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High-resolution numerical and experimental study of dense jets

by

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Declaration of Authorship

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Abstract

The rapid global expansion of seawater desalination has emerged as a critical solution to freshwater scarcity, yet it generates large volumes of saline and thermal effluents that pose challenges for coastal and marine environments. The near field hydrodynamics and mixing of desalination discharges are governed by the delicate interplay between jet momentum, buoyancy, and ambient conditions. An accurate prediction of these processes is vital for designing outfalls that ensure regulatory compliance and minimize ecological impacts. Despite significant progress in experimental and numerical modeling, notable knowledge gaps remain in (i) the specification of realistic boundary conditions for high-fidelity simulations, (ii) the representation of jet behavior in complex stratified and crossflow environments, and (iii) the integration of experimental and numerical data within predictive, computationally efficient modeling frameworks. This thesis addresses these challenges through a coordinated program of advanced experiments, high-resolution simulations, and multi-fidelity statistical modeling. The first part of the thesis investigates the role of inlet boundary conditions in Large Eddy Simulation (LES) of negatively buoyant jets relevant to desalination outfalls. Multiple inflow turbulence treatments, including mapped, synthetic, and stochastic methods, were systematically compared against high-resolution Particle Image Velocimetry (PIV) measurements. The study demonstrated that mapped inflow and synthetic turbulence approaches are most effective in reproducing near-field turbulence generation, velocity statistics, and dilution performance, while oversimplified uniform inflows led to systematic underprediction of mixing. This highlights the decisive role of physically consistent boundary specification for LES reliability.

The second part examines dense jets in crossflow and stably stratified environments using LES. A suite of simulations covering a wide parameter space of densimetric Froude numbers, velocity ratios, and stratification strengths was conducted. Results revealed that ambient stratification strongly suppresses vertical penetration and enhances asymmetric entrainment, while crossflow drives trajectory deflection and modifies coherent turbulent structures. These findings extend the current understanding of jet–ambient interactions and provide physically grounded benchmarks for the design of desalination outfalls in variable environments.

The third component of the thesis develops a Bayesian hierarchical multi-fidelity framework that combines low-fidelity Reynolds Averaged Navier-Stokes (RANS), high-fidelity LES, and experimental Particle Image Velocimetry (PIV) and Laser Induced Fluorescence (LIF) data within a Gaussian Process Regression (GPR) model. This approach exploits the complementary strengths of different fidelities, achieving robust predictions of terminal rise height, return point dilution, and centerline concentration while substantially reducing computational cost. The framework demonstrates the feasibility of integrating simulation and measurement data into unified, uncertainty-aware predictive models for environmental engineering applications. Finally, Direct Numerical Simulation (DNS) of a positively buoyant thermal jet is presented as a benchmark. The DNS resolves turbulence and scalar transport at all relevant scales, producing high-fidelity datasets of mean flow, turbulence statistics, and entrainment. These results elucidate fundamental turbulence–buoyancy interactions and serve both as validation for LES subgrid-scale models and as calibration input for the multi-fidelity framework.

The thesis makes four main contributions: (1) it establishes best practices for LES inlet boundary conditions in desalination jet simulations; (2) it quantifies the interplay between

crossflow, stratification, and dense jet dynamics; (3) it introduces and validates a Bayesian multi-fidelity modeling framework for efficient prediction of discharge behavior; and (4) it generates high-resolution DNS datasets of thermal jets that advance physical understanding and provide a benchmark for future model development. Collectively, these contributions enhance predictive capabilities for desalination discharges, offering methodological and physical insights that support the design of environmentally sustainable outfalls.

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Chapter 1

Introduction and Study Objectives

1.1 Background and Motivation

The demand for freshwater has increased globally as a result of industrialisation, population growth, and climate change. In response, seawater desalination has emerged as a dependable source of water in many water stressed areas. Over the past two decades, desalination capacity has grown rapidly, with more than 16,000 plants now operating across 177 countries, producing on the order of 10^8 m³/day of freshwater [5]. While desalination provides water supply, it also generates a substantial wastewater in the form of saline or thermal discharges. Desalination effluent also release chemical substantial that impact the receiving environment. The discharge of seawater reverse osmosis (SWRO) plants usually has a salinity that is 1.5–2 times higher than the intake seawater [6]. On the other hand, thermal desalination methods like multi-stage flash or multi-effect distillation generate even more brine per unit of freshwater and discharge it at higher temperatures, typically 5-10 °C above room temperature [5, 6]. Particularly in shallow coastal zones or semi-enclosed seas where dilution is restricted, the confluence of hypersalinity and excessive heat can worsen stress on the receiving waters. Furthermore, residual chemicals from pre-treatment and operation, including chlorine, chloramines, anti-scalants, and trace metals from corrosion, may be present in desalination effluents [6]. Beyond the immediate near field, insufficient initial dilution can result in hypersaline or thermal plumes persisting over hundreds of meters, increasing salinity and temperature above ambient levels and potentially affecting benthic habitats, water column stratification, and coastal ecosystems, particularly in shallow or weakly flushed environments [6, 176].

The behavior of discharges from desalination is governed by the relative balance between initial momentum and buoyancy forces. The behavior of desalination discharges is determined by the interaction between discharge momentum and buoyancy forces. When the buoyancy force acts in the same direction as the discharge momentum, the jet is classified as positively buoyant, as in the case of thermal effluents where reduced density drives the flow upward toward the free surface. Conversely, when the buoyancy force opposes the discharge momentum, the jet is classified as negatively buoyant, as occurs with dense brine discharges, which sink under gravity and spread along the seabed as a bottom attached plume. Both types of effluents can adversely affect marine ecosystems, hypersaline plumes elevate bottom salinity and may induce oxygen depleted layers near the seabed, whereas thermal discharges increase

surface temperatures and modify the ambient stratification [7, 8]. To minimize environmental impacts, regulations often require desalination outfalls to achieve sufficient dilution within the near-field so that the salinity and temperature of the effluent return close to ambient levels. In practice, this is commonly achieved through engineered outfall systems equipped with different type of diffusers [9, 9–11]. These diffusers discharge the wastewater as a series of high-velocity jets, typically inclined upwards, which entrain ambient water and enhance mixing [12–14]. By increasing initial dilution, such designs reduce the extent of salinity elevation and prevent the formation of dense bottom layers on the seabed [15, 16]. Inclined dense jets have therefore become a widely adopted engineering solution to effectively dissipate hypersaline effluents and protect marine ecosystems [17, 18]. Optimizing diffuser design and predicting their performance, however, requires a detailed understanding of the hydrodynamics of turbulent buoyant jets. This need has driven research over the past 15 years, including high-resolution laboratory experiments using Laser Induced Fluorescence (LIF) and Particle Image Velocimetry (PIV) [14, 19, 19–22] as well as advanced numerical simulations based on Reynolds Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) [17, 23–26].

1.2 Experimental studies

Laser based optical diagnostics have become the most widely adopted tools for investigating desalination jet mixing, with the ability to provide high-resolution, non-intrusive measurements in laboratory environments. Among these, Laser Induced Fluorescence (LIF) is the primary method for quantifying concentration fields. In LIF experiments, a fluorescent dye is added to the effluent, and a thin laser sheet illuminates the flow, exciting the dye molecules to emit light at a longer wavelength, which is recorded by cameras. The emitted fluorescence intensity is directly proportional to the local dye concentration under controlled conditions. To obtain quantitative concentration maps, the measured light intensity is calibrated against reference images of known dye concentrations, thereby compensating for non-uniform laser sheet intensity, optical distortions, and camera sensitivity. This calibration procedure enables accurate mapping of scalar fields and dilution patterns within the jet. Consequently, LIF provides detailed visualization of jet mixing processes, which are critical for evaluating desalination discharge performance and for validating numerical models [27–30]. Particle Image Velocimetry (PIV) is a laser based measurement method used to obtain velocity fields in fluid flows. The flow is seeded with neutrally buoyant particles that act as tracers of the motion. A thin laser sheet illuminates the seeded region, and the scattered light from the particles is recorded by one or more cameras. The images are subdivided into interrogation windows, and particle displacements between successive frames are evaluated through cross-correlation analysis. These displacements are then converted into velocity vectors, yielding a spatially resolved representation of the flow field. The dual-frame and time resolved are primary methods of PIV for quantifying mean flow structures and turbulence statistics. In the dual-frame (double-pulse) approach, two images are recorded with a short time while time resolve PIV employs continuous sequences of particle images for measuring the velocity. The combined LIF, PIV provides simultaneous measurements of velocity and scalar concentration fields, thereby providing a comprehensive characterization of momentum and mass transport [31, 32].

Laboratory investigations of dense jets was conducted by advanced optical and intrusive diagnostic methods to resolve the complex interplay between momentum and buoyancy. Early experimental approaches were primarily qualitative, performed by dye visualization and shadow graph techniques [33, 34], which provided limited information on trajectory and terminal rise height. The development of quantitative optical method, particularly LIF and PIV, transformed the field by enabling non-intrusive measurements of concentration and velocity with high spatial and temporal resolution. Roberts et al. were among the first to apply planar LIF to inclined dense jets, reporting dilution and trajectory data that have since served as reference benchmarks. Their results established key scaling relations for terminal rise height and return point dilution. Later studies by [36] extended LIF to three-dimensional scanning, highlighting the asymmetry of concentration profiles caused by detrainment on the inner side of the jet. More recent work [14, 37] eliminated bottom boundary effects, and used high-quality LIF datasets to measure behavior of different jet angles. In parallel, intrusive methods such as micro-conductivity probes have been employed to obtain pointwise concentration data at high frequency. Papakonstantis et al. [15, 38] used a micro-scale conductivity and temperature instrument to measure mean and fluctuating concentration fields in inclined dense jets. These measurements confirmed the asymmetric nature of vertical concentration distributions, with Gaussian profiles above the centerline and flatter profiles below, and showed that turbulent concentration fluctuations peak above the jet axis. Lai et al. [13, 39] combined LIF and PIV to obtain simultaneous velocity and concentration fields of inclined dense jets, enabling direct investigation of momentum scalar coupling, entrainment, and coherent structures. Crowe et al. [2, 16] employed particle tracking velocimetry (PTV), a variant of PIV, to measure velocity fields at multiple inclination angles. Their results provided accurate velocity distributions at the terminal rise and return point, thereby clarifying the role of detrainment and inner side instabilities.

1.3 Numerical studies

Computational fluid dynamics (CFD) has become an indispensable tool for investigating complex flow phenomena that are often difficult to access experimentally. By numerically solving the governing equations of fluid motion, CFD enables researchers to examine detailed flow structures, turbulence dynamics, and mixing processes across a wide range of scales and configurations [40, 41]. In environmental hydraulics, CFD provides valuable insights into buoyant and negatively buoyant jets, sediment transport, and effluent discharges, complementing laboratory and field studies and allowing for systematic exploration of parameter spaces that would otherwise be infeasible. At the core of CFD lies the challenge of turbulence modelling. The Navier-Stokes equations describe fluid motion exactly, but for turbulent flows the equations involve fluctuating quantities that cannot be resolved analytically in most practical situations. When the governing equations are averaged (in time, space, or filtered), additional unknown terms appear in the form of Reynolds stresses or subgrid stresses. This creates the *closure problem*, whereby the number of unknowns exceeds the number of equations, requiring additional modelling assumptions [40].

Different strategies have been developed to address the closure problem, each with distinct strengths and limitations:

- **Reynolds Averaged Navier-Stokes (RANS):** RANS models solve for the mean flow field, with turbulence effects represented through closure relations such as the k - ε or k - ω models. These approaches are computationally inexpensive and suitable for engineering applications requiring rapid design iterations. However, they often struggle to capture unsteady turbulent structures, leading to inaccuracies in flows where coherent eddies strongly influence mixing [40, 42].
- **Large Eddy Simulation (LES):** LES resolves the larger, energy-containing turbulent structures directly while modelling only the smaller subgrid scales. This provides a more accurate representation of turbulence dynamics, particularly for unsteady mixing processes, at a significantly higher computational cost than RANS. LES has been shown to reproduce flow structures, entrainment, and instabilities with higher fidelity, making it a valuable tool for research and high-resolution analysis [41, 43].
- **Direct Numerical Simulation (DNS):** DNS resolves all scales of turbulence by directly integrating the Navier-Stokes equations without modelling assumptions. It provides the most accurate representation of turbulence but requires computational resources, rendering it feasible only for low Reynolds number flows [44].

RANS remains the most practical approach for routine engineering and environmental applications due to its efficiency, but its accuracy depends heavily on the choice and calibration of turbulence closure models. LES offers a balance between fidelity and cost, capturing coherent turbulent structures and providing more reliable predictions for complex jets and mixing flows. DNS, while computationally prohibitive for real-scale problems, serves as the benchmark for turbulence research and model development. Together, these approaches form a hierarchy of modelling strategies, allowing researchers to select the appropriate method depending on the scale, objectives, and available computational resources.

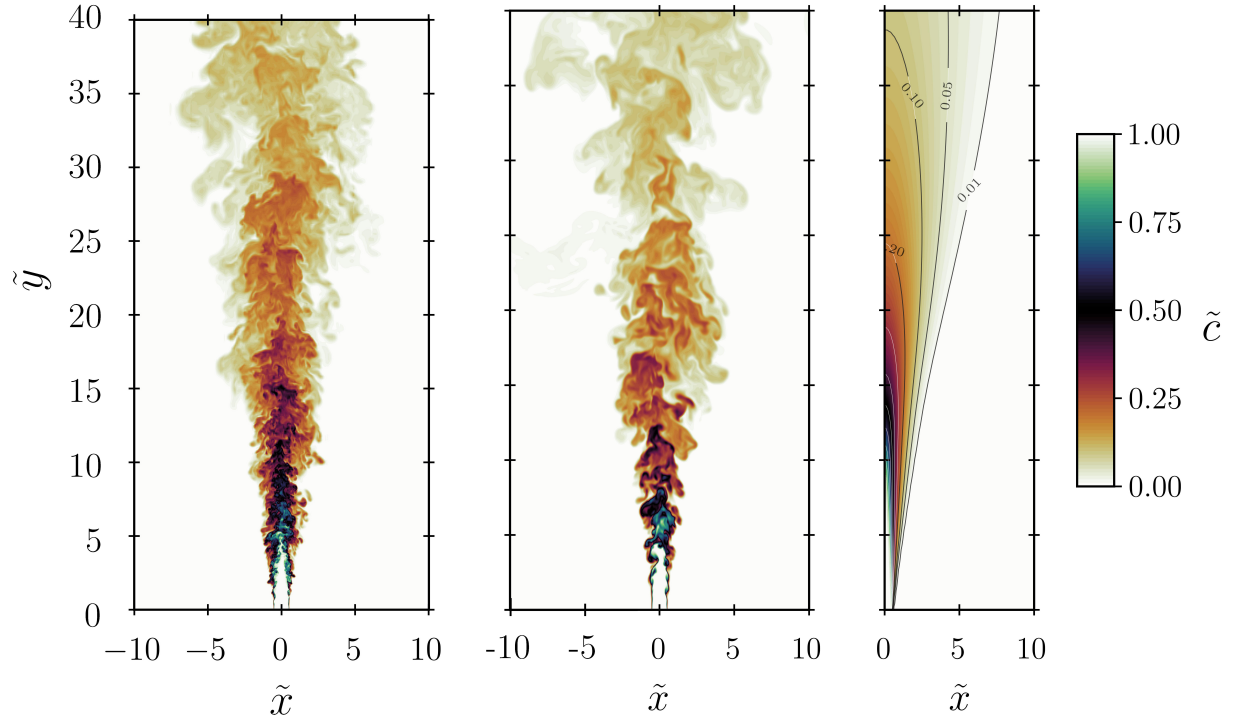


Figure 1.1: Comparison of thermal jet simulations using three turbulence modelling approaches: (right) RANS, (middle) LES, and (left) DNS.

The differences between RANS, LES, and DNS are illustrated in Figure 1.1, which compares their predictions for a thermal jet. RANS provides only the time-averaged field, smoothing out coherent turbulent structures and leading to diffused concentration distributions. LES resolves the large eddies responsible for entrainment and mixing, thereby capturing more realistic turbulence dynamics and plume development. DNS offers the highest level of fidelity by resolving all turbulence scales, clearly reproducing fine-scale vortical structures and scalar mixing.

RANS models have been widely employed to investigate the mixing dynamics of inclined negatively buoyant jets, given their balance between computational efficiency and predictive capability. Early applications focused on evaluating the suitability of linear and nonlinear eddy viscosity closures, as well as Reynolds stress models, in reproducing the complex trajectory and dilution behavior of dense effluents. Kheirkhah Gildeh et al. [17] simulated 30° and 45° inclined dense jets using OpenFOAM with five turbulence closures, ranging from realizable $k-\varepsilon$ to Reynolds stress models. Their results highlighted that the LRR and realizable $k-\varepsilon$ models achieved better agreement with experimental data, particularly in predicting terminal rise height, return point, and centerline trajectory. This study established the importance of turbulence anisotropy representation in RANS frameworks. Subsequent efforts explored the sensitivity of RANS predictions to scalar transport modeling. Tahmooreesi and Ahmad-yar systematically examined the role of the turbulent Schmidt number (Sc_t) in simulations of 45° jets. They demonstrated that adopting reduced values of Sc_t (0.4–0.6) significantly enhanced dilution predictions, though at the cost of trajectory accuracy. To overcome this limitation, they proposed a Regional Turbulent Schmidt Number (RTSN) approach, where

Sc_t was varied spatially according to jet-plume regions. This methodology improved return point dilution while retaining the accuracy of geometric parameters, underscoring the critical coupling between scalar transport and turbulence closures. The challenges of modeling discharges in shallow waters were addressed by Kheirkhah Gildeh et al., who reported three discharge regimes full submergence, plume contact, and centerline impingement using five RANS closures. Their findings confirmed that Reynolds stress models (LRR and SSG) outperformed two-equation models, as they better accounted for turbulence anisotropy in cases of surface attachment. More recent studies have focused on advancing scalar flux modeling beyond the classical gradient diffusion hypothesis. Tahmooresi and Ahmadyar implemented a Reynolds scalar flux model yielding markedly improved predictions of return point dilution and concentration fields compared with conventional RANS closures. This approach reduced average errors in mixing parameters to approximately 4%, in contrast to nearly 20% for standard gradient diffusion based RANS simulations. Extending this direction, Tahmooresi et al. further analyzed the full transport equation of scalar fluxes, providing new insights into the contribution of buoyancy production and pressure scalar correlations. Their results emphasized that scalar flux modeling significantly enhances the capability of RANS to capture both mean concentration fields and fluctuations. Law et al. applied dynamic formulations of the turbulent Schmidt number to reduce model biases. Law et al. extracted Sc_t distributions from validated LES data and implemented a dynamic turbulent Schmidt number approach in RANS simulations. While this method moderately improved dilution predictions, especially in the ascending part of the jet, it remained limited in capturing the descending jet dilution. The study highlighted the sensitivity of RANS predictions to the characterization of Sc_t . LES has become an increasingly valuable tool for studying dense jet discharges, bridging the gap between Direct Numerical Simulation (DNS) and Reynolds averaged approaches by resolving the large energy containing structures while modeling only the subgrid-scale motions. Owing to its capacity to capture coherent turbulent structures and unsteady entrainment processes, LES has been extensively applied to inclined negatively buoyant jets, providing new insights into their near-field dynamics and mixing performance. Among the primary LES studies of inclined dense jets were conducted by Zhang et al., who examined 45° jets using both the Smagorinsky and dynamic Smagorinsky subgrid models. Their simulations reproduced the geometric trajectory with reasonable accuracy, including the terminal rise height and return point, but consistently underpredicted dilution. This shortfall was attributed to insufficient resolution of buoyancy-induced instabilities, which play a central role in convective mixing. Extending this line of work, Zhang et al. performed LES of 45° and 60° jets with bottom impact, adopting near-wall modeling to resolve spreading layers along the seabed. Their results captured the localized concentration build-up at the impact point reported in experiments, but underestimated impact dilution by approximately 20%, highlighting the challenge of wall jet interaction in LES frameworks. Subsequent studies refined inlet and boundary condition treatments to address these limitations. Jiang et al. and later investigations incorporated turbulent velocity inlets to enhance near nozzle turbulence generation, though discrepancies remained in reproducing terminal rise and dilution. LES has also been applied to assess geometric effects on dense jets. Studies by [50] and [48] investigated the role of nozzle inclination and multiport configurations, showing that LES can resolve asymmetric spreading and port port interactions beyond the reach of integral or RANS models.

1.4 Research Questions and Objectives

The aim of this thesis is to advance the understanding and predictive capabilities of desalination discharges and dense jets through high-fidelity simulations, experimental validation, and multi-fidelity modeling frameworks. In pursuit of this aim, the following key research questions are addressed:

Research Questions

1. How does the specification of inlet boundary conditions influence turbulence generation, mixing efficiency, and the overall predictive performance of Large Eddy Simulation (LES) for desalination jets when validated against high-resolution Particle Image Velocimetry (PIV) data?
2. What are the dominant flow structures, entrainment mechanisms, and stratification effects that govern dense jet behavior in crossflow and stably stratified ambient environments, and how effectively can LES resolve these complex dynamics?
3. In what ways can multi-fidelity modeling, combining Reynolds Averaged Navier-Stokes (RANS), LES, and LIF within a Gaussian Process Regression (GPR) framework, improve predictive accuracy and computational efficiency for buoyant jet?
4. What fundamental insights into turbulence, entrainment, and thermal transport can be derived from DNS of buoyant thermal jets, and how can these findings be leveraged to refine and validate LES and multi-fidelity models?

Research Objectives and Novelty

To answer the above questions, this thesis pursues the following specific objectives:

1. To systematically assess alternative inflow boundary treatments for LES of desalination jets, quantifying their effect on near-field turbulence development, jet dilution, and comparison with PIV benchmarks.
2. To perform high-resolution LES of dense jets in crossflow and stratified conditions, examining how ambient stratification and crossflow alter jet trajectory, dilution, and coherent turbulent structures.
3. To design and apply a multi-fidelity Gaussian Process Regression framework that integrates RANS, LES, and LIF data, thereby producing robust surrogate models capable of accurate predictions at reduced computational cost.
4. To carry out DNS of buoyant thermal jets in order to generate benchmark data on turbulence and scalar transport, and to exploit these results for evaluating and enhancing LES and multi-fidelity modeling strategies.

1.5 Thesis Outline

This thesis is organized into six chapters, each addressing a distinct component of the investigation of dense and buoyant jets, with emphasis on desalination discharges:

- **Chapter 1** introduces the motivation and scope of the research. The challenges posed by desalination discharges are discussed, and the research questions and objectives are formulated in the context of existing knowledge gaps.
- **Chapter 2** investigates the role of inlet boundary conditions in LES of desalination jets. Different inflow turbulence treatments are implemented and validated against high-resolution PIV data, highlighting their decisive influence on near-field turbulence and scalar mixing.
- **Chapter 3** examines dense jets in crossflow and stratified environments using LES. The chapter elucidates the interplay between ambient stratification, crossflow, and jet entrainment, yielding new insights into complex discharge dynamics.
- **Chapter 4** develops a multi-fidelity Gaussian Process Regression framework that uses RANS, LES, and LIF data. The framework is shown to enable accurate and computationally efficient predictions of jet mixing under diverse conditions.
- **Chapter 5** summarises the principal findings, highlights the thesis contributions to both methodology and physical understanding, and proposes avenues for future research.
- **Chapter A** compares the impact of the inlet boundary condition on LES results of desalination jet.
- **Chapter B** presents DNS of buoyant thermal jets, generating reference data on turbulence and scalar transport. These results are used both for benchmarking LES and for enriching the multi-fidelity framework.
- **Chapter C** Explores numerical scheme impact on convection term in LES.
- **Chapter D** explains the non-dimensionalization method applied in OpenFOAM solver developed for the desalination jet.

1.6 List of publications

The following peer-reviewed publications have been produced as direct outcomes of the present research and are incorporated into this thesis:

- Goodarzi, D., Mohammadian, A., & Rezaeiravesh, S. (2025). Numerical simulation of desalination brine discharges: Effects of inlet boundary conditions. *Desalination*, 119389. <https://doi.org/10.1016/j.desal.2025.119389> Chapter 2.

- Goodarzi, D., Mohammadian, A., & Tahmoressi, S. (2025). Numerical Simulation of Negatively Buoyant Jets in Stratified Crossflow. *Under preparation*. Chapter 3.
- Goodarzi, D., Mohammadian, A., & Tahmoressi, S. (2023). Numerical Simulation of Buoyant Jet in Linearly Stratified Flowing Ambient. In *Proceedings of the 40th IAHR World Congress*, Vienna, Austria. https://doi.org/10.3850/978-90-833476-1-5_iahr40wc-p0605-cd Chapter 3.
- Goodarzi, D. & Mohammadian, A., (2025). Multifidelity Numerical Modeling and Bayesian Hierarchical Prediction of the Desalination Discharges. *Desalination*, 119737. <https://doi.org/10.1016/j.desal.2025.119737> Chapter 4.
- Goodarzi, D. (2024). Comment on “Venturi nozzles for desalination brine discharges” [Amiri, N.S., Abessi, O., & Roberts, P.J., *Desalination* 573 (2024) 117193]. *Desalination*, 592, 118105. <https://doi.org/10.1016/j.desal.2024.118105> Appendix A.
- Goodarzi, D., Mohammadian, A., & Dutta, S., (2025). Direct Numerical Simulation of thermal jet. *Under Preparation*. Appendix B.

Chapter 2

Numerical simulation of desalination brine discharges: effects of inlet boundary conditions

2.1 Introduction

The study of brine discharges using computational fluid dynamics has gained significant attention due to its accuracy, time efficiency, and cost-effectiveness. Traditionally, the Reynolds-averaged Navier-Stokes (RANS) approach has been widely employed for predicting time-averaged quantities, such as mean concentration and velocity fields, primarily due to past limitations in computational resources. However, RANS models inherently lack the ability to resolve the full spectrum of turbulent scales, which are critical for accurately capturing complex flow characteristics [51, 52]. In contrast, direct numerical simulation (DNS) can fully resolve all relevant turbulent scales and capture the true physics of turbulent flows, but its extremely high computational cost makes it impractical for most real-world applications [53]. Large Eddy Simulation (LES) offers a compromise between accuracy and computational efficiency. LES resolves the large, energy-containing eddies while modeling the smaller subgrid-scale structures, resulting in better accuracy than RANS and requiring fewer computational resources than DNS [43]. Advancements in high-performance computing have improved the feasibility of LES for a broader range of environmental and industrial flows across various Reynolds numbers (Re). However, performing accurate LES remains challenging due to the complex, non-linear interaction between numerical discretization and turbulence modeling effects [54]. Beyond employing a high-resolution mesh and appropriate numerical schemes, the implementation of realistic inlet boundary conditions is critical for ensuring the accuracy of LES predictions [55]. The accuracy of LES is highly sensitive to the specification of boundary conditions, such as the inlet, as the temporal and spatial structure of inflow turbulence strongly influences downstream flow development [56–58]. Inadequate or overly simplified inflow conditions can result in distortion of flow dynamics, leading to either artificial amplification or suppression of important flow features, particularly in regions of interest [43, 59]. This study focuses on inclined desalination discharges, also referred to as inclined negatively buoyant jets, where a dense fluid is discharged into a lighter ambient fluid through a nozzle

oriented at an angle to the horizontal. The terms desalination discharge and negatively buoyant jet are used interchangeably in this manuscript. The term negative refers to the fact that the buoyancy force acts in the opposite direction of the jet's vertical momentum. Buoyant jets such as these are encountered in a variety of industrial and natural processes, including brine discharge from desalination plants, volcanic eruptions, and thermal plumes [4, 60–68]. In desalination systems, both single-port and multi-port discharges are employed to enhance mixing and reduce the environmental impact of brine in the receiving water body [69, 70]. As such, a deep understanding of jet dynamics and scalar mixing processes is essential for the design, optimization, and environmental management of desalination discharge systems. The dynamics of a desalination jet are determined by the interaction between momentum and buoyancy forces [12], and are quantitatively characterized by the dimensionless parameter known as the densimetric Froude number (Fr_d), defined as:

$$Fr_d = \frac{U_0}{\sqrt{g'd_0}} \quad (2.1)$$

where U_0 denotes the jet velocity (i.e., characteristic velocity of the jet also referred to as the bulk velocity), d_0 is the jet diameter (i.e., the characteristic length scale), and g' represents the initial reduced gravity, calculated as:

$$g' = g \frac{\rho_0 - \rho_a}{\rho_a} \quad (2.2)$$

Here, g is the gravitational acceleration ($0, -9.81, 0$), and ρ_0 and ρ_a are the densities of the jet and ambient fluid, respectively.

