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Insight into mass transfer mechanism of CO₂–N₂ mixed gas with oil

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ABSTRACT

The appropriate selection of CO₂–N₂ mixed gas is critical for cost-effective and efficient gas flooding in enhanced oil recovery. Optimizing this process requires a molecular-level understanding of the interfacial mass transfer mechanisms and their governing factors. This study employs molecular dynamics simulations to reinvestigate the classical surface renewal theory from a molecular perspective, develop a quantitative characterization method for the renewal frequency of surface voids, and elucidate the underlying micro-mechanisms of interfacial mass transfer. It was found that the renewal frequency of surface voids serves as the dominant factor influencing mass transfer, governed by the competition between the gas–oil interaction and the oil–oil interaction. The crude oil extraction efficiency improves with a higher CO₂ mole fraction in the mixed gas. A critical mole fraction (CMF) of CO₂ was identified for different alkane systems, beyond which the mass transfer performance improves significantly. Alkane systems with longer chain lengths are associated with higher CMF values. These results are attributed to the higher molecular density and stronger gas–oil interactions in CO₂-rich mixed gases. Therefore, optimizing the CO₂–N₂ mixed gases with a CO₂ fraction above the system-specific CMF can achieve high mass transfer efficiency while enhancing economic feasibility by reducing reliance on pure CO₂ with high economic costs, providing a foundation and molecular-scale insights for designing gas injection processes.

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1. Introduction

Gas flooding has gained widespread application as an effective enhanced oil recovery (EOR) technique in oilfields around the world. In China, annual oil production from gas flooding has reached millions of tons and is anticipated to grow to tens of millions of tons within the next decade (Lyu et al., 2025; Zhang et al., 2025a,b). Common gases used in gas flooding include CO₂, hydrocarbon gases, N₂, associated gas, and oxygen-reduced air (Jia et al., 2023; Li et al., 2025; Liu et al., 2025; Wan et al., 2024; Zhang et al., 2025a,b). Due to their distinct interaction mechanisms with crude oil, these gases are suited to different reservoir conditions and exhibit varying EOR performances. CO₂ is currently the most widely used medium. Under most reservoir conditions, CO₂

reaches a supercritical state and demonstrates strong mass transfer capacity, effectively extracting residual oil that remains after water flooding. When miscibility is achieved, displacement efficiency can exceed 90% theoretically, highlighting its exceptional capacity for EOR (Kumar et al., 2022; Prasad et al., 2023). N₂, valued for its chemical inertness, wide availability, and ability to maintain reservoir pressure, is also commonly employed (Li et al., 2018).

Despite the technical benefits of CO₂, its high cost, particularly in China, limits large-scale application (Wang et al., 2025). In contrast, the United States has fostered a robust CO₂-EOR industry over the past seven decades, supported by policy incentives and a mature Carbon Capture, Utilization, and Storage (CCUS) infrastructure, which includes large-scale capture facilities and long-distance CO₂ pipelines, thereby reducing overall gas cost. Since a significant portion of captured CO₂ originates from industrial exhaust streams (typically containing CO₂ and N₂), the purification of CO₂ to high levels entails substantially increased costs, particularly beyond the 90% purity threshold (Sänger et al., 1994;

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Sinanan and Budri, 2012). As suggested (Lin et al., 2024), impure CO₂ streams mixed with N₂ may offer a viable compromise between economic feasibility and displacement performance. Thus, a fundamental understanding of the interaction mechanisms between CO₂–N₂ mixed gases and crude oil is essential to identify the critical CO₂ mole fraction that balances cost with recovery efficiency.

Extensive research has been conducted on the interactions of pure CO₂ or N₂ with crude oil, primarily through phase behavior experiments and molecular simulations. CO₂ plays a critical role in enhancing oil recovery within shale and nanoporous media, as recent studies (He et al., 2024; Song et al., 2024) have demonstrated its effectiveness through mechanisms influenced by nanoconfinement and oil composition, and through the accurate prediction of its minimum miscible pressure under nanoscale conditions. Qian et al. (2019) conducted swelling and dissolution tests on CO₂–crude oil systems, identifying the minimum extraction pressure (MEP), as the equilibrium pressure at which the oil swelling factor begins to decrease rapidly during the process of increasing equilibrium pressure, below which oil swelling dominates and above which significant extraction of heavier components occurs. Notably, the extraction rate decreases as the molecular weight of oil components increases. Molecular dynamics (MD) simulations have been effectively employed to investigate the mechanisms of CO₂–enhanced oil recovery within shale and nanoporous media (Bao et al., 2025; Wu et al., 2024). Luo et al. (2023) combined pressure–volume–temperature (PVT) experiments, equations of state, and molecular dynamics simulations to analyze mass transfer near the gas–oil interface, analyzing the diffusion of CO₂ and crude oil components near the oil–gas interface with pressure decay experiments. They reported that the diffusion coefficient of CO₂ decreases with increasing CO₂ mole fraction in the hydrocarbon mixture and that of light oil exhibits enhancement near the interface compared to the bulk phase of oil. Wang et al. (2021) used MD to compare the miscibility of different gases (CO₂, N₂, CH₄, C₃H₈) in crude oil. The solubility and miscibility capacity of nonpolar alkanes with these gases were found to follow the order: C₃H₈ > CO₂ > CH₄ > N₂. Although solubility in both CO₂ and N₂ decreases with increasing alkane chain length, the interaction energy with CO₂ and N₂ increases and decreases, respectively. They attributed CO₂'s superiority to smaller molecular mass differences rather than interaction energy. Xue et al. (2015) applied MD to nitrogen flooding in shale reservoirs, evaluating the effects of pressure, pore size, rock type, nitrogen injection volume, and temperature. They identified that the mobilization of crude oil is governed by the interplay between crude oil–rock adsorption strength, quantified by interaction energy, and gas driving force. These studies collectively analyzed the influence of environmental conditions, crude oil composition, and gas type on mass transfer efficiency. Although MD has proven reliable in probing these mechanisms, current models often lack comprehensive theoretical treatment of non-equilibrium processes and tend to overlook the role of oil–oil component interactions in mass transfer.

In comparison, research on CO₂–N₂ mixed gas systems remains limited, particularly concerning non-equilibrium mass transfer mechanisms. Existing studies have mainly focused on the effects of CO₂ mole fraction on physical properties and displacement efficiency. Gajbhiye (2020) investigated the influence of the CO₂ mole fraction in CO₂–N₂ mixed gas on oil–gas interfacial tension (IFT) using the pendant drop technique. It was demonstrated that an increase in the CO₂ mole fraction reduces IFT, with CO₂ exhibiting a more significant effect than N₂. Zhang et al. (2025a,b) found that the reduction in IFT between CO₂–N₂ mixed gas and crude oil nonlinearly correlates with changes in the CO₂ mole fraction. They

