

Modeling of near-source conditions of alkalinity injection in marine environment for precipitation assessment

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ABSTRACT

The permanent sequestration of carbon dioxide via Ocean Alkalinity Enhancement offers a promising pathway for large-scale climate mitigation. However, the operational safety of alkaline discharges is contingent upon avoiding secondary calcium carbonate precipitation, which occurs when the seawater aragonite saturation state exceeds critical thresholds. This study investigates the near-field mixing dynamics of bicarbonate-enriched effluents using high-resolution Large Eddy Simulations across various seasonal stratification and buoyancy regimes.

We implement a methodological framework that couples passive scalar transport of Total Alkalinity and Dissolved Inorganic Carbon with an equilibrium chemistry approach. By leveraging the linearity of transport equations and established Reynolds number independence, we present a non-dimensional formulation that allows for the scaling of results across diverse plant capacities and injection concentrations without the need for additional computational fluid dynamics runs.

Our results indicate that while the spatial decay of the saturation state under threshold safety values are primarily governed by jet momentum, the residence time within the supersaturated zone is strongly modulated by ambient buoyancy and stratification. Even when accounting for turbulent fluctuations, via a conservative 95th-percentile analysis, the maximum residence times observed remained, for representative industrial scales, orders of magnitude below than the timescales required for carbonate nucleation and precipitation kinetics reported in the literature. These findings suggest that the risk of runaway secondary precipitation in the near-source region is negligible under the examined conditions, providing a scalable quantitative foundation for the design and environmental safety assessment of ocean alkalinity enhancement technologies.

1. Introduction

Anthropogenic carbon dioxide (CO₂) emissions are driving ocean acidification and global warming (Intergovernmental Panel on Climate Change (IPCC), 2023). To mitigate these impacts, Ocean Alkalinity Enhancement (OAE) has emerged as a promising strategy for long-term carbon sequestration (Moras et al., 2022). Among OAE technologies, Buffered Accelerated Weathering of Limestone (BAWL) (Caserini et al., 2021) offers a scalable approach by reacting CO₂ with seawater and carbonate minerals to produce a bicarbonate-enriched solution. This process, further optimized for industrial application by Limenet®, injects a pH-balanced effluent into the marine environment to facilitate carbon storage while buffering local ocean acidification (Fakhraee et al., 2023). However, the operational safety and efficiency of alkaline discharges are strictly contingent upon avoiding secondary calcium carbonate (CaCO₃) precipitation, a process where dissolved calcium and

carbonate ions recombine into solid minerals. Secondary precipitation shifts the carbonate equilibrium, leading to the degassing of previously sequestered CO₂ gas back into the atmosphere and causing a severe reduction in net carbon removal efficiency (Moras et al., 2022; Varliero et al., 2024). The thermodynamic propensity for this chemical reaction is governed by the aragonite saturation state (Ω_a), defined as the ratio of the ion concentration product of dissolved Ca²⁺ and CO₃²⁻ to their stoichiometric solubility product (K'_{sp}):

$$\Omega_a = \frac{[\text{Ca}^{2+}][\text{CO}_3^{2-}]}{K'_{sp}} \quad (1)$$

Seawater pH directly dictates this equilibrium: higher pH levels shift dissolved inorganic carbon species toward carbonate ions ([CO₃²⁻]), which in turn raises Ω_a . While typical open-ocean background values range between $\Omega_a \approx 2$ and 4, recent empirical findings demonstrate that exceeding a critical design threshold of $\Omega_a = 7$ rapidly

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accelerates nucleation kinetics (the initial formation and growth of solid mineral seeds via homogeneous or heterogeneous pathways), triggering uncontrollable secondary CaCO_3 precipitation (Varliero et al., 2024). Given projected industrial operational discharge rates of up to 1 ton/h of dissolved alkalinity, ensuring rapid hydrodynamic mixing and scalar dilution below this critical threshold ($\Omega_a < 7$) is a primary engineering challenge for offshore outfall systems. While existing studies have explored OAE in controlled open ocean environments, called *mesocosms* (Groppelli et al., 2026), the hydrodynamics of full-scale discharge through pipelines, framed as a free round jet problem, remains poorly understood in dynamic, inherently turbulent marine environments. Current literature on wastewater outfalls often focuses on regimes that are not directly comparable; for instance, many numerical studies operate at low Reynolds numbers ($\text{Re} \approx 10^3$) or high stratification frequencies that do not represent high-momentum injections ($\text{Re} \approx 10^5$) characteristic of industrial OAE plants (He et al., 2022). Computational Fluid Dynamics (CFD) is essential for evaluating these systems where *in situ* experiments are constrained by logistical or regulatory hurdles. In this study, we employ Large Eddy Simulation (LES) within the OpenFOAM framework to resolve the turbulent mixing of the jet. Unlike traditional Reynolds-Averaged Navier–Stokes (RANS) approaches, LES provides a superior description of unsteady entrainment processes and the evolution of scalar concentrations in stratified flows. To bridge fluid mechanics with marine carbonate chemistry without incurring prohibitive computational costs, ocean chemistry is coupled via an equilibrium thermodynamic framework. Rather than solving stiff chemical kinetic differential equations, we track Dissolved Inorganic Carbon (DIC, representing the sum of all inorganic carbon species $[\text{CO}_2^*] + [\text{HCO}_3^-] + [\text{CO}_3^{2-}]$) and Total Alkalinity (TA, representing the net charge balance of weak acid anions) as conservative passive scalar tracers (Zeebe and Wolf-Gladrow, 2001). From the resolved local DIC and TA fields, local values of pH (reported in total scale) and Ω_a are calculated as diagnostic parameters. Furthermore, to evaluate whether fluid parcels remain within supersaturated “hotspots” ($\Omega_a > 7$) long enough to initiate mineral formation, we compute the local fluid residence time (τ), defined as the temporal duration a fluid element spends within the critical zone prior to dilution, and compare it against the characteristic kinetic time scales required for CaCO_3 nucleation and degassing reported in available literature. By leveraging an established Reynolds number independence assessment and a scalable non-dimensional problem formulation, this work provides a generalized framework for assessing the risk of secondary CaCO_3 precipitation. This approach enables the evaluation of diverse engineering designs (varying effluent flow rates and alkalinity dosage concentrations) through post-processing, avoiding the need for multiple, computationally prohibitive CFD runs. The primary objectives of this research are:

- to identify near-source saturation “hotspots” exceeding the critical safety threshold ($\Omega_a = 7$) under diverse discharge and seasonal stratification regimes;
- to quantify the maximum residence times (τ) of water parcels within these critical supersaturated zones and evaluate the physical risk of bicarbonate nucleation;
- to elucidate the competing effects of momentum, seasonal thermal stratification, and ambient buoyancy forces on near-field plume mixing and scalar dispersion.

The paper is organized as follows: Section 2 describes the methodology proposed, in terms of chemistry modeling, numerical setup, cases simulated and assessment of the validity of the dataset; Section 3 presents the analysis of the discharge scenarios; finally, Section 4 draws the conclusions.

