

Original Paper

Molecular dynamics study on the diffusion and dissolution of heavy oil in supercritical CO₂ under high-temperature and high-pressure conditionsKe-Xin Du^{a,b}, Song-Yan Li^{a,b,*}, Fa-Kun Li^{a,b}, Jia-Wei Zhao^{a,b}, Yu Zhang^{a,b}^a National Key Laboratory of Deep Oil and Gas, China University of Petroleum (East China), Qingdao, 266580, Shandong, China^b School of Petroleum Engineering, China University of Petroleum (East China), Qingdao, 266580, Shandong, China

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ABSTRACT

CO₂-assisted steam thermal recovery is an efficient CO₂-enhanced oil recovery (CO₂-EOR) technique, increases heavy oil production while storing CO₂. To elucidate heavy oil and supercritical CO₂ interactions under high-temperature and high-pressure conditions, PVT experiments were conducted, and molecular dynamics (MD) simulations were used to examine the effects of temperature and pressure on diffusion and dissolution in CO₂. The analysis considered oil and gas density distributions, interaction energies between SARA fractions and CO₂, radial distribution functions (RDFs), and diffusion coefficients obtained from mean square displacement (MSD). The results show that increasing temperature reduces the dissolved gas–oil ratio but enhances the volume coefficient. Light components such as saturates and aromatics interact most strongly with CO₂ and dissolve fastest, whereas heavy components such as resins and asphaltenes have lower interaction energies and dissolve more slowly because of strong π – π association. The interaction energy between CO₂ and light components is 2–4 times stronger than that with heavy components in the temperature range 373–523 K and pressure range 5–20 MPa. The CO₂–SARA interaction energy decreases by about 30%–40% with increasing temperature, but increases by about 50%–60% with increasing pressure. The diffusion rate of SARA molecules is fastest at 523 K and 20 MPa, with diffusion coefficients of 34.8×10^{-9} , 20.4×10^{-9} , 6.2×10^{-9} , and 4.7×10^{-9} m²/s, respectively. Overall, an injection temperature close to 250 °C combined with pressures exceeding 10 MPa provides optimal conditions for CO₂ diffusion and dissolution, thereby facilitating the extraction of light fractions and maximizing viscosity reduction and thermal recovery performance.

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1. Introduction

As global warming intensifies, carbon capture, utilization and storage (CCUS) technology has emerged as a pivotal solution for addressing greenhouse gas emissions and achieving carbon neutrality and peak carbon targets. This technology can capture CO₂ generated during industrial and energy production processes and inject it into the ground for permanent storage, effectively reducing greenhouse gas emissions and driving the global transition to a low-carbon future. The Paris Agreement has set strict

control standards for global temperature change, with the core objective of limiting the global average temperature rise to below 2 °C, and striving to keep it within 1.5 °C (Wang et al., 2025; Schleussner et al., 2016; Li et al., 2024). The combustion of fossil fuels, including coal, oil, and natural gas, is one of the primary sources of global CO₂ emissions. According to data from the International Energy Agency (IEA) and the United Nations Framework Convention on Climate Change, approximately 75% of global greenhouse gas emissions originate from carbon dioxide produced by the combustion of fossil fuels (IEA, 2025; Li, 2025). As an important component of fossil fuels, oil development is closely linked to global carbon emissions (Lin et al., 2025; Wang et al., 2026), with the majority of carbon emissions originating from the upstream stage of crude oil production—heavy oil development.

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Owing to the presence of heteroatoms such as N, O, S, and other metal elements in heavy oil molecules, their complex molecular configurations increase intermolecular interaction forces, resulting in the high viscosity and low fluidity of heavy oil. Therefore, thermal recovery methods that reduce the viscosity of heavy oil and increase its fluidity have become the primary means for the efficient development of heavy oil (Sun et al., 2023; Zhang et al., 2024; Guan et al., 2025). Currently, commonly used thermal recovery methods include cyclic steam stimulation (CSS), steam flooding, and steam-assisted gravity drainage (SAGD) (Guo et al., 2016; Cui et al., 2022; Alvarez and Han, 2013). These methods are all energy- and CO₂-intensive production methods that generate a large amount of CO₂ during the development process, thereby significantly increasing carbon intensity (Masnadi et al., 2018). In addition, these thermal recovery methods often face issues such as high energy consumption and low steam heat utilization efficiency in the later stages of development, resulting in lower oil production and a higher water cut. Therefore, to achieve low-carbon green development, reduce carbon emissions, and significantly increase heavy oil recovery, there is an urgent need to innovate and optimize conventional thermal recovery methods. In recent years, CCUS technology has been widely applied in the field of oil extraction, particularly in CO₂-EOR technology, as a key means to achieve this goal (Lin et al., 2025; Du et al., 2026; Zhao et al., 2024; Xiong et al., 2024). CO₂-EOR technology not only enhances oil recovery but also effectively reduces CO₂ emissions, promoting the green and low-carbon transformation of the petroleum industry (Zhang et al., 2025). On the basis of CO₂-EOR technology, some scholars have proposed a CO₂-assisted steam thermal recovery method, which utilizes viscosity reduction and the heat carrying capacity and expands the sweep effects of CO₂ to reduce steam energy consumption and improve thermal recovery efficiency (Du et al., 2024; Feng et al., 2020; Liu et al., 2023). In addition, CO₂ can not only prevent steam channelling and overlap but also enhance the heat utilization efficiency of steam and reduce greenhouse gas emissions, thereby achieving CCUS. Among them, solution trapping and residual trapping are the primary methods of CCUS in the process of CO₂-assisted steam thermal recovery (Li et al., 2026).

During the CO₂-assisted steam thermal recovery process, the temperature of the injection well can reach 300 °C, and the injection pressure approaches 10 MPa. In this environment, CO₂ is in a supercritical state and has a stronger diffusion capability. A series of interactions between CO₂ and heavy oil occur at the swept front, thus changing the physical properties of heavy oil. These interactions include the dissolution and diffusion of heavy oil in CO₂, as well as the extraction of light components from heavy oil by CO₂. Some experiments have shown that after CO₂-assisted steam flooding, the viscosity reduction rate of heavy oil increases, and the content of light components in the produced oil increases while the content of heavy components decreases (Xi et al., 2019; Liu et al., 2023, 2024). To investigate the changes in the physical properties of heavy oil after dissolving CO₂ under high-temperature conditions, numerous studies have conducted high-temperature and high-pressure PVT experiments. The saturation pressure, volume factor, and viscosity reduction rate of heavy oil dissolving CO₂ were measured using a PVT device (Li et al., 2018; Zhao et al., 2018; Liu et al., 2020).

However, conventional laboratory experiments can only capture the physical property changes of heavy oil and fluids after mutual dissolution from a macroscopic perspective, making it difficult to characterize the interaction between heavy oil SARA molecules and fluids during the dissolution process from a microscopic perspective. In recent years, with technological advancements and enhanced computational capabilities, MD

simulation, as a powerful computational tool, has been widely applied in the fields of materials science, biology, and chemistry. MD simulations can provide precise descriptions at the atomic level, revealing intermolecular interactions, diffusion behaviour, and thermodynamic properties (Seyyedattar et al., 2019). In the field of petroleum and natural gas, MD simulations have become important for studying the behaviour of oil–water–gas interfaces and fluid–solid interactions (Huang et al., 2024). Currently, some studies have reported the dissolution and diffusion behaviour of heavy oil in supercritical water. As an environmentally friendly hydrocarbon solvent, supercritical water possesses strong dissolution and diffusion capabilities, enabling the dissolution of heavy oil (Li et al., 2023; Zhang et al., 2019). The critical temperature and pressure of supercritical water are 647 K and 22.1 MPa, respectively. Supercritical water exhibits extremely strong thermodynamic properties under these conditions. Xin et al. (2016) studied the aggregation behaviour of asphaltenes in supercritical water through MD simulations. The results indicated that owing to the high van der Waals (vdW) repulsion, supercritical water and asphaltenes mutually repel each other, making asphaltenes prone to aggregation. Ding et al. (2021) studied the dissolution process of heavy polycyclic aromatic hydrocarbons (PAHs) in supercritical water under different hydrogen contents and densities through MD simulations. They reported that as the hydrogen content and density of supercritical water increased, the degree of dissolution of PAHs also increased. Qu et al. (2019) studied the dissolution behaviour of polycyclic aromatic hydrocarbon mixtures in supercritical water under different densities and temperatures through MD simulations. The results indicated that as the temperature and SCW density increased, electrostatic attraction intensified, leading to a greater degree of dissolution of PAHs.

In the context of CCUS, supercritical CO₂ has garnered widespread attention as a crucial carbon sequestration medium (Zhang et al., 2017; Qin et al., 2022; Lin et al., 2025). Supercritical CO₂ possesses unique physicochemical properties, exhibiting both the high diffusivity of a gas and the high density of a liquid at its critical temperature of 304.13 K and critical pressure of 7.38 MPa. Therefore, supercritical CO₂ has excellent effects on crude oil extraction and dissolution. Wang et al. (2024) studied the diffusion behaviour of PAHs in supercritical CO₂ through MD simulations under conditions of 313–373 K and 10–30 MPa and calculated the diffusion coefficients of heavy PAHs under different temperatures and pressures. They reported that the diffusion coefficient of heavy PAHs increased with increasing temperature and decreased with increasing pressure, reaching a maximum at 373 K and 10 MPa. Wu et al. (2016) studied the extraction behaviour of supercritical CO₂ on kerogen adsorbed on the surface of shale at 333–373 K through MD simulations. They reported that the extraction capacity of supercritical CO₂ increased with increasing pressure and that the amount of kerogen adsorbed on the shale surface decreased. Li et al. (2025) employed MD simulations to investigate the extraction behaviour of polar and nonpolar molecules in shale oil by supercritical CO₂ at 338 K and calculated the diffusion coefficients of polar and nonpolar molecules through the MSD. The results indicated that CO₂ exhibited the highest extraction rate for the nonpolar molecule C₈H₁₈, whereas the extraction rate for the nonpolar molecule C₆H₁₄N₂O₂ was very low.

In summary, existing research has preliminarily revealed the dissolution phenomena of PAHs and heavy oil in supercritical water and supercritical CO₂. In CO₂-assisted steam thermal recovery, fluids are exposed to high-temperature and high-pressure environments. The current experimental conditions make it difficult to study the microscopic interactions between CO₂ and heavy oil at the swept front. MD simulations can be used to study the microscopic interactions between heavy oil and CO₂ at the atomic/

molecular level. However, previous studies have been limited to the dissolution and extraction of PAHs in supercritical CO₂ under conventional reservoir conditions, and the diffusion and dissolution behaviour of heavy oil in CO₂ remains unclear under high-temperature and high-pressure conditions. Therefore, systematically characterizing the diffusion and dissolution behaviour of heavy oil molecules, especially SARA molecules, in supercritical CO₂ at high temperatures and pressures is essential for understanding the mechanism of heavy oil thermal recovery and carbon sequestration. The objective of this study is to investigate the diffusion and dissolution behaviour of heavy oil SARA molecules in supercritical CO₂ under high-temperature and high-pressure conditions by MD simulations. First, PVT experiments were conducted under high-temperature and high-pressure conditions to test the physical properties of heavy oil after dissolving CO₂. MD simulations were subsequently performed using Material Studio software. The density distribution of heavy oil and CO₂, the interaction energy between heavy oil SARA molecules and CO₂, the RDF of CO₂ molecules and heavy oil SARA molecules, and the diffusion coefficient of SARA molecules in CO₂ were analysed. The results elucidate the diffusion and dissolution mechanism of heavy oil in supercritical CO₂ under high-temperature and high-pressure conditions, providing important guidance for improving the thermal recovery efficiency of heavy oil and understanding the microscopic interactions between CO₂ and heavy oil.

2. Experimental and simulation methods

2.1. Experimental methods

2.1.1. Materials

The oil sample was from the heavy crude oil in Block Cao 4 of the Shengli Oilfield. The relationships among viscosity, density, and temperature were measured by a rheometer and a density bottle after the oil sample was dehydrated. The carbon number of the heavy oil was tested by gas chromatography, providing basic physical property parameters for subsequent experimental analysis. The viscosity, density, and carbon number distribution of the heavy oil are shown in Fig. 1. The heavy oil in this block is classified as ordinary heavy oil. The viscosity of heavy oil is sensitive to temperature and decreases sharply as the temperature increases. The decreasing trend of viscosity slows down at a temperature of 40 °C, with the oil viscosity being 18642.75 mPa s. The oil viscosity rapidly decreases to 393.68 mPa s at a temperature of 100 °C. The oil density decreases from 946.83 to 889.02 kg/m³ as the temperature increases from 20 to 100 °C. The carbon number distribution reveals that the content of light components in the heavy

oil is low, whereas the contents of medium and heavy components are relatively high. The mass fraction of light components with a carbon number $\leq C_{20}$ is 14.64%, the mass fraction of medium components such as C₂₁–C₄₀ is 24.4%, and the mass fraction of heavy components such as C₄₁–C₁₁₀ is 60.96%. The elemental content in the heavy oil was tested through elemental analysis, and the results are listed in Table 1. According to Table 1, the oil sample is primarily composed of C and H, with contents of 80.21% and 10.76%, respectively. Additionally, the heavy oil contains small amounts of impurities such as S, N, and O, with a total content of 8.25%. The gas used in the experiments was provided by Qingdao Tianyuan Gas Co., Ltd., with a purity greater than 99.99%.

