

Interface-mediated gas exchange in turbulent multiphase flowSimone Di Giorgio  and Alessandro Iafrati *Istituto di Ingegneria del Mare, Consiglio Nazionale delle Ricerche (INM-CNR),
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This paper is associated with a video winner of a 2024 American Physical Society's Division of Fluid Dynamics (DFD) Milton van Dyke Award for work presented at the DFD Gallery of Fluid Motion. The original video is available online at the Gallery of Fluid Motion, <https://doi.org/10.1103/APS.DFD.2024.GFM.V2694489>.

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Gas exchange at the ocean surface is a key process in Earth's climate system, as oceans represent a significant carbon sink, accounting for approximately 26% of global carbon budget [1,2]. The physics behind this process spans a wide range of length scales, from the mesoscale of the ocean surface, going through the meter scale of waves and the centimeter/millimeter scale of bubbles generated during wave breaking, and finally down to the very thin sea surface microlayer where molecular diffusion plays a role [3,4]. Reportedly [5], the larger proportion of gas exchange occurs in the upper ocean, and particularly during wave breaking events, when turbulence and bubble production are maximized. Despite its importance, this process is characterized by extremely complex physics and remains poorly understood [5]. So far, most of the research has focused on correlating gas transfer velocity with wind speed (e.g., Ref. [6]). Yet, the fundamental mechanisms driving gas exchange processes are not fully elucidated.

The first part of our award-winning video showcases a numerical simulation of a wave breaking event, highlighting the close coupling between interface deformation and gas transfer mechanisms that occurs during this intricate process. Figure 1 visualizes a typical wave breaking event, highlighting how gas concentration evolves across the air-water interface.

The sequence of snapshots shows the evolution of gas transfer during wave breaking under controlled initial conditions. The wave is initialized following established methods from [7–9], with wavelength λ and gravitational acceleration g resulting in reference velocity $U_R = (g\lambda)^{1/2}$.

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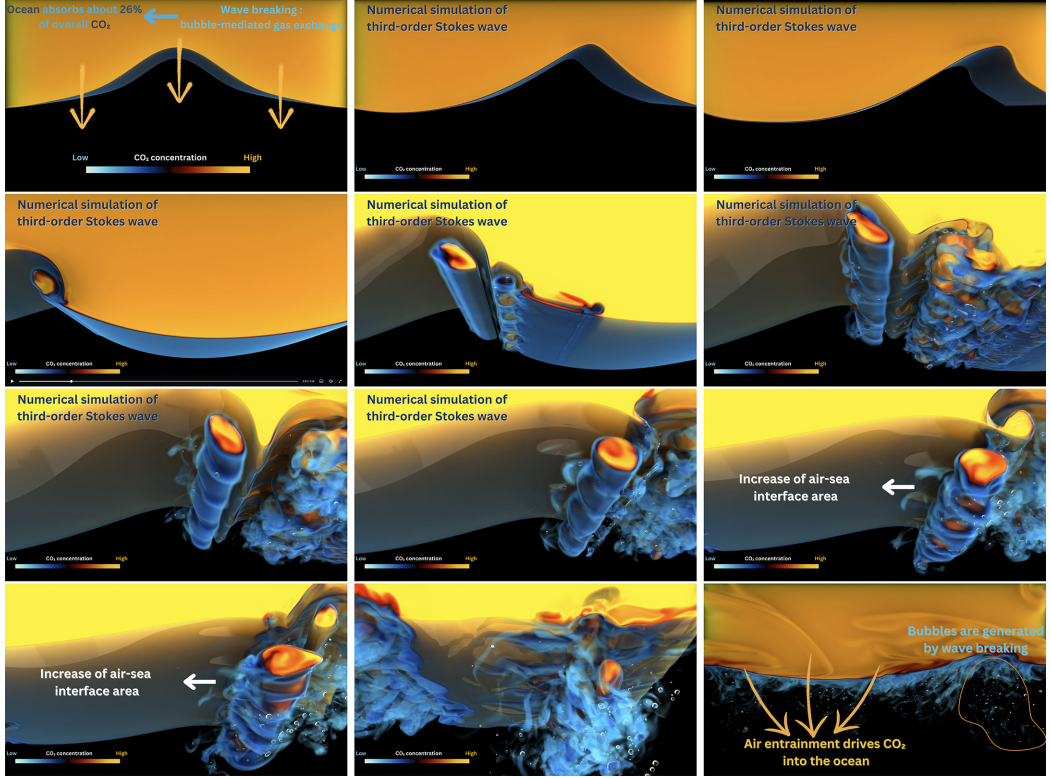


