STUDY OF DISSOLUTION OF CO_2 BUBBLE INTO SEAWATER

● LOI HOANG HUY PHUOC PHAM - AN NGUYEN SI XUAN

ABSTRACT:

Carbon capture and storage (CCS) is a critical technology designed to reduce CO_2 emissions from industrial sources such as fossil fuel power plants, oil refineries, and cement plants. A key aspect of CCS involves the injection of CO_2 into sub-seabed geological formations. However, potential CO_2 leakage poses a risk to the marine environment, necessitating careful monitoring. This study investigates the mass transfer process of CO_2 bubbles released from shallow subsea storage using computational fluid dynamics (CFD) simulations. The CFD-Fluent code was employed to simulate the rise and dissolution of CO_2 bubbles in seawater under varying current conditions. The simulations were validated against experimental data from the Quantifying and Monitoring Potential Ecosystem Impacts of Geological Carbon Storage (QICS) project. The results demonstrate that the CFD model accurately predicts the behaviors of released CO_2 bubbles in seawater, offering a valuable tool for assessing the risks associated with CCS operations.

Keywords: CO_2 bubble, release, mass transfer, current, computational fluid dynamics, dissolution.

1. Introduction

The Intergovernmental Panel on Climate Change (IPCC) has identified carbon capture and storage (CCS) as a vital strategy to mitigate these emissions [1]. CCS involves three primary processes: capturing CO_2 at the source, transporting it to storage sites, and injecting it into underground or subsea geological formations [2]. By 2050, CCS is expected to contribute to a 14% reduction in global CO_2 emissions. After capture, the CO_2 gas will be transported through onshore and offshore pipelines or by ships to geological storage sites across different regions and population centers [3].

The primary concern is the leakage of CO_2 from storage sites, which could acidify seawater and harm marine ecosystems [4]. The 1986 Lake Nyos disaster, where natural CO_2 release led to over 1,700 fatalities, underscores the need for robust risk assessment and monitoring of CCS sites [5].

When CO_2 leaks into the ocean, it forms droplets or bubbles, depending on the depth, which rise and dissolve, creating a plume [6]. This process, influenced by factors such as bubble size, rising velocity, and regional currents, can alter water quality and contribute to ocean acidification [7].

Previous models studying CO_2 bubbles rising in seawater have identified a gap in understanding the effects of current and turbulence on their ascent after leakage [8]. A new integrated model combining CFD-FLUENT and a population balance model (PBM) has been developed to study the hydrodynamics of these bubbles [9]. However, this model uses a simplified approach to current velocity and body forces, relying on constant current velocity and drag and lift coefficients, which may not accurately represent the variety of bubble shapes [10]. This paper aims to investigate these factors, including the CO2 bubble dissolution process in seawater, to improve simulation accuracy.

2. Methodology

2.1. QICS experiment overview

The Quantifying and Monitoring Potential Ecosystem Impacts of Geological Carbon Storage (QICS) experiment, conducted in the Scottish sea at Ardmucknish Bay in 2012, served as the basis for validating the CFD simulations in this study [11]. The QICS experiment involved the release of 4.2 tonnes of CO_2 at a depth of 9-12 meters over 37 days, producing 35 pockmarks on the seabed. Data collected included bubble size, rising velocity, pCO_2, and leakage rates, with a focus on three specific pockmark locations [11].

2.2. CFD model development

2.2.1. Hydrodynamic model

The Eulerian model [12] enables the modeling of bubble-liquid flow by employing the Euler-Euler approach, where continuous (primary) and discrete (secondary) phases are mathematically treated as interpenetrating continua.

2.2.2. Interphase mass transfer

The interphase mass transfer of a bubble with radius R_b is considered to be driven by the mass fraction gradient. The mass fraction of a chemical species j in the liquid bulk and bubble are represented by Y_e^j and Y_b^j, respectively, while the value of both quantities at each side of the bubble-liquid interface is given by Y_e^{j*} and Y_b^{j*}.

The mass transfer rate of a bubble due to a mass fraction gradient of species j is represented as:

$$m_b^j = k_e^j A_b \rho_e (Y_e^{j*} - Y_e^j) \qquad (1)$$

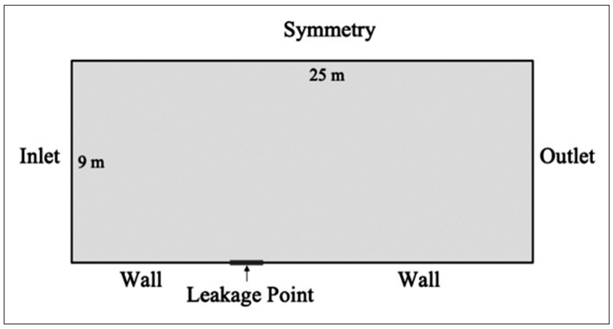
where $A_b = \pi R_b^2$ is the interfacial area of the bubble and k_e^j is the mass transfer coefficient for chemical species *j*, ρ is density (kg/m³), b is bubble and l is liquid.