2.1.2. Apparatus

The experimental setup consisted of a high-temperature and high-pressure piston-type PVT analyser, a falling ball viscometer, an ISCO pump, a pressure gauge, and back pressure regulators (BPRs). The high-temperature and high-pressure PVT analyser was produced by Jiangsu Huaan Technology Co., Ltd., with a temperature upper limit of 300 °C and a pressure upper limit of 60 MPa. The falling ball viscometer was provided by Beijing Uliber Technology Co., Ltd., with an upper temperature limit of 280 °C and an upper pressure limit of 50 MPa. The experimental flow chart is shown in Fig. 2.

2.1.3. Experimental procedures

- (1) After vacuuming, a certain volume of degassed crude oil was added to the high-temperature and high-pressure PVT cell. The temperature was increased to the experimental temperature and stabilized for 2 h until the temperature was stable.
- (2) The oil was pressurized to the top by a hand pump, and the initial reading V_1 was recorded after withdrawing 100 mL from the pump. CO₂ with a certain dissolved gas–oil ratio was injected, and the reading V_2 of the hand pump was recorded.
- (3) The pump was pressurized to 3–4 MPa above the predicted saturation pressure, and the PVT chamber was rotated to a stable pressure. A series of corresponding volumes and pressures were plotted on coordinate paper, and the

Table 1
Elemental composition of heavy oil.

Element types	C	H	S	N	O
Element content, %	80.99	10.76	3.12	3.51	1.62

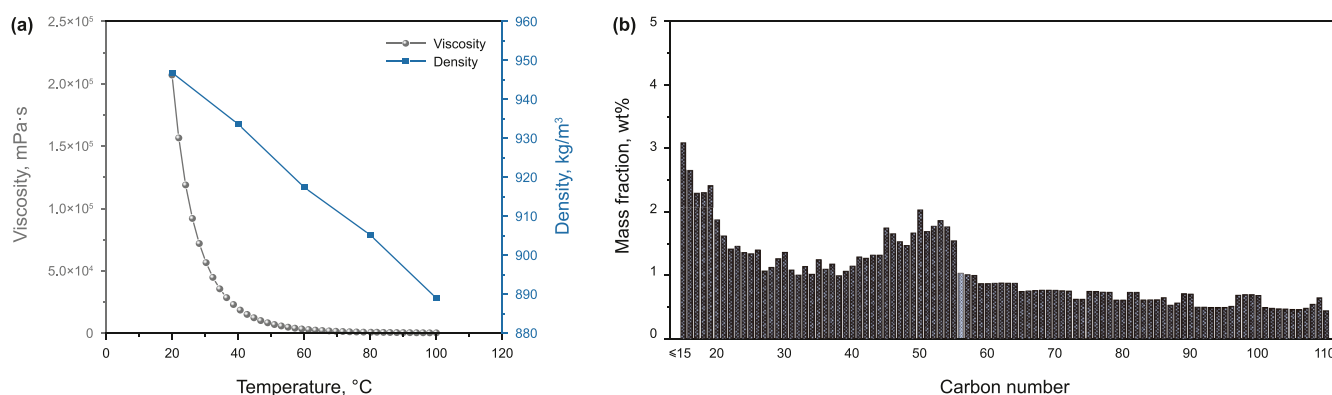


Fig. 1. The basic physical properties of heavy oil. (a) Curves of the viscosity and density of heavy oil with respect to temperature, (b) the distribution of carbon numbers.

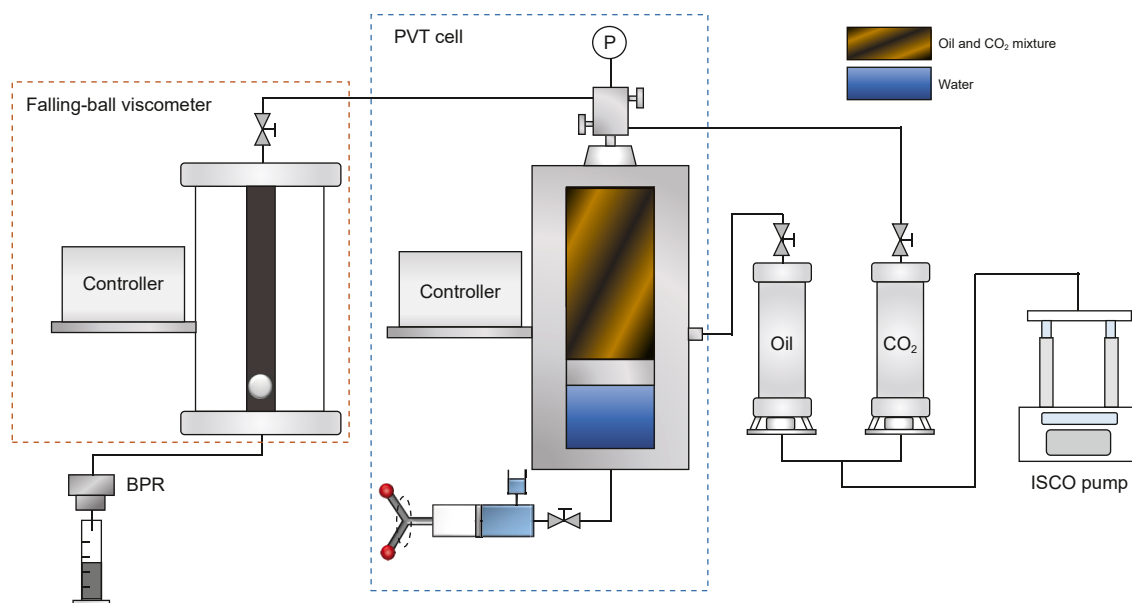


Fig. 2. Schematic diagram of heavy oil dissolution in CO₂.

pressure corresponding to the inflection point of the curve was the saturation pressure at the gas content.

- (4) A high-pressure metering pump was used to inject the oil–gas mixture into a high-temperature and high-pressure falling ball viscometer through a high-pressure pipeline at a back pressure higher than the saturation pressure. The viscosity of the mixture at different temperatures was measured by setting the heating temperature of the falling ball viscometer. The test was repeated three times, and the results were averaged.
- (5) The experimental pressure was changed, and steps (1)–(4) were repeated.

2.2. Simulation methods

2.2.1. Model construction

All molecular models and simulations were performed in Materials Studio 2020 using the COMPASS III force field, which has been widely validated for condensed-phase hydrocarbon systems (Zhong et al., 2013; Huang et al., 2024; Wang et al., 2023). SARA fraction was used to represent heavy oil components in order to comprehensively characterize the unique properties of resins and asphaltenes macromolecules in heavy oil (De León et al., 2017; Verstraete et al., 2010). On the basis of previous work (Wu et al., 2015; Mullins, 2011; Tang et al., 2018), SARA molecular models for heavy oil were established and compared with the experimentally measured four-component content of heavy oil, as shown in Table 2. As shown in Table 2, the SARA content from the simulation was close to the test value, with an error within 2%, indicating the accuracy of the model. The relative molecular mass

of SARA gradually increased, with a molecular weight range of 170.33–1149.69 g/mol. Resins and asphaltenes with high molecular weights accounted for the high viscosity and high density of heavy oil. The molecular configuration of SARA is shown in Fig. 3. The saturates were represented by a straight-chain alkane (C₁₂H₂₆), while the aromatics consisted of three benzene rings and two straight-chain alkanes. The molecular model of the resins was represented by that extracted from Athabasca oil sands by Murgich et al. (1999). The molecular model of asphaltenes was represented by the classic continental model proposed by Speight and Moschopedis (1979). In this work, all molecular models were constructed using an all-atom (AA) representation. The COMPASS III force field provided fully atomistic parameters. All atoms, including hydrogen atoms in hydrocarbon chains and heteroatoms in resins and asphaltenes, were explicitly considered. The simulated and measured values of density and viscosity of oil sample at 40 °C are shown in Table 3. The results show that the simulated values of oil density and viscosity are close to the measured values, and the relative errors are 0.77% and 2.12%, respectively.

First, CO₂ and SARA molecules were constructed using the Visualizer Tools module. The molecules were then geometrically optimized using the smart algorithm in the Forcite module to minimize their energy. Subsequently, the amorphous cell module was employed to construct heavy oil boxes with dimensions of 46.72 Å × 46.72 Å × 46.72 Å, and five configurations were output. The configuration with the minimum energy was selected for geometric optimization, and three cycles of annealing were performed using the NPT ensemble based on the experimental temperature and pressure to obtain a stable heavy oil box structure. Afterwards, an oil droplet with a radius of 20 Å was extracted from

Table 2
The SARA molecular number of heavy oil.

Component	Chemical formula	Number	Mass fraction, wt%		Molecular weight, g/mol	Reference
			Test value	Simulated value		
Saturates	C ₁₂ H ₂₆	78	30.55	30.81	170.33	Tang et al. (2018)
Aromatics	C ₁₉ H ₂₄	52	30.16	30.24	252.16	Zhang et al. (2019)
Resins	C ₅₀ H ₈₀ S	21	35.21	34.48	713.25	Tang et al. (2018)
Asphaltenes	C ₇₉ H ₉₂ N ₂ OS ₂	2	4.08	4.47	1149.69	Speight and Moschopedis (1979)

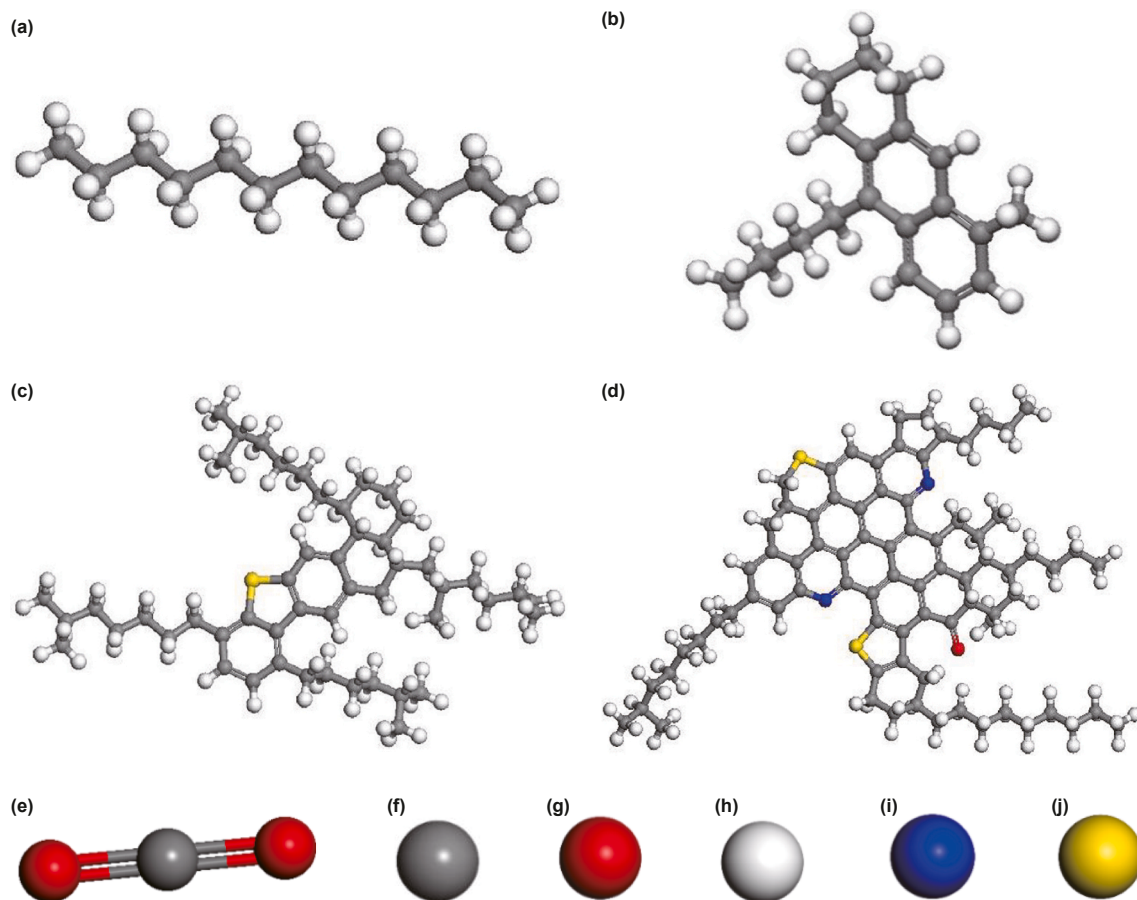


Fig. 3. The average SARA and CO₂ molecular model. (a) Saturates, (b) aromatics, (c) resins, (d) asphaltenes, (e) CO₂, (f) C, (g) O, (h) H, (i) N, (j) S.