A schematic of the trajectory of a desalination jet released from an inclined discharge is illustrated in Figure 2.1. This configuration is common for discharging brine into the environment and is also referred to as submerged desalination discharges. Upon entering the ambient environment, the jet undergoes two distinct dynamic phases. Initially, the jet is governed by its discharge momentum, ascending while progressively decelerating until the momentum is fully dissipated. Thereafter, the buoyancy force becomes dominant, causing the jet to reverse direction and descend toward the bed. To characterize the behavior of a dense jet, the concentration centerline, defined as the path along which the jet develops and the saline concentration reaches its maximum, serves as a reference for assessing both the jet trajectory and the mixing dynamics [20, 45]. The vertical distance reached by the centerline and the jet plume are referred to as the centerline peak and terminal rise, respectively, and are denoted by y_m and y_t , as illustrated in Figure 2.1. The horizontal distances from the nozzle to the terminal rise and the return point are denoted by x_m and x_r , respectively. The corresponding dilution levels, expressed as the ratio of the initial jet concentration ($C_0 = 1$) to the local concentration C_0/c , are denoted by s_m at the centerline peak and s_r at the return point.

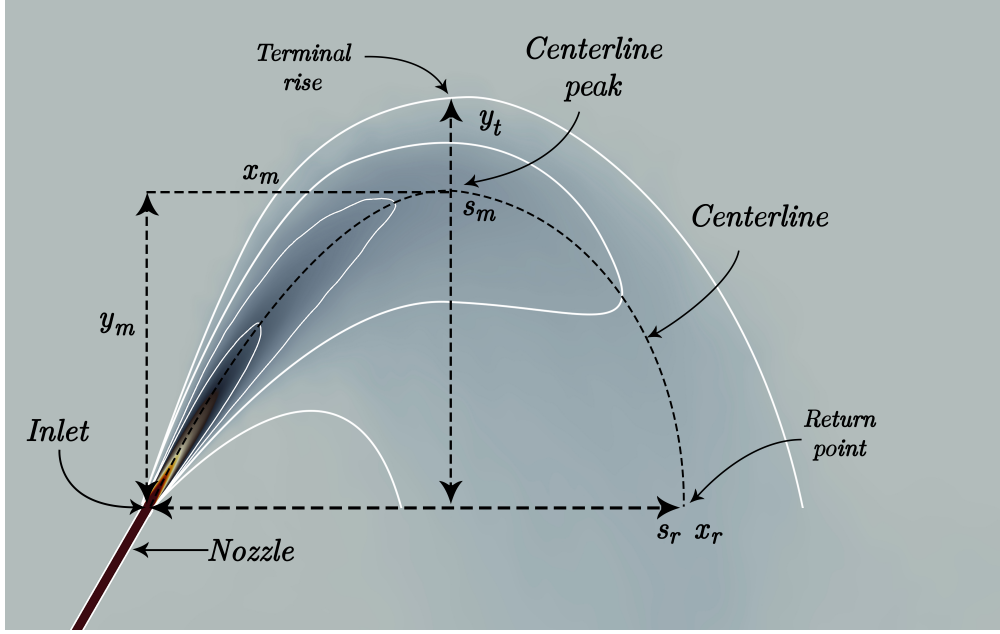


Figure 2.1: A schematic of a 60-degree dense jet representing geometrical characteristics.

To date, a large number of studies have investigated the behavior of buoyant jets through experimental, analytical, and numerical models [10, 22, 48, 71, 72]. Early numerical studies on buoyant jet simulations predominantly utilized RANS models. While these models contributed significantly to advancing the understanding of flow dynamics, they exhibited inherent limitations in accurately capturing the mixing processes and trajectory of buoyant jets. A recent study conducted by Galeshi et al. [73] highlighted a significant discrepancy between their RANS simulations and experimental observations. In contrast, previous research employing RANS models (e.g., [7, 17, 18, 74–77]) indicated comparatively lower errors. Among the different RANS models, Tahmooresi and Ahmadyar [26, 47] demonstrated significant improvements over traditional gradient-type models using Scalar Flux Modeling for predicting dynamics of an inclined negatively buoyant jet. Given the discrepancies observed in previous studies (e.g., [45]) between numerical simulations employing RANS models and experimental results, it is evident that RANS models may not be efficient in accurately predicting the behavior of buoyant jets.

Based on previous studies on desalination discharges using LES, three inlet boundary conditions of uniform velocity (UV), turbulent velocity (TV), and fully developed constant velocity (FDCV) have been applied in the literature (summarized in Table 2.1). Studies by [23, 50, 79–81, 83, 84] utilized the UV boundary condition and consistently reported an underestimation of jet trajectory evolution and mixing characteristics compared to experimental results. These discrepancies may arise from the inability of the UV boundary condition to generate realistic physical inflow, fluctuations, and turbulent eddy structures, thus limiting the accuracy in predicting jet behavior. Tofghian et al. [82] also reported an underestimation of the dense jet trajectory, including both the terminal rise and the return point, despite implementing the FDCV, which generates a fully developed laminar flow at the inlet. Several LES studies have used the TV boundary condition to generate a more physically realistic inflow for dense jets. However, considering the nature of turbulent flows and the theoretical foundations of

Table 2.1: A summary of the previous studies using Large Eddy Simulation (LES) modeling the desalination jets

No.	Study	Jet inlet boundary condition	Code	Nozzle	Inlet geometry	Inlet inclination method
1	Zhang et al. (2015) [23]	UV	ANSYS Fluent	Not Modeled*	Circle	No inclination
2	Zhang et al. (2016) [24]	TV (10%)	OpenFOAM	Not Modeled	Circle	Explicit
3	Zhang et al. (2017) [25]	TV (10%)	OpenFOAM	Not Modeled	Circle	Explicit
4	Jiang et al. (2019) [49]	TV (5-10%)	OpenFOAM	Not Modeled	Circle	Explicit
5	Cintolesi et al. (2019) [50]	UV	OpenFOAM	Not Modeled	Circle	No inclination
6	Songa et al. (2020) [78]	TV (10%)	OpenFOAM	Not Modeled	Circle	No inclination
7	Vafa et al. (2021) [79]	UV	OpenFOAM	Not Modeled	Square	Implicit
8	Azadi and Firoozabadi (2022) [80]	UV	OpenFOAM	Not Modeled	Not mentioned	Implicit
9	Habibi et al. (2022) [81]	UV	OpenFOAM	Not Modeled	Not mentioned	Implicit
10	Tofghian et al. (2022) [82]	FDCV	OpenFOAM	Not Modeled	Circle	Explicit
11	Habibi et al. (2023) [83]	UV	OpenFOAM	Not Modeled	Not mentioned	Implicit
12	Law et al. (2023) [48]	TV (10%)	OpenFOAM	Not Modeled	Circle	Explicit
13	Amiri et al. (2023) [84]	UV	OpenFOAM	Not Modeled	Circle	Explicit
14	Goodarzi (2024) [85]	MI	OpenFOAM	Modeled	Circle	Explicit

* “Not Modeled” indicates that the nozzle geometry was not explicitly included in the computational domain. In these cases, the inlet boundary conditions were directly applied at the domain entry without simulating the internal flow development within a nozzle or a pipe.

LES, simply superimposing random fluctuations at the inlet, as done in the TV boundary condition, may be insufficient. For LES to accurately resolve the energy containing eddies that govern turbulent mixing, the inflow should enable the natural formation of coherent turbulent structures. Nonetheless, despite these theoretical shortcomings, some studies have reported good agreement between LES predictions using the TV boundary condition and experimental observations, particularly in terms of jet trajectory and mixing behavior. In contrast, other investigations have found that the TV condition leads to overestimation of jet rise and underprediction of dilution [24, 25, 78]. These conflicting outcomes are not solely attributable to the inherent suitability of the TV boundary condition itself, but are likely influenced by factors such as mesh resolution and the specific implementation details of the boundary configuration. In a commentary, Goodarzi [85] investigated the impact of inlet boundary conditions on LES accuracy for a dense jet, emphasizing that the UV boundary condition used in [84] led to a considerable underestimation of jet development and mixing efficiency. Goodarzi’s analysis suggests that the mapped inlet (MI) condition, which more accurately captures turbulent fluctuations, should be prioritized to improve LES accuracy in buoyant jet simulations. However, to date, no study has systematically compared the effects of various inlet boundary conditions to establish a robust approach for inflow generation in modeling desalination discharges.

Numerical simulations have demonstrated the capability of LES in accurately capturing the behavior of turbulent dense jets; however, discrepancies remain when compared with experimental data. Furthermore, notable variations exist among numerical studies modeling identical dense jet configurations, which are likely attributable to differences in LES setup. These inconsistencies primarily arise from variations in grid resolution, numerical schemes, and the specification of boundary conditions. This study investigates the influence of inlet boundary conditions and nozzle representation methods on the dynamics of desalination jets using a robust, non-dimensional numerical framework. Two approaches for nozzle representation are considered: an explicit model incorporating a nozzle length of $20d_0$, and an implicit model in which the nozzle geometry is omitted. These configurations are evaluated in conjunction with various inflow boundary conditions, including MI, UV, TV, FDCV, and divergence-free synthetic eddy method (DFSEM). To enable rigorous validation, a high-resolution particle image velocimetry (PIV) experiment is conducted, providing reference data for comparison with the LES results. The remainder of this paper is organized as follows: §2.2 describes the numerical methodology used to model the dense jets; §2.3 presents and discusses the results of the numerical simulations; and §2.5 summarizes the key findings and conclusions drawn from the study.

2.2 Methodology

2.2.1 Governing equations

In this study, the transport of momentum and mass is governed by the incompressible Navier-Stokes equations coupled with an advection-diffusion equation for scalar transport. The LES approach employing implicit filtering is implemented using the Finite Volume Method [86]. The coupling of momentum and buoyancy forces is conducted based on the Boussinesq ap-

proximation, as the density difference between the dense jet and ambient fluid is relatively low [87]. The simulations are conducted using a non-dimensionalized form of equations based on [85], which eliminates dependence on specific dimensional parameters, ensuring the results are scalable across different physical conditions and experimental setups. This approach allows the model to be governed by Fr_d and Re , which control the characteristics of the desalination jet. The non-dimensional governing equations are expressed as follows [40, 88]:

$$\frac{\partial \tilde{u}_i}{\partial \tilde{x}_i} = 0, \quad (2.3)$$

$$\frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j \partial \tilde{x}_j} - \frac{\partial \tilde{\tau}_{ij}}{\partial \tilde{x}_j} + e_i^g \frac{1}{Fr_d^2} \tilde{c}, \quad (2.4)$$

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{c}}{\partial \tilde{x}_i} = \frac{1}{ReSc} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}_i \partial \tilde{x}_i} - \frac{\partial \tilde{\tau}_i^c}{\partial \tilde{x}_i}, \quad (2.5)$$

where $i, j = 1, 2, 3$, p is the pressure, u_i is the i -th velocity component, t is the time, and τ_{ij} denotes the subgrid-scale (SGS) stress tensor and τ_i^c denotes the SGS scalar flux. e_i^g is the direction of the gravitational acceleration, which is $(0, -1, 0)$, and c is the salinity concentration. In this study, the symbol $\sim$ indicates dimensionless variables. The Reynolds number (Re) is defined as $Re = U_0 d_0 / \nu$ [89–92]. The Schmidt number (Sc) is defined as $Sc = \nu / D$. The constant values of kinematic viscosity (i.e., momentum diffusivity) and mass diffusivity (e.g., salt), ν and D , were set as 1×10^{-6} and 1.5×10^{-9} , respectively [93, 94]. Dimensionless variables are defined based on the characteristic length, velocity, and time scales, as detailed in Table 2.2.

Table 2.2: Definition of non-dimensionalization used in this work.

Parameter	Non-dimensionalization
Spatial coordinates	$\tilde{x}_i = x_i / d_0$
Velocity	$\tilde{u}_i = u_i / U_0$
Time	$\tilde{t} = (U_0 / d_0) t$
Pressure	$\partial \tilde{p} / \partial \tilde{x}_i = (d_0 / \rho_a U_0^2) \partial p / \partial x_i$
Subgrid-scale stress tensor	$\partial \tilde{\tau}_{ij} / \partial \tilde{x}_j = (d_0 / U_0^2) \partial \tau_{ij} / \partial x_j$
Salinity	$\tilde{c} = c / C_0$

In this study, the Wall-Adapting Local Eddy-Viscosity (WALE) model is employed for SGS modeling. The WALE model is widely chosen for LES due to its ability to accurately predict near-wall turbulence by accounting for both strain and rotation rates, which are critical in wall-bounded flows. Furthermore, its capability to minimize eddy viscosity in laminar regions allows for better representation of laminar to turbulent transitions and complex flow phenomena such as separation and recirculation [88]. The SGS stress tensor $\tilde{\tau}_{ij}$, is given as:

$$\tilde{\tau}_{ij} = 2\nu_{sgs} S_{ij} + \frac{1}{3} \tau_{kk} \delta_{ij}, \quad (2.6)$$

where S_{ij} denotes the resolved strain-rate tensor, δ_{ij} is the Kronecker delta and ν_{sgs} represents the subgrid-scale eddy viscosity, computed as:

$$S_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} + \frac{\partial \tilde{u}_j}{\partial \tilde{x}_i} \right), \quad (2.7)$$

$$\nu_{sgs} = (C_w \Delta)^2 \frac{(S_{ij}^d S_{ij}^d)^{3/2}}{(S_{ij} S_{ij})^{5/2} + (S_{ij}^d S_{ij}^d)^{5/4}}, \quad (2.8)$$

where C_w represents the model constant, Δ denotes the filter width, and S_{ij}^d is the deviatoric part of the strain rate tensor. The filter width Δ determines the cutoff scale between resolved and modeled turbulence, defined based on the local grid size as $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$, where Δx , Δy , and Δz are the grid spacing in each direction. A detailed formulation of the methodology is provided in [43, 88].

2.2.2 Simulation setup and parameters

The simulations in this study were performed using a modified version of the standard OpenFOAM solver, *pimpleFoam*, for incompressible flow, coupled with an advection-diffusion equation. The governing equations for fluid and salinity transport were solved by the PIMPLE algorithm in nondimensional form, as explained in §2.2.1. Readers are referred to [95–97] for further information about the PIMPLE algorithm and OpenFOAM. The time derivative terms were discretized using a backward scheme to achieve second-order accuracy. Similarly, gradient terms were treated with the Gauss linear method, ensuring second-order accuracy. Divergence terms were discretized using the Gauss-limitedLinear scheme, while viscous terms employed the Gauss-linear scheme, and for the Laplacian terms, the Gauss-linear uncorrected scheme was utilized [98–100]. To enhance stability and accuracy during the simulations, the maximum Courant-Friedrichs-Lewy (CFL) number was maintained below 0.5 using adaptive time stepping. Each simulation was conducted until a statistically stationary state was achieved; thereafter, flow quantities were averaged over a period of 30,000 to 40,000 nondimensional time units. The statistically stationary state is considered when the time-averaged statistical properties, such as the mean and variance of flow quantities, exhibit negligible variation over time.

In the numerical domain, the jet is positioned at the center with a 60-degree inclination relative to the horizontal, as illustrated in the schematic in Figure 2.2. The geometry was generated in nondimensional form using the diameter of the jet d_0 as the characteristic length scale ($d_0 = 1$). The domain was configured as a rectangular tank, characterized by dimensions $l_x = 450d_0$ in length, $l_z = 250d_0$ in width, and $l_y = 180d_0$ in depth, with a circular nozzle placed at $l_y = 40d_0$ from the bottom. The nozzle, with diameter d_0 , extends to a length of $l_p = 20d_0$ in cases where the nozzle is explicitly modeled. A stagnant flow condition ($\tilde{u} = 0$, $\tilde{c} = 0$) was imposed as the initial state within the tank. The bottom, sides, front, and back boundaries of the domain were assigned an inlet-outlet condition, allowing fluid to enter or exit based on the instantaneous pressure and velocity fields. To simplify the modeling, free surface effects were neglected, and the top boundary was treated as a slip condition to approximate an open boundary, as its distance from the jet is sufficiently large.

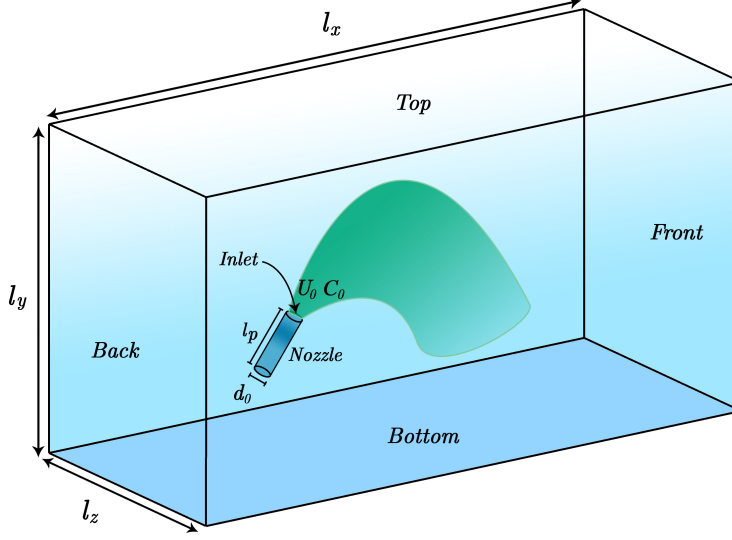


Figure 2.2: Schematic of the computational domain (not to scale). The inlet center is located at $(x = 0, y = 0, z = 0)$.

The numerical domain was discretized into hexahedral cells, comprising a total of 18.4 million cells, as illustrated in Figure 2.3. The mesh generation process was performed using a multi-level refinement method via the open-source tool Gmsh, where the resolution was selectively enhanced in critical regions of interest [101]. Hexahedral cells were used to ensure accuracy and facilitate smooth transitions from the round nozzle to the rectangular domain. In this study, the adequacy of the mesh was evaluated using the LES index, a quantitative criterion defined as the ratio of resolved turbulent kinetic energy (TKE) to total TKE ($LES_{\text{index}} = \text{TKE}_{\text{resolved}} / \text{TKE}_{\text{total}}$) [40, 85, 102]. The mesh resolution was systematically refined to ensure that more than 95% of the TKE was resolved, corresponding to an LES index of $LES_{\text{index}} = 0.95$, in critical regions of the jet flow, including the interior part of the pipe and the jet development region downstream of the nozzle. It should be noted that Batchelor scales were not resolved in this study. Figure 2.A1 shows the distribution of LES_{index} in the middle of the domain for the Mapped Inlet (MI) case, which is shown here as it exhibited the highest TKE among all boundary conditions considered. The results demonstrate that most of the domain maintains LES_{index} values exceeding 0.95, indicating sufficient resolution for a reliable LES. Data over four lines are plotted in key regions of the jet, illustrating the spatial variation in LES_{index} . These profiles confirm that TKE is well resolved throughout the critical region of the jet.

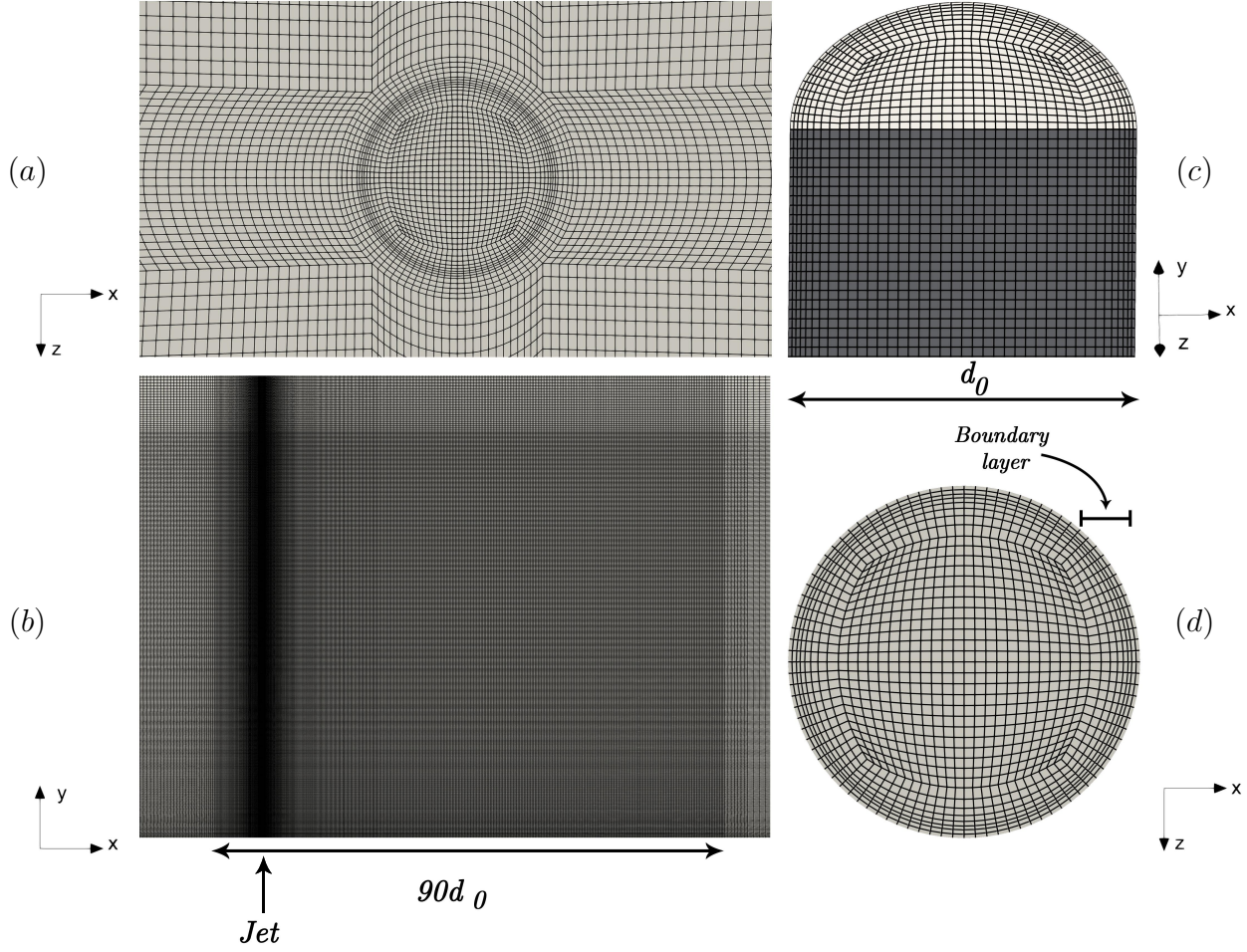


Figure 2.3: Visualization of the computational mesh used for the simulation, illustrating the hexahedral cell structure and refinement near the critical regions.

Figure 2.3 illustrates the areas of interest where the jet develops and data are gathered within the domain (for clarity, only this area is shown, as the full 3D computational domain is significantly larger.): (a) depicts the expanding horizontal surface (x - z) above the jet, (b) shows the streamwise area where the jet develops, and (c) and (d) highlight the nozzle pipe, detailing the mesh and boundary layer refinements. The O-grid method was employed to discretize the circular cross-section of the jet as a straight pipe, ensuring an accurate representation of the nozzle shape. The nozzle cross-section was discretized into 40 cells with near-wall refinements. The area of interest in the x -direction was divided into more than 400 cells, the y -direction into 300 cells, and the z -direction into 120 cells. This resolution corresponds approximately to the area of interest shown in Figure 2.3 and does not represent the total number of cells in the entire computational domain. The total number of cells in the domain with explicit nozzle modeling, including the pipe, is approximately 21 million while, cases employing implicit nozzle modeling, in which the pipe is not geometrically represented, contain approximately 18.4 million cells. This indicates that the pipe region accounts for roughly 2.6 million cells. Additionally, regions beyond the primary area of interest contribute an estimated 4 million cells. The cell size progressively increased by a factor of 1.025 in both

the streamwise and spanwise directions outside the nozzle area. The progressive increase in mesh size led to the smallest cell size of $0.03d_0$ near the nozzle area, which expanded to the largest cell size of $0.5d_0$ in downstream regions for $l_x > 200d_0$. To achieve a 60-degree discharge angle, the OpenFOAM tool *rotateMesh* was used to rotate the entire domain. A sample script for generating a desalination jet mesh using Gmsh is available for reference¹. In a wall-resolved LES, imposing a sufficient resolution near the walls is essential, and the location of the first off-wall cell center should be within the viscous sub-layer such that $y^+ < 1$, where superscript $+$ denotes wall-units. This non-dimensional distance is defined as:

$$y^+ = \frac{u_\tau y_d}{\nu}, \quad (2.9)$$

where u_τ denotes the friction velocity and y_d is the distance of the first off-wall cell center from the wall [40]. For the cases with a modeled nozzle, the final mesh was refined to ensure y^+ values remained below 1 within the nozzle.

To examine the impact of inlet configuration and boundary conditions on the behavior of desalination discharges, seven LES cases are considered, as detailed in Table 2.3. The simulations, categorized by the method of nozzle representation, are divided into explicit and implicit approaches. For the explicit method of nozzle modeling, four boundary conditions of Uniform Velocity (UV), Divergence-Free Synthetic Eddy Method (DFSEM), Mapped Inlet (MI), and Turbulent Velocity (TV) are examined. For the cases using the implicit method, three boundary conditions of UV, Fully Developed Constant Velocity (FDCV), and TV are considered. The UV and TV boundary conditions are compatible with both explicit and implicit nozzle modeling, as they can be directly imposed at the inlet without requiring a developed flow profile. Conversely, the DFSEM and MI boundary conditions necessitate a nozzle to allow for proper flow development and are therefore applied only in the explicit modeling cases. The FDCV boundary condition, designed to represent a fully developed velocity profile typically established in a long pipe, is exclusively used in the implicit modeling approach. For clarity, the UV and TV cases are labeled by “-p” when using the explicit method and “-np” when using the implicit method.

¹For a simple example of mesh generation for a desalination jet using Gmsh, see: https://github.com/HydroCFD/buoyant_jet/blob/main/Gmsh/inlcined_jet/.

Table 2.3: Summary of the parameters for different simulation scenarios.

Case name	Inlet boundary condition	Turbulent intensity (%)	Jet modeling method	Fr_d	Re
MI	Mapped Inlet (MI)	calculated	Pipe - $20d_0$ ¹	20	5300
DFSEM	Divergence-Free Synthetic Eddy Method (DFSEM)	calculated	Pipe - $20d_0$	20	5300
UV-p	Uniform Velocity (UV)	0%	Pipe - $20d_0$	20	5300
TV-p	Turbulent Velocity (TV)	10%	Pipe - $20d_0$	20	5300
UV-np	UV	0%	Not Modeled ²	20	5300
TV-np	TV	10%	Not Modeled	20	5300
FDCV	Fully Developed Constant Velocity (FDCV)	0%	Not Modeled	20	5300

¹ Explicit method: The nozzle geometry is modeled in the computational domain, with a pipe length of $20d_0$.

² Implicit method: The nozzle is not explicitly modeled, and inlet conditions are applied directly at the jet entry without any pipe.

2.2.3 Jet inlet boundary conditions

Uniform Velocity (UV)

UV is a Dirichlet boundary condition, where the velocity at the boundary is specified and remains constant spatially and temporally. In other words, the magnitude and direction of the velocity vectors across the entire surface of the boundary remain equal and constant. The UV boundary condition has been utilized in many RANS studies, see [17, 18, 103–106], where the analyses were predominantly focused on the mean flow. Mathematically, the UV boundary condition (which in OpenFOAM is known as *fixedValue*) sets the surface to a given reference velocity.