2.2.3. Simulation set-up

2.2.3.1. Computational domain and mesh

During the QICS test on day 33 [11], the rising velocity and size of CO_2 bubbles leaking at a 9-meter depth in seawater were measured at three pockmark locations, with the pockmarks being evaluated at 16.78 cm in size. To study the CO_2 leakage at each pockmark, a two-dimensional (2D) computational domain was created. This 2D domain is often used to track fluid flow trajectories from the seabed to the sea surface, as it provides accurate maximum horizontal migration distances with minimal CPU load and shorter simulation times. The computational domain was designed as a rectangle with a height of 9 meters and a length of 25 meters, using the design modeler package. The height corresponds to the seawater depth during the test, while the length was selected to prevent any interruptions in the simulation. Figure 1 presents the generated boundary conditions for the computational domain.

Figure 1: Photo of generated boundary conditions.



Source: Analysis by authors

2.2.3.2. Boundary conditions

The boundary conditions for the domain were defined as follows:

a) Inlet boundary condition

A velocity inlet was specified on the left side of the domain to allow seawater to enter. The current velocity was set to 0.05 m/s.

b) Outflow boundary condition

The outflow condition was placed at the right boundary, as specific flow velocity and pressure values were not provided.

c) Symmetry boundary conditions

Symmetry boundary conditions with zero flow gradients were applied to both sides and the top of the domain to reflect this assumption.

d) Wall boundary condition

The seabed floor (bottom boundary) was modeled using a standard wall function to impose a no-slip condition, resulting in a zero velocity at this boundary.

e) CO_2 bubbles release

CO_2 bubbles were introduced through the pockmark at a steady flow rate of 1.296 kg/h, with an initial bubble diameter of 10 mm.

2.2.3.3. Solution method

The ANSYS Fluent Phase Coupled SIMPLE algorithm was applied in this study to solve complex multiphase flow problems, specifically focusing on the interaction between seawater and CO_2 leakage. By employing different discretization schemes, the algorithm ensured accurate simulations of volume fractions, momentum, and turbulence. Initially, a steady-state simulation modeled seawater flow, and then the algorithm was used to simulate CO_2 leakage by adjusting boundary conditions. The transient nature of CO_2 bubble formation and movement was captured using a time step of 0.001 seconds, with convergence achieved within 70-120 iterations. This application provided valuable insights into the behavior of CO_2 in marine environments, which is crucial for understanding leakage scenarios.

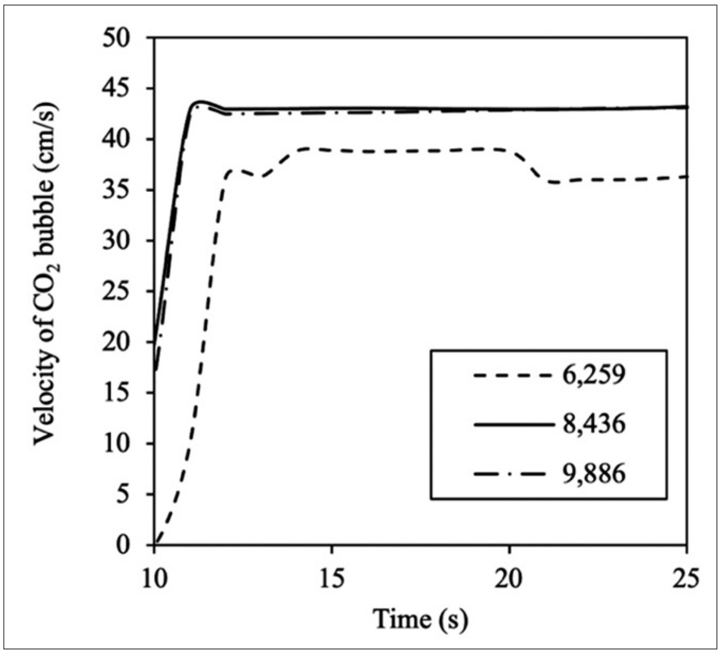
3. Results

3.1. Grid dependency

Mesh generation is a crucial step in the pre-processing of CFD simulations. In this study, the computational domain was divided into discrete volume elements using ANSYS Workbench Meshing software, with a finer mesh applied near the seabed and a coarser one near the top. To ensure the simulation results were independent of mesh size, three different meshes were created, containing 6,259, 8,436, and 9,886 elements.