2. Methodology

The parameter space governing the hydrodynamics of a buoyant jet in a marine environment is extensive. In the absence of buoyancy forces, the flow is unequivocally described by a single dimensionless group, the Reynolds number (Re), which relates the jet inlet velocity U , the nozzle diameter D , and the kinematic viscosity ν . The Reynolds number represents the ratio of inertial forces to viscous forces within the fluid, dictating the degree of flow turbulence (Pope, 2000). However, when buoyancy is considered due to density variations, the density difference between the effluent (ρ_j) and the ambient fluid (ρ_∞) introduces additional complexity, typically characterized by the Richardson number (Ri), which quantifies the relative importance of buoyancy forces over flow shear dynamics. In a stratified marine environment, the flow is further influenced by the density gradient $d\rho/dz$, or equivalently the Brunt–Väisälä frequency N (the static stability frequency of the water column governing internal gravity wave oscillations), and the depth at which the injection of alkaline seawater occurs, denoted as z_j . While real-world marine stratification is often non-linear (i.e., $N = N(z)$), assuming a linear distribution is a common and robust practice in current literature (Chubarenko and Hutter (2005), Yang et al. (2017)). Although linear profiles capture first-order stratification effects, we acknowledge that more complex, exponentially decaying profiles may be required to reproduce extreme summer scenarios with low vertical mixing (Fairall et al., 1996). Under the Boussinesq approximation, which introduces an error of less than 1% for the temperature ranges considered in this study (by treating density differences as negligible except where they appear in terms multiplied by gravitational acceleration g), the density gradient remains constant with depth. This allows for the definition of three fundamental dimensionless groups, derived from the Navier–Stokes equation (Vallis, 2017), that fully parameterize the flow physics:

$$\text{Re} = \frac{UD}{\nu} \quad (2)$$

$$N^2 = \frac{g}{\rho_0} \left| \frac{\partial \rho}{\partial z} \right| = \frac{g}{\rho_0} \frac{\rho(z_j) - \rho(0)}{z_j} \quad (3)$$

$$\text{Ri} = \frac{gD(\rho_j - \rho(z_j))}{\rho_0 U^2} \quad (4)$$

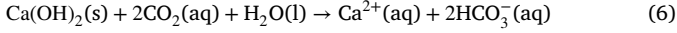
where ρ_0 is the reference density of seawater. Note that z indicates the vertical coordinate, positive pointing downwards, while x and y coordinates define the axial and transversal directions, respectively. Hence, density can be defined with respect to the vertical coordinate z . In this study, we assume a realistic operational scenario where the jet discharges seawater at the same temperature as the surface intake, such that $\rho_j = \rho(0)$. Physically, this represents a system where surface seawater is drawn in, enriched with alkaline minerals, and re-injected at depth z_j without significant thermal manipulation. This assumption couples N and Ri via the injection depth z_j , yielding:

$$\text{Ri} = \frac{N^2 z_j D}{U^2} \quad (5)$$

Consequently, N models the regional oceanographic conditions, while Re and Ri encapsulate the primary engineering design variables (U, D, z_j). It is worth noting that while the nozzle diameter D serves as the characteristic length scale for the local velocity shear (U/D), the injection depth z_j dictates the vertical density deficit $\Delta\rho = \rho_j - \rho(z_j)$ under linear stratification. Consequently, the injection depth z_j is implicitly embedded within the density difference term of Eq. (4), yielding the explicit coupled dependence $\text{Ri} = N^2 z_j D / U^2$ shown in Eq. (5). This approach ensures the scalability of our results; for instance, doubling the jet diameter produces an effect equivalent to doubling the injection depth or reducing the inlet velocity by a factor of $\sqrt{2}$ for Re -independent quantities.

2.1. Chemistry modeling and scalar transport

The BAWL process is based on the following chemical reaction:



which results in an injection of TA and DIC into the marine environment through a pH-equilibrated solution. To model this process, it becomes essential to represent the interaction of these added quantities with the marine carbonate system, a non-trivial task due to the numerical stiffness of the governing equations. A full kinetic representation would require solving seven coupled differential equations (Zeebe and Wolf-Gladrow, 2001), which is computationally prohibitive for high-resolution LES. To ensure feasibility without sacrificing accuracy in the near-field, we adopt an equilibrium chemistry approach. Since any two variables are sufficient to define the carbonate system at equilibrium, we track DIC and TA as conservative passive scalars:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \nabla \cdot (D_{eff} \nabla \phi) \quad (7)$$

where $\phi \in \{\text{DIC}, \text{TA}\}$ is a general scalar tracer and D_{eff} is the effective diffusivity (molecular plus turbulent). By leveraging the linearity of passive scalar advection-diffusion transport, we formulate a non-dimensional scalar tracer $\phi^* \in [0, 1]$ normalized by the inlet injection value (ϕ_{inj}) and the depth-dependent ambient background value ($\phi_{\infty}(z)$):

$$\phi^* = \frac{\phi - \phi_{\infty}(z)}{\phi_{inj} - \phi_{\infty}(z)} \quad (8)$$

Under non-dimensional spatial ($\mathbf{x}^* = \mathbf{x}/D$), velocity ($\mathbf{u}^* = \mathbf{u}/U$), and temporal ($t^* = tU/D$) coordinates, the scalar transport equation simplifies to:

$$\frac{\partial \phi^*}{\partial t^*} + \nabla^* \cdot (\mathbf{u}^* \phi^*) = \frac{1}{\text{ReSc}_{eff}} \nabla^{*2} \phi^* \quad (9)$$

where Sc_{eff} is the effective Schmidt number combining molecular and sub-grid scale turbulent diffusivities. This formulation provides a powerful computational advantage: for any solved hydrodynamic flow field governed by dimensionless parameters (Re , Ri , N), the non-dimensional scalar field $\phi^*(\mathbf{x}^*, t^*)$ is resolved once. Physical concentration fields for Total Alkalinity (TA) and Dissolved Inorganic Carbon (DIC) for any arbitrary plant capacity or chemical dosing dosage (TA_{added} , DIC_{added}) can be retrieved a posteriori via direct linear scaling:

$$\text{TA}(\mathbf{x}, t) = \text{TA}_{\infty}(z) + \phi^*(\mathbf{x}^*, t^*) \cdot \text{TA}_{added} \quad (10)$$

$$\text{DIC}(\mathbf{x}, t) = \text{DIC}_{\infty}(z) + \phi^*(\mathbf{x}^*, t^*) \cdot \text{DIC}_{added} \quad (11)$$

This simplification allows the saturation state (Ω_a) and pH to be computed as a post-processing step for any time instant using the *pyCO2SYS* library (Humphreys et al., 2022) by passing the linearly scaled physical concentrations directly into the thermodynamic model, completely bypassing the need for additional computationally expensive CFD runs. The carbonate system equilibrium is defined using the dissociation constants K_1 and K_2 from Lueker et al. (2000), while the bisulfate dissociation constant ($K_{\text{HSO}_4^-}$) follows Dickson (1990). The total boron concentration is estimated from salinity using the ratio provided by Uppström (1974). Solubility products (K_{sp}) for the calculation of calcite and aragonite saturation states are based on Mucci (1983), with all pH values reported on the total scale (pH_T). This methodology assumes that biological feedbacks and air-sea gas exchange are negligible over the short spatiotemporal scales characteristic of the discharge point (minutes to hours). Furthermore, while this approach cannot explicitly predict the kinetics of CaCO_3 precipitation, it provides diagnostic tendency maps. To address the risk of secondary precipitation, we introduce a tracking of the residence time (τ) (Ghirelli and Leckner, 2004), modeled by the equation:

$$\frac{\partial \Theta}{\partial t} + \nabla \cdot (\Theta \mathbf{u}) = \nu_t \nabla^2 \Theta + \phi \quad (12)$$

with $\Theta = \phi \tau$ being the quantity of residence time. By identifying regions where $\Omega_a > 7$ and quantifying the duration the effluent spends in these “hotspots”, we can evaluate the potential for bicarbonate precipitation as discussed in Section 3.1.