Table 3

Simulated value and measured value of oil sample at 40 °C.

	Measured value	Simulated value	Relative error, %
Density, kg/m ³	946.83	954.27	0.77
Viscosity, mPa·s	18642.75	19038.56	2.12

the initial heavy oil box and placed at the centre of the cubic box. The side length of the cubic box containing the oil droplet was 80 Å. Finally, the amorphous cell module was utilized to fill the remaining space inside the box with CO₂ molecules, the number of which depended on the density value under the experimental conditions. The entire modelling and MD simulation process is illustrated in Fig. 4.

2.2.2. MD simulation

A series of MD simulations were performed on the final model through the Forcite module. First, an NPT ensemble was used for a 0.5 ns MD simulation to quickly bring the system to the preset pressure. Subsequently, an equilibrium phase MD simulation lasting for 19.5 ns was conducted using the NVT ensemble. The total simulation time was 20 ns, with a time step of 1 fs, and trajectories were saved and output every 1 ps. The Nosé–Hoover–Langevin (NHL) algorithm (Qu et al., 2019) was used to control the simulated temperature, while the Berendsen algorithm (Berendsen et al., 1984) was employed to control the simulated pressure. The Ewald method was employed to handle long-range electrostatic interactions, whereas the Atom-based method was utilized to address short-range vdW interactions

(Tosi, 1964). The quality precision for the entire modelling and MD process was set to fine, with a cut-off distance of 1.2 nm.

3. Results and discussion

3.1. Physical properties of heavy oil after dissolving CO₂

3.1.1. Dissolved gas–oil ratio

The dissolved gas–oil ratio of the heavy oil after dissolving CO₂ was measured under different temperature and pressure conditions, as shown in Fig. 5. The dissolved gas–oil ratio increases with increasing pressure at the same temperature. According to Henry's law, the solubility of a gas in a liquid is directly proportional to the partial pressure of that gas acting on the liquid (Staudinger and Roberts, 1996). Under reservoir conditions, an increase in pressure signifies a greater partial pressure of CO₂ on the oil phase, leading to the dissolution of more CO₂ molecules into the oil. CO₂ is strongly soluble in heavy oil. At a temperature of 373 K, as the pressure increases from 5 to 20 MPa, the dissolved gas–oil ratio increases from 23.41 to 97.46 sm³/m³. In the low-pressure region (5–10 MPa), the internal space of the oil-phase molecules is abundant, which can accommodate more CO₂ molecules, and the dissolved gas–oil ratio increases rapidly with increasing pressure. In the high-pressure zone (15–20 MPa), the internal space of oil-phase molecules decreases, the CO₂ solubility approaches saturation, and the dissolved gas–oil ratio increases slowly. The solubility of CO₂ in the oil phase increases as the system pressure increases, and the amount of CO₂ dissolved per unit volume of oil increases, thereby increasing the dissolved gas–oil ratio. The

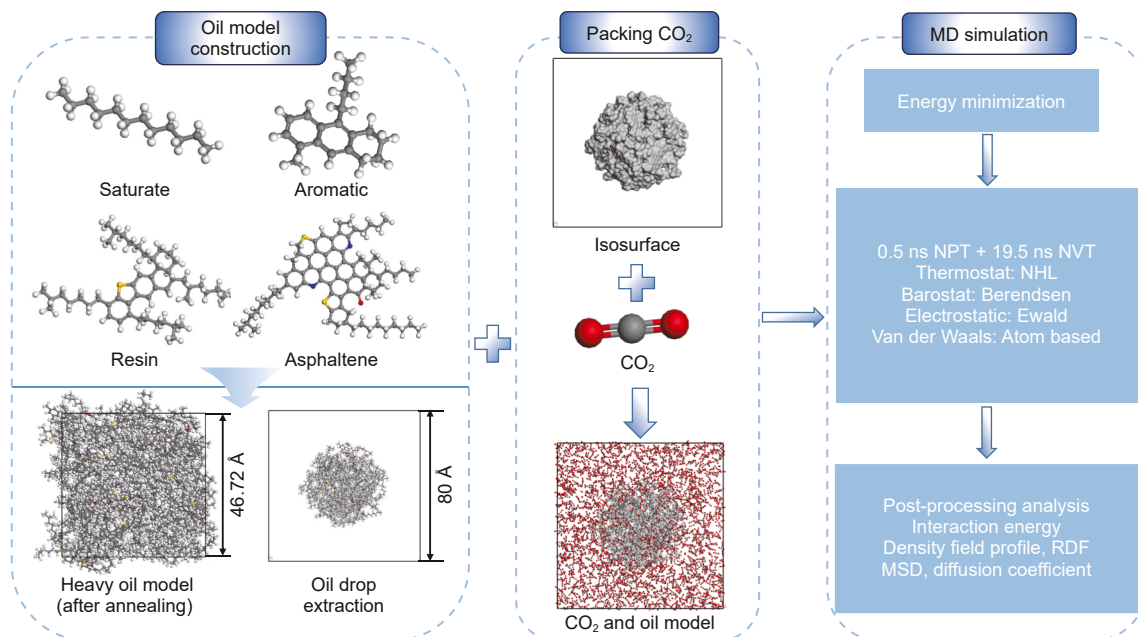


Fig. 4. Flowchart of model construction and MD simulation.

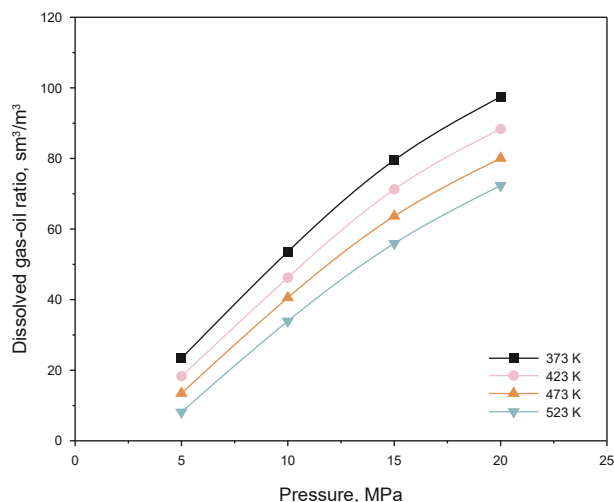


Fig. 5. Relationships between the dissolved gas-oil ratio and saturation pressure at different temperatures.

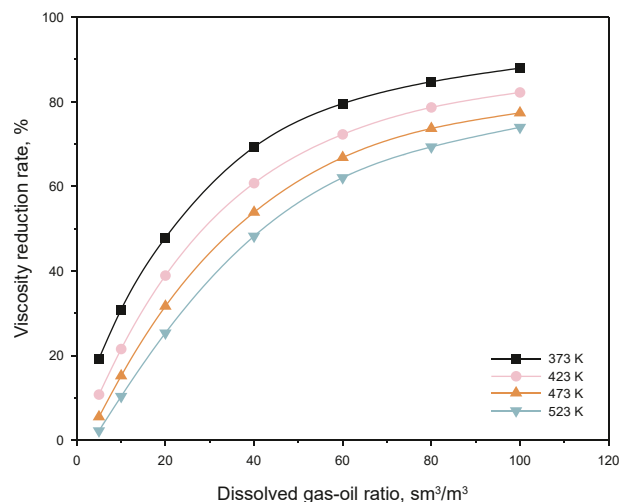


Fig. 6. Relationships between the viscosity reduction rate and dissolved gas-oil ratio at different temperatures.

dissolved gas-oil ratio decreases with increasing temperature under the same pressure. When the pressure is 15 MPa and the temperature increases from 373 to 523 K, the dissolved gas-oil ratio decreases from 79.53 to 55.91 sm^3/m^3 . An increase in temperature disrupts the equilibrium of dissolution, promoting the escape of gas molecules from the liquid phase, leading to a decrease in CO_2 solubility and subsequently a reduction in the dissolved gas-oil ratio.

3.1.2. Viscosity reduction rate

The viscosity of the heavy oil after dissolving CO_2 was tested, and the viscosity reduction rate was calculated. The viscosity reduction rate is expressed by Eq. (1) (Li et al., 2017).

$$Y = \frac{X_1 - X_2}{X_1} \times 100\% \quad (1)$$

where Y is the viscosity reduction rate, %; X_1 is the initial viscosity of the heavy oil, mPa·s; and X_2 is the viscosity of the heavy oil after dissolving CO_2 , mPa·s.

The relationship curve between the viscosity reduction rate and dissolved gas-oil ratio at different temperatures is shown in Fig. 6. As the dissolved gas-oil ratio increases, the viscosity reduction rate rapidly increases but then stabilizes. The dissolved gas-oil ratio increases from 5 to 40 sm^3/m^3 at a temperature of 373 K, and the viscosity reduction rate increases from 19.32% to 69.24%, representing a 49.92% increase. The dissolved gas-oil ratio increases from 40 to 100 sm^3/m^3 , and the viscosity reduction rate increases from 69.24% to 87.87%, an increase of only 18.63%. CO_2 first reacts with the light components in heavy oil under a low dissolved gas-oil ratio. CO_2 molecules gradually permeate into the interior of heavy components and interact with them during the dissolution process. This interaction progressively disrupts the

intermolecular forces between oil molecules, such as vdW forces and hydrogen bonds, leading to the destruction of the aggregation structure among heavy components and a significant decrease in viscosity. The dissolved CO₂ content approaches saturation at high dissolved gas–oil ratios, weakening the interaction between the resin and asphaltene macromolecules. Further increasing the CO₂ concentration cannot continue to disrupt the aggregation structure of these macromolecules. In addition, CO₂ primarily exerts a swelling effect on heavy oil under a high dissolved gas–oil ratio, increasing the average distance between oil molecules and weakening the intermolecular forces between them, thereby slowly reducing the oil viscosity. When the dissolved gas–oil ratio is 80 sm³/m³ and as the temperature increases from 373 to 523 K, the viscosity reduction rate decreases from 84.65% to 69.29%. An increase in temperature significantly reduces oil viscosity, while the viscosity changes after dissolving CO₂.

3.1.3. Volume factor

The relationship curve between the volume factor and the dissolved gas–oil ratio after heavy oil dissolves CO₂ at different temperatures is shown in Fig. 7. The experimental results indicate that the volume of heavy oil significantly expands after dissolving CO₂. After expansion, the remaining oil can effectively overcome the constraints of the formation and rock surface, thereby transforming into movable oil, reducing the residual oil saturation, and increasing the recovery rate of crude oil. The volume factor of heavy oil after dissolving CO₂ increases linearly with increasing dissolved gas–oil ratio. The dissolved gas–oil ratio increases from 5 to 100 sm³/m³ at 373 K, and the volume factor increases from 1.022 to 1.288. Previous studies have shown that the volume factor of light oil after dissolving CO₂ can increase to more than twice the initial oil volume (Welker, 1963). Compared with that of light oil, the volume factor of heavy oil after dissolving CO₂ at 373 K changed slightly and was only 1.26 times the original value. At the same dissolved gas–oil ratio, the volume factor increases with increasing temperature. When the dissolved gas–oil ratio is 80 sm³/m³ and the temperature increases from 373 to 523 K, the volume factor increases from 1.232 to 1.306. An increase in temperature causes the volume of heavy oil to expand in the case of insoluble CO₂, and the thermal motion of molecules intensifies. The dissolved CO₂ molecules occupy the space of the heavy oil molecules, further increasing the volume of the heavy oil after CO₂

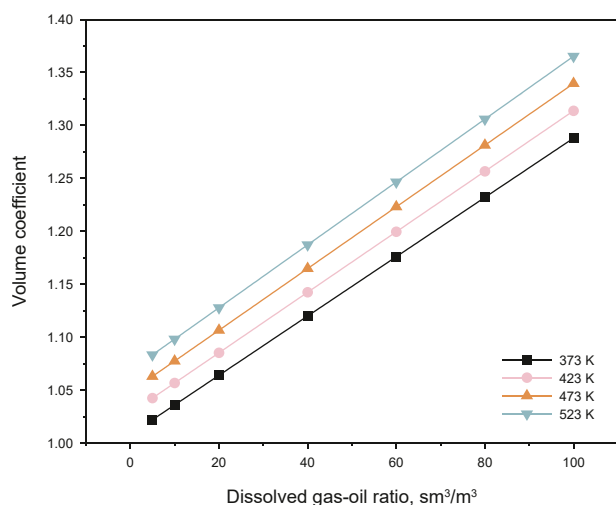


Fig. 7. Relationships between the volume factor and dissolved gas–oil ratio at different temperatures.

is dissolved. In addition, the increase in temperature leads to an increase in the distance between heavy oil molecules, weakening the intermolecular forces. Dissolved CO₂ molecules are more likely to push away the surrounding oil molecules and occupy a larger space, resulting in an increase in the volume expansion per unit of dissolved CO₂ in heavy oil.

