CO₂ Diffusion and Dispersion in Porous Media: Review of Advances in Experimental Measurements and Mathematical Models

Mohamed Gamal Rezk, Jalal Foroozesh, Ahmed Abdulrahman, Jebraeel Gholinezhad

Abstract

CO₂ molecular diffusion in subsurface porous media is one of the key mechanisms in high pressure-high temperature CO₂ geo-sequestration and CO₂ based enhanced oil recovery (EOR) projects. Mass transfer rate of the injected supercritical CO₂ and its dissolution in reservoir fluids are mainly described by gas diffusion coefficient. Over the past decades, numerous efforts have been made to investigate the CO₂ molecular diffusion process in both hydrocarbon reservoirs and saline aquifers. However, various experimental methods and mathematical models with simplified assumptions were used to determine the CO₂ diffusivity, which sometimes lead to inaccurate or contradicting results. Hence, it is essential to critically review and compare the CO₂ diffusion related literature for better application in geoscience, chemical and petroleum engineering fields. In this article, we critically review the physics of CO₂ diffusion in porous and nano-porous media including diffusion theory, factors affecting CO₂ diffusion coefficient in hydrocarbon reservoirs and
saline aquifers, analyzing laboratory measurements methods; their advantages and disadvantages, and limitations, and also evaluating previously developed mathematical models and their uncertainties and empirical correlations in detail. Additionally, we briefly discuss CO2 dispersion in porous media from various aspects. Finally, potential research areas related to CO2 diffusion in porous media are proposed.

Keywords: Molecular Diffusion; Knudsen diffusion; Dispersion; CO2 mass transfer; Porous media; CO2 geo-sequestration; EOR; CO2 impurities

1. Introduction

It is a consensus that, the increasing concentrations of anthropogenic CO2 greenhouse gas in the atmosphere is the main reason of the global warming problem and the subsequent climate changes [1]. Therefore, the intergovernmental panel on climate change (IPCC) recommended to reduce CO2 concentration by 80% before 2050 year [2]. Several options were suggested in the IPCC report [3] to reduce the CO2 concentration in the atmosphere and mitigate the climate changes, such as: (1) improving energy efficiency that can result in reducing CO2 emission from fossil fuel, (2) replacing high carbon fuel (e.g. coal) by low carbon fuel (e.g. natural gas) that would be cost effective and also reduce the CO2 concentration by 50%, (3) switching to near zero carbon fuels (e.g. renewable energies and nuclear power) that can result in a significant reduction in the amounts of CO2, (4) enhancing natural and biological sinks, such as forests and soils, to store CO2 and reduce its concentration in the atmosphere, however, the sequestration may not be permanent, and (5) increasing carbon capture and storage (CCS) projects which can store large amounts of CO2 underground. Among the above-mentioned options to mitigate the climate change,
CCS projects have received much attention as the transition from fossil fuels to near-zero carbon fuels still needs further investigation and research. The CCS process includes capturing of CO₂ generated by anthropogenic activities (e.g., fuel combustion and industrial processes), followed by storing the captured CO₂ in underground formations for a long time. Saline aquifers and depleted hydrocarbon reservoirs are considered as the main formations used for CO₂ storage due to their relatively high storage capacity compared to other types of geological formations.

There are four main trapping mechanisms for CO₂ storage in underground formations, known as (1) structural, (2) residual, (3) dissolution, and (4) mineral trapping [4]. Structural or stratigraphic trapping is the most dominant trapping mechanism where injected CO₂ rises to the top of geological structures but remains trapped in the formation by an impermeable caprock. The residual trapping is controlled by capillary forces that can trap CO₂ bubbles in micro-pores as an immobile phase [5-7]. In solubility trapping, CO₂ dissolves in the formation fluids and becomes immobile, reducing the volume of free CO₂ [8]. For the mineral trapping mechanism, CO₂ is trapped by geochemical reactions where CO₂ reacts with brine and formation minerals, and consequently, precipitates as a solid mineral phase in the reservoir [9]. CO₂ leakage is one of the main threats to any CCS project where abandoned wells and geological faults can be potential leakage pathways for CO₂, therefore, numerous efforts have been made to develop efficient technology to monitor CO₂ storage sites to ensure the security of the project and the safety of environment and public [10]. Cost-efficient monitoring sensors are the main solution for proper CO₂ monitoring. Techno-economic study is needed to evaluate technology performance and the cost involved in any CCS project. Also, proper uncertainty analysis is needed to provide a
valuable insight into the impacts of assumptions and give an indication of the study quality and robustness, as well as the reliability of the study output [11-14]. There are many techno-economic models for CCS techno-economic analysis, some of them are very simple and they are mainly used to get a quick and a rough idea of technical and economic feasibility of the project. On the other hand, there are some other rigorous technology models and also detailed “bottom-up” cost models [15].

Other than its environmental impact, CO₂ has shown a high capability to improve the oil recovery in mature oil fields for more than six decades [16] that considered to be an added-value to CCS project if implemented in hydrocarbon reservoirs. CO₂ can be injected into oil reservoirs for enhanced oil recovery (EOR) purposes on its own (conventional injection) or together with water under water alternating gas (WAG) or carbonated water injection (CWI) strategies. Additionally, cyclic CO₂ injection, i.e., CO₂ Huff and Puff, can be applied in reservoirs with limited drainage areas and in unconventional reservoirs [17, 18]. Some other CO₂ injection strategies have also received attentions such as CO₂ simultaneous water and gas injection (CO₂-SWAG), CO₂ gas assisted gravity drainage (GAGD), and CO₂ vapor extraction (CO₂-VAPEX) which is applied in heavy oil reservoirs.

Regardless of the applied CO₂-EOR injection strategy, the oil recovery is improved through various complex mechanisms. The origin of most of these recovery mechanisms is the high solubility and diffusivity of CO₂ into the reservoir fluid, i.e., crude oil and formation water, at reservoir conditions [19]. Additionally, during CO₂ sequestration in underground formations, CO₂ solubility trapping provides a high gas storage security within a short time period [20]. Hence, both the CO₂ dissolution and diffusion play an
important role in successful long-term CO$_2$ sequestration projects. The dissolution of the CO$_2$ injected into a reservoir with the reservoir fluids, i.e. oil and or water, is controlled by: molecular diffusion due to concentrating difference over distance, mechanical mixing due to fluid velocity variation in the porous medium (known as dispersion), and natural convection which is driven by the density difference that exists due to gas dissolution and diffusion in reservoir fluids [21]. It was found that the performance of any CO$_2$-EOR or carbon sequestration project mainly depends on the mass transfer rates of CO$_2$ into the reservoir fluids [22]. Hence, based on the above-mentioned significant role of CO$_2$ diffusion in fluid transport properties, it is essential to determine the mass transfer parameters, e.g., diffusion coefficient, with high accuracy. Several studies in the literature have developed experimental methods, mathematical models, and empirical correlations to obtain the gas diffusivity in various fluid-fluid systems, and in both conventional and unconventional reservoirs, i.e., shale and coal formations. However, the methods proposed in the literature to determine the gas diffusion coefficient have resulted in different values even for the same gas-liquid system at similar operating conditions. This can be due to the oversimplified procedures and assumptions followed in the laboratory measurements and the developed mathematical models without considering the realistic nature of the diffusion process. As a consequence, there is a high uncertainty in the data available for CO$_2$ diffusivity reported in the literature which can result in significant errors in simulating the process of CO$_2$ injection in porous media. Hence, more studies are needed to evaluate the currently available diffusion models and experimental measurement methods. In this article, we review previous methods used to measure and determine the CO$_2$ diffusivity in reservoir fluids, and their applications and impact on hydrocarbon recovery and carbon
storage. The theory of CO$_2$ dispersion in porous media and determination of the gas dispersion coefficient are also briefly reviewed in this paper. More specifically, this study encapsulates the following sections:

- Discussing the theory of gas diffusion and dispersion in bulk fluids and in porous media.
- Illustrating the factors controlling CO$_2$ diffusion in hydrocarbon reservoirs and saline aquifers, and their subsequent impact on the measured CO$_2$ diffusion coefficient.
- Summarizing previously applied experimental methods to measure the CO$_2$ diffusivity in laboratory and identifying their limitations.
- Defining mathematical models available in the literature to determine the CO$_2$ diffusion coefficient and summarizing the values of CO$_2$ mass transfer parameters reported in the literature in both light and heavy oil reservoirs at various reservoir conditions.
- Summarizing previously developed CO$_2$ diffusion coefficient empirical correlations and previous work studied molecular dynamics simulation in gas diffusion application.
- Defining current challenges and future research areas related to gas diffusion in porous media.

2. CO$_2$ diffusion in porous media

Generally, the diffusion process in porous media has been described based upon an analogy with thermal and electrical conduction theories [23]. Nevertheless, the irregular shapes and distributions of rock grains and pore spaces (complex heterogeneous pore
structure) [24, 25], and the heterogeneous mineral composition, make the investigation of
the diffusion phenomenon in porous rocks a challenging process. Hence, the measured
values of diffusion coefficients highly depend on the properties of the solute (e.g., \( \text{CO}_2 \) gas), solvent (e.g., resident liquid), as well as the porous medium and the thermodynamic
properties of the system.

2.1 Brownian motion and mass transfer by concentration gradient

Robert Brown [26] described the mass transport by the random motion of pollen
grained on a surface of water. He noticed that, by using a microscope, the molecules are
on continuous random motion, i.e., known as Brownian motion. Later, Einstein [27] tried
to further investigate this phenomenon. He introduced the term diffusion coefficient of a
particle, which is related to temperature of the system, viscosity of fluid, and geometry of
the particle. Adolf Fick [28] found that flux caused by diffusion is mainly dependent on
the difference in concentration of the species in solution. Fick continued to study the
diffusion process by introducing Fick’s first law [29]. By analogy with the laws of heat
conduction, Fick explained the diffusion phenomenon in terms of concentration gradient.
The molecules movement is driven by the concentration gradient, i.e. from high
concentration to low concentration regions, until equilibrium state is reached in the system
[30]. Fick developed a 1-D relation between the mass flux (\( J \)), and the concentration
gradient as shown in Eq. (1). \( D \) is defined as the Fickian diffusion coefficient and is used
to quantify the molecular diffusion within phases. The diffusion coefficient, \( D \), is
describing the diffusing mass through a unit surface area per unit time. Fick also developed
the second law to define the molecular diffusion process as a time-dependent unsteady state
process. Fick’s second law is defined in Eq. (2) [31]. As described in Eq. (2), the diffusion
process depends on the diffusion length, \( z \), the contact time, \( t \), and the rate of diffusion, which is described by the diffusion coefficient, \( D \). Although the diffusion coefficient was found to be concentration dependent, \( D \) is considered constant in most of the mass transfer applications to avoid the complexity of the mathematical models describing the diffusion process.

\[
J = -D \frac{\partial c}{\partial z} \quad (1)
\]

\[
\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial z^2} \quad (2)
\]

where \( J \) is the mass flux, \( c \) is the concentration, \( t \) is the time, and \( z \) is the distance.

It is important to mention here that mass diffusion is not only controlled by concentration gradient, but other conditions like temperature, chemical potential, magnetic and electric fields can cause the mass transfer to occur opposite to the concentration gradient direction [32, 33].

2.2 Knudsen diffusion coefficient versus molecular diffusion coefficient

Knudsen and molecular diffusion are two primary diffusion mechanisms that can take place during fluid flow in porous media. In general, during gas injection, the molecular diffusion occurs due to the collision between the molecules of the gas. While, Knudsen diffusion occurs when the gas molecules collide with the rock wall and get reflected back by the rock particles [34, 35]. Hence, the Knudsen diffusion is dominant when the pore
diameter is less than or nearly equals to the free path of the molecules. Consequently, the Knudsen diffusion is more likely to occur in tight reservoirs with permeability less than $10^{-14}$ m$^2$ [36]. On the other side, the molecular diffusion is more dominant in systems where the pore diameter is larger than the free path of gas molecules, thus the gas molecules will colloid with themselves [37]. Li et al. [38] categorized the CO$_2$ diffusion types in oil reservoirs based on pore radius ($r_p$). They showed that bulk diffusion can take place at $r_p>1\mu$m. While, at $1\mu$m>$r_p>0.01\mu$m, both bulk and Knudsen diffusion coexist. Only Knudsen diffusion occur at pore radius less than 0.01$\mu$m. Fig. 1 shows a schematic diagram of a molecule moving in a cylindrical pore of diameter (d).