2.2. Test matrix and scenario design

The comprehensive dataset was generated according to the test matrix presented in Table 1, with scenarios categorized to isolate specific physical effects. The unstratified scenario (W) serves as a baseline representing a non-buoyant, non-stratified turbulent round jet. In contrast, the stratified scenarios (S) are characterized by the interplay of buoyancy and stratification, featuring high stratification (HN, $N = 0.03$ rad/s) and low stratification (LN, $N = 0.02$ rad/s) conditions. Within the high-stratification regime, buoyancy variations are further explored through low Richardson (LR, $Ri = 0.006$) and high Richardson (HR, $Ri = 0.012$) numbers. Finally, in Appendix A, the assumption of Reynolds number independence is critically assessed by comparing the 120×10^3 baseline with a dedicated low-Reynolds simulation (WL, $Re = 60 \times 10^3$).

It is worth noting that the range of tests conducted in terms of N and Ri could be further expanded to more buoyancy dominated jets and higher stratification conditions, but in order to maintain a certain degree of fidelity with respect to real operational injection scenarios, broadening the range of applicability is left for future work. While the fluid dynamics are governed by these dimensionless groups, the chemical behavior is absolute and depends on specific concentration values. Therefore, physical concentrations are retrieved *a posteriori*. For all cases, the seabed temperature is fixed at 20 °C, while surface temperatures are 30 °C for $N = 0.3$ and 25 °C for $N = 0.2$. Ambient profiles for pH and Ω_a (Fig. 1) were computed using the *pyCO2SYS* library, based on tropical open-ocean datasets (E.U. Copernicus Marine Service Information, 2019), assuming a constant salinity of 35 PSU.

To assess also potential differences due to injection values of DIC and TA, two different operational plant conditions have been examined, presented in Table 2. A more complete description of how these values have been computed is given in Appendix B.

2.3. Numerical setup

The CFD setup is based on the open-source suite OpenFoam v12 (Weller et al., 1998). Buoyancy effects are added to the set of equations through the Boussinesq approximation, based on the chosen Ri , and the hydrostatic pressure effect due to stratification was also accounted for through the static solution of the pressure equation:

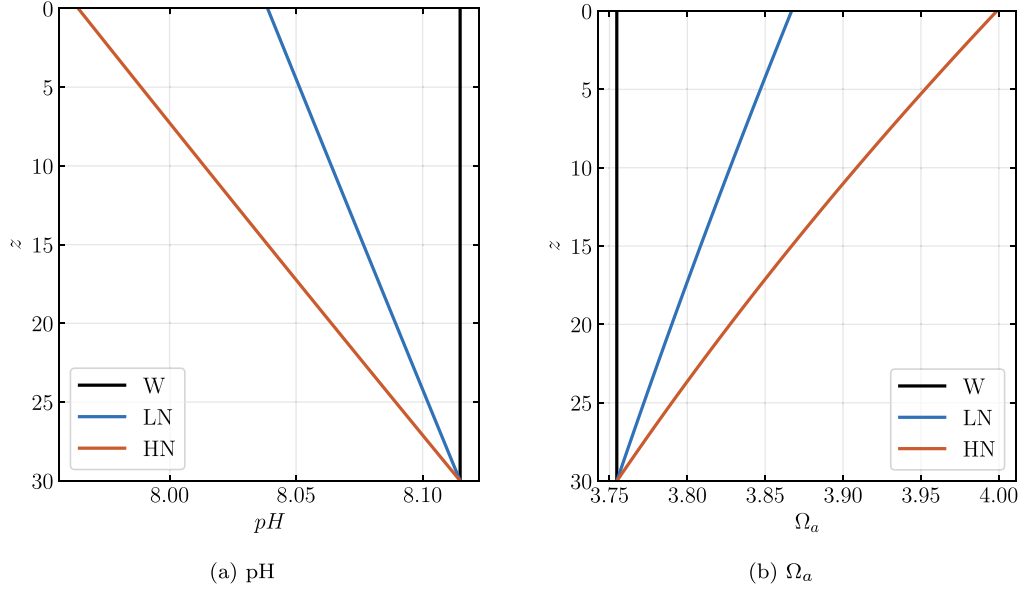
$$\frac{dp}{dz} = \rho(z)g \quad (13)$$

The stratification was imposed at the beginning of the simulation, and open-mixed boundary conditions (*pressureInletOutletVelocity*) were applied at the outlet and the sides. These allow for the flux to both enter and exit the domain, while prescribing that the inlet flux must respect the imposed stratification. Slip conditions were imposed to the top and bottom, and a turbulent velocity profile was prescribed at the inlet, taken from the experimental setup of Xu and Chen (2012), superimposed with random fluctuations around the mean profile with a magnitude of 0.5% of the mean velocity, a conservative low value according to present literature Ghaisas et al. (2015), Kuan et al. (2023a), that prevents from overestimating the core-length. In fact, according to Or et al. (2011), Bogey and Bailly (2006), the core length of the jet, a preliminary zone in which centerline velocity and scalar concentrations do not decay, is influenced by both external and inlet conditions. Capturing the instability process that leads to the establishment of a fully turbulent jet is no trivial task, and it lies out of the scope of this work. However, since the definition of a critical length under which uncontrolled precipitation is avoided can be influenced by the core length, it is important to take into account this source of uncertainty.

Table 1

Test matrix of the simulated cases. T_{bot} and T_{top} denote bottom and top temperatures ($^{\circ}\text{C}$); z_j/D is injection depth. Naming: W = Unstratified, S = Stratified, L/H = Low/High, R = Ri, N = N .

Case	Description	Re	Ri	N [rad/s]	T_{bot}	T_{top}	z_j/D
WL	Unstratified, Low Re	60×10^3	0	0	20	20	12
W	Unstratified Baseline	120×10^3	0	0	20	20	12
SHRHN	Stratified, High Ri, High N	120×10^3	0.012	0.03	20	30	24
SLRHN	Stratified, Low Ri, High N	120×10^3	0.006	0.03	20	30	12
SLRLN	Stratified, Low Ri, Low N	120×10^3	0.006	0.02	20	25	27.2

**Fig. 1.** Ambient profiles of pH (a) and Ω_a (b) in the simulated domain.**Table 2**

Operational Plants considered for the precipitation assessment analysis. TA and DIC values indicate added and absolute values at the inlet. Ω values are referred to aragonite saturation state at the inlet, for reference. For each plant, the nominal storing capacity of the plant is reported.