suggested that at high temperatures, a lower CO₂ mole fraction could achieve the most economical IFT reduction. Yu et al. (2022) employed MD simulations to characterize the process of crude oil stripped by CO₂–N₂ mixed gas on the surface of residual oil. They analyzed the patterns of phase changes, distribution characteristics, microstructural evolution, and interaction energy in the oil–gas system under the action of CO₂, N₂, and mixed gas. The retention of residual oil on pore surfaces was explained based on intermolecular forces among different components. Wang et al. (2024) used MD simulations to study the differences in EOR and storage efficiency among CO₂, N₂, and H₂S. Their results indicated that N₂ has an adverse effect on both oil displacement and CO₂ storage, owing to its weaker interactions with crude oil and rock surfaces, which hinder gas dissolution in oil and competitive adsorption on the rock. Lin et al. (2024) conducted core flooding experiments to evaluate the oil displacement efficiency and production costs of CO₂–N₂ mixed gas injection. They observed a significant decline in recovery efficiency when the N₂ content exceeded 17.2% (i.e., CO₂ mole fraction less than 82.8%). Yu et al. (2022a) employed MD simulations to examine variations in oil–gas interfacial thickness across three systems—pure CO₂, pure N₂, and mixed gas of CO₂:N₂ = 1:1—under varying pressure conditions. The results suggested that a higher CO₂ fraction in gas phase leads to a broader interfacial region and enhanced oil–gas mixing. However, the influence of the range of gas compositions was not systematically investigated in their work. Zhang et al. (2025a,b) utilized LF-NMR-coupled core flooding to investigate the displacement behavior of N₂–CO₂ mixtures in porous cores. They observed a reduction in residual oil saturation within large pores, which was attributed to the synergistic effect of gas dissolution and non-miscible flooding at an optimal N₂ ratio. CO₂ dissolution plays a crucial role in oil displacement (Y. Wang et al., 2023; Chen et al., 2025). This ratio was associated with the gas dissolution thresholds under the experimental pressure conditions. Yu et al. (2022b) examined the capacity of N₂–CO₂ mixtures with varying fractions to dissolve and strip decane within hydroxylated quartz nanopores. Their findings indicate that gas mixtures with a CO₂ mole ratio of 25% effectively dissolved into the oil film, while a higher CO₂ content of 75% was required to achieve effective stripping of the decane layer. Z. Wang et al. (2023) conducted cyclic steam stimulation experiments assisted by N₂–CO₂ mixtures with varying ratios. The results demonstrated that the recovery factor varies with the N₂/CO₂ ratio, exhibiting an increasing trend from 1:0 to 2:1, followed by a decrease from 2:1 to 0:1. The initial increase is primarily attributed to viscosity reduction of heavy oil due to CO₂ dissolution, whereas the subsequent decline is governed by the elevation of formation energy resulting from N₂ expansion. The optimal recovery performance was achieved at an N₂/CO₂ injection ratio of 2:1. These findings reveal a gap in the mechanistic understanding of dynamic mass transfer processes between CO₂–N₂ mixed gas and crude oil, particularly under non-equilibrium conditions.

The above studies offer valuable foundational insights into gas–crude oil interactions. Due to the considerable variability in the properties of crude oil in reservoirs suitable for gas flooding for enhanced oil recovery (EOR), selecting an appropriate injection gas type—especially mixed gases—is essential to achieving an optimal balance between high recovery efficiency and economic viability. A fundamental scientific challenge involves elucidating the molecular-scale interactions between different gases and crude oil, as well as identifying the dominant factors that govern mass transfer behavior.

To address this challenge, this study integrates molecular dynamics simulations with a molecular-level reinterpretation of the Surface Renewal Theory. This approach enables quantitative

characterization of microscopic oil–gas interaction features during dynamic non-equilibrium mass transfer processes. The surface renewal frequency is identified as the dominant factor controlling mass transfer. This work establishes a conceptual framework in which oil–gas mass transfer is interpreted as a competition between driving and resisting forces at the molecular level. By extending the gas medium from pure gases to CO₂–N₂ mixed gases, we introduce the concept of a critical CO₂ mole fraction (CMF), which corresponds to a rapid recovery enhancement across different crude oil types. These findings provide an important foundation and molecular-scale insights for the scalable and cost-effective application of gas flooding EOR technology.

2. Models and methodology

2.1. Model construction and simulation details

To investigate the mass transfer mechanisms between CO₂/N₂ and crude oil, a molecular-level oil–gas mass transfer model was constructed and performed with the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator, version: 29 August 2024) software package. As illustrated in Fig. 1, the system comprises a spherical oil droplet surrounded by a gas phase within a cubic simulation box with an edge length of 120 Å. The oil droplet, centered at (60 Å, 60 Å, 60 Å) with a radius of 40 Å, is composed of alkane molecules—C₆, C₁₀, C₁₅, and C₂₀, respectively—representing different crude oil types. The remaining volume is occupied by the gas molecules as gas phase. The spherical interface used in this model, while simplifying the influence of complex geometries on interfacial mass transfer to some extent, effectively captures the overall trends of mass transfer. The system was maintained at 90 °C and 15 MPa to simulate typical reservoir conditions. Six CO₂–N₂ mixed gases with CO₂ mole fractions of 100%, 85%, 70%, 50%, 15%, and 0% were considered.

The TraPPE (Transferable Potentials for Phase Equilibria) force field was employed for CO₂ and N₂ molecules, while the OPLS-AA (Optimized Potentials for Liquid Simulations-All Atom) force field was applied to the alkane molecules. Both force fields are widely adopted in gas–oil simulation studies (Bi et al., 2026; Jorgensen et al., 1996; Potoff and Siepmann, 2001). Non-bonded interactions (E) were described using the Lennard-Jones 12–6

potential (E_{LJ}) and Coulombic interactions (E_{coul}), as given by Eq. (1). A cut-off distance of 14 Å was applied for short-range interactions. Long-range electrostatic interactions were treated using the Particle-Particle Particle-Mesh (PPPM) method with an accuracy of 10^{-4} . The Nosé-Hoover thermostat was used to regulate temperature, and periodic boundary conditions were applied in all three directions.

$$E = E_{LJ} + E_{coul} = 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \quad (1)$$

where r_{ij} represents the distance between atoms i and j . ϵ_{ij} and σ_{ij} stand for the LJ well depth and zero-potential distance between atoms i and atoms j , respectively. q_i and q_j are the charge of atoms i and atoms j , respectively. ϵ_0 is the vacuum permittivity.

The oil droplet and gas phase were first pre-equilibrated separately under the isothermal-isobaric (NPT, constant number of atoms, pressure, and temperature) ensemble to achieve thermodynamically stable configurations. Subsequently, the combined system was simulated for 2 ns in the isothermal-isovolumetric (NVT, constant number of atoms, volume, and temperature) ensemble using a time step of 1 fs to capture the mass transfer process from non-equilibrium to equilibrium. Equilibration was considered complete when the fluctuation of the total potential energy fell below a threshold over a 100 ps window.

Due to the gas dissolution and oil swelling in a result of mass transfer, the spherical surface of the oil droplet (radius 40 Å, centered at (60 Å, 60 Å, 60 Å)) was defined as the initial interface to ensure a uniform benchmark for comparison of different systems. Any molecule crossing this boundary was considered to have undergone mass transfer—either dissolution of gas molecules into the oil phase or extraction of oil molecules into the gas phase.

