamics (MD) method

Molecular dynamics simulation method was established by Alder and Wainwright[2]in 1957. Molecular dynamics method is a method to simulate the motion of molecular system by solving the classical Newton mechanics equation. MD is to change the molecular coordinate and momentum by intermolecular force, and obtain the dynamic information of the whole system by integrating the Newton motion equation. The internal principle of simulation is the classical Newton equation of motion, see formula (1). Where $\overrightarrow{a}(t)$ is the acceleration at time t, $\overrightarrow{r}(t)$ is the position vector at time t, $\overrightarrow{F}(t)$ is the force of the atom under a specific potential field, and $m_i$ is the mass of the atom.

$$\overrightarrow{a}(t) = \frac{d^2 \overrightarrow{r}(t)}{dt^2} = \frac{\overrightarrow{F}(t)}{m_i}$$ (1)

The steps of molecular dynamics simulation can be summarized as follows:

![Figure 1. Molecular simulation step diagram.](image)

Molecular dynamics, as a product of the comprehensive development of statistical mathematics, physics and chemistry, plays an important role in exploring the mechanism of the microscopic world. It can limit the temperature, pressure and other parameters of the target structure, further optimize the molecular structure and calculate the energy, and analyze the various structural parameters and
dynamic properties of the system, especially suitable for the study of organic and inorganic small molecules, polymer, nanoporous materials and crystal structure. In this paper, we focus on the application of molecular dynamics method in the oil industry.

2.3. Introduction to related software
The application of simulation calculation method cannot be separated from the support of computer software. With the rapid rise of computer science, the types of software used for simulation calculation have mushroomed in large numbers, with their respective advantages. Molecular simulation can be divided into atomic simulation, coarse-grained simulation and mesoscopic simulation according to the scale of simulation. The calculation software is also divided into the following categories. The first is mainly used to study the problems related to electronic effects, such as Gaussian and VASP. The theories involved include ab initio method, first-principles and density functional theory. The second kind mainly simulates the molecular system motion, such as GROMACS, AMBER, LAMMPS and Material Studio. The main theoretical basis is molecular mechanics, focusing on the macroscopic properties of the system. Of course, there are also simulations using both methods, such as CHARMM, NAMD, etc.

Table 1. Introduction of various software.

| Software name | Range of application | Research content | Merit | Defect |
|---------------|----------------------|------------------|-------|--------|
| Gaussian      | Studies in molecular and partial chemistry | Instantaneous reaction intermediates and transition structures, influence of substituents, chemical reaction mechanism, potential energy surface and excitation energy | High calculation accuracy | The computation is tedious and takes a long time, so it only applies to small systems |
| VASP          | Study on Solid, Surface and molecular systems | Kohn-Sham equation can be solved within the framework of density functional theory | Good optimization algorithm and fast calculation speed | You need to compile and run in Linux, slow entry |
| GROMACS       | Study on dynamic molecular systems for simulating millions of particles Studies on biological systems and general chemical molecular systems | Solving macromolecular system by classical Newton mechanics equation | Rich function, fast calculation speed, strong compatibility, good maintenance service | Poor compatibility |
| AMBER         | Research on molecular modeling | Whole modeling of particles in liquid, solid, or gas states can be done with few | Compatible with most current potential energy models, advanced | Low computational efficiency, slow running speed, payable purchase |
| LAMMPS        | Research on molecular modeling | - | | No tools for establishing molecular systems, no |
particles to simulate two- or three-dimensional systems or millions of billions of particles programming and high computational efficiency automatic force field parameters, no output data mapping, poor maintenance

| Material Studio | Research for materials science | Property prediction, polymer modeling, X-ray diffraction simulation | Support multiple platform operation, advanced algorithm, simple operation, friendly interface | High price, poor openness and low parallel efficiency

| CHARMM | Study on biological and chemical materials system | - | The potential energy model updates quickly, customizes the new model conveniently, maintains well High level of program design, high efficiency, strong compatibility and good maintenance service | Slow computing speed, low computational efficiency, paid purchase

| NAMD | Study on biological and chemical soft materials | - | - |

3. Application of molecular simulation technology in petroleum industry

Oil is the blood of industry and plays an important role in energy. Molecular simulation technology has now been applied to various aspects of oil industry production, ranging from microscopic mechanism research (adsorption and desorption process, interaction between minerals and fluid) to increasing oil and gas well production and ultimate recovery (surfactant flooding, polymer flooding).