3.2. MD simulation of the dissolution and diffusion of heavy oil in CO₂

3.2.1. The process of heavy oil dissolution and the distribution of SARA

During the thermal-composite development process of heavy oil, the injected CO₂ is in a supercritical state under high-temperature and high-pressure conditions, and its strong dissolving ability significantly affects the properties and morphology of heavy oil. In this section, the MD method is employed to simulate the diffusion and dissolution process of heavy oil in CO₂ under different temperatures and pressures. To better observe the morphology of the heavy oil clusters at different stages, specifically the motion state of the SARA molecules, Fig. 8 displays images from the MD simulations at 0, 5, 10, 15 and 20 ns. A snapshot of the diffusion and dissolution process of heavy oil in CO₂ at 373–523 K and 20 MPa is shown in Fig. 8(a).

Taking 373 K as an example, at a dissolution time of 0 ns, the initial model of the research system consists of an oil droplet cluster at the centre of the box, surrounded by CO₂. The SARA molecules and CO₂ molecules are in a separated state at this moment. The CO₂ molecules are relatively concentrated and evenly distributed, while the SARA molecules are concentrated in a smaller area, indicating that dissolution has not yet occurred. With a dissolution time of 5 ns, CO₂ strongly interacts with saturates and aromatic molecules, causing a large amount of saturates to detach from the droplets and diffuse and dissolve into the CO₂ phase, ultimately diffusing to the box boundary. At this point, the volume of the oil droplet gradually expands. The interaction between aromatics and CO₂ is weaker compared to saturates and CO₂, some aromatics diffuse into CO₂, and the volume of oil droplets continues to increase. At this stage, due to the π - π interaction, resin and asphaltene molecules have strong intermolecular forces and remain in a tightly connected cluster state (Rashid et al., 2019). When the dissolution time is 10 ns, the interaction between aromatic molecules and CO₂ molecules reaches its maximum, and most saturate and aromatic molecules diffuse to the boundary of the box. The diffusion of light components increases the contact area between CO₂ molecules and heavy component molecules. CO₂ permeates into the heavy molecular weight, enhancing the interaction with the heavy molecular weight. At this point, a small portion of resin molecules detach from the heavy oil clusters and diffuse and dissolve into CO₂. The dissolution time is 15–20 ns, and the dissolution diffusion of the resins reaches equilibrium, while some loosely connected heavy component aggregates still exist. At this point, the volume of the oil droplet reaches the maximum and is in a loose state. Asphaltene molecules have strong hydrogen bonds and π - π interactions, and the cohesive energy of heavy oil clusters is relatively high. In addition, CO₂ has limited solvation ability for asphaltenes, and its interaction with asphaltenes is mainly concentrated in the alkyl side chains, outer resin, and aromatic components, making it difficult to effectively compete and disrupt the aromatic stacking and polar network structure of the core (Lv et al., 2023).

As the temperature increases, the number of CO₂ molecules in the box decreases, but the diffusion and dissolution of the heavy oil droplet become more pronounced. A significant expansion of the oil droplet volume can be observed compared with that at

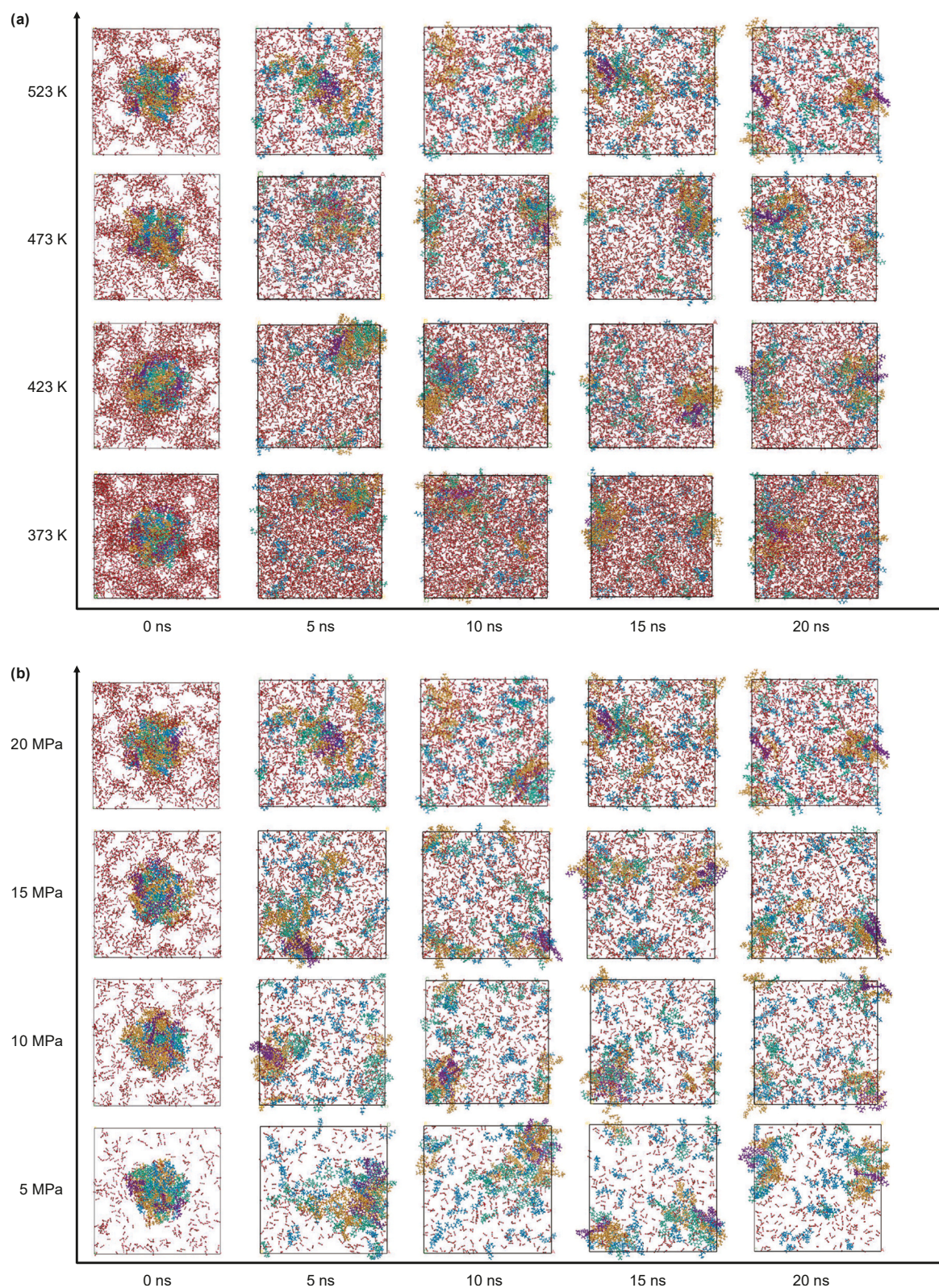


Fig. 8. Diffusion and dissolution processes of heavy oil in supercritical CO₂ under different pressure and temperature conditions. (a) 373–523 K, 20 MPa; (b) 5–20 MPa, 523 K.

373 K. Under the strong interaction of CO₂, the saturate and aromatic molecules inside the oil droplet begin to expand and straighten from the bent state. The mutual unwrapping between these light components can even lead to an increase in the volume

of oil droplets, making it easier for CO₂ molecules to enter the interior of the cluster and accelerating the dissolution of light components (Li et al., 2023). Some saturate and aromatic molecules are completely detached from the oil droplet and move to the

box boundary at 5 ns. At this time, CO₂ has permeated into the cluster and interacts with the resin and asphaltene macromolecules, causing the macromolecules to detach from the cluster. When the temperature is 523 and 573 K, the initial dissolution and diffusion of oil droplets are similar to 373 and 423 K, but the dissolution rate of light components is accelerated. Most light component molecules rapidly diffuse and dissolve into the CO₂ phase in the initial stage, while some resins and asphaltenes remain in the clusters. Dissolve for 10 ns, some resin and asphaltene molecules separate from the oil droplets and gradually diffuse towards the edge of the box, while the remaining large molecular clusters move towards the edge of the box. High temperature increases the thermal motion and solubility of CO₂ molecules compared with low temperature, allowing them to penetrate more effectively between resin and asphaltene molecules, and interact with aromatic ring structures and alkyl chain parts (Yang et al., 2024). In addition, the π - π interactions and hydrogen bonds between resin and asphaltene molecules are weakened at high temperatures, thereby reducing the stability of the aggregates. The originally tight structure is disrupted, and CO₂ gradually dissolves the internal molecules, leading to the dissociation of large molecular clusters.

A snapshot of the diffusion and dissolution process of the heavy oil cluster in CO₂ at 523 K and 5–20 MPa is shown in Fig. 8(b). The density of CO₂ is relatively low at 5 MPa, and its ability to dissolve the heavy oil cluster is the weakest. Although CO₂ molecules still permeate into the oil droplet, the dissolution rate of SARA molecules is the slowest, and the structure of the oil droplet cluster remains relatively tight. The solubility of CO₂ is enhanced at 10 MPa. CO₂ molecules still effectively permeate into the aggregation region of resin and asphaltene molecules in the later stage, leading to an increased depolymerization rate of the oil droplet cluster (Li et al., 2019). The density of CO₂ is relatively high at 15 MPa, allowing CO₂ molecules to interact more effectively with the resin and asphaltene molecules in heavy oil. The diffusion and dissolution ability of the heavy oil cluster in CO₂ increases with increasing pressure compared to 5 MPa. The diffusion and dissolution rate of SARA molecules increase significantly.

MD simulations under different temperature and pressure conditions indicate that the SARA molecules that have not been fully dissolved form a loose cluster and undergo random motion within the simulation box. In addition, dissolved resin molecules tend to entangle and aggregate with light component molecules to form small clusters (Zhu et al., 2021). Temperature has a significant effect on the diffusion and dissolution of heavy oil in CO₂. Although an increase in temperature reduces the density of CO₂, it can significantly decrease the viscosity of heavy oil and the intermolecular interaction forces between large molecules. The thermodynamic driving force for the dissolution of resin and asphaltene molecules is insufficient under low-temperature conditions. Although CO₂ has good solubility, the interaction between it and the heavy component molecules is weak, which leads to incomplete depolymerization of the resin and asphaltene molecules. Additionally, low temperature reduces the collision frequency and reaction rate between macromolecules and CO₂ molecules, preventing CO₂ molecules from rapidly permeating the interior of macromolecular clusters. Consequently, they can only exert a stretching effect on the outside, promoting the local dissolution of macromolecular molecules rather than complete depolymerization. Compared with temperature, pressure has a weaker effect on the diffusion and dissolution of heavy oil in CO₂. The inherent properties of heavy oil, such as viscosity and density, are more sensitive to temperature. High temperatures significantly reduce the viscosity and density of heavy oil and provide sufficient energy to overcome the interaction forces between the resin and

asphaltene molecules (Jin et al., 2022; Luo and Gu, 2007; Ghanavati et al., 2013).

3.2.2. Density field profiles of oil and CO₂

The diffusion and dissolution of heavy oil in CO₂ can be better understood by studying the density distribution curves of the heavy oil cluster and CO₂. The mass density distribution curves of heavy oil and CO₂ at different temperatures and pressures are shown in Figs. 9 and 10, respectively. The trends of change under various temperature and pressure conditions are similar. The heavy oil cluster is in the range of 17.5–62.5 Å, while the CO₂ phase surrounding the heavy oil clusters is in the ranges of 0–17.5 Å and 62.5–80 Å. The oil phase density decreases in region I and increases in region II. The movement of CO₂ into the heavy oil molecules leads to the increase of CO₂ density in region I. Resin molecules further diffuse and dissolve from the heavy oil clusters at the last moment of 20 ns, and the oil phase density in region I reaches the minimum, while that in region II reaches the maximum. The undissolved heavy oil clusters move randomly in the box, resulting in the shift of peak density of oil phase. Currently, the density of CO₂ is evenly distributed in the whole box, indicating that a large amount of CO₂ has penetrated the oil phase. The penetrated CO₂ molecules occupy the interstitial spaces within the heavy oil clusters, which increases the free volume of system and effectively screens the strong short-range vdW attractions between the asphaltene molecules, thereby inducing significant volume swelling and structural loosening (Dastjerdi et al., 2023; Lu et al., 2022; Wang et al., 2022).

Taking 373 K as an example, when the initial time is 0 ns, the heavy oil molecules have not expanded to CO₂ phase, and the oil phase density in zone II is 0. The oil phase density in zone I is the highest, and the CO₂ density in zone II is slightly higher than that in zone I, the tight oil mass in zone I occupies part of the space and reduces the CO₂ density. Light components such as saturated hydrocarbons and aromatic hydrocarbons have been uniformly diffused into CO₂ in 10 ns. The oil phase density decreases in zone I and increases in zone II. The movement of CO₂ into the heavy oil molecules leads to the increase of CO₂ density in zone I. at the last moment of 20 ns, resin molecules further diffuse and dissolve from the heavy oil clusters, and the oil phase density in zone I reaches the minimum, while that in zone II reaches the maximum. The undissolved heavy oil clusters move randomly in the box, resulting in the shift of peak density of oil phase. Currently, the density of CO₂ is evenly distributed in the whole box, indicating that a large amount of CO₂ has penetrated the oil phase.