2.2. Fluid characteristics and model validation

The number of molecules for both oil and gas phases was determined based on their equations of state (Eq. (2)). Key parameters for the gas and crude oil are listed in Tables 1 and 2, respectively. The validity of the fluid models was confirmed by comparing simulated densities with reference data from the NIST

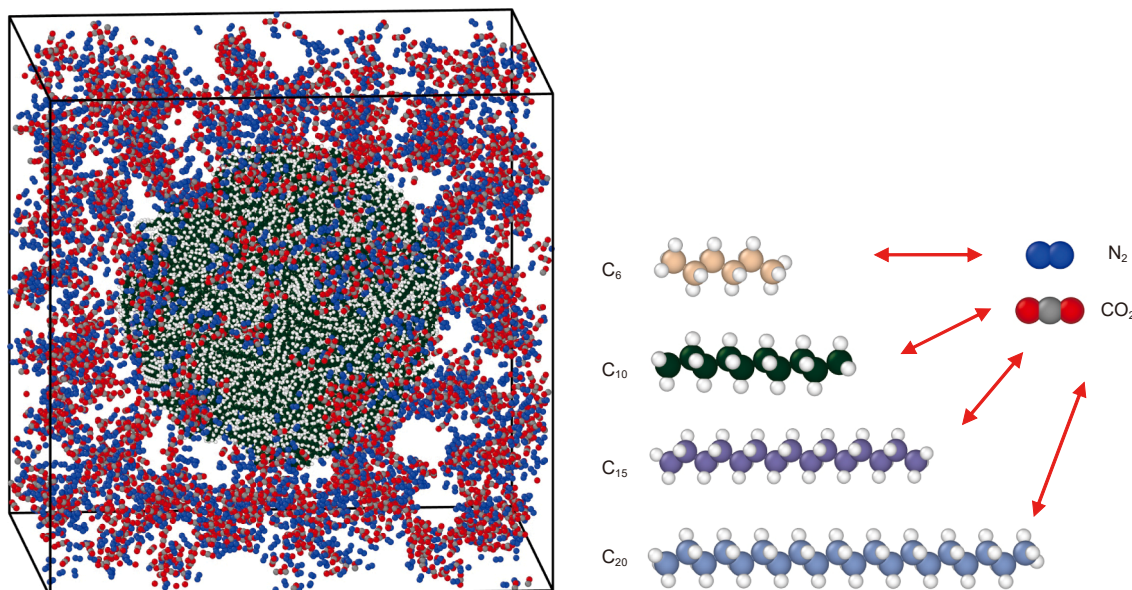


Fig. 1. Schematic structure of the mass transfer model (illustrated with the CO₂/N₂–C₁₀ system) and fluid molecules.

Table 1
Gas system parameters and validation.

CO ₂ mole fraction, mol%	Compressibility factor	Molecular number <i>N</i>		Density, g/cm ³		
		CO ₂	N ₂	MD	NIST	Deviation, %
100	0.5882	7424	0	0.3692	0.3717	−0.6726
85	0.7167	5180	914	0.2895	0.2884	0.3814
70	0.8106	3771	1616	0.2510	0.2403	4.4528
50	0.9052	2412	2412	0.1911	0.1976	−3.2895
15	1.0197	642	3641	0.1543	0.1482	4.1161
0	1.0552	0	4139	0.1311	0.1319	−0.6065

Table 2
Crude oil system parameters and validation.

Oil droplet	Molecular number	Density, g/cm ³		
		MD	NIST	Deviation, %
C ₆	1154	0.6155	0.6164	−0.1460
C ₁₀	784	0.6906	0.6920	−0.2023
C ₁₅	557	0.7324	0.7328	−0.0546
C ₂₀	431	0.7533	0.7550	−0.22517

(National Institute of Standards and Technology) database of U.S. Additionally, oil–gas interactions were verified by comparing the simulated diffusion coefficients of CO₂ in the oil phase against experimental values, as summarized in Table 3. Due to variations in experimental temperature, pressure, and sample conditions, the average CO₂ diffusion coefficients obtained in this study exhibit a deviation of 25.35% from the average values reported in the literature. Nevertheless, the data agree in order of magnitude, confirming the robustness of the model and its ability to reproduce physically plausible mass transfer behavior in gas–alkane systems.

$$PV = ZnRT \quad (2)$$

3. Results and discussion

3.1. Molecular mass transfer mechanisms of CO₂/N₂ with crude oil

3.1.1. Mass transfer characteristics of CO₂/N₂ with oil droplets

For systems consisting of pure CO₂ or N₂ with four types of alkane droplets, the quantities of extracted alkane molecules and dissolved gas molecules after mass transfer equilibrium are presented in Fig. 2. As the alkane chain length increases, both alkane extraction and gas dissolution decrease, following the order: C₆ > C₁₀ > C₁₅ > C₂₀. Compared to N₂, CO₂ yields significantly greater extraction of alkanes into the gas phase and dissolution of gas into the oil droplet. For systems involving longer-chain alkanes (C₁₀, C₁₅, and C₂₀), the average number of extracted alkane molecules and dissolved gas molecules in CO₂-containing systems are 1.58 and 2.88 times higher, respectively, than those in N₂-containing systems. These results clearly indicate that CO₂–alkane systems exhibit superior mass transfer efficiency relative to N₂–alkane systems.

Table 3
Comparison of simulated gas diffusion coefficients of CO₂ in this study with published literature data.

Data source	Pressure, MPa	Temperature, °C	Gas diffusion coefficient, 10 ^{−8} m ² /s
In this study	15.00	90.00	0.49–0.58
Zhang et al. (2000)	3.47	21.00	0.48
Renner (1988)	1.44–5.83	37.85	0.73–1.26
Kavousi et al. (2014)	1.73–4.48	22.00–32.00	0.036–0.090
Dong et al. (2018)	2.17	63.00	1.29

*The average CO₂ diffusion coefficient determined in this study is 0.53, which corresponds to a deviation of 25.35% from the literature average value of 0.71.

Fig. 3(a) illustrates the non-equilibrium mass transfer process at the interface, exemplified by a C₁₀ alkane droplet in the presence of CO₂. Initially, CO₂ molecules penetrate into intermolecular voids within the oil phase, disrupting the arrangement of alkane chains and facilitating further void expansion. This allows additional CO₂ molecules to enter the oil, thereby enhancing CO₂ dissolution. Subsequently, dissolved CO₂ molecules promote the stripping of surface alkanes, releasing them into the gas phase. A distinct mass transfer zone develops near the interface where both dissolution and extraction occur efficiently. Finally, the continuous expansion of this mass transfer zone increases the effective interfacial area, thereby augmenting overall mass transfer rates.

In contrast, as shown in Fig. 3(b), N₂ molecules penetrate only slowly into the oil phase without substantially widening the existing voids. A prolonged accumulation of N₂ molecules on the droplet surface is required to disentangle and partially straighten some alkane chains before extraction can occur. This results in markedly slower mass transfer between oil and gas, with significantly fewer molecules exchanged between phases. Consequently, no well-defined mass transfer zone is formed in N₂–alkane systems.

3.1.2. Surface renewal theory and dominant factors in molecular mass transfer

Interfacial mass transfer between oil and gas is a complex process influenced by both thermodynamic and kinetic factors. The Surface Renewal Theory (SRT), introduced by Danckwerts (1951), provides a robust framework for analyzing such systems. This study demonstrates that a molecular-level reinterpretation of SRT effectively explains the non-equilibrium mass transfer process at oil–gas interfaces. A comparison between molecular and macroscopic interpretations of SRT is summarized in Table 4.