Plant	TA_{added} [$\mu\text{mol/kg}$]	DIC_{added} [$\mu\text{mol/kg}$]	TA_{tot} [$\mu\text{mol/kg}$]	DIC_{tot} [$\mu\text{mol/kg}$]	Ω_{inlet}	$CO_{2,\text{stored}}$ [kg/h]
P1	3832	3397	6477	5715	10.5	120
P2	6962	6258	9607	8576	15	270

Together with the verification process we conduct in this work (Section 2.4), the choice of inlet conditions complying with a fully turbulent injection scenario and the high Reynolds number simulated, we believe that our current analyses are in line with present literature, yielding a core length of approximately 4 diameters. The *local dynamic k-equation* model (Kim and Menon, 1995) was chosen to model the sub-grid scales, together with the assumption of constant turbulent Prandtl and Schumann number for the transport of temperature and passive scalars. The domain length and span, relative to inlet diameter, are fixed to $x = [-2, 48] D$, $y = [-12, 12] D$, while the domain height z changes depending on buoyancy: distance from the boundaries has been imposed through a series of preliminary simulations in order to ensure that no influence is observed due to the interaction with them. The jet inlet position changes according to Table 1. Simulations were conducted using a basic cartesian grid with Adaptive Mesh Refinement (AMR). For the W cases, a starting grid size for simulations was chosen based on the available High-Re literature Bogey and Bailly (2006), which was then scaled to the present work Re numbers using Kolmogorov length scaling (Pope, 2000):

$$\Delta/\Delta_0 = (Re/Re_0)^{3/4} \quad (14)$$

This results in a grid size range $\Delta = [0.035, 0.27] D$ for the W case, and $\Delta = [0.059, 0.23] D$ for the WL case, progressively unrefined further away

from the inlet. For the stratified cases, as the jet trajectory is not known apriori, AMR was used to locally double the resolution in zones where scalar concentration was higher than 5% of the inlet value. This results in a mesh resolution up to $\Delta = 0.05D$ for the reference grid, and up to $\Delta = 0.025D$ for the finer grid used for validation purposes (Section 2.4). In Fig. 2, an example of the generated mesh is presented for reference.

Simulations were performed for $t^* = 4000$ in all S cases, and $t^* = 1200$ for the W ones, as the underlying symmetry of the latter substantially reduces the time necessary for data convergence.

2.4. Verification

To ensure the reliability of the LES results and their independence from grid resolution, a systematic verification process was conducted. Comprehensive validation is currently constrained by the lack of experimental datasets at high Reynolds numbers ($Re \approx 10^5$) for buoyant jets in stratified environments. Furthermore, comparing stratified scenarios with classical integral models, such as those proposed by Fan and Brooks (1969), presents significant challenges. While non-buoyant jets in homogeneous environments follow well-established physical laws (e.g., centerline velocity decay rates), momentum-dominated buoyant jets in stratified media involve complex regime transitions that hinder the direct application of simple power laws. A similar limitation was

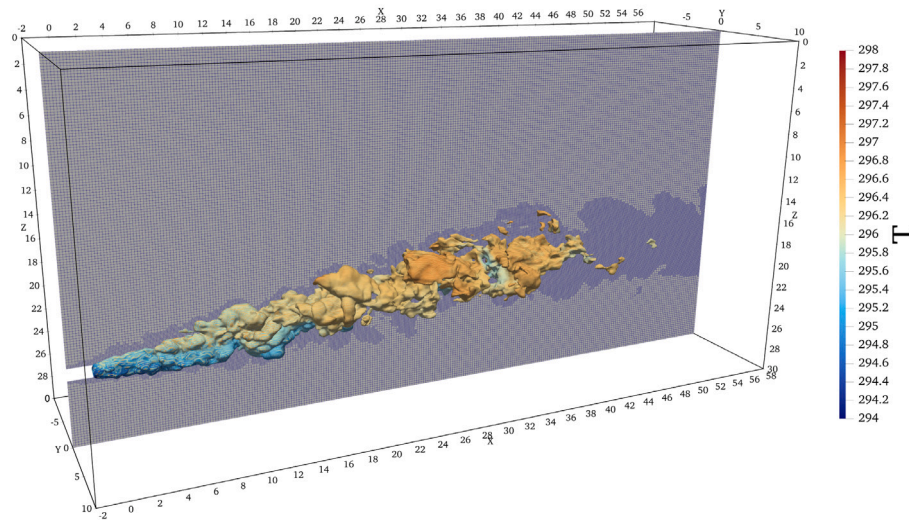


Fig. 2. Mesh generated for reference showing the action of Adaptive Mesh Refinement. In Figure iso-contours at fixed concentration colored with temperature field.

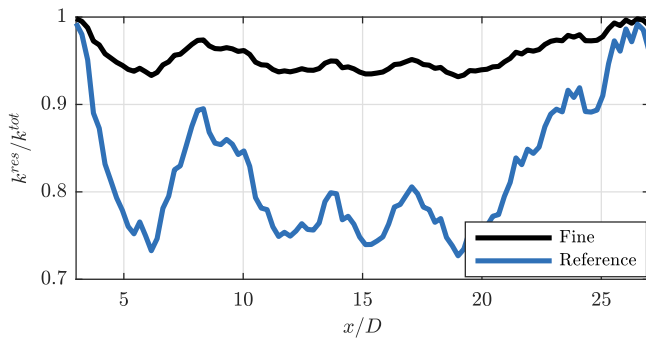


Fig. 3. Ratio of resolved to total turbulent kinetic energy (k_{res}/k_{tot}) along the jet centerline, for the SLRHN scenario.

noted by Papanicolaou et al. (2008), who demonstrated that traditional integral models often overpredict the entrainment coefficient α (the non-dimensional ratio relating ambient entrainment velocity to local centerline velocity, $u_e = \alpha U_c$) for momentum-driven buoyant jets; they suggested a lower value of $\alpha \approx 0.03$ for a more accurate prediction of the terminal height (the maximum vertical overshoot reached by the jet momentum before stabilizing at its neutral buoyancy level).

In Appendix A, a proof of validation of the unstratified case is given, together with a discussion on Reynolds number independence that helps broadening the validity of the dataset. For the stratified simulations, a robust metric to assess LES performance is the ratio of resolved turbulent kinetic energy (k_{res}) to the total turbulent kinetic energy (k_{tot}) as proposed by Celik et al. (2005). This index quantifies the contribution of the sub-grid scale (SGS) model to the overall turbulence: as k_{res} approaches k_{tot} , the simulation tends toward a Direct Numerical Simulation (DNS). According to the criterion established by Celik et al. (2005), a “good LES” is achieved when the resolved portion accounts for approximately 80% of the total kinetic energy. This criterion was applied to the SLRHN case by comparing the reference grid (blue line in Fig. 3) to a finer one, with halved grid spacing (black line).

The ratio k_{res}/k_{tot} , computed along the centerline of the jet, demonstrates that the resolution quality remains well above the recommended threshold throughout the region of interest for the finer mesh, being able to resolve the larger scales of turbulence, and representing a solid reference point. The employed grid, on the other hand, presents portions where the ratio of resolved energy falls to about 75%, slightly

below the conventional ‘adequate’ value of 80%. Given that the present work does not involve any higher order moments, focusing on first order quantities like scalar and velocity decay not meeting the 80% threshold is not an inherent indication of under-resolvedness. In fact, comparing the velocity and scalar centerline decay profile for the two resolutions (Fig. 4), it is apparent that the two simulation differ only for the core length (which is a product of the inflow conditions and their stability). The kinetic energy ratio k_{res}/k_{tot} confirms that the finer mesh provides an excellent benchmark resolution. Because no meaningful differences in primary quantities (velocity and scalar fields) are observed between the two resolutions, the reference grid is sufficiently accurate and can be safely employed for all subsequent simulations at this Reynolds number.