3.1. Study on microscopic adsorption and desorption process

Molecular simulation technology has been widely used to study molecular microscopic adsorption and desorption process. In 1998, Murguch et al.[3] studied the atomic interaction between asphaltene and resin adsorption on kaolinite, and found that the interaction between resin and kaolinite surface was stronger than that between asphaltene. In 2014, Xu[4] analyzed the displacement mechanism of oil displacement agent by molecular dynamics method. Zhang et al.[5] studied the desorption mechanism of oil on hydrophobic / hydrophilic silica surface in 2016. Sun et al.[6] in 2017 stretched asphaltenes from calcite to quantify the binding force of the interface to determine the adsorption capacity of asphaltenes on solid surfaces. In 2018, Meng et al.[7] used MD to simulate various interactions between components in heavy oil and rough SiO$_2$ surface. The roughness of SiO$_2$ surface of SiO$_2$ surface is conducive to the adsorption of oil droplets due to the Van der Waals force interaction. Bai et al.[8] studied the adsorption and desorption of asphaltene SiO$_2$ surface containing heteroatoms in 2019. It was found that N, Q and S heteroatoms promoted asphaltene adsorption and hindered desorption. In 2020, Ji[9] used MD to study the polymerization and adsorption of heavy oil molecules on different hydrophilic SiO$_2$ surfaces. Although molecular dynamics simulation has been widely used to study the adsorption mechanism of heavy oil on SiO$_2$ surface. However, there is a lack of understanding of the adsorption mechanism of heavy oil at different hydrophobic SiO$_2$ interfaces.
In addition, a large number of studies have been carried out on the microscopic adsorption of shale gas. In 2006, Tenney[10]simulated the adsorption of gas in graphene slit holes with functional groups on the surface, and found that the adsorption amount of gas increased with the increase of oxygen content on the pore surface. In 2012, Amborse et al.[11]found that different adsorption potential could lead to uneven distribution of hydrocarbons in nanopores, which strengthened the adsorption of fluid molecules on the wall and promoted the flow of alkanes. In 2013, Mosher et al.[12]used MC method to predict the adsorption characteristics under different pore sizes and different temperature and pressure conditions and simulated and predicted excess adsorption. In 2014, Etminan et al.[13] found through MD simulation that the expansion of compressed gas in shale nanopores would promote the gas desorption on the inner surface of pores and the release of dissolved gas in amorphous kerogen. Wang[14]simulated the adsorption and transport process of shale oil in organic and inorganic nanopores in 2016, and established a model to describe the flow behavior of liquid alkanes based on the simulation results. In 2017, Xiong et al.[15]simulated the adsorption of CH4 in kaolinite slit pores, compared the effects of different temperatures, pressures and pore sizes on the adsorption amount of CH4, adsorption heat and the potential energy of interaction between CH4 molecules and pore walls, and also compared the adsorption capacities of kaolinite for CH4, N2 and CO2. In 2018, Zhang et al.[16]studied the adsorption law of CH4 in shale inorganic matter. The results show that pore size has an important influence on the adsorption of shale gas. The smaller the pore size, the stronger the adsorption of organic matter on CH4. Lu Zhaolan et al.[17]simulated the adsorption behavior of CH4 on clay minerals in 2019. The results showed that the adsorption capacity of three clay minerals for CH4 was in the order of montmorillonite>illite/montmorillonite mixed layer>illite. Wang[18]simulated the effects of water content, pore size and temperature of shale on the adsorption of CH4 and CO2, and found that shale first adsorbed CO2 and then adsorbed CH4. In 2020, Huang Tao et al.[19]used MC and MD methods to construct the microscopic models of illite, montmorillonite and kaolinite (Figure 2) to study the adsorption of CH4 by three clay minerals under different pressures and pore size spaces. With the increase of pore size and pressure, the adsorption amount of CH4 gas between the three clay minerals gradually increases and the adsorption stability gradually increases. These studies tend to simplify shale models to single substances such as minerals (quartz) or organic matter (illite, montmorillonite models) without considering shale heterogeneity. In addition, shale gas is simplified to CH4 and other alkanes are rarely studied. Therefore, more in-depth research is needed in these two aspects.

