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Invited review

A mini-review of ReaxFF molecular simulation in the heavy oil enhancing oil recovery: Development, challenges and prospects

Lu Zhang[1,2]*, Jingang Fu[2], Mingda Dong[2]*, Wei Yu[3], Shuyu Sun[1]

[1]*School of Mathematical Sciences, Tongji University, Shanghai 200092, P. R. China*
[2]*School of Petroleum Engineering, Chongqing University of Science and Technology, Chongqing 401331, P. R. China*
[3]*School of Aerospace Engineering, Civil Aviation Flight University of China, Sichuan 618307, P. R. China*

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Abstract:
Heavy oil plays a vital role in unconventional oil resources, receiving increasing attention. Owing to the high viscosity and high density, the complex components from heavy oil such as asphaltene and resin faces significant challenges in enhanced oil rate. ReaxFF molecular dynamic simulation (RMDS) as a powerful tool to reveal the chemical reaction process at the atomic scale has demonstrated great potential in the research of the mechanism of enhanced oil recovery (EOR) for heavy oil. This review systematically summarizes the application of RMDS in enhanced heavy oil recovery. The basic theory of the ReaxFF force field and the development of its force field parameters suitable for heavy oil simulation were introduced. The applications of RMDS in heavy oil structure and aggregation, thermal pyrolysis and catalytic mechanisms, as well as in situ combustion and oxidation were presented. The challenges of RMDS are mainly the accuracy and universality of force field parameters, limitations of simulation time and space scales, and the construction of the real heavy oil complex models. In the future, by combining machine learning potential functions, RMDS is expected to transform from an advanced tool into a key force for promoting breakthroughs in enhanced heavy oil recovery technology.

1. Introduction

With the decreasing of global light crude oil reserves, heavy oil-accounting for approximately 70% of total global oil resources-has drawn increasing attention from the petroleum industry regarding its effective development and utilization (Temizel et al., 2018; Yatimi et al., 2024). Heavy oil is widely distributed throughout the world, with significant reserves found in countries such as Canada, the United States, Russia, Venezuela, China, and Indonesia (Li et al., 2025). Heavy oil typically refers to crude oil characterized by high viscosity (typically greater than 100 mPa·s) and high density (API gravity less than 20°) under reservoir conditions. It contains substantial amounts of asphaltene and kerogen, along with high concentrations of sulfur, nitrogen, oxygen, nickel, vanadium, and other heteroatoms and metal compounds. These properties render heavy oil extremely difficult to transport through reservoir formations under natural energy or conventional displacement mechanisms. Consequently, the primary recovery factor of heavy oil relying solely on natural energy is usually less than 10%. Enhanced oil recovery theories and technologies must be implemented to reduce viscosity, improve fluidity, and thereby increase the ultimate recovery factor.

Currently, the enhanced oil recovery (EOR) technologies for heavy oil can be classified into three main categories (Guo et al., 2016): thermal oil recovery (Wu and Liu, 2019) (steam flooding, steam injection, and fire-assisted oil recovery), chemical oil recovery (Thomas et al., 2001) (polymer flooding and surfactant flooding), and solvent extraction (Li et al., 2020)

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*Corresponding author.
E-mail address: luzhang422@tongji.edu.cn (L. Zhang); fujg@cqust.edu.cn (J. Fu,); 2019063@cqust.edu.cn (M. Dong); 785914648@qq.com (W. Yu); suns@tongji.edu.cn (S. Sun).
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(CO_2 injection and hydrocarbon solvent injection). Although these technologies are technically feasible in field applications, their underlying mechanisms remain incompletely understood. In recent years, enhancing the recovery rate of heavy oil has received extensive attention. The most critical mechanism involves the kinetics of thermal decomposition reactions of heavy oil. Furthermore, for reaction processes, traditional experimental analysis methods-such as nuclear magnetic resonance and mass spectrometry-can provide average structural information, but often fail to capture reaction intermediates and transient processes. In thermal oil recovery processes, numerical simulations rely heavily on constitutive equations and reaction kinetics parameters, which in turn depend on accurate analysis of dynamic reaction processes. The limitations in understanding these transient phenomena present significant challenges for optimizing recovery operations and developing more accurate predictive models.