Based on the characteristics of mass transfer at the oil–gas molecular interface, the equations associated with the SRT (Danckwerts, 1951) reinterpreted from a molecular perspective are given by Eq. (3) to Eq. (5) below:

$$\phi(\theta) = s \cdot e^{-s\theta} \quad (3)$$

where ϕ represents distribution function of surface voids in the oil phase, indicating the probability that a void among oil molecules remains exposed for gas–molecular penetration over time θ . s

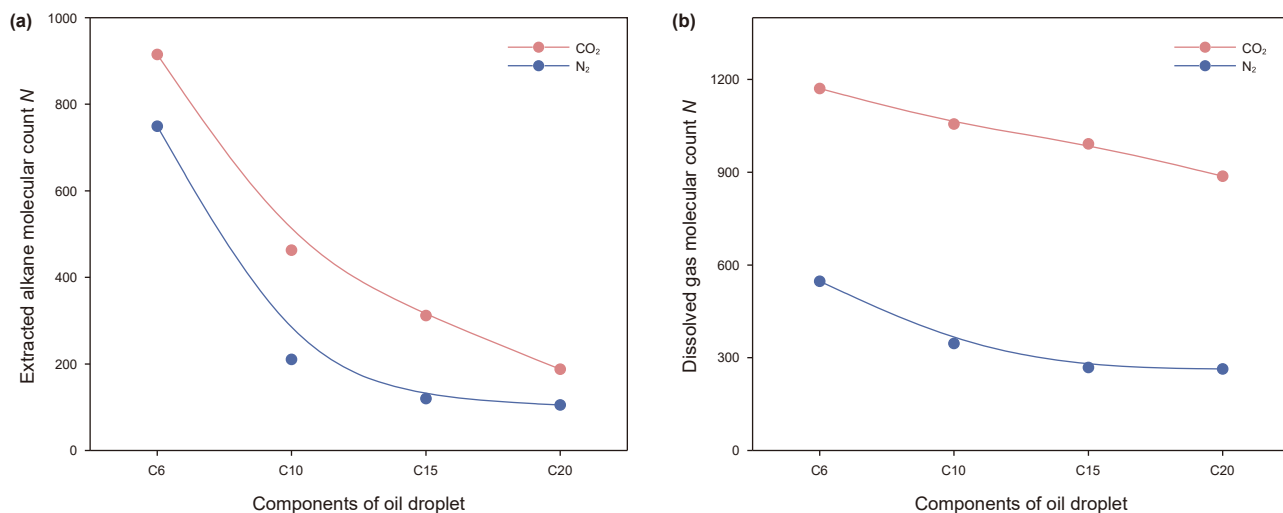


Fig. 2. (a) Equilibrium number of extracted alkane molecules in the gas phase to total alkane molecules for CO₂ or N₂ system. (b) Equilibrium number of dissolved CO₂ or N₂ molecules in the oil droplet at equilibrium to the total number of corresponding gas molecules.

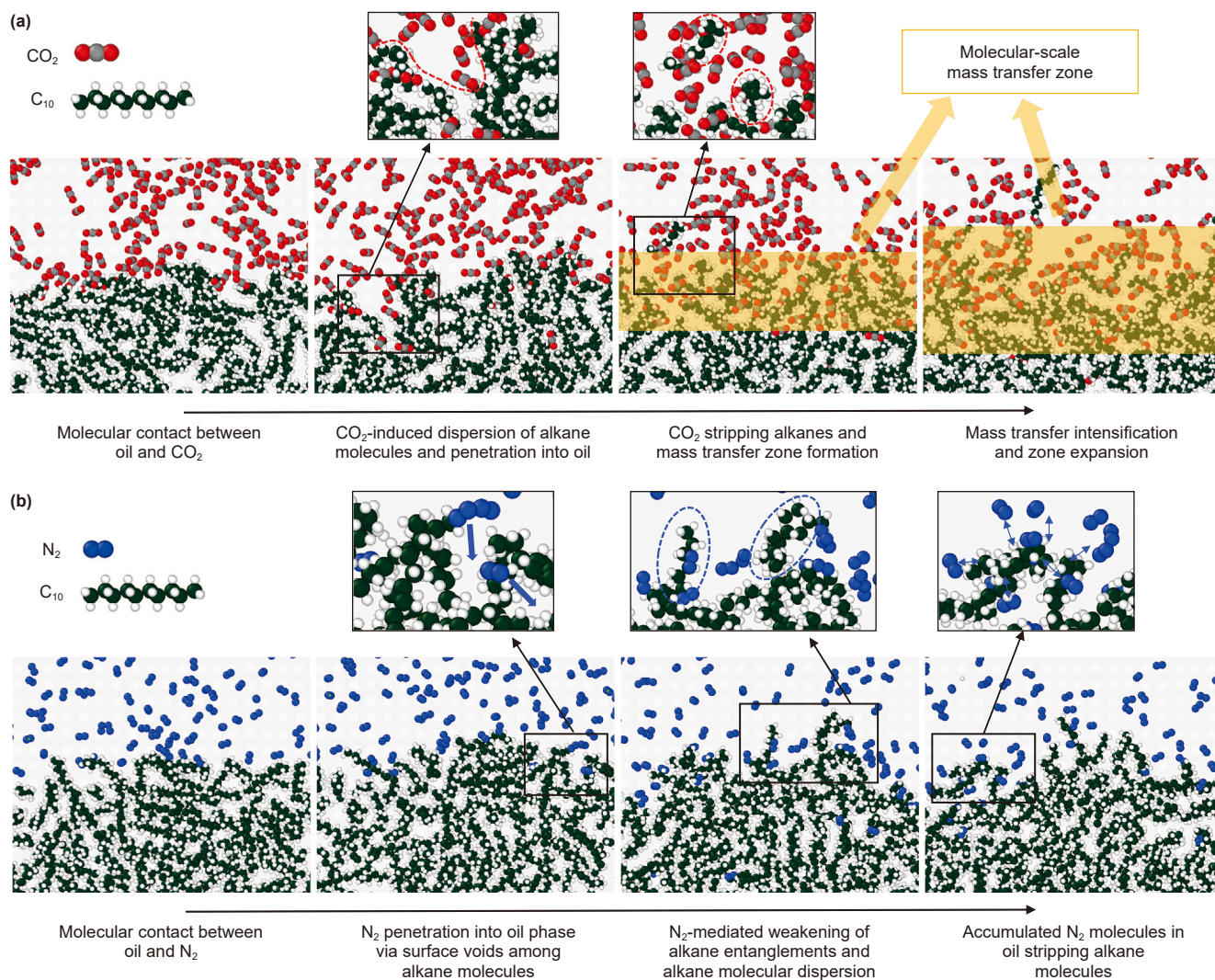


Fig. 3. Microscopic interaction characteristics between gas and alkane molecules on a C₁₀ droplet surface: (a) CO₂, (b) N₂.

Table 4
Molecular Reinterpretation of SRT: From bulk phase to fluid molecules.

Scale of perspective	Focus	Mass transfer direction	Driving force
Molecular scale	Individual fluid molecules	Gas to oil and oil to gas	Intermolecular interactions
Macroscopic scale	Continuum liquid elements	Gas dissolution	Concentration gradient

denotes the renewal frequency of surface voids, s^{-1} ; and θ is the time for which a void has been exposed to gas molecules, s .

$$R = \Delta F \cdot \sqrt{D} \int_0^\infty \frac{se^{-s\theta}}{\sqrt{\pi\theta}} d\theta = \Delta F \cdot \sqrt{Ds} \quad (4)$$

where R is mean mass transfer rate per unit area of molecules. ΔF and D represent the mass transfer driving force provided by intermolecular interactions, kcal/mol; and diffusion coefficient of molecules in the other phase, m^2/s , respectively.

$$K = \sqrt{Ds} \quad (5)$$

where K is mass transfer coefficient, m/s ; which represents the capacity of molecular mass transfer. Thus, the mass transfer capacity of molecules is jointly determined by the diffusion coefficient D and renewal frequency of surface voids s of the corresponding component.

Due to the dynamic nature of the interface, s is challenging to measure experimentally (Gao, 2009). Fig. 4(a) shows the interfacial structure of four alkane droplets under CO_2 and N_2 exposure. As alkane chain length increases, surface void space decreases, leading to a reduction in s in the order: $C_6 > C_{10} > C_{15} > C_{20}$.

Moreover, CO_2 –alkane systems exhibit more dispersed surface alkane molecules and greater void availability compared to N_2 systems, resulting in a higher s for CO_2 . Consequently, systems containing CO_2 exhibit a higher s than those with N_2 .