3.2. Study on the interaction between reservoir minerals and CO2
Molecular simulation technology is a powerful tool for studying the microscopic interaction between reservoir clay minerals and CO2 fluid. In 2004, Palandri[20]found that HCO3− in rocks originated from the dissolution of calcite through experiments, but his simulation only considered the interaction between CO2 or water and clay without considering other influencing factors, which had certain limitations. Botan et al.[21]simulated the adsorption of CO2 between montmorillonite layers by
GCMC and MD methods in 2010, and found that CO₂ can stably exist in different hydration states of montmorillonite and the adsorption of CO₂ will inhibit the diffusion of other molecules. In 2012, Yang[22]carried out the experiment of anhydrous CO₂ insertion into montmorillonite, the results show that the collapse of montmorillonite interlayer is not caused by low pressure CO₂. In 2014, Lee et al.[23]found that the first layer of hydrated montmorillonite would expand due to expansion due to the insertion of CO₂, while the second layer of hydrated montmorillonite would reduce the interlayer spacing after adsorbing CO₂. In 2015, Makaremi et al.[24]explored the adsorption of CO₂ and water by clay minerals by GCMC and MD methods, and concluded that CO₂ had high solubility between montmorillonite layers. In 2016 Rao et al.[25]simulated CO₂ fluid in montmorillonite nanopores by the same method, and found CO₂ dimer configuration in two layers of hydrated montmorillonite. In addition, they also discussed the influence of different charged clays on supercritical CO₂ adsorption, and obtained that clays with high charged were more likely to adsorb water molecules to achieve the transformation of hydration morphology. In 2017, Gadikota et al.[26]calculated the distribution coefficient of CO₂ in interlayer pores and intergranular pores of montmorillonite by MD simulation and adsorption experiment, but mainly analyzed the diffusion coefficient and solubility of CO₂. At present, the research of scholars mainly focuses on the adsorption position and diffusion of CO₂, and there is no in-depth study on the dynamic process and energy change of CO₂ entering the interlayer of montmorillonite. Therefore, in 2019, Li Qin[27]studied the interaction between montmorillonite and different concentrations of CO₂ fluid under geological temperature was simulated, and the microstructure, diffusion properties of CO₂ fluid on the surface of montmorillonite and the energy change into the interlayer of montmorillonite were revealed.

3.3. Study on surfactant flooding

The adsorption characteristics of surfactants on the interface have been studied by molecular simulation. In 2000, Laradji[28]used the MD method to study the elastic properties of surfactant on the liquid/liquid interface. It was found that the interfacial tension decreased with the increase of surfactant or chain length on the interface. When the surfactant was less, the flexural modulus decreased with the increase of surfactant concentration, and increased with the increase of surfactant concentration after reaching a certain concentration. In 2002, Yuan et al.[29]studied the adsorption structure, kinetic properties and phase diagram of sodium dodecyl sulfonate and sodium bis (2-ethylhexyl) succinate (AOT) on the interface by MD method. In 2003, Rekvig et al.[30]studied the staggered binding and phase transition characteristics of the surfactant bimolecular layer, and simulated the effects of the order parameters of a single surfactant, the area occupied by the molecule, the thickness of the bimolecular layer, and the structure of the surfactant on these properties. In 2005, Peng et al.[31]calculated the number of adsorbed molecules, oil-water interfacial tension, interfacial film thickness and the time required for the equilibrium of the system to study the adsorption characteristics of star polymers on the oil-water interface. In 2006, Khurana et al.[32]used the MD method to study the monolayers formed by a series of Gemini surfactants on the air-water interface, and found that only when the carbon number of the hydrophobic chain length of the surfactant was 12 and 14, a stable monolayer could be formed on the interface. When the surfactant was less, the flexural modulus decreased with the increase of surfactant concentration, and increased with the increase of surfactant concentration after reaching a certain concentration. In 2007, Hantal et al.[33]studied the effect of anti-ion species and surface concentration on the adsorption of ionic surfactants at the gas-liquid interface, and found that the larger the size of the anti-ion, the greater the interface thickness. Other researchers studied the MD simulation of self-assembly behavior of nanoparticles and SDS at water/trichloroethylene (TCE) interface, and concluded that the interfacial properties of the system were only affected by surfactant and had nothing to do with nanoparticles. In 2010, Gang et al.[34]used MD simulation to study the interfacial properties of surface active peptide derivatives at the n-alkane/water interface with low coverage. The molecular direction of the surface active peptide, the structural change of the cyclic main chain of the amino acid, the area of the interfacial molecule, and the motion properties were further studied. Shi[35]studied the structure and interfacial properties
of three SDS surfactants with different structures at the water/trichloroethylene interface by MD simulation, and analyzed the effect of surfactant chain length on these properties. Guo Yingyan[36] used MD method to discuss the effect of molecular structure on the aggregation behavior of surfactant at oil-water interface, the effect of polymer on the aggregation behavior of surfactant at oil-water interface, and the effect of polymer with different polymerization degree on the aggregation behavior of surfactant at oil-water interface. It can be seen that in previous studies, the aggregation behavior of surfactant on the interface was mainly studied by molecular simulation. However, in the simulation of surfactant systems, there are still some shortcomings in how to select simulation data, obtain relevant thermodynamic quantities and define appropriate potential energy functions. In particular, the current aggregation system of molecular simulation is relatively small, and some problems cannot be fully explained, which requires a larger time scale, especially in the treatment of long-range forces, which is one of the main reasons for less research on surfactant/oil/water complex systems.