The Reaxff molecular dynamics simulation (RMDS) has become a tool for directly revealing these complex processes of chemical reaction at the atomic scale. Based on the ReaxFF force field, it is proposed by Van Duin et al. (2001) and achieved the dynamic description of chemical bond formation and breakage by using a continuous potential function based on bond orders. It can simulate chemical reactions in complex systems consisting of thousands to millions of atoms. Over the past decade, RMDS has been widely applied in combustion, materials science, and catalysis, and has gradually become a powerful means for studying the complex behaviors of oil systems, especially heavy oil systems.

This review aims to systematically summarize the application progress of ReaxFF molecular simulation in the research of heavy oil enhanced oil recovery (EOR), deeply analyze the main challenges currently faced, and strategically envision its future development trends, with the expectation of providing theoretical support and direction guidance for promoting the leap from microscopic mechanism understanding to macroscopic technological innovation in this field.

2. ReaxFF molecular simulation

Classical molecular dynamics force fields describe the energy of a system through interatomic potentials expressed as functions of the relative positions of atoms, making them suitable for characterizing non-reactive interactions. In contrast, reactive molecular dynamics force fields build upon classical force fields by incorporating terms that account for bond dissociation and formation, thereby enabling the simulation of chemical reaction processes. Currently, widely used reactive force fields include VALBOND (Firman and Landis, 2001), BEBO (Johnston and Parr, 1963), and ReaxFF (Van Duin et al., 2001). Among these, ReaxFF has become one of the most employed force fields in this domain, owing to its broad applicability and relatively high simulation accuracy.

2.1 ReaxFF basic theory

The ReaxFF force field was developed by Professor van Duin's research group in 2001, introducing the concept of bond order to describe chemical bond breaking and formation. In ReaxFF simulations, the total potential energy of the system is expressed as follows (Van Duin et al., 2001):

$$\begin{aligned}E_{\text{system}} &= E_{\text{bond}} + E_{\text{val}} + E_{\text{over}} + E_{\text{angle}} + E_{\text{tors}} \\ &\quad + E_{\text{conj}} + E_{\text{vdWaals}} + E_{\text{Coulomb}} + E_{\text{specific}}\end{aligned}$$

where E_{bond}, E_{val} and E_{tors} respectively represent the contributions of bond stretching vibration, bond angle vibration and dihedral torsion to the energy of the system. All three belong to the bond interaction energy. E_{angle} is the energies associated with three-body valence angle strain. E_{conj} represents the four-body conjugation energy in the benzene and aromatic hydrocarbon systems. E_{over} represents the energy compensation of atomic over-coordination. E_{vdWaals} and E_{Coulomb} respectively represent the van der Waals potential energy and Coulomb electrostatic potential energy, which belong to non-bond interaction energy. E_{specific} represents system specific terms that are not generally included, such as lone-pair, conjugation, hydrogen binding, and C_2 corrections (the properties to system).

2.2 ReaxFF force field of heavy oil

After more than 20 years of development, hundreds of ReaxFF force fields have been developed, covering most of the elements in the first five periods of the periodic table (Senftle et al., 2016), shown in Fig. 1. The ReaxFF reaction dynamics simulation technology has been widely applied in various fields, such as the pyrolysis of aviation fuels (Kwon et al., 2020), coal (Bhoi et al., 2014), biomass (Rismilleroi et al., 2018), and rubber (Wang et al., 2021), etc. However, it should be noted that the ReaxFF force field is not a universal force field. Its accuracy in describing the chemical behavior of different types of systems highly depends on the quality and scope of the training set. Therefore, it is crucial to select the appropriate force field for the specific system being studied. The accuracy of ReaxFF force field is highly dependent on its force field parameters. These parameters are obtained by fitting high-precision quantum mechanical calculation data (such as structure, energy, vibration frequency, reaction barrier, etc.). Due to the complexity and particularity of the heavy oil system, researchers have developed and optimized a series of specialized force field parameter sets. The summary was conducted on the force fields that are publicly available in the literature and involve elements C/H/O/N/S and are related to chemical reactions, which is shown in Table 1.