Mapped Inlet (MI)

MI is a three-dimensional, space- and time-dependent turbulent inflow technique proposed by Lund, Wu, and Squires [107]. In this approach, the flow characteristics are derived from a similar cross-section within the interior, at a designated downstream location, and are then imposed at the inlet [108]. The MI approach is a recycling simulation method that is integrated directly into the solution domain. As a result, the turbulent flow is generated in the main computational domain by the dominant flow mechanism.

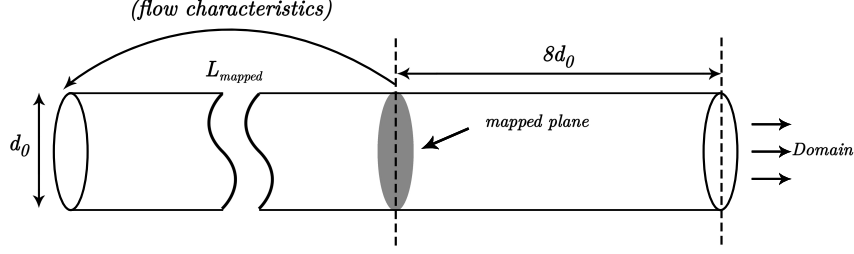


Figure 2.4: Schematic of the mapped inlet configuration (the figure is not drawn to scale).

The mapped plane (interior cross-section) within the domain must be positioned at an optimal distance from the inlet boundary, ensuring sufficient length for eddy formation, while also being adequately distanced from the downstream area to prevent reusing any extra perturbation originating from that region [59]. In this study, MI is generated by a pipe connected to the domain, and the mapped length L_{mapped} within the pipe is set to $12d_0$, with the distance from the mapped plane (interior cross-section) to the main domain set to $8d_0$, based on [109, 110], as shown in Figure 2.4.

Divergence-Free Synthetic Eddy Method (DFSEM)

DFSEM generates synthetic eddies that represent a set of velocity fluctuations at the inlet patch. Synthetic eddies, defined by their centers and the distribution of velocity fluctuations around them, are convected at each time step by the local mean velocity. After being convected into the domain, new eddies are generated at random locations across the inlet. The method is capable of accurately reproducing characteristic length and time scales of a target inlet turbulent flow. Further details on the generation of synthetic eddies can be found in [111–113]. The fluctuations are computed as:

$$u'_\beta(x) = \sqrt{\frac{1}{N}} \sum_{k=1}^N \sigma_\beta^k [1 - (d^k)^2] \epsilon_{\beta jl} r_j^k \alpha_l^k. \quad (2.10)$$

Here, $u'_\beta(x)$ is the fluctuating component of the velocity field in the β -th direction at position x , N is the number of synthetic eddies, σ_β^k is the k -th eddy's length scale in the β -th direction, representing the size of the eddy in that direction, $\epsilon_{\beta jl}$ is the Levi-Civita symbol (used to represent permutations in tensor notation), α_l^k is the intensity of the k -th eddy in the l -th direction, and d^k is defined as:

$$d^k = \sqrt{(r_j^k)^2}, \quad (2.11)$$

where r_j^k is the normalized distance vector between the point x and the k -th eddy:

$$r_j^k = \frac{x_j - x_j^k}{\sigma_j}. \quad (2.12)$$

Turbulent Velocity (TV)

This boundary condition generates a velocity field that varies both spatially and temporally by adding a series of pseudo-random numbers to a mean velocity profile. Pseudo-random

numbers are generated according to the probability density function of the uniform distribution, ranging from 0 to 1. The seed for the random number generator is fixed to produce the same sequence of random numbers at every execution.

$$u = (1 - \alpha)u^{n-1} + \alpha(u_{\text{ref}} + c_{tv}sR|u_{\text{ref}}|) , \quad (2.13)$$

where u is the velocity magnitude, u_{ref} is the spatiotemporal-invariant mean velocity, n is the time step, α is a scalar used to build two-temporal-point correlations, c_{tv} is a heuristically determined correction term (calculated to compensate for energy losses associated with the scalar α), R is a pseudo-random number, and s is the fluctuation scale. In this study, TV is established with a characteristic velocity $U_0 = 1$ (i.e., in Equation 2.13, $u_{\text{ref}} = 1$), and a variation of 10% is considered (i.e., $cs = 0.1$) [97, 114, 115].

2.2.4 Experimental setup

A high-resolution PIV experiment [116] was conducted to provide reference data for assessing the impact of buoyant jet inlet boundary conditions on the characteristics of the buoyant jet using LES. The experiment was conducted in a glass-walled water tank, with dimensions of 3 m in length, 1.2 m in width, and 1 m in depth. An aluminum apparatus was installed in the tank to provide a 60-degree jet by using two sliding parts. A solid polymer pipe with a diameter of 6 mm and a straight length equivalent to $40d_0$ was utilized for the jet, as depicted in Figure 2.5. A constant flow rate was applied using a head tank located above the test tank, which was continuously supplied with homogeneous saline water from a storage tank. To maintain the uniformity of the saline water, two mixing pumps were utilized within the storage tank. The density and temperature of saline and freshwater were measured using the portable density meter DMA 35 (Anton Paar), with an accuracy of 0.001 g/cm^3 . In this experiment, the density of the saline jet was established at $\rho_0 = 1027.6 \text{ kg/m}^3$, and the flow rate was set to 85 L/hr, resulting in $Fr_d = 20$ and $Re = 5010$.

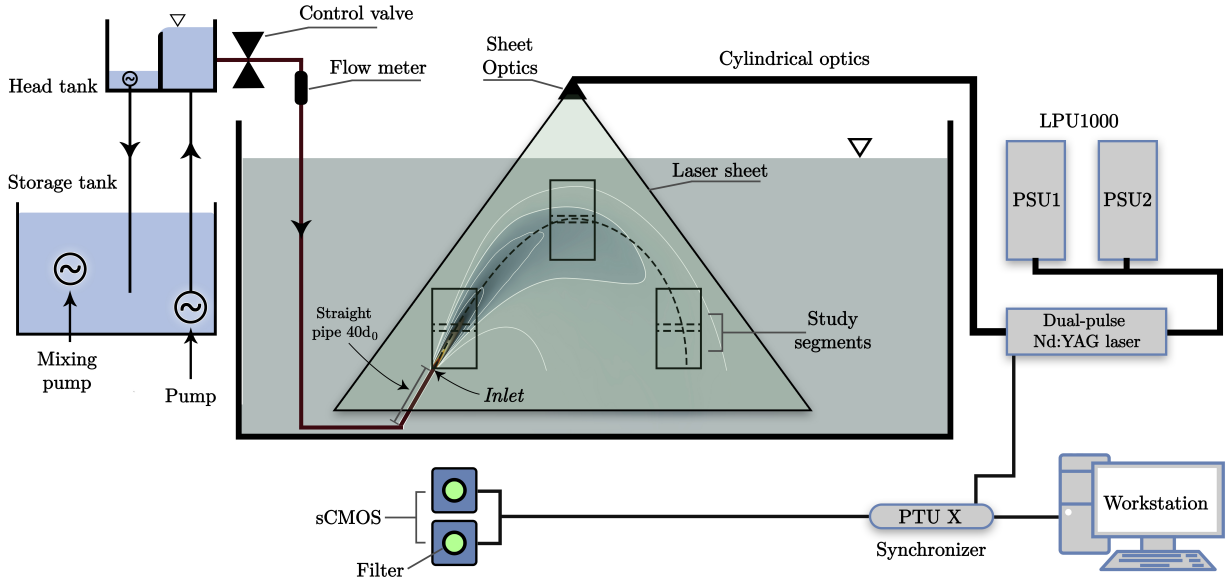


Figure 2.5: Schematic of the PIV configuration.

Both the dense and light fluids were homogeneously seeded with hollow non-porous microspheres (glass seeds), characterized by a size of $9\text{ }\mu\text{m}$ and a specific gravity of 1.1 g/cm^3 . A dual-pulse Nd:YAG laser with a wavelength of 532 nm was utilized to produce laser light and delivered through an articulated light arm. Sheet optics were used to create a 1 mm thick laser sheet. The images were captured using two dual-frame sCMOS cameras (side-by-side, 2D2C configuration), each with a resolution of 2560×2160 pixels, operating at a frequency of 5 Hz over a duration of 600 seconds , yielding a total of 3000 images. The cameras were positioned vertically, each covering an area of 105 mm in the x -direction and 180 mm in the y -direction, with 10% overlap, resulting in approximately 24 pixels per millimeter. The camera lenses had a focal length of 50 mm , an aperture of $f/1.8$, and were equipped with a bandpass filter centered at 532 nm with a bandwidth of 10 nm to prevent ambient light. The time delay between the two pulses varied from $250\text{ }\mu\text{s}$ to $1000\text{ }\mu\text{s}$ depending on the average flow velocity within the sampling area, ensuring that particles did not move more than $1/4$ of the interrogation window size. Cross-correlation algorithms were utilized to determine the two-dimensional velocity distribution within 32×32 pixel interrogation windows. To obtain high-resolution data, the experiment was structured into three distinct data acquisition phases, focusing on measurements near the nozzle, at the terminal rise, and at the return point, as shown in Figure 2.5. Following each data acquisition phase, the tank was emptied, filled with fresh water, and reseeded to eliminate any residual salinity effects on the jet characteristics. Data acquisition and post-processing of the PIV measurements were conducted using the LaVision system and DaVis 10.2.1 software on a workstation equipped with an Intel(R) Xeon(R) W-3235 CPU @ 3.30 GHz and 128 GB of RAM. The experiments were repeated in each phase to reduce error and uncertainty as reported by the DaVis software. Furthermore, all PIV experiments were performed in accordance with the standard methodology recommended by LaVision², ensuring the quality of the data acquisition process. A detailed assessment of measurement uncertainty associated with the PIV processing is provided in Appendix B.

2.3 Results

The numerical and experimental data were post-processed using open-source Python libraries of Matplotlib³, PyVista⁴, and Pandas⁵ and Davis 10. The bar symbol ($\bar{}$) denotes the time-averaged data in the results section.

2.3.1 Flow characteristics inside the pipe

To assess the flow characteristics within the modeled pipe for explicit method cases employing MI, DFSEM, UV-p, and TV-p boundary conditions, four separate simulations were conducted using the same numerical solver and mesh configuration, without buoyancy effects. Since PIV measurements were not possible for the authors inside the pipe due to laboratory limitations,

²<https://www.lavision.de/en/downloads/manuals/>

³<https://matplotlib.org/>

⁴<https://pyvista.org/>

⁵<https://pandas.pydata.org/>

the DNS data of pipe flow from [1]⁶ with $Re = 5300$ is utilized for comparing the time-averaged velocity and time-averaged dimensionless root-mean-square (RMS) values of the fluctuating velocity components in three directions, $\overline{\tilde{u}'_{rms}}$, $\overline{\tilde{v}'_{rms}}$, and $\overline{\tilde{w}'_{rms}}$, defined as:

$$\overline{\tilde{u}'_{rms}} = \sqrt{\overline{\tilde{u}'\tilde{u}'}}, \quad \overline{\tilde{v}'_{rms}} = \sqrt{\overline{\tilde{v}'\tilde{v}'}}, \quad \overline{\tilde{w}'_{rms}} = \sqrt{\overline{\tilde{w}'\tilde{w}'}} \quad (2.14)$$

$$\overline{\tilde{u}'_{rms}^+} = \frac{\overline{\tilde{u}'_{rms}}}{\tilde{u}_\tau}, \quad \overline{\tilde{v}'_{rms}^+} = \frac{\overline{\tilde{v}'_{rms}}}{\tilde{u}_\tau}, \quad \overline{\tilde{w}'_{rms}^+} = \frac{\overline{\tilde{w}'_{rms}}}{\tilde{u}_\tau} \quad (2.15)$$

where u_τ is the friction velocity (see [40] for more details on equations). Simulations were conducted in nondimensionalized mode as explained in §2.2.1.

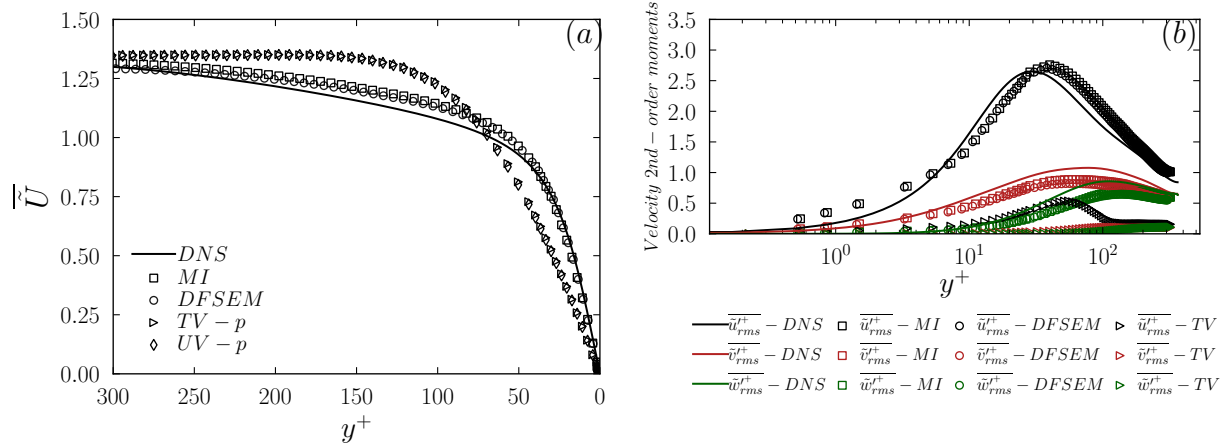


Figure 2.6: Nondimensional time-averaged velocity and turbulence statistics for the flow in the pipe and reference DNS data by [1].

Figure 2.6 - a compares the nondimensional time-averaged velocity profiles for different boundary conditions applied in the pipe flow simulations. Data were interpolated along a line from the center of the pipe to the wall, perpendicular to the flow direction. In Figure 2.6 - b, $\overline{\tilde{u}'_{rms}^+}$ represents the stream-wise RMS of velocity fluctuations, $\overline{\tilde{v}'_{rms}^+}$ denotes the radial component, and $\overline{\tilde{w}'_{rms}^+}$ indicates the fluctuation perpendicular to both the radial and stream-wise directions. The profile of time-averaged velocity indicates that the MI and DFSEM boundary conditions closely align with the DNS data, with a slight overprediction. In contrast, the TV-p and UV-p boundary conditions deviate significantly from the DNS data. The maximum of velocity for the TV-p and UV-p is higher, while the near-wall velocity is lower than that of the DNS, resulting in an overall velocity distribution that does not match the reference. The MI and DFSEM cases exhibit RMS values that match the DNS data, with a slight overestimation in the stream-wise component and underestimation in the radial and transverse components as shown in Figure 2.6 - b. This suggests that these boundary conditions effectively capture turbulent velocity fluctuations. In contrast, the TV-p condition, while introducing some turbulence, shows larger discrepancies across all three components.

⁶Data are available at: <https://ctr.stanford.edu/about-center-turbulence-research/research-data>

This is attributed to the nature of the TV-p condition, which generates random velocity fluctuations rather than coherent three-dimensional turbulent structures. As a result, the fluctuations fail to evolve into sustained turbulence. The RMS values for the UV-p condition remain on the order of 1×10^{-3} and are therefore omitted from the plot. This condition fails to generate turbulence or meaningful velocity fluctuations, leading to an unrealistic representation of the flow field. These findings highlight the importance of boundary conditions that incorporate physically realistic turbulence generation mechanisms, such as MI and DFSEM, for achieving accurate velocity predictions in pipe flow simulations.

2.3.2 Velocity field

Figure 2.7 presents the near nozzle time-averaged velocity profiles for all boundary conditions and PIV measurements, normalized by the centerline velocity ($\tilde{U}/\tilde{U}_c$). Here, $\tilde{U}_c$ refers to the maximum of velocity along the jet centerline at each corresponding cross-section. The profiles are extracted along lines perpendicular to the centerline at distances of $8d_0$, $10d_0$, and $15d_0$ downstream from the inlet (i.e., from $x = 0$, $y = 0$, and $z = 0$). Negative r/d_0 values, r denotes the radial distance measured perpendicular to the jet centerline within each cross-sectional plane, correspond to positions below the centerline, whereas positive values denote positions above it. Among the four simulated cases, UV-p consistently exhibits an underdeveloped velocity distribution across all examined locations. The profile remains narrow and approximately parabolic, characterized by steep velocity gradients and limited radial spreading. This nonphysical behavior indicates that the flow remains laminar or weakly transitional, resulting in velocity confinement along the centerline and inadequate dispersion across the jet cross-section. The MI and DFSEM boundary conditions both yield velocity profiles that closely resemble the experimentally observed behavior. These profiles exhibit symmetric, bell-shaped distributions with physical lateral spreading, consistent with PIV. At $8d_0$, DFSEM offers a closer match to the PIV data in the shear-layer regions, likely due to its ability to generate turbulence synthetically without relying on a long development length. This leads to earlier shear-layer growth and more rapid transition. However, at $10d_0$ and $15d_0$, the MI boundary condition shows comparable agreement with the PIV results across the full radial extent. TV-p exhibits a slightly lower average velocity distribution that partially resembles PIV profile and slightly underpredicts the velocity distribution at $8d_0$. This underestimation suggests a delayed transition to turbulence and weaker initial perturbations compared to MI and DFSEM. Although the profile improves downstream at $10d_0$ and $15d_0$, it continues to underestimate lateral spreading relative to the experimental data. At $15d_0$, the velocity profiles for the MI, DFSEM, and TV-p boundary conditions exhibit a lateral extent reaching approximately $3.5 r/d_0$ in inner layer and $3 r/d_0$ in outer layer, consistent with the spreading observed in the PIV measurements. This distribution indicates well-developed shear layers and active entrainment, particularly in the lower half of the jet, where the negative buoyancy force enhances downward momentum and increases vertical deflection. In contrast, the UV-p case shows a confined profile, with a sharp velocity gradient limited to $1.5 r/d_0$ below and $1 r/d_0$ above the centerline. This limited extent and asymmetry reflect the poor development of shear layers and the absence of adequate turbulence at the inlet, which in turn hinders ambient entrainment and limits the jet's capacity to expand under buoyancy force.

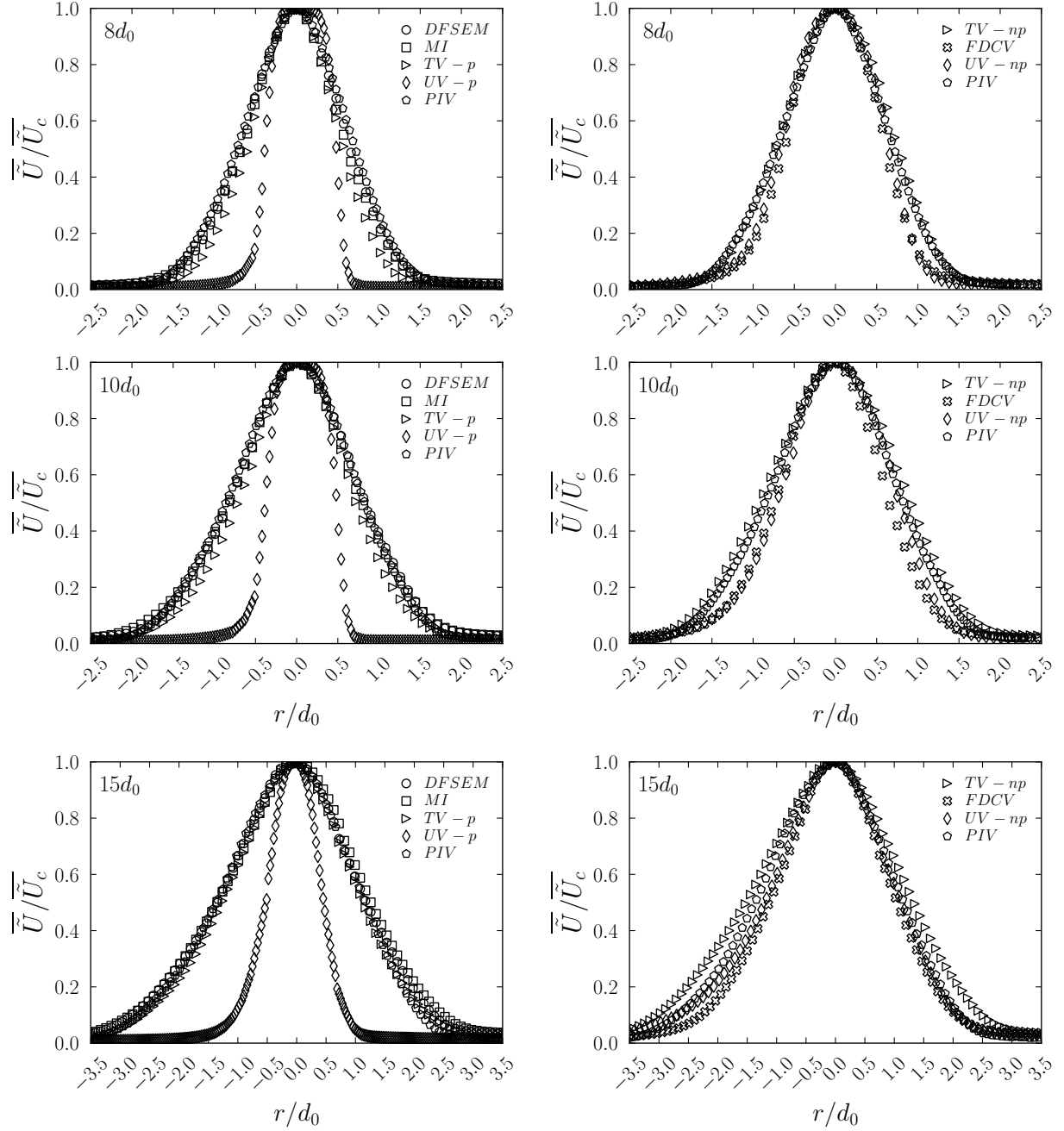


Figure 2.7: Distribution of normalized time-averaged velocity profiles $\bar{U}/\bar{U}_c$ at distances of $8d_0$, $10d_0$, and $15d_0$.

Comparison of the implicit nozzle modeling for UV-np and FDCV with PIV shows higher discrepancies across all measured sections near the nozzle. At $8d_0$, all three cases produce symmetric profiles about the centerline; however, distinct differences emerge in the shape and distribution of the normalized velocity field. TV-np reasonably captures the general profile shape, while FDCV presents a more confined distribution, indicating a narrower spread of momentum. UV-np shows the steepest gradients near the centerline and the most abrupt

decay, reflecting limited shear-layer growth similar to UV-p. At $10d_0$, UV-np and FDCV exhibit increased radial expansion compared, however, their distributions still deviate from the PIV profile in the outer regions. TV-np slightly overpredicts the extent of the velocity distribution, suggesting enhanced lateral spreading relative to PIV. By $15d_0$, TV-np exhibits the broadest velocity distribution, slightly overestimating the radial extent relative to the PIV data. FDCV shows moderate improvement, with reasonable agreement in the upper layer, although it underpredicts the extent of the lower layer. UV-np remains the most confined, with limited lateral development.

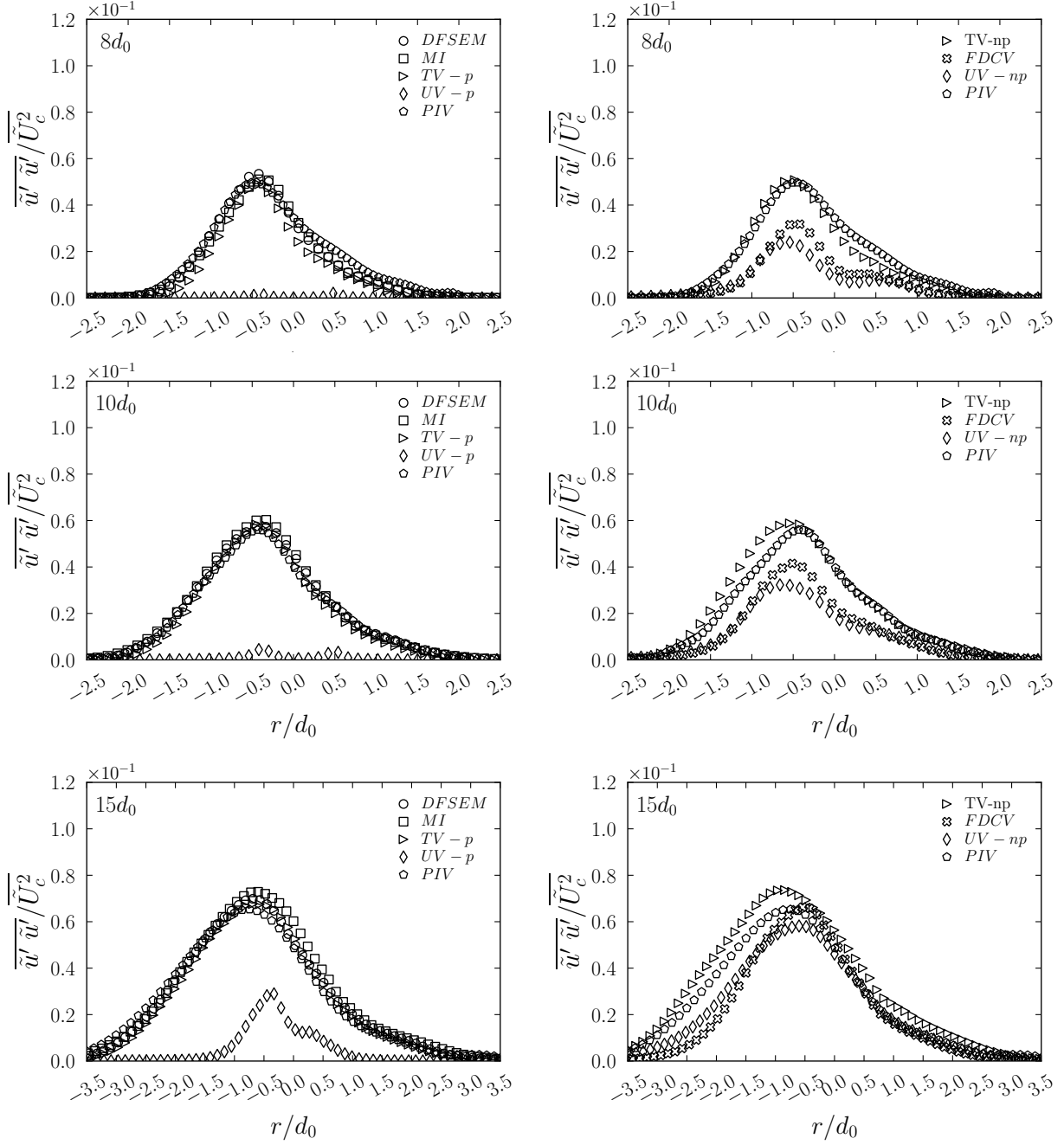


Figure 2.8: Distribution of normalized time-averaged velocity component fluctuations $\overline{u'u'}/\overline{U_c^2}$ at distances of $8d_0$, $10d_0$, and $15d_0$.