FIG. 1. Evolution of wave breaking and CO_2 gas exchange from initial time to postbreaking time. The rendering highlights the air-water interface, showing the wave profile evolution and bubbles entrained in water. The color map indicates CO_2 concentration: Transparent/blue represents zero/low concentration (initially zero in water), while red/yellow represents high concentration (initially unitary in air). The sequence demonstrates how a steep third-order Stokes wave ($\epsilon = 0.5$) transitions from stable propagation (top panels) to violent plunging breaking (second row of panels), entraining large air pockets that fragment into smaller bubbles. This fragmentation dramatically increases the interfacial area available for gas transfer; the gas is transferred from air to water, with colors showing the distribution of CO_2 advected by the flow. Simulation parameters: $\text{Re} = 40\,000$, $\text{We} = 12\,000$, $\text{Fr} = 1$.

The simulation is performed under specific dimensionless conditions. The Weber number $\text{We} = (\rho_w U_R^2 \lambda) / \sigma = 12\,000$, with σ the surface tension coefficient, represents the ratio of inertial forces to surface tension effects, corresponding to waves with $\lambda \simeq 30$ cm. The Reynolds number $\text{Re} = (\rho_w U_R \lambda) / \mu_w \simeq 500\,000$, and represents the inertia to viscous forces ratio; however, computational constraints require reducing this to $\text{Re} = 40\,000$ to resolve the essential flow structures. The Froude number, i.e., the inertia to gravity forces ratio, is $\text{Fr} = U_r / \sqrt{g\lambda} = 1$. The dissolving gas parameters are Schmidt number $\text{Sc}_w = 4$ (momentum-to-mass diffusivity ratio), air-to-water diffusivity ratio $D_a/D_w = 100$, and solubility $\alpha = 0.33$. The reduced value of Sc compared to real oceanic CO_2 ($\text{Sc} \approx 660$) enables grid resolution while preserving key gas transfer mechanisms. Simulations are performed using a two-phase Navier-Stokes solver coupled with a volume of fluid (VOF) approach to accurately track the interfaces between air and water [9–11]. In addition, we account for the gas exchange process by solving an advection-diffusion equation for the chemical species. The details and validations of the numerical method can be found in Refs. [12,13], in particular the gas transfer velocity is overestimated by approximately 8% for bubbles with a diameter smaller than 25 grid cells, which account for less than 4% of the total air volume entrained in the simulation reported

here. The computational domain is discretized using $N_x = 1152$, $N_z = 576$, $N_y = 768$ collocation points, uniformly distributed in the x and z directions, and in the y direction between $y = -\lambda/4$ and $y = +\lambda/4$ (well-resolved region). The size of the grid is the same in all directions in the uniform grid region, while the size of the cell increases toward the bottom and top boundaries according to a hyperbolic tangent function [14].

The atmosphere above the wave is fully saturated with gas (CO_2 concentration = 1, shown in yellow), while the water below contains initially no gas (CO_2 concentration = 0). More details about this simulation are provided in Ref. [13]. The frames capture the complete evolution of a third-order Stokes wave from its initial steep configuration to violent breaking. The high wave steepness ($\epsilon = 0.5$) produces an energetic plunging breaker, where the wave crest curls over and impacts the water surface ahead of the wave. The breaking process occurs in distinct phases. As the steep wave becomes unstable, its crest overturns and entrains a large, cylindrical volume of gas-rich air beneath the surface. The violent turbulence generated by wave breaking subsequently fragments this trapped air mass into a number of smaller bubbles of varying sizes. This fragmentation process is critical for gas exchange efficiency. When large air pockets break into smaller bubbles, the total interfacial area available for gas transfer increases substantially. Each new interface represents a location where concentration gradients drive CO_2 transfer from the air phase into the water. The final panels of Fig. 1 illustrate this interface increase, with the color gradient showing CO_2 beginning to transfer from bubbles into the surrounding water. The breaking wave simultaneously generates turbulent eddies across multiple length scales—from large, wave-scale circulations to small, submillimeter vortices that enhance mixing and accelerate gas transfer into the water column.

The wave breaking phenomenon described above is also responsible for most of the energy dissipation occurring in the ocean, and there is clear evidence that this dissipation is strongly related to air entrainment, as already documented in the literature [9,15].

