

Review

A Review of CO₂ Plume Dispersion Modeling for Application to Offshore Carbon Capture and Storage

Yong-Hoon Kim ¹ and Young-Gyu Park ^{2,*} ¹ Department of Earth and Space Sciences, West Chester University of Pennsylvania, West Chester, PA 19383, USA; ykim@wcupa.edu² Ocean Circulation and Climate Research Department, Korea Institute of Ocean Science and Technology, Busan 49111, Republic of Korea

* Correspondence: ypark@kiost.ac.kr

Abstract: The exponential increase in greenhouse gas emissions necessitates urgent measures to mitigate climate change impacts. Carbon capture and storage (CCS) has emerged as a promising solution, capturing CO₂ from industrial processes and storing it underground. However, CCS implementation poses risks that demand sophisticated modeling. This review focuses on the numerical modeling of CO₂ plume dispersion from reservoir leaks during offshore CCS projects, including near- and far-field modeling and the comparison between Lagrangian and Eulerian modeling in particular. Near-field modeling examines CO₂ behavior in jet plume, considering depth-related changes. Far-field modeling, employing Eulerian and Lagrangian methods, evaluates dispersion in marine environments. Case studies illustrate the complexity and uniqueness of CO₂ dispersion events. The Lagrangian approach emphasizes gas bubble tracking, while the Eulerian approach employs fixed grid systems for detailed hydrodynamic modeling. Both approaches contribute valuable insights, with Eulerian models excelling in site-specific complexities and Lagrangian models offering computational efficiency. A hybrid approach may offer a comprehensive understanding of CO₂ dispersion.

Keywords: CCS; CO₂; Eulerian modeling; Lagrangian modeling; bubble tracking



Citation: Kim, Y.-H.; Park, Y.-G. A Review of CO₂ Plume Dispersion Modeling for Application to Offshore Carbon Capture and Storage. *J. Mar. Sci. Eng.* **2024**, *12*, 38. <https://doi.org/10.3390/jmse12010038>

Academic Editor: Valery M. Abramov

Received: 30 November 2023

Revised: 19 December 2023

Accepted: 20 December 2023

Published: 22 December 2023



Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

The exponential rise in greenhouse gas emissions has spurred an urgent need for innovative measures to mitigate climate change's adverse impacts. As part of such active mitigation efforts, carbon capture and storage (CCS) has emerged as a promising solution in reducing CO₂ emissions significantly [1]. CCS involves capturing CO₂ from industrial processes and storing it permanently underground, primarily in depleted oil and gas reservoirs or deep saline formations [2–5]. However, despite its potential, the deployment of CCS entails certain risks and complexities that necessitate thorough and sophisticated modeling for effective implementation and regulation [6].

The need for comprehensive modeling efforts to bolster CCS initiatives is multi-faceted. It spans across understanding the dynamic movements of CO₂ plumes under offshore conditions to predict potential leak scenarios and assess their environmental implications [7]. The fundamental objective is to ensure the safe and secure storage of the captured CO₂ without compromising the ecological integrity of marine ecosystems [8,9]. Additionally, the existing regulatory frameworks surrounding CCS demand precise, science-driven modeling to meet stringent standards, ensuring operational safety and environmental protections [10–13].

Foremost among the concerns within the domain of CCS is the potential risk arising from leaks in the CO₂ storage reservoirs [14]. Once the leaked CO₂ reaches the boundary between the seabed and ocean water, simulating the dispersion of CO₂ plumes in the offshore environment is essential to predict the behavior of released CO₂, especially its

interaction with marine sediments and water columns. Understanding the differences between the movement of CO₂ in sediment and water is crucial for estimating the possible impacts on biodiversity, ecosystems, and the overall marine environment. Modeling techniques play a pivotal role in analyzing and simulating the dispersion of CO₂ plumes with the perspective of both near-field (i.e., close to the source) and far-field (i.e., broader extent). When considering far-field simulation, two predominant approaches, Lagrangian and Eulerian models, offer different strategies for studying fluid flow and dispersion behavior. The choice between these methodologies significantly impacts the accuracy and comprehensiveness of CO₂ plume dispersion predictions, thus influencing the risk assessment associated with CCS implementations.

This review paper aims to delve into the diverse aspects of CO₂ plume dispersion modeling concerning risks related to reservoir leak events during and after offshore CCS projects. It scrutinizes the significance of modeling efforts, addresses the potential risks, explores the requirements outlined in CCS regulations, dissects the contrasting behavior of CO₂ movement in sediment versus water, and evaluates the pivotal choice between Lagrangian and Eulerian modeling techniques. By synthesizing and evaluating existing research, this review intends to provide a comprehensive understanding of the complexities and challenges associated with CO₂ plume dispersion modeling in the offshore environment for effective CCS implementation and regulation.

2. Offshore CCS and Modeling of CO₂ Dispersion in the Ocean

Since its proposal by Marchetti [15], CCS has led to the development of various technological scenarios for the capture, transport, and injection of CO₂. The most effective method involves transportation via ships or deep-sea pipelines and injecting it into subsea geological structures or deep-sea locations [2–4]. In the early 2000s, large-scale CCS projects started to take shape, such as the Sleipner Project in Norway, which involved the injection of captured CO₂ into geological formations beneath the North Sea [4,5]. Since then, various pilot projects and initiatives worldwide have aimed to test and advance different aspects of CCS, from capture technologies to transportation and storage methods.

The method of direct injection into the seawater could cause adverse effects on the marine environment; hence, subsurface storage methods are preferred. Although the direct injection approach may have fewer environmental impacts compared to other methods, once the CO₂ compound is stored, a leakage from the stored point or damage to pipelines could result in dissolution into the seawater, causing chemical reactions in the surrounding waters [16–18]. The dissolved CO₂, through the deionization of [H⁺] ions, leads to the acidification of seawater [3,18]. Despite the seawater's internal buffering mechanism (carbonate buffering system) to prevent significant changes in [H⁺] concentration, localized and short-term increases in acidity beyond natural levels have a considerable impact on deep-sea organisms [3,19]. Moreover, it is evident that an excess of carbonic acid concentration would affect the ecological environment.

However, despite the potential dangers and harm caused by large-scale CO₂ leakages into the marine environment due to leaks or accidents, CCS has progressed to almost operational stages in many countries without appropriate environmental assessments. This is mainly due to the limited understanding of CO₂ itself within seawater. Hence, research that comprehends the physical behavior of liquid CO₂ under various leakage conditions is highly necessary.

In the realm of CO₂ plume dispersion modeling, several key considerations merit detailed exploration to ensure accurate assessments and a comprehensive understanding. The geological characteristics of the storage site play a pivotal role in determining the behavior of the leaked CO₂. Variations in geological formations, such as the presence of faults, fractures, or porous reservoirs, significantly impact the migration and dispersion patterns of the plume [4,5]. Understanding the geology is crucial for predicting potential pathways, rates of migration, and the interaction of CO₂ with subsurface structures.

Additionally, the modeling process must encompass a spectrum of leakage scenarios to account for diverse situations that may arise [5,8,9]. These scenarios should include variations in leak duration, volume, and depth as well as considerations for different environmental conditions, such as tidal influences and seasonal variations. Evaluating the impact of CO₂ leakages under a range of scenarios ensures a robust understanding of the potential outcomes and aids in the development of tailored mitigation and monitoring strategies.

In the event of a CO₂ subsurface storage leakage incident, it is known that leaked CO₂ compounds dissolve into seawater, inducing chemical reactions in the surrounding waters [16,17]. The behavior of initially leaked liquid CO₂ is evident through the emergence of plume and jet forms, depending on the CO₂ volume, momentum, and buoyancy flux. Additionally, the behavior of CO₂ is intricately complex, contingent upon its inherent properties, such as solubility, temperature, density, leakage angle, and discharge momentum. The movement of CO₂ can be determined by environmental conditions including pressure, temperature, stratification degree, background flow, and seawater turbulence [2,4,20]. Chemical reaction modeling should integrate the complex interplay of CO₂ with seawater, considering factors such as pH alterations, carbonate chemistry dynamics, and the potential impact on marine ecosystems [10–14,16–18]. Accurate representation of these chemical reactions enhances the reliability of predictions regarding the environmental consequences of CO₂ leaks.