To quantify s , we propose an indirect metric based on the reasoning that a higher s implies more dynamic rearrangement of alkane molecules at the interface, which in turn creates a larger transient space available for gas molecules to access and interact with the oil phase. Therefore, we quantified the number of gas molecules within a 6 Å radius of alkane molecules. Fig. 4(b) shows that the number of CO_2 molecules around the alkane molecules consistently follows the order: $C_6 > C_{10} > C_{15} > C_{20}$ during the mass transfer process. Fig. 4(c) demonstrates a similar trend for N_2 –alkane systems. However, the number of N_2 molecules participating in mass transfer is considerably lower than that of CO_2 , as reflected by substantially fewer interfacial voids on the oil droplet surface in the N_2 system compared to the CO_2 system. The radial distance of these CO_2 molecules from the droplet center at 100 ps and non-equilibrium process are shown in Fig. 4(d) and Fig. S1. It can be observed that the oil–gas interactions primarily occur at the initial interface position. Furthermore, in systems with shorter-chain alkanes, a greater number of CO_2 molecules

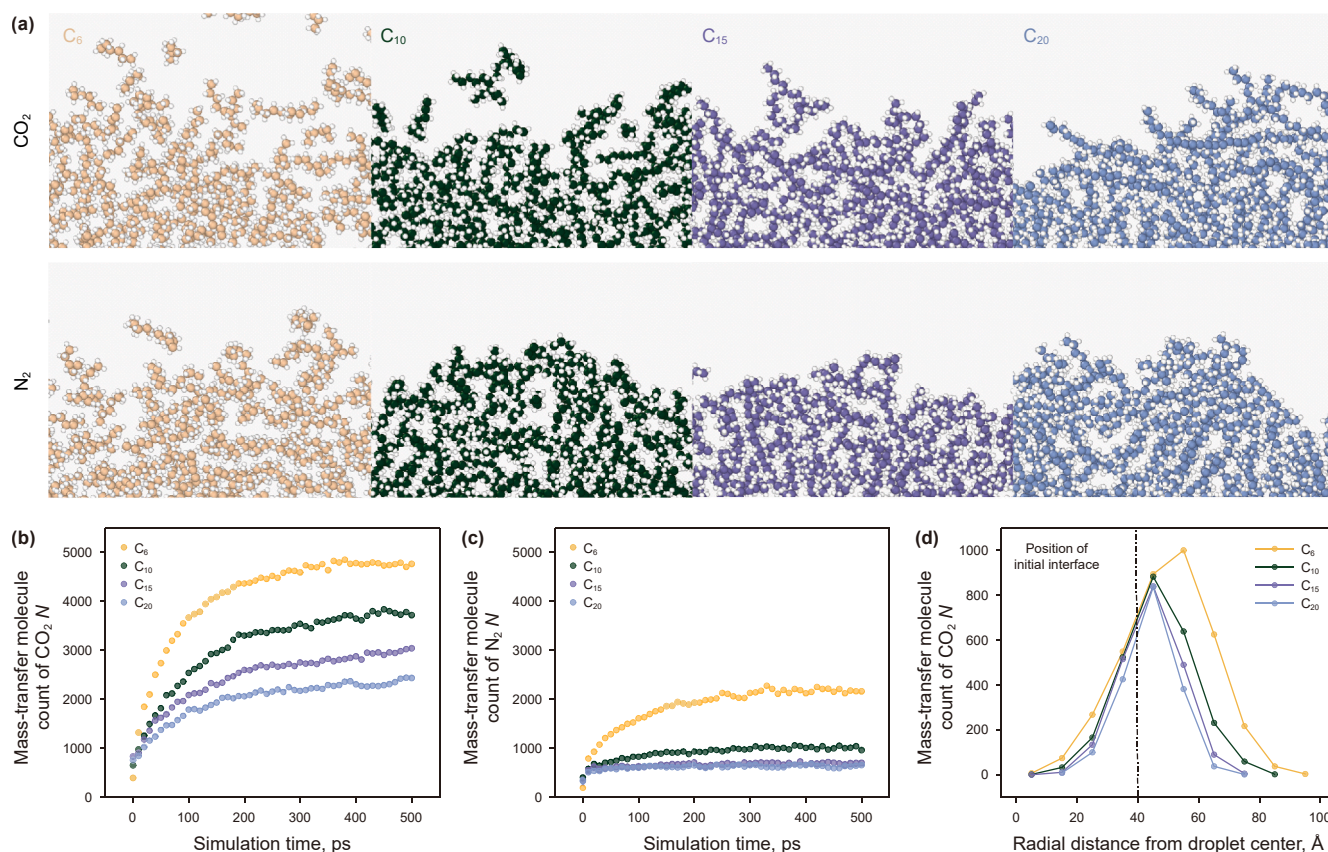


Fig. 4. (a) Distribution of alkane molecules in oil droplet surface under CO_2/N_2 exposure. Temporal evolution of interacting molecule count of (b) CO_2 and (c) N_2 during mass transfer process. (d) Radial distance of interacting molecule count of CO_2 during mass transfer process at 100 ps.

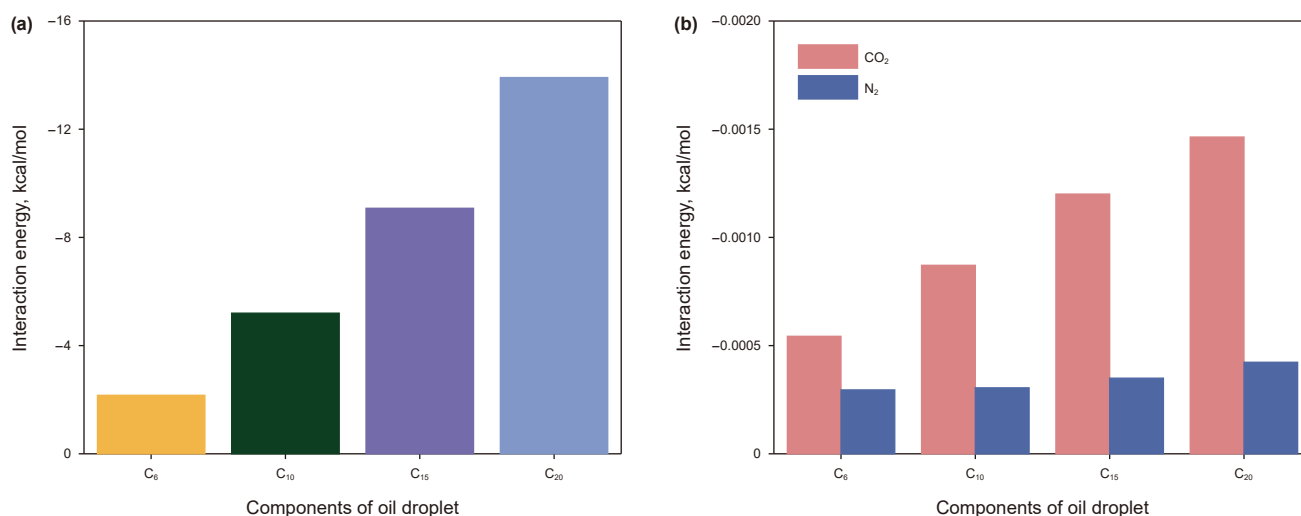


Fig. 5. Interaction energy per molecule: (a) alkane-alkane interactions and (b) gas-alkane interactions.