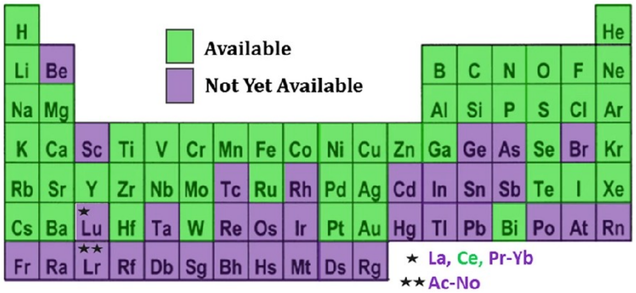


Fig. 1. Elements currently described in available parameter sets (Senftle et al., 2016).

Table 1. The ReaxFF force field suitable for heavy oil simulation.

Year	Element	Application Scope	Reference
2005	C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co	Hydrocarbons containing metallic elements	Nielson et al. (2005)
2009	C/H/O/N/S/Si	The combustion and explosion behavior of high-energy fuels	Zhang et al. (2009)
2012	C/H/O/N/S/B	Applicable to combustion reactions of biomass such as coal	Zhang et al. (2015)
2012	Si/C/O/H/N/S	Oxygen-containing combustion	Newsome et al. (2012)
2013	C/H/O/N/S/Mg/P/Na/Ti/Cl/F	The reaction behavior of solutions containing ions	Kim et al. (2013)
2013	C/H/O/N/Si/S	The interaction between hydrocarbons and SiO_2	Kulkarni et al. (2013)
2021	C/H/O/N/S/Si	Combustion of high-carbon compounds with oxygen	Liu et al. (2011)

3. ReaxFF molecular simulation applied and development in heavy oil EOR

The application of reaction molecular dynamics simulation in enhancing oil recovery from heavy oil mainly consists of three parts, such as the structural stability of heavy oil molecules, thermal oil recovery, and the thermal cracking and oxidation mechanisms that occur during in-situ combustion processes.

3.1 Heavy oil structure and aggregation

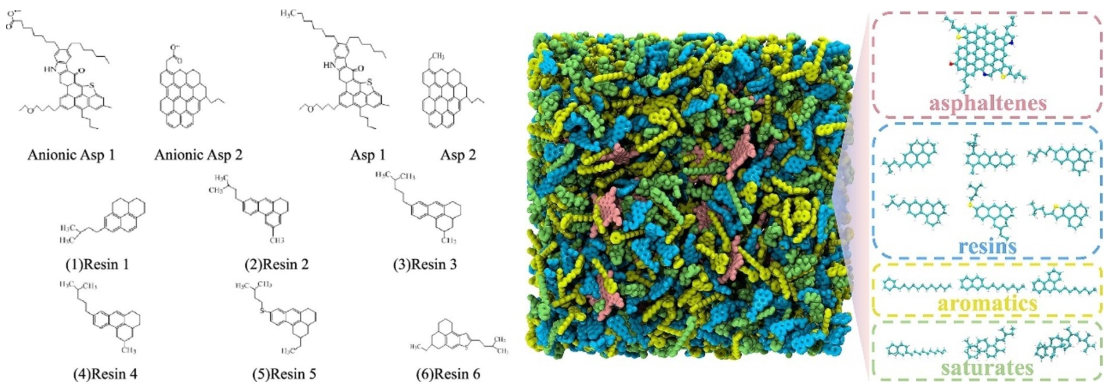
The high viscosity and tendency to deposit heavy oil mainly result from its rich content of heavy components such as asphaltene and colloidal matter (Su et al., 2019; Zhang et al., 2024), shown in Fig. 2. Understanding the molecular structure, interactions, and initial aggregation behavior of these components is crucial for predicting and controlling their macroscopic deposition. Compared with OPLS-AA force field, the research of ReaxFF force field used in heavy oil structure mainly focuses on revealing the chemical driving forces for molecular structure stability and initial aggregation from the perspective of chemical reactions (Morrow and Harrison, 2021). RMDS results show that the branched molecular structures usually exhibit higher thermal stability due to steric effects (Chen et al., 2017; Li et al., 2021). Throughout the oxidation process, asphaltene mainly involves changes in C-O, H-O, and S-O bonds, and in the presence of oxygen, it generates ketones (Hu et al., 2020). To study adhesion properties, the RMD method (Shishehbor et al., 2018) was used to analyze the aggregation behavior of saturated substances, asphaltene, resin, and aromatic (SARA) components with silica (SiO_2) at different temperatures, and it was found that due to hydrogen bonding and covalent bond breakage, the adhesion properties of asphaltene molecules are higher than those of other components (Xu et al., 2021). Asphaltene molecules (Sedghi et al., 2013) will rapidly aggregate through π-π stacking, hydrogen bonds, and van der Waals forces to form nano aggregates, which is highly consistent with the flocculation phenomenon observed experimentally.