This information signifies the intricate and varied behavior of CO₂ leakages in subsea environments. It emphasizes the significance of factors such as depth, pressure, and various properties of CO₂, shedding light on the complex mechanisms involved during a potential CO₂ subsurface storage leakage incident. Understanding these complex interactions and the influence of multiple environmental conditions is crucial for planning and mitigating the potential adverse effects and managing such situations effectively in marine ecosystems.

This study employs two primary approaches, near-field and far-field modeling, to investigate the transport and fate of CO₂ in oceanic environments. Subsequent chapters elaborate on the significant discoveries resulting from these recent modeling methods.

3. Near-Field Modeling

The behavior of leaked liquid CO₂ from reservoirs manifests in plumes and jet forms, which warrant an understanding, particularly in CO₂ volume, momentum, and buoyancy flux [21]. The behavior of CO₂ becomes highly intricate due to its inherent characteristics, such as solubility, temperature, density, leakage angle, and discharge momentum. Furthermore, the behavior of CO₂ can be influenced by environmental conditions, such as pressure, temperature, stratification degree, background flow, and seawater turbulence. Particularly, the depth at which CO₂ is injected into the deep sea is closely related to seawater density due to its pressure, becoming a crucial variable in determining the state characteristics of CO₂ [2,4,20,21].

Figure 1 illustrates a schematic representation of the movement state of CO₂ depending on the distance from the leakage as well as water depth. Typically, when gas plumes are discharged from the seafloor, they initially manifest as jet plumes, driven by the momentum of the discharge point [22]. These jet plumes tend to maintain their shape only within a short distance of several meters from the discharge point. As these plumes rise, they lose momentum from the jet, and the subsequent movement of the plume is determined by the buoyancy arising from the density contrast between the gas within the plume and the surrounding seawater [23,24]. Gas-induced buoyancy, being significantly more substantial, is commonly the primary consideration in Lagrangian numerical modeling.

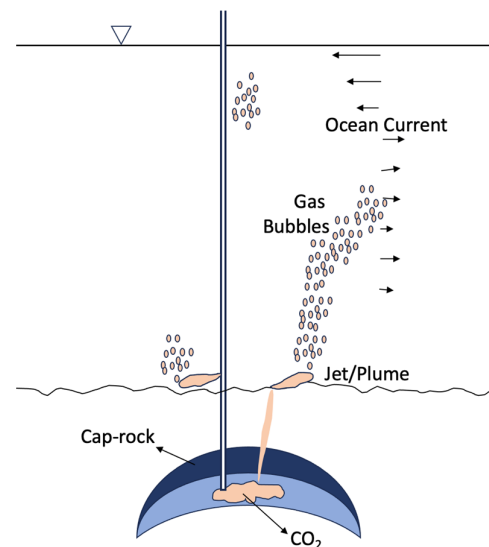


Figure 1. Schematic diagram showing the behavior of leaked CO₂ depending on ocean depth. Triangle represents water surface and vertical line shows a hypothetical pipeline.

In oceanic subsurface storage, there is a risk of a pressurized CO₂ leakage through small cracks or sediments, leading to the formation of vertical jets or plumes due to the elevated pressure in the reservoir system [4]. The dynamics of these jets or plumes can be simulated considering both single-phase and multiphase scenarios, involving liquid–liquid and liquid–gas interactions within the plumes [21]. In the near-field zone, where the leakage occurs, multiphase hydraulics play a crucial role, influencing turbulence through churn flow and affecting the conditions for the formation of bubbles or droplets. Previous modeling studies have explored both single-phase and multiphase liquid systems, addressing phenomena such as churn flow, droplet formation, and heat and mass transfer. Accurate modeling, particularly considering aspects such as churn flow, has become increasingly important.

The advancement of models designed to predict the behavior of gas and oil mixtures leaking at different depths, coupled with multiphase integral modeling, has significantly improved our ability to anticipate subsea blowout dynamics [21]. Substantial progress has been achieved in both experimental and computational fluid dynamic (CFD) modeling. Advanced CFD models, employing Eulerian–Eulerian and Eulerian–Lagrangian formulations, can simulate centimeter-scale hydrodynamics and the transport of oil droplets and gas bubbles in particular. These models serve as a crucial link between laboratory experiments and real-world oceanic dynamics, offering valuable insights into the behavior of multiphase plumes. Various types of computational fluid dynamics (CFD) models, involving the numerical solution of three-dimensional Navier–Stokes equations, have been employed to simulate multiphase flows, including incidents such as oil/natural gas blowouts or CO₂ leakages. For instance, Boufadel et al. [25] utilized a large eddy simulation (LES) to replicate churn flow in the Deepwater Horizon blowout. Gao et al. [26] applied CFD with Reynolds Averaged Navier–Stokes (RANS) equations to reproduce velocity components, turbulence kinetic energy, and the turbulence dissipation rate from underwater oil jet experimental measurements. Another type of CFD, direct numerical simulation (DNS), aims to directly resolve turbulence motions and, despite its high computational cost, has demonstrated promising results in simulating multiphase plumes [27].

As for one of the case study examples, a numerical simulation using Fluent, a commercial software developed by Ansys Inc., was applied to evaluate the complex behavior and formation of liquid CO₂ jets/plumes in the deep-sea condition [28]. This approach utilized finite volume methods to solve 3D Navier–Stokes equations, incorporating various computational modules for turbulence, heat transfer, chemical reactions, and multiple phases, enabling the simulation of various physical flow scenarios, including low-speed

incompressible and high-speed compressible flows. The governing equation used in the simulation is:

$$\frac{\partial}{\partial t}(\rho_t \vec{v}_t) + \nabla \cdot (\rho_t \vec{v}_t \vec{v}_t) = -\nabla p + \nabla \cdot \left[\mu_t \left(\nabla \vec{t}_t + \nabla \vec{t}_t^T \right) \right] + \rho_t \vec{g} + \vec{F} + \nabla \cdot \left(\alpha_{H_2O} \rho_{H_2O} \vec{v}_{H_2O} + \alpha_{CO_2} \rho_{CO_2} \vec{v}_{CO_2} \right), \quad (1)$$

where ρ_t = total density of the mixture, $\vec{v}_t$ = averaged velocity of the mixture, t = time, p = pressure, μ_t = dynamic viscosity of the mixture, T = transpose matrix, α_{H_2O} = ratio of water, ρ_{H_2O} = density of water, $\vec{v}_{H_2O}$ = velocity of water, α_{CO_2} = ratio of CO_2 , ρ_{CO_2} = density of CO_2 , and $\vec{v}_{CO_2}$ = velocity of CO_2 [20,28].

The numerical experimental results verified the occurrence of peculiar behaviors, such as the bifurcation phenomenon in fluid buoyancy entering the transverse flow [28]. Calculations involved the trajectory of jets/plumes, changes in cross-sectional size with flow development, the distance of the complete dissolution of liquid CO_2 , turbulence intensity, and extinction rates regarding the behavior of CO_2 .

4. Far-Field Modeling

As leaked CO_2 ascends from a jet plume in the ocean, its trajectory undergoes a critical shift influenced by the dissipation of momentum from the initial jet. The subsequent movement of the plume is intricately governed by buoyancy, arising from the density disparity between the CO_2 within the plume and the encompassing seawater. Within this context, far-field modeling emerges as a pivotal tool for comprehending the dispersion dynamics in the larger expanse. This modeling approach, particularly in the far field, is adaptable through both Eulerian and Lagrangian frameworks, offering nuanced perspectives on the complex interactions between the rising CO_2 plume and the surrounding marine environment.

4.1. Eulerian Approach

The Eulerian approach in CO_2 leakage modeling involves utilizing a fixed grid system to track the dispersion and transport of CO_2 in the marine environment. The approach is detailed in the context of a fine-scale model of marine hydrodynamics designed to understand the environmental impact of leaks from CCS systems. The model simulates a range of hypothetical leak scenarios, considering tidal variability and different model configurations [10,11,29]. These studies emphasized the significance of comprehending the environmental impact of CCS system leaks and underscored the necessity for designing effective monitoring tools. Moreover, they recognized the challenges posed by the natural, tidally driven dynamics of regions such as the North Sea, highlighting the complexity of CO_2 dispersion in such environments.