![Diagram of a molecule moving in a cylindrical pore](image)

Figure 1. A schematic diagram of a molecule moving in a cylindrical pore of diameter ‘d’, ‘l’ is the free path of the molecule.

Experimentally, the Knudsen diffusion coefficient, $D_K$, is determined through conducting gas flow experiments and relating the $D_K$, the gas permeability, and Klinkenberg parameter [39]. Knudsen diffusion coefficient for a gas can be determined using Eq. (3) [40].
\[ D_K = \frac{2 \phi \, d_p \, \mu \, M}{3 \times 10^{-3} \, \tau \, R \, T \, \rho^2} \sqrt{\frac{8RT}{\pi M}} \]  

where \( \phi \) is the porosity, \( d_p \) is the pore diameter, \( \mu \) is the gas viscosity, \( \tau \) is the tortuosity of the porous media, \( \rho \) is the gas density, \( T \) is the temperature, \( R \) is the gas constant, and \( M \) is the gas molecular weight. It should be noted that accurate determination of both the molecular diffusion and Knudsen diffusion coefficients are equally important for gas transport in porous media, especially in tight formations.

### 2.3 Effective diffusion coefficient

The molecular diffusion process in a porous medium behaves differently compared to gas diffusion in a bulk liquid [41]. This different behavior of gas diffusion is due to both the tortious nature of the porous medium and the lower cross-sectional area available for the diffusion process. The porous medium reduces the diffusion coefficient as the molecules of the fluid have to travel longer paths through the pores and also the contact area between the fluids is not as large as in the case of non-porous systems, as can be clearly shown in Fig. 2. In porous media, the diffusion length depends on the properties of the rock and the formation heterogeneity [42]. It was found that effective gas diffusion coefficient is significantly dependent on the pore size and pore structure of the reservoir rock. Higher permeability formations and less tortuous pore structure were proved to facilitate the gas diffusion in reservoir fluids [43]. The diffusive flux in porous media can be described by the same equations of Fick’s laws, i.e., Eqs (1) and (2), but with replacing the bulk phase diffusion coefficient or the Fickian diffusion coefficient, \( D \), with an effective diffusion coefficient, \( D_e \).
Figure 2. Effect of formation properties, i.e., porosity and tortuosity, on the paths of molecules during the diffusion process.

Fried et al. [44] argued that molecular diffusion is similar to the conduction of electricity where the molecular concentration, mass flux, and diffusion coefficient are analogous to electrical potential, intensity and conductivity, respectively. They proposed the following correlation (Eq. 4) for the effective diffusion coefficient.

\[ D_e = \frac{D}{F \cdot \phi} \]  

where \( F \) is the formation resistivity factor which is defined as the ratio of resistivity of rock saturated with brine \( (R_o) \) to the resistivity of the saturating brine \( (R_w) \). \( \phi \) is the formation porosity. \( F \) also can be described in terms of formation porosity \( (\phi) \) and \((m)\) which is a constant called the cementation factor, and \((a)\) which is an empirical constant. Hence, \( F \) can be defined using the following equation: \( F = \frac{a}{\phi^m} \) [45]. A published data showed that the value \((F \cdot \phi)\) typically ranges from 1.25 to 1.65 depending on the texture of the medium [46].
The resistivity factor-porosity term ($F\phi$) can be described by the diffusive tortuosity factor ($\tau$). The diffusive tortuosity factor is defined as the square of the average length of diffusive pathway $l_d$ between two points to the shortest distance $l$ of those points in a porous medium as shown in Eq. (5) [47]. Similarly, many studies have proposed analytical and empirical correlations that can be used to calculate the diffusive tortuosity [48-51].

\[ \tau = \left( \frac{l_d}{l} \right)^2 \]  

(5)

Ullman and Aller [52] introduced a correlation for the effective diffusion coefficient by considering the formation diffusive tortuosity as can be shown in Eq. (6).

\[ D_e = \frac{D}{\tau^2} \]  

(6)

where the formation tortuosity can be related to formation porosity and formation resistivity using the following empirical correlation, Eq. (7) [53].

\[ \tau^2 = (F\phi)^n = (a\phi^{1-m})^n \]  

(7)

For shale free sandstone formations, $m$ ranges from 1.8 to 2. $a$ and $n$ are empirical constants, which can be assumed equal to 1 [54].

From equations 6 and 7, and with assuming $a = n = 1$, the effective diffusion coefficient can be calculated directly from Eq. (8).

\[ D_e = D \phi^{m-1} \]  

(8)

Additionally, Darvish [55] proposed a correlation where the effective diffusion can be calculated using formation tortuosity and formation properties as shown in Eq. (9).
\[ D_e = \frac{D \phi_{eff} \delta}{\tau} \tag{9} \]

where \( \phi_{eff} \) is the effective porosity which accounts for the reduced cross-sectional area available for diffusion in the pore space (\( \phi_{eff} \) equals to the overall porosity \( \phi \) if the total pore space in isotropic media is available for the diffusion process). \( \delta (\leq 1) \) is the dimensionless constrictivity and it is an important parameter in the case of chemical interactions because the path may become inaccessible for the large diffusing particles [23, 56].

### 2.4 Surface diffusion coefficient

During gas injection in underground formations, surface diffusion can exist in addition to the bulk diffusion (molecular diffusion that is controlled by concentration gradient). It turned out that the gas molecules can move as foreign particles along the pore walls directly after being adsorbed on the pore surface, which is known as the surface diffusion process [34]. Fig. 3 illustrates both the bulk diffusion and surface diffusion in a porous medium. It can be observed that the particles are being caught by the strong potential field of adsorption near to the pore surface. It is also found that the surface diffusion coefficient is much less than the bulk diffusion coefficient as the movement is a two-dimensional system which is relatively slower compared to that in a space, i.e., three-dimensional system. Karacan et al. [57] investigated the CO\(_2\) diffusion in both pore surface and pore space in coal seams using X-ray computerized tomography (CT). They found that the surface diffusion coefficient of CO\(_2\) is an order of magnitude lower than the determined value of pore diffusion coefficient. Nevertheless, the surface diffusivity of a gas still has a
significant effect on the mass transfer process especially in formations with high adsorption potential such as coal. Hence, potential of the surface diffusion is mainly dependent on mineralogy of the surface, interactions between the adsorbed material and surface atoms, and lateral interactions between the diffusion molecules. Additionally, surface coverage, i.e. adsorbed atoms concentration with respect to concentration of substrate surface atoms, is another important factor affecting the behavior of the surface diffusion process [58]. It is important to mention here that, in this paper, we focus on investigating of the gas molecular diffusion process form various aspects as it will be demonstrated in the following sections.

![Molecular diffusion and surface diffusion process in a porous medium](image)

Figure 3. Explanation of molecular diffusion and surface diffusion process in a porous medium.

2.5 Impact of CO₂ thermodynamic state and operating conditions on gas diffusion

Many previous studies investigated the thermodynamic properties for both pure CO₂ and CO₂ mixtures [59-62]. The thermodynamic and transport properties of supercritical CO₂ and its various applications were comprehensively reviewed by Nikolai et al. [62]. It was found that the mass transfer rate of CO₂ into a crude oil is significantly affected by the
thermodynamic state of the CO\textsubscript{2}. The thermodynamic properties of a CO\textsubscript{2}-oil system are function of the thermodynamic conditions, i.e., system pressure and temperature. CO\textsubscript{2} has advantageous transport and thermodynamic properties in its supercritical state. Rezk and Foroozesh [63] have experimentally investigated the mass transfer rates of CO\textsubscript{2}, at both gas and supercritical states, into a light crude oil. They could obtain the CO\textsubscript{2} diffusion coefficients using a developed mathematical model. Whereas the experiments were run at an isothermal condition, two different test pressures were selected to investigate the diffusion of gas and supercritical CO\textsubscript{2}. They found that the obtained mass transfer parameters were higher in case of supercritical CO\textsubscript{2} (SC CO\textsubscript{2}) compared to CO\textsubscript{2} at gas state. Additionally, the advantageous thermodynamic properties of the SC CO\textsubscript{2} resulted in a higher diffusivity of CO\textsubscript{2} in crude oil and faster improvements in the oil properties. Several previous studies have investigated the effect of operating pressure and temperature on the measured CO\textsubscript{2} diffusion coefficient in bulk liquids and porous media [64-70]. Li et al. [64] investigated the CO\textsubscript{2} diffusion in low permeability cores saturated with oil under reservoir conditions. They tested the effect of operating pressure and temperature along with oil saturation and core permeability. Their results showed that the diffusion coefficient of CO\textsubscript{2} in supercritical state is much greater than its value in case of CO\textsubscript{2} at gas and liquid states. The experimental results showed that at pressure 6.49 MPa and temperature 130 °C (CO\textsubscript{2} at gas phase), the D coefficient was found to be $2.407 \times 10^{-10}$ m\textsuperscript{2}/sec. Whereas, by increase in the pressure to 9.615MPa at the same temperature, the CO\textsubscript{2} phase became under supercritical state and the D coefficient increased to $7.628 \times 10^{-10}$ m\textsuperscript{2}/sec. That shows higher mass transfer rates of the supercritical CO\textsubscript{2} in oil saturated porous media. By further increasing the operating pressure, the rate of increase in the D coefficient gradually slowed
down. Similarly, their results showed that increasing the operating temperature resulted in a significant increase in the obtained CO₂ D coefficient. Increasing the oil saturation and core permeability also showed positive impacts on the CO₂ diffusivity. Ssebadduka et al. [65] estimated both gas and supercritical CO₂ diffusion coefficients in crude oils. They found that the D coefficients of the supercritical CO₂ in crude oil are more than two-fold higher than their values in case of subcritical CO₂ gas range. Zhou et al. [66] reviewed the mechanisms of CO₂ Huff and Puff in heavy oil EOR. They highlighted that CO₂ diffusion is the dominant mechanism during the soaking period. From the available data in the literature, they concluded that D coefficient of CO₂ in heavy oils increases with increasing operating pressure and temperature. Shu et al. [67] investigated the effect of operating conditions on the measured CO₂ diffusion coefficients in a carbonated water-oil system. Their results showed that both saturation pressure and temperature had positive impacts on increasing the CO₂ diffusion coefficient values. The diffusion coefficients were increased two-fold by rising the temperature from 20°C to 40°C. Li et al. [68] results shown similar impacts for the operating pressure and temperature during measuring CO₂ diffusion coefficients in tight oil reservoirs. They concluded that lower oil viscosities and higher operating pressures and temperatures resulted in a significant improvement in the CO₂ diffusivity into the crude oil even in tight reservoir conditions.