As the temperature increases, the densities of both heavy oil and CO₂ decrease, and the density of heavy oil in zone I decreases more obviously. As shown in Fig. 7, higher temperature promotes diffusion and dissolution of light components, which leave the cluster and migrate towards the box boundaries, leading to a marked increase in oil density in region II. The elevated temperature imparts higher kinetic energy to the light component molecules, enabling them to overcome the potential energy barriers associated with the dense heavy component molecules. Consequently, the dense heavy oil cluster expands, causing the SARA molecules within the oil phase to undergo thermal migration and rearrangement (Guo et al., 2022). In contrast, lower pressure reduces CO₂ density and its ability to penetrate the heavy-oil cluster, so the diffusion and dissolution of SARA are suppressed. Most of the heavy component molecules are still concentrated in the centre of region I, and the density of oil and carbon dioxide changes little.

3.2.3. The interaction energy of CO₂ molecules with SARA molecules

In this section, the interaction energies of CO₂ and SARA molecules are calculated at different temperatures and pressures, and

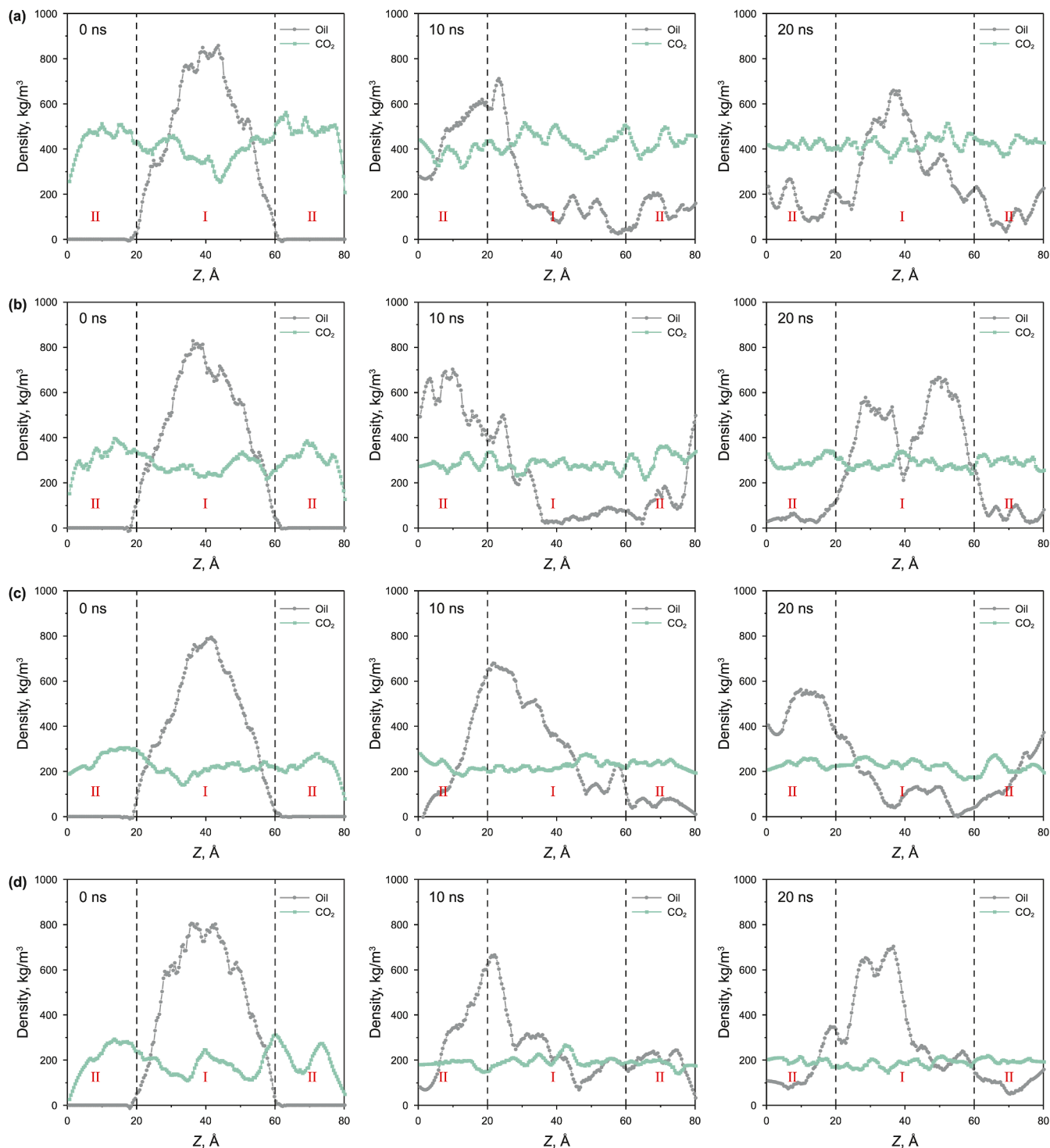


Fig. 9. Density profiles of CO₂ and oil at different temperatures. (a) 373 K, (b) 423 K, (c) 473 K, (d) 523 K.

the diffusion and dissolution mechanisms of heavy oil molecules in CO₂ are further analysed from the perspective of intermolecular interactions. The interaction energy can reflect the association strength of CO₂ and SARA (Li et al., 2022). The higher the absolute value of the interaction energy is, the greater the degree of intermolecular interaction and attraction. The equation for calculating the interaction energy between CO₂ and SARA molecules is as follows:

$$E_{\text{Inter}} = E_{\text{Total}} - (E_{\text{CO}_2} + E_{\text{SARA}}) \quad (2)$$

where E_{Inter} is the interaction energy between CO₂ and SARA molecules, kcal/mol; E_{Total} is the total energy between CO₂ and SARA molecules, kcal/mol; and E_{CO_2} and E_{SARA} are the energies of CO₂ molecules and SARA molecules, respectively, kcal/mol.

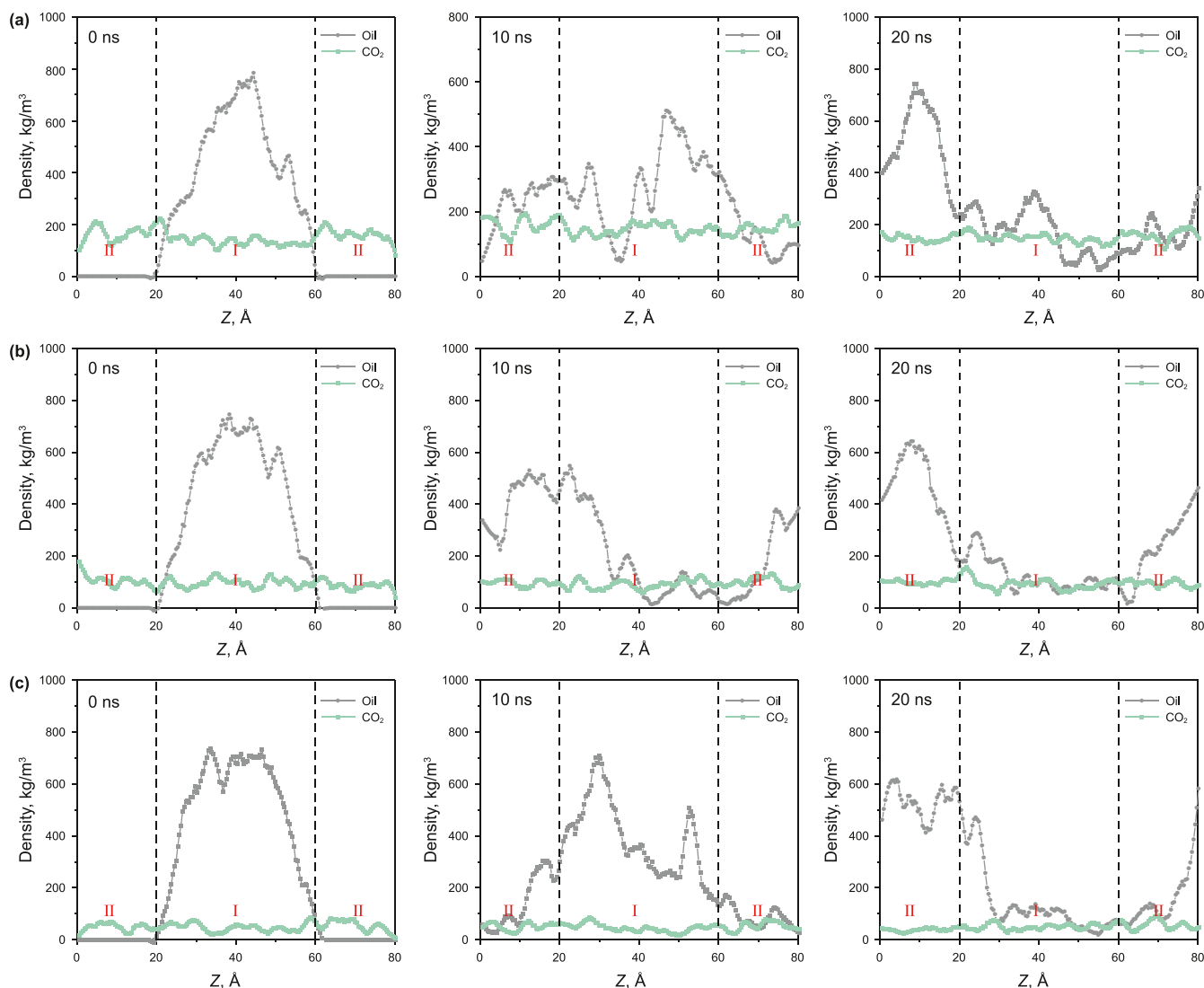


Fig. 10. Density profiles of CO₂ and oil at different pressures. (a) 15 MPa, (b) 10 MPa, (c) 5 MPa.

The time evolution of the interaction energy between CO₂ and each SARA fraction at different temperatures and pressures is shown in Figs. 11 and 12. For all systems, the interaction energy is negative over the whole simulation, indicating attractive interactions. The absolute value of interaction energy initially increases with time and then reaches a plateau after equilibration. The equilibration time depends on the component: CO₂–saturates and CO₂–aromatics interactions stabilize after about 2 ns, CO₂–resin after about 5 ns, and CO₂–asphaltene after about 10 ns, reflecting the easier penetration of CO₂ into low-molecular-weight saturates and aromatics compared with the more strongly associated resins and asphaltenes. Resins and asphaltenes with high molecular weight have strong intermolecular forces, and it takes longer for CO₂ to permeate into the molecules. The temporal difference is attributed to different steric hindrances and molecular configurations. Unlike the flexible aliphatic chain of saturates fraction, asphaltene fraction has dense polyaromatic nuclei and is stabilized by a strong π – π stacking network, which creates an important potential energy barrier for CO₂ intercalation, thus delaying the diffusion process.

At equilibrium, the magnitude of the interaction energy follows saturates > aromatics > resins > asphaltenes, consistent with previous work (Lu et al., 2025). CO₂ therefore interacts most strongly with the light components mainly through vdW forces, whereas the strong self-association within resins and asphaltenes aggregates reduces their net interaction with CO₂. The absolute value of the interaction energy decreases with increasing temperature and increases with increasing pressure. The decrease of interaction energy caused by temperature is attributed to the increase of thermal kinetic energy, which destroys the weak vdW gravity and reduces the residence time of CO₂ molecules in the first solvated shell of heavy oil clusters (Lu et al., 2024; Xu and Wang, 2017). On the contrary, the pressure induced interaction can be enhanced due to the reduction of the free volume of the system. The increased pressure forces CO₂ molecules into the pores of the oil phase, thus reducing the average intermolecular distance, thus maximizing the short-range dispersion interaction.