The rising velocity was analyzed across these meshes, focusing on drag and lift forces without considering interaction effects. With a maximum current velocity of 5 cm/s, the results from all three meshes were consistent, confirming grid independence, as shown in Figure 2. Balancing computational cost with the need for accuracy, the mesh with 8,436 elements was selected for further analysis.

Figure 2: Study of mesh dependency



Source: Analysis by authors

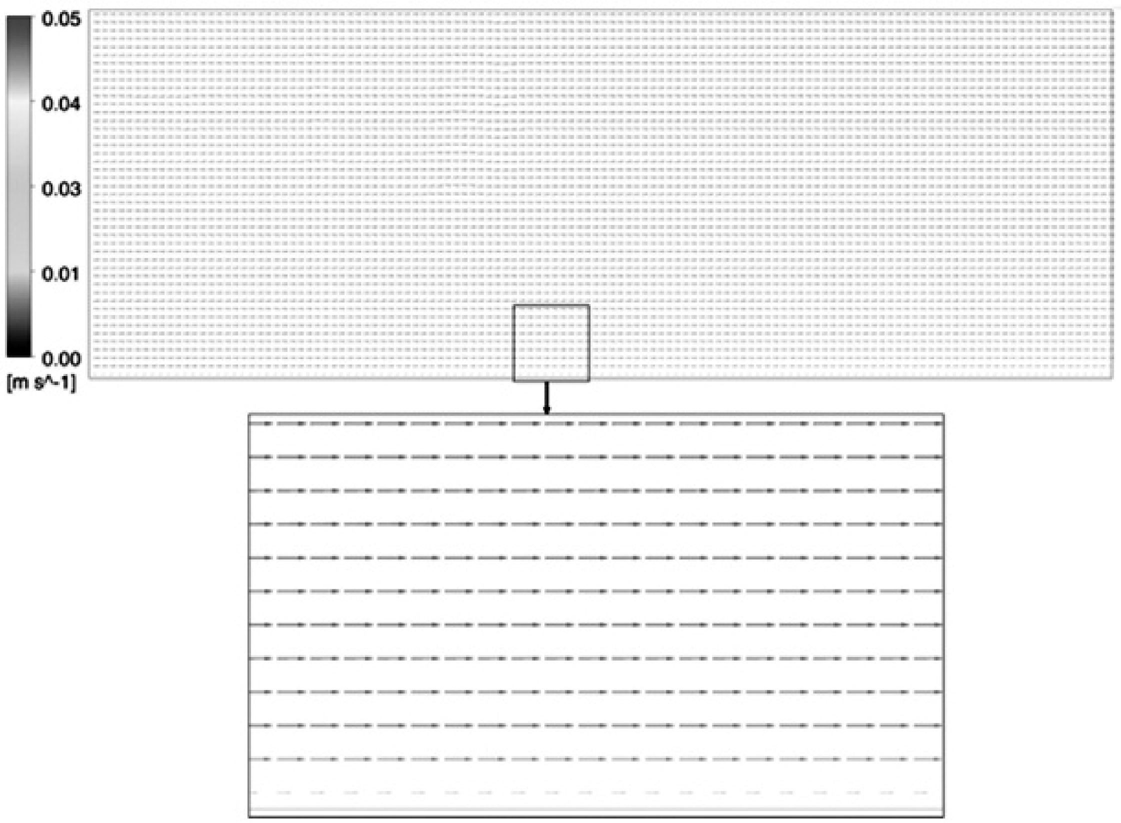
3.2. Prediction of current velocity

This section details the computation and analysis of ocean current velocity, shown in Figure 3 as a contour plot. The plot displays the shear velocity distribution at the sea surface, with a maximum velocity of 0.05 m/s, aligning with real-world observations. A zoomed-in section highlights local velocity variations, underscoring the accuracy of the computational model in predicting ocean currents.