3. Results

This section aims to analyze the dispersion characteristics of the jet, both from a fluid-dynamic and chemical perspective, under the various environmental conditions described in Section 2.2. Starting from a qualitative perspective, it is worth noting the different behaviors that can be found among the different cases. In Fig. 5, vertical slices representing the Ω_a field are reported. As expected, the unstratified case represents the well known round free-jet since no buoyancy or stratification is present. On the other hand, the presence of stratification introduces a bending of the jet itself, due to the density difference at the inlet. As entrainment starts to introduce ambient seawater inside the jet, density difference itself reduces, thus diminishing the buoyancy effect and stabilizing the jet at a certain terminal height, also defined in literature as neutral height (Chen et al., 2021), corresponding to the depth at which the average local density of the jet meets the local ambient value of the water column. This will be crucial for the subsequent analysis, since no ambient value regarding pH, temperature or saturation state can be addressed, if not the local one of the water column located at terminal height.

To further characterize the spatial dispersion physics around the jet centerline, transverse (y - z) cross-sections of the aragonite saturation field (Ω_a) are evaluated at two distinct axial locations representing different physical regimes (Fig. 6): $x/D = 8$ (within the momentum-dominated near-field) and $x/D = 28$ (within the buoyancy- and stratification-influenced region near the neutral height). For brevity, since similar flow physics is present among the scenarios, only SLRHN is presented. At $x/D = 8$, the scalar distribution displays a concentrated core where values exceed the critical threshold ($\Omega_a > 7$), explicitly

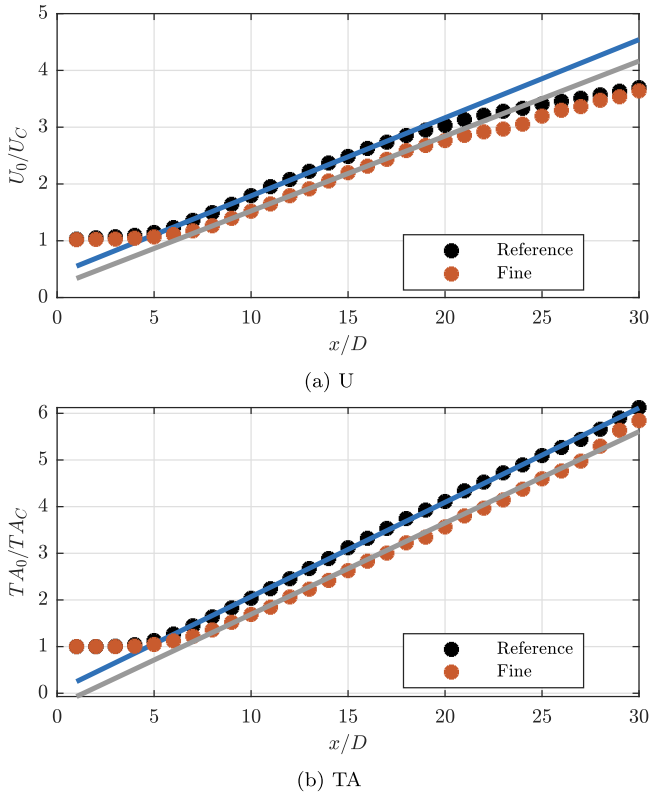


Fig. 4. Comparisons of decay ratio for (a) centerline velocity and (b) scalar concentration (b) for the two resolutions tested on SLRHN case.

highlighted by the red iso-line. The cross-section exhibits a slight vertical asymmetry (teardrop shape) as positive thermal buoyancy begins to act on the upper boundary of the jet. By $x/D = 28$, intense turbulent mixing and lateral spreading broaden the plume footprint significantly, as stratification inhibits vertical spreading. At this downstream location, the maximum saturation value drops to $\Omega_a \approx 5.5$, well below the critical safety threshold, confirming that the potential for secondary precipitation is completely confined to the near-field momentum core before the jet stabilizes within the ambient stratification layer.

A more quantitative study can be done by following the quantities of interest along the centerline of the jet, as is commonly done in tracer injection analyses (Gao et al., 2017; Otoo et al., 2023): this allows for the identification of the maximum values attained by the dispersion process moving away from the jet origin. In Fig. 7, the evolution and decay of the mean values of pH (total scale) and aragonite saturation state (Ω_a) are shown. It is observed that Ω_a falls below the critical value of 7 after a distance, that we will define from now on as X_{crit} , of approximately 9–11D for plant P1 (Fig. 7(a)) and 14–18D for plant P2 (Fig. 7(b)), depending on stratification and inlet temperature. The decay of omega aragonite seems to be poorly influenced by stratification and buoyancy forces, at least within the test matrix and non-dimensional number proposed. We can observe however how the spread of values seems to increase with plant P2. This can be explained by the fact that momentum dominates a significant portion of the phenomenon, in which less influence is given by buoyancy forces, allowing for the identification of the crossing point of supersaturation within a relatively small range of non-dimensional distances; with higher alkalinity injected, a larger area is needed to reach the same dilution, progressively moving further from momentum dominated areas and reaching distances from the inlet in which buoyancy and stratification influence the physics, thus influencing the different decay rates.

The spatial variations of both Ω_a and pH along the jet axis can be reconciled through a single cohesive mechanism: the turbulent entrainment of ambient seawater, which continuously drives both chemical

properties toward the local ambient values dictated by the terminal neutral height of the jet trajectory. The apparent difference in the axial trends between Ω_a and pH arises from the difference in their initial perturbation magnitudes relative to background conditions. For aragonite saturation, the injected solution introduces a significant perturbation ($\Omega_{a,inlet} \approx 10.5$ –15 compared to background values of $\Omega_{a,\infty} \approx 3.75$). Consequently, the initial decay of Ω_a is dominated by high-momentum scalar dilution near the nozzle, masking subtle stratification effects until further downstream. In contrast, because the BAWL technology utilizes a pH-equilibrated solution, the initial pH perturbation at the inlet is very small relative to ambient seawater. As turbulent mixing dilutes this small initial offset within a few nozzle diameters, the centerline pH becomes highly sensitive to, and directly mirrors, the vertical ambient pH gradient of the water column as positive buoyancy elevates the jet toward its neutral height (where ambient pH is higher due to warmer surface waters). Thus, both quantities seamlessly transition toward local ambient conditions at the height of the jet; this shift is simply manifested immediately in pH due to the near-ambient inlet condition, whereas Ω_a requires longer physical distances to dilute its large initial scalar excess. In this sense, it can be inferred that Ω_a and pH values closely return to local ambient conditions, requiring more than 40 diameters to fully return to an unperturbed pre-injection state; a larger domain could effectively show the space required to asymptotically reach the ambient values, but the computational cost would have been prohibitive. Since the scope of the project is to identify possible precipitation-prone areas, the results have been considered satisfactory for the present work.

3.1. Precipitation assessment

As discussed in Section 2.1, the proposed model cannot explicitly quantify the occurrence of precipitation; therefore, this must be evaluated through alternative reliable metrics. This is addressed by evaluating the residence time of a water parcel within a specified region. Precipitation is not an instantaneous phenomenon; it requires an initial nucleation stage, which can occur with or without the presence of solid surfaces in the water (Moras et al., 2022). The subsequent growth phase represents a complex mechanism (Suitner et al., 2024) influenced by numerous factors that may either promote or inhibit the process. This stage can lead to runaway precipitation if the saturation state exceeds a critical threshold, identified as $\Omega_a = 7$ by Varliero et al. (2024). In this study, the likelihood of precipitation is estimated by evaluating the residence time of water parcels within the critical zone (Section 2.1). Since current literature suggests that precipitation processes occur on timescales of hours or days, the significant difference in orders of magnitude between residence time and precipitation kinetics allows for meaningful and reliable conclusions at a reasonable computational cost.