2.6 Effect of impurities on CO₂ diffusion in reservoir fluids

The CO₂ gas captured from different sources and injected underground is usually impure due to the need to lower the capture costs [71]. High purity requires additional cost and more energy. Hence, a trade-off between cost and environmental, legal, and safety aspects is recommended. The presence of impurities such as nitrogen, oxygen, argon,
hydrogen sulfide, and methane affect the CO$_2$ phase diagram and the mixture critical properties [72]. Concentration ranges of carbon dioxide impurities are listed in Table 1. Several previous studies have investigated the thermodynamic properties of CO$_2$ mixtures, i.e., binary or multicomponent system [73-75]. The impacts of impurities on CO$_2$ density, viscosity, isothermal compressibility, and critical point (critical pressure and temperature) were comprehensively studied by Al-Siyabi [75]. Li at al. [76] reviewed the available experimental data and the theoretical models related to obtaining diffusion coefficients of CO$_2$ mixtures, i.e. impure CO$_2$. Most of the experimental work and diffusion data available were found for binary impure CO$_2$ systems, e.g., CO$_2$/N$_2$, CO$_2$/Ar, CO$_2$/CH$_4$, etc. [77]. The data available for experimental measurements of molecular diffusion of impure CO$_2$ in multicomponent crude oils are very rare in the literature as most of the previous studies considered pure CO$_2$-oil systems in their diffusion experiments. Lansangan and Smith [78] investigated the viscosity, density, and phase behavior of an impure CO$_2$ (CO$_2$/N$_2$)-crude oil system. Their results showed that even small concentrations of N$_2$ in the CO$_2$ stream resulted in an adverse effect on the gas mixture-crude oil miscibility as the N$_2$ gas increased the minimum miscibility pressure (MMP). Additionally, CO$_2$ solubility in the oil phase was lowered by adding N$_2$ gas. Similarly, the viscosity and density of the impure CO$_2$ (CO$_2$+N$_2$) were found to be significantly lowered compared to pure CO$_2$, which directly affects the extraction capabilities of hydrocarbon components by CO$_2$, i.e., reduces mass transfer rates. They also found that the existence of N$_2$ gas, even at low concentrations, in the CO$_2$ steam reduces the diffusion of the gas mixture in the crude oil. This reduction in the mass transfer occurred as N$_2$ creates a stagnant phase which CO$_2$ must diffuse through before transferring into the oil phase. Nguyen [79] investigated the effect of CO$_2$ impurities
on the gas molecular diffusion process in a heavy oil sample. The molecular diffusion coefficient of pure CO$_2$, mixture 1 (15 mole% N$_2$ and 85 mole% CO$_2$), and mixture 2 (30 mole% N$_2$ and 70 mole% CO$_2$) were measured experimentally in a CO$_2$ mixture-heavy oil system. The results showed that pure CO$_2$ has a higher diffusion coefficient and mass transfer rate into the crude oil. Additionally, increasing the N$_2$ concentration had a negative effect on the gas mixture diffusion coefficient as the average gas D coefficient in the oil decreased three-fold and fourteen-fold when N$_2$ concentration in CO$_2$ was increased to 15 mol% and 30 mol%, respectively. Shi et al. [80] obtained the individual diffusion coefficients of alkane solvent-CO$_2$-heavy oil systems. They concluded that the diffusivity of CO$_2$ in crude oil is much lower than C$_3$H$_8$ and n-C$_4$H$_{10}$ under the same operating pressure and temperature. Hence, adding alkane solvent to the CO$_2$ gas improves the mass transfer process, and consequently, enhances oil swelling [81, 82]. It should be noted that the crude oils in CO$_2$ mixture-oil systems are treated as one pseudo-component in most of the previous CO$_2$ diffusion studies. Zhao et al. [83] investigated the diffusion process of CO$_2$ mixture in heavy oils. Their results showed that the D coefficients of C$_3$H$_8$ and CO$_2$ in crude oils, measured at the same conditions, are larger than the CH$_4$ diffusion coefficient. In a different study, Li et al. [84] investigated the effect of CH$_4$ gas dissolved in a crude oil sample, i.e., live oil, on CO$_2$ diffusion process. Their results showed that the presence of dissolved gases in the crude oil lowers the mass transfer rates of CO$_2$ into the oil phase. Based on the above-mentioned results obtained from previous studies, it is clearly shown that the presence of impurities in the CO$_2$ stream used in EOR or carbon storage applications highly affects the gas mass transfer rates into reservoir fluids. Thus, a reliable
and accurate measurement of the effect of the impurities, listed in Table 1, on the CO$_2$ mass transfer process is highly recommended to be investigated in the future works.

Table 1. Concentration ranges of carbon dioxide impurities (after Li et al. [76] and Li et al. [85])

<table>
<thead>
<tr>
<th>Component</th>
<th>Minimum concentration (mol%)</th>
<th>Maximum concentration (mol %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$</td>
<td>75</td>
<td>99</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>0.7</td>
<td>4</td>
</tr>
<tr>
<td>N$_2$</td>
<td>0.02</td>
<td>10</td>
</tr>
<tr>
<td>Ar</td>
<td>0.005</td>
<td>3.5</td>
</tr>
<tr>
<td>CO</td>
<td>&lt;0.001</td>
<td>0.2</td>
</tr>
<tr>
<td>H$_2$</td>
<td>0.06</td>
<td>4</td>
</tr>
<tr>
<td>SO$_2$</td>
<td>&lt;0.001</td>
<td>1.5</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>0.005</td>
<td>6.5</td>
</tr>
<tr>
<td>NO$_x$</td>
<td>&lt;0.002</td>
<td>0.3</td>
</tr>
<tr>
<td>NH$_3$</td>
<td>&lt;0.001</td>
<td>3</td>
</tr>
<tr>
<td>O$_2$</td>
<td>0.04</td>
<td>5</td>
</tr>
<tr>
<td>H$_2$S + COS</td>
<td>0.01</td>
<td>1.5</td>
</tr>
<tr>
<td>Amines</td>
<td>&lt;0.001</td>
<td>0.01</td>
</tr>
</tbody>
</table>

2.7 CO$_2$ diffusion in saline aquifers
CO₂ geo-sequestration in saline aquifers can occur through different stages. At first, when CO₂ is injected into porous media, it migrates upward by the effect of buoyancy forces until it is trapped by an impermeable cap rock, i.e., structure trapping. After the CO₂ is trapped at the top of the reservoir, it starts to diffuse into the underlying brine, i.e., dissolution trapping. The CO₂ diffusion at the interface separating the two phases (CO₂ and brine), causes an increase in the density of brine which creates instabilities in the system, i.e., convective currents or density driven natural convection, that accelerates the mass transfer process [8]. Hence, accurate estimation of CO₂ diffusion coefficients in brine is important in order to understand CO₂ transport properties in aquifers. The process of CO₂ diffusion into saline aquifers is controlled by several factors, such as pressure, temperature, and brine salinity and composition [86-91]. Azin et al. [88] have studied CO₂ diffusion into a saline aquifer at reservoir conditions. Their results showed that increasing operating pressure and temperature had a positive impact on the measured CO₂ diffusion coefficients in a brine with salinity of 207000 ppm. Zhang et al. [90] conducted a series of experimental tests, using a diffusion cell, to investigate the effect of system temperature and pressure, and brine salinity on CO₂ diffusion coefficient in a brine sample. D coefficients were measured at temperature range of 25-70 °C and under a pressure of 1 MPa. CO₂ diffusion coefficients were found to increase with the system temperature. The operating pressure had also a positive effect as the measured CO₂ diffusion coefficients were increased by increasing the pressure from 0.5 MPa up to 2 MPa. Nevertheless, they highlighted that the effect of pressure on the gas diffusion becomes minor when the pressure rises above certain value due to the increase in the gas viscosity. The total dissolved solids (TDS) was found to have an adverse effect on the measured CO₂ diffusion coefficient values. The impact of
salt type (ion types) was also included in their study by testing 4 types of salts: Na$_2$SO$_4$, NaHCO$_3$, MgCl$_2$, and CaCl$_2$. The results showed that the CO$_2$ diffusion coefficients in MgCl$_2$ and CaCl$_2$ based-brines were the highest compared to other two types of brine. While the CO$_2$ diffusion coefficient in NaHCO$_3$ solution was the lowest. Omrani et al. [89] investigated the effect of pressure, temperature, brine salinity, and brine composition on CO$_2$ diffusion in brine by employing Molecular Dynamics (MD) simulation. They found that increasing the temperature in the range of 294-423 K resulted in higher values of D coefficients. While, increasing NaCl salinity reduced the CO$_2$ diffusivity. However, the simulation results showed an insignificant effect of the system pressure on the obtained CO$_2$ diffusion coefficients at pressure range of 10-30 MPa. The effect of various types of salts, such as MgCl$_2$, CaCl$_2$, Na$_2$SO$_4$, and KCl, on the CO$_2$ diffusivity was also included in their study. The results showed that CaCl$_2$ and KCl had the most and the least effect on the CO$_2$ diffusion coefficients respectively when compared to CO$_2$ diffusion coefficient in pure water. To conclude the above results, the CO$_2$ diffusion coefficient in saline aquifers was found to be significantly increasing with higher system pressures and temperatures. However, the effect of pressure on CO$_2$ diffusivity in brine becomes minor at relatively high pressures. The brine salinity has a negative effect on the CO$_2$ diffusivity, while the CO$_2$ diffusion process in saline aquifers was proved to be highly dependent on the brine compositions and salt types.

3. Experimental measurement of CO$_2$ diffusion coefficients

Previous studies on mass transfer by molecular diffusion have proposed different laboratory methods for measuring the gas diffusion in liquid phases and in porous media
saturated with different reservoir fluids. The proposed experimental methods are divided into conventional (direct) and non-conventional (indirect) methods. In the direct methods, the gas diffusion coefficients are obtained through compositional measurements of fluid mixtures collected during running the diffusion test. On the other side, the indirect methods (non-conventional methods) require less time compared to the conventional methods. The molecular diffusion coefficients are estimated indirectly by measuring a property of a gas-oil system during performing a designed mass transfer experiment. This can be done because the diffusion process can change various properties of the oil-gas system such as: interfacial tension [92, 93], gas pressure [94, 95], gas volume [96], or position of the interface between oil and gas inside a capillary tube [42]. Additionally, the gas diffusion process can be monitored by using the X-ray computer tomography (CT) scan technology to determine the gas distribution inside the liquid phase [97].

In this section, most of the previously used experimental measurements of gas diffusivity are reviewed in different aspects including technical description, limitations, advantages, and equipment used in the test.

3.1 Conventional methods

The conventional methods, also called direct methods, directly obtain the gas concentration distribution by performing compositional analysis of gas-liquid mixtures collected at various locations and times during running the diffusion test [98, 99]. These methods require a special type of PVT cell to be used in measuring the gas diffusion into liquid systems as shown in Fig. 4.a. Various samples can be collected during running the diffusion experiment at different locations, through the valves shown in Fig 4.a. Then,
chromatographic analysis is used to determine the gas concentrations in liquid at different times. This technique, besides being very expensive, is considered to be time consuming and system-intrusive which can lead to experimental errors. Sigmund [98] was one of the pioneers who studied gas diffusion. He used a diffusion cell to measure binary molecular diffusion coefficients of gas mixtures at reservoir conditions. Juarez et al. [100] measured the effective diffusion coefficient of a gas, i.e. nitrogen, in a sand packed setup saturated with hexane by directly measure the concentrations of fluid samples collected at various times and distances during running the test. The direct method for estimating the gas effective diffusion coefficients in hexane showed acceptable results compared to a non-conventional method, i.e. pressure decay method, that will be explained in the next section.

3.2 Pressure decay method

The pressure decay method is considered the most applicable indirect method for measuring the gas diffusion in liquids. This method was first proposed by Riazi in 1996 [95]. This process of measuring the gas diffusion in any liquid starts with monitoring the decay in pressure of gas which is in a direct contact with a liquid. The system, i.e., gas and liquid, is sealed in a diffusion or PVT cell under isothermal conditions. The position of the interface separating the gas and liquid is also monitored as it can be changed due to gas dissolution and liquid swelling. Fig. 4.b shows the components of the PVT system used in running the pressure decay experiments. Recently, Janiga at al. [101] modified the pressure decay method by using acoustic pulse-echo technique along with measuring the pressure and volume changes in a gas-liquid system. The pulse-echo technique adds an advantage of measuring the location of the boundary/interface between two fluids of different densities, i.e., gas and liquid, though transmitting a wave and detecting its echo. Hence, the
volume changes due to gas diffusion into the underlying liquid can be easily measured. The main advantages of the pressure decay method are the simplicity of the application in laboratory and also it can be implemented over a wide range of gas types, i.e., solvents, and various liquids.