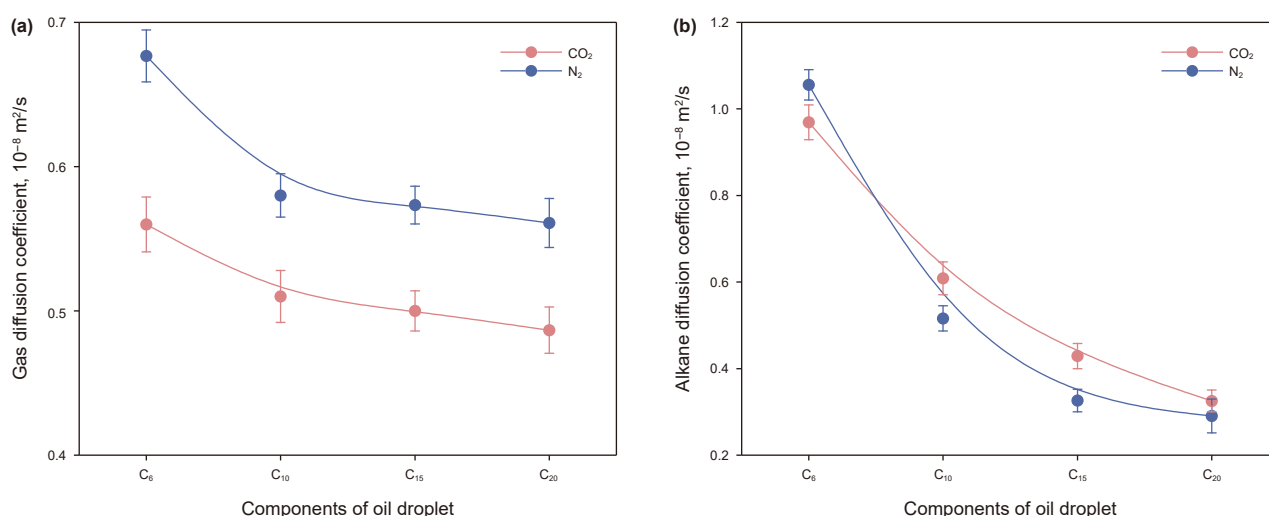


Fig. 6. Diffusion coefficients of (a) gas molecules in the oil phase and (b) alkane molecules in the gas phase.

participate in the interactions and strip alkane molecules from the droplet surface.

Fig. 5(a) presents the interaction energy between alkane molecules, which increases with chain length, thereby resisting their mass transfer with gas molecules. Fig. 5(b) shows the interaction energy between gas-alkane molecules, indicating that CO₂ exhibits stronger interactions with alkanes than N₂, promoting penetration of CO₂ into the oil and facilitating alkane extraction. Thus, molecular mass transfer is governed by the competition between the driving force from gas-alkane interactions and the resisting force from alkane-alkane interactions. The distinct trends in Fig. 5(b) are attributed to different intermolecular interaction mechanisms, although both involve dispersive interactions. CO₂, with its significant quadrupole moment, generates strong instantaneous induced dipoles with alkane molecules. This induction-driven attraction intensifies with alkane polarizability, which increases with chain length, causing the marked rise in interaction energy. In contrast, N₂, being simple non-polar, interacts mainly via weaker dispersion interactions without strong instantaneous induced dipoles, resulting in lower energy and reduced sensitivity to chain length.

After initial mass transfer, gas and alkane molecules have migrated into the opposing phase. Molecular diffusion becomes the controlling factor. The diffusion coefficient D is calculated from the mean squared displacement (MSD) using Eqs. (6) and (7):

$$\text{MSD} = \langle |x(t_0 + t) - x(t_0)|^2 \rangle \quad (6)$$

$$D = \frac{\text{MSD}}{6t} \quad (7)$$

where MSD denotes the mean squared displacement of target molecules (Å²). Here, $x(t_0)$ and $x(t_0 + t)$ represent the position of a particle at the initial time t_0 and its position after an elapsed time t , respectively. The MSD curves for alkane and gas molecules in the other phase (Fig. S2 and S3) indicate that the slopes—and thus D —remain constant throughout the mass transfer process, consistent with the findings of Guindon (2015). According to Eq. (7), this indicates that D of each component remains constant during both non-equilibrium and equilibrium states.

Fig. 6(a) shows D for CO_2 and N_2 within the oil phase. As alkane chain length increases, D decreases for both gases. Notably, D for N_2 is higher than for CO_2 , due to stronger CO_2 –alkane interactions restricting its mobility. Despite its lower D , CO_2 achieves higher dissolution due to a higher s , indicating that renewal frequency s is the dominant factor for gas dissolution.

Fig. 6(b) displays D for alkane molecules in the gas phase. Longer-chain alkanes exhibit lower D , due to higher molecular mass which hinders its mobility in gas phase. The similar D values in CO_2 and N_2 indicate that gas type has relatively minimal influence on alkane diffusion. Since alkane extraction is primarily and much earlier governed by interfacial interactions (reflected in s) rather than diffusion in the gas phase, and given that the amount of extracted oil is much smaller than dissolved gas, we conclude that s is the dominant factor for oil molecule extraction. In

summary, the renewal frequency of surface voids s is identified as the primary factor controlling mass transfer between oil and gas.

3.2. Mass transfer behavior of CO_2 – N_2 mixed gas with oil

3.2.1. Mass transfer characteristics of CO_2 – N_2 mixed gas with oil droplets

Fig. 7(a) presents snapshots at 100 ps of alkane droplets exposed to CO_2 – N_2 mixed gases with varying CO_2 mole fractions (note: mass transfer equilibrium is attained after 300 ps, and gas molecules are hidden for clarity). As the CO_2 mole fraction increases, a greater number of alkane molecules are released from the main oil droplet into the gas phase. Consequently, the interfacial region of oil becomes more blurred, indicating enhanced molecular dispersion.