Having established that the mean Ω_a decays below 7 within 9–11 jet diameters of the injection point, thereby identifying the critical saturation region (Varliero et al., 2024), the analysis now focuses on the residence time of water parcels within this high- Ω_a zone. Fig. 8 shows, alongside the decay of the saturation state, the residence time as defined by Ghirelli and Leckner (2004), providing a more dynamic characterization of the injection process.

Here, the trends are more dependent on environmental conditions: the dataset highlights how residence strongly decreases with buoyancy forces, i.e., by raising Richardson number or stratification stability, expressed by N . This is a rather interesting consequence given by the presence of buoyancy. Without it, the round jet dilutes the alkalinity introduced but also loses velocity, leaving the tracers to stagnate. On the other hand, the buoyant cases dilute the tracer and keep the water mass moving, since the momentum flux is constantly increasing. Moreover, by looking at dimensional analysis, we can see how the decay of velocity and tracer concentration are higher for non-buoyant cases with respect to buoyant ones, as shown in Fischer et al.

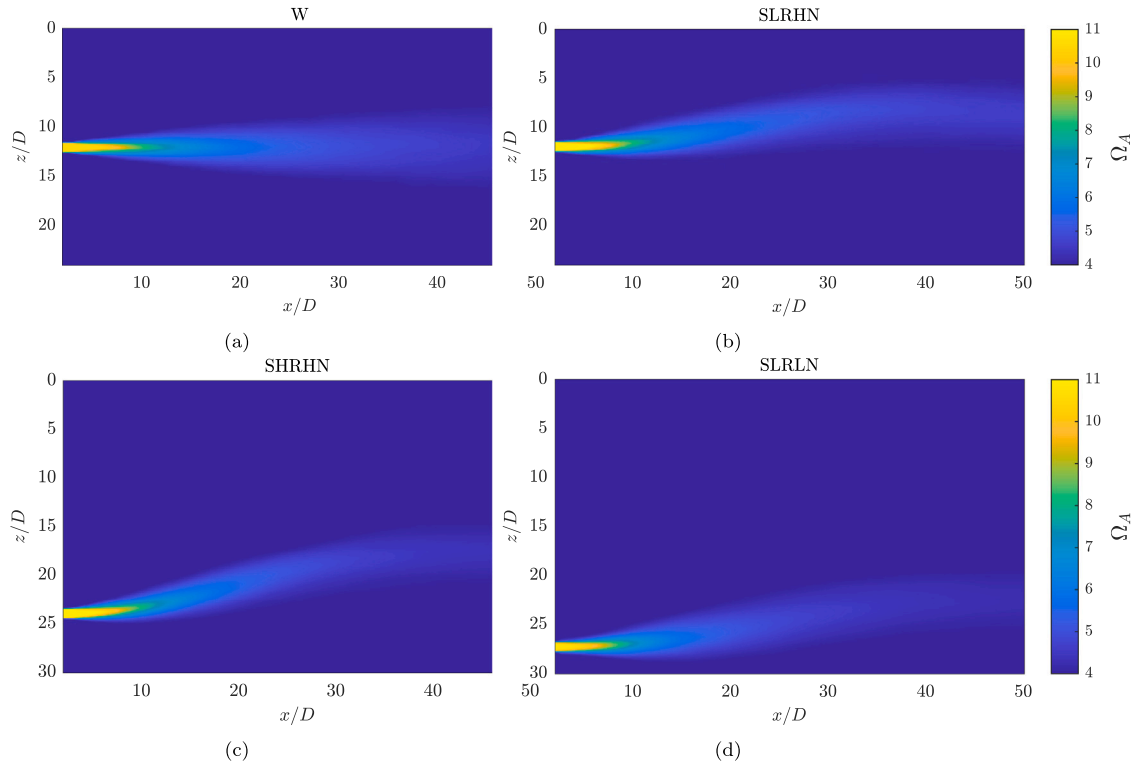


Fig. 5. Vertical slices indicating aragonite saturation levels for each simulation. Note: the spatial extent of some simulations, such as SLRLN, is broader than what is shown to ensure results are not influenced by boundary wall interactions.

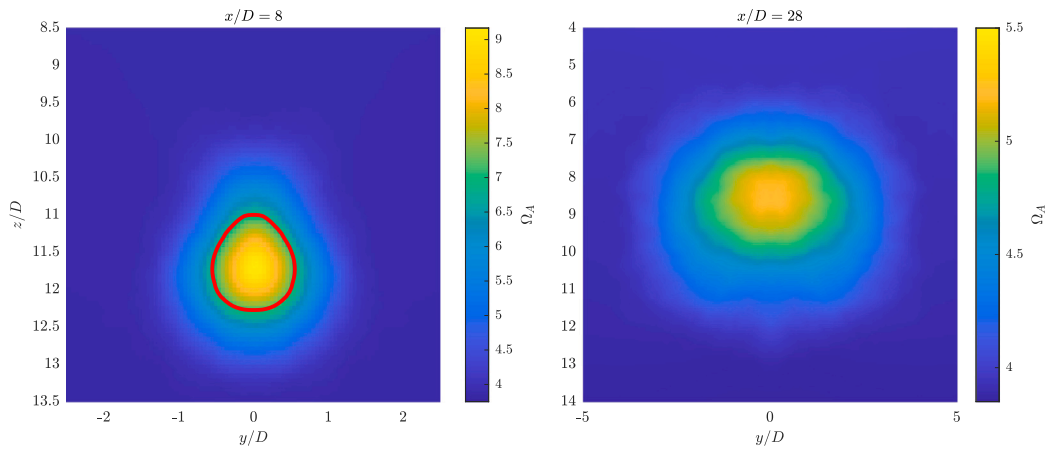


Fig. 6. Transversal slices indicating aragonite saturation levels Ω_a for SLRHN case.

(1979). It is also observed that an increase in stratification stability leads to a major decrease in residence time compared to the effect of buoyancy forces. Between the two plants P1 and P2 trends are identical as expected, differing only in absolute values reached. This is expected as decay rates are prescribed by the flow physics under analysis: however, by raising the injected alkalinity, falling below the critical threshold of 7 interests a larger portion of space, hence a longer residence time if the high saturation zone stretches until the buoyancy dominated zone, in which differences between un-stratified and stratified injection scenarios become evident and different decay rates are observed. Overall, non-dimensional times across cases span between 15/20 units for P1 and 30/40 units for P2. In order to provide a dimensional interpretation, we assume operating with a 330 mm pipe

for the injection. With a mass flow rate of 900 m³/h, the inlet velocity is equal to 2.92 m/s, indicating residence times on the order of 2 to 3 s for P1 and 4 to 6 s for P2. These short timescales make the precipitation of bicarbonates and the degassing of carbon dioxide extremely unlikely, compared to the day-scale experiments of Varliero et al. (2024). It is safe to assess, according to Morse et al. (2007), that in this short time ranges nucleation does not have time to occur, hence avoiding the risk of runaway precipitation.