3.3 Constant pressure method

The constant pressure method or volume changing measurement was used by Renner to measure the diffusivity of CO$_2$ in both decane and brine [96]. The volume changing method is similar to the pressure decay method in the procedure. However, the only difference is that the gas is continuously supplied into the diffusion cell to keep the pressure of the system constant by pressurizing the gas cap and compensating the amount of gas dissolved into the liquid due to the diffusion and dissolution processes. While the amount of gas injected is monitored by recording the position of the pump, i.e., piston position, used to inject the gas from the supply cell or accumulator into the diffusion cell. The velocity of the interface separating the gas and liquid can be also measured to describe the diffusion process. The pressure changes in the supply cell are also monitored in this method. By the end of the experiment, the cumulative mass of gas withdrawn from the supply cell is calculated. The PVT setup shown in Fig. 4.b can be used to measure gas diffusion using the constant pressure method and the pressure decay method as well. The advantage of this method is that the boundary condition at the interface separating gas and liquid is not changing with time that makes the mathematical model used to interpret the experimental results more easier to solve [102].

3.4 Dynamic pendant drop shape/volume analysis method
The shape and the volume of a pendant drop of liquid surrounded by any type of gas are changing with time by the effect of gas diffusion. Gas diffusion also causes a change in the interfacial tension in a gas-liquid system. Yang and Gu introduced a new method to measure solvent diffusivity in heavy oils by using the dynamic pendant drop shape analysis (DPDSA) method [93]. In the DPDSA method, the dynamic changes in solvent concentrations inside the liquid phase, i.e., pendant drop, due to the diffusion process is related to the dynamic changes in the liquid drop shape and gas-liquid interfacial tension (IFT). In a later study, Yang and Gu could obtain the mass transfer parameters of CO₂ gas in a CO₂-crude oil by relating only the dynamic change in the interfacial tension (IFT) directly to the time-dependent CO₂ concentration distribution inside the oil phase [92]. One of the advantages of the DPDSA method is that a single test can be run within short time, e.g., one hour, and a small amount of liquid, e.g., oil or brine, is needed to run the test. Fig. 4.c shows the axisymmetric drop shape analysis system that is used to measure the IFT and determine the dynamic change in drop volume with time, and hence quantify gas diffusivity in liquids.

3.5 NMR and X-ray CT Methods

Nuclear magnetic resonance (NMR) and X-ray computed tomography (X-ray CT) methods are widely used to investigate dynamic process of fluid flow and also to observe the gas diffusion process in saturated porous media. Teng et al. [103] obtained the diffusion coefficient of CO₂ gas in n-decane saturated porous medium using variant NMR system. They could obtain the fluid concentrations from the monitored signal intensities. Then, image processing was used to determine the diffusion coefficients for different tests. Similarly, in X-ray CT method, the X-ray attenuation through the porous media is
measured by the CT and time-averaged images of density distributions in the porous medium are produced. Hence, fluids saturation profiles can be determined from the CT numbers of the rock samples saturated with different kinds of fluids [97, 104, 105]. The equipment the is usually used in these methods is a core flooding system equipped with CT scanner, as can be shown in Fig. 4.d. It should be noted that X-ray CT technology can easily distinguish between gas and liquid based on fluid densities during fluid flow compared to other imaging methods.

Table 2 summarizes most of the experimental methods used to measure gas diffusion in liquids. Additionally, limitations and advantages of each method are also listed in Table 2. It is important to mention here that the estimation of diffusion coefficient of solvent, e.g., CO₂ gas, in the liquid phase is interpreted by matching the results of a mathematical model describing the gas diffusion process in liquid with the experimentally measured data obtained from one of the above-mentioned laboratory methods. It should be also noted that most of the mathematical diffusion models are based on Fick’s law. In the following section, we briefly describe and summarize the mathematical models reported in the literature describing the gas molecular diffusion process.
Figure 4. Schematic diagrams of various experimental setups used in measuring gas diffusion: (a) PVT cell used in conventional measurements, (b) PVT setup used to run the pressure decay test (Reproduced with permission from [106]. Copyright [2019] Elsevier), (c) IFT and pendant drop shape measurement setup (Reproduced with permission from [106]. Copyright [2019] Elsevier), and (d) Core flooding system equipped with CT scan (Reproduced with permission from [19]. Copyright [2019] Elsevier).

Table 2. Commonly used experimental methods in measuring CO₂ diffusion coefficients.

<table>
<thead>
<tr>
<th>Experimental method</th>
<th>Description</th>
<th>Equipment</th>
<th>Limitations</th>
<th>Advantage</th>
<th>Reference</th>
</tr>
</thead>
</table>
| Concentration measurements           | The changes in gas concentration are measured versus time though | PVT cell (Fig. 4.a) | • System-intrusive.  
• Expensive.  
• Time consuming. | • Directly measure gas concentration distribution in a liquid phase. | [98, 100, 107]  |
<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
<th>Advantages</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure decay method</td>
<td>The decrease in the pressure of gas in a direct contact with a liquid is measured at a constant temperature. The pressure decay data is matched with a mathematical model to obtain the gas diffusion coefficient.</td>
<td>• Cannot detect small concentration changes. • The experiment can last for several days as in case of gas-heavy oil systems. • Natural convection can affect the diffusion results as in case of fluids such as light oil or saline water, or by introducing high gas injection rates into the diffusion cell during running the test. • Very sensitive to pressure and temperature fluctuation.</td>
<td>[84, 94, 108-112]</td>
</tr>
<tr>
<td>Volume changing measurement</td>
<td>The pressure is kept constant by continuously injecting the gas from the supply cell.</td>
<td>• Gas diffusivity measurement can take several days to acquire one set of volume/time · The mathematical model is easier to solve as the interface boundary</td>
<td>[96, 102]</td>
</tr>
</tbody>
</table>
| Dynamic pendant drop shape/volume analysis (DPDSA, DPDVA) | The dynamic and equilibrium IFT between liquid and surrounding solvent are measured and correlated to the change in solvent concentration with axisymmetric drop shape analysis system (Fig. 4.c) | Axisymmetric drop shape analysis | • Limited application at high pressures due to difficulty of holding the pendant drop.  
• Image analysis is needed to obtain accurate drop volume. | • Gas diffusion measurement duration is relatively low, i.e., several minutes or few hours.  
• Require small volumes of fluids in small volumes of fluid. | [92, 93, 113] |
time. Hence, the solvent diffusivity is obtained at certain conditions, i.e., pressure and temperature.

- Liquid vaporization cannot be ignored at high pressures, e.g., in CO$_2$-oil application.
- The measured oil volume changes due to gas diffusion make the numerical solution more complex.

| Nuclear magnetic resonance (NMR) and X-ray computed tomography (X-ray CT) methods |
| Gas diffusion process is observed by using NMR or CT to obtain dynamic fluid saturation profiles that are used to obtain fluid concentrations. |
| Core flooding system equipped with CT scan (Fig. 4.d). |
| Needs high resolution capabilities to be able to detect the diffusion process. |
| Requires image processing to accurately distinguish different phases. |
| The obtained results are highly dependent on the accuracy of the mixture density and gas concentration relationship. |
| Can be applied to measure gas diffusion during fluid flow in saturated porous media. |
| Fluid saturations and concentration profiles can be easily obtained from the measured data. |
| Does not require large volume of fluids to run a diffusion test. |

[103-105]
4. Mathematical models of gas diffusion

Gases and liquids are usually multi-component phases and when a gas and a liquid are in contact, the concentration gradient in the two separate phases causes the gas components to move into the liquid phase and vice versa, which is known as the two-way mass transfer process. Three stages can describe the molecular diffusion process in a gas-liquid system. First, a pure gas component tends to move towards the interface separating the gas and liquid phases. This stage is directly related to the diffusion coefficient within the gas phase. Then, the gas component crosses the gas-liquid interface towards the liquid phase. The mass transfer process across the interface is controlled by a parameter called interface mass transfer coefficient, \( k \), that describes the resistance at the interface [114]. The final stage is the gas diffusion within liquid phase which is controlled by the diffusion coefficient within the liquid phase, the \( D \) coefficient. The values of both coefficients (\( k \) and \( D \)) are essential to calculate the rate of gas dissolution in a liquid phase.

The mathematical models used to study the mass transfer process, i.e., molecular diffusion, are based on a set of governing partial differential equations (PDE) solved numerically or analytically by applying some specific boundary conditions. It was found that the accuracy of the mathematical model describing the diffusion process is considered to have the most influence on the value of the calculated gas diffusion coefficient. Therefore, the value of \( D \) coefficient mainly depends on the assumptions defined to develop the diffusion model. Unfortunately, most of the previously developed diffusion models defined oversimplified assumptions which directly affect the accuracy of the results.
and caused significant discrepancies in the reported mass transfer values even for the same systems [66].

Here, in this paper, we summarize the most common assumptions used in the previously developed diffusion models for various gas-oil systems, as shown in Fig. 5. The main assumption is for the operating temperature. Most of the diffusion models assumed an isothermal condition to follow the conditions of the applied experimental method. Although the liquids and gases are multi-component phases, they are considered as pure components or one pseudo-components in most of the previous models [93, 113, 115]. Limited studies considered the multicomponent system. Li et al. developed a mathematical model to obtain the individual diffusion coefficient of each component in a solvent mixture, i.e. CO₂ and C₃H₈ mixture, in CO₂-C₃H₈-heavy oil system [116]. They found that the presence of propane with carbon dioxide in the gas mixture resulted in a faster diffusion of CO₂ into the liquid phase. Li et al. [38] investigated CO₂ diffusion in a tight oil reservoir. Their results showed that characterizing the crude oil with three pseudo-components improved the diffusion model accuracy. Ignoring the oil swelling due to gas diffusion can lead to significant errors in the determined gas diffusion coefficients. Few studies in the literature have considered the oil swelling during investigating gas diffusion in crude oils [95, 115-118]. Zheng et al. developed a one-way mass transfer model to obtain the diffusion coefficient of gas mixture in heavy oil with considering the oil swelling effect [117]. They obtained both the apparent and individual diffusion coefficient of each component in the gas mixture by minimizing an objective function, i.e., root-mean-square relative error between the experimentally measured and numerically calculated oil swelling factors at various times during running the diffusion test. Rezk and Foroozesh developed a
model to accurately obtain mass transfer parameters and oil swelling rate at both supercritical and subcritical conditions by interpreting data of pressure decay tests with considering the mass transfer resistance at the gas-liquid interface [115]. They found that the values of mass transfer coefficients of gas are relatively higher in light oil compared to heavy oil. Additionally, considering the oil swelling highly affected the obtained mass transfer parameters. Although the diffusion coefficient (D) is dependent on the pressure, temperature, and the composition of the phases, that is more noticeable at supercritical conditions, D can be considered constant in petroleum engineering applications. This is because the reservoir temperature is usually constant and the order of magnitude of the pressure change in the reservoirs has a minor effect on the diffusion coefficient [119]. Nevertheless, limited studies investigated the concentration-dependent diffusion coefficient [95, 119-121]. Riazi developed a semi-analytical model to obtain a set of gas and liquid diffusion coefficients at various pressures and compositions [95]. The diffusion coefficient is not considered constant in his study, but pressure dependent. It can be noticed form the reported results in Riazi’s study that the variation of the diffusion coefficient value within the range of the experimental pressures is around 35% for both gas and liquid phases. Guo et al. [121] developed a mutual diffusion model to measure the diffusion coefficients in a gas-light oil system. Their model considers no resistance at the gas-oil interface (boundary condition at the interface). Their results showed that the diffusion coefficients, for N₂, CH₄, and CO₂, did not show a significant change within the pressure range of the experiments, i.e., 1-1.4 %. Although the developed model aimed to find the diffusion coefficient in gas and light oil phases, they could not determine the gas-liquid interface velocity due the change in the volume of oil. Ghaderi et al. investigated the
mathematical modeling of gas diffusion process through an approximate analytical model with concentration-dependent diffusion coefficient [120]. The non-linear diffusion problem was solved using the Heat Integral Method and the results were verified using numerical solutions. One of the most important and argumentative assumption considered in the literature is the boundary condition at the gas-liquid interface. In general, three types of boundary conditions were assumed at the liquid-gas interface. The first type is called the equilibrium boundary condition. That is, the concentration of gas at the interface is assumed to be equal to the saturation concentration of gas at equilibrium pressure, $C_{\text{sat}}(P_{\text{eq}})$ [96, 122]. The second case is called quasi-equilibrium boundary condition and assumes that the interface will be saturated with the gas based on the system pressure. That is, the concentration of gas at the liquid-gas interface depends on the pressure of the system which changes with time [94, 119]. The third type, which is called non-equilibrium boundary condition, the flux of the mass transfer of gas at the liquid-gas interface is directly proportional to the difference between the concentration of gas at the equilibrium condition, $C_{\text{sat}}(P_{\text{eq}})$, and the concentration of gas at current conditions, $C(x,t)$. The non-equilibrium boundary condition is also known as Robin boundary condition [123, 124]. The non-equilibrium boundary condition is the most reliable boundary condition at the gas-liquid interface as it considers the resistance to the gas diffusion across the interface.
Figure 5. Mathematical model assumptions used in the previously developed diffusion models for gas-oil systems.