3.4. Study on polymer flooding
Analytical simulation techniques have been applied to polymers since 1978, Rapaport[37], MD simulation of polymer chains containing 50 units. In 1986, Muhammad[38] used MC method to simulate the diffusion of single-phase and two-phase fluids in two-dimensional and three-dimensional network models. After 1990, Hall[39] assumed the polymer as a hard sphere chain, calculated its thermodynamic and transport properties, and determined the basic properties of diffusion rate, viscosity and thermal conductivity. In 1991, Sorbie[40] used MC method to simulate the movement of tracer and xanthan gum in porous media, and concluded that macromolecules were easier to diffuse than small molecules in a certain flow rate area. In 1999, Clark et al.[41] simulated the diffusion coefficient of alkanes in octahedral zeolite by equilibrium molecular dynamics method. In 2000, Sanborn[42] used this method to discuss the diffusion coefficient of CF4 and alkanes mixture in octahedral zeolite micropores. In 2002, Lu[43] simulated the diffusion coefficient of organic matter in supercritical CO2 by MD method, and proposed a generalized diffusion coefficient prediction equation. After 2003, Zhang[44] systematically studied the transport properties in micropores, and analyzed the diffusion properties of CH4, H2O, CO2 and other molecules in simplified porous media. In 2004 Song Kaoping[45] explained the mechanism of enhanced oil recovery by polymer flooding with MD method. The driving force of oil displacement is the thrust and friction of crude oil formed by the collision and vibration of the injection agent and crude oil molecules. The process of water flooding or polymer flooding is actually the collision and vibration of the injection agent and crude oil molecules. In 2010, Wang Xiaoan[46] studied the molecular aggregation structure (Figure 3), rheological properties, seepage characteristics, molecular wire size and its mechanism of action of oil displacement agent from both micro and macro aspects. Dong Shijin[47] studied many processes and various physical and chemical properties in polymer blend system, polymer surfactant solution system and polymer inorganic particle system in 2011. The molecular dynamics simulation of chitosan and polyethylene oxide blend system was carried out, and the compatibility of chitosan and polyethylene oxide binary system was studied from two aspects of parameters and glass transition temperature. The effects of temperature and concentration on the aqueous solution of triblock polymer surfactant were studied by all-atom molecular dynamics simulation. In 2012, Lv[48] used the method of combining MD and DPD simulation to simulate the non-equilibrium state of polyethylene melt, and studied the variation of viscosity with shear rate in the simulation system. Zhou et al.[49] studied the effect of hypercrosslinked polymer on the change of copolymer in 2015. It was found that the glass transition temperature and chain hardness increased with the increase of crosslinking degree. In 2018, Kupgan et al.[50] reviewed the progress of different molecules in simulating and describing CO2 capture and separation capabilities of polymer materials. In the application of molecular dynamics method to study the transfer properties, at present, only the diffusion of simple fluid in simplified geometric micropores can be simulated. The above scientific research on the microscopic seepage of polymer flooding has obtained important theoretical results. However, foreign scholars mainly study the light hydrocarbon...
diffusion and polymer viscoelasticity by molecular dynamics method, and there are few studies on the flow law of polymer macromolecular flooding, while domestic scholars mainly focus on the diffusion properties of inorganic small molecules in pores at the pore level. These studies do not involve the microscopic mechanism of polymer chain molecular displacing oil molecular process, and the influence of different chain structures on the seepage mechanism and intermolecular interaction in polymer displacing process, and these mechanisms and influence laws are just important data of macroscopic polymer flooding. Therefore, it is urgent to carry out more in-depth research on microscopic theory and study the microscopic diffusion law of molecules in rock pores from the molecular level of polymer, which provides a solid theoretical basis for polymer flooding in complex reservoirs in China.