One key takeaway is the acknowledgment of the uniqueness of each CO_2 leak event, influenced by dynamic factors, such as the tidal state, wind-driven mixing, the geographical location, and the leak amount and duration. The model results suggested that the dispersion of a CO_2 leak is intricate and, also, that rapid dispersion tends to mitigate extreme impacts through dilution. Validation of the model against field data is identified as crucial to enhance confidence in its results, although the scarcity of available datasets for validation is acknowledged.

For example, Blackford et al. [10] adapted a fine-scale model of marine hydrodynamics, NW European Shelf POLCOMS, and coupled it with FVCOM to include processes relevant to CO_2 dispersion in seawater. The study simulated a range of hypothetical leak scenarios to assess the dispersal of CO_2 plumes in the North Sea. Tidal dynamics, a significant factor in the North Sea, are considered to account for the non-trivial nature of CO_2 dispersion. Tidal dynamics, a significant factor in the North Sea, are considered to account for the non-trivial nature of CO_2 dispersion [10]. In addition, the impact of different model configurations, including the model resolution, on simulated leak scenarios is examined, contributing to a comprehensive understanding of dispersion dynamics.

The model results revealed that, in NW European shelf seas with strong tidal mixing, the dispersion of a CO₂ leak will be complex, posing a challenge for monitoring. Rapid dispersion, driven by tidal forces, was identified as a mitigating factor against extreme impacts through dilution. In addition, the comparison of each scenario showed that any CO₂ leak event is expected to be unique, influenced by factors such as the tidal state, wind-driven mixing, the geographical location, and the leak amount and duration. Therefore, bespoke modeling of a comprehensive range of plausible scenarios is recommended for each storage site to develop specific monitoring strategies and impact assessments. Based on simulation results, Blackford et al. [10] concluded that high natural variability in dissolved CO₂ in seawater and related factors, such as pH, is observed in regions such as the NW European Shelf.

Another extensive case study illustrating the Eulerian approach of CO₂ leakage modeling was conducted in the North Sea region to assess potential carbon sequestration site leakages. Phelps et al. [11] implemented a three-dimensional hydrodynamic model (POLCOMS) coupled with a CO₂ speciation model. The CO₂ system is simulated using an iterative speciation model with dissolved inorganic carbon (DIC) and total alkalinity (TA) as master variables. This study simulated large-scale leakages from two distinct release sites, examining seasonal, inter-annual, and spatial variability in CO₂ leakages within the North Sea ecosystem [11].

The hydrodynamic model, POLCOMS, renowned for its successful application in various studies, including those in the North Sea [29–31], was utilized. Phelps et al. [11] specifically employed the high-resolution continental shelf (HRCS) setup, featuring a horizontal resolution of 1.8 km and 32 vertical σ -coordinate layers. Their grid spans the entirety of the North Sea, and the designated impact area extends up to 200 km horizontally, a range not easily addressed by the Lagrangian Approach.

Assessing the impact of CO₂ leakages, Phelps et al. [11] simulated pH alterations resulting from CO₂ additions. Scenarios were designed to encompass short-term and long-term perspectives. In short-term simulations, CO₂ was assumed to be emitted steadily at 5000 tons per day from the two leakage sites for a single day. The results indicated that, in the short term, CO₂ plumes from leakages are highly localized in the North Sea, with minimal perturbations beyond 10 km from the release sites. The significant impact was generally confined to changes weaker than 0.1 pH units, with the extreme case showing a maximum change of 1.92 pH units. In addition, the CO₂ concentration decreases rapidly after the release period, primarily due to advection and tidal mixing, with pH reductions weaker than 0.1 units within 5–8 days. In contrast, long-term simulations involved continuous CO₂ injection over a year, simulating scenarios of prolonged failure in carbon sequestration reservoirs. Long-term scenarios with higher release rates result in extensive, persistent plumes of highly acidified water that extend from the source locations. The simulation results show that the greatest pH reductions are 2.67 and 2.32 units at the north and south sites, with large regions of calcite undersaturation up to 70 km from the source.

Phelps et al. [11] contextualized predicted acidification within the natural pH variability of the North Sea, noting potential consequences for marine fauna and flora. It highlighted the importance of considering the future environmental conditions, such as increased atmospheric CO₂ and surface temperatures, in assessing the carbonate system's response to CO₂ leakages. While their study provided insights into the physical and chemical impacts of large CO₂ additions, it also acknowledged that assessing the marine ecosystem's response depends on resident biota tolerance [11]. When compared with previous studies [29], Phelps et al.'s [11] study revealed the differences attributed to model improvements, especially in local pH perturbations.

In order to simulate oceanic carbon cycling in the Ulleung Basin area in the East Sea, Korea, KIOST [28] implemented a numerical model by combining the regional ocean modeling system (ROMS) with Fennel's model [32]. The target area for numerical experiments spans from longitude 128.5° to 132.5° E and latitude 35° to 38° N, with a horizontal resolution of approximately 1/30° (about 3 km) in both the longitude and latitude directions, and

the vertical direction consists of 50 layers. The biogeochemical model used is based on the nitrogen cycling model developed by Fennel et al. [32] and the carbon chemistry model based on the theory of Zeebe and Wolf-Gladrow [33].

Numerical experiments calculate the movement and diffusion of variables between grid units, as the model is constructed on a grid-by-grid basis. Therefore, each grid has a uniform variable value. In the numerical model implemented in KIOST [28], it was assumed that the carbon dioxide introduced into a grid is uniformly distributed within that grid. Consequently, carbon dioxide leaked from an offshore subsurface storage facility and, entering the marine environment, became more diluted in larger grids, resulting in lower concentrations within the grid. To simulate the movement and diffusion of carbon dioxide more precisely and reduce the initial dilution ratio, they applied a higher-resolution numerical model by increasing the resolution of the grid up to $1/108^\circ$ for the detailed Ulleung Basin model area.

The results of carbon leakage dispersion experiments for six different scenarios were analyzed in terms of the total dissolved inorganic carbon (DIC) category, which directly increases in concentration with the carbon leakage, and the pH category, which is expected to be most sensitively affected by changes in the marine environment and biology [28]. For example, when simulating the scenario of 10% of the storage capacity leaked as a short-term event, the model results showed an increase in DIC of over 50 mmol/m^3 and a pH decrease of over 0.5 with seasonal variability (Figure 2). In contrast, for the case of 10% of the storage capacity leaked as a short-term event, the results exhibited intermittent increases in DIC of 5 mmol/m^3 or less and pH decreases of 0.01 or less.

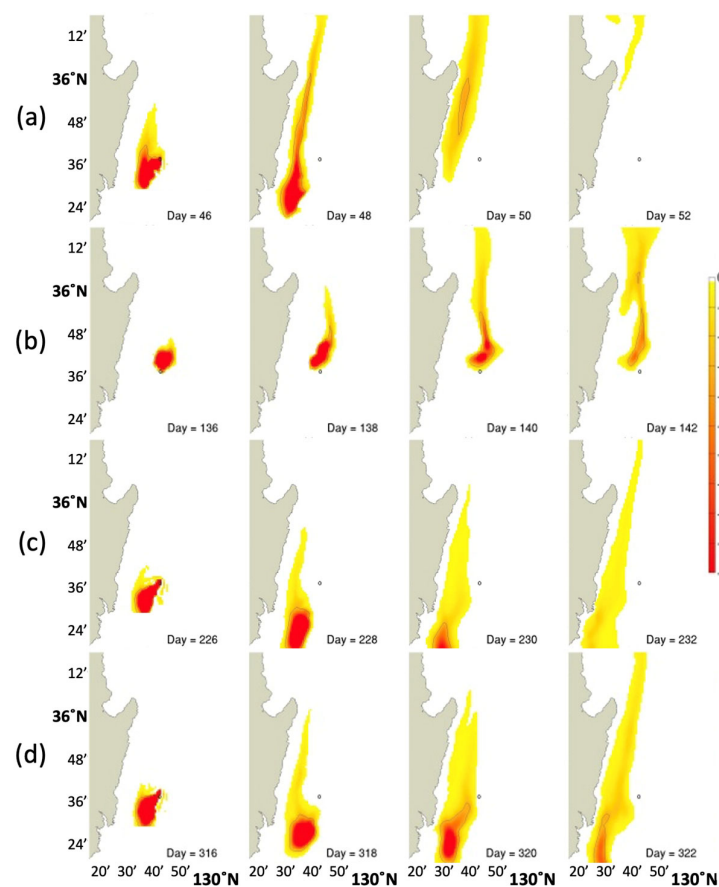


Figure 2. Time evolution of pH change due to CO_2 leakages during and after CCS extent of pH change due to CO_2 leakages at the seabed during winter (a), spring (b), summer (c), and fall (d) (Reprinted/adapted with permission from ref. [28]). The day number in the figure represents the year dates.