3.2 Thermal pyrolysis and catalytic mechanism

Thermal oil recovery methods and in-situ combustion technologies involve thermal pyrolysis and oxidation reactions of heavy oil at high temperatures. Over the past 20 years of research, RMD (Wang et al., 2011) has been widely used to simulate the thermal decomposition behavior of heavy oil model compounds at high temperatures, which can visually display the preferential breakage of weak bonds (such as C-S, C-Alkyl bonds) at the initial stage of the reaction, generating radical intermediates, followed by a series of reactions such as β-scission, hydrogen transfer, radical recombination, etc., ultimately generating small molecule products such as light hydrocarbons, alkenes, H_2, H_2S, etc. (Zhang et al., 2015). Catalytic pyrolysis is another method to accelerate the reaction of heavy oil. The catalyst can reduce the cracking conditions of heavy oil. RMD is used to study the cracking mechanism of heavy oil on the surface of acidic catalysts. The Brønsted acid sites on the catalyst surface can protonate hydrocarbon molecules, initiating carbocation reactions, thereby promoting cracking, isomerization and aromatization reactions, and generating higher-value light products (Chen et al., 2017). In addition, simulations can also study the catalytic effect of minerals under hydrothermal conditions (Li et al., 2025), as well as the promoting effect of metal nanoparticles on hydrogenation desulfurization reactions.

3.3 In-situ combustion and low-temperature oxidation

The oil combustion layer technology involves complex high-temperature combustion reactions and low-temperature oxidation mechanisms that are difficult to directly capture the behavior through experiments. High-temperature combustion typically occurs under high-temperature reaction conditions, and the RMD simulation can clearly show the deep oxidation process of hydrocarbon molecules, generating CO, CO_2, and H_2O (Li et al., 2013). By analyzing the oxidation activity of different hydrocarbon structures, it can provide guidance for optimizing gas injection processes and improving combustion efficiency. The C-C bond in n-heptane is easier to break than the C-H bond, and the C_2-C_3 bond is the easiest to break, generating C_2H_5 and C_5H_{11} radicals. Single-molecule dissociation is the main pathway for the decomposition of n-heptane, and the C-C bond in the middle dissociates before the terminal C-C bond. Through RMD simulation (Chen et al., 2017) for the high-temperature pyrolysis reaction of C_{16}, it was found that carbon-carbon bonds are preferentially broken



(a)

Fig. 2. Asphaltene and resin molecules used in the simulation (Su et al., 2019) and Molecular topological structures of SARA components (Zhang et al., 2024).

under high-temperature conditions, and the pyrolysis process is completed in a short time. In addition, low-temperature oxidation has been the main approach to improve oil recovery rate and by-products. One of the main reaction processes in the in-situ combustion of heavy oil technology in the low-temperature zone is the in-situ combustion of heavy oil. Using RMD method to study the low-temperature oxidation (LTO) of heavy oil by Jin et al. (2025), it was demonstrated that long carbon chains are preferentially decomposed in the low-temperature oxidation process, forming peroxide radicals, small carbon fragments produce carbon dioxide, and the final residual products include polycyclic aromatic hydrocarbons and aromatic compounds. Using RMD simulation to study the in-situ combustion gasification (ISCG) process of heavy oil by Chen et al. (2025), it was found that hydrogen is mainly generated through the reaction of hydrogen radicals with water, and during the in-situ combustion process, sulfur first forms carbonyl sulfide (COS), which is then converted into hydroxy sulfide hydroxyl (HOS) and hydrogen sulfide ions (HS) under the action of water and oxygen, and subsequently converted into H_2S and SO_2.