3.2. Quartile analysis and uncertainty propagation

Relying solely on mean quantities may lead to an underestimation of transient conditions, particularly in instances where Ω_a drops below

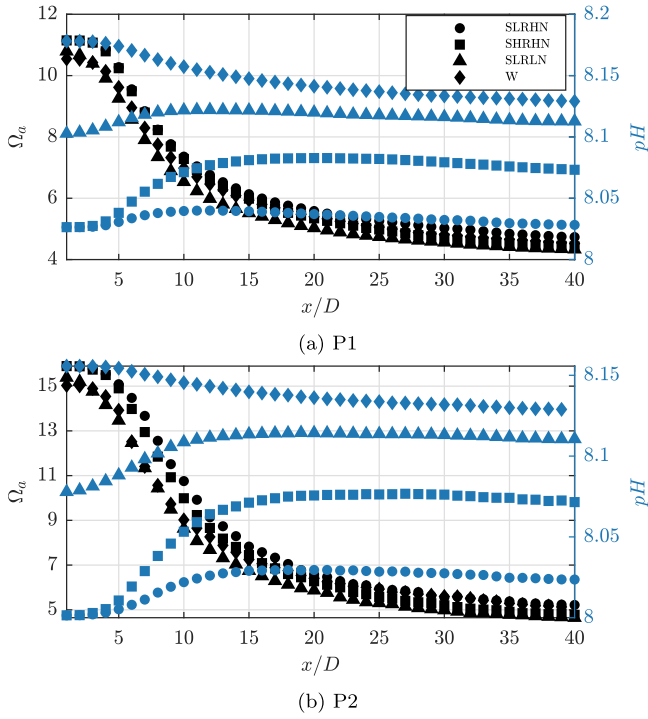


Fig. 7. Decay of Ω_a and pH (total scale) along the jet axis. Black symbols represent Ω_a , while blue ones correspond to pH values, with different markers for the various simulated environmental conditions. (a) and (b) indicates trends for P1 and P2 cases, respectively.

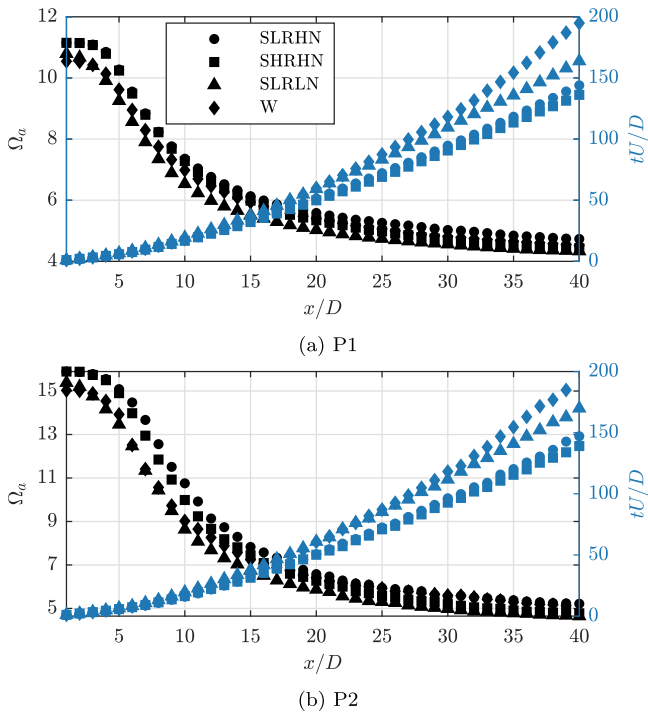


Fig. 8. Decay of Ω_a and water age along the jet axis. Black symbols represent Ω_a , while blue ones indicate water age values, with different markers corresponding to the simulated environmental conditions. (a) and (b) indicates trends for P1 and P2 cases, respectively.

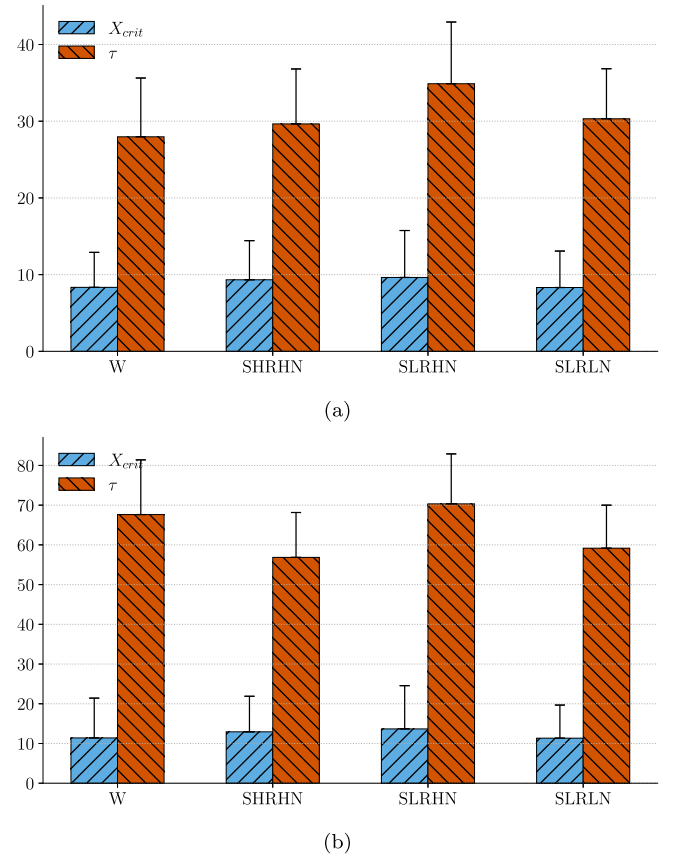


Fig. 9. Bar chart showing the mean critical length X_{crit} (blue) and corresponding residence time τ (orange) across the simulated environmental scenarios. Error bars indicate the conservative 95th percentile values for each parameter to account for turbulent unsteadiness. Panels (a) and (b) correspond to Plant P1 and Plant P2 operational configurations, respectively.. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the threshold of 7 beyond the calculated average length. In such scenarios, a water parcel might remain within the critical zone longer than predicted by an analysis based on mean values. To establish more robust safety ranges and threshold values, the distribution of Ω_a and residence times are evaluated through a percentile-based approach.

In Fig. 9, a bar chart compares the mean critical length X_{crit} (blue bars) and the residence time τ (orange bars) across all simulated environmental configurations (W, SHRHN, SLRHN, SLRLN). To account for turbulent fluctuations and establish a robust engineering safety margin, black error bars display the 95th percentile values for X_{crit} . At this conservative distance, the resulting residence time τ is evaluated, with its own error bar representing its 95th percentile. This visualization highlights the propagation of uncertainty stemming from the inherent unsteadiness of the turbulent jet mixing process.

The results indicate that for Plant P1, the maximum X_{crit} ranges between 13 and 15D, whereas for P2, the critical area extends up to 21–25D. Consequently, these distances yield residence times of up to 40 units for P1 and 80 units for P2. Interestingly, the residence time is strongly influenced by ambient conditions when the critical area extends beyond the momentum-dominated region. This behavior is evident when comparing Figs. 9(a) and 9(b), particularly for the W case. Notably, while the W case shows intermediate values in the P1 scenario, it reaches residence times comparable to the highest recorded cases when moving to the P2 configuration. As shown in Fig. 8, the residence time increases at a significantly higher rate compared to buoyant cases.

4. Conclusions

This study investigated the near-field mixing dynamics of alkalinity injection in marine environments to assess the risk of secondary calcium carbonate precipitation. Through LES, the research characterized the evolution of the bicarbonate-enriched effluent under various seasonal stratification and buoyancy regimes.