4.2. Lagrangian Approach

The numerical simulation of the movement of subsea-released CO₂ gas in the marine environment encompasses various modeling methods. Techniques based on Lagrangian particle tracking-models have been developed to compute particle behavior. These models play a vital role in predicting the movement and dispersion of CO₂ plumes, essential for predicting their potential impact on marine ecosystems and environments.

Modeling the movement of a CO₂ leakage involves utilizing Lagrangian CO₂ gas bubble-tracking models, which are numerical methods based on computational results from 2D or 3D fluid dynamics models. An analysis of the developed models reveals that the Lagrangian modeling method offers a simplified computational process compared to conventional grid-based modeling, allowing for swift numerical modeling.

During the movement of the plume driven by gas-induced buoyancy, the plume's speed results in the entrainment of seawater, reducing the plume's ascent rate and enlarging its size [23,34,35]. Additionally, the plume can be divided into two layers: an inner region densely packed with gas bubbles and an outer layer mixed with incoming seawater due to turbulent conditions within the plume. This turbulence causes the gas bubbles within the plume to break into smaller units, ranging from microns to millimeters.

Depending on the depth of the gas release and the ascent rate of the gas plume, scenarios arise where the plume reaches the sea surface or becomes trapped at a certain depth. Ultimately, when the gas bubbles dissolve entirely, lose buoyancy, or reduce in size due to dissolution, the plume ceases to ascend further and instead moves horizontally [24,35,36]. When the depth of the gas emission area exceeds 200 m, the influence of water pressure acting on the gas bubbles within the plume becomes more substantial, creating a complex relationship due to increased compressibility. Consequently, this affects changes in the ascent rate and dissolution characteristics of the plume.

The modeling of CO₂ gas migration should accommodate changes in bubble sizes due to dissolution and model the resulting plume's diffusive horizontal spread as gas density matches the surrounding seawater. The most critical factor affecting the movement of the plume due to buoyancy is the bubble size, intrinsically linked to dissolution [35,36]. The dissolution mass transfer rate $\frac{dm}{dt}$ for CO₂ gas bubble is calculated by the following:

$$\frac{dm}{dt} = K \cdot M \cdot A \cdot (C_s - C_0), \quad (2)$$

where m = mass of gas bubble, t = time, K = mass transfer coefficient, M = molecular weight of gas, A = surface area of a gas bubble, C_0 = concentration of dissolved gas, and C_s = saturated value of C_0 [23]. The computation tracks the movement of gas bubbles considering advection, mixing, and gas transport in seawater. The gas solubility, dictated by the quantity of gas released and the initial bubble size formed upon release, influences the bubble size. Consequently, as the plume ascends, the reducing gas bubble size contributes to the reduction of plume buoyancy and an increase in dissolved CO₂ within the plume. The effects of the reduced bubble size due to dissolution and increased bubble size due to ascent-induced decompression at deeper depths must be considered.

For example, the OCEAN_CO₂ model based on MEGADEEP (MEthane GAs in DEEP-water), a simulator focusing on the movement and diffusion of gas and hydrates released in deep-sea environments, was implemented to model the impact of a CO₂ release in Kagoshima Bay, Japan [35]. As gas leaks from the seabed, it interacts with the surrounding seawater, acting as a jet plume. To simulate this, computational processes consider momentum changes and buoyancy. One of the crucial factors determining the buoyancy of the gas is the size of the gas bubbles, making the accurate calculation of gas solubility essential. Additionally, as the gas rises, it loses its jet momentum and eventually drifts horizontally with the current. The simulation in OCEAN_CO₂ also accurately predicts the intermediate process where the jet transitions into a rising plume. Various parameters are accounted for in OCEAN_CO₂, including the dissolution of gas bubbles, mass conversion rates, heat

transfer rates, and changes in the size of gas bubbles. The rising terminal velocity, U_T , depends on the shape and size of bubbles as follows [35]:

$$U_T = Re \frac{\mu}{\rho \cdot d} \quad \text{for Spherical shape (small size)} \quad (3)$$

$$U_T = \frac{\mu \cdot M^{-0.149} \cdot (J - 0.857)}{\rho \cdot d_e} \quad \text{for Ellipsoidal shape (intermediate size)} \quad (4)$$

$$U_T = 0.711 \sqrt{g \cdot d_e \frac{\Delta \rho}{\rho}} \quad \text{for Spherical – cap shape (large size),} \quad (5)$$

where Re = Reynolds number, μ = dynamic viscosity of ambient fluid, ρ = density of ambient fluid, d = bubble diameter, $M = g\mu^4\Delta\rho/\rho^2\sigma^3$, σ = interfacial tension, $J = 0.94 \cdot H^{0.757}$, $H = 0.75 \cdot E_0 \cdot M^{-0.149} \cdot (\mu/\mu_w)^{-0.14}$, $E_0 = g\Delta\rho d_e^2/\sigma$, g = gravitational acceleration coefficient, and d_e = equivalent diameter. The modeling results show that the effect of CO₂ leakages on pH change is limited to the lower 50–70 m depth in Kagoshima Bay, and higher discharge rates may not raise dissolved CO₂ to higher elevations because the plume height is controlled by the dissolution rate and thus bubble size [35].

Kano et al. [37,38] used a numerical model based on a Eulerian–Lagrangian two-phase model, with a finite difference method for the continuous seawater phase and individual bubble or droplet motion analysis. The model considers mass, momentum, and energy conservation equations for the continuous phase and mass conservation and motion equations for each dispersed phase. Advection–diffusion equations for salinity and total CO₂ (TCO₂) are also solved. The model accounts for factors such as turbulence, drag, lift forces, and mass transfer coefficients. In Kano et al.’s [37,38] implementation around Japan, various simulation cases were conducted, considering different seabed depths, inflow velocities, initial diameters of bubbles/droplets, temperature, salinity, and TCO₂ profiles, considering realistic conditions with tidal currents and topography. The simulations involve a multi-scale ocean model that combines a mesoscale hydrostatic model and a small-scale, fully 3D, two-phase model. The latter includes a Eulerian–Lagrangian two-phase model to analyze the movement of CO₂ bubbles.

The results from Kano et al. [37] showed that, despite differences in the initial conditions, most leaked CO₂ dissolves within 150 m. Factors influencing the dissolved CO₂ concentration included the initial diameter of bubbles/droplets, inflow velocity, temperature, and TCO₂ background. Their study emphasized the importance of considering background TCO₂ levels, temperature, and seawater conditions in understanding the behavior of leaked CO₂. The calculated $\Delta p\text{CO}_2$ profiles generally aligned with ΔTCO_2 profiles, with background TCO₂ having a significant impact. Kano et al. [38] evaluated two leakage-rate scenarios: an extreme case with a rate of 94,600 tons per year, assuming a large fault connection, and a reasonable case with a rate of 3800 tons per year, based on an existing enhanced oil recovery (EOR) site. The results suggested that, even in the extreme case, the impact on floating organisms is limited, with experienced $\Delta p\text{CO}_2$ values below the proposed safety thresholds.

To optimize the leak detection probability, Ali et al. [12] applied the Bergen ocean model (BOM) in simulating spatial and temporal signals of elevated CO₂ concentration away from seep locations, considering factors such as currents, natural gas seeps, and biogeochemical parameters. The research discussed a case study involving leak scenarios in the central North Sea, emphasizing the importance of proper baseline data and a long-time series for designing a comprehensive monitoring program.