Figures 2.8 and 2.9 illustrate the normalized time-averaged velocity fluctuations of components, $\overline{u'u'}/\overline{U_c^2}$ and $\overline{v'v'}/\overline{U_c^2}$, at distances of $8d_0$, $10d_0$, and $15d_0$ for different inlet boundary conditions under both implicit and explicit nozzle modeling methods and compare them with the PIV. At $8d_0$ (Figure 2.8), the DFSEM and MI cases closely match the PIV data, particularly within the shear-layer region. Both conditions slightly underpredict velocity fluctuations in the jet core ($-0.5 < r/d_0 < 0.5$) but maintain a comparable profile shape,

capturing the peak location and asymmetry reasonably well. The TV-p condition exhibits a modest underestimation of fluctuation across the profile, suggesting a weaker generation of turbulence. In contrast, UV-p produces a nearly flat distribution, indicating a failure to initiate physically realistic turbulence structures; this reflects the absence of sufficient formation of three dimensional eddies at the inlet, resulting in a nonphysical laminar core and suppressed shear-layer development. At a downstream location of $10d_0$, the DFSEM and MI inlet conditions exhibit velocity fluctuation profiles that remain in close agreement with the PIV measurements, with MI slightly overpredicting the magnitude in the jet core region ($-0.5 < r/d_0 < 0.5$). This modest overestimation is likely to be attributable to the sustained coherence of the inflow structures retained from the mapped velocity fields. The TV-p condition agrees well with the experimental data, though it consistently underestimates magnitude across the entire radial profile, suggesting incomplete development of large-scale structures. UV-p condition continues to demonstrate a significant deficiency in turbulence generation, reflecting the inherent limitations of uniform velocity profiles in replicating realistic inflow turbulence dynamics. At a downstream location of $15d_0$, DFSEM, MI, and TV-p inlet conditions reproduce the general shape of the PIV velocity fluctuations profile, but all exhibit a visibly elevated peak in the core region, suggesting a moderate overprediction of turbulence. Among these, the MI condition shows the highest peak, indicating the largest overestimation relative to PIV, followed by DFSEM and then TV-p. This gradation suggests varying degrees of excess turbulence generation introduced by the different inflow treatments. The UV-p condition, although slightly improved compared to upstream, continues to significantly underpredict velocity fluctuations magnitude. Figure 2.A3 presents the time-averaged velocity fluctuation contours ($\tilde{u}'\tilde{u}'$), showing similar velocity fluctuation patterns for the DFSEM, MI, and TV-p cases, with peak intensity near the nozzle and a broad spread. In contrast, the UV-p case exhibits nonphysical flow characteristics, forming a laminar region immediately after the nozzle and delayed shear layer formation, resulting in a displaced and diffused turbulence peak.

At a distance of $8d_0$, the $\overline{\tilde{u}'\tilde{u}'}/\overline{U_c^2}$ profiles for the implicit nozzle modeling cases (without pipe) show significant differences in their capability to capture realistic velocity fluctuations compared to the PIV data. The TV-np condition demonstrates closer alignment with the PIV data in capturing the maximum of $\overline{\tilde{u}'\tilde{u}'}/\overline{U_c^2}$, though it slightly underestimates velocity fluctuations magnitude in the core jet. In contrast, FDCV and UV-np conditions both exhibit lower velocity fluctuations magnitude across the entire radial extent, with the UV-np condition showing the most significant underprediction, suggesting nonphysical turbulence generation. At a distance of $10d_0$, a similar trend is observed and TV-np condition maintains a closer alignment with the PIV data, albeit with an observable overprediction of velocity fluctuations magnitude in the lower shear layer of jet ($-2 < r/d_0 < -0.5$). Both FDCV and UV-np conditions continue to significantly underpredict the velocity fluctuations magnitude across the profile, reflecting a persistent underestimation in capturing the resolved turbulent fluctuations. By $15d_0$, the UV-np and FDCV conditions show improved agreement with the PIV data; however, they continue to underpredict velocity fluctuations magnitude, particularly within the lower shear layer and the outer radial regions of the jet. In contrast, the overprediction observed with the TV-np condition intensifies, exceeding the PIV data across all regions. This trend is consistent with the time-averaged velocity profiles Figure 2.7. Figure

2.A4 illustrates the time-averaged velocity fluctuation contours for the TV-np, FDCV, and UV-np boundary conditions. Compared to the explicit method, these cases exhibit weaker and more confined formation of shear layers near the centerline. FDCV condition generates more intense fluctuations that extend further downstream from the nozzle. This behavior is attributed to the enhanced shear layer development initiated by the parabolic inflow velocity profile.

At $8d_0$, the DFSEM and MI boundary conditions closely reproduce the PIV measurements across the core and shear-layer regions. Both profiles display peak intensities in the upper shear layer ($0.0 < r/d_0 < 0.5$), slightly overestimating the measured velocity fluctuations magnitude (Figure 2.9). TV-p case exhibits a similar profile shape but with reduced magnitude compared to MI and DFSEM more close to PIV. In contrast, UV-p condition significantly underpredicts velocity fluctuations magnitude across the entire radial extent, indicating a lack of realistic turbulence generation in the vertical direction. By $10d_0$, the DFSEM, MI, and TV-p cases exhibit good agreement with the PIV, though they slightly overpredict within the core and upper shear layers. Among them, the MI condition shows the highest degree of overestimation, followed by DFSEM, while the TV-p condition presents the closest match. In contrast, the UV-p boundary condition continues to produce a flat and attenuated profile, failing to replicate the spatial variability in velocity fluctuations magnitude. At $15d_0$, the DFSEM, MI, and TV-p profiles remain in agreement with the PIV measurements. The MI and DFSEM cases exhibit a slight overprediction of velocity fluctuations magnitude near the jet core, while the TV-p condition shows a modest underprediction. The UV-p boundary condition, although still significantly underestimating the fluctuations, begins to exhibit the onset of turbulence generation at this distance. Figure 2.A5 depicts the near-field distribution of the vertical velocity fluctuations, $\overline{\tilde{v}'\tilde{v}'}$, for the DFSEM, MI, TV-p, and UV-p boundary conditions. In all three turbulence generating cases, DFSEM, MI, and TV-p the fluctuation magnitude is confined near the jet origin and gradually spreads outward the jet path. Among these, the DFSEM condition produces the earliest onset of peak fluctuations immediately after the nozzle, followed by MI and TV-p, where the maxima shift slightly farther downstream, indicating a delayed turbulence development. While the UV-p case exhibits a fluctuation magnitude comparable to MI in the far field, it lacks early turbulence formation near the nozzle due to the extended laminar region.

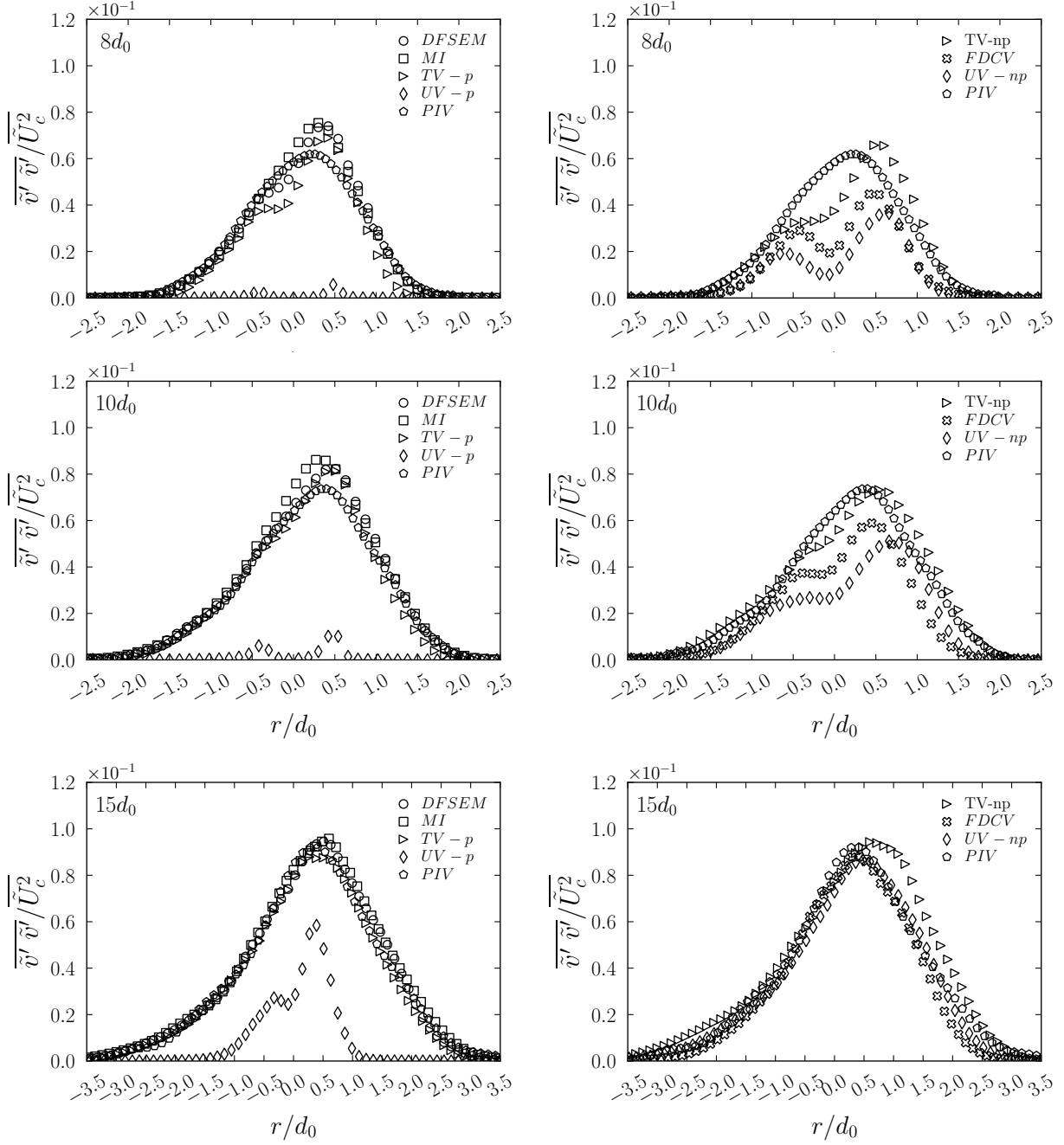


Figure 2.9: Distribution of normalized time-averaged velocity component fluctuations $\overline{\tilde{v}'\tilde{v}'} / \tilde{U}_c^2$ at distances of $8d_0$, $10d_0$, and $15d_0$.

At $8d_0$ (Figure 2.9), none of the simulated cases fully captures the velocity fluctuation profile observed in the PIV measurements. Among the tested conditions, only the TV-np case demonstrates a partial resemblance in terms of magnitude and spatial distribution. However, the structure of the shear layer does not align with the experimental data, with the peak fluctuations appearing at a higher radial position than those captured by PIV. At $10d_0$, FDCV and UV-np conditions display lower velocity fluctuation magnitude across the profile, indi-

cating limited turbulence generation and delayed shear-layer development. TV-np boundary condition continues to align most closely with experimental data, although its profile exhibits a broader peak, suggesting excess vertical fluctuations that may be sustained due to insufficient dissipation of turbulence in the absence of an explicit pipe. By $15d_0$, TV-np case shows overprediction across the entire upper shear layer, with fluctuations exceeding those measured by PIV. Conversely, while FDCV and UV-np show slight improvements compared to closer distances, they continue to underpredict the velocity fluctuations magnitude across the profile. Figure 2.A6 illustrates the near-field distribution of the vertical velocity fluctuations, $\tilde{v}'\tilde{v}'$, TV-np, UV-np and FDCV conditions. The FDCV case exhibits the highest intensity of vertical velocity fluctuations among the three cases, characterized by a distinct region of elevated turbulence originating near the nozzle and extending along the developing shear layers. In contrast, the TV-np case produces a broader yet more diffuse distribution of fluctuations, indicative of sustained but less localized turbulent generation along the jet trajectory. The UV-np case displays markedly weaker fluctuation magnitudes, with low intensities formed far from the nozzle and minimal lateral spread. This distribution suggests delayed turbulence onset and underdeveloped shear layers, consistent with the uniform inflow conditions and absence of imposed perturbations or initial eddy structures.

Figure 2.10 illustrates the distribution of total TKE, normalized by the square of the centerline velocity ($\tilde{U}_c$). At $8d_0$, the turbulent kinetic energy (TKE) profiles for the DFSEM, MI, and TV-p boundary conditions show a generally good agreement with the PIV data in terms of profile shape, but all exhibit varying degrees of underprediction in magnitude. Among them, the TV-p condition demonstrates the lowest turbulence level near the centerline, indicating reduced energy associated with velocity fluctuations. The DFSEM and MI conditions perform comparably, with the MI case slightly closer to the PIV, particularly in capturing the peak TKE values across the shear layer. The DFSEM condition follows the profile trend but with a marginal underprediction. In contrast, the UV-p boundary condition severely underpredicts TKE across the entire cross-section, resulting a nearly flat distribution that highlights the absence of resolved turbulent structures. This behavior proves previous observations of the UV-p case's laminar core and delayed shear-layer development. At $10d_0$, the TKE profiles for the DFSEM, MI, and TV-p boundary conditions continue to follow the experimental data with good agreement, maintaining the general profile shape and peak location observed in the PIV measurements. Among these, MI condition exhibits a slight overprediction of the TKE peak at the centerline, indicating enhanced turbulence retention along the jet core. DFSEM case, while capturing the peak location with reasonable accuracy, slightly underpredicts turbulence levels within the core region but demonstrates an overestimation within the range $0.5 < r/d_0 < 1.5$, showing a higher magnitude in lower the shear layer. TV-p exhibits a larger underprediction compared to DFSEM near the jet core and remains within acceptable agreement across the shear layers. TKE profile of PIV data is more clearly replicated by MI and DFSEM, whereas TV-p underestimates the intensity in the lower shear region. In contrast, the UV-p condition, although showing a modest increase compared to its performance at $8d_0$, still significantly underpredicts TKE throughout the cross-section. By $15d_0$, the DFSEM, MI, and TV-p boundary conditions exhibit strong agreement with the PIV data, accurately reproducing the shape and magnitude of the TKE distribution across the jet cross-section. The MI condition demonstrates the closest match to the experimental results, whereas DFSEM and TV-p slightly underpredict the turbulence levels. The UV-p

condition, despite a modest increase in TKE compared to upstream locations, continues to significantly underpredict turbulence intensity, particularly within the shear layers, reflecting a delayed transition to a fully developed turbulent state. Figure 2.A7 illustrates the near-field distribution of TKE for cases with explicit nozzle modeling. The MI condition generates the highest turbulence levels, with the two peak layers merging more closely. The DFSEM and TV-p conditions exhibit similar layer structures, though in the TV-p case, the peak turbulence layers develop further downstream, consistent with the distributions of $\overline{\tilde{u}'\tilde{u}'}$ and $\overline{\tilde{v}'\tilde{v}'}$ for this boundary condition. In contrast, the UV-p condition displays delayed turbulence development, characterized by an asymmetric distribution in which the upper shear layer shows higher intensity than the lower one.

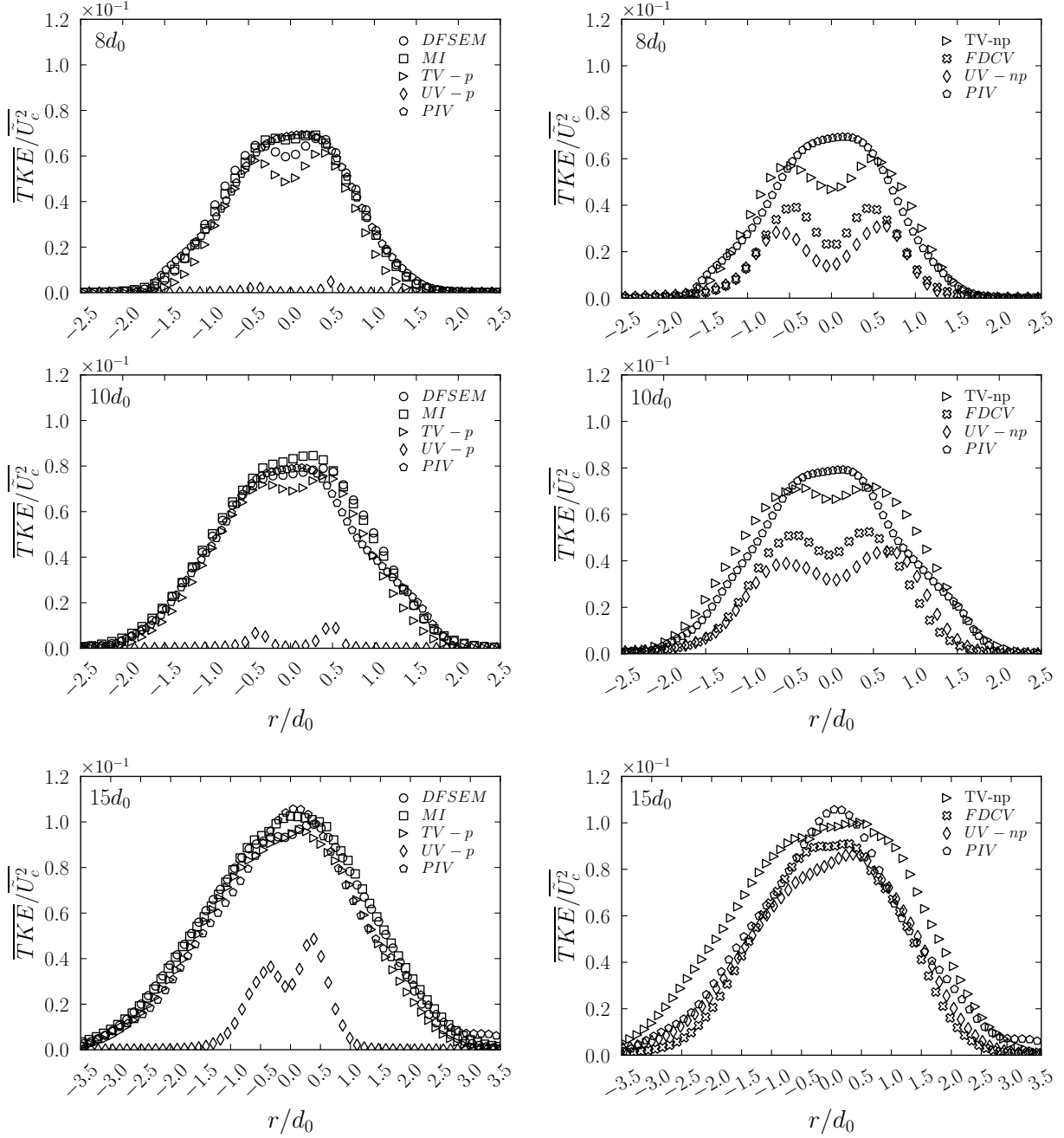


Figure 2.10: Distribution of turbulent kinetic energy (TKE), normalized by the square of the centerline velocity $\overline{TKE}/\tilde{U}_c^2$, at distances of $8d_0$, $10d_0$, and $15d_0$.

At $8d_0$ (Figure 2.10), TV-np condition underpredicts the peak of TKE compared to the PIV data but reproduces the general shape and spread of the profile with marginal discrepancies. The FDCV and UV-np cases both significantly underpredict the TKE across the entire cross-section. At $10d_0$ (Figure 2.10), the TV-np condition underestimates the peak TKE relative to the PIV reference but remains the most consistent in capturing both the magnitude and spatial distribution among the implicit inlet conditions. In contrast, the FDCV and UV-np

cases significantly underpredict turbulence levels across the entire jet profile, with the largest discrepancies observed near the centerline. At $15d_0$, the TV-np condition begins to overpredict the TKE magnitude, both in the core jet and shear layers. In contrast, the FDCV and UV-np conditions continue to exhibit lower TKE levels across the profile. Although the UV-np case shows a modest increase in turbulence intensity compared to upstream positions, its distribution remains inconsistent with the PIV reference, indicating a delayed and incomplete transition to fully developed turbulence. Figure 2.A8 illustrates the near-field distribution of TKE for simulations using implicit nozzle modeling. The TV-np condition exhibits a wider spatial spread of turbulence but with comparatively low intensity throughout the domain. In contrast, both FDCV and UV-np cases display non-uniform turbulence patterns, elevated TKE magnitudes appear close to the nozzle, followed by a decline and subsequent secondary growth downstream. Among them, FDCV produces the highest localized TKE in the shear layers but lacks uniform development across the jet width.

Figure 2.11 presents the normalized time-averaged velocity profiles at the jet's terminal rise y_t . For the explicit nozzle modeling cases, MI, DFSEM, and TV-p produced well-developed velocity profiles that closely matched the PIV data across most of the jet cross-section. MI provided the best match in the core region ($-5 < r/d_0 < 5$), with improved symmetry and sharper decay, while DFSEM slightly underpredicted velocities in the lower shear layer ($r/d_0 < -7.5$). TV-p also reproduced the general shape with only minor deviations. In contrast, UV-p substantially overpredicted velocities in both the inner and outer layers, resulting in an overly broadened distribution. For the implicit nozzle modeling cases, FDCV exhibited a similar trend to UV-p, with inflated velocities across the profile. UV-np captured the general shape on the upper side but showed significant discrepancies in the lower region, overpredicting velocity for $-10 < r/d_0 < 0$ and underpredicting for $r/d_0 < -10$. The TV-np case consistently underpredicted velocity across the entire span, failing to reproduce the peak magnitude and lateral spreading observed in the PIV data.

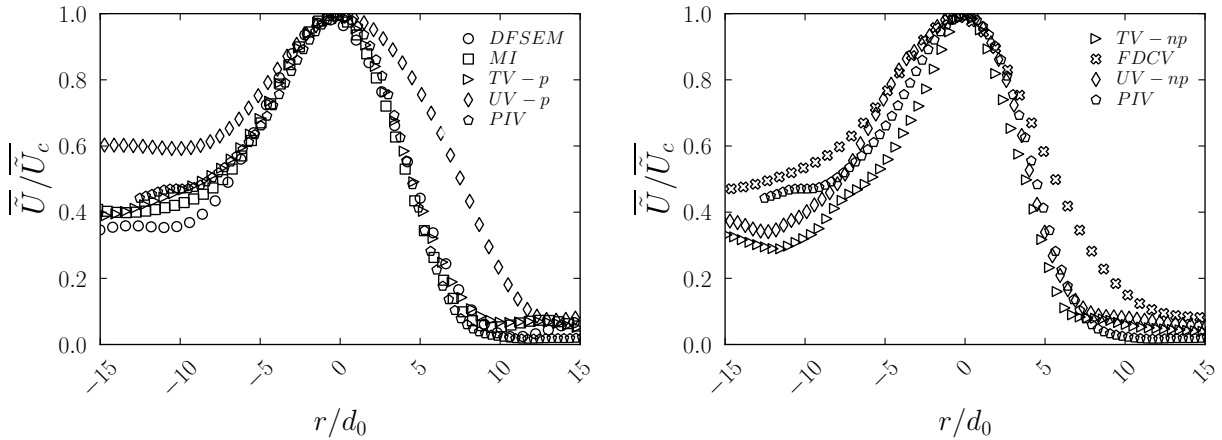


Figure 2.11: Distribution of normalized time-averaged velocity profiles $\tilde{U}/\tilde{U}_c$ at terminal rise.

Figure 2.12 illustrates the time-averaged velocity component fluctuations $\overline{\tilde{u}'\tilde{u}'} / \tilde{U}_c^2$ at the terminal rise (y_t) for both explicit and implicit nozzle modeling cases, compared with experimental PIV data. In the explicit pipe cases, the DFSEM, MI, and TV-p boundary conditions

slightly underpredict the peak fluctuations near the centerline ($-5 < r/d_0 < 5$), resulting in lower turbulence intensity than measured experimentally. In contrast, the UV-p condition markedly over-predicts the fluctuations across the entire profile, indicating excessive turbulence generation. For implicit modeling, the FDCV condition also significantly overestimates the velocity fluctuations, while the TV-np and UV-np conditions under-predict turbulence levels, failing to capture the peak intensities observed in the PIV data.

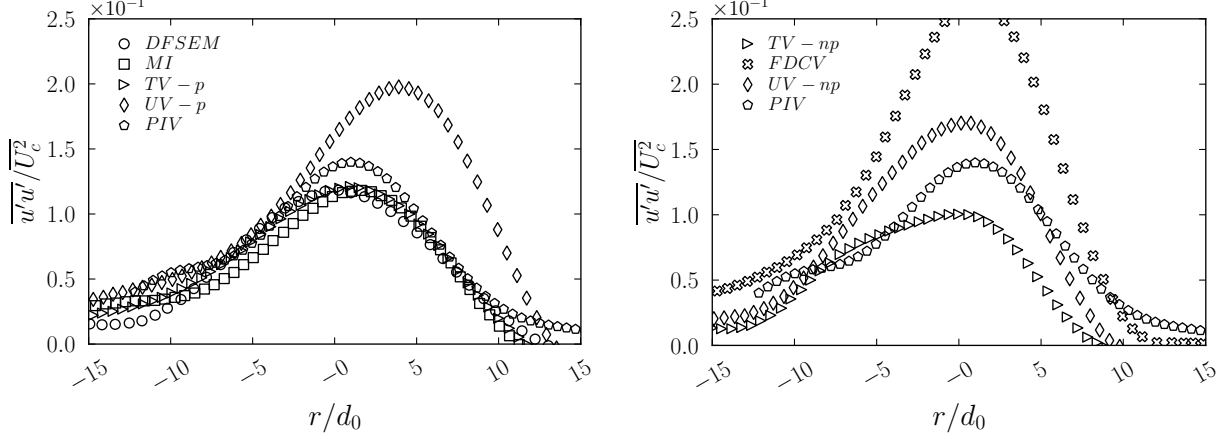


Figure 2.12: Distribution of normalized time-averaged velocity component fluctuations $\overline{u'u'}/\tilde{U}_c^2$ at terminal rise.

Figure 2.13 shows the normalized time-averaged cross-stream velocity fluctuations, $\overline{\tilde{v}'\tilde{v}'}/\tilde{U}_c^2$, at the terminal rise location. In the explicit nozzle modeling cases, the DFSEM, MI, and TV-p boundary conditions exhibit similar trends but generally under-predict the fluctuation levels across the profile. The UV-p condition shows larger deviation, compared to the PIV data. In the implicit nozzle modeling, the FDCV condition considerably over-predicts the fluctuation magnitudes, while the TV-np condition underestimates $(\overline{\tilde{v}'\tilde{v}'}/\tilde{U}_c^2)$, particularly at the peak locations. The UV-np condition generally follows the trend of the FDCV profile but exhibits a noticeable underestimation in the region $r/d_0 < 5$.

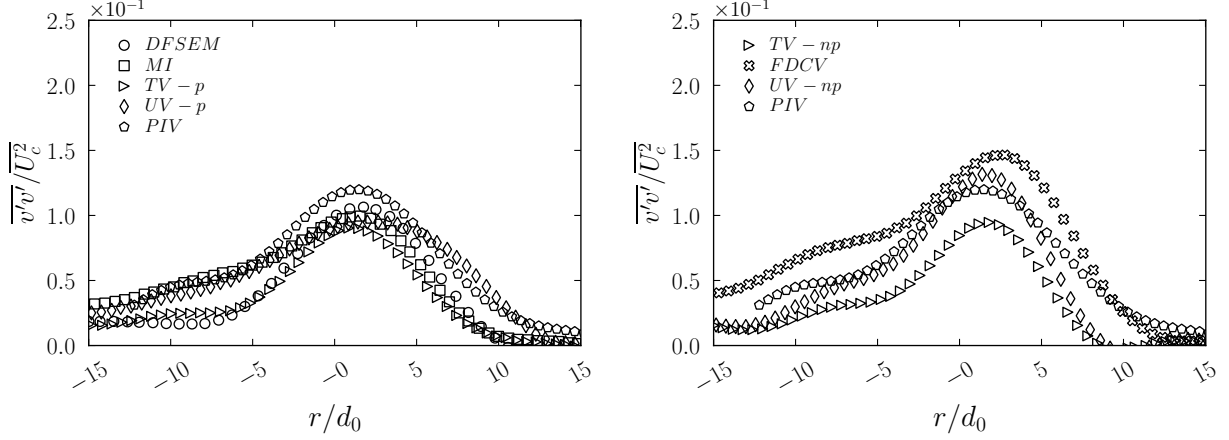


Figure 2.13: Distribution of normalized time-averaged velocity component fluctuations $\overline{v'v'}/\overline{U_c^2}$ at terminal rise.

Figure 2.14 presents the normalized time-averaged velocity profiles at the return point of the jet. Among the explicit nozzle modeling cases, all boundary conditions reproduce the general trend of the PIV data near the jet centerline ($0 < r/d_0 < 5$). However, deviations become more apparent in the outer regions. The MI and DFSEM conditions maintain closer agreement with the PIV profile across the full span, while the TV-p case slightly underestimates velocity beyond $r/d_0 > 5$. A more detailed examination indicates that the MI condition slightly overpredicts the velocity within $0 < r/d_0 < 10$ and underpredicts it beyond this region. In contrast, the DFSEM case exhibits the opposite behavior, underestimating velocity in the inner region and overestimating it in the outer shear layer ($r/d_0 > 10$). This inverse trend implies that, although both models are capable to capture the overall velocity distribution, they diverge in their characterization of velocity.