The average interaction energy of CO₂–SARA at 15–20 ns at different temperatures and pressures is shown in Fig. 13. At each

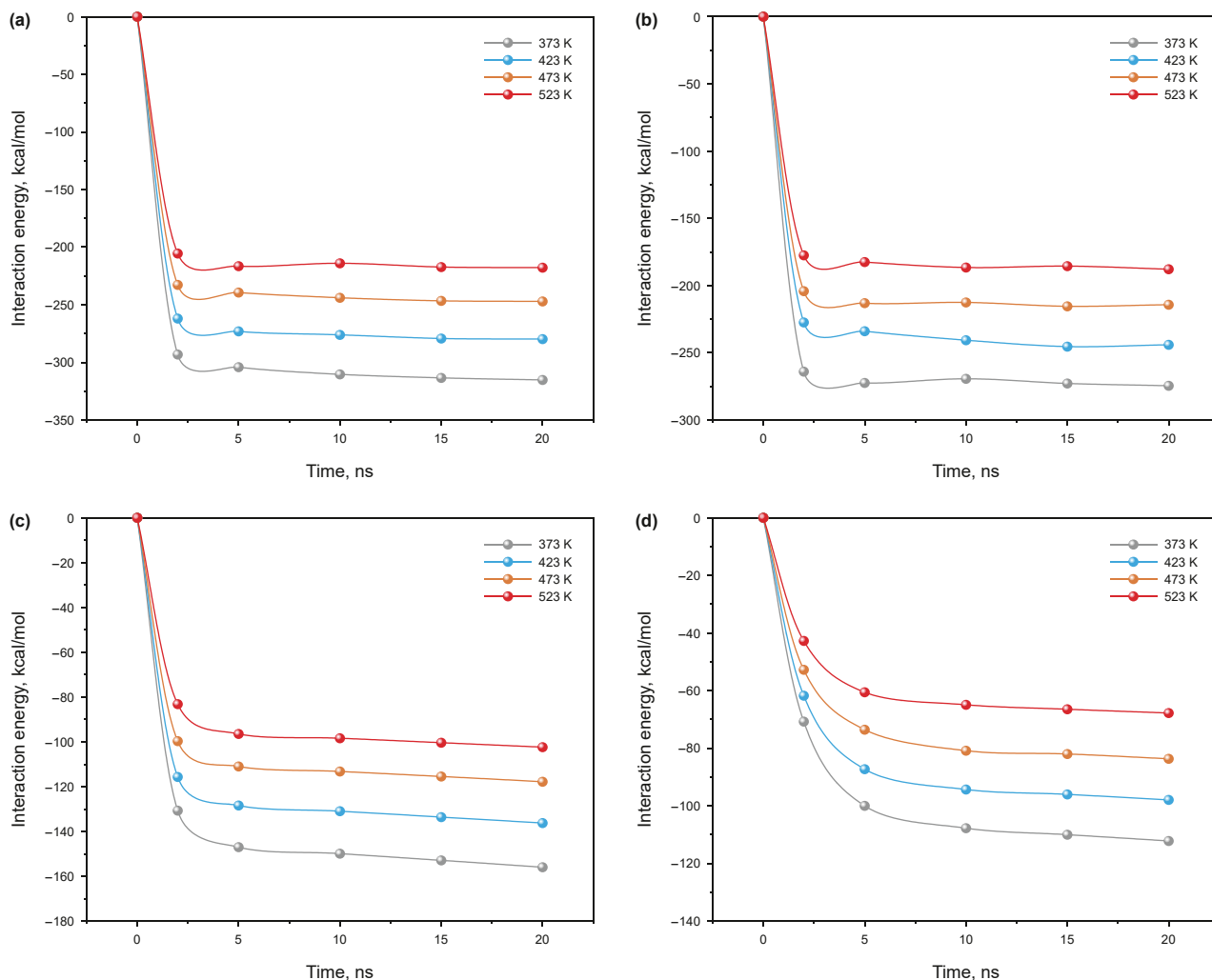


Fig. 11. Variation in the interaction energy of CO₂-SARA with time at different temperatures. (a) CO₂-saturates, (b) CO₂-aromatics, (c) CO₂-resins, (d) CO₂-asphaltenes.

temperature and pressure, the absolute values of the interaction energy between saturates and aromatics and CO₂ are greater than those of the other components, and the absolute value of the interaction energy decreases with increasing temperature and decreasing pressure. When the temperature increases from 523 to 373 K, the interaction energies of SARA and CO₂ range from −217.36 to −315.44 kcal/mol, −187.28 to −274.31 kcal/mol, −102.46 to −155.65 kcal/mol, and −67.79 to −112.21 kcal/mol, respectively. When the pressure increases from 5 to 20 MPa, the absolute values of the interaction energy between SARA and CO₂ range from −143.23 to −217.36 kcal/mol, −128.87 to −187.37 kcal/mol, −75.43 to −102.39 kcal/mol, and −42.69 to −67.44 kcal/mol, respectively. Although the interaction energy between SARA and CO₂ decreases with increasing temperature, the intermolecular force of SARA is greatly reduced, and its flow and diffusion ability are enhanced. An increase in pressure enhances the interaction between CO₂ and SARA molecules and promotes the diffusion and dissolution of SARA molecules.

3.2.4. The RDF of CO₂ molecules with SARA molecules

The distribution of SARA molecules around CO₂ molecules was described by the RDF to better understand the interaction between

CO₂ molecules and SARA molecules. The RDF describes the normalized probability that the target example appears around the reference particle at a certain distance r in a certain system (Hu et al., 2015). The formula for calculating the RDF is as follows (Ahmadi and Chen, 2022):

$$g(r) = \frac{1}{4\pi r^2 \rho dr} \frac{\sum_{j=1}^N \Delta N(r \rightarrow r + \Delta r)}{N} \quad (3)$$

where $g(r)$ is the RDF strength, ρ is the density of target particles in the system, N is the number of target particles in the system, r is the distance between the reference particle and the target particle centroid, and ΔN is the number of target particles from r to $r + \Delta r$ around the reference particle.

The RDF curves of CO₂-SARA under different temperatures and pressures are shown in Figs. 14 and 15. The RDF trends of the CO₂-SARA of each component are essentially similar under different temperatures and pressures, and the peak value of the curve is in the range of 0.5–0.6 nm. Previous studies have shown that the RDF peaks of heavy oil components in the range of 0.4–0.6 nm are caused mainly by intermolecular vdW interactions and π - π interactions (Wang et al., 2024). In particular, the peak intensity is

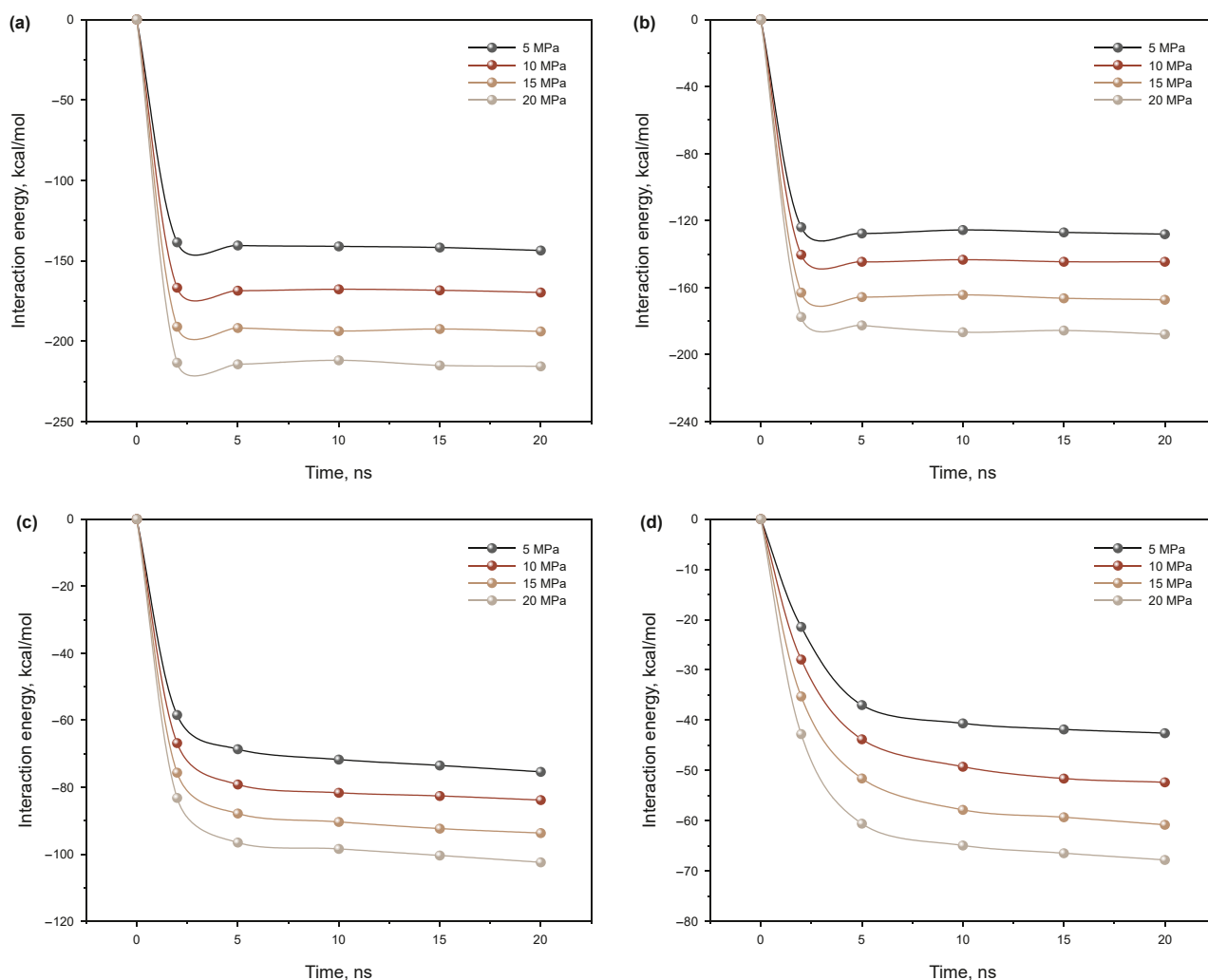


Fig. 12. Variation in the interaction energy of CO₂-SARA with time at different pressures. (a) CO₂-saturates, (b) CO₂-aromatics, (c) CO₂-resins, (d) CO₂-asphaltenes.

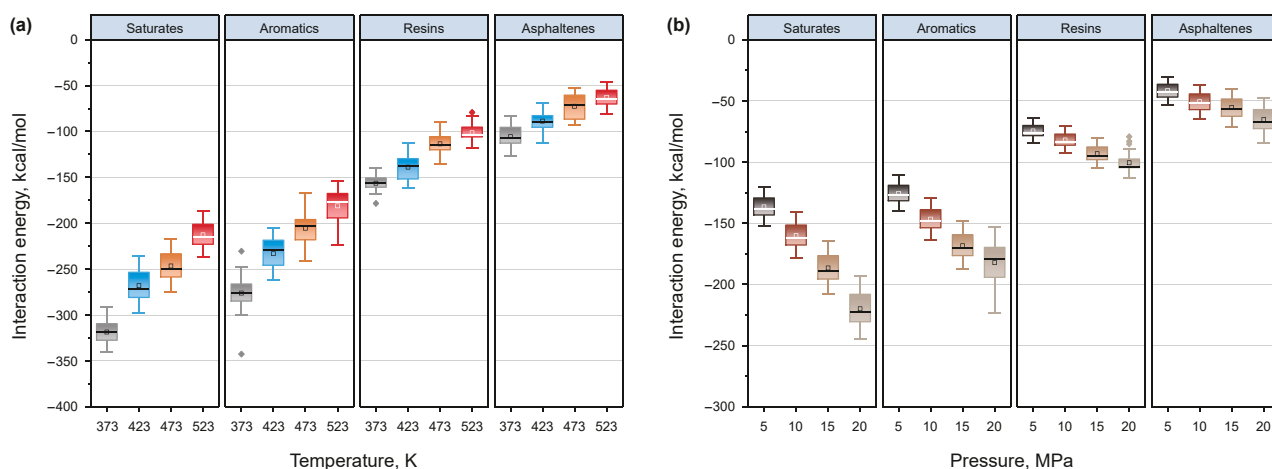


Fig. 13. The average interaction energies of SARA under different temperatures and pressures at 15–20 ns. (a) Interaction energies at different temperatures, (b) interaction energies at different pressures.

positively correlated with temperature and pressure. Although high temperature usually reduces the bulk fluid density, the increase in peak height observed here indicates an increase in the local concentration of SARA molecules around CO₂. From the

perspective of dynamics, high temperature provides the kinetic energy required to destroy the self-accumulation of heavy oil. The destruction increases the volume of SARA molecules, making CO₂ penetrate more effectively and form a denser coordination shell.