4. Challenges and perspectives

4.1 The accuracy and universality of field parameters

The force field parameters are vital for the accuracy of the simulation results. The existing ReaxFF force field parameters are mostly fitted based on the calculation results of simple compounds. Although the main components of heavy oil can be classified into four types, the real heavy oil components contain different structural molecules. It is necessary to build an exclusive ReaxFF force field for real heavy oil. The accuracy of the existing ReaxFF force field in describing heavy oil needs to be systematically verified. Moreover, the elements of heavy oil components include S, N, O, etc., but the reactions between multiple elements are complex and variable. The current trained ReaxFF force field has limited accuracy and high simulated temperature for reactions involving mixed atoms, especially for cases involving metal atoms. Currently, the training and fitting process of the ReaxFF force field is not taken the thermodynamic properties of mixed systems into consideration. Therefore, when using the ReaxFF force field to predict the gas-liquid, liquid-liquid phase equilibrium and thermodynamic properties of multi-component mixtures of heavy oil, its limited accuracy seriously affects the quantitative prediction ability of thermodynamic and kinetic processes after pyrolysis. In the future, combined with machine learning potential functions, the force field parameters of the representative molecular structures identified in heavy oil are refitted and systematically verified. It can maintain quantum mechanical accuracy while significantly improving computational efficiency, and larger systems and longer simulation times with the same computing resources.

4.2 Simulated spatial and temporal scales

Many processes in heavy oil EOR are lengthy. The aggregation of asphaltenes, the diffusion of heavy components, and low-temperature oxidation reactions have characteristic times ranging from microseconds to hours. RMDS are at the nanosecond scale. Even with enhanced sampling techniques, it is difficult to cover the entire timescale of these slow processes. A real asphaltene aggregate or micelle may contain hundreds of molecules and have a size of several tens of nanometers. But the current conventional ReaxFF simulation systems usually can only accommodate a few to several dozen asphaltene molecules, making it difficult to fully reproduce their true aggregation state structure and size distribution. When simulating porous media, only highly idealized nanopore models can be constructed. Therefore, the approach of further enhancing the spatial and temporal scales is necessary to improve the practicality of the simulation.

4.3 Establishment of the true heavy oil model

Most of the RMD simulations are designed to be computationally feasible by using a single or a few model compounds to represent the entire heavy oil system. This undoubtedly neglects the synergistic or antagonistic effects brought about by the diversity of components and is far from the actual situation. The real reservoir environment includes formation water, various minerals, pressure and temperature gradients, etc. Most current simulations are conducted under uniform and constant conditions, which are unable to reflect the complex multi-field coupling effects under real geological conditions.

5. Summary and conclusions

ReaxFF molecular dynamics simulations have evolved into an indispensable tool for understanding the complex physical and chemical mechanisms in the process of enhanced oil recovery (EOR) of heavy oil at the atomic scale. It provides microscopic insights that are difficult to obtain through experiments in aspects such as the aggregation behavior of heavy oil components, thermal cracking and catalytic upgrading pathways, and in-situ combustion reaction kinetics. This has greatly deepened our understanding of the essence of EOR method. However, when applied to the extremely complex system of heavy oil, ReaxFF faces severe challenges in terms of force field accuracy, spatial and temporal scales, model authenticity, and computational efficiency. Future breakthroughs will rely on the deep cross-fusion of computational science, chemistry, petroleum engineering, and artificial intelligence. By developing more precise specialized force fields, ReaxFF simulations will surely transform from an advanced research tool into breakthroughs in heavy oil EOR technology, laying a foundation for the efficient development of heavy oil resources.

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Conflict of interest

The authors declare no competing interest.

References

Bhoi, S., Banerjee, T., Mohanty, K. Molecular dynamic simulation of spontaneous combustion and pyrolysis of brown coal using ReaxFF. Fuel, 2014, 136: 326-333.

Chen, Z., Sun, W., Zhao, L. High-temperature and high-pressure pyrolysis of hexadecane: molecular dynamic simulation based on reactive force field (ReaxFF). The Journal of Physical Chemistry A, 2017, 121(10): 2069-2078.