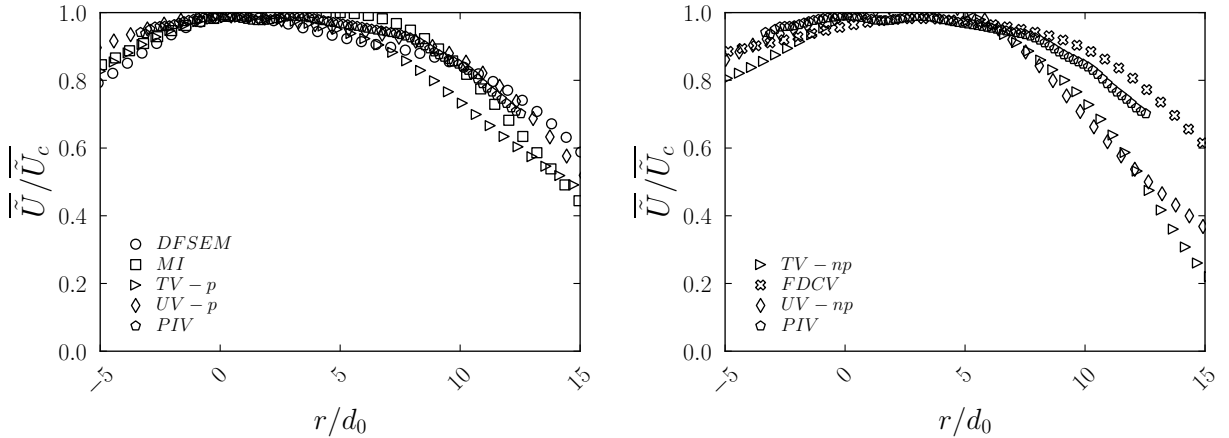


Figure 2.14: Distribution of normalized time-averaged velocity profiles ($\overline{\tilde{U}}/\overline{U_c}$) at return point.

For the implicit nozzle modeling cases, the FDCV boundary condition exhibits the closest agreement with the PIV data with a overprediction in $r/d_0 > 10$. In contrast, both TV-np

and UV-np cases underpredict the velocity in the outer region ($r/d_0 > 5$), suggesting that these conditions do not fully reproduce the lateral spreading of the jet observed in the PIV data.

2.3.3 Concentration field

Figure 2.15 presents the time-averaged concentration profiles, normalized by the centerline concentration ($\tilde{c}_c$). At $8d_0$, the concentration profiles exhibit a smooth radial decay from the jet centerline, reflecting entrainment and mixing with the ambient fluid. While all cases maintain a broadly similar shape, notable differences emerge in the gradient steepness and spread, particularly between the explicit and implicit nozzle modeling approaches, indicating difference in mixing efficiency and turbulence development. As the distance from the nozzle increases, the concentration profiles broaden for all boundary conditions, showing an increase in entrainment and dilution of jet. Among the explicit nozzle modeling cases, both DFSEM and MI produce relatively symmetric profiles with wide spreading at all measured distances, signifying well-developed turbulent mixing. The UV-p condition shows narrow concentration distributions centered around the core due to inadequate turbulence generation and delayed transition, which is consistent with its previously observed laminar behavior and subdued fluctuation intensity. While TV-p aligns moderately well with DFSEM and MI in terms of spread, it shows lower concentrations in the shear layers. For implicit nozzle modeling, the TV-np boundary condition generates the broadest concentration profiles, particularly at $15d_0$, indicating an overestimated dispersion and lateral expansion of jet. In contrast, the FDCV and UV-np conditions yield narrower distributions with sharper concentration gradients near the centerline, reflecting constrained turbulent entrainment and limited lateral mixing. This behavior is consistent with the previously discussed velocity field distributions and turbulence intensities, where both FDCV and UV-np exhibited lower levels of resolved fluctuations and reduced shear layer development.

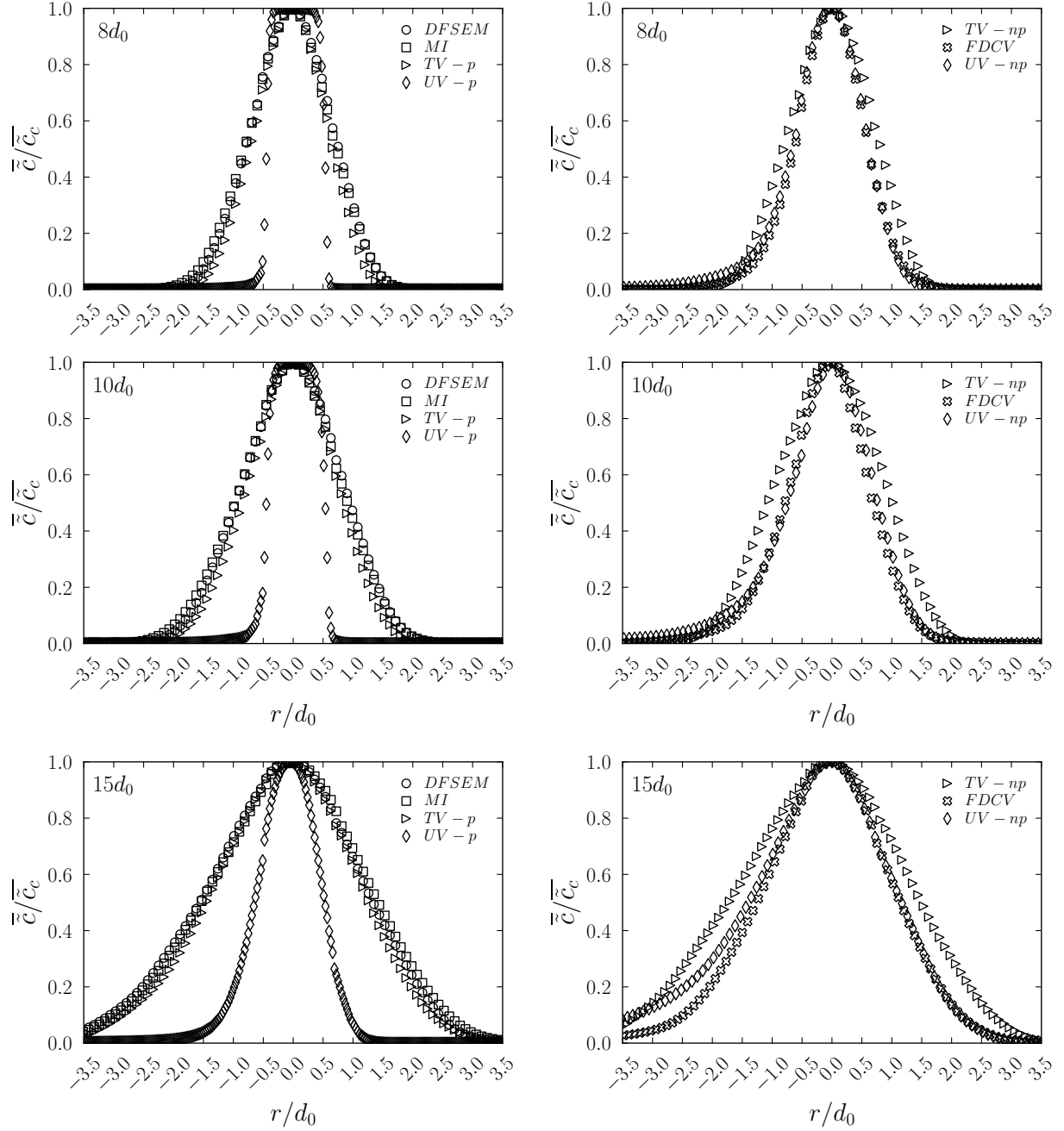


Figure 2.15: Distribution of normalized time-averaged concentration profiles $\bar{\tilde{c}}/\bar{\tilde{c}}_c$ at distances of $8d_0$, $10d_0$, and $15d_0$.

Figure 2.16 presents the distribution of concentration fluctuations, normalized by the square of centerline concentration ($\tilde{c}_c$) for both explicit and implicit nozzle modeling approaches. In the explicit cases, distinct discrepancies emerge between the UV-p condition and the turbulence generating inlets (DFSEM, MI, and TV-p). At $6d_0$, the DFSEM and MI conditions exhibit elevated fluctuation magnitudes in both shear layers, reflecting robust turbulent mixing and enhanced scalar dispersion. The TV-p profile also demonstrates a well-distributed

fluctuation field, albeit with slightly reduced peak values compared to DFSEM and MI. In contrast, the UV-p condition produces a confined and dampened profile, characterized by a limited spread and low peak values, indicating poor mixing due to the delayed onset of turbulence. As the flow evolves downstream to $8d_0$, $10d_0$, and $15d_0$, the DFSEM and MI conditions sustain higher concentration fluctuation levels across the jet width, with broader and more symmetric profiles. The TV-p condition follows a similar trend but remains consistently lower in magnitude. Meanwhile, the UV-p condition shows minimal improvement with distance, retaining its narrow fluctuation zone and low peak amplitude.

At $x = 6d_0$, the TV-np inflow generates high concentration fluctuation peaks in the upper and lower shear layers at $-0.5 < r/d_0 < 0.5$, with values reaching $6.5 \times 10^{-2} \tilde{c}_c^{-2}$, indicating strong shear-induced mixing. In contrast, both FDCV and UV-np cases exhibit weaker fluctuations and narrower profiles, with limited radial spread. As the jet develops downstream ($x = 8d_0$ and $10d_0$), TV-np maintains a broader and higher fluctuation field, while FDCV and UV-np show delayed growth and reduced intensity. By $x = 15d_0$, TV-np achieves the widest concentration distribution across the centerline, whereas FDCV partially recovers in width but remains lower in amplitude, and UV-np continues to underpredict mixing. These trends align with previous velocity and turbulence metrics, highlighting TV-np's enhanced capability in promoting concentration fluctuation development without explicit pipe modeling.

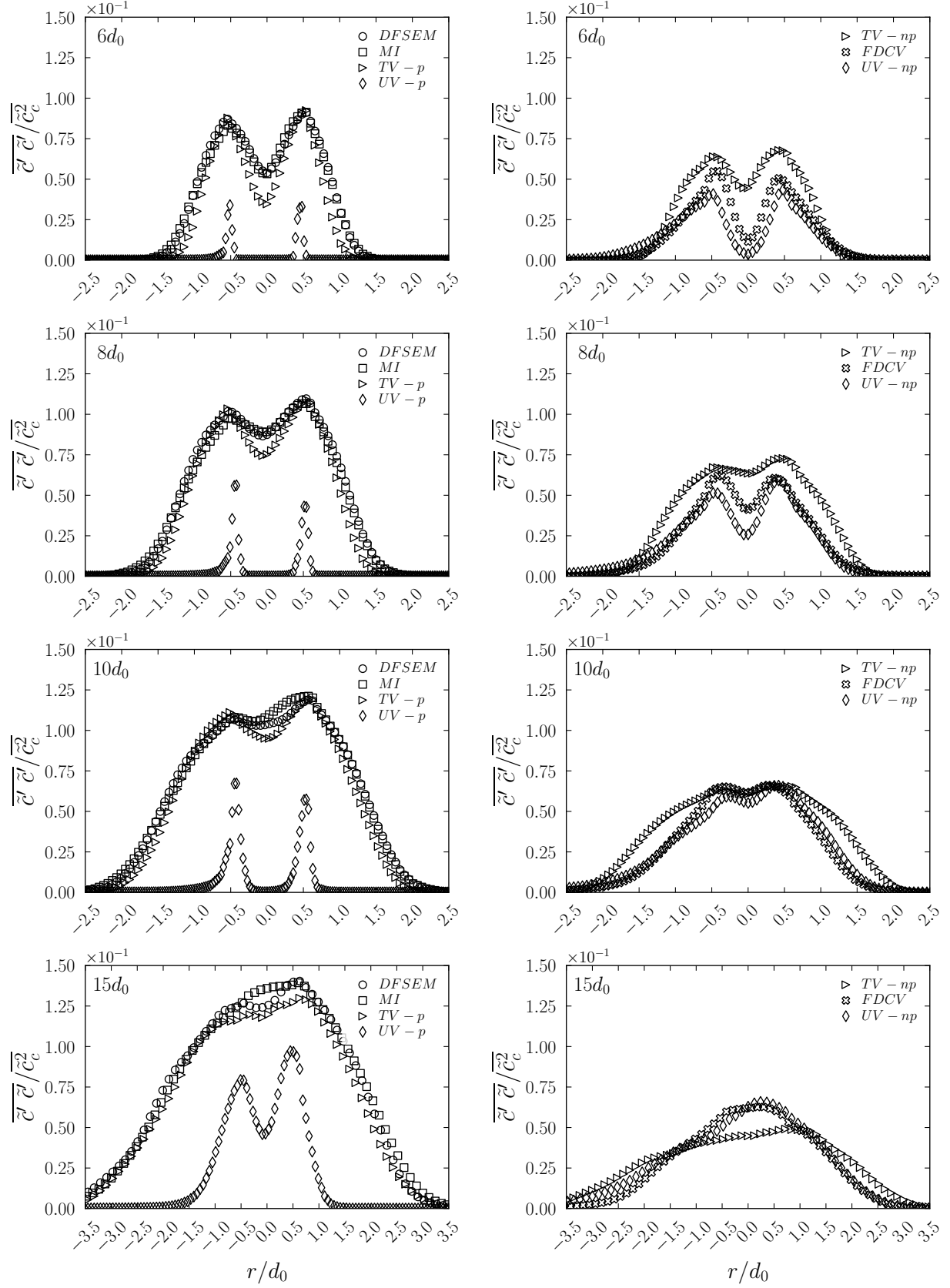


Figure 2.16: Distribution of normalized time-averaged concentration fluctuations profiles $\overline{c'c'}/\overline{c_c^2}$ at distances of $6d_0$, $8d_0$, $10d_0$, and $15d_0$.

Figure 2.17 shows the normalized time-averaged concentration profiles, $\tilde{c}/\tilde{c}_c$, at the terminal rise height for all boundary conditions. In the explicit nozzle modeling cases, DFSEM, MI, and TV-p produce comparable profiles near the centerline, with DFSEM and TV-p showing slightly broader dispersion in the upper layer compared to MI. The UV-p case exhibits large lateral spread across both layers, indicative of enhanced concentration transport. For implicit nozzle modeling, FDCV produces the widest distribution, particularly in the upper shear layer, whereas TV-np and UV-np result in narrower, steeper profiles, reflecting weaker entrainment and mixing, consistent with prior velocity field observations.

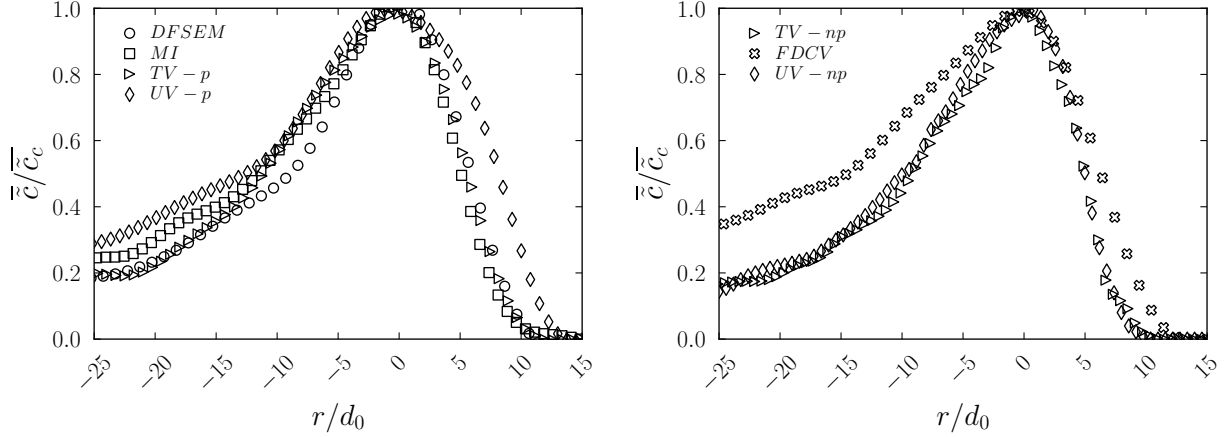


Figure 2.17: Distribution of normalized time-averaged concentration profiles $\tilde{c}/\tilde{c}_c$ at terminal rise.

Figure 2.18 presents the time-averaged concentration fluctuation profiles, $\overline{c'c'}/\overline{c_c^2}$, at the terminal rise. In the explicit nozzle modeling cases, the DFSEM, MI, and TV-p boundary conditions exhibit relatively consistent distributions across the jet cross-section, with peak fluctuations forming in the upper layer. The UV-p condition displays a broader distribution of fluctuations, particularly beyond $r/d_0 > 5$, differing from the other boundary conditions. In the implicit nozzle modeling group, the FDCV condition results in a wider and more intense fluctuation profile across the domain. The TV-np and UV-np conditions show similar distributions to each other, with lower fluctuation levels compared to those observed under the DFSEM, MI, and TV-p conditions in the explicit modeling cases.

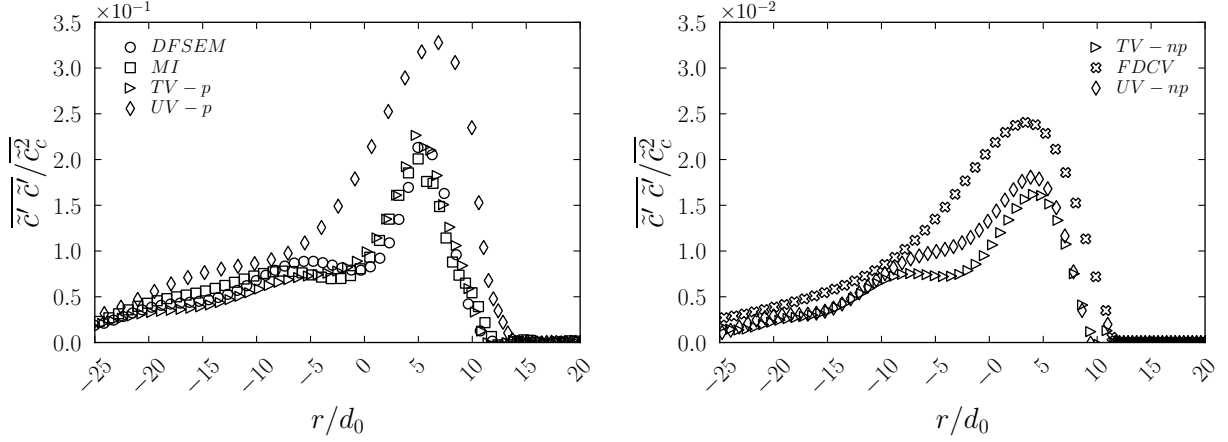


Figure 2.18: Distribution of normalized time-averaged concentration fluctuations profiles $\overline{\tilde{c}'^2}/\overline{\tilde{c}_c^2}$ at terminal rise.

Figure 2.19 illustrates the distribution of normalized time-averaged concentration profiles, $\overline{\tilde{c}}/\overline{\tilde{c}_c}$, at the return point. In the explicit modeling cases, the MI boundary condition yields higher concentration levels in the inner region of the jet, while the DFSEM condition shows the lowest values in the lower layer. In the upper layer, both the DFSEM and UV-p conditions exhibit higher concentrations relative to the MI and TV-p cases. For the implicit nozzle modeling approach, the FDCV condition produces a broader concentration profile in both the upper and lower layers, while maintaining a similar overall shape to the other conditions. The TV-np and UV-np conditions display similar trends, both exhibiting slightly lower concentration values across the jet cross-section.

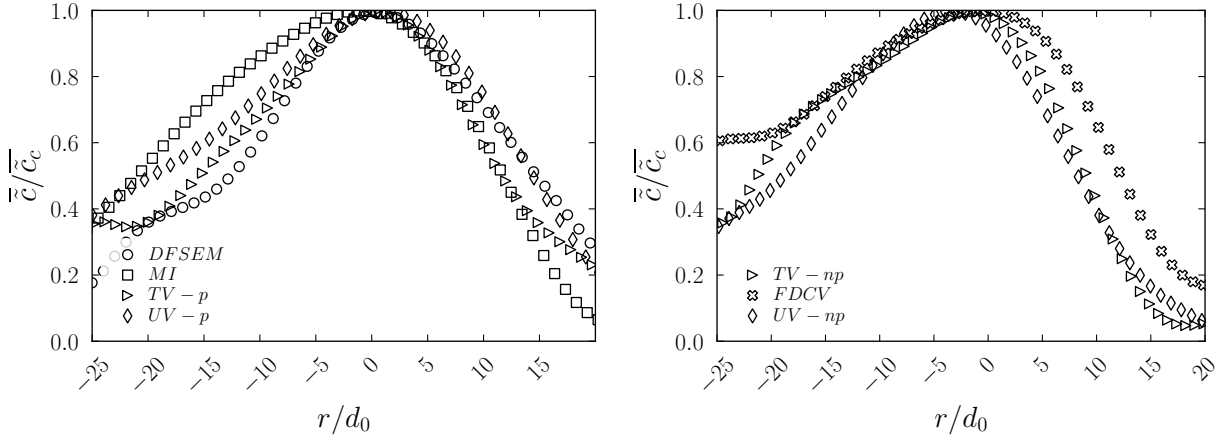


Figure 2.19: Distribution of normalized time-averaged concentration profiles $\overline{\tilde{c}}/\overline{\tilde{c}_c}$ at return point.

2.3.4 POD of the concentration field

Proper orthogonal decomposition (POD) is a mathematical technique commonly applied in fluid dynamics to extract dominant coherent structures existing in complex turbulent

flows [117, 118]. By decomposing the flow field into a set of orthogonal spatial modes that are ranked according to their energy content, POD offers an optimal representation of the flow’s most dominant features. These modes provide critical insights into the interaction between the jet and its surrounding environment, particularly the role of boundary conditions in shaping flow structures. This method operates by taking a series of flow field snapshots, forming a data matrix, and applying Singular Value Decomposition to decompose the data into spatial modes with corresponding temporal coefficients. The resulting eigenvalues provide a direct measure of the energy captured by each mode. For a more detailed explanation of POD, readers are referred to [119–123]. In this study, POD is applied to the concentration field to identify the dominant mixing structures across various boundary conditions. The extracted coherent structures reflect underlying physical mechanisms governing jet development and scalar transport. The most commonly identified features include shear-layer modes, associated with instabilities along the jet edges, and global column modes, which represent large-scale oscillatory motion of the jet core. Near the nozzle, the axisymmetric mode is generally dominant; however, farther downstream, alternating lobed patterns often emerge, consistent with the development of azimuthal or helical modes. These alternating patterns, characterized by periodic sign changes in the transverse direction, are indicative of rotating or swirling structures, a sign of helical instabilities, previously reported in studies of jet dynamics and turbulent entrainment [121, 124–126]. The first three POD modes were extracted for all boundary conditions under both explicit and implicit nozzle modeling configurations. Mode 1, representing the most energetic structures in the flow field for the explicit modeling cases, reveals significant differences among the boundary conditions (see Figure 2.20). DFSEM and MI cases exhibit well-defined, helical structures of alternating positive and negative lobes along the jet axis, indicative of strong coherent vortical structures [124, 127]. These patterns suggest a well-developed turbulence structure with clear helical periodicity in the streamwise direction. In contrast, the TV-p and UV-p conditions show different spatial structures from those observed in the DFSEM and MI cases. Instead of the alternating lobe patterns associated with helical instabilities, these conditions produce weaker, more symmetric distributions with elongated structures forming farther downstream, suggesting the emergence of less coherent modes near the nozzle region. Thus, while DFSEM and MI capture the expected structures, TV-p and UV-p cases demonstrate significant discrepancies, with UV-p showing the poorest representation of flow features in the near nozzle region [121, 124–126]. Near the nozzle, strong shear and velocity gradients along the jet boundary create conditions for the development of azimuthal instabilities. These instabilities lead to the formation of helical structures, which enhance entrainment and mixing, as shown in recent experimental studies [22]. In Mode 2, both the DFSEM and MI inflow conditions exhibit distinctly periodic, alternating lobe structures, consistent with the presence of coherent helical vortical modes. These large-scale structures maintain their periodicity, highlighting a strong turbulence field. The TV-p condition shows a similar pattern, but with slightly more diffused lobes compared to DFSEM and MI, suggesting some reduction in the turbulence intensity and coherence of flow. In contrast, the UV-p condition produces significantly reduced lobe formations, diminished spatial structures, and increased diffusion, indicative of weakened turbulence structures and rapid energy dissipation. Mode 3 further illustrates the differences in turbulence structures among the boundary conditions. The DFSEM case shows slightly diffused structures compared to MI, though both maintain strong, coherent structures with

clear periodicity, preserving the helical patterns observed in the previous modes. The TV-p condition shows more diffuse and less coherent structures compared to DFSEM and MI, indicating further energy dissipation and loss of turbulence coherence. The UV-p condition exhibits the most diffused and least coherent structures, with very weak lobe formations that indicate a significant reduction in turbulence energy and coherence.

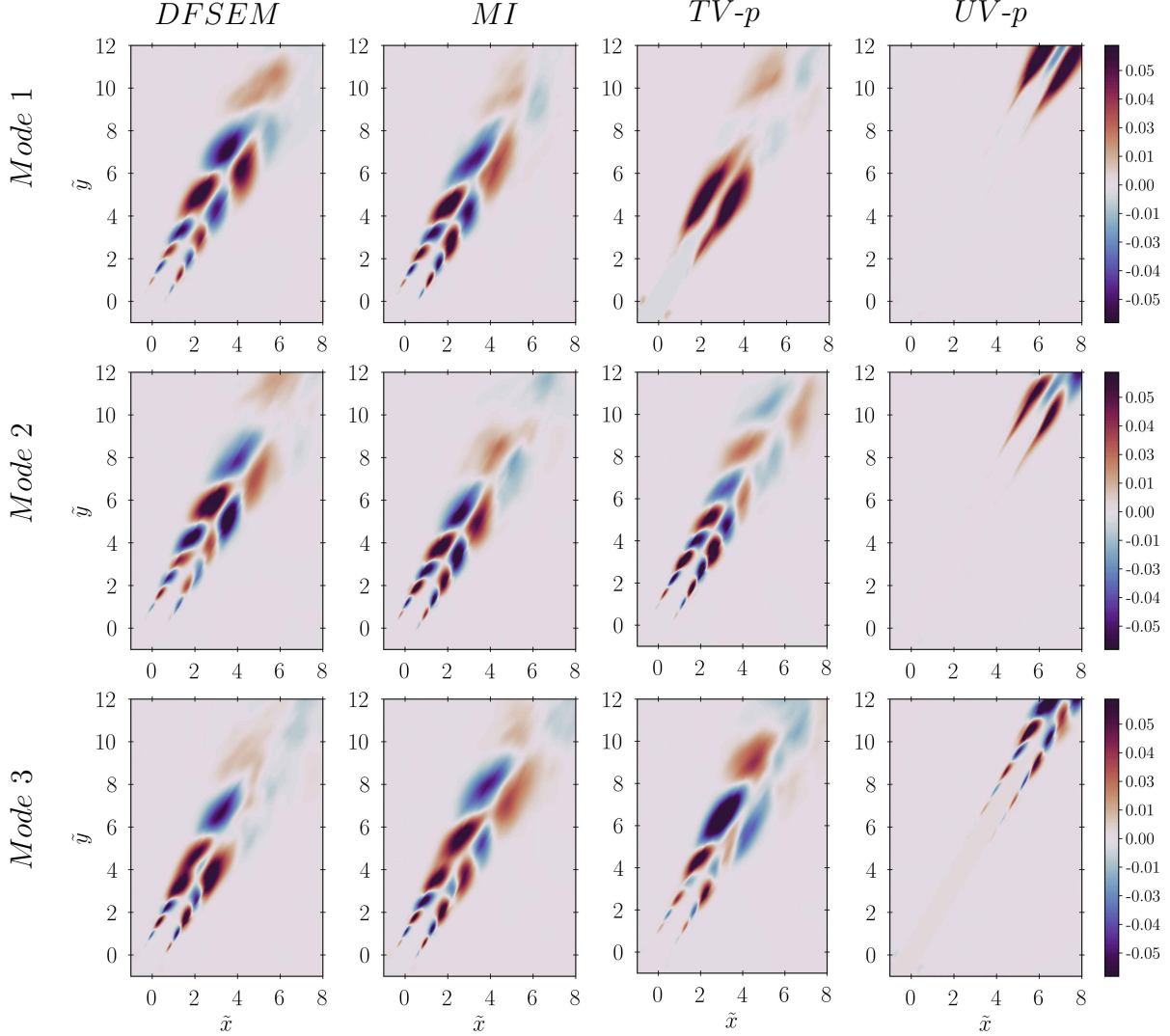


Figure 2.20: Spatial patterns of the first three POD modes for the explicit nozzle modeling cases (DFSEM, MI, TV-p, UV-p).