Ali et al.’s [12] modeling focused on developing probable footprints of a seep to the water column achieved through modeling. The authors demonstrated the use of high-resolution models. The BOM, a three-dimensional, terrain-following ocean model, was set to include an 800 m horizontal grid resolution, 41 σ -coordinate layers vertical, and various forcing data, such as wind, atmospheric pressure, tidal constituents, and river

runoff. The vertical distribution of CO₂ is based on results from the Heriot–Watt University (HWU) bubble plume model. Seep simulations were conducted by introducing CO₂ sources at nine different locations around Sleipner, and the concentrations were modeled as a passive tracer [12]. The results illustrated the spatial dependency and variability in concentration signals, emphasizing the influence of current conditions and local topography on monitoring designs.

Dewar et al. [39] showed a demonstration of integrating a multi-phase leakage model, PLUME, into a high-resolution hydrodynamic model linked to a carbonate system for a CO₂ analysis in the North Sea region. The system was constructed on the unstructured-grid finite-volume community ocean model (FVCOM) to capture local and regional hydrodynamics [40], and the nested domains ranged from 2.5 km at the boundaries to 0.5–1.0 m at the release sites. The predicting leakage using multi-phase equations (PLUME) model was integrated as a two-way plume modeling system. This integration enabled the examination of localized physicochemical impacts, utilizing the carbonate system from the European regional seas ecosystem model (ERSEM) for an ecosystem impact analysis [41]. The efficacy of the PLUME model was demonstrated at the STEMM-CCS and QICS sites, showing the model's ability to predict the observed pCO₂ and pH changes within acceptable errors.

The PLUME model uses a Lagrangian approach to simulate the dynamics of bubbles, droplets, or particles interacting with seawater [39]. The model accounts for mass and momentum exchanges between these entities and the surrounding fluids. The modeling system setup involves a nested configuration within FVCOM to account for tidal and coastal currents. The simulations included an analysis of bubble plume dynamics, dissolved carbon plume distribution, and impacts on pH and pCO₂ in the water column. Different experiments, QICS and STEMM-CCS, were simulated to explore the fate of CO₂ bubbles and dissolved solutions. Specific findings included the accumulation of CO₂ solutions at release locations during low current speeds, the prevention of significant vertical movements due to stratification or well-mixed conditions, and limited horizontal transport beyond ~100 m from the release site [39].

The results from Dewar et al. [39] showed the importance of considering local dynamics for predicting the impacts of CO₂ leakages in marine environments, showcasing the capabilities of the integrated modeling system in capturing these dynamics at different scales. Their findings highlighted the significant impact of water currents and resolution on local effects, revealing momentary spikes in pCO₂ and pH reductions due to tidal oscillation. In summary, it provided insights into the behavior of CO₂ bubbles and dissolved solutions, aiding in the assessment of potential environmental impacts.

Another well-established Lagrangian approach-based modeling framework is SIMAP, an environmental impact assessment model developed by Applied Science Associates in the mid-1990s. Used in over 40 countries, SIMAP was applied to numerous oil spill and gas leak incidents, including the 2010 Mexican Gulf oil spill, earning high trust in the model's outcomes [24]. Although its primary focus is for oil droplets and hydrocarbon bubbles, SIMAP is also capable of simulating the transport and fate of gas bubbles and was applied for CO₂ bubble transport [28]. The core of SIMAP's simulation is the numerical assessment of the movement and diffusion of gas released from the seafloor, where Lagrangian particles undergo evaporation, seawater inflow, dissolution, and adsorption of sediments.

KIOST [28] implemented SIMAP to assess the movement and fate of CO₂ from Korean CCS project in the East Sea. The trajectory calculations of particles within an offline particle-tracking model depend on previously computed numerical model results. This characteristic enables the model to calculate particle movements efficiently without influencing the physical values of the seawater. The model uses various data types for gas bubble movement, such as the velocity field, sea temperature, and salinity data. Each variable is computed from the temporal and spatial positions within the model's own framework. The particle-tracking model accounts for changing particle characteristics along their pathways, recording details such as the particle's location, physical properties (e.g., sea temperature, salinity), and the particle's age. Optional characteristics can include

the chemical properties of particles, which is essential for assessing the transformation of particles into a gaseous state and their further chemical alterations.

Park et al. [36] applied a gas bubble-tracking model to assist the environmental impact assessment procedure for a potential CCS project in southwestern Ulleung Basin, the East Sea, Korea. The methodology primarily encompasses a Lagrangian simulation, enabling the intricate modeling of individual CO₂ bubbles, their movement, and dissolution. The dissolution of gas bubbles, as a function of gas solubility, initiates the reduction of bubble size. As the plume ascends, reducing the bubble sizes affects buoyancy, reducing the plume's upward movement. This process increases the dissolved CO₂ content within the plume. Conversely, factors such as a reduced bubble size due to dissolution and an increased bubble size due to ascent-induced decompression in deeper waters create relative complexity, necessitating consideration in the model. The plume's behavior and the influences affecting its movement, such as dissolution dynamics, gas bubble size variations, and the switch from a jet- to buoyancy-driven phase, are crucial in formulating predictive models for CO₂ gas dispersion in marine environments.

The Lagrangian CO₂ bubble transport model introduced in Park et al.'s study [36] encompassed the transport and fate of CO₂ bubbles in three dimensions, considering factors such as the wind drift, ocean currents, and vertical movement. Their model incorporated the rising of gas bubbles, CO₂ gas dissolution, and chemical reactions of CO₂ in seawater. The model employed a dissolution mass transfer rate formula based on the molecular weight of the gas, mass transfer coefficient, bubble surface area, and temperature-dependent solubility. Chemical reactions of CO₂, including a grid data analysis, DIC change determination, and pH calculation using DIC, total alkalinity, temperature, and salinity, were also included in the simulation. Based on Park et al.'s [36] approach, we reproduced a numerical model to simulate the impact of CO₂ leakages on seawater, particularly focusing on changes in dissolved inorganic carbon (DIC) levels and pH (Figure 3).

The results from Park et al. [36] showed the dependence of terminal velocity on carbon dioxide particle size, 3D trajectories of gas bubbles, changes in bubble size distribution, and pH variability in a deep ocean environment. As part of a sensitivity test, the dissolution amount of carbon dioxide is simulated for varying leakage scenarios. Their study concludes that leaked CO₂ would be confined to a specific volume, resulting in a minimal drop in pH, even with significant amounts of CO₂ leakages.