Because of the prominent role played by bubbles in gas exchange occurring at the ocean surface, we have also directed our attention to the problem of interface-mediated gas exchange.

The wave breaking simulations reveal the complex multiphase dynamics of gas exchange, but the chaotic nature of the process makes it difficult to isolate individual drop/bubble contributions. Moreover, our simplified setup cannot capture real-world complexities such as the much larger Reynolds and Schmidt numbers in oceanic conditions, complex wave spectra, temperature gradients, and salinity variations.

To better understand the fundamental mechanism of the gas transfer across the interface, we have focused on a simplified configuration that allows us to study the fundamental physical mechanisms in a controlled and reproducible environment. Hence, we conducted direct numerical simulations (DNSs) of a wall-bounded turbulent channel flow upon injection of CO_2 laden drops.

The DNSs are carried out by imposing a constant mass flow rate at bulk Reynolds number $\text{Re} = 10\,000$, where the reference length is the half channel height, $\tilde{L} = h$. The size of the computational domain is $L_x \times L_y \times L_z = 4\pi h \times 2h \times 2\pi h$ in the streamwise, wall-normal, and spanwise directions, respectively. The grid spacing is uniform in the streamwise and spanwise direction, where the flow is periodic, while it is nonuniform in the wall-normal direction where no-slip conditions are enforced at the top and bottom walls and then natural grid stretching [16] is used to cluster collocations points towards the channel walls. The grid resolution for each case is $\Delta x^+ = \Delta z^+ \approx 3.27$, while Δy^+ ranges between 0.046 and 3.06. Hereinafter, and for ease of notation, we will use the subscript d to refer to drops, and the subscript c to refer to the carrier flow. All simulations are initialized by injecting two horizontal layers of regularly spaced spherical drops. The drops have an initial diameter of $d = 0.4h$ with their centers located at a distance of $y_{d,0} = 0.5h$ from the top and bottom wall, respectively (128 drops in each planar distribution). The volume fraction of the drops is $V_d/(V_d + V_c) = 5.4\%$, with V_d and V_c the total volume of the drops and the carrier phase, respectively. The initial condition of the species concentration field is such that all drops are initially saturated with an initial concentration $c_d = 1$, while the carrier phase is initially empty, with an initial concentration $c_c = 0$.

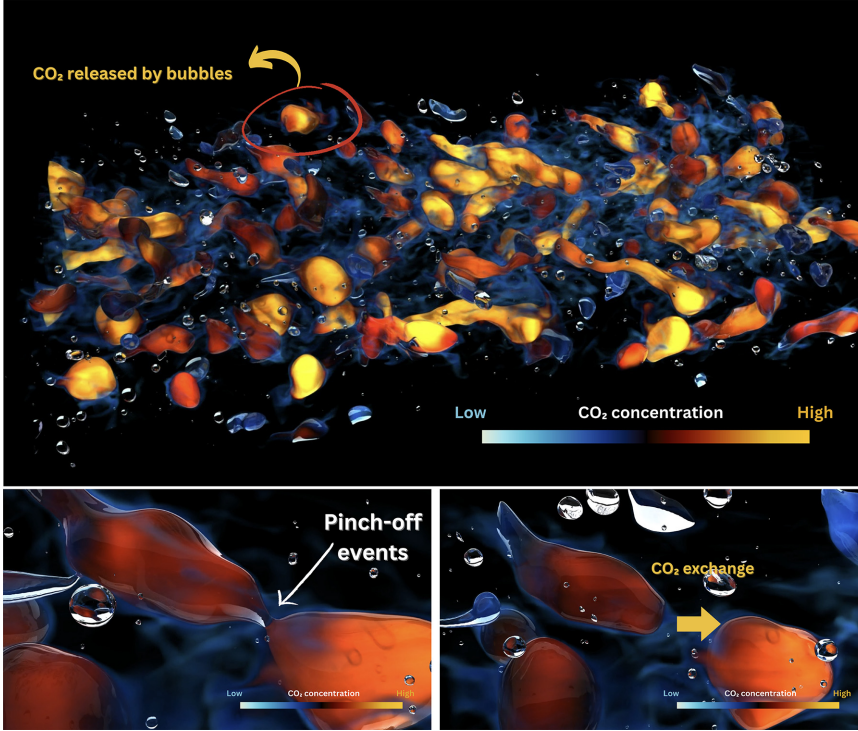


FIG. 2. Drop dynamics and CO_2 transfer in turbulent channel flow ($\text{Re} = 10\,000$). Top panel: Multiple deformable drops with CO_2 concentration shown as volume rendering (transparent/blue = zero/low concentration, red/yellow = high concentration). Bottom panels: Detailed pinch-off event showing drop breakup (left) and corresponding CO_2 exchange with interface increase (right). The fragmentation process increase interfacial area for enhanced mass transfer, with colors indicating CO_2 distribution in the turbulent flow.