A summary of lab measurement method, experimental conditions, and molecular diffusion models, used in previous studies to measure CO$_2$ diffusivity in light and heavy crude oils, is tabulated in Table 3. It is obvious from Table 3 that most of the previous studies used the pressure decay method to measure CO$_2$ diffusion in liquids. The molecular diffusion models, summarized in Table 3, are all based on Fick’s model. Most of the previous studies that used the pressure decay method considered the diffusion process in a 1-D cartesian coordinate system. While, other studies used the dynamic pendant drop method, considered gas diffusion into liquids in 2-D cylindrical coordinate system. The
mathematical solution to the diffusion model is divided between analytical and numerical methods. The mass transfer parameters are obtained through minimizing an objective function that represents the error between the experimentally measured and theoretically calculated system property such as: system pressure, mass of gas dissolved in liquid phase, mole fraction of gas component in the liquid, and dynamic volume of liquid or swelling factor, as can be shown in Table 3. Previous studies showed that the CO₂ diffusion coefficient in crude oils is related to system conditions, i.e., pressure and temperature, and oil composition, i.e., light or heavy oil. It was clearly proved that the CO₂ diffusion coefficient increases with pressure and the effect of pressure on the diffusion coefficient is more sensitive at high temperatures. Nevertheless, at very high pressure values, the density and viscosity of the liquids increase that can lead to a decrease in the diffusion coefficient [69]. Increasing the system temperature also shows a positive effect on the calculated gas diffusion coefficients in crude oils. That can be justified by the reduction in oil viscosity at higher temperatures which leads to easier mass transfer of gas across the gas-oil interface. Hence, CO₂ diffusion coefficient is higher in CO₂-light oil systems compared to CO₂-heavy oil, as can be seen in Table 3. It is important to mention here that not only the system conditions, oil composition, and lab measurement method affect the CO₂ diffusion coefficient, the mathematical model assumptions and the used objective function can also lead to a significant difference in the obtained D coefficients [125].

One can notice from Table 3 that most of the diffusion tests were carried out using heavy oil samples (presented in the top rows), while the data available for light oils (presented in the bottom rows) are very rare. Furthermore, the effect of oil swelling has been ignored in most of the previous diffusion models. It has been also noticed that limited
studies considered both the effect of oil swelling due to CO$_2$ diffusion and the resistance across the CO$_2$-oil interface, i.e. non-equilibrium boundary condition at the interface, in a diffusion model [115].
Table 3. Summary of experimental conditions, diffusion models, and calculated mass transfer parameters of CO₂ in heavy and light crude oils.

<table>
<thead>
<tr>
<th>Researcher, reference</th>
<th>Test method</th>
<th>Mathematical model</th>
<th>Governing Equation</th>
<th>Objective function, E</th>
<th>Interface boundary condition</th>
<th>Oil sample, API gravity</th>
<th>Oil viscosity (cP)</th>
<th>Pressure (KPa), Temperature (°C)</th>
<th>Calculated diffusion coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yang and Gu [93]</td>
<td>Pendant Drop</td>
<td>Numerical</td>
<td>( \frac{\partial C}{\partial \tau} = \frac{1}{R} \frac{\partial}{\partial R} \left( R \frac{\partial C}{\partial R} \right) + \frac{\partial^2 C}{\partial Z^2} )</td>
<td>( E = \frac{1}{N \times M} \sum_{j=1}^{M} \sum_{i=1}^{N} d \left[ \left( r_{m} \left( t_{j} \right), z_{m} \left( t_{j} \right) \right) \right] )</td>
<td>Non-equilibrium</td>
<td>Heavy oil, 23.8 API</td>
<td>/</td>
<td>2900 KPa, 25°C</td>
<td>( D = 1.14 \times 10^{-9} ) m²/s</td>
</tr>
<tr>
<td>Sheikha et al. [126]</td>
<td>Pressure decay</td>
<td>Analytical</td>
<td>( P(t) = P_i \exp \left( \frac{\sqrt{D ZRT \sqrt{E}}}{LMK_h} \right)^2 \text{erf} \left( \frac{\sqrt{D ZRT \sqrt{E}}}{LMK_h} \right) )</td>
<td>Relative error in the predicted pressure data versus time.</td>
<td>Quasi-equilibrium</td>
<td>Bitumen, 8.6 API</td>
<td>106000</td>
<td>4000, 3960 KPa, 75, 90 °C</td>
<td>( D = 0.46, 0.79 \times 10^{-9} ) m²/s</td>
</tr>
<tr>
<td>Upreti and Mehrotra [127]</td>
<td>Pressure decay</td>
<td>Numerical</td>
<td>( \frac{\partial C}{\partial \tau} = D \left( 1 + \frac{C}{\rho_b} \right) \frac{\partial^2 C}{\partial Z^2} + \left( 1 + \frac{C}{\rho_b} \right) \frac{\partial D}{\partial C} + \frac{D}{\rho_b} \left( \frac{\partial C}{\partial Z} \right)^2 )</td>
<td>( E = \frac{1}{t} \int_0^t \left[ \frac{\left( m_{b,calc} \right)^2}{m_{b,exp}} \right] dt )</td>
<td>Quasi-equilibrium</td>
<td>Bitumen, 9.1 API</td>
<td>767</td>
<td>4000 KPa, 25-90 °C</td>
<td>( D^* = 0.16-0.47 \times 10^{-9} ) m²/s</td>
</tr>
<tr>
<td>Upreti and Mehrotra [119]</td>
<td>Pressure decay</td>
<td>Numerical</td>
<td>( \frac{\partial C}{\partial \tau} = D \left( 1 + \frac{C}{\rho_b} \right) \frac{\partial^2 C}{\partial Z^2} + \left( 1 + \frac{C}{\rho_b} \right) \frac{\partial D}{\partial C} + \frac{D}{\rho_b} \left( \frac{\partial C}{\partial Z} \right)^2 )</td>
<td>/</td>
<td>Quasi-equilibrium</td>
<td>Bitumen, 9.1 API</td>
<td>821000</td>
<td>4000 KPa, 25-90 °C</td>
<td>( D^* = 0.13-0.43 \times 10^{-9} ) m²/s</td>
</tr>
<tr>
<td>Authors</td>
<td>Type</td>
<td>Method</td>
<td>Equation</td>
<td>Equilibrium</td>
<td>Bitumen</td>
<td>Pressure</td>
<td>Bitumen</td>
<td>Temperature</td>
<td>Temperature</td>
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</tr>
<tr>
<td>Etminan et al. [102]</td>
<td>Constant pressure</td>
<td>Analytical</td>
<td>( \frac{dm_{gb}}{dt} = -D A \frac{\partial c}{\partial z} ) at interface</td>
<td></td>
<td></td>
<td></td>
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<td></td>
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<td>( m_{gb} ) is mass of gas diffuse to the liquid phase</td>
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<td></td>
<td></td>
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<td>( E = \sum_{i=1}^{n_g} (m_{gfr}(t_i) - m_{gb}(t_i))^2 )</td>
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<td></td>
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<td></td>
<td>( m_{gfr} ) is mass of gas transferred to diffusion cell</td>
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<tr>
<td>Li and Yang [128]</td>
<td>Pressure decay</td>
<td>Numerical</td>
<td>( \frac{\partial c_1}{\partial t} = D_{11} \frac{\partial^2 c_1}{\partial x^2} + D_{12} \frac{\partial^2 c_1}{\partial x^2} )</td>
<td>Quasi-equilibrium</td>
<td></td>
<td>10 API</td>
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<td>( \frac{\partial c_2}{\partial t} = D_{21} \frac{\partial^2 c_1}{\partial x^2} + D_{22} \frac{\partial^2 c_2}{\partial x^2} )</td>
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<tr>
<td></td>
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<td></td>
<td>The subscripts 1 and 2 stand for CO₂ and solvent gases, respectively.</td>
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</tr>
<tr>
<td>Yang and Gu [113]</td>
<td>Pendant Drop</td>
<td>Numerical</td>
<td>( \frac{\partial C}{\partial \tau} = \frac{1}{R} \frac{\partial}{\partial R} \left( R \frac{\partial C}{\partial R} \right) + \frac{\partial^2 C}{\partial Z^2} )</td>
<td>Equilibrium</td>
<td>Lloydminster</td>
<td>11.7 API</td>
<td>24 °C</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( E = \sum_{i=1}^{m} \left[ x_{cal}(i) - x_{exp}(i) \right]^2 )</td>
<td></td>
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<td></td>
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<td></td>
<td>( n_g ) is the number of gas phase components.</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>( x_{cal} ) and ( x_{exp} ) are the calculated and measured mole fractions of ith component in the liquid phase at the end of the test.</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Zhang et al. [94]</td>
<td>Pressure decay</td>
<td>Analytical</td>
<td>( \frac{dC}{dt} = D \frac{\partial^2 C}{\partial Z^2} )</td>
<td>Equilibrium</td>
<td>Heavy oil</td>
<td>5000</td>
<td>3510 KPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>C is the molar concentration of gas in oil.</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>Numerical curve fitting of measured pressure data.</td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unatrakarn et al. [129]</td>
<td>Pressure decay</td>
<td>Analytical</td>
<td>( \frac{dC}{dt} = D \frac{\partial^2 C}{\partial X^2} )</td>
<td>Non-equilibrium</td>
<td>Heavy oil 1</td>
<td>21285</td>
<td>2666-2415 KPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>( E = \Delta P_{av} = \sqrt{\frac{1}{m} \sum_{i=1}^{m} \left[ P_{cal}(t) - P_{exp}(t) \right]^2} )</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>( m ) is the number of measured pressure points.</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