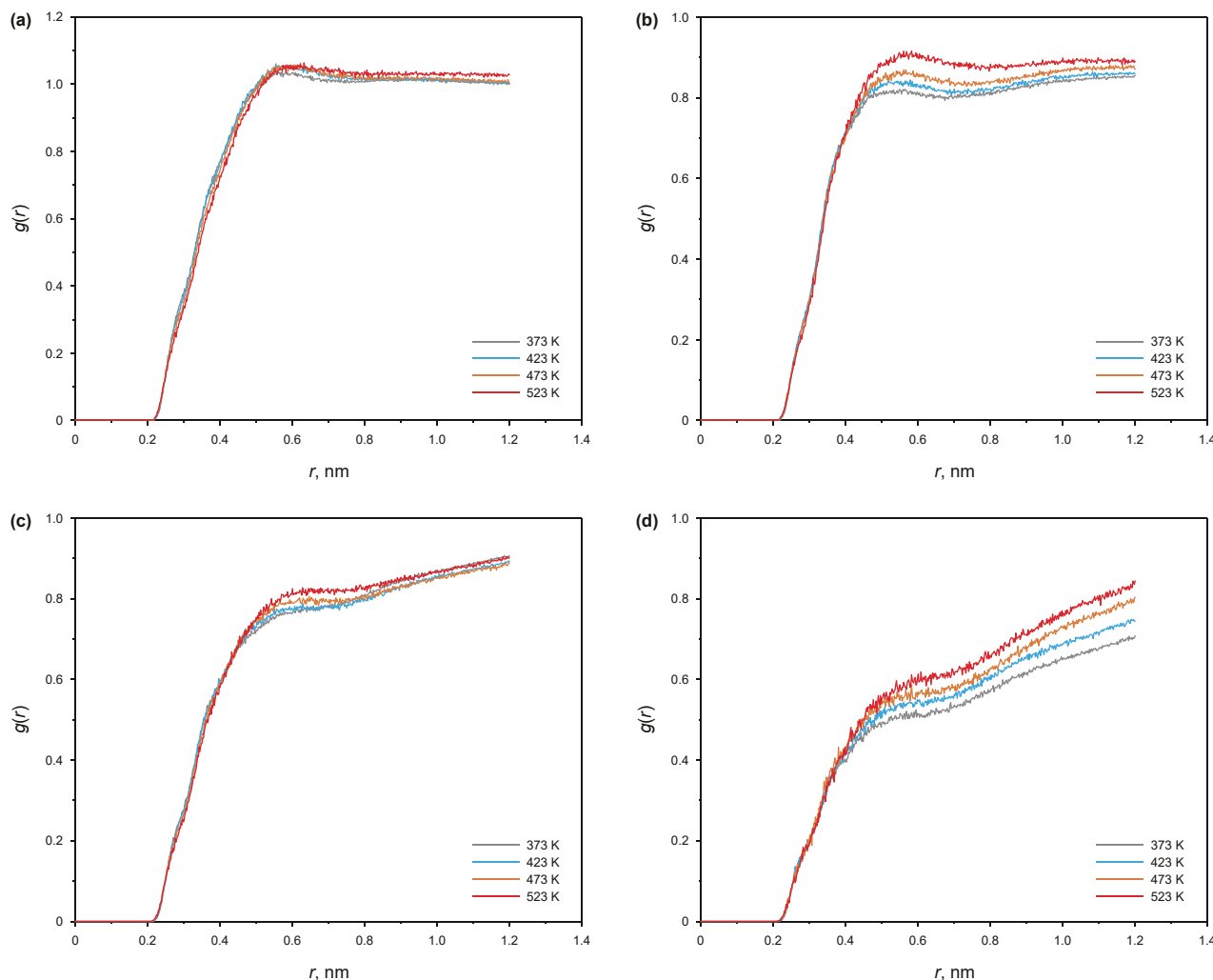


Fig. 14. The RDF of SARA with time at different temperatures. (a) CO₂-saturates, (b) CO₂-aromatics, (c) CO₂-resins, (d) CO₂-asphaltenes.

Similarly, the pressure-induced peak enhancement confirmed that higher CO₂ density promoted the solvation of heavy components by increasing the collision frequency and reducing the average free path (Long et al., 2021).

The contribution of the short-range E_{vdW} and long-range E_{elect} to the CO₂-SARA molecular interaction energy is analysed in Table 4 to understand the influence of intermolecular interactions on the RDF peaks. For the light components, the interaction energy is dominated by E_{vdW} , as both CO₂ and the saturate/aromatic fractions are essentially nonpolar, and the mutual interaction is therefore governed primarily by dispersion forces. For resins and asphaltenes, E_{vdW} and E_{elect} make comparable contributions, and the relative importance of E_{elect} is increased at higher temperatures, indicating that electrostatic interactions between CO₂ and the polar moieties of these macromolecules are strengthened. When the pressure is decreased, the CO₂ density is reduced and both contributions are weakened, resulting in smaller overall interaction energies. Consistent with the RDF analysis, the peaks for CO₂ and light components are controlled predominantly by short-range E_{vdW} , whereas those for CO₂ and heavy component are influenced by

both E_{vdW} and E_{elect} . The gradual increase of the CO₂-resin and asphaltene RDF beyond 0.8 nm indicates that appreciable electrostatic attraction is still exerted at larger distance.

3.2.5. The MSD and diffusion coefficient of heavy oil in CO₂

The MSD of the SARA molecule can reflect the diffusion and dissolution behaviour of heavy oil clusters. MSD can be used to derive the estimated values of motion parameters, such as the diffusion coefficient of free diffusing particles. The calculation equation for the MSD is as follows (Einstein, 1905):

$$\text{MSD}(\Delta t) = \frac{1}{\tau - \Delta t} \int_0^{\tau - \Delta t} [r(t - \Delta t) - r(t)]^2 dt$$

$$= \langle [r(t - \Delta t) - r(t)]^2 \rangle \quad (4)$$

where MSD is the mean square displacement of the particle at time interval Δt , Å²; τ is the total simulation time, s; Δt is the time interval; $r(t)$ is the position vector of the particle at time t ; and

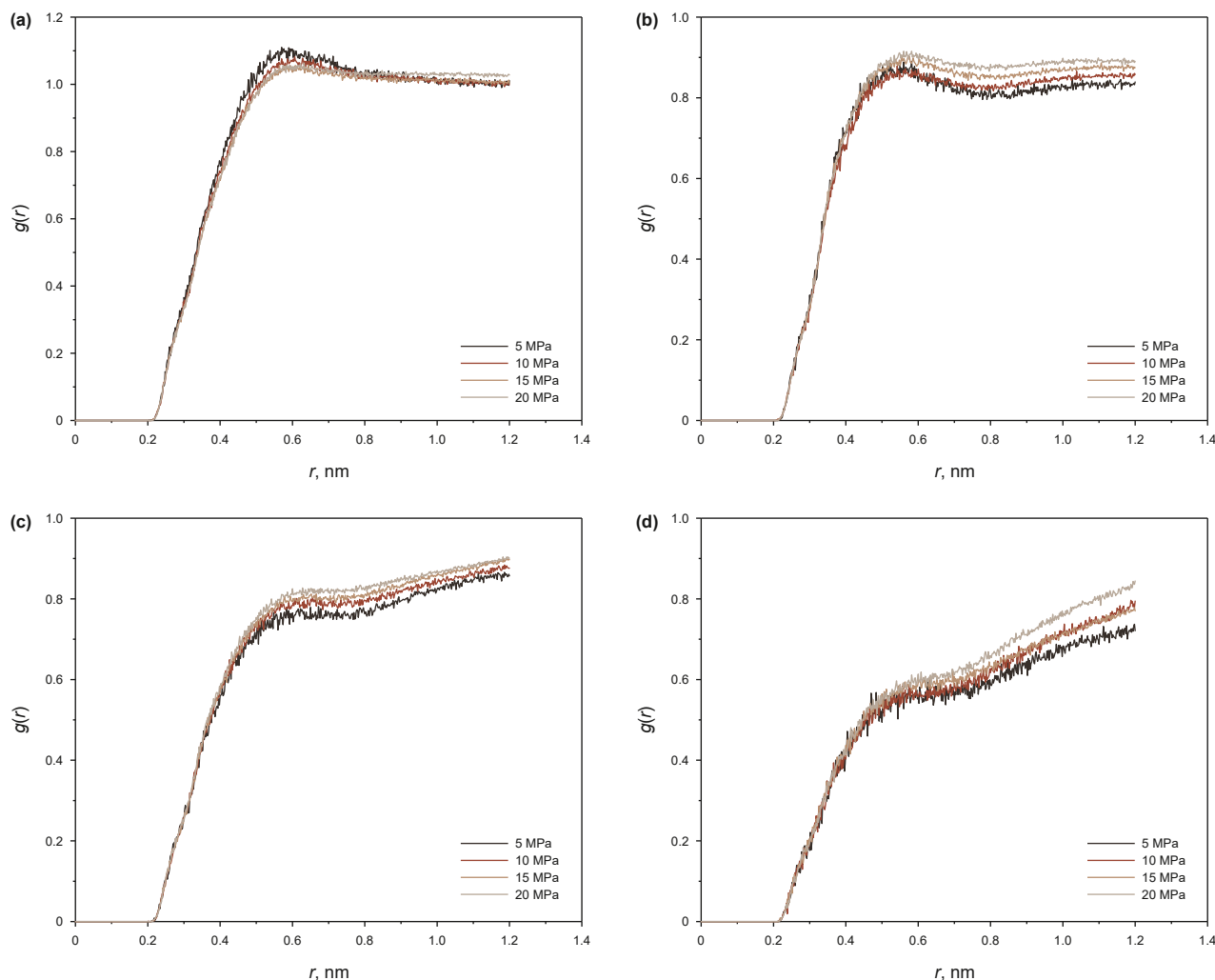


Fig. 15. Variation in the RDF of SARA with time at different pressures. (a) CO₂-saturates, (b) CO₂-aromatics, (c) CO₂-resins, (d) CO₂-asphaltenes.

Table 4

The contributions of different energies to the interaction energy of CO₂-SARA under different temperatures and pressures.

Temperature/Pressure	Saturates		Aromatics		Resins		Asphaltenes	
	E _{vdW} , kcal/mol	E _{elect} , kcal/mol	E _{vdW} , kcal/mol	E _{elect} , kcal/mol	E _{vdW} , kcal/mol	E _{elect} , kcal/mol	E _{vdW} , kcal/mol	E _{elect} , kcal/mol
373 K	−219.46	−95.98	−186.54	−87.77	−83.95	−71.70	−61.34	−50.87
423 K	−215.22	−53.78	−178.36	−55.64	−75.39	−63.61	−53.20	−35.80
473 K	−196.28	−51.72	−158.84	−47.16	−54.67	−58.33	−43.41	−28.59
523 K	−176.50	−40.86	−139.36	−47.92	−40.85	−61.61	−41.36	−26.43
15 MPa	−165.59	−21.41	−139.78	−29.22	−24.68	−68.32	−34.07	−23.93
10 MPa	−155.82	−6.18	−118.09	−28.91	−1.38	−81.62	−23.39	−27.61
5 MPa	−120.44	−22.79	−96.37	−32.50	−27.13	−48.30	−19.36	−23.33

$r(t-\Delta t)$ is the position vector of the particle at time $t-\Delta t$. The diffusion coefficient of SARA can be determined by the Einstein equation (Ahmadi et al., 2020).

$$D = \frac{1}{6} \lim_{\Delta t \rightarrow \infty} \frac{dMSD}{d\Delta t} \quad (5)$$

In this section, the MSD curve of the 20 ns is selected for analysis. The MSD results of the SARA molecules at different

temperatures and pressures are shown in Figs. 16 and 17. The fit is restricted to the 5–15 ns time interval for all SARA components, avoiding the initial non-diffusive state and the late-time high-noise region. Saturates and aromatics, with simpler molecular structures, diffuse rapidly and uniformly in CO₂, showing better linearity and larger slopes. The behaviour reflects their favorable interaction with CO₂, which facilitates diffusion. In contrast, resins and asphaltenes exhibit slower and uneven diffusion due to their

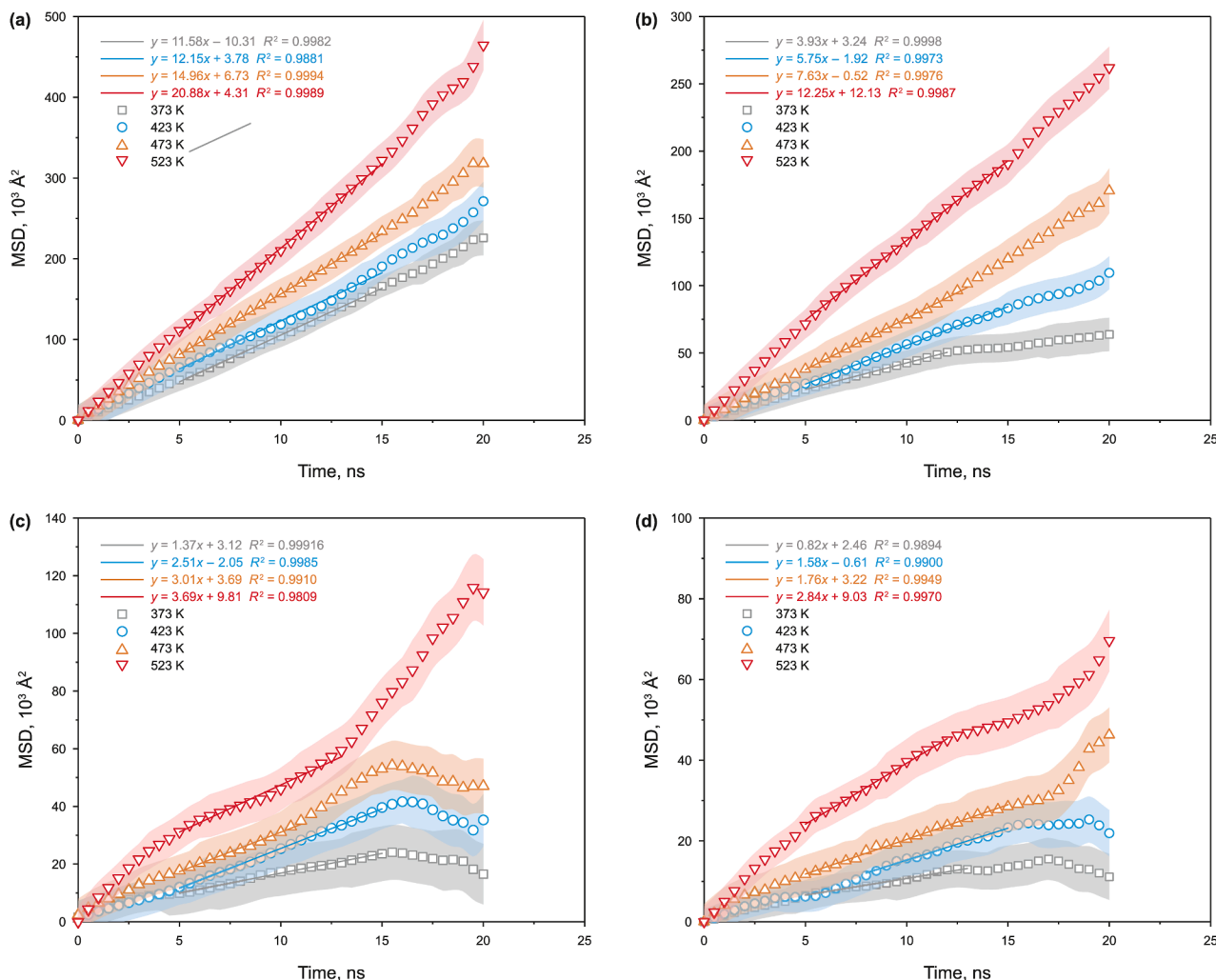


Fig. 16. Variation in the MSD of SARA with time at different temperatures. (a) Saturates, (b) aromatics, (c) resins, (d) asphaltenes.

complex molecular structures, strong self-association, and cohesive forces, which hinder CO₂ penetration and diffusion.