3.3. Prediction of dissolution process

Figure 4 illustrates the temporal evolution of the partial pressure of CO_2 (pCO_2 when a CO_2 bubble is

Figure 3: Contour of the shear velocity distribution of current



Source: Analysis by authors

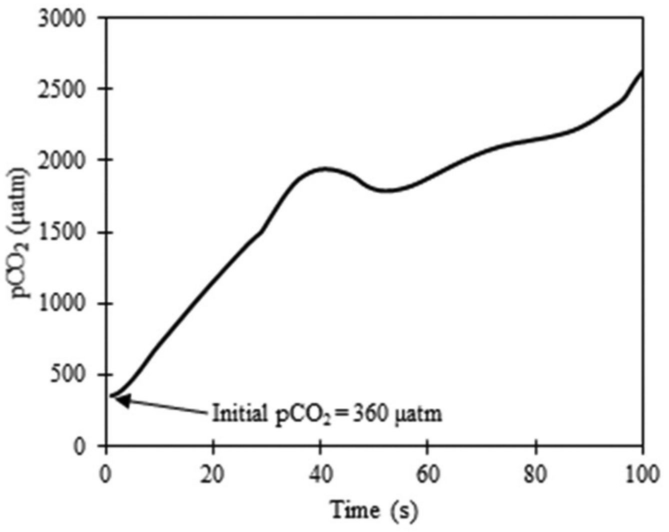
introduced into seawater. The x-axis represents time in seconds, while the y-axis represents the pCO_2 in microatmospheres (µatm). The initial pCO_2 level is marked at 360 µatm.

As shown in the Figure 4, there is a rapid increase in pCO_2 shortly after the CO_2 bubble is released, indicating the dissolution of CO_2 into the seawater.

3.4. Prediction of bubble size distribution

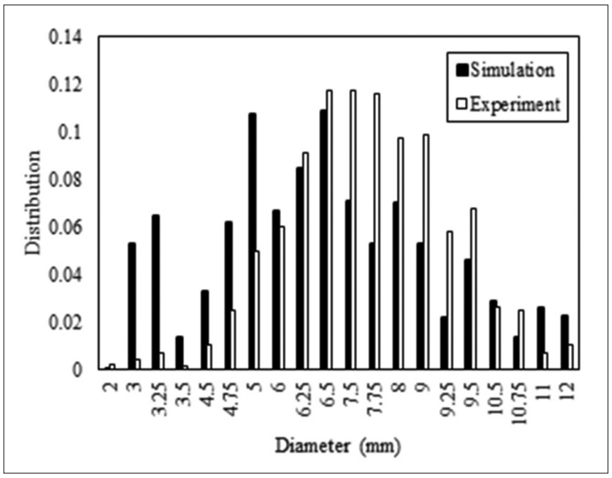
Figure 5 compares the predicted and experimental distributions of CO_2 bubble sizes, demonstrating a close correlation between the two, with bubble sizes ranging from 2.0 mm to 12.0 mm. This distribution highlights the prevalent bubble sizes and indicates that the model effectively simulates the bubble

Figure 4: Prediction of pCO_2 at a point of X = 5.6 m and Y = 0.3 m



Source: Analysis by authors

Figure 5: Prediction of bubble size distribution of released CO_2 bubbles



Source: Analysis by authors

formation process. The size of CO_2 bubbles is a critical factor in determining dissolution rates; smaller bubbles exhibit faster dissolution due to their higher surface area-to-volume ratio, resulting in variations in CO_2 dissolution across different bubble sizes.

4. Conclusion

This study found that the predictions are independent of mesh size, justifying the use of a medium mesh for the remainder of the analyses. The predicted current velocity was consistent with observed data, while the pCO_2 values were overestimated. Bubble size distribution was forecasted to fall within the 2.0-12 mm range. The reaction between dissolved CO_2 and seawater was not considered, potentially leading to the overestimation of pCO_2 since the dissolved CO_2 concentration remained unchanged. Future research should include this reaction to enhance the accuracy of seawater pH and pCO_2 predictions. Moreover, further validation of the CFD model through comparison with experimental data is recommended ■

Acknowledgment:

We acknowledge Ho Chi Minh City University of Technology (HCMUT), VNU-HCM for supporting this study.

REFERENCES:

1. J. Wilcox (2012). Carbon Capture: Springer-Verlag, New York.

2. GCCSI (2017). Understanding CCS-storage.

3. J. Koornneef, M. Spruijt, M. Molag, A. Ramírez, W. Turkenburg, and A. Faaij (2010). Quantitative risk assessment of CO_2 transport by pipelines—A review of uncertainties and their impacts. Journal of Hazardous Materials, 177, 12–27.

4. R. R. P. Noble, L. Stalker, S. A. Wakelin, B. Pejcic, M. I. Leybourne, A. L. Hortle, and K. Michael (2012). Biological monitoring for carbon capture and storage – A review and potential future developments. International Journal of Greenhouse Gas Control, 10, 520-535.