Figure 2.21 presents the first three POD modes for the implicit nozzle modeling cases, revealing notable differences in coherent structure across the boundary conditions. In Mode 1, the TV-np exhibits distinct, spatially periodic lobes of alternating sign aligned along the jet axis, indicative of a well-developed helical mode with strong coherence in the near and intermediate fields. These structures display clear azimuthal asymmetry, consistent with shear-layer instabilities driving large-scale vortical motion. The FDCV condition, by con-

trast, produces elongated, streamwise oriented regions of uniform sign with minimal lateral undulation, reflecting a more diffused scalar field and reduced three-dimensional vortex. The UV-np condition shows a combination of both tendencies, regions of elevated amplitude with partial axisymmetry, but lacking the regular lobe spacing characteristic of fully developed helical modes. In Mode 2, TV-np maintain its helical structure, though with slightly reduced amplitude and a shift of the dominant lobes downstream, suggesting persistence of large-scale coherent motion. The FDCV condition continues to display stretched, quasi-axisymmetric regions with minimal transverse variation, indicative of weakened azimuthal instability and diminished eddy formation. UV-np condition demonstrates irregular lobe compared to Mode 1, with greater downstream spread but less periodicity than TV-np. Mode 3 for the TV-np condition still displays coherent structures but weaker. The alternating lobe structure remains identifiable, albeit with reduced coherence and more pronounced attenuation in the far field. FDCV structures appear highly diffused, with no clear periodic arrangement, underscoring the limited ability of this condition to sustain organized coherent structures. UV-np displays a fragmented spatial pattern, with localized alternating regions interspersed with diffused zones, reflecting intermediate turbulence coherence and partial helical mode formation relative to the other cases.

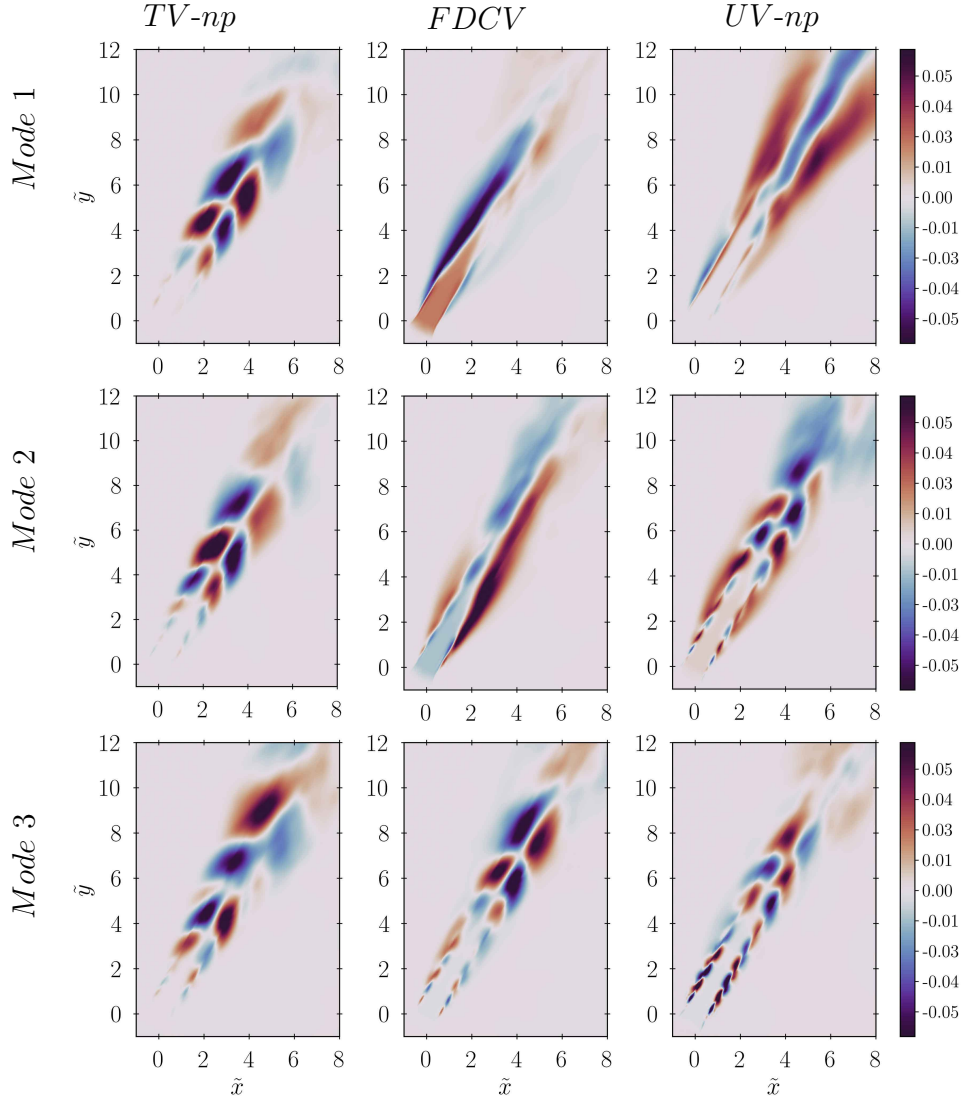


Figure 2.21: Spatial patterns of the first three POD modes for the implicit nozzle modeling cases (TV-np, FDCV, UV-np).

Figure 2.A9 represents the normalized magnitude of eigenvalues (λ) associated with the POD modes for all boundary conditions (refer to [123] for details of the calculation procedure). The eigenvalues quantify the relative energy content captured by each mode, providing a direct measure of the contribution of the corresponding spatial structures to the total variance of the concentration field. Higher eigenvalues in the leading modes indicate that a larger fraction of the flow's energetic content is concentrated in the dominant coherent structures, such as large-scale shear-layer instabilities or global column modes. Conversely, a more gradual decay of eigenvalues with increasing mode number suggests a broader distribution of energy across multiple scales, indicative of more complex, multi-scale turbulence. The vertical axis shows the normalized eigenvalues, indicating the proportion of total energy captured by each mode, while the horizontal axis denotes the mode number (n). The inlet boundary conditions TV-np, UV-np, and FDCV display significantly higher normalized eigenvalues in the first three modes, suggesting that the flow dynamics in these cases are dominated by

large-scale structures as shown in Figure 2.21. This behavior aligns with a scenario in which the inlet conditions develop an intermittent flow regime, concentrating energy in the lower modes. In contrast, the cases of DFSEM, MI, TV-p, and UV-p exhibit lower eigenvalues for the first mode and a more gradual decline across the higher modes. For the lower-order modes (modes 1 to 3), the UV-np case exhibits a higher eigenvalue in mode 1 and lower eigenvalues in modes 2 and 3 compared to other boundary conditions. This suggests that the UV-np inlet configuration results in reduced contributions from smaller-scale flow features, while the elevated eigenvalue in mode 1 indicates a dominant contribution from large-scale structures. The eigenvalue profiles for DFSEM, MI, and TV-p are elevated for modes beyond 2, indicating a greater contribution from smaller-scale flow structures. This suggests a more even distribution of energy across the modes, indicative of a more complex and turbulent flow structure. Under these boundary conditions, the flow field demonstrates greater variability, with smaller-scale structures contributing more significantly to the overall energy distribution. For higher modes ($n > 3$), the normalized eigenvalues converge towards lower values across all cases, suggesting that the finer, smaller-scale structures are captured by these modes. Despite the initial differences in the first few modes, the inlet boundary conditions show similar behavior in the higher modes, indicating that the higher-order flow structures are less sensitive to the inlet conditions and are likely associated with smaller, more isotropic turbulence features.

2.3.5 Geometrical characteristic of jet

Figure 2.22 compares the non-dimensionalized jet trajectories calculated using both explicit and implicit modeling methods, alongside various boundary conditions, against the experimental concentration data of [2]. DFSEM and MI show close alignment with the experimental data in both the initial rise and descent of the jet trajectory, while TV-p slightly underpredicts the trajectory. UV-p exhibits the most significant deviation, overpredicting the jet rise and failing to capture the descent phase accurately. All boundary conditions in the implicit modeling group deviate substantially from the non-dimensionalized experimental data. FDCV overpredicts both the rise and descent phases, while TV-np and UV-np underpredict the trajectory, showing notable discrepancies and failing to capture the jet's overall path. The underprediction of the trajectory by TV-np and UV-np has also been reported by [48] and [84], respectively.

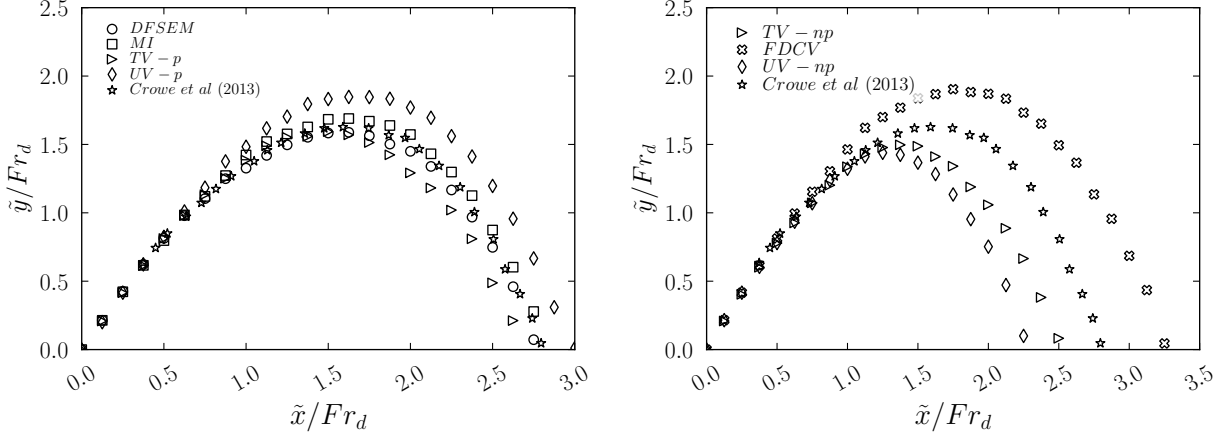


Figure 2.22: Comparison of the centerline trajectory of LES and experimental data of [2]. The left graph represents cases with explicit nozzle modeling, and the right graph shows cases with implicit nozzle modeling.

Table 2.4 provides a detailed comparison of numerical simulations using various boundary conditions against experimental data from different studies. The parameters considered include the centerline peak height ($\tilde{y}_m/Fr_d$), terminal rise height ($\tilde{y}_t/Fr_d$), return point ($\tilde{x}_r/Fr_d$), dilution at centerline peak ($\tilde{s}_m/Fr_d$), and dilution at the return point ($\tilde{s}_r/Fr_d$). It is evident that the MI and DFSEM boundary conditions align closely with experimental data, exhibiting minor deviations and thus indicating their performance in accurately capturing the jet trajectory. In contrast, the UV-p boundary condition significantly overestimates the trajectory parameters, suggesting a lower level of accuracy. The TV-p boundary condition, while demonstrating a performance close to that of MI and DFSEM, still shows a slight reduction in accuracy. For the implicit methods, the results show greater divergence. The FDCV boundary condition tends to overestimate most trajectory parameters, particularly the return point and horizontal spread. In contrast, the TV-np boundary condition underestimates these parameters, reflecting lower values than most explicit methods. Similarly, the UV-np boundary condition also underestimates trajectory parameters, though not as pronounced as the TV-np condition.

Table 2.4: Summary of numerical results compared with previous experimental data.

Inlet boundary condition	$\tilde{y}_m/Fr_d$	$\tilde{y}_t/Fr_d$	$\tilde{x}_r/Fr_d$	$\tilde{s}_m/Fr_d$	$\tilde{s}_r/Fr_d$
DFSEM	1.61	2.08	2.68	0.55	1.49
MI	1.65	2.25	2.79	0.58	1.57
TV-p	1.57	2.06	2.61	0.58	1.51
UV-p	1.85	2.49	3.03	0.76	2.27
TV-np	1.50	1.82	2.55	0.45	1.42
FDCV	1.91	2.44	3.26	0.82	2.50
UV-np	1.44	1.91	2.33	0.47	1.36
Crowe [2] (Exp., 60° , $Fr_d = 19.1$)	1.62	2.12	2.81	–	–
Oliver et al. [14]	1.61	2.21	2.76	0.42	1.55
Ferrari and Querzoli [128]	1.67	–	2.67	–	–
Kikkert [129]	1.76	2.45	2.67	–	–
Papakonstantis et al. [15, 38]	1.68	2.15	2.75	–	1.68

2.4 Discussion

To evaluate the performance of the applied inlet boundary conditions, two quantitative error metrics were employed, the root mean square error (RMSE), which captures the deviation between numerical predictions and PIV measurements; and the cross-correlation coefficient, which assesses the structural similarity of the velocity profiles, with particular emphasis on their shape. These metrics characterize both the numerical accuracy and the spatial coherence of the simulated velocity fields relative to the PIV data and are computed as follows [130, 131]:

$$RMSE = \sqrt{\frac{1}{N_e} \sum_{i=1}^{N_e} \left(\tilde{U}_i^{\text{sim}} - \overline{\tilde{U}^{\text{sim}}} \right)^2} \quad (2.16)$$

$$\text{cross-correlation} = \frac{\sum_{i=1}^{N_e} \left(\tilde{U}_i^{\text{sim}} - \overline{\tilde{U}^{\text{sim}}} \right) \left(\tilde{U}_i^{\text{PIV}} - \overline{\tilde{U}^{\text{PIV}}} \right)}{\sqrt{\sum_{i=1}^{N_e} \left(\tilde{U}_i^{\text{sim}} - \overline{\tilde{U}^{\text{sim}}} \right)^2} \sqrt{\sum_{i=1}^{N_e} \left(\tilde{U}_i^{\text{PIV}} - \overline{\tilde{U}^{\text{PIV}}} \right)^2}} \quad (2.17)$$

here, $\tilde{U}_i^{\text{sim}}$ and $\tilde{U}_i^{\text{PIV}}$ represent the time-averaged velocity values at the i^{th} spatial point, obtained from the simulation and PIV measurements, respectively. The variables $\overline{\tilde{U}^{\text{sim}}}$ and $\overline{\tilde{U}^{\text{PIV}}}$ denote the spatial averages of the corresponding time-averaged velocity profiles. The index i runs from 1 to N_e , where N_e is the total number of discrete sampling points across the profile.

Table 2.5 presents the RMSE and cross-correlation coefficient values across five locations of $\tilde{x} = 8, 10, 15$, the terminal rise, and the return point as reported in §2.3. Among all tested inlet boundary conditions, the MI and DFSEM boundary conditions demonstrate better performance in replicating experimental velocity profiles. As reported in Table 2.5,

both cases achieve consistently low RMSE values and high cross-correlation coefficients at all measured locations. At $\tilde{x} = 8$, DFSEM and MI yield RMSE values of 0.0478 and 0.0503, respectively, with corresponding cross-correlation coefficients of 0.9885 and 0.9875. This trend holds throughout the jet trajectory, with both methods preserving velocity magnitude and flow structure similarity to the PIV data. Notably, DFSEM slightly outperforms MI in the far field, particularly at $\tilde{x} = 15$, where it achieves the lowest RMSE of 0.0115 and highest correlation of 0.9991 among all cases. Despite their comparable performance in terms of accuracy, DFSEM and MI differ significantly in their implementation requirements and practical considerations. The MI approach is straightforward, it employs a precursor simulation to generate a statistically converged turbulent flow, which is subsequently mapped onto the inlet of the main domain. This method requires the application of a precursor pipe section to allow the imposed turbulence to evolve into a physically realistic inflow before entering the main computational domain. Some studies have suggested that a pipe length of at least $7.5d_0$ is typically sufficient for achieving statistically developed turbulence at the outlet [109, 132]. However, it is advisable to compare the evolving velocity and turbulence profiles within the pipe against high-fidelity reference data, such as available DNS benchmarks (e.g., [132]), in order to determine the appropriate development length for each specific simulation setup. While easy to set up, this additional pipe length increases the total domain size and computational cost. However, MI compatibility with standard OpenFOAM utilities and its ability to produce physically consistent turbulent inflow make it a robust choice for high-fidelity simulations. In contrast, the DFSEM condition employs a synthetic eddy generation technique that introduces coherent turbulent structures directly at the inlet without the need for a precursor simulation. This boundary condition requires configuration of turbulent quantities such as the Reynolds stress tensor, mean velocity, and length scale, as well as optional parameters like eddy count per cell and reference velocity. This added configuration complexity demands a more detailed understanding of the inflow turbulence characteristics and needs comparison with DNS data. Nevertheless, DFSEM offers greater computational efficiency by eliminating the need for an extended inlet pipe, making it advantageous for domains with space constraints or when computational resources are limited. Nevertheless, DFSEM offers better computational efficiency by eliminating the need for an extended inlet pipe, making it advantageous for domains with space constraints or when computational resources are limited. As recommended by [107, 111, 113, 133], a short pipe of approximately $3d_0$ to $10d_0$ is sufficient to allow eddy interaction and stabilization before entering the main domain. This reduced length is adequate because the DFSEM method discharge synthetic eddies at the boundary, bypassing the need for full flow development through an upstream section. In terms of overall cost-performance tradeoff, MI and DFSEM remain the most accurate boundary conditions tested in this study. However, when computational efficiency is prioritized over exact physical realism, the TV-np condition may serve as a reasonable alternative. Though it lacks detailed turbulent structure and exhibits higher RMSE in downstream regions, its implementation is straightforward and does not require precursor simulations or complex parameter tuning.

Table 2.5: Error metrics for time-averaged velocity of different boundary conditions compared to PIV.

Metric	Location	DFSEM	MI	TV-p	UV-p	TV-np	FDCV	UV-np
RMSE	$8d_0$	0.0478	0.0503	0.0895	0.2689	0.0943	0.1675	0.1239
	$10d_0$	0.0304	0.0313	0.0613	0.2311	0.0683	0.1547	0.1095
	$15d_0$	0.0115	0.0148	0.0498	0.1871	0.0506	0.0858	0.0814
	Terminal rise	0.0468	0.0452	0.0646	0.1948	0.1083	0.1160	0.1555
	Return point	0.0404	0.0549	0.0824	0.0878	0.1782	0.1599	0.2330
Cross-correlation	$8d_0$	0.9885	0.9875	0.9604	0.8268	0.9503	0.9415	0.9219
	$10d_0$	0.9934	0.9936	0.9707	0.8159	0.9412	0.9597	0.9163
	$15d_0$	0.9991	0.9972	0.9785	0.8149	0.9358	0.9323	0.8973
	Terminal rise	0.9512	0.9554	0.9472	0.9017	0.9134	0.9028	0.8887
	Return point	0.9565	0.9453	0.9487	0.9105	0.9231	0.9087	0.8728

A comparison between the TV-p and TV-np boundary conditions highlights the impact of explicit nozzle modeling on the turbulent inlet. Both conditions apply synthetic velocity fluctuations without inherent spatial or temporal coherence; however, the presence of the nozzle in TV-p approach provides a region for partial evolution of turbulent structures prior to entering the main domain. Consequently, TV-p demonstrates improved performance at certain downstream locations (e.g., at $\tilde{x} = 15$, RMSE=0.0498, cross-correlation=0.9785) relative to TV-np (RMSE=0.0506, cross-correlation=0.9358). As illustrated in Figure 2.6-b, TV-p supports the formation of small-scale turbulence within the inlet region, enhancing structural alignment with the DNS profiles. In contrast, TV-np lacks such a transitional zone, resulting in higher downstream RMSE and reduced correlation, indicative of weaker turbulence development. The UV-p, UV-np, and FDCV boundary conditions demonstrate significant limitations in reproducing the jet velocity field, as reflected by high RMSE and relatively low cross-correlation coefficients. Despite modeling the nozzle, UV-p yields the highest RMSE (0.2689 at $\tilde{x} = 8$) and consistently low cross-correlation (below 0.83 in the near field), indicating inadequate turbulence generation and delayed transition from laminar inflow conditions. This deficiency results in geometrically excessive jet spreading, as observed in Table 2.4. UV-np shows marginally better near-field accuracy (RMSE of 0.1239 at $\tilde{x} = 8$) but fails downstream due to insufficient shear-layer instability development. Similarly, FDCV, while imposing a fully-developed velocity profile, does not incorporate turbulent fluctuations; consequently, it achieves slightly improved initial performance (cross-correlation of 0.9415 at $\tilde{x} = 8$) but deteriorates downstream, exhibiting elevated RMSE (0.1599) and decreased correlation (0.9087) at the return point.

The performance of the UV-p, UV-np, and FDCV boundary conditions reveals their inability to reproduce the velocity field with acceptable accuracy across the jet domain. Despite the inclusion of a pipe in UV-p, the boundary condition yields the highest RMSE values among all configurations, reaching 0.2689 at $\tilde{x} = 8$ and remaining elevated throughout the domain. This deficiency is also reflected in the geometrical characteristics of the jet, as presented in Table 2.4, where UV-p results in overestimated spreading due to its inability to generate or sustain realistic turbulent structures. The corresponding cross-correlation coefficients remain below 0.83 in the near field and do not exceed 0.92 in any location. These results indicate

that the presence of a nozzle does not compensate for the fundamental limitation of UV-p, namely its imposition of a uniform velocity profile with no synthetic fluctuations or eddy content. As a result, the flow remains largely laminar upon entering the domain. UV-np, which also prescribes a uniform velocity profile but without a pipe, exhibits slightly improved accuracy in the near field, achieving an RMSE of 0.1239 at $\tilde{x} = 8$ compared to 0.2689 for UV-p. However, the absence of both a turbulent inflow and a transitional region severely limits its ability to generate shear-layer instabilities. Consequently, performance declines downstream, with an RMSE of 0.2330 and a correlation coefficient of just 0.8728 at the return point. FDCV presents a distinct but similarly limited case. This approach prescribes a fully developed velocity profile, assuming equilibrium turbulence conditions at the inlet. However, this steady-state approximation fails to introduce dynamic fluctuations or coherent turbulent structures necessary for shear-layer growth. Although FDCV performs slightly better than UV approaches in the near field, with a cross-correlation of 0.9415 at $\tilde{x} = 8$, its RMSE remains high throughout the domain, and its performance degrades significantly downstream (e.g., RMSE = 0.1599 and correlation = 0.9087 at the return point). All three boundary conditions, UV-p, UV-np, and FDCV, demonstrate substantial limitations due to their failure to introduce physically meaningful turbulent structures. Whether due to the absence of fluctuations (UV-p, UV-np) or the imposition of fixed turbulent properties (FDCV), these methods fall short in reproducing the amplitude and spatial structure of the jet, emphasizing the need for dynamic and physically consistent inflow strategies such as DFSEM and MI.

The studies summarized in Table 2 of [82] report a considerable variation in experimental results for an identical jet configuration (e.g., a 60-degree negatively buoyant jet). For instance, terminal rise values span from 2.08 to 2.86, and return point (or impact point) values range from 2.67 to 3.70. This wide range of dense jet characteristics in experimental data implies that numerical simulations even obtained under unsuitable modeling approaches, such as inadequate mesh resolution, low order numerical schemes, or improper inlet boundary conditions, may still agree with certain experimental datasets. Therefore, validation of a numerical simulation cannot rely only on comparison of geometrical jet characteristics, such as terminal rise or return point. A robust inlet boundary condition that preserves the physical realism of the resolved turbulent structures in LES of dense jets is essential for accurately capturing the jet physics.

2.5 Conclusion

This study compared LES results with high-resolution PIV to investigate the impact of different inlet boundary conditions on the performance of LES for 60-degree desalination discharges. The inlet boundary conditions of UV, MI, DFSEM, TV, and FDCV were evaluated for both explicit and implicit nozzle modeling approaches. The results demonstrate the importance of application of physically realistic inlet boundary condition in accurately capturing the jet dynamics and mixing behavior for a reliable numerical modeling approach of desalination discharge systems.

For the explicit nozzle modeling cases, the normalized time-averaged velocity and turbulence statistics of the pipe were compared against reference DNS data. The MI and DFSEM

boundary conditions showed the best performance in capturing the time-averaged velocity and turbulence statistics in the pipe (i.e., nozzle). In contrast, the UV and TV boundary conditions were unable to generate realistic flow in the pipe and showed large deviations from the DNS data. In the dense jet simulations using the explicit nozzle approach, the normalized time-averaged velocity, turbulent kinetic energy (TKE), and Reynolds stress components ($\tilde{u}'\tilde{u}'$, $\tilde{v}'\tilde{v}'$) were compared with PIV measurements. The MI and DFSEM cases provided the closest match to the PIV data, with DFSEM performing marginally better overall. The TV-p case reproduced the general flow features with only minor discrepancies, whereas UV-p consistently underestimated all metrics, showing large errors in velocity, TKE, and Reynolds stresses. Time-averaged concentration fields from the explicit nozzle simulations revealed that MI, DFSEM, and TV-p produced similarly broad distributions, indicative of effective scalar spreading, while UV-p generated a narrower jet distribution near the nozzle. In terms of concentration fluctuations ($\tilde{c}'\tilde{c}'$), MI, DFSEM, and TV-p displayed higher fluctuation intensities consistent with well-developed turbulent mixing, whereas UV-p exhibited weaker scalar variability. The TV-np condition showed the most accurate predictions of time-averaged velocity and turbulence statistics, closely matching the PIV reference among the implicit nozzle modeling cases. UV-np and FDCV showed significant discrepancies from the PIV data. A similar pattern was observed for TKE and Reynolds stresses for the TV-np case, while UV-np and FDCV underestimated both the magnitude and radial extent of turbulence. Similarly, concentration fields from the implicit cases showed TV-np producing broader concentration and fluctuation profiles, whereas UV-np and FDCV yielded weaker and more confined concentration distributions. POD was applied to the scalar concentration field to extract the first three modes and evaluate the influence of different inlet boundary conditions on the spatial coherent structures. MI and DFSEM boundary conditions generated alternating helical structures periodically along the jet axis, indicative of large-scale coherent structures that govern turbulent entrainment and mixing. These results reflected the ability of MI and DFSEM to replicate realistic physical mechanisms responsible for scalar transport in buoyant turbulent jets. TV-p and TV-np conditions also captured large-scale structures, albeit with reduced spatial coherence and more diffuse mode shapes, indicating partial diffusion of turbulent structures. In contrast, the coherent structures generated by UV-p, UV-np, and FDCV conditions were predominantly diffused and did not form the expected lobe patterns associated with shear-layer instabilities. The jet trajectory and dilution of MI, DFSEM and TV-p boundary conditions showed a close agreement with the experimental data of [2], while the UV-p condition overestimated the trajectory and dilution of the jet. For the implicit method, UV-np and TV-np underestimated the trajectory, whereas FDCV had a significant overestimation of trajectory and dilution.

This study provided a nondimensionalization framework that facilitates the numerical simulation of dense jets, reduces input related errors, and improves numerical stability. By formulating the simulations independently of specific physical scales, the proposed framework enhances the generality and applicability of the results. Based on the findings, the MI and DFSEM boundary conditions are recommended for LES of dense jets, while TV-p and TV-np are acceptable alternatives when configuration or computational limitations prevent the use of the former. Future studies should perform comprehensive DNS of dense jets to establish consistent and comparable reference values for various jet configurations as the current body of literature is not uniform for different jet configurations. Additional studies

should explore other applicable inlet boundary conditions for LES, such as digital filters or direct values obtained from DNS studies, to examine their impact on dense jet dynamics. Furthermore, future work should be focused on accurately quantifying time-averaging uncertainties [134, 135] as well as detailed assessment of uncertainties in the LES and PIV experiments of dense jets [136].