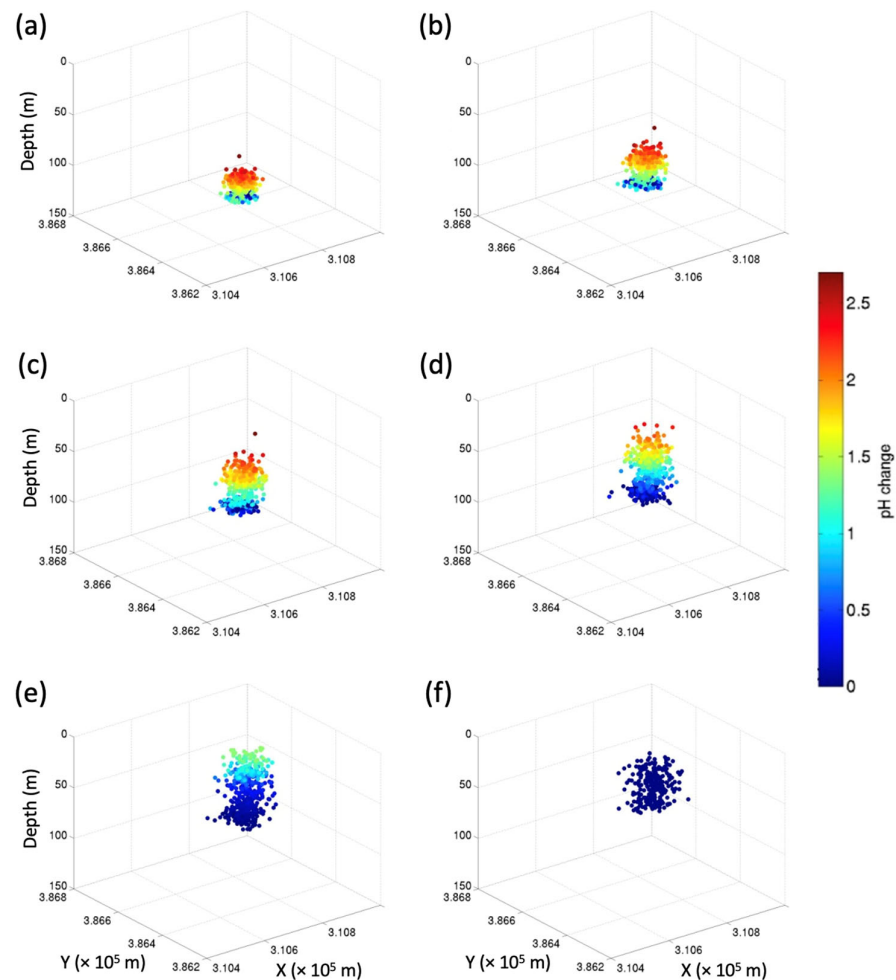


Figure 3. Time evolution of pH change due to CO₂ leakage during and after CCS. Each plot represents 15 min (a), 20 min (b), 25 min (c), 30 min (d), 35 min (e), and 40 min (f) after the leakage.

5. Discussion

5.1. Eulerian vs. Lagrangian Approach

The objective of most modeling efforts reviewed in this paper is to understand the environmental impacts of leaks from carbon capture and storage (CCS) systems. Two representative modeling approaches, Eulerian and Lagrangian, were employed to simulate CO₂ dispersion in marine ecosystems. The Eulerian approach mostly involved a fixed grid system to track the dispersion of CO₂, while the Lagrangian approach used particle-tracking models exclusively.

The Eulerian approach introduced in this study employed a fine-scale model of marine hydrodynamics, such as the NW European Shelf POLCOMS model, to simulate hypothetical CO₂ leak scenarios. Those studies considered tidal variability, geographical location, and different model configurations to capture the intricacies of CO₂ dispersion in regions such as the North Sea. Two case studies, one by Blackford et al. [10] and another by Phelps et al. [11], demonstrated the pros and cons of the Eulerian approach. Blackford et al. [10] simulated CO₂ plume dispersal in the North Sea, considering tidal dynamics and different model configurations. Phelps et al. [11] focused on large-scale leakages in the North Sea, assessing pH alterations over short- and long-term scenarios, highlighting the importance of considering future environmental conditions.

The Lagrangian approach involves tracking gas bubbles using numerical methods based on fluid dynamic models. Gas bubbles initially form jet plumes, transitioning to a buoyancy-driven ascent, influencing their movement and dissolution. Key factors include bubble size, dissolution dynamics, and the transition from jet- to buoyancy-driven

motion. Most Lagrangian simulations introduced in this study involved predicting CO₂ movements by considering dissolution, bubble size variations, and the transition from jet-to buoyancy-driven motion. Those simulations incorporated advanced computational techniques, mathematical models, and a thorough understanding of gas dissolution dynamics, buoyancy effects, and gas hydrate formation. Various studies, including the Quantifying and Monitoring Potential Ecosystem Impacts of Geological Carbon Storage (QICS) project and the Strategies for Environmental Monitoring of Marine Carbon Capture and Storage (STEMM-CCS) project, utilize Lagrangian models [39]. The Bergen ocean model (BOM) and MEGADEEP simulate CO₂ concentration signals, emphasizing the importance of baseline data and proper monitoring strategies [12].

Both Eulerian and Lagrangian approaches are capable of contributing valuable insights to CO₂ leakage modeling. Eulerian models excel in capturing site-specific complexities, while Lagrangian models provide efficiency in simulating individual gas bubble dynamics. The Eulerian approach involves the use of a fixed grid system, enabling the fine-scale modeling of marine hydrodynamics. This allows for a detailed understanding of the environmental impact of CO₂ leaks. In addition, the Eulerian approach takes into account dynamic factors, such as the tidal state, wind-driven mixing, the geographical location, and the leak amount and duration. This comprehensive consideration acknowledges the uniqueness of each CO₂ leak event. Case studies, such as those in the North Sea [10,11], provide insights into the dispersion of CO₂ plumes in real-world scenarios, considering seasonal, inter-annual, and spatial variability. However, the scalability of Eulerian models may be constrained by computational resources, especially when simulating large-scale scenarios. The fine-scale models, such as NW European Shelf POLCOMS coupled with FVCOM, used by Blackford et al. [10], provide valuable insights into the environmental impact of leaks but may face limitations when extrapolating results to broader oceanic scales. The accuracy of Eulerian models is highly dependent on the chosen grid resolution. Simulations with coarse grids may overlook small-scale features, impacting the reliability of the results. However, increasing resolution comes at the cost of higher computational demands. It should be noted that the validation against field data is identified as crucial, but the scarcity of available datasets for validation is acknowledged, posing a challenge to building confidence in model results.

The Lagrangian modeling method offers a simplified computational process compared to conventional grid-based modeling, allowing for swift numerical modeling [35,36,39]. The approach simulates the movement of gas plumes, accounting for factors such as buoyancy, dissolution, and the transition from jet- to buoyancy-driven motion. Lagrangian particle-tracking models enable the detailed tracking of gas bubbles, considering advection, mixing, and gas transport in seawater. Lagrangian approaches, such as the one implemented in [28,36], offer a more computationally efficient solution. Lagrangian models, while generally more computationally efficient, still require substantial resources, especially when dealing with large-scale or longer-term simulations. However, the accuracy of the model relies mostly on assumptions related to the initial size and behavior of gas bubbles in seawater, which are not yet well known. The trade-off involves making certain assumptions about the behavior of individual particles, and the results might lack the detailed spatial information that Eulerian models can offer.

The far-field modeling of CO₂ dispersion in the ocean presents challenges and opportunities in terms of scalability. For example, KIOST [28] utilized both Eulerian and Lagrangian methodologies to model the consequences of CO₂ leakages in the East/Japan Sea. Using the Eulerian approach, simulations of the leakage scenario extended over periods ranging from 7 to 10 days, or even up to several months, with the impact reaching a length of up to 200 km (Figure 2). In contrast, outcomes from the Lagrangian approach depicted a scale of less than a kilometer within hours of the leakage event (Figure 3). Regarding computational demands, the Lagrangian model was processed within a few dozen minutes on a personal computer, whereas the Eulerian simulation necessitated several days of execution on a high-performance computing server.

The choice between Eulerian and Lagrangian approaches depends on the specific goals of the modeling study, the available data, and the computational resources. Eulerian approaches provide detailed insights into the environmental impact, while Lagrangian approaches offer advantages in terms of computational efficiency and detailed particle tracking. A hybrid approach integrating the strengths of both methods could potentially offer a comprehensive understanding of CO₂ dispersion in marine environments [42,43].

5.2. Challenges

The oceanic subsurface storage of CO₂ involves not only securing large-scale reservoirs but also prioritizes environmental risk management [6]. It is essential to systematically identify and quantify various hazardous factors based on monitoring and modeling data for marine hazard and safety management. Environmental impact monitoring and modeling aim to observe and simulate any changes or impacts on the marine environment due to CO₂ oceanic subsurface storage, particularly focusing on marine ecosystems and biodiversity [7]. The focus lies in obtaining data to assist in devising response strategies, determining the spread and concentration under various leakage scenarios, or assessing the sensitivity of diverse marine organisms to leaked CO₂ [7]. Recognizing the sensitivity of key species inhabiting the targeted operational area and establishing a database is crucial for future ecological risk assessments. However, the comprehensive examination on the impact of CO₂ leaks on marine ecosystems and biodiversity is beyond the scope of this study and merits consideration in a forthcoming manuscript.