5. G. W. Kling, M. A. Clark, G. N. Wagner, H. R. Compton, A. M. Humphrey, J. D. Devine, W. C. Evans, J. P. Lockwood, M. L. Tuttle, and E. J. Koenigsberg, (1987). The 1986 Lake Nyos Gas Disaster in Cameroon, West Africa, Science, 236, 169-175.

6. P. G. Brewer, E. T. Peltzer, G. Friederich, and G. Rehder (2002). Experimental determination of the fate of rising CO2 droplets in seawater. Environmental Science & Technology, 36, 5441–5446.

7. G. Alendal and H. Drange (2002). Two-phase, near-field modeling of purposefully released CO_2 in the ocean. Journal of Geophysical Research: Oceans - Wiley Online Library, 106, 1085–1096.

8. Y. Kano, T. Sato, J. Kita, S. Hirabayashi, and S. Tabeta (2009). Model prediction on the rise of pCO_2in uniform flows by leakage of CO_2 purposefully stored under the seabed. International Journal of Greenhouse Gas Control, 3, 617-625.

9. L. H. H. P. Pham, R. Rusli, and L. K. Keong (2016). Consequence Study of CO_2 Leakage from Ocean Storage, Procedia Eng., 148, 1081-1088.

10. L. Schiller and Z. Naumann, Z. (1935). A Drag Coefficient Corre-lation. VDI Zeitung, 77, 318-320.

11. K. Shitashima, Y. Maeda, and A. Sakamoto (2015). Detection and monitoring of leaked CO_2 through sediment, water column and atmosphere in a sub-seabed CCS experiment. International Journal of Greenhouse Gas Control, 38, 135-142.

12. ANSYS Inc. (2024). ANSYS Fluent Theory Guide. ANSYS Inc., USA, 15317, 746.

Received date: August 10, 2024
Reviewed date: August 12, 2024
Accepted date: August 27, 2024

Authors information:
1. LOI HOANG HUY PHUOC PHAM[1,2]
2. AN NGUYEN SI XUAN[1,2]
[1]Department of Process and Equipment, Faculty of Chemical Engineering, Ho Chi Minh City University of Technology (HCMUT), 268 Ly Thuong Kiet Street, District 10, Ho Chi Minh City, Vietnam
[2]Vietnam National University Ho Chi Minh City, Linh Trung Ward, Thu Duc City, Ho Chi Minh City, Vietnam

NGHIÊN CỨU VỀ QUÁ TRÌNH HÒA TAN CỦA BỌT KHÍ CO_2 VÀO NƯỚC BIỂN

● **LỢI HOÀNG HUY PHƯỚC PHẠM[1,2]**
● **ÂN NGUYỄN SĨ XUÂN[1,2]**
[1]Bộ môn Quá trình và Thiết bị, Khoa Kỹ thuật Hoá học, Trường Đại học Bách khoa Tp. Hồ Chí Minh
[2]Đại học Quốc gia Thành phố Hồ Chí Minh

TÓM TẮT:

Công nghệ thu giữ và lưu trữ khí cacbonic (CCS) là một công nghệ quan trọng được thiết kế nhằm giảm thiểu khí thải CO_2 từ các nguồn công nghiệp như nhà máy nhiệt điện dùng nhiên liệu hóa thạch, nhà máy lọc dầu và nhà máy xi măng. Một khía cạnh chính của CCS liên quan đến việc lưu trữ CO_2 vào các tầng địa chất dưới đáy biển là khả năng rò rỉ khí CO_2 có thể gây rủi ro cho môi trường biển, do đó cần phải giám sát cẩn thận. Nghiên cứu này đánh giá quá trình chuyển khối của các bọt khí CO_2 được rò rỉ từ kho lưu trữ dưới đáy biển bằng cách sử dụng các mô phỏng động lực học chất lỏng tính toán (CFD). Phần mềm CFD-Fluent đã được sử dụng để mô phỏng sự thoát ra và hòa tan của các bọt khí CO_2 trong nước biển dưới các điều kiện dòng chảy khác nhau. Các mô phỏng đã được xác thực dựa trên dữ liệu thực nghiệm từ dự án định lượng và giám sát tác động có thể xảy ra đến hệ sinh thái biển khi lưu trữ khí cacbonic ở các tầng địa chất dưới đáy biển (QICS). Kết quả cho thấy mô hình CFD dự đoán chính xác đặc tính của bọt khí CO_2 được rò rỉ trong nước biển, cung cấp một công cụ hữu ích để đánh giá các rủi ro liên quan đến các hoạt động CCS.

Từ khóa: Bọt khí CO_2, rò rỉ, chuyển khối, dòng chảy, động lực học chất lỏng tính toán, hòa tan.