Acknowledgments

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Data Availability

The solver, Gmsh mesh generation script, and a simple example of the non-dimensional modeling approach developed in this study are publicly available at the following link: https://github.com/HydroCFD/buoyant_jet. This repository provides the necessary tools to reproduce the simulation setup and facilitates the application of the proposed methodology in related studies.

Nomenclature

Symbol

C_0	Jet initial constant concentration ($= 1$)
C_w	Model constant
D	Diffusivity coefficient
Fr_d	Densimetric Froude number
L_{mapped}	Mapped length
N	Number of synthetic eddies
N_e	Number of sampling points across the velocity profile
R	Pseudo-random number
Re	Reynolds number
S_{ij}^d	Deviatoric part of strain rate tensor
S_{ij}	Resolved strain tensor
Sc	Schmidt number
U_0	Jet velocity
$\langle \tilde{U}^{\text{PIV}} \rangle$	Spatial averaged of PIV normalized velocity profile
$\langle \tilde{U}^{\text{sim}} \rangle$	Spatial averaged of simulated normalized velocity profile
$\tilde{U}_c$	Centerline velocity
$\tilde{U}_{\text{center}}$	Maximum of velocity along the jet centerline
$\tilde{U}_i^{\text{sim}}$	Normalized streamwise velocity from simulation at point i
$\tilde{c}, \tilde{c}_c$	Salinity concentration, centerline value
c_{tv}	Heuristic correction term
d_0	Jet diameter
d_k	Magnitude of r_k
$\delta\tilde{U}$	Nondimensional velocity uncertainty
e_{gi}	Direction of gravity acceleration
g	Gravitational acceleration
l_p	Pipe length
l_x, l_y, l_z	Domain size in x, y and z directions
n	Time level
$\tilde{p}$	Pressure
r	Radial distance measured perpendicular to the jet centerline
r_{kj}	Normalized distance vector to k^{th} eddy
s	Fluctuation scale
s_m, s_r	Dilution at peak and return point
$\tilde{t}$	Nondimensional time
u	Velocity magnitude
$u'_\beta(x)$	Fluctuating velocity at position x in direction β
u'^+_{rms}	RMS of velocity fluctuation in x-direction
u_τ	Friction velocity
u_{ref}	Mean velocity
$\tilde{u}_i$	Nondimensional velocity in direction i
v'^+_{rms}	RMS of velocity fluctuation in y-direction
w'^+_{rms}	RMS of velocity fluctuation in z-direction
x_k	Position of k^{th} eddy
x_m, x_r	Horizontal distances of centerline peak (or terminal rise), and return point
y^+	Wall distance
y_d	Distance of the first off-wall cell center from the wall
y_m, y_t	Vertical distance of centerline peak, and terminal rise

Greek Symbol

α	Scalar for temporal correlation
α_l^k	Intensity of k^{th} eddy in l^{th} direction
β	Direction index
Δ	Spatial filter width
Δy	Grid spacing in y-direction
$\epsilon^{\beta j l}$	Levi-Civita symbol
λ	Normalized eigenvalues
ν	Kinematic viscosity
ν_{SGS}	SGS eddy viscosity
ρ_0	Jet fluid density
ρ_a	Ambient fluid density
σ_β^k	Eddy length scale in β^{th} direction
$\tilde{\tau}_{ij}$	Subgrid-scale stress tensor

Abbreviations

CFL	Courant-Friedrichs-Lewy number
DFSEM	Divergence Free Synthetic Eddy Method
DNS	Direct Numerical Simulation
FDCV	Fully Developed Constant Velocity
LES	Large Eddy Simulation
MI	Mapped Inlet
OpenFOAM	Open Source Field Operation and Manipulation
PIV	Particle Image Velocimetry
POD	Proper Orthogonal Decomposition
RANS	Reynolds-Averaged Navier Stokes
RMS	Root Mean Square
RMSE	Root Mean Square Error
SGS	subgrid-scale
TKE	Turbulent Kinetic Energy
TV	Turbulent Velocity
UV	Uniform Velocity
WALE	Wall-Adapting Local Eddy-viscosity

Appendix - A

Figure 2.A1 presents the spatial distribution of the time-averaged LES_{index} for the MI case, serving as a quantitative measure of the fraction of turbulence energy resolved by the LES. Values approaching unity indicate a high degree of resolution of the turbulent eddies, whereas lower values correspond to regions where subgrid-scale contributions are more significant. The contour reveals that the core and shear-layer regions of the jet maintain LES_{index} values above 0.95, confirming that the large-scale turbulent structures are predominantly resolved. The profiles along Lines 1-4 further confirm the high resolution of the applied mesh, showing the radial variation of LES_{index} and revealing small drops in resolution within the shear layers, where strong velocity gradients and intense mixing occur.

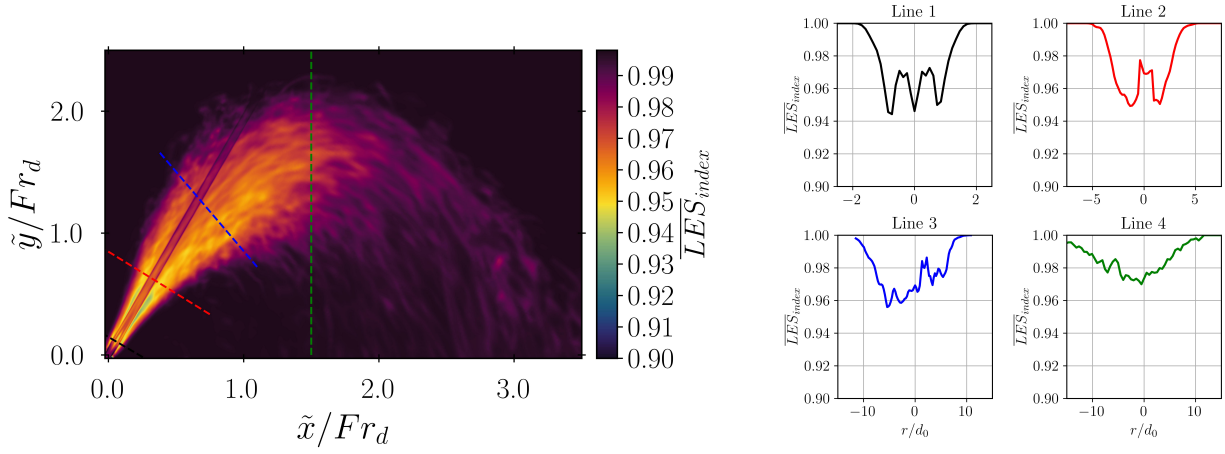


Figure 2.A1: Time-averaged LES_{index} for the case MI.

Figure 2.A2 compares the present LES and PIV measurements at the terminal rise location with the experimental dataset of Crowe [2], which has a $Fr \approx 19$ comparable to the present study but a different Re . In the Crowe [2] PIV, the radial coordinate is normalized by b , defined as the radial distance from the centerline to the location where the axial velocity component in the cross-section drops to $e^{-1}U_c$. Therefore, to enable a direct comparison, the present dataset was also normalized using b following the same definition. The dataset of Crowe [2] represents the only available PIV measurement for a 60° inclined dense buoyant jet that reports velocity profiles exclusively at the terminal rise, without measurements at other locations along the jet trajectory. Despite these differences in Re , the present PIV measurements show strong agreement with Crowe [2], supporting the reliability and validity of the current PIV measurement.

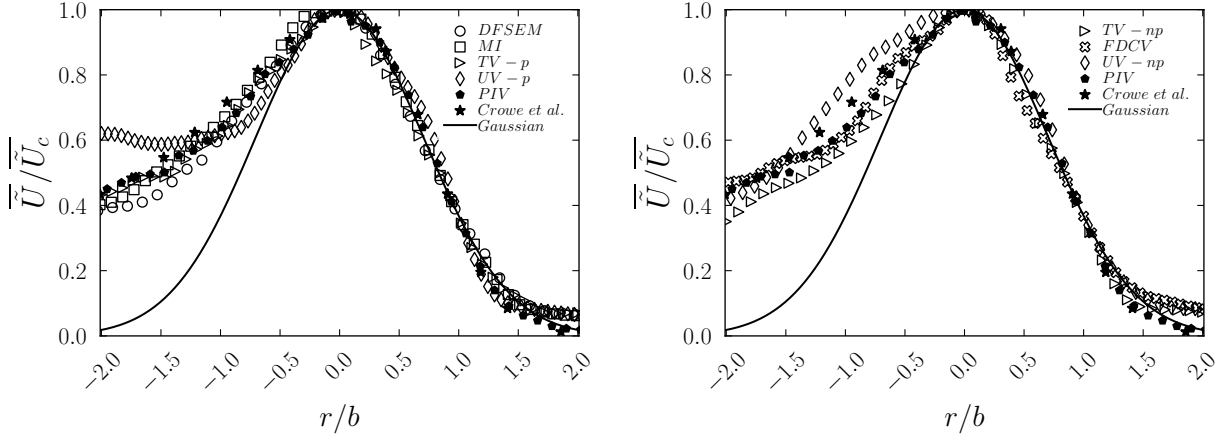


Figure 2.A2: Distribution of normalized time-averaged velocity profiles $\tilde{U}/\tilde{U}_c$ at terminal rise.

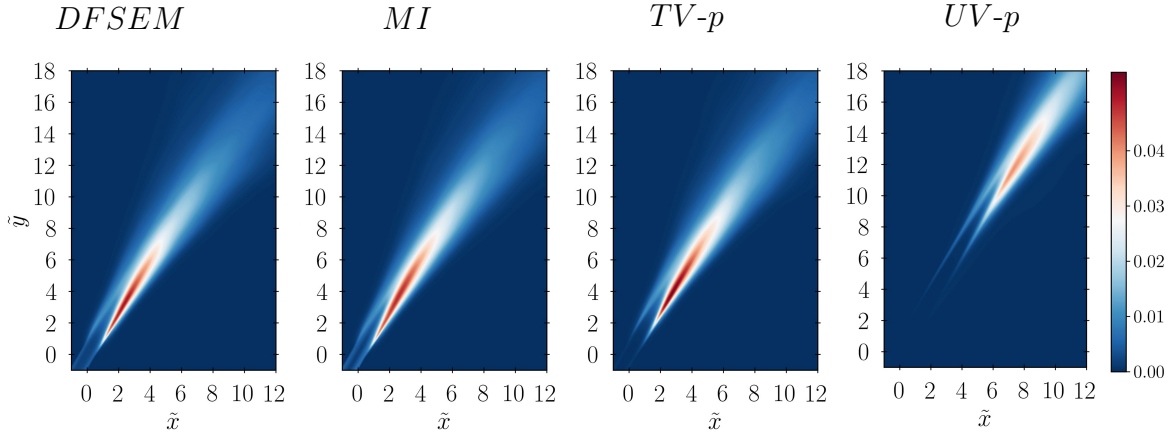


Figure 2.A3: Near-field distribution of the time-averaged velocity fluctuations $\tilde{u}'\tilde{u}'$ for cases with explicit nozzle modeling using various boundary conditions (DFSEM, MI, TV-p, UV-p).

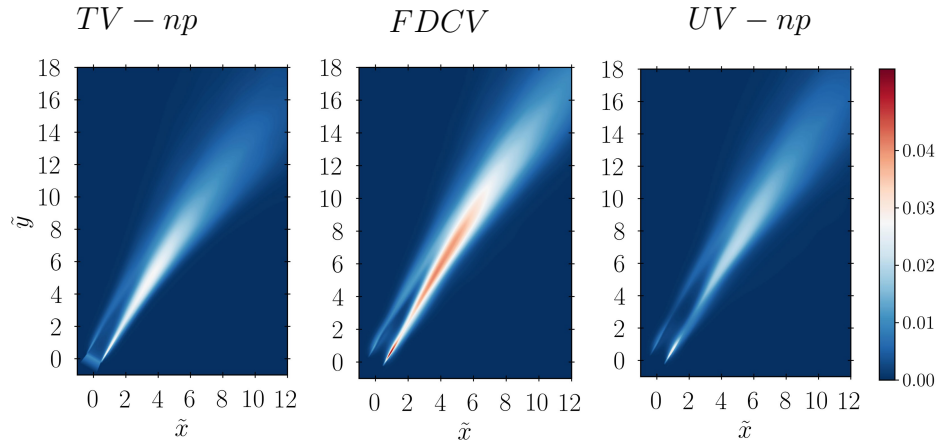


Figure 2.A4: Near-field distribution of the time-averaged velocity fluctuations $\tilde{u}'\tilde{u}'$ for cases with implicit nozzle modeling using various boundary conditions (TV-np, FDCV, UV-np).

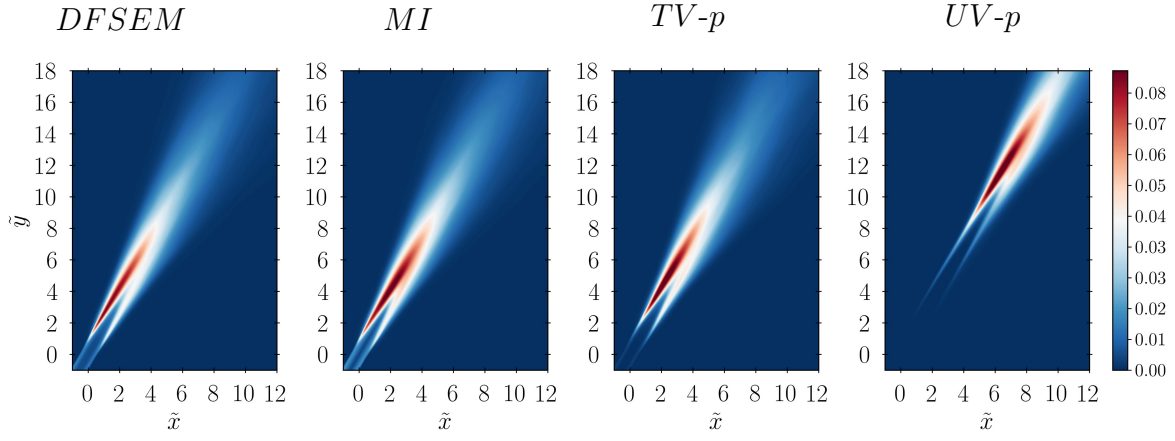


Figure 2.A5: Near-field distribution of the time-averaged velocity fluctuations $\overline{\tilde{v}'\tilde{v}'}$ for cases with explicit nozzle modeling using various boundary conditions (DFSEM, MI, TV-p, UV-p).

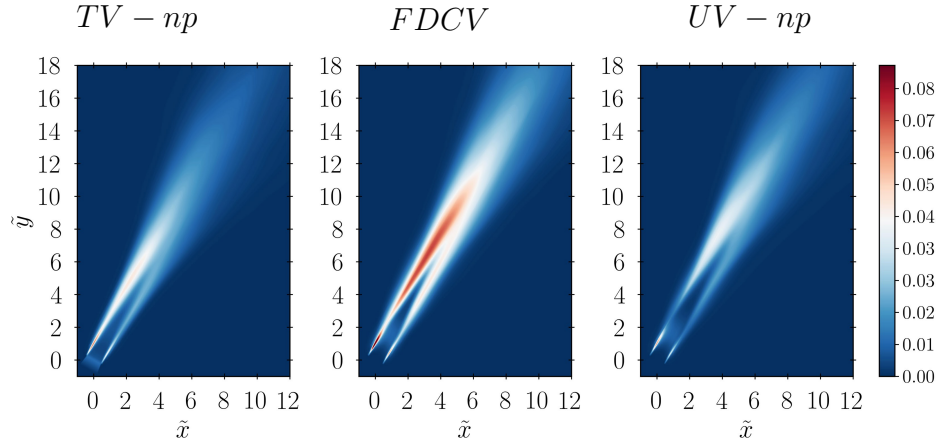


Figure 2.A6: Near-field distribution of the time-averaged velocity fluctuations $\overline{\tilde{v}'\tilde{v}'}$ for cases with implicit nozzle modeling using various boundary conditions (TV-np, FDCV, UV-np).

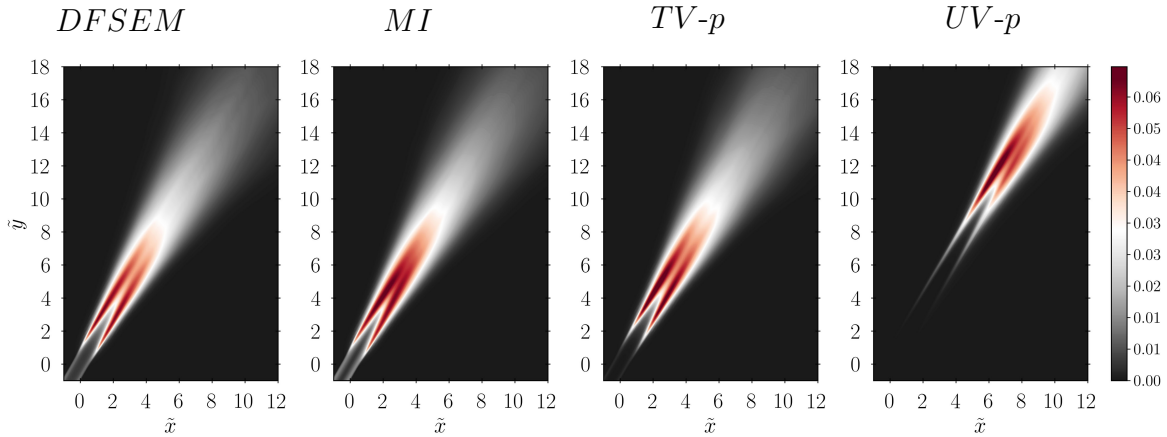


Figure 2.A7: Near-field distribution of time-averaged turbulent kinetic energy (TKE) for cases with explicit nozzle modeling using various boundary conditions (DFSEM, MI, TV-p, UV-p).

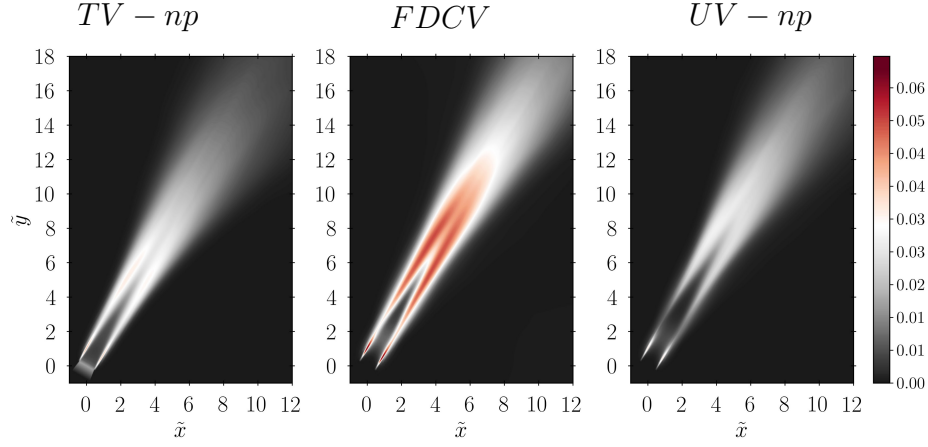


Figure 2.A8: Near-field distribution of time-averaged turbulent kinetic energy (TKE) for cases with implicit nozzle modeling using various boundary conditions (TV-np, FDCV, UV-np).

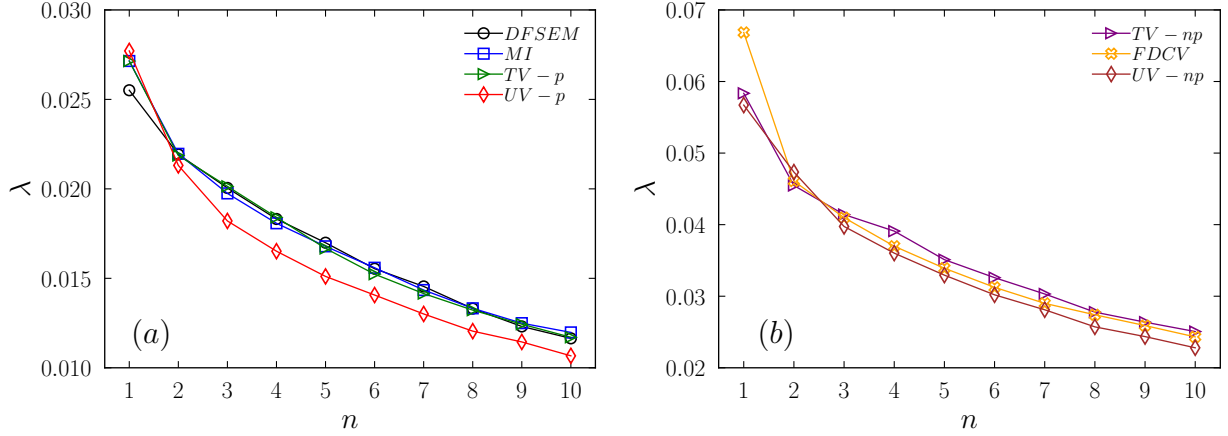


Figure 2.A9: Normalized eigenvalues of the first ten POD modes for cases with: (a) implicit nozzle modeling using various boundary conditions (TV-np, FDCV, UV-np), and (b) explicit nozzle modeling using various boundary conditions (TV-p, FDCV, UV-p).

Appendix B. Estimation of PIV measurement uncertainty

The accuracy and reliability of PIV measurements are governed by a range of uncertainty sources that originate from both the experimental apparatus and the post-processing methodology. In this study, planar PIV with dual-camera acquisition was employed, and the velocity fields were obtained using correlation-based algorithms implemented in DaVis (LaVision GmbH). Several factors contribute to measurement uncertainty, including particle-related issues such as out-of-plane motion and local fluctuations in seeding concentration, despite using neutrally buoyant tracer particles provided by the manufacturer. On the illumination

side, imperfections in laser sheet uniformity and minor pulse timing variations may introduce spatial inconsistency in the recorded particle displacements. Limitations in imaging performance, such as sensor noise, optical aberrations, and focus imperfections, can further reduce the fidelity of the captured images. During data processing, choices related to interrogation window configuration, sub-pixel peak detection, and the handling of spurious vectors influence the precision of the final velocity field. In the present study, all relevant sources of uncertainty were systematically addressed through careful experimental design and parameter control. The laser sheet thickness and alignment were optimized to ensure uniform illumination, and synchronization hardware was used to maintain precise pulse timing. The imaging system was calibrated to minimize optical distortions, and high-resolution sensors with appropriate lens configurations were selected to enhance image quality. Particle seeding was adjusted to maintain adequate density throughout the measurement domain, while multi-pass window deformation, robust validation criteria, and correlation peak fitting techniques were applied to enhance vector accuracy. Through these combined measures, the influence of uncertainty on the final velocity field was significantly reduced, ensuring the reliability of the experimental data and its suitability for comparison with high-fidelity numerical simulations. All experimental procedures and processing settings were configured according to LaVision's technical guidelines and best practices⁷.

The uncertainty of the PIV velocity fields was estimated using the correlation statistics method proposed by [137, 138] and implemented in the DaVis software (LaVision GmbH). This technique quantifies the local asymmetry of the cross-correlation peak by analyzing residual intensity mismatches between the original and dewarped particle images, enabling a vector-wise estimation of displacement uncertainty. As a nonintrusive, a posteriori method, it is applicable to any PIV dataset and does not require synthetic calibration images or ensemble statistics. A comprehensive description of the methodology and its validation can be found in [137–139]. Figure 2.B1 illustrates the time-averaged nondimensional velocity uncertainty ($\delta\tilde{U} = \delta U/U_0$) fields stemming from the post-processing procedures applied to the PIV measurements. Figure 2.B1 - a shows the uncertainty profiles at three locations of $x/d_0 = 8, 10$, and 15 in the near field. These sections correspond to the developing region of the jet, where shear layers and out-of-plane motion contribute to increased uncertainty. The peak uncertainty reaches approximately 4×10^{-3} m/s, with broader distributions observed farther downstream as the jet evolves. Figure 2.B1 - b presents the distribution of velocity uncertainty at the terminal rise of the jet, where the jet reaches its maximum vertical location before transitioning to downward motion. A pronounced peak is observed near the centerline, indicating a localized region of higher uncertainty associated with vertical deceleration and increased flow instability at this stage of the jet's trajectory. Figure 2.B1 - c shows the uncertainty profile at the return point, where the jet momentum has significantly decayed. As expected, the uncertainty levels are lower and relatively uniform across the span, reflecting more stable flow conditions and reduced velocity gradients. These profiles illustrate the spatial variation in post-processed measurement uncertainty and provide a quantitative indication of the local reliability of the PIV data throughout the jet's development.

⁷<https://www.lavision.de/en/downloads/manuals/>

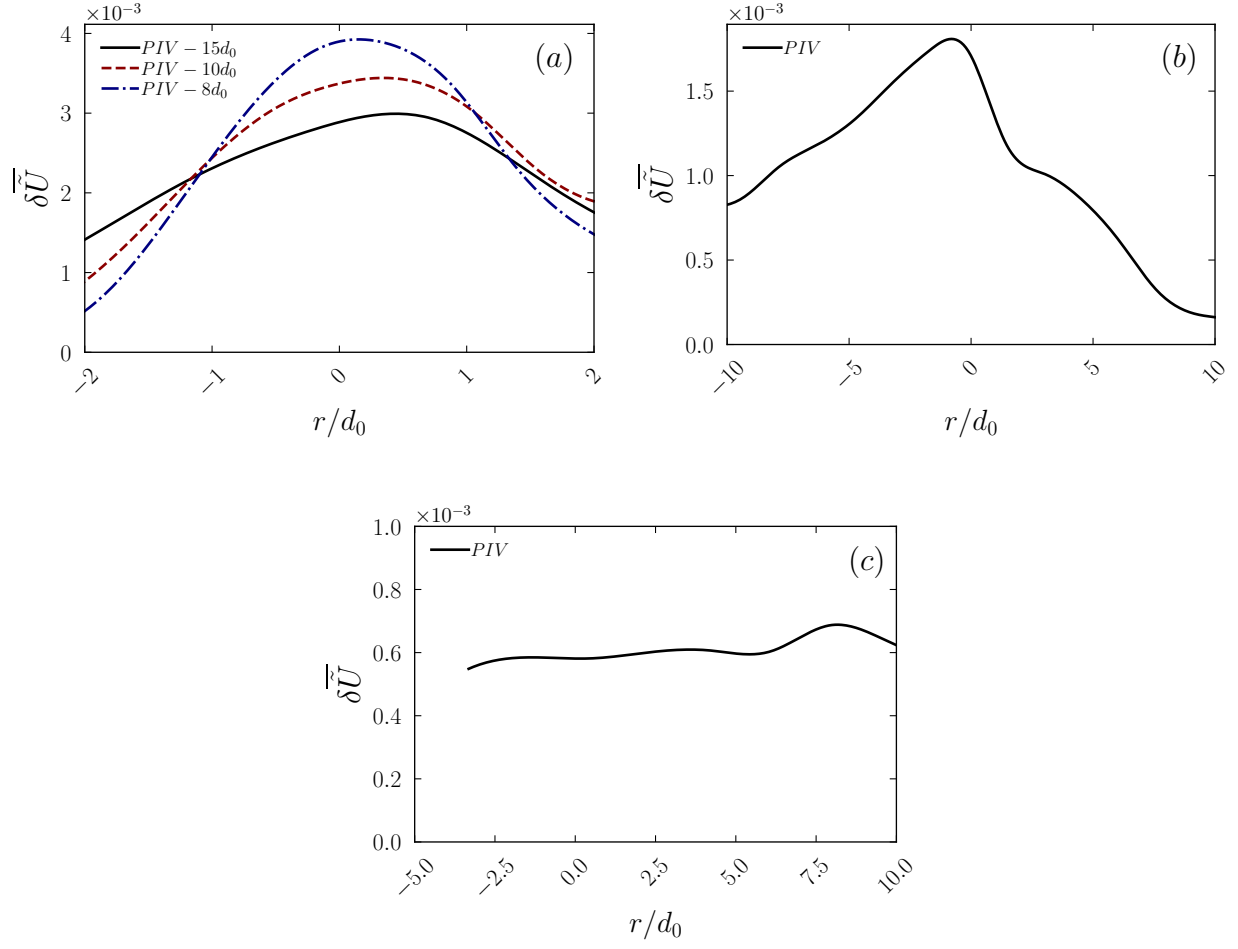


Figure 2.B1: Time-averaged normalized velocity uncertainty obtained from DaVis post-processing (a) cross-section at $x/d_0 = 8, 10, \text{ and } 15$; (b) terminal rise; (c) return point.