![Crosslink structure diagram of polymer gels](image)

(a) Intermolecular crosslinking          (b) Intra-molecular cross-linked

Figure 3. Crosslink structure diagram of polymer gels[47]

### 3.5. Other studies

In 2004, Nyden et al.[51] simulated the pyrolysis process of polyethylene, polypropylene and isobutylene, providing a new idea for the study of thermal reactivity of macromolecules and nanostructures. In 2005, Lan Jianhui[52] ignored the electronic polarization effect and could not describe the nature of chemical bond formation or fracture based on MD simulation, and discussed the ab initio molecular dynamics method and its application in detail. In 2009, Li[53] used MD and DPD methods to simulate the multi-scale coalescence of polymer condensed states at micro and meso scales, and studied how to simulate the coarse-grained model of polymer. In 2010, Hu Yuanzhong[54] studied the rheological law of lubricating oil by molecular dynamics method, and obtained the conclusion that the critical pressure of solid-liquid phase change decreased with the film thinning, and the lubricant showed solid or solid-like properties in nano-film. In 2014, Collell et al.[55] constructed a new three-dimensional molecular model of oil shale oil matrix, optimized the molecular structure through molecular dynamics annealing, and simulated the real existence conditions of oil matrix molecules. In 2015, Wang[56] simulated the occurrence state of liquid alkanes in shale organic matter pores based on OPLS force field. In 2016, Ning Yaqian[57] studied the effect of temperature and nanoparticle addition on clean fracturing fluid formed by surfactant and salt using molecular dynamics method. Appropriate addition of NaSal can promote micelle formation and improve the rheological properties of clean fracturing fluid system. In 2019, Xue Ping[58] took the random copolymer of supercritical CO2 thickener poly ( PVAEE ) as the breakthrough point to study the positive effect mechanism of adding thickener on CO2 flooding and the basic mechanism of CO2 flooding technology in essence. In 2020, Wang Lei[59] established a molecular model to study the influence of water, ethanol and acetone penetrating into PVC system on its glass transition temperature. It was found that fine spherical particles reduced the glass transition temperature of the material, resulting in the softening of the material. In the same year, Wei Yaoyao[60] used MD simulation to study the phase transition behavior of gas-liquid interface film of sodium dodecyl sulfate caused by surface coverage change from the...
perspective of molecular configuration entropy. At the molecular level, the collapse mode of interfacial film from gas-liquid interfacial monolayer to micelle in solution is described in detail.

4. Conclusion and foresight

- With most of the onshore oilfields in China entering the middle and late stages of mining, the difficulty gradually increases, and the traditional research methods are difficult to analyze the complex formation conditions. Therefore, it is crucial to develop reliable methods for predicting fluid flow conditions and measures. Molecular simulation is one of the hotspots in the study of microscopic seepage mechanism and enhanced oil recovery because it can study the underground situation at atomic and molecular scales.
- In the process of studying adsorption and desorption, molecular simulation pays more attention to the study of adsorption location and diffusion information, and lacks the dynamic process and energy change between reservoir rocks. In addition, the constructed model is simple, generally single substance or gas, unable to accurately express the actual situation. Therefore, the complexity of the model and the diversification of gas molecules are the focus of future research.
- In the aspect of surfactant molecular simulation, scholars mainly focus on the analysis of aggregation behavior on the interface. However, there are few studies on how to select the data, how to obtain the relevant thermodynamic quantities and define the appropriate potential energy function, and there are some deficiencies in the study of surfactant/oil/water complex system. Therefore, considering multiple factors to make the results closer to the actual situation and persuasiveness is the focus of scholars’ next work.
- The research on micro-seepage of polymer flooding focuses on light hydrocarbon diffusion and small molecular diffusion, but the research on micro-seepage mechanism and diffusion law of polymer macromolecular flooding is less. Therefore, we should make full use of the previous research results, on the basis of continuous innovation to open up new research directions, and more systematically and comprehensively explain the seepage phenomenon of polymer macromolecules.
- With the continuous development of science and technology, the interdisciplinary interaction becomes more and more obvious. As a relatively new field direction, the application of molecular simulation in the oil industry has many problems to be solved.

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