Despite the significant strides, this review highlights crucial unknowns that warrant further investigation in CO₂ fate modeling in the ocean. The input condition of a CO₂ leakage could be one major controlling factor, but there are not many field or lab studies that documented various impacts from the initial bubble size. Detailed measurements are called for to characterize plume hydrodynamics and gas bubble size distribution at various locations within the plume [39]. The incorporation of high-fidelity CFD models, particularly large eddy simulations (LES), is deemed essential for synergistic validation and the extension of experimental databases for near-field modeling. In addition, the gaps in understanding bubble-generated turbulence and the dynamics of multiphase plumes in the presence of stratification and crossflow in the far-field domain remain challenging areas that require further exploration. New datasets to calibrate and validate engineering-type models would be required more to ultimately advance our understanding of field-scale multiphase plume dynamics.

The numerical simulation approach for analyzing CO₂ leakage scenarios, which would provide input parameters for the CO₂ dispersion modeling, is deemed significantly crucial. Quantitative numerical simulations for CO₂ leakages are broadly divisible into CO₂ fluid-movement models within the sediment and dispersion models for CO₂ released into the seawater. Understanding the movement paths of CO₂ released from subsurface storage requires computational calculations of groundwater and CO₂ flow to track the CO₂'s trajectory. Eventually, CO₂ passing through the sediment reaches the seafloor and is discharged into the seawater, where employing CO₂ bubble-movement diffusion models for numerical simulations becomes essential.

6. Conclusions

This manuscript thoroughly examines the critical aspects of CO₂ plume dispersion modeling concerning the risks associated with offshore CCS projects. Recognizing the multifaceted challenges associated with predicting CO₂ plume dispersion and understanding potential leak scenarios, this review emphasizes the significance of precise, science-driven modeling for ensuring the secure storage of captured CO₂ without compromising marine ecosystems. Of particular concern is the risk of leaks in CO₂ storage reservoirs and the subsequent dispersion of CO₂ plumes in the offshore environment.

In the realm of near-field modeling, where the intricacies of CO₂ behavior in the initial stages of a leakage are crucial, this paper explores the dynamics of jet plumes,

multiphase hydraulics, and the role of computational fluid dynamic (CFD) models. The discussion extends to the advancements in showcasing the progress achieved through experimental and computational approaches, including a large eddy simulation (LES) and direct numerical simulation (DNS).

Furthermore, the far-field modeling approach, utilizing both Eulerian and Lagrangian frameworks, is discussed. The Eulerian approach involves a fixed grid system to track CO₂ dispersion, as demonstrated in studies simulating hypothetical leak scenarios in the North Sea. These simulations emphasize the complexity of CO₂ dispersion, the importance of rapid dispersion in mitigating impacts, and the uniqueness of each CO₂ leak event. The Lagrangian approach, employing particle-tracking models, is crucial for predicting the movement and dispersion of CO₂ plumes. Various modeling frameworks, including OCEAN_CO₂, are discussed in the context of simulating the fate of CO₂ bubbles. These models consider factors such as bubble size, dissolution dynamics, and the influence of subsurface currents on plume dynamics.

The paper evaluates the merits of Eulerian and Lagrangian approaches. Through case studies and simulations, it becomes evident that Eulerian models excel in capturing site-specific complexities, considering dynamic factors such as the tidal state, wind-driven mixing, and the geographical location. On the other hand, Lagrangian models, with their efficiency in simulating individual gas bubble dynamics, offer valuable insights into the movement and dispersion of CO₂ plumes with higher precision.

The review recognizes the challenges inherent in CO₂ fate modeling, highlighting crucial unknowns that demand further investigation. It emphasizes the importance of detailed measurements to characterize plume hydrodynamics and gas bubble size distribution, particularly in the context of the initial bubble size impact. The integration of high-fidelity computational fluid dynamic (CFD) models, especially large eddy simulations (LES), is deemed essential for the validation and extension of experimental databases. Moreover, the manuscript identifies gaps in understanding bubble-generated turbulence and the dynamics of multiphase plumes in the presence of stratification and crossflow in the far-field domain. It calls for new datasets to calibrate and validate engineering-type models, ultimately contributing to an enhanced understanding of field-scale multiphase plume dynamics.

In essence, this comprehensive review serves as a valuable resource for researchers, policymakers, and stakeholders involved in offshore CCS projects, offering insights, challenges, and future directions for effective CO₂ plume dispersion modeling and regulatory compliance.

Author Contributions: Conceptualization, Y.-H.K. and Y.-G.P.; investigation, Y.-H.K. and Y.-G.P.; writing—original draft preparation, Y.-H.K.; writing—review and editing, Y.-H.K. and Y.-G.P.; supervision, Y.-G.P.; project administration, Y.-G.P.; funding acquisition, Y.-G.P. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by the Korea Institute of Energy Technology Evaluation and Planning (KETEP) and the Ministry of Trade, Industry, and Energy (MOTIE) of the Republic of Korea (No. 20214710100060).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data are contained within the article.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. IPCC. *Climate Change 2023: Synthesis Report*; IPCC: Geneva, Switzerland, 2023; p. 184.
2. Liro, C.; Adams, E.; Herzog, H. Modelling the releases of CO₂ in the deep ocean. *Energy Convers. Manag.* **1992**, *33*, 667–674. [[CrossRef](#)]
3. Auerbach, D.I.; Caulfield, J.A.; Adams, E.E.; Herzog, H.J. Impacts of ocean CO₂ disposal on marine life: I. A toxicological assessment integrating constant-concentration laboratory assay data with variable-concentration field exposure. *Environ. Model. Assess.* **1997**, *2*, 333–343. [[CrossRef](#)]