A significant methodological contribution of this work is the implementation of an equilibrium chemistry approach coupled with passive scalar transport. By tracking TA and DIC as conservative tracers, the stiff kinetics of the carbonate system were bypassed, allowing for a computationally efficient yet accurate diagnostic of the aragonite saturation state (Ω_a) in the near-field. This approach, combined with a non-dimensional formulation and the assessment of Reynolds number independence, establishes a scalable framework for OAE engineering. Specifically, the linearity of the transport equations for passive scalars enables the evaluation of diverse operational scenarios, varying injection concentrations or plant capacities, through simple post-processing and rescaling of the resolved scalar fields, without the need for additional costly CFD runs.

The analysis of the critical saturation zone ($\Omega_a > 7$) reveals that while the critical length X_{crit} is primarily governed by jet momentum, the residence time within this region is strongly modulated by ambient stratification and buoyancy forces. Even when considering a conservative 95th-percentile analysis to account for turbulent fluctuations, the maximum observed residence times remained below 80 non-dimensional units. For representative industrial scales, these values translate to timescales of only a few tenths of seconds. Given that literature-reported precipitation and nucleation kinetics occur over several hours to days, the results suggest that the risk of runaway secondary precipitation in the near-source region is negligible under the examined operational conditions.

Despite these findings, certain limitations remain. The current model assumes chemical equilibrium and does not explicitly resolve the complex multi-phase kinetics of carbonate precipitation or the potential role of heterogeneous nucleation on suspended particles. Furthermore, the far-field evolution and the cumulative effects of multiple injection points were outside the scope of this study.

CRedit authorship contribution statement

Bindoni Diego: Writing – original draft, Resources, Methodology, Investigation, Formal analysis, Conceptualization. **Francesco Esposito:** Writing – review & editing, Visualization, Methodology, Formal analysis. **Abbà Antonella:** Writing – review & editing, Supervision.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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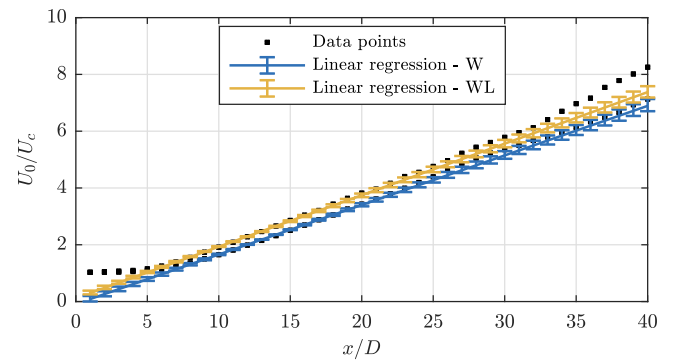


Fig. A.10. Centerline velocity decay for the W cases and uncertainties estimation due to regression.

Appendix A. Reynolds independency

A universal (i.e. *Re*-independent) parameter that characterizes turbulent round jets is the centerline velocity decay rate B , defined as

$$B = \frac{U_c(x) (x - x_o)}{U_o D} \quad (\text{A.1})$$

Experiments and simulation agree that such a linear decay law does indeed exist, and its value is typically taken to be $B \approx 5.9$ (Pope, 2000). While the existence of a certain spread around this value is indeed acknowledged, even in numerical simulation, due to reasonable differences in setup conditions, like modeling effect and the presence of co-flows.

Another possible source of uncertainty comes from the linear regression employed to compute B , and its quantification in particular regarding the choice of interpolation range, has not attempted before for this specific issue as far as the author's knowledge. While a more serious effort at both proving a stronger assessment of the value of the B constant and its uncertainty is outside of the scope of this work, an effort is made here to provide an overview of the expected variability of this parameter. Furthermore, it is shown that even seemingly significant variations in B have a relatively minor impact on the jet's diffusion characteristics.

Data from the W case is considered, together with two reference LES, by Salkhordeh et al. (2019), Kuan et al. (2023a). The decay rate sampled data is treated through a piecewise spline interpolation to alleviate discrete sampling effect. Once reasonable bounds of the linear region were identified for each simulation, the interpolated curve was subdivided in overlapping segments of various length (but no shorter than one-fifth of the whole linear region), and the starting and ending point of the regression region was systematically varied. This results in a distribution of regression coefficient B for each simulation, which account for the arbitrary differences in regression. Each distribution includes values consistent with those reported in the respective studies, confirming that the method successfully reproduces plausible regression choices. The standard deviation of the coefficient was then calculated for the present dataset and the references (Table A.3). It can be seen that the B is associated with a significant deviation across all datasets, indicating that the value is strongly affected by the choice of integration extrema. However, as illustrated in Fig. A.10, even relatively large variances for B do not correspond to equally large discrepancies in the actual decay behavior. This cements the idea that, even if the B coefficient is predicted with significant error (order of 5%), the overall diffusion characteristics are still correctly captured.

Table A.3

B and its variance. For the reference works, B is the one reported by the authors; while the standard deviation σ has been calculated as described above.

	Kuan et al. (2023a)	Salkhordeh et al. (2019)	W	WL
B	5.87	6.07	5.73	5.54
σ	0.194	0.254	0.229	0.157

Appendix B. Methodology for inlet DIC and TA derivation

This appendix describes the stoichiometric framework used to determine DIC and TA values within the test matrix, focusing on the chemical signature of atmospheric CO₂ removal. The methodology utilizes a mass balance approach to simulate the enrichment of seawater through the addition of alkalinity and the subsequent capture of ambient carbon.

The baseline chemical properties for the seawater are defined by a density $\rho = 1025 \text{ kg/m}^3$, alongside representative far-field values for DIC and TA. The inlet conditions for the test matrix, as reported in Table 2, are derived from the stoichiometric requirements of capturing atmospheric CO₂ and the dosage of calcium hydroxide (Ca(OH)₂) required to stabilize the inorganic carbon in the aqueous phase.

The total concentration of DIC (DIC_{tot}) is calculated by assuming the quantitative conversion of captured atmospheric CO₂ into bicarbonate species:

$$DIC_{tot} = DIC_{initial} + \frac{\dot{m}_{CO_2, atm}}{M_{CO_2} \cdot Q_{sw}} \quad (B.1)$$

where $\dot{m}_{CO_2, atm}$ represents the mass flow of carbon dioxide removed from the atmosphere and Q_{sw} is the seawater mass flow. Simultaneously, the alkalinity enhancement is determined by the dosage of Ca(OH)₂. Given that each mole of hydroxide yields two equivalents of alkalinity, the Total Alkalinity (TA_{tot}) is defined as:

$$TA_{tot} = TA_{initial} + 2 \cdot \left(\frac{\dot{m}_{Ca(OH)_2}}{M_{Ca(OH)_2} \cdot Q_{sw}} \right) \quad (B.2)$$

Second terms in both equations will be referred in the present work as DIC_{added} and TA_{added} , respectively. The seawater mass flow (Q_{sw}) used to compute the test matrix is set at 900 m³/h, consistent with an hypothetical industrial configuration utilizing a standard 330 mm diameter pipe. Due to the inherent scalability and non-dimensional formulation of the proposed model, these conditions are intended to provide a robust framework for informed design studies rather than imposing a rigid operational standard.

Data availability

The model simulation data supporting the findings of this study are available from the corresponding author upon request.

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