Chen, Z., Zhao, P., Zhao, L., et al. Molecular simulation of the catalytic cracking of hexadecane on ZSM-5 catalysts based on reactive force field (ReaxFF). Energy & Fuels, 2017, 31(10): 10515-10524.

Chen, Q., Tang, X., Pu, W., et al. ReaxFF molecular dynamics study on hydrogen generation from heavy oil in-situ combustion gasification. Geoenergy Science and Engineering, 2025, 249: 213786.

Firman, T. K., Landis, C. R. Valence bond concepts applied to the molecular mechanics description of molecular shapes. 4. transition metals with π-bonds. Journal of the American Chemical Society, 2001, 123(47): 11728-11742.

Guo, K., Li, H., Yu, Z. In-situ heavy and extra-heavy oil recovery: A review. Fuel, 2016, 185: 886-902.

Hu, D., Gu, X., Cui, B., et al. Modeling the oxidative aging kinetics and pathways of asphalt: A ReaxFF molecular dynamics study. Energy & Fuels, 2020, 34(3): 3601-3613.

Johnston, H. S., Parr, C. Activation energies from bond energies. I. Hydrogen transfer reactions. Journal of the American Chemical Society, 1963, 85(17): 2544-2551.

Jin, X., Tang, X., Pu, W., et al. Study on the characteristics and mechanism of low-temperature oxidation of heavy oil using ReaxFF molecular dynamics simulation. Computational and Theoretical Chemistry, 2025, 1244: 115070.

Kwon, H., Shabnam, S., van Duin, A. C., et al. Numerical simulations of yield-based sooting tendencies of aromatic fuels using ReaxFF molecular dynamics. Fuel, 2020, 262: 116545.

Kim, S. Y., Van Duin, A. C., Kubicki, J. D. Molecular dynamics simulations of the interactions between TiO_2 nanoparticles and water with Na^+ and Cl^-, methanol, and formic acid using a reactive force field. Journal of Materials Research, 2013, 28(3): 513-520.

Kulkarni, A. D., Truhlar, D. G., Goverapet Srinivasan, S., et al. Oxygen interactions with silica surfaces: Coupled cluster and density functional investigation and the development of a new ReaxFF potential. The Journal of Physical Chemistry C, 2013, 117(1): 258-269.

Li, X., Zhou, W., Zhou, Y., et al. Review on molecular dynamics simulations for understanding mechanisms of enhanced heavy oil recovery: Recent progress, challenges, and prospects. Energy & Fuels, 2025, 39(35): 16628-16651.

Li, X., Berg, S., Castellanos-Diaz, O., et al. Solvent-dependent recovery characteristic and asphaltene deposition during solvent extraction of heavy oil. Fuel, 2020, 263: 116716.

Liu, L., Liu, Y., Zybin, S. V., et al. ReaxFF-lg: Correction of the ReaxFF reactive force field for London dispersion, with applications to the equations of state for energetic materials. The Journal of Physical Chemistry A, 2011, 115(40): 11016-11022.

Li, W., Yu, S., Zhang, L., et al. ReaxFF molecular dynamics simulations of n-eicosane reaction mechanisms during pyrolysis and combustion. International Journal of Hydrogen Energy, 2021, 46(78): 38854-38870.

Li, Y., Han, H., Xu, Z., et al. Mechanism of the Effect of Al Nanoparticles on n-Decane Cracking: An Experimental and ReaxFF Simulation Study. Industrial & Engineering Chemistry Research, 2025, 64(24): 11851-11867.

Li, J. Q., Wang, F., Cheng, X. M., et al. Reactive Molecular

Dynamics Simulation on Thermal Decomposition of n-Heptane. Chinese Journal of Chemical Physics, 2013, 26(2): 211-219.

Morrow, B. H., Harrison, J. A. Evaluating the ability of selected force fields to simulate hydrocarbons as a function of temperature and pressure using molecular dynamics. Energy & Fuels, 2021, 35(5): 3742-3752.

Nielson, K. D., Van Duin, A. C., Oxgaard, J., et al. Development of the ReaxFF reactive force field for describing transition metal catalyzed reactions, with application to the initial stages of the catalytic formation of carbon nanotubes. The Journal of Physical Chemistry A, 2005, 109(3): 493-499.