For simplicity, the bubbles are assumed to have the same density and viscosity as the carrier fluid, allowing the analysis to focus on the effects of deformation, breakage, and coalescence on gas exchange. Turbulence strongly affects the drops dynamics, causing interface deformation and enhancing the gas transfer between drops and the surrounding fluid. Figure 2 illustrates how bubbles release CO_2 into the water, with the color map representing gas concentration (blue for low concentration, red/yellow for high concentration). The top panel shows a complex field with drops of various shapes and dimensions, whose individual and collective dynamics control the overall distribution of gas concentration. Our simulations capture two critical phenomena that significantly impact gas exchange rates: drop breakup and coalescence. The left-bottom panel in Fig. 2 highlights “pinch-off events,” during which larger drops break into smaller ones. These events are particularly effective at enhancing gas transfer, as they generate fresh interfaces (increase of the total interface area) with high concentration gradients (see the right-bottom panel of Fig. 2).

Equally important are the coalescence events shown in Fig. 3, and representing the merger of two drops with different gas concentrations and dimensions. The sequence of snapshots during a coalescence event (Fig. 3) shows that two approaching bubbles initially retain very different gas concentrations, but, upon merging, rapidly develop a uniform internal gas concentration as a result of internal diffusion and advection processes. This represents a physical building block through which gas concentration interacts with drops dynamics and redistributes gases in oceanic environments.

In summary, our high-fidelity numerical simulations reveal the intricate interactions among turbulence, interface dynamics, and mass transfer at small scales, which collectively impact the global

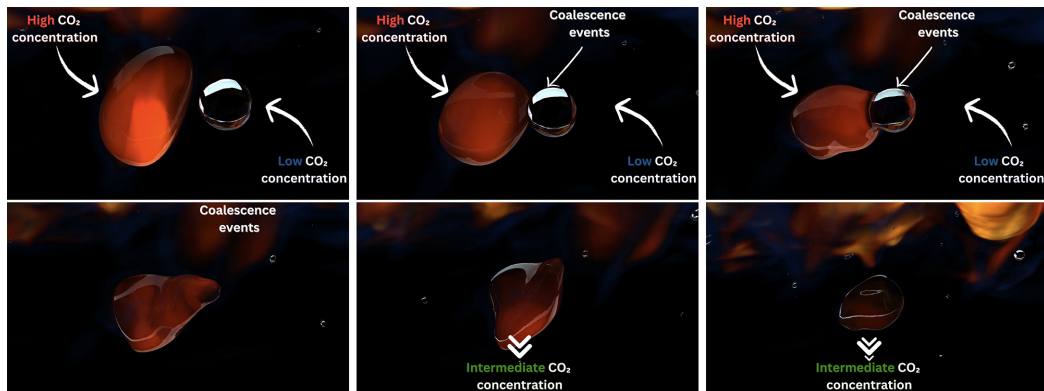


FIG. 3. Coalescence sequence of two drops with different initial CO_2 concentrations and sizes. The sequence shows approach (top-left panel), merging (top-right panel), and final uniform mixing (bottom panel). Gas concentration: transparent/blue = zero/low, red/yellow = high. The process demonstrates how coalescence redistributes gas concentration through internal mixing, impacting overall mass transfer in turbulent multiphase flows.

carbon cycle. Furthermore, these findings underscore the critical importance of accurately modeling bubble/drop-mediated gas-exchange processes within turbulent environments. Our analysis demonstrates that breaking waves entrain air, generate bubbles, and enhance gas transfer through increased interface area and turbulent mixing. The detailed resolution of phenomena such as bubbles/drops breakup and coalescence provides unprecedented insight into the fundamental mechanisms controlling air-sea gas exchange. These findings emphasize the need for improved parametrizations in climate models that account for the multiscale, multiphase nature of ocean-atmosphere gas exchange. By better understanding the microscale processes governing interface-mediated transfer, we aim to develop more accurate models of CO_2 absorption by the oceans, thus helping improved predictions of climate change impacts and more effective environmental policies.

Data availability. The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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