The MSD slope for all SARA components increases with temperature and pressure. Higher temperatures and pressures reduce the self-association of resins and asphaltenes, allowing CO₂ to penetrate more effectively, weaken molecular cohesion, and enhance diffusion. In the later stage of dissolution (15–20 ns), the MSD curves deviate from linearity due to boundary effects, as the residual droplet reaches a more stable state, slowing down further diffusion (Ahmadi and Chen, 2022). The diffusion coefficients of SARA molecules are calculated in CO₂ at different temperatures and pressures by Eq. (5), and the results are shown in Fig. 18. For all conditions, the diffusion ability follows the order saturates > aromatics > resins > asphaltenes, and the coefficients increase systematically with temperature and, to a lesser extent, with pressure. The diffusion rate of SARA molecules is fastest at 523 K and 20 MPa, with diffusion coefficients of 34.8×10^{-9} , 20.4×10^{-9} , 6.2×10^{-9} , and 4.7×10^{-9} m²/s, respectively. Higher temperature and pressure enhance the CO₂–SARA interactions and facilitate the detachment of SARA molecules from the heavy-oil aggregate, thereby promoting their diffusion into the CO₂ phase.

CO₂ injection can not only increase the fluidity of heavy oil but also reduce steam energy consumption and carbon emissions during the process of CO₂-assisted steam thermal recovery. MD simulations can analyse the diffusion and dissolution behaviour of heavy oil in CO₂ at the molecular level, providing a theoretical basis for the optimization of the injection temperature, pressure, and other parameters during actual reservoir development. The results of the diffusion and dissolution of heavy oil in CO₂ at different temperatures and pressures reveal the microscopic interactions between CO₂ and heavy oil and their potential impact on thermal recovery efficiency. Moreover, the alteration in the interaction energy, RDF, and diffusion coefficient of SARA molecules reflects the dissolution characteristics of different components in a supercritical CO₂ environment, especially the diffusion behaviour of resins and asphaltenes under high temperature and high pressure. These results provide theoretical guidance for the application of CO₂-EOR technology, enable the application of CCUS technology in heavy oil thermal recovery, and promote the transformation of the oil and gas industry towards low-carbon and sustainable development.

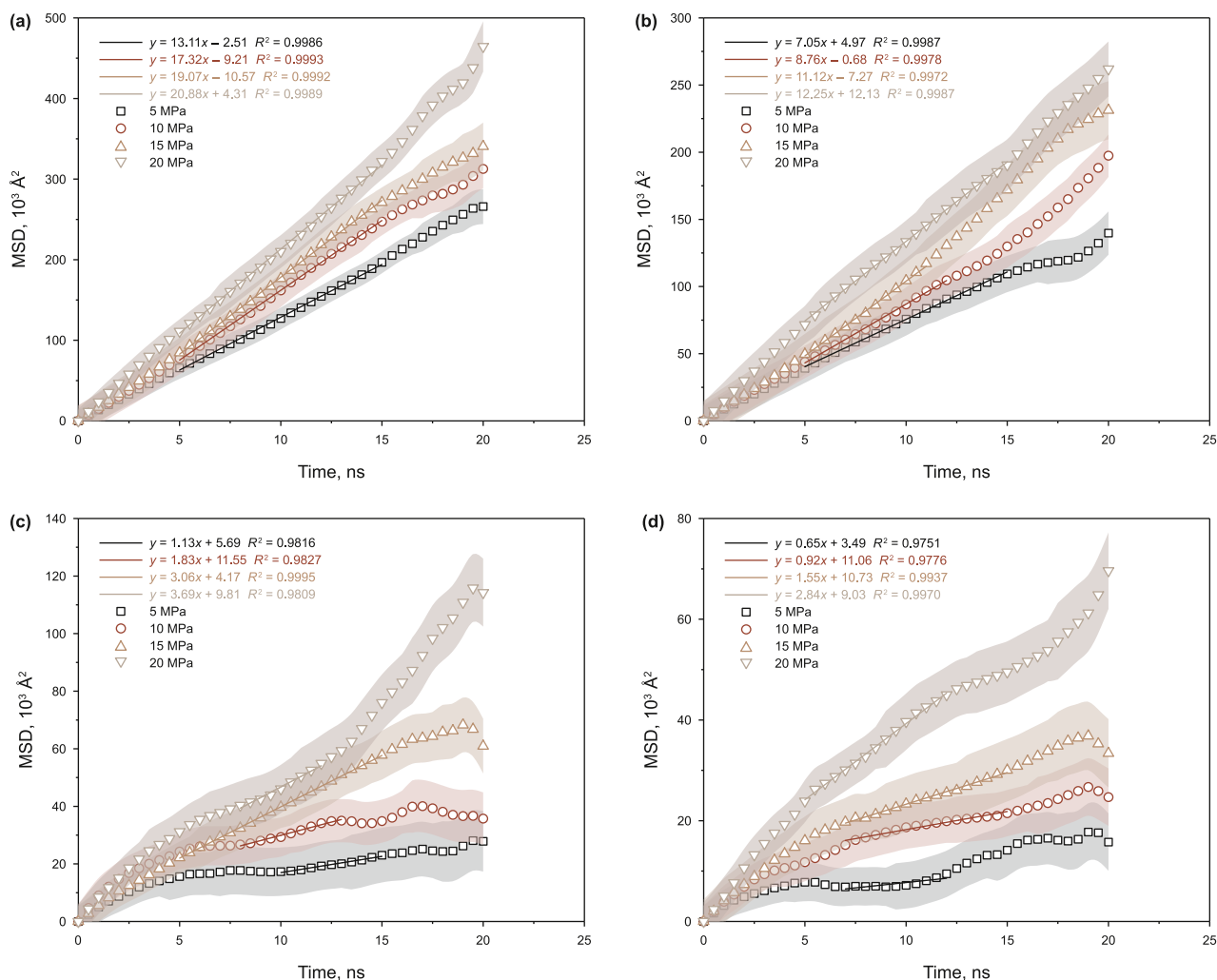


Fig. 17. Variation in the MSD of SARA with time at different pressures. (a) Saturates, (b) aromatics, (c) resins, (d) asphaltenes.

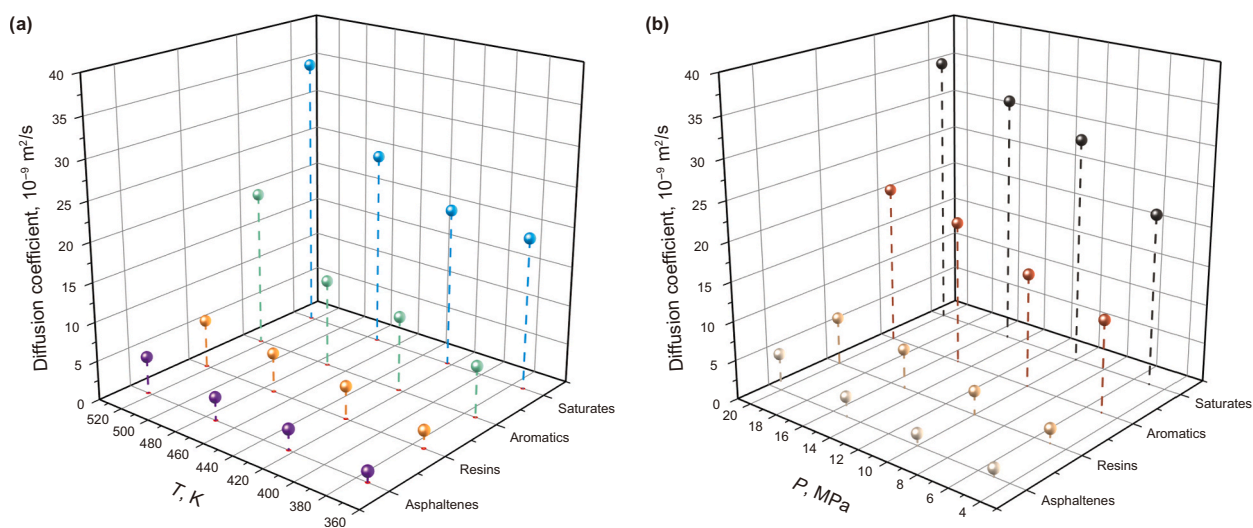


Fig. 18. Diffusion coefficient of SARA at different temperatures and pressures. (a) Diffusion coefficients at different temperatures, (b) diffusion coefficients at different pressures.

4. Conclusion

In this paper, tests were conducted on the high-pressure physical properties of heavy oil after dissolving CO₂, and the diffusion and dissolution behaviours of heavy oil in CO₂ under high-temperature and high-pressure conditions were investigated through MD simulations. The main results are as follows:

- (1) The dissolved gas–oil ratio increased gradually with increasing CO₂ pressure. The dissolution expansion and extraction of CO₂ effectively reduced the viscosity of the heavy oil and increased its volume factor after dissolution of CO₂. The viscosity of the heavy oil decreased and the volume factor of the heavy oil increased with increasing temperature under the same dissolved gas–oil ratio. The dissolved gas–oil ratio was close to 100 sm³/m³, and the viscosity reduction rate was as high as 90% at 373 K.
- (2) MD snapshots over 0–20 ns reveal a sequential dissolution process in which light components such as saturates and aromatics first unwind, straighten, and detach from the droplet to rapidly diffuse into the CO₂ phase, while resins and asphaltenes dissolve more slowly and remain partially aggregated. This preferential extraction leads to a progressive decrease in oil-phase density in the central region and an increase near the CO₂-rich boundary. Elevated temperature and pressure further weaken the intermolecular cohesion of the heavy-oil cluster and enhance CO₂ penetration, thereby accelerating the diffusion and dissolution of heavy oil.
- (3) Within 373–523 K and 5–20 MPa, the interaction energy of CO₂–saturates is typically 2–3 times stronger than that with resins and up to 4 times stronger than that with asphaltenes. The absolute values of the CO₂–SARA interaction energies decrease by approximately 30%–40% when the temperature is raised from 373 to 523 K, whereas they increase by about 50%–60% when the pressure is elevated from 5 MPa to 20 MPa. Over the entire range of temperatures and pressures investigated, the RDF peak values of the CO₂–SARA lie within 1.0–1.1, 0.8–0.9, 0.7–0.8, and 0.5–0.6, respectively. The influence of temperature on RDF is more significant than that of pressure, indicating a stronger local enrichment of SARA around CO₂ under high-temperature conditions.
- (4) The diffusion coefficients of saturates and aromatics were much greater than those of resins and asphaltenes. The diffusion coefficients of SARA molecules increased with increasing temperature and pressure. At 523 K, the diffusion coefficients of saturates and aromatics were 34.8×10^{-9} and 20.4×10^{-9} m²/s, respectively, while the diffusion coefficients of resins and asphaltenes were 6.2×10^{-9} and 4.7×10^{-9} m²/s, respectively. The increase in temperature and pressure enhanced the thermal motion of CO₂ molecules, increasing the collision frequency between SARA molecules and CO₂ molecules and thereby increasing the diffusion coefficient.

CRediT authorship contribution statement

Ke-Xin Du: Writing – original draft, Software, Investigation, Formal analysis. **Song-Yan Li:** Validation, Supervision. **Fa-Kun Li:** Investigation. **Jia-Wei Zhao:** Investigation. **Yu Zhang:** Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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