4. IPCC. *Carbon Dioxide Capture and Storage*; Cambridge University Press: Cambridge, UK, 2005; p. 431.
5. IOGP. The Potential for CCS and CCU in Europe. 2019. Available online: https://iogpeurope.org/wp-content/uploads/2021/09/IOGP_The-potential-for-CCS-and-CCU-in-Europe_reportstudy.pdf (accessed on 1 November 2023).
6. Van Noorden, R. Carbon sequestration: Buried trouble. *Nature* **2010**, *463*, 871–873. [CrossRef] [PubMed]
7. Kim, H.W.; Kim, Y.H.; Kang, S.-G.; Park, Y.-G. Development of environmental impact monitoring protocol for offshore carbon capture and storage (CCS): A biological perspective. *Environ. Impact Assess. Rev.* **2016**, *57*, 139–150. [CrossRef]
8. IEAGHG. *Review of Offshore Monitoring for CCS Project*; IEAGHG: Cheltenham, UK, 2015; p. 153.
9. IEAGHG. *Monitoring and Modelling of CO₂ Storage: The Potential for Improving the Cost-Benefit Ratio of Reducing Risk*; IEAGHG: Cheltenham, UK, 2020; p. 89.
10. Blackford, J.C.; Torres, R.; Cazanave, P.; Artioli, Y. Modelling dispersion of CO₂ plumes in sea water as an aid to monitoring and understanding ecological impact. *Energy Procedia* **2013**, *37*, 3379–3386. [CrossRef]
11. Phelps, J.J.C.; Blackford, J.C.; Holt, J.T.; Polton, J.A. Modelling large-scale CO₂ leakages in the North Sea. *Int. J. Greenh. Gas Control* **2015**, *38*, 210–220. [CrossRef]
12. Ali, A.; Frøysa, H.G.; Avlesen, H.; Alendal, G. Simulating spatial and temporal varying CO₂ signals from sources at the seafloor to help designing risk-based monitoring programs. *J. Geophys. Res. Ocean.* **2016**, *121*, 745–757. [CrossRef]
13. Jeong, S.-M.; Ko, S.; Sean, W.-Y. Numerical Prediction of the Behavior of CO₂ Bubbles Leaked from Seafloor and Their Convection and Diffusion near Southeastern Coast of Korea. *Appl. Sci.* **2020**, *10*, 4237. [CrossRef]
14. Alcalde, J.; Flude, S.; Wilkinson, M.; Johnson, G.; Edmann, K.; Bond, C.E.; Scott, V.; Gilfillan, M.V.; Ogaya, X.; Haszeldine, R. Estimating geological CO₂ storage security to deliver on climate mitigation. *Nat. Commun.* **2018**, *9*, 2201. [CrossRef]
15. Marchetti, C.; Nakicenovic, N. *The Dynamics of Energy Systems and the Logistic Substitution Model*; IIASA: Laxenburg, Austria, 1979; p. 73.
16. Teng, H.; Yamasaki, A.; Shindo, Y. The fate of liquid CO₂ disposed in the ocean. *Int. Energy* **1996**, *21*, 765–774. [CrossRef]
17. Sato, T. Numerical Simulation of Biological Impact Caused by Direct Injection of Carbon Dioxide in the ocean. *J. Oceanogr.* **2004**, *60*, 807–816. [CrossRef]
18. Sato, T.; Sato, K. Numerical Prediction of the Dilution Process and its Biological Impacts in CO₂ Ocean Sequestration. *J. Mar. Sci. Technol.* **2002**, *6*, 169–180. [CrossRef]
19. Barry, J.P.; Buck, K.R.; Lovera, C.F.; Kuhn, L.; Whaling, P.J.; Peltzer, E.T.; Walz, P.; Brewer, P.G. Effects of Direct Ocean CO₂ Injection on Deep-Sea Meiofauna. *J. Oceanogr.* **2004**, *60*, 759–766. [CrossRef]
20. Alendal, G.; Drange, H. Two-phase, near-field modeling of purposefully released CO₂ in the ocean. *J. Geophys. Res. Ocean.* **2001**, *106*, 1085–1096. [CrossRef]
21. Boufadel, M.C.; Socolofsky, S.; Katz, J.; Yang, D.; Daskiran, C.; Dewar, W. A review on multiphase underwater jets and plumes: Droplets, hydrodynamics, and chemistry. *Rev. Geophys.* **2020**, *58*, e2020RG000703. [CrossRef]
22. Levine, J.; Haljasmaa, I.; Lynn, R.; Shaffer, F.; Warzinski, R.P. *Detection of Hydrates on Gas Bubbles during a Subsea Oil/Gas Leak*; National Energy Technology Laboratory: Pittsburgh, PA, USA, 2015; p. 36.
23. Zheng, L.; Yapa, P.D.; Chen, F.H. A Model for Simulating Deepwater Oil and Gas Blowouts—Part I: Theory and Model Formulation. *J. Hydraul. Res.* **2003**, *41*, 339–351. [CrossRef]
24. French-McCay, D.P.; Jayko, K.; Li, Z.; Spaulding, M.L.; Crowley, D.; Mendelsohn, D.; Horn, M.; Isaji, T.; Kim, Y.H.; Fontenault, J.; et al. Oil fate and mass balance for the Deepwater Horizon Oil Spill. *Mar. Pollut. Bull.* **2021**, *171*, 112681. [CrossRef]
25. Boufadel, M.C.; Gao, F.; Zhao, L.; Özgökmen, T.; Miller, R.; King, T.; Robinson, B.; Lee, K.; Leifer, I. Was the Deepwater Horizon well discharge churn flow? Implications on the estimation of the oil discharge and droplet size distribution. *Geophys. Res. Lett.* **2018**, *45*, 2396–2403. [CrossRef]
26. Gao, F.; Zhao, L.; Boufadel, M.; King, T.; Robinson, B.; Conmy, R.; Miller, R. Hydrodynamics of oil jets without and with dispersant: Experimental and numerical characterization. *Appl. Ocean Res.* **2017**, *68*, 77–90. [CrossRef]
27. Roghair, I.; Mercado, J.M.; Annaland, M.V.S.; Kuipers, H.; Sun, C.; Lohse, D. Energy spectra and bubble velocity distributions in pseudo-turbulence: Numerical simulations vs. experiments. *Int. J. Multiph. Flow* **2011**, *37*, 1093–1098. [CrossRef]
28. KIOST. *Development of Technology for CO₂ Offshore Geological Storage*; Korea Ministry of Oceans and Fisheries: Seoul, Republic of Korea, 2016; p. 4800.
29. Blackford, J.C.; Jones, N.; Proctor, R.; Holt, J. Regional scale impacts of distinct CO₂ additions in the North Sea. *Mar. Pollut. Bull.* **2008**, *56*, 1461–1468. [CrossRef] [PubMed]
30. Holt, J.T.; James, I.D. An s coordinate density evolving model of the northwest European continental shelf—1, model description and density structure. *J. Geophys. Res. Ocean.* **2001**, *106*, 14015–14034. [CrossRef]
31. Holt, J.; Proctor, R. The seasonal circulation and volume transport on the northwest European continental shelf: A fine-resolution model study. *J. Geophys. Res. Ocean.* **2008**, *113*, C06021. [CrossRef]
32. Fennel, K.; Wilkin, J.; Levin, J.; Moisan, J.; O'Reilly, J.; Haidvogel, D. Nitrogen cycling in the Middle Atlantic Bight: Results from a three-dimensional model and implications for the North Atlantic nitrogen budget. *Glob. Biogeochem. Cycles* **2006**, *20*, BG3007. [CrossRef]
33. Zeebe, R.E.; Wof-Gladrow, D. *CO₂ in Seawater: Equilibrium, Kinetics, Isotopes*; Elsevier: Amsterdam, The Netherlands, 2001; p. 360.
34. Zheng, L.; Yapa, P.D. Modeling Gas Dissolution in Deepwater Oil/Gas Spills. *J. Mar. Syst.* **2002**, *31*, 299–309. [CrossRef]

35. Dissanayake, A.L.; De Graff, J.A., Jr.; Yapa, P.D.; Nakata, K.; Ishihara, Y.; Yabe, I. Modeling the Impact of CO₂ Releases in Kagoshima Bay, Japan. *J. Hydro-Environ. Res.* **2012**, *6*, 195–208. [[CrossRef](#)]
36. Park, Y.-G.; Kim, Y.H.; Seo, S.; Hwang, J.H.; Ha, H.K. Environmental impact assessment of carbon storage using a CO₂ bubble model. *J. Coast. Res.* **2020**, *95*, 138–142. [[CrossRef](#)]
37. Kano, Y.; Sato, T.; Kita, J.; Hirabayashi, S.; Tabeta, S. Model prediction on the rise of pCO₂ in uniform flows by leakage of CO₂ purposefully stored under the seabed. *Int. J. Greenh. Gas Control* **2009**, *3*, 617–625. [[CrossRef](#)]
38. Kano, Y.; Sato, T.; Kita, J.; Hirabayashi, S.; Tabeta, S. Multi-scale modelling of CO₂ dispersion leaked from seafloor off the Japanese coast. *Mar. Pollut. Bull.* **2010**, *60*, 215–224. [[CrossRef](#)]
39. Dewar, M.; Saleem, U.; Flohr, A.; Schaap, A.; Strong, J.; Li, J.; Roche, B.; Bull, J.M.; Chen, B.; Blackford, J. Analysis of the physicochemical detectability and impacts of offshore CO₂ leakage through multi-scale modelling of in-situ experimental data using the PLUME model. *Int. J. Greenh. Gas Control* **2021**, *110*, 103441. [[CrossRef](#)]
40. Chen, C.; Liu, H.; Beardsley, R.C. An Unstructured Grid, Finite-Volume, Three-Dimensional, Primitive Equations Ocean Model: Application to Coastal Ocean and Estuaries. *J. Atmos. Ocean. Technol.* **2003**, *20*, 159–186. [[CrossRef](#)]
41. Artioli, Y.; Blackford, J.C.; Butenschon, M.; Holt, J.T.; Wakelin, S.L.; Thomas, H.; Borges, A.V.; Allen, J.I. The carbonate system in the North Sea: Sensitivity and model validation. *J. Mar. Syst.* **2012**, *102–104*, 1–13. [[CrossRef](#)]
42. Olsen, J.E.; Skjetne, P. Summarizing an Eulerian–Lagrangian model for subsea gas release and comparing release of CO₂ with CH₄. *Appl. Math. Model.* **2020**, *79*, 672–684. [[CrossRef](#)]
43. Fraga, B.; Stoesser, T.; Lai, C.C.K.; Socolofsky, S.A. A LES-based Eulerian–Lagrangian approach to predict the dynamics of bubble plumes. *Ocean Model.* **2016**, *97*, 27–36. [[CrossRef](#)]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.