**Note:** The table provides a summary of various experimental setups and the equations used to analyze the pressure decay data. The authors and their respective methods are listed, along with the equations used to calculate the mass transfer, equilibrium conditions, and pressure decay rates. The table also includes the bitumen properties and pressure decay data for different conditions.
<table>
<thead>
<tr>
<th>Name</th>
<th>Method</th>
<th>Equation</th>
<th>Type</th>
<th>Pressure</th>
<th>Temperature</th>
<th>Diameter D</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Janiga et al. [101]</td>
<td>Pulse-echo pressure-volume decay</td>
<td>$\frac{\partial C(z, t)}{\partial t} = D \frac{\partial^2 C(z, t)}{\partial z^2}$</td>
<td>Equilibrium</td>
<td>Heavy oil, 17.3 API</td>
<td>1050</td>
<td>4100 KPa</td>
<td>D = 58-68 x $10^{-9}$ m/s</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$O(t) =</td>
<td>n^c(t) - n^o(t)</td>
<td>$</td>
<td></td>
<td>23 °C, 30 °C, 40 °C</td>
<td></td>
</tr>
<tr>
<td>Zhou et al. [130]</td>
<td>Pressure decay</td>
<td>$\frac{c(x, t)}{c_{sat}(P_{eq})} = 1 - \sum_{n=1}^{\infty} \frac{\sin(\lambda_n)}{2\lambda_n + \sin(\lambda_n)} \cos(\lambda_n x L) e^{-D \lambda_n^2 t}$</td>
<td>Non-equilibrium</td>
<td>Heavy oil, 14.2 API</td>
<td>2200</td>
<td>5000 KPa</td>
<td>D = 5.778 x $10^{-9}$ m/s</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$E = \Delta P_{ave} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (P_{i}^{calc} - P_{i}^{lab})^2}$</td>
<td></td>
<td>21 °C</td>
<td></td>
<td>De = 3.22 x $10^{-9}$ m/s</td>
<td></td>
</tr>
<tr>
<td>Jang et al. [131]</td>
<td>Dynamic volume analysis</td>
<td>$\frac{dc}{dt} = \frac{\partial}{\partial x} \left[ D(c) \frac{dc}{dx} \right]$</td>
<td>Equilibrium Lloydminster heavy oil</td>
<td>/</td>
<td>3950 kPa</td>
<td>D* = 2.51 - 8.62 x $10^{-10}$ m/s</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(constant pressure method)</td>
<td>$E = AARD = \frac{1}{ND} \sum_{m=1}^{N} \frac{</td>
<td>x_{calc}^{m} - x_{exp}^{m}</td>
<td>}{x_{exp}^{m}} \times 100%$</td>
<td></td>
<td>21.4 °C</td>
<td></td>
</tr>
</tbody>
</table>
| Fayazi and Kantzas [132] | Constant pressure method | Numerical | Fick’s first law and continuity equation | $E = O(D_{so}, D_{os}) = \sum_j \sum_i w_s^{exp}(x_i, t_j) - w_s^{model}(x_i, t_j)$ | Equilibrium | Heavy oil | 2859, 4238, and 5617 KPa | 35 ℃ | For P = 2859 KPa, $D_{os}$ and $D_{so} = 1.15$ and $2.7 \times 10^{-9}$ m$^2$/s
For P = 4238 KPa, $D_{os}$ and $D_{so} = 0.95$ and $2.7 \times 10^{-9}$ m$^2$/s
For P = 2859 KPa, $D_{os}$ and $D_{so} = 0.75$ and $2.7 \times 10^{-9}$ m$^2$/s |
<p>| Ssebadduka et al. [65] | Swelling-time curve | Analytical | $R(t) = 1 - \frac{8}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{(2n - 1)^2} \exp(-D\lambda^2t)$ | $R(t)$ unit ratio of cumulative dissolved gas at t, $\lambda$ is variable (m$^{-1}$) | Equilibrium | Medium and heavy dead oil samples (API = 35-97) | 100 KPa | 50 ℃ | $D_{medium \ oil} = 35-97 \times 10^{-9}$ m$^2$/s |</p>
<table>
<thead>
<tr>
<th>Authors</th>
<th>Type</th>
<th>Equation</th>
<th>Description</th>
<th>Pressure (KPa)</th>
<th>Temperature (°C)</th>
<th>Diffusivity (m²/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wang and Hou [110]</td>
<td>Pressure decay Analytical</td>
<td>( \frac{\partial C(t, h)}{\partial t} = D \frac{\partial^2 C(t, h)}{\partial x^2} )</td>
<td>Equilibrium Crude oil</td>
<td>40.27, 13.06</td>
<td></td>
<td>0.61 - 1.6 x 10⁻⁹ m²/s</td>
</tr>
<tr>
<td>Rezk and Foroozesh [63]</td>
<td>Pressure decay Numerical</td>
<td>( \frac{\partial C_{CO_2}(x, t)}{\partial t} = D \frac{\partial^2 C_{CO_2}(x, t)}{\partial x^2} ), ( 0 \leq x \leq L(t) ) and ( t &gt; 0 ) ( \frac{dL(t)}{dt} = \frac{M_{wt_{CO_2}}}{\rho_{CO_2}} D \frac{\partial C_{CO_2}(x, t)}{\partial x} )</td>
<td>Non-equilibrium Light oil</td>
<td>2.21</td>
<td>6340, 13730 KPa</td>
<td>D = 57 - 80 x 10⁻⁹ m²/s</td>
</tr>
<tr>
<td>Guo et al. [121]</td>
<td>Pressure decay Numerical</td>
<td>( \frac{dC_{oi}}{dt} = \frac{\partial}{\partial x_o} \left[ D_{oi} \frac{dC_{oi}}{dx_o} \right] ), ( \frac{dC_{gi}}{dt} = \frac{\partial}{\partial x_g} \left[ D_{gi} \frac{dC_{gi}}{dx_g} \right] )</td>
<td>Equilibrium Light oil</td>
<td>/</td>
<td>20000 KPa</td>
<td>D² = 0.01852 - 0.01869 x 10⁻⁹ m²/s</td>
</tr>
<tr>
<td>Araujo et al. [104]</td>
<td>Pressure decay Analytical</td>
<td>( \frac{dC}{dt} = D \frac{\partial^2 C}{\partial Z^2} )</td>
<td>Non-equilibrium Light oil</td>
<td>/</td>
<td>2760 - 28960 KPa</td>
<td>D = 62.1 - 29.1 x 10⁻⁹ m²/s</td>
</tr>
</tbody>
</table>
\[
\frac{dC_i}{dt} = D_{ii} \frac{\partial^2 C_i}{\partial X_i^2} \\
\frac{dC_g}{dt} = D_g \frac{\partial^2 C_g}{\partial X_g^2} \\
SF(t) = \frac{V(t)}{V_o} \times \frac{1}{1 - s(t)}
\]

\(C_i, C_g\) are the concentration of \(i\)th component in oil and concentration of oil in gas phase, respectively. 
\(D_{ii}, D_g\) are the diffusion coefficient of \(i\)th component in oil, and diffusion coefficient of oil in gas, respectively. 
\(SF(t)\) is the dynamic swelling factor, \(V_o\) is the initial volume of oil, \(V(t)\) is the volume of oil + diluted solvent, and \(s(t)\) is the mole fraction of gas components diluted in the oil.

\[
E_1 = \sqrt{\frac{1}{ND} \sum_{i=1}^{NG} \left( \frac{SF_{calc} - SF_{exp}}{SF_{exp}} \right)^2}
\]

\[
E_2 = \sqrt{\frac{1}{NG} \sum_{i=1}^{NG} \left( \frac{y_{calc} - y_{exp}}{y_{exp}} \right)^2}
\]

\(ND\) and \(NG\) are the number of measured dynamic swelling factors points collected, and number of gas components in the gas phase. 
\(SF_{calc}\) and \(SF_{exp}\) are the calculated and measured dynamic swelling factors for the \(i\)th measured data point, respectively. 
\(y_{calc}\) and \(y_{exp}\) are the calculated and measured gas composition of the \(i\)th component, respectively.

* concentration-dependent diffusion coefficient
5. Empirical correlations of gas diffusion coefficients

In general, empirical correlations are widely used in practice due to their simplicity compared to numerical and analytical solutions to diffusion equations. Diffusion coefficients of gases in liquids can be calculated by using empirical correlations which is based on binary diffusion coefficients and system properties. The proposed correlations in the literature were derived from experimental measurements at different conditions and based on different mathematical models with various assumptions. Thus, large discrepancies can be observed between different correlations even for the same system. Some of the commonly used correlations to find gas diffusion coefficients in liquids are shown in Table 4.

It is important to note that the empirical correlations are developed based on limited experimental conditions and experimental data. Additionally, some correlations show contradicting trends for the effect of pressure and temperature on the gas diffusivity. For example, in Table 4, Renner showed an increasing trend of D coefficient with pressure, while Wilke and Chang reported that the diffusion coefficient is not directly dependent on the operating pressure. Therefore, it can be concluded that more experimental efforts are needed to accurately determine the gas diffusivity in crude oils during EOR processes and correctly predict oil recoveries. Nevertheless, empirical correlations can be used when experimental tests cannot be carried out.
Table 4. Empirical correlations of gas diffusion coefficient in liquids.

<table>
<thead>
<tr>
<th>Researcher, reference</th>
<th>Correlation</th>
<th>Main controlling variables</th>
</tr>
</thead>
</table>
| Wilke and Chang [134] | $D_{im} = \frac{7.4 \times 10^{-6} M_{im}^{0.5} T}{\mu_m V_{bi}^{0.6}}$ | • Molecular weight  
• Temperature  
• Mixture viscosity  
• Partial molar volume |
|                       | $M_{im} = \frac{\sum_j y_{jm} M_j}{1 - y_{im}}$, $V_{bi} = 0.285 V_c^{1.048}$ | |
|                       | $D_{im}$ is the diffusion coefficient of component $i$ in a mixture, i.e., multi-component system.  
$M_{im}$ and $V_{bi}$ are the molecular weight and the partial molar volume at the boiling point of component $i$, respectively. $\mu_m$ and $T$ are the mixture viscosity (cp) and the temperature (K), respectively. $y_{im}$ is the mole fraction of component $i$, and $V_c$ is the critical volume. | |
| Sigmund [98]          | $\frac{\rho_M D_{ij}}{\rho_{bi} \ D_{ij}^0} = 0.99589 + 0.096016 \rho_{Mr} - 0.22035 \rho_{Mr}^2 + 0.032874 \rho_{Mr}^3$ | • Pressure  
• Temperature  
• Pseudoreduced mixture density |
|                       | $\rho_{Mr} = \rho_M \frac{\sum_i y_{im} v_{ci}^{5/3}}{\sum_i y_{im} v_{ci}^{2/3}}$ | |
|                       | $\rho_M D_{ij}^0 = \frac{2.2648 \times 10^{-5} T^{0.5} \delta_{ij} \Omega_{ij}}{\sigma_{ij}^{0.5} \Omega_{ij}} \left[\frac{1}{M_i} + \frac{1}{M_j}\right]^{0.5}$ | |
|                       | where $\rho_M D_{ij}$ is the mixture density and diffusion coefficient product, the superscript 0 indicates a low pressure, and $\rho_{Mr}$ is the pseudoreduced mixture density, $n_c$ is the components number, $v_{ci}$ is the critical volume of component $i$, and $\rho_M$ is the density of the mixture. $\sigma_{ij}$ is the Leonard-Jones potential of components $i$ and $j$, $M$ is the molecular weight, and $\Omega_{ij}$ is the collision integral of components $i$ and $j$. | |
| Chapman and Cowling [37] | $D = \frac{1.86 \times 10^{-3} T^{2} \frac{2}{M_1} + \frac{1}{M_2}^{0.5}}{P \delta_{12}^{2} \omega}$ | • Pressure  
• Temperature |
Their theory is based on the concept that collisions occurred between two molecules at the same time during diffusion interaction.

Renner [96] Generalized equation to estimate the effective diffusion coefficient of CO\textsubscript{2} and light hydrocarbons in reservoir fluids:

\[ D_i = 10^{-9} \mu_o^{-0.4562} M_i^{-0.6898} \rho_{Mi}^{1.706} T^{4.524} P^{-1.83} \]

where \( D_i \) is the diffusion coefficient of component \( i \) in cm\(^2\)/s, \( \mu_o \) is the viscosity of oil in cp, \( M_i \) is the molecular weight of component \( i \), \( \rho_{Mi} \) is molar density of component \( i \) in gmol/cm\(^3\), \( T \) is reservoir temperature in K, and \( P \) is reservoir pressure in psia.

Empirical equation to measure the diffusivity of CO\textsubscript{2} in a brine phase:

\[ D_{CO2-H2O} = 6391 \mu_{CO2}^{-0.1584} \mu_{H2O}^{6.911} \]

where \( \mu_{CO2} \) and \( \mu_{H2O} \) are the viscosities of carbon dioxide and water, respectively.

Lv et al. [135] Empirical equation for the supercritical CO\textsubscript{2} diffusion coefficient in n-decane-saturated porous media:

\[ D = 10^{-10} \times P^{3.1078} \times T^{0.9337} \times \mu^{-2.6558} \]

\( P \) denotes the pressure, MPa; \( T \) presents the temperature, K, \( \mu \) is hydrocarbon viscosity, cp.