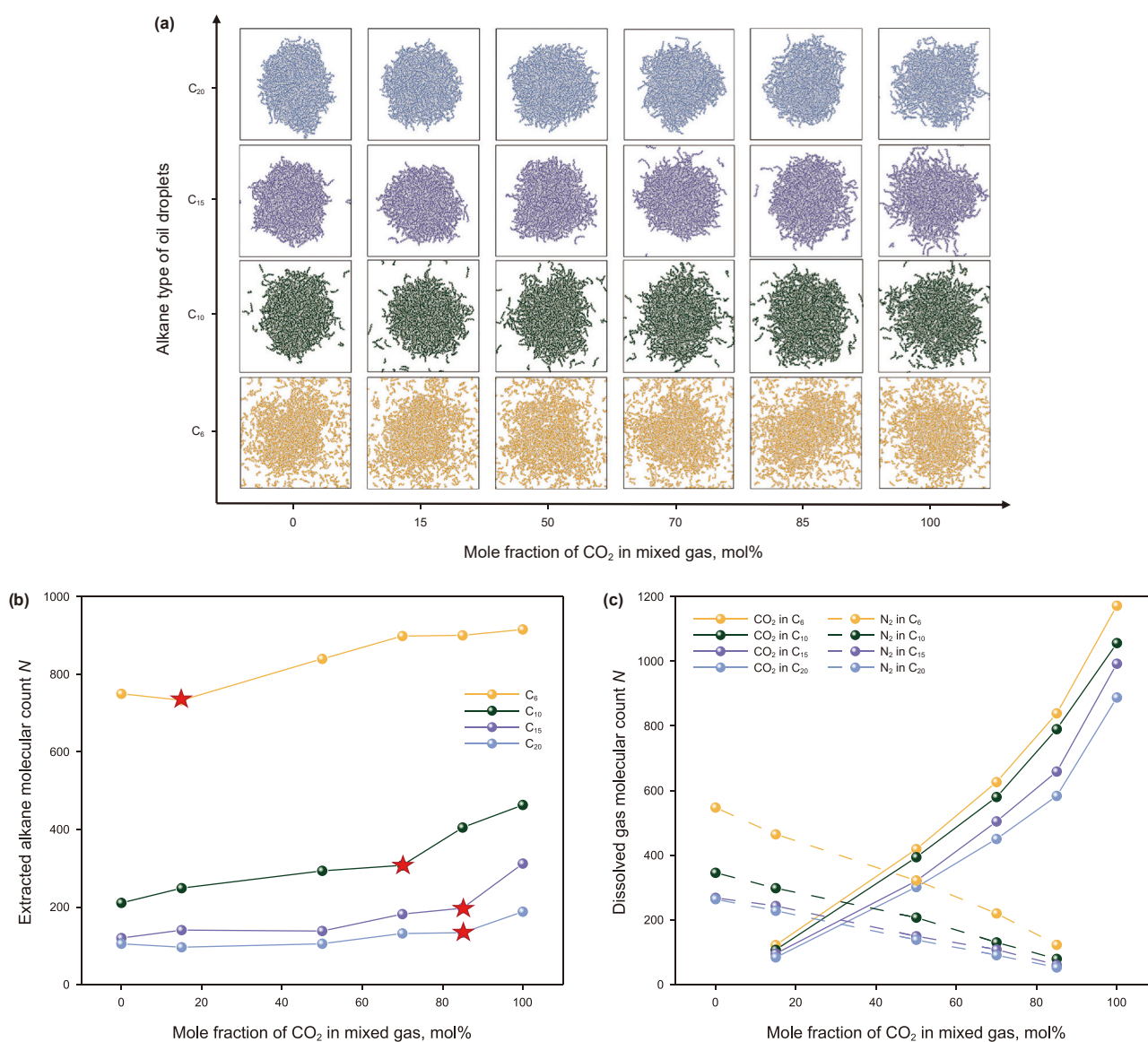


Fig. 7. (a) Morphological states of alkane droplets under different CO_2 – N_2 mixed gas at 100 ps. (b) Equilibrium number of extracted alkane molecules for different mixed gas. (c) Equilibrium number of dissolved gas molecules in the oil droplets (CO_2 : solid line, N_2 : dashed line).

The equilibrium quantities of alkane molecules extracted into the gas phase are shown in Fig. 7(b). For all four alkanes, the extent of extraction increases with the CO₂ mole fraction, following the consistent order: C₆ > C₁₀ > C₁₅ > C₂₀. These results indicate that higher CO₂ mole fraction in the mixed gas enhances extraction efficiency.

Notably for each alkane system, a critical mole fraction (CMF) was identified as the mole fraction of CO₂ in mixed gases, beyond which oil extraction increases substantially. The CMF values for C₆, C₁₀, C₁₅, and C₂₀—where a significant increase in the slope of the extraction curve was observed in Fig. 7(b)—are 15, 70, 85, and 85 mol%, respectively. Longer-chain alkanes exhibit higher CMF values. Thus, maintaining the CO₂ mole fraction above the system-specific CMF—rather than using pure CO₂—can significantly improve mass transfer efficiency while reducing capture costs.

Fig. 7(c) shows the equilibrium number of CO₂ and N₂ molecules dissolved into the oil droplets. The dissolution of each gas component increases with its respective mole fraction in the mixed gases. Notably, N₂ dissolution increases approximately linearly with its mole fraction, whereas CO₂ dissolution rises exponentially with its mole fraction. This demonstrates that systems with higher CO₂ mole fraction facilitate considerably greater cumulative gas dissolution, thereby enhancing overall mass transfer.

The diffusion coefficients *D* of alkanes in the gas phase and gas molecules in the oil phase are presented in Fig. 8. As the CO₂ mole fraction increases, the *D* value of C₆ decreases slightly, while those of C₁₀, C₁₅, and C₂₀ increase. In contrast, the *D* values of gas components remain largely unaffected by composition of mixed gas.

These diffusion trends do not fully explain the mass transfer behavior shown in Fig. 7(b, c). Instead, the renewal frequency of surface voids *s*, which increases with CO₂ content, aligns well with the enhanced mass transfer efficiency. This supports the conclusion that *s* is the dominant factor governing interfacial mass transfer and is influenced by both oil and gas properties.

3.2.2. Mass transfer mechanisms of CO₂–N₂ mixed gas with oil

Fig. 9(a) shows the number of CO₂ and N₂ molecules within the simulation volume for each mixed gas system, consistent with the dissolution trends in Fig. 7(c). Owing to its higher compressibility (see Table 1), CO₂-rich mixed gases exhibit a lower compressibility factor (*Z*), enabling a greater number of gas molecules per unit

volume. This higher gas molecular density with more CO₂ molecules promotes stronger gas–oil interactions and enhances mass transfer. This study primarily examines the influence of gas composition under constant temperature and pressure. It should be noted that temperature and pressure also significantly impact mass transfer, largely by altering the gas-phase density (Chen et al., 2022; Franklin and AuthorAnonymous, 1987).

The interaction energies among alkane molecules at initial and equilibrium states are provided in Fig. S5, and their proportional reduction is summarized in Fig. 9(b). As the CO₂ mole fraction increases, the reduction in alkane–alkane interaction energy becomes more pronounced, consistent with the enhanced extraction observed in Fig. 7(b). This weakening of cohesive forces between alkane molecules results from strong gas–oil interactions of mixed gases with higher CO₂ mole fraction, leading to increased intermolecular spacing.

To quantitatively validate the competition mechanism between the driving force from gas and resisting force of oil, the temporal evolution of the interaction energy in C₁₀ system is analyzed. Fig. 9(c) illustrates that the strengthening of the gas–alkane intermolecular interaction is accompanied by a weakening of the alkane–alkane interaction during mass transfer. Furthermore, CO₂ molecules contribute significantly more to mass transfer than N₂. In the system with a CO₂ mole fraction of 50%, the CO₂–C₁₀ interaction energy surpasses that of N₂–C₁₀ by a factor of about 2.8.

In mixed gases with high CO₂ mole fraction, the number of CO₂ molecules per unit volume increases significantly due to both higher mole fraction and reduced compressibility. Once the gas–oil interaction energy exceeds the cohesive energy among alkane molecules at the interface, efficient mass transfer is initiated. The CO₂ mole fraction at which this occurs is identified as the critical mole fraction (CMF) for the system.

The enhancement of mass transfer with increasing CO₂ mole fraction is consistent with the established trend of reduced oil–gas interfacial tension (IFT) (Gajbhiye, 2020; Yu et al., 2022). While IFT is a crucial macroscopic property that controls initial phase contact, it fundamentally represents an equilibrium thermodynamic state. Our study reveals the underlying non-equilibrium processes: the dynamic renewal of interfacial voids and the competition between gas–oil and oil–oil intermolecular interactions. These mechanisms directly govern the molecular penetration and