Newsome, D. A., Sengupta, D., Foroutan, H., et al. Oxidation of silicon carbide by O_2 and H_2O: A ReaxFF reactive molecular dynamics study, Part I. The Journal of Physical Chemistry C, 2012, 116(30): 16111-16121.

Rismiller, S. C., Groves, M. M., Meng, M., et al. Water assisted liquefaction of lignocellulose biomass by ReaxFF based molecular dynamic simulations. Fuel, 2018, 215: 835-843.

Senftle, T. P., Hong, S., Islam, M. M., et al. The ReaxFF reactive force-field: Development, applications and future directions. npj Computational Materials, 2016, 2(1): 1-14.

Su, G., Zhang, H., Geng, T., et al. Effect of SDS on reducing the viscosity of heavy oil: A molecular dynamics study. Energy & Fuels, 2019, 33(6): 4921-4930.

Shishehbor, M., Pouranian, M. R., Imaninasab, R. Evaluating the adhesion properties of crude oil fractions on mineral aggregates at different temperatures through reactive molecular dynamics. Petroleum Science and Technology, 2018, 36(24): 2084-2090.

Sedghi, M., Goual, L., Welch, W., et al. Effect of asphaltene structure on association and aggregation using molecular dynamics. The Journal of Physical Chemistry B, 2013, 117(18): 5765-5776.

Thomas, S., Ali, S. F., Scoular, J. R., et al. Chemical methods for heavy oil recovery. Journal of Canadian Petroleum Technology, 2001, 40(3).

Temizel, C., Canbaz, C. H., Tran, M., et al. A comprehensive review heavy oil reservoirs, latest techniques, discoveries, technologies and applications in the oil and gas industry. Paper SPE 193646 Presented at SPE International Heavy Oil Conference and Exhibition, Kuwait City, Kuwait, 10-12 December 2018.

Van Duin, A. C., Dasgupta, S., Lorant, F., et al. ReaxFF: A reactive force field for hydrocarbons. The Journal of Physical Chemistry A, 2001, 105(41): 9396-9409.

Wu, Z., Liu, H. Investigation of hot-water flooding after steam injection to improve oil recovery in thin heavy-oil reservoir. Journal of Petroleum Exploration and Production Technology, 2019, 9(2): 1547-1554.

Wang, Y., Yao, S., Wang, W., et al. Pyrolysis of vulcanized styrene-butadiene rubber via ReaxFF molecular dynamics simulation. Chinese Journal of Chemical Engineering, 2021, 31: 94-102.

Wang, Q. D., Wang, J. B., Li, J. Q., et al. Reactive molecular dynamics simulation and chemical kinetic modeling of pyrolysis and combustion of n-dodecane. Combustion and Flame, 2011, 158(2): 217-226.

Xu, Z., Wang, Y., Cao, J., et al. Adhesion between asphalt molecules and acid aggregates under extreme temperature: A ReaxFF reactive molecular dynamics study. Construction and Building Materials, 2021, 285: 122882.

Yatimi, Y., Mendil, J., Marafi, M., et al. Advancement in heavy oil upgrading and sustainable exploration emerging technologies. Arabian Journal of Chemistry, 2024, 17(3): 105610.

Zhang, L., Zybin, S. V., Van Duin, A. C., et al. Carbon cluster formation during thermal decomposition of octahydro-1, 3, 5, 7-tetranitro-1, 3, 5, 7-tetrazocine and 1, 3, 5-triamino-2, 4, 6-trinitrobenzene high explosives from ReaxFF reactive molecular dynamics simulations. The Journal of Physical Chemistry A, 2009, 113(40): 10619-10640.

Zhang, Y., Wang, X., Li, Q., et al. A ReaxFF molecular dynamics study of the pyrolysis mechanism of oleic-type triglycerides. Energy & Fuels, 2015, 29(8): 5056-5068.

Zhang, J., Zhu, B., Yuan, H., et al. Nonlinear relationship between heavy oil viscosity and asphaltene dispersion: A molecular dynamics simulation study. Chemical Engineering Science, 2024, 295: 120173.