Li et al. [136] Empirical equation for the CO\textsubscript{2} diffusion coefficient in brine saturated core at reservoir conditions

- Oil viscosity
- Molecular weight
- Molar density
- Temperature
- Pressure
- Brine viscosity
- CO\textsubscript{2} viscosity
- Pressure
- Temperature
- Viscosity
- Pressure
- Temperature
<table>
<thead>
<tr>
<th>Ssebadduka et al. [65]</th>
<th>Empirical equation used to estimate the CO₂ gas diffusion coefficient using the oil viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ D = 0.19122 \times T^{0.4681} \times P^{0.51717} ]</td>
<td></td>
</tr>
<tr>
<td>P denotes the pressure, MPa; T presents the temperature, °C</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>McManamey and Woollen [137]</th>
<th>Empirical equation used to estimate the CO₂ gas diffusion coefficient using oil viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ D = 36.24 \times 10^{-6} \mu_\text{oil}^{-0.47} ]</td>
<td></td>
</tr>
<tr>
<td>( \mu_\text{oil} ) is the oil viscosity (cP)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Thomas and Adams [138]</th>
<th>Empirical equation used to estimate the CO₂ gas diffusion coefficient using in water</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ D = 5.72 \times 10^{-8} \frac{T}{\mu_\text{water}} ]</td>
<td></td>
</tr>
<tr>
<td>T is the temperature of the system (K), ( \mu_\text{water} ) is the water viscosity (cP)</td>
<td></td>
</tr>
</tbody>
</table>

6. **Determination of gas diffusivity using molecular dynamics simulation**

Molecular dynamics simulation (MD) is a computer simulation method for analyzing the physical movements of atoms and molecules. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic "evolution" of the system. In the most common version, the trajectories of atoms and molecules are determined by
numerically solving Newton's equations of motion for a system of interacting particles, where forces between the particles and their potential energies are often calculated using interatomic potentials or molecular mechanics force fields. MD simulation is used by many researchers in the oil and gas industry as an alternative economical method for the measurement of CO$_2$ diffusion at different pressure and temperature variation, also the effect of rock mineral, water content, and ions can be easily controlled in the MD simulation [139-146].

Two types of diffusion coefficients can be measured using the MD simulation, namely self-diffusion coefficient ($D_s$) and Fickian diffusion coefficient ($D_t$). The self-diffusion coefficient is generally measured by microscopic techniques, which cover the average mean-square displacement (MSD) of individual molecules over time. It can also be calculated based on the Einstein diffusion Eq. (10).

$$D_s = \frac{1}{6N} \lim_{t \to \infty} \frac{1}{t} \left\langle \sum_{i=1}^{N} [r_i(t) - r_i(0)]^2 \right\rangle$$

(10)

where $D_s$ represents the self-diffusion coefficient, $N$ is the number of diffusing molecules, $r_i(t)$ is the displacement vector of the molecule $i$ at time $t$, and the angular bracket means that the quantity is an ensemble average property. On the other hand, the transport or Fickian diffusion coefficient ($D_t$) is mostly used for practical applications and it is typically measured by macroscopic techniques, and it can be related to the self-diffusion coefficient as below in Eq. (11).
\[ D_t = D_s \times \frac{\partial \ln f}{\partial \ln c} \bigg|_t \]  
(11)

where \( \frac{\partial \ln f}{\partial \ln c} \bigg|_t \) is a thermodynamic factor.

In the literature, many efforts have been made to measure the self-diffusion coefficient of CO\(_2\) at different temperatures, pressures, and formation types. Zhao et al. [141, 142] and Hu et al. [143] found that the self-diffusion coefficient of CO\(_2\) in coal increased with temperature while conflicting findings were reported about the effect of pressure on CO\(_2\) diffusion in coal [140-142]. Similarly, Aliu et al. [145] studied self-diffusion coefficient of CO\(_2\) in oil-brine-sandstone systems at various pressures and temperatures and the sole CO\(_2\) diffusion coefficient in brine with different ions at a fixed temperature and pressure. They found that an increase in pressure and temperature leads to an increase in the diffusion coefficient of CO\(_2\) in oil-brine-sandstone systems. On the other hand, in the CO\(_2\)-brine system, the variations of ions affected CO\(_2\) diffusion, and the Ca ion appeared to result in the highest diffusivity of CO\(_2\) in brine. Babaei et al. [144] used MD simulation to determine composition-dependent self-diffusion coefficients for a multicomponent fluid system in a synthetic fractured reservoir during CO\(_2\) injection and similar effort made by Zabala et al. [139] using MD simulation to determine the Fickian diffusion coefficient of CO\(_2\)/n-alkane binary liquid mixtures. It worth mentioning that the MD simulation is not widely used in the oil industry yet as it is mathematically ill-conditioned generating cumulative errors in numerical calculation, thus proper selection of the algorithms and parameters is still needed.

7. CO\(_2\) dispersion in porous media
Dispersion is one of the mass transport mechanisms which contributes to the mixing process between the solute and resident fluid in porous media. There are two main phenomena causing solute dispersion, which are, diffusion and mechanical mixing [44, 147]. Diffusion is solute-dependent, while mechanical mixing is solute-independent. The mechanical mixing is governed by the physical properties of the porous medium, i.e., porosity, and dispersivity, and flow velocity [147]. The dispersion coefficient is a function of the solute diffusion and mechanical mixing within the solvent, and it can be written mathematically as shown in Eq. (12).

\[ D_{dis} = D^\ast + \alpha v_i^n \]  

(12)

Where \( D_{dis} \) is the dispersion coefficient \((L^2.T^{-1})\), \( D^\ast \) the effective diffusion coefficient \((L^2.T^{-1})\), \( \alpha \) is formation dispersivity \((L)\), i.e., a measure of the physical heterogeneity of the media, and \( v_i \) is the advective velocity in the direction of maximum flow \((L.T^{-1})\), \( n \) is an empirically constant, and usually has the value between 1 to 2 [148]. In most applications, the exponent, \( n \), is assumed to be unity where dispersion coefficient is a linear function of fluid velocity. However, \( n \) may be greater than unity in many situations [149].

In the case of low permeability formations (e.g., shale or tight formations), dispersion is governed mainly by molecular diffusion since zero or small velocity is reported. On the other side, when the reservoir permeability is high, dispersion is governed by mechanical mixing since usually they have substantial value compared to diffusion coefficient [147]. Mechanical mixing is defined as the spatial spreading of a solute inside a porous medium, due to velocity variations and the splitting of the flow path, i.e., formation tortuosity. When a fluid flows through a porous medium, its velocity distribution is not uniform due to boundary effects; i.e., the velocity is zero on the solid surface, which creates a velocity
gradient in the fluid phase [44, 147]. Fig. 6 illustrates the factors that control the mechanical dispersion in porous media. The mechanical mixing can be in the direction of bulk flow (longitudinal mechanical mixing), and in the directions orthogonal to the bulk flow (transverse mechanical mixing), however, under most conditions transverse mechanical mixing is observed to be much less significant than longitudinal mechanical mixing [147, 150, 151].

Figure 6. Factors lead to mechanical mixing in a porous medium. a,b) nonuniform velocity profiles along individual pores, and c) tortuosity of flow paths.

Hughes et al. [152] have conducted some lab experiments to measure CO$_2$-CH$_4$ longitudinal dispersion coefficient ($k_l$) during enhanced gas recovery (EGR) process over a range of temperature, pressure, velocity, and rock core permeability values [152]. They have used two Berea core samples (one long, one short) and two Donnybrook core samples (one long, one short). The apparent $k_l$ was measured at a horizontal level by matching CO$_2$ production profile to the prediction by the one-dimensional advective–dispersion equation. The dispersivity constant $\alpha_L$ was calculated using a corrected dispersion coefficient ($k_{corr}$) and it is values was found to be 0.0001 m and 0.00025 m for the Berea core and the Donnybrook core, respectively. This low dispersivity values indicates that excessive mixing will not occur in EGR scenarios in the absence of conformance effects such as
heterogeneity coupled with injection well pattern [152]. Honari et al. [153] have repeated the same experiments using a pulse injection measurement apparatus as to minimize the effects of density and concentration gradients. The dispersivity values for the Berea and the Donnybrook rocks were found to be 0.00035 m and 0.00131 m, respectively.

Uddin et al. [154] used a mathematical modeling approach to accurately predict the long-term partitioning and distributions of CO$_2$ in a selected simultaneous but separate injection of water and gas (SSWG) area of 2.15 km$^2$ in the Weyburn CO$_2$-EOR field. The CO$_2$ dispersion was predicted using the compositional CMG-GEM simulator with brine chemistry and semi-reactive transport options. In the simulations, the total dispersion coefficient was predicted for every time step by combining diffusion and mechanical mixing processes. Diffusion was relatively small whereas the mechanical dispersion could vary by a few orders of magnitude depending on the flow velocity and flow length (scale dependent). The matching parameters for primary and secondary water-flood were based on tuning of capillary pressure and relative permeability, while the dispersion parameters, i.e., longitudinal and transverse dispersivity, were dominant in history matching of the field CO$_2$ plumes and they were found to be 10 m and 2 m, respectively. The numerical simulations systematically demonstrated that the mechanical dispersion plays a critical role in the performances of CO$_2$-EOR and subsequent CO$_2$ geological storage [154]. Coats et al. [155] explained why rock physical dispersivity should be considered in reservoir numerical simulation studies. They have mentioned that the physical dispersivity ($\alpha_p$) is a rock property in the order of 0.01 ft for consolidated rocks and is significantly smaller for unconsolidated sand packs. $\alpha$ reflects microscale heterogeneity and is independent of time and scale, regardless of whether the scale is defined as system length, distance traveled, or
scale of heterogeneity. They have introduced the term apparent dispersivity \( (\alpha_a) \) which reflects (macroscale) heterogeneity and is scale-dependent and it is obtained by matching the observed or a numerically calculated effluent concentration curve to the prediction of 1D convective-diffusive equation. It reflects areal and vertical conformance that both are dependent upon well pattern, completion intervals, heterogeneity, and drift. \( \alpha_a \) can be expressed mathematically as \( \alpha_a = \alpha_p + \alpha_{ac} \), where \( \alpha_{ac} \) is the apparent dispersivity due to conformance.

Mahadevan et al. [156] have used three types of dispersion mixing in permeable porous media to obtain realistic estimates at field scale dispersion. The different types included echo dispersivity which was measured from single well tracer test (SWTT), transmission dispersivity which was a result from layering in the formation, and local dispersivity which was the mixing observed at a point as tracer flows past. They have employed reservoir simulation to perform an injection and production on a 2D uniformly layered permeable medium. Each layer was homogenous with an input longitudinal dispersivity equal to 0.46 m and an input transverse dispersivity equal to 0.046 m. The history match of concentration equation gave transmission dispersion of 2.47 m which was relatively larger than the simulator longitudinal dispersivity. They found that the local dispersivity is always less than the transmission dispersivity and greater than the echo dispersivity. John et al. [157] used the idea of flow reversal to resolve the ambiguity between convective spreading driven by permeability heterogeneity and the in-situ mixing (mechanical dispersion). They have simulated flow-reversal tests (echo dispersivity) for tracer transport in several permeability realizations using particle-tracking simulations along with 3D high-resolution models at the field-scale. They have studied the influence
of permeability heterogeneity, permeability anisotropy, core-scale, and residence time on in-situ mixing. Likewise, they have compared the dispersivities estimated from their simulations to those measured from field tests. They have shown that convective spreading, even without local mixing, can result in dispersion-like mixing-zone because of permeability heterogeneity. However, for such cases, the dispersivity estimated on flow reversal was zero. With local mixing (diffusion or core-scale dispersion), the dispersivity value on flow reversal was nonzero and much larger than that in typical core values. Additionally, they have reported that layering in permeability, while increasing the convective contribution to transport, also enhances mixing by providing a larger area in the transverse direction for diffusion to act. They concluded that dispersivity values increase with scale mainly because of the increases in the connections in the permeability field.