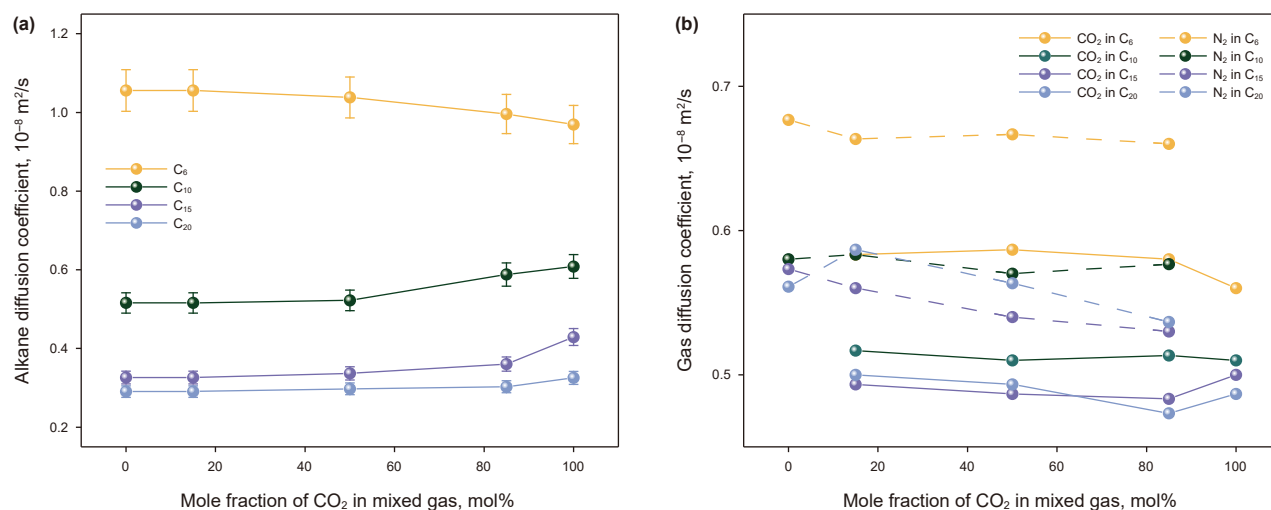


Fig. 8. (a) Diffusion coefficients of alkane molecules in different mixed gases. (b) Diffusion coefficients of mixed gas components in various alkane droplets (comprehensive error analysis is provided in Fig. S4).

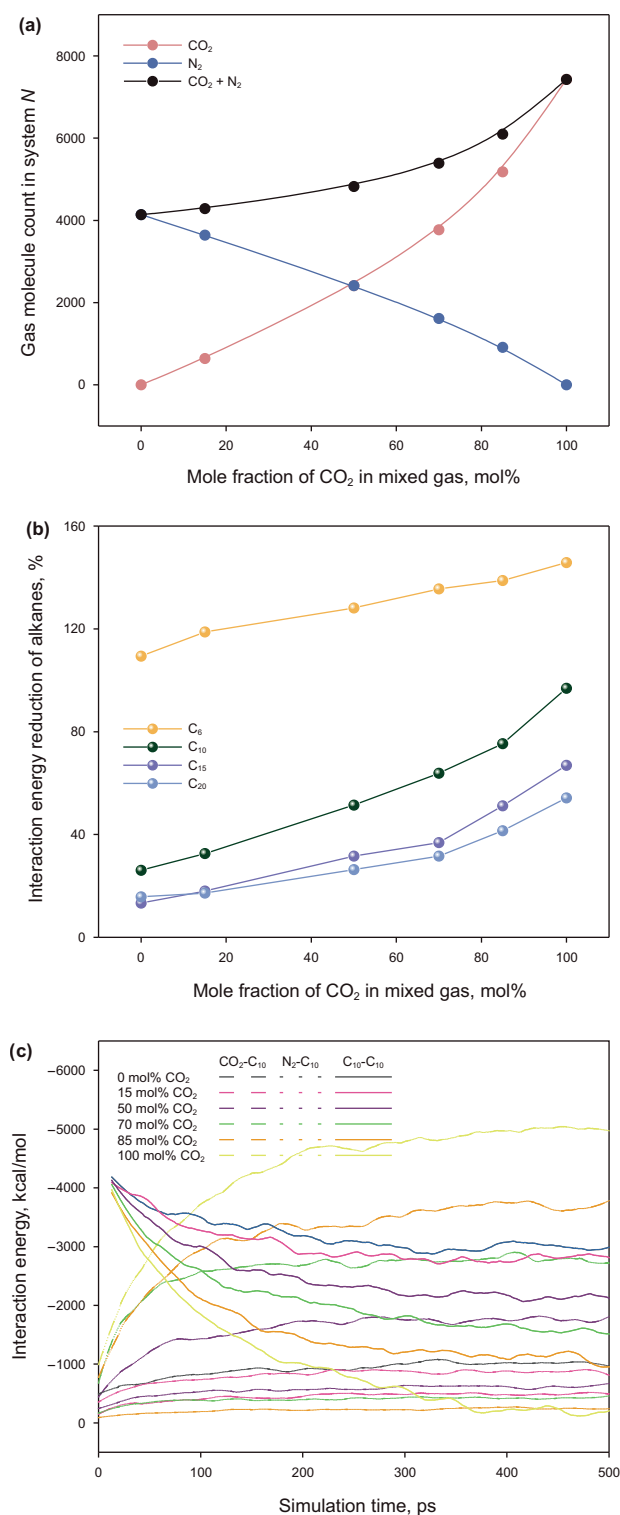


Fig. 9. (a) Molecular counts of CO₂ and N₂ in mixed gases with different mole fraction of components. (b) Reduction ratio of interaction energy between alkane molecules from initial to equilibrium state. (c) Temporal evolution of the interaction energy in C₁₀ system.

exchange rates of gas and oil, acting as the microscopic driver for the macroscopic outcome of IFT reduction and the associated mass transfer efficiency. Therefore, the surface renewal mechanism in molecular scale provides a more fundamental, kinetic explanation for the observed properties of gas–oil interactions.

4. Conclusions

The interfacial mass transfer between gas and crude oil is effectively characterized through a molecular reinterpretation of the Surface Renewal Theory. This process is governed by two key parameters: the renewal frequency of surface voids s and the molecular diffusion coefficient D , with s playing the dominant role. Fundamentally, the mass transfer is determined by the competition between the driving force arising from gas–oil interactions and the resisting force resulting from cohesive interactions among oil molecules.

The mass transfer efficiency of CO₂ significantly exceeds that of N₂. Specifically, CO₂ facilitates the formation of an efficient mass transfer zone at the interface, leading to markedly enhanced extraction and dissolution. CO₂–N₂ mixed gases with higher CO₂ mole fractions exhibit superior mass transfer performance. A critical mole fraction (CMF) of CO₂ exists for each gas–oil system, beyond which mass transfer improves substantially. Furthermore, longer-chain alkanes are associated with higher CMF values.

The mass transfer behavior of CO₂–N₂ mixed gases is influenced by both the strength of total gas–oil interactions and the molecular density of the gas phase. In mixed gases with high CO₂ mole fraction, the number of CO₂ molecules per unit volume increases considerably due to a lower compressibility factor and higher mole fraction. This elevated molecular density enhances the frequency of effective interactions and promotes mass transfer.

Optimizing injected gas composition using CO₂–N₂ mixed gases with high CO₂ content enhances mass transfer efficiency while reducing costs. The key to this strategy is determining the critical mole fraction (CMF) specific to the reservoir's oil components. Injected gases above this threshold significantly improve mass transfer during enhanced oil recovery. This insight provides a crucial foundation for gas flooding schemes with an optimal balance between EOR performance and economic viability, particularly in cases where CO₂ sourcing is costly.

Our study establishes fundamental molecular-scale insights into gas–oil interactions, creating a foundation for bridging these findings with field-scale engineering parameters. Our ongoing research builds directly on this work by: (1) extending the research to realistic crude oil systems; and (2) establishing quantitative correlations between molecular descriptors like CMF and key engineering parameters like minimum miscibility pressure (MMP).

CRediT authorship contribution statement

Jia-Hao Gao: Writing – original draft. **Yu Zhang:** Data curation. **Ming-Yuan Wang:** Supervision. **Ke Zhang:** Data curation. **Ning-Hong Jia:** Investigation. **Wei-Feng Lyu:** Resources.

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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Supplementary data

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