Schulze-Makuch [158] have compiled longitudinal dispersivity ($\alpha$) of 307 determinations retrieved from a total of 109 different studies for different types of geological media. The data were subdivided into different subsets. Dispersivity values for consolidated media were subdivided as basalts, granites, sandstones, and carbonate rocks, while unconsolidated sediments were subdivided into three reliability classes (low, intermediate, high) based on certain criteria. The objective is to provide a tool for groundwater modelers to help estimate the range of dispersivities to expect when performing “upscaling” procedures. Additionally, their work considers whether the observed increase in dispersivity with scale is related to the type of geological medium. They have found that the relationship that empirically best described the dispersivity data regarding scale of measurement was in the form of a power law and it can be expressed as $\alpha = c(L)^m$. Where $\alpha$ is longitudinal dispersivity, $c$ is a parameter related to the characteristics of a geological
medium, L is the flow distance, and m is the scaling exponent. Based on the 307 data pairs analyzed, the mean scaling exponent appeared to be 0.5, with no statistically significant difference between various geological media. The parameter c varies between 0.01 m for sandstones and unconsolidated media, and 0.8 m for carbonate rocks. Delgado [159] have proposed several empirical correlations to calculate longitudinal and transverse dispersion coefficient in porous media at different dispersion regimes [44, 56, 160]. These empirical correlations were made using a set of experimental dispersion data in beds of mono-sized particles of constant voidage [161-163].

Mechanical mixing is an important mechanism that has a significant effect on CO₂ dissolution in deep saline aquifers. The value of dispersivity is expected to be in the order of meters [164], thereby significantly affecting CO₂ transport and mixing. Hidalgo and Carrera [165] have used a numerical analysis to investigate if activating hydrodynamic dispersion, i.e., mechanical mixing, transport mechanism can accelerate CO₂ dissolution in saline aquifers. The hydrodynamic dispersion has been activated in the advective–diffusive-dispersive transport equations which govern CO₂ dissolution in a saline aquifer and the used longitudinal and transvers dispersivity ranged between 0-0.5 m and 0-0.05 m, respectively. Hidalgo and Carrera [165] found that hydrodynamic dispersion accelerates significantly CO₂ dissolution time when convection becomes the dominant transport mechanism reaching values around 100 times shorter than those of purely diffusive cases. In a different study, Ghesmat et al. [166] have used a nonlinear simulation to investigate how anisotropic dispersion may influence the CO₂ sequestration process in saline aquifers. They found that the dissolution of CO₂ increases as dispersion degree increases. They also
reported that the medium dispersivity ratios slightly affect the mixing, while having an impact on the fingering pattern.

To summarize the above discussion, dispersion is one of the main transport mechanisms in porous media where the solute spreads spatially inside the solvent due to the combined effect of molecular diffusion and mechanical mixing. In low permeability formations (having small flow velocity) diffusion is dominant, while in high permeability formations (having large flow velocity) mechanical mixing is the main process and diffusion has little or no effect. Mechanical mixing is calculated using formation dispersivity which is mainly a rock property and does not get affected by formation fluid. The dispersivity is defined in both transverse and longitudinal direction and usually the transverse dispersivity has a smaller value compared to longitudinal one. Most of the dispersivity measurements have been done by history matching the concentration profile of the solute using the convective-dispersive equation. The majority of the literature argued that dispersivity is scale-dependent where its value increases as the travel length increases. Therefore, the reported core-scale dispersivity is relatively small compared to field-scale dispersivity. Moreover, it was found in the literature that the solute dispersion is a function of formation conformance (homogeneity), i.e., the more heterogeneous the reservoir the higher the effect of dispersion. Additionally, it was found that dispersion in carbonate formations is higher than solute dispersion in sandstone rocks. Finally, several previous studies have found that mechanical mixing accelerates significantly the CO₂ dissolution in saline aquifers, when convection was found to be the dominant transport mechanism.
8. Challenges and future perspectives

The evaluation of gas diffusivity in liquids and determination of gas diffusion coefficients are found to be diverse and complex task, as it was discussed in this paper. Various experimental methods and mathematical models have been used in the literature to measure and calculate gas diffusion coefficients in reservoir fluids. First of all, despite the variety of available gas diffusion experimental measurement methods, various sources of errors should be considered. For instance, conventional measurement methods are system-intrusive due to the continuous sampling during running the diffusion test that is a common source of error. Pressure and temperature fluctuations during the experimental measurements can increase the level of noise in the measured data, and hence will affect the obtained results. Additionally, some of the present diffusion measurement methods cannot detect several vital physical phenomena such as the dynamic process of oil swelling in gas-oil systems. Furthermore, most of the available gas diffusion measurement methods are applied in gas-liquid systems. Therefore, the obtained gas diffusion coefficients still need to be converted to their effective values in porous media. This creates an additional source of error and uncertainty as the effective diffusion coefficient is function of the formation tortuosity value, formation resistivity, and empirical constants, that all need to be determined with a high level of accuracy. Secondly, a reliable mathematical model is the key to obtain accurate gas diffusion coefficients since the experimental measurements cannot directly obtain the gas diffusion coefficient. The mathematical model assumptions have a potential impact on the physical reliability of the obtained results. As demonstrated above, various assumptions in mathematical models can result in various values of gas diffusion coefficients and mass transfer rates, even when the same set of experimental data
for a particular diffusion test has been used. For the sake of simplicity, most of the available developed diffusion models have considered oversimplified assumptions with ignoring parameter changes due to the diffusion process. Additionally, the solution method applied, i.e., analytical or numerical method, can itself cause discrepancy in the obtained results. The phase behavior of a CO₂-oil system was found to be significantly different if reservoir permeability and pore radius are less than 0.001 mD and 0.1 µm, respectively [38, 167]. Hence, diffusion models with high accuracy are required to be developed in future studies in order to correctly describe gas diffusion in tight reservoirs. CO₂ impurities were also found to have a significant impact on the phase behavior, mass transfer and thermodynamic properties of CO₂ mixtures. Therefore, it is essential to investigate the effect of various types of CO₂ impurities, with various concentrations, on the measured CO₂ diffusion coefficient in CO₂ mixture-crude oil systems at typical reservoir conditions. Empirical correlations are based on various data sets of experimental results. The controlling parameters of gas diffusion coefficients are different for every correlation which can lead sometimes to contradicting results. Furthermore, since empirical correlations are based on experimental data, the previously mentioned experimental errors highly affect the correlations accuracy. The uncertainty in the measured value of gas diffusion coefficient can result in significant impacts on the simulated oil recovery by CO₂ injection and gas storage efficiency. Hence, reliable experimental measurement methods and comprehensive mathematical models with assumptions that accurately describe the diffusion process and its underlying physical relations, are highly essential to be investigated in future work. Additionally, various approaches to quantify the uncertainties in the gas diffusion coefficients, and weight of different factors and sources of errors lead to the evaluated
uncertainty, still need to be developed. The impact of D coefficient uncertainties for various strategies of gas flooding and its effect on the oil recovery process and gas storage application are also important to be quantified in the future research works. For CO₂ geo-sequestration projects, the operating conditions, i.e., aquifer pressure and temperature, brine salinity, and salt type highly affect the CO₂ diffusion coefficient in brine. Hence, more research work is needed to investigate the effect of various types of salt in brine at wide ranges of reservoir pressures and temperatures, and salt concentrations in order to improve the security of CO₂ sequestration in saline aquifers.

9. Conclusions

In this review article, we comprehensively discussed and summarized gas diffusion process in porous media. Gas dispersion in porous media was also reviewed briefly from various aspects. The review encompassed various topics including theory of mass transfer for various forms of diffusion: molecular diffusion in bulk fluids and porous media, Knudsen diffusion, and surface diffusion. The impacts of various factors affecting gas diffusion in porous media such as the effect of CO₂ thermodynamic state, operational parameters, and impurities in CO₂ mixtures on the gas diffusion process were also included. Additionally, factors affecting CO₂ diffusion during CO₂ geo-sequestration in saline aquifers were reviewed. Furthermore, previous experimental methods used to measure gas diffusion in both gas-liquid systems and porous media, were comprehensively reviewed including comparing them with one another from various aspects such as equipment used, their pros and cons, and limitations. Previous mathematical models describing the diffusion process were also presented with focusing on the model assumptions and their subsequent
impact on the gas diffusion process. Additionally, the applied mathematical model, the objective functions used in determining CO₂ diffusion coefficient in both light and heavy oils at various experimental conditions, and the obtained values of D coefficients were summarized and discussed. Empirical correlations and the application of molecular dynamics simulation in obtaining gas diffusion coefficient in liquids were also discussed in this article. To investigate the discrepancies in the reported values of CO₂ diffusion coefficients in the literature for similar systems at reservoir conditions, current challenges of laboratory measurements and diffusion modeling were highlighted, and also the future research areas related to gas diffusion in porous media were clearly addressed. Based on this review, the following conclusions and remarks can be drawn:

- Multiple types of gas diffusion can coexist in hydrocarbon reservoirs and saline aquifers. Their impacts on the mass transfer process are mainly controlled by formation and fluid properties, and reservoir conditions.
- CO₂ diffusion in reservoir fluids is highly dependent on the thermodynamic state of CO₂, i.e., supercritical, liquid, or gas state. For instance, supercritical CO₂ has a higher diffusivity in crude oils and faster improvements in the oil properties compared to CO₂ at gas state.
- Higher operating pressures and temperatures have positive impacts on CO₂ diffusion into both crude oils and brine. However, crude oil viscosity and brine salinity have adverse effects on the CO₂ diffusion coefficient in oil reservoirs and saline aquifers, respectively. Furthermore, the effect of salts concentration on the CO₂ diffusivity in brine varies with the type of brine salts.
• The presence of impurities in the CO₂ stream used in EOR or carbon storage applications highly affects the gas mass transfer rates into reservoir fluids. The effect of the impurities of the CO₂ mixture, i.e., positive or negative effect, on the CO₂ diffusion coefficient is a function of the type of impurities in the gas stream, e.g., N₂, CH₄, Ar, etc., and their concentrations.

• Not all diffusion laboratory measurement methods are suitable for every system. However, the experimental method used to measure the diffusivity of gas need to be selected based on fluid type (light oil, heavy oil, or saline water), operating conditions (pressure and temperature), and saturation conditions (static or dynamic flow). For instance, the pressure decay method was found to be the most applicable experimental method to measure the gas diffusion process, however, natural convections can lead to measurement errors especially in brine water and light oil systems. Additionally, despite the dynamic pendant drop method was successfully applied in various CO₂-liquid systems, oil vaporization and challenges of IFT measurement at high pressures cannot be ignored.

• Mathematical diffusion model assumptions were proved to highly affect the obtained values of CO₂ diffusion coefficient. Most of the available models in the literature neither adequately represent the conducted diffusion laboratory test nor accurately describe the molecular diffusion process. For instance, oil vaporization, i.e., two-ways mass transfer, dynamic process of oil swelling due to diffusion, multicomponent gas-oil system, and non-equilibrium boundary condition at the gas-liquid interface are rarely included in a single diffusion model.
• Wide ranges of CO₂ diffusion coefficient at reservoir conditions are reported in the literature even for similar CO₂-fluid systems. This is due to the various experimental methods, mathematical models, numerical solutions, and objective functions applied to determine the gas diffusion coefficient. Further research is needed to investigate different experimental measurement methods and mathematical models for the same gas-liquid system to produce reliable results.

• The empirical correlations of gas diffusion available in the literature are function of different parameters which occasionally lead to contradicting results. Furthermore, empirical correlations are mainly based on experimental data and mathematical models, hence measurement and numerical solution errors should be considered whenever these correlations are used.

• Molecular dynamics simulation was found to be an effective tool to estimate gas diffusion coefficients at various scales, i.e., microscopic, and macroscopic scales.

• Mechanical dispersion can be an important mass transfer mechanism in high permeability formations and is highly affected by the formation heterogeneity. Additionally, fluid dispersivity was found to be scale-dependent, i.e., core-scale dispersivity is relatively small compared to field-scale dispersivity.

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