Chapter 3

Numerical Simulation of Negatively Buoyant Jets in Stratified Crossflow

3.1 Introduction

Buoyant jets are observed in both natural environments, e.g., volcanic eruptions and cumulonimbus convection in the atmosphere, and a diverse range of industrial applications, e.g., building ventilation systems, electronic component cooling, chimney smoke dispersion, and the discharge of brine, heated water from desalination plants, or treated wastewater from sewage treatment facilities [60, 62–69, 140, 141]. The release of waste through jets is engineered to efficiently mix the waste with the ambient, ultimately mitigating potential environment impacts [142]. A buoyant jet is formed by the steady release of a volume of fluid with a density of ρ_0 into an environment with a different density of ρ_a through outlets (e.g., orifices, nozzles, or cracks) [143, 144]. The dynamics of buoyant jets are shaped by the interplay between momentum and buoyancy forces, stemming from the differences in density between the source fluid and the receiving fluid. This complex interaction categorizes buoyant jets into either negative or positive, based on the direction of the buoyancy force relative to the jet’s momentum. A positively buoyant jet is formed when the buoyancy force acts in the same direction as the jet’s momentum, while a negatively buoyant jet is formed when the buoyancy force opposes the jet’s initial momentum [145]. While the Reynolds number, densimetric Froude number, and release angle are primary parameters governing the behavior of a buoyant jet, the characteristics of the receiving environment into which the jet is discharged also play a significant role in shaping its dynamics [146–151]. Therefore, understanding the impact of ambient conditions on buoyant jet dynamics and mixing processes is essential.

The interaction between a buoyant jet and non-stratified uniform crossflow has been extensively studied in various engineering and environmental applications [34, 50, 152–158]. The jet in a stratified crossflow is expected to result in a more complex dynamic compared to a homogeneous ambient [3, 147, 159–167]. The current body of literature predominantly concentrates on the investigation of buoyant jets discharged into non-stratified crossflow environments, with extensive studies utilizing experimental and numerical approaches to examine positive and negative buoyant jet trajectory and mixing characteristics (e.g., [12, 16, 20, 25, 151, 168]). However, the effects of crossflow stratification on jet trajectory, the locations of terminal rise and return points, and dilution of the jet remain poorly understood, especially under different

stratification intensities and discharge configurations. Several theoretical and mathematical models have been developed to advance the understanding of buoyant jet dynamics in both stagnant and crossflow environments. Fan and Brooks [169] provided analytical solutions for different types of turbulent buoyant jets under uniform and stratified ambient conditions. Their work was extended by Bemporad [170], who introduced a model incorporating the effects of crossflow velocity and stratification. Further developments include models by Schatzmann [171] and Jirka [172], which account for submerged jets and three-dimensional behavior using conservation equations and entrainment formulations. Papanicolaou et al. [173] adapted existing integral models for negatively buoyant jets in stratified environments, highlighting the role of entrainment coefficients in improving dilution predictions. Additional contributions by Mehaddi et al. [174] and Sarasua et al. [175] focused on vertical fountains, offering analytical expressions and identifying collapse conditions in linearly stratified ambient settings.

Gungor and Roberts [176] investigated turbulent vertical dense jets in crossflow using three-dimensional laser-induced fluorescence. Their results showed that jet behavior is governed by the velocity ratio of crossflow to jet (R) and the densimetric Froude number (Fr_d). Ben Meftah et al. [177] examined the hydrodynamic behavior of dense jets in shallow crossflow, with a focus on mixing processes. Experimental observations revealed structures of vortex associated with ascent and descent phases. In another study, Ben Meftah and Mossa [178] investigated the turbulence characteristics of a dense jet in crossflow, including jet trajectory, turbulence intensity, turbulent kinetic energy, and dispersion coefficients. By introducing a new trajectory scaling, the study highlights the anisotropic nature of the jet flow and its impact on dispersion behavior. Wright [179] analyzed the maximum and equilibrium heights of vertical jets discharged into a linearly stratified crossflow and proposed analytical approximations to estimate the maximum rise and the corresponding minimum dilution. The experimental study by Roberts and Matthews [180] revealed that jets discharged horizontally into a linearly stratified fluid undergo an initial growth phase followed by a sudden vertical collapse, forming horizontal density currents. The findings suggest that the collapse of the jet occurs when the time scale of the entraining eddies near the jet's edge becomes comparable to the buoyancy period. This phenomenon is believed to be associated with the dissipation of energy through internal waves. Yan et al. [74] numerically studied the dynamics of inclined jets in a linearly stratified environment. Their Reynolds-averaged Navier Stokes (RANS) model provided acceptable predictions for the variables of interest. New empirical functions were derived from dimensional analysis, providing a framework for estimating important parameters for jets discharged into a linearly stratified stagnant ambient.

Previous studies have primarily focused on buoyant jets in homogeneous ambient environments. However, the combined influence of crossflow parameters, including stratification intensity and velocity, on the trajectory, geometric evolution, and mixing behavior of negatively buoyant jets remains insufficiently understood. Advancing this understanding is essential for reliable environmental assessments and for the effective design and optimization of discharge systems. This study addresses this knowledge gap by applying high-resolution Large Eddy Simulation (LES) to systematically examine the influence of key nondimensional parameters of the densimetric Froude number (Fr_d), the crossflow-to-jet velocity ratio (R), and the stratification intensity ($\tilde{N}$). Unlike prior work that has focused on isolated effects or simplified conditions, this investigation covers a broad and structured parametric space, en-

abling a comprehensive analysis of how these factors govern jet dynamics dilution efficiency, and scalar transport in linearly stratified environments. The LES approach is selected for its ability to capture unsteady turbulent structures and coherent jet behavior, which are critical in accurately resolving mixing in stratified flows. Validation against physical models confirms the reliability of the numerical framework. The structure of this paper is as follows: §3.2 outlines the numerical methodology, §3.3 presents and interprets the simulation results, and §3.4 summarizes the key findings and implications for environmental flow modeling.

3.2 Methodology

Figure 3.1 illustrates a schematic of a negatively buoyant jet discharged into a linearly stratified crossflow. A negatively buoyant jet discharged into a stratified crossflow undergoes four distinct dynamic phases: ascent, descent, fluctuating, and stabilization. In the ascent phase, the jet momentum dominates over the downward buoyancy force, driving the jet upward into the crossflow. As the jet rises, it gradually decelerates and reaches a terminal height, denoted by $\tilde{y}_t$. The crossflow imposes a transverse force that deflects the jet from its initial vertical trajectory, resulting in a horizontal displacement of the terminal rise point, defined by $\tilde{x}_t$. In the descent phase, the buoyancy force becomes dominant, causing the jet to bend downward. The descending jet continues to decelerate until the upward buoyancy force from the ambient stratification counteracts the motion, marking the return point at a vertical location $\tilde{y}_r$ and a horizontal distance $\tilde{x}_r$ from the jet. During the fluctuating phase, the interaction between the ambient and jet buoyancy forces creates a fluctuating flow pattern. This flow pattern arises from the continuous mixing of the jet with the ambient flow. The height corresponding to the second terminal rise in the upward motion is indicated by $\tilde{y}_r^*$.

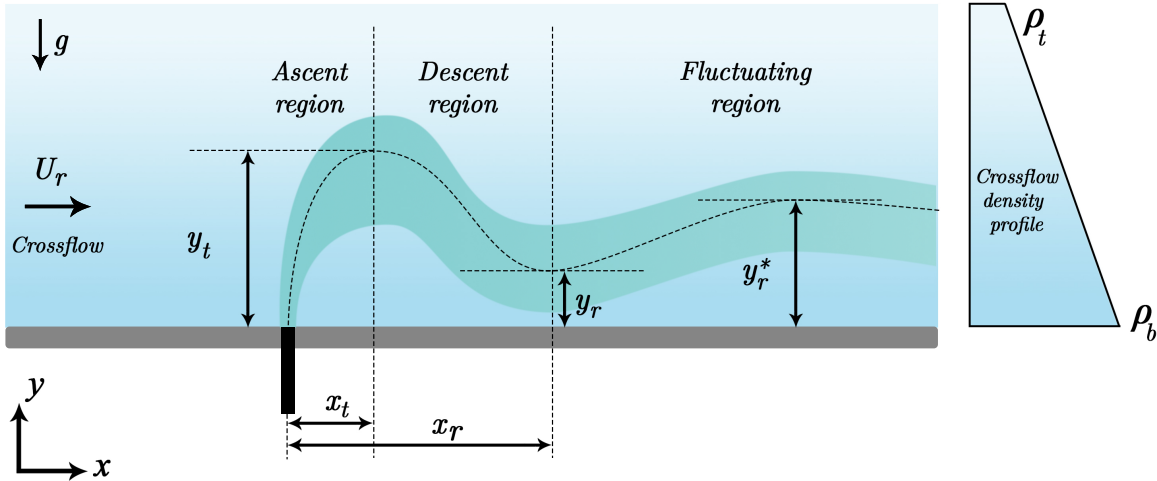


Figure 3.1: Schematic representation of a negatively buoyant jet discharged perpendicularly into a linearly stratified crossflow. (Note: All geometric characteristics are based on the centerline of concentration.)

In the final phase, progressive mixing of the jet with the crossflow reduces the jet's density

until it equilibrates within a layer of comparable crossflow density. At this stage, a balance is achieved between the buoyancy forces exerted by the ambient and the jet.

3.2.1 Non-Dimensional Parameters

The flow characteristics of a jet are determined by the Reynolds number, with laminar flows at low Reynolds numbers exhibiting markedly different behavior from turbulent flows at high Reynolds numbers [89–92]. A notable difference between the two is the large-scale entrainment of ambient fluid observed in turbulent flows. In this study, the jet Reynolds number (Re) is defined as follows:

$$Re = \frac{U_0 d_0}{\nu} \quad (3.1)$$

where U_0 is the characteristic velocity of the jet, d_0 is the characteristic length scale (i.e., diameter of the jet), and ν is the kinematic viscosity (the viscosity of the source fluid was considered as $\nu = 1 \times 10^{-6}$). The relation between buoyancy and inertial forces is defined by the dimensionless parameter densimetric Froude Number (Fr_d), which is defined as:

$$Fr_d = \frac{U_0}{\sqrt{g' d_0}} \quad (3.2)$$

here, g' denotes the reduced gravity and is given by $g' = g \frac{\rho_0 - \rho_b}{\rho_b}$, where g is the acceleration due to gravity, ρ_0 is the jet density, and ρ_b is the channel bed density. The ratio of momentum diffusivity (kinematic viscosity, ν) to mass diffusivity (molecular diffusivity, D) is defined as the Schmidt number (Sc) [181]:

$$Sc = \frac{\nu}{D} \quad (3.3)$$

The ambient density stratification is quantified N , which is a measure of the strength of the stratification induced by the density difference between the top (ρ_t) and channel bed (ρ_b) of the crossflow. The N is calculated using the following equation [182]:

$$N = \sqrt{\frac{g}{\rho_b} \frac{d\rho}{dy}}, \quad (3.4)$$

where $\frac{d\rho}{dy}$ is the vertical gradient of the density at the height of the crossflow. The magnitude of N is directly proportional to the strength of the ambient density stratification and has a significant impact on the mixing behavior of turbulent vertical dense jets in a crossflow.

3.2.2 Governing equations

The incompressible filtered Navier-Stokes equations coupled with a mass transport equation are utilized to compute the dynamics of the negatively buoyant jet. The Boussinesq approximation is employed to incorporate coupling, and the LES turbulence model is utilized to spatially filter the equations. Through the filtering process, large eddies are computed directly, whereas small eddies are modeled using a subgrid-scale model. The governing equations are expressed in a filtered nondimensional form as follows [40, 43, 143]:

$$\frac{\partial \tilde{u}_i}{\partial \tilde{x}_i} = 0, \quad (3.5)$$

$$\frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j \partial \tilde{x}_j} - \frac{\partial \tilde{\tau}_{ij}}{\partial \tilde{x}_j} + e_i^g \frac{1}{Fr^2} \tilde{c}, \quad (3.6)$$

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{c}}{\partial \tilde{x}_i} = \frac{1}{ReSc} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}_i \partial \tilde{x}_i} - \frac{\partial \tilde{\tau}_i^c}{\partial \tilde{x}_i}, \quad (3.7)$$

where $\tilde{p}$ is pressure, $\tilde{u}_i$ is the velocity component in the i -th direction, $\tilde{t}$ is time, $\tilde{\tau}_{ij}$ represents the subgrid-scale stress tensor, $\tilde{c}$ is the concentration, and e_i^g is the direction of the gravitational acceleration $(0, -1, 0)$. Here, the tilde symbol ($\sim$) represents dimensionless variable. The nondimensionalization resulted in three key nondimensional parameters of Reynolds number (Re) (Eq. 3.1), densimetric Froude number (Fr_d) (Eq. 3.2), and Schmidt number (Sc) (Eq. 3.3). The nondimensionalized variables are defined in detail in Table 3.1.

Table 3.1: Definitions of nondimensionalizations used in this study.

Parameter	Nondimensionalization
Length	$\tilde{x} = x/d_0, \tilde{y} = y/d_0$
Velocity	$\tilde{u} = u/U_0$
Time	$\tilde{t} = (U_0/d_0)t$
Pressure	$\partial \tilde{p}/\partial \tilde{x}_i = (d_0/\rho_a U_0^2) \partial p/\partial x_i$
Subgrid-scale stress tensor	$\partial \tilde{\tau}_{ij}/\partial \tilde{x}_j = (d_0/U_0^2) \partial \tau_{ij}/\partial x_j$
Concentration	$\tilde{c} = c/C_0$

The effect of unresolved flow structures, smaller than the local filter length scale, is accounted for by the subgrid-scale (SGS) stress tensor, denoted by $\tilde{\tau}_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$, and the SGS scalar flux, denoted by $\tau_i^c = \overline{u_j c} - \bar{u}_j \bar{c}$. The SGS eddy viscosity (ν_{SGS}) is calculated using the standard Smagorinsky subgrid-scale model [43, 183, 184], which is expressed as:

$$\tau_{ij} = -2\nu_{SGS} \overline{S_{ij}^s} \quad (3.8)$$

$$\tau_i^c = \frac{\nu_{SGS}}{Sc_{SGS}} \frac{\partial \bar{c}}{\partial x_j} \quad (3.9)$$

$$\overline{S_{ij}^s} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (3.10)$$

$$\nu_{SGS} = (C_s \Delta)^2 \sqrt{\overline{S_{ij}^s} \overline{S_{ij}^s}} \quad (3.11)$$

where the strain tensor of the filtered eddies is denoted by S_{ij} , the subgrid scale Schmidt number is denoted by Sc_{SGS} , and is set to a value of 1.0 [45, 81, 83]. The Smagorinsky coefficient, denoted by C_s , varies in the literature from $C_s = 0.065$ to $C_s = 0.25$ [40, 185], in this study a value of $C_s = 0.18$ is used. The numerical constants employed are established values derived from prior research, as referenced in [25] and [23]. The filter width, denoted by Δ , is determined from the cell volume and is defined as:

$$\Delta = \sqrt[3]{(\Delta_x \Delta_y \Delta_z)} \quad (3.12)$$

The local filter length scales in the x , y , and z directions, denoted as Δ_x , Δ_y , and Δ_z , respectively, were determined by the size of the cells in each respective dimension. The OpenFOAM code used in this study filters the turbulent scales based on the cell size, with the local filter length scales equal to the resolution of the cells in the discretized numerical domain. Scales larger than the cell size were directly resolved, whereas smaller scales were modeled using the subgrid-scale (SGS) model.

3.2.3 Numerical setup and parameters

The simulations in this study were performed in a nondimensionalized form utilizing the modified pimpleFoam incompressible flow solver coupled with an advection-diffusion equation. The governing equations were solved using the open-source code OpenFOAM, which utilizes the Finite Volume Method (FVM) to discretize and solve the equations governing equations. The proposed solver employs the PIMPLE algorithm, which combines the PISO and SIMPLE algorithms, for the simultaneous solution of the pressure-velocity coupling of the Navier-Stokes equations. For further details on the PIMPLE algorithm and OpenFOAM, readers are referred to [95, 96]. The diffusion terms were discretized using the second-order accurate central differencing scheme, while the convection terms were discretized using the Gauss-filtered Linear scheme, a second-order central differencing method [98–100]. The temporal terms were discretized using the Second-Order Backward scheme. To ensure higher stability and accuracy, the maximum CFL number was kept below 0.5 throughout the simulation process, with a corresponding temporal interval of approximately 1×10^{-4} nondimensional time unit. Each simulation was continued until a quasi-steady flow condition was achieved. A quasi-steady state refers to a condition where the flow variables no longer exhibit significant changes over time, even though the flow remains technically unsteady. This was ensured by monitoring flow characteristics, such as velocity and scalar concentrations, at various locations within the domain during simulations. In various simulation scenarios, the time required to attain a quasi-steady flow condition varied. To account for this variability, all simulations were extended for a minimum duration of 40,000 nondimensional time units. Following this, the flow characteristics were averaged over a subsequent period of 20,000 nondimensional time units to obtain time-averaged fields.

3.2.4 Flow configuration, boundary conditions, and grid

The present study simulated a jet in crossflow configuration, similar to [3], to investigate the behavior of a negatively buoyant jet. The jet is located at the bed of a channel, releasing a dense fluid into a crossflow with a linear density stratification. To avoid formation of any wake and disrupting the stratification of the crossflow, tip of the pipe is aligned with the plane of the channel bed. Figure 3.2 illustrates a schematic representation of the geometry of the numerical domain. The geometry of the numerical domain was nondimensionalized using the jet diameter (d). The domain consists of a rectangular channel section with dimensions of $l_x = 500d_0$, $l_z = 300d_0$, and $l_y = 150d_0$, and a round jet at the bed with a diameter of $d_0 = 1$ (length unit) and a length of $l_p = 40d_0$. A fully developed velocity, denoted as $\tilde{u}_r$, was applied at the crossflow inlet, along with a stable linear density stratification, characterized by a top nondimensional concentration ($\tilde{c}_t$) and a bed nondimensional concentration ($\tilde{c}_b$). A passive

scalar was introduced through the jet only after the flow field had reached a statistically steady state. It was not present in the initial condition and was injected solely from the jet once the flow had stabilized. Various techniques could be used to simulate turbulent inflow fluctuations that emulate the temporal and spatial correlations of eddies larger than the grid filter size [108]. A recycling technique (known as *mapped inlet* in OpenFOAM) was employed, as explained in [8, 85], for both the crossflow inlet and jet nozzle to introduce the effects of inlet turbulence based on the characteristics of the inflow. In this approach, the velocity of the inlet boundary is mapped from an internal plane where turbulent fluctuations are generated. The recycling plane for the crossflow is located at $x_t = -150d_0$, corresponding to a distance of $50d_0$ upstream of the crossflow inlet patch located at $x_t = -200d_0$. For the jet, the recycling plane is set at $y_t = -7.5d_0$, maintaining a distance of $12.5d_0$ from the jet inlet located at $y_t = -20d_0$ (based on [85, 109]). Within the numerical domain, the side walls were treated as cyclic boundary conditions to ensure continuity of the flow without any reflection. The bed boundary was treated as a solid wall with a no-slip condition, where the fluid velocity is assumed to be zero at the wall. The top boundary was modeled using a slip condition to represent an open surface, while the influence of free-surface effects was neglected.

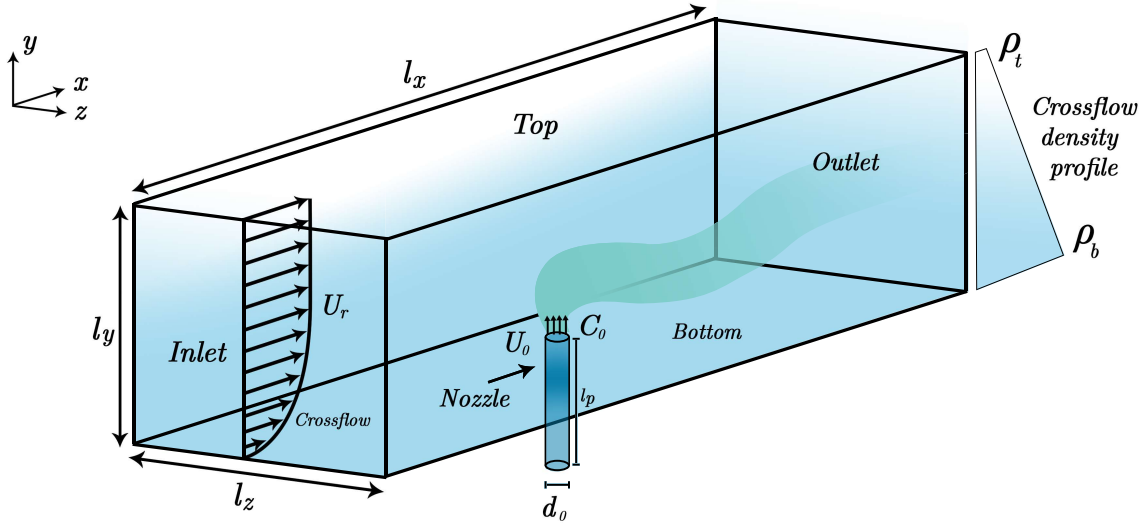


Figure 3.2: Schematic of the computational domain configuration.

Beside the boundary conditions, the grid resolution is a critical factor in determining the precision of simulation results. An inadequate grid resolution can introduce errors and inaccuracies into the simulations, while an excessively fine resolution can lead to unnecessary increases in computational time and resource consumption. Therefore, careful consideration of grid resolution is essential to achieve an optimal balance between accuracy and efficiency. The LES Index of Resolution (LES_{Index}) can be used to assess the quality of the resolution, which is mathematically expressed as:

$$LES_{Index} = \frac{k_{Resolved}}{k_{Resolved} + k_{SGS}} \quad (3.13)$$

where k_{resolved} denotes the resolved and k_{sgs} represents the unresolved (sub-grid) scale portions of the turbulence kinetic energy. The resolved component of the turbulence kinetic energy corresponds to the energy present within the flow structures that are directly captured by the simulation, whereas the sub-grid scale component pertains to the energy inherent in flow structures that are smaller than the filter length scale utilized in large eddy simulation. According to [40, 186], it is essential to refine the grid resolution of the simulation to capture at least 80% of the turbulence kinetic energy. While [187] recommended a mesh with a cell size of approximately 0.1 times the diameter of the jet, the use of such criteria may result in a coarse mesh, potentially leading to inaccuracies in LES. Therefore, we employed the LES_{Index} to evaluate the resolution quality of our mesh for the case with the highest Re . The mesh was then refined iteratively until a minimum of 80% of the turbulence kinetic energy was resolved directly. Figure 3.3 displays the LES_{Index} of the case with the highest $Re = 4800$ at various distances from the nozzle (from $2.5d_0$ to $70d_0$) in the middle of the domain. It is observed that for all locations, more than 80% of the total turbulence kinetic energy was resolved directly by the computational grid. The increase in the cell sizes was controlled to maintain a reasonable value for the ratio of resolved turbulence kinetic energy to total turbulence kinetic energy. This was performed to avoid over-refinement of the computational grid, which can lead to unnecessary computational costs. Overall, the results suggest that the chosen grid resolution is suitable for capturing the key features of the turbulent flow field and generating reliable large eddy simulation results.

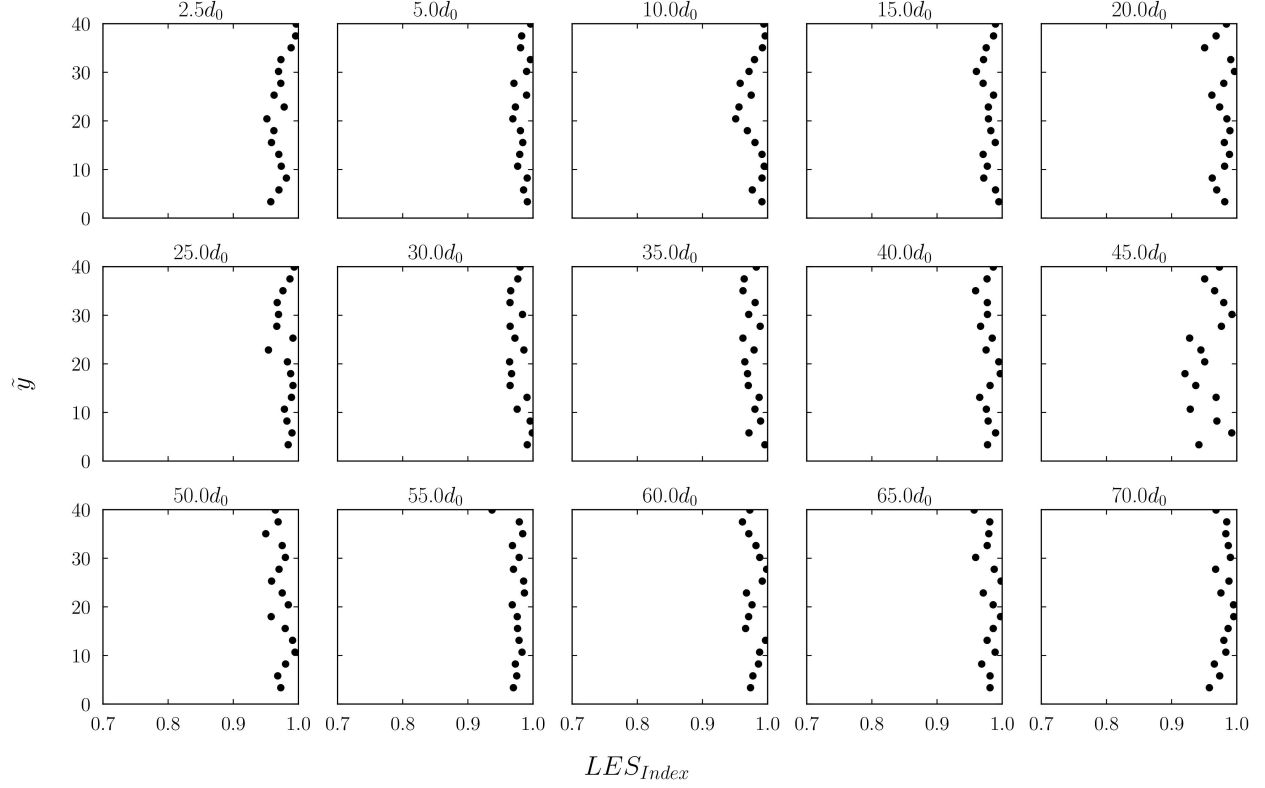


Figure 3.3: The ratio of the resolved TKE and the total TKE in the middle of the channel in y direction at different distances of $2.5d_0$, $5.0d_0$, $15.0d_0$, $25.0d_0$, $35.0d_0$, $45.0d_0$, $55.0d_0$, $65.0d_0$, and $70.0d_0$.

The numerical domain was discretized using hexahedral cells, incorporating a total of 23 million cells, as depicted in Figure 3.4. The hexahedral cells were employed to ensure accuracy and enhance smooth transitions from the round nozzle to the rectangular channel section. The O-grid method was utilized to mesh the nozzle geometry for a precise representation of the nozzle's shape and features, as illustrated in Figure 3.4. The nozzle was divided into 32 cells with a minimum size of $0.02d$ near the nozzle wall. The depth of the channel was divided into more than 180 cells with a minimum size of $0.05d$ close to the bed. In the channel, the cell size increased by a factor of 1.01 in both the streamwise and spanwise directions. This variation resulted in the smallest cell size of $0.03d_0$ near the nozzle vicinity and the largest cell size of $0.5d_0$ further downstream for $l_x > 200d_0$. The applied meshing approach ensures a balance between resolving small-scale flow structures and minimizing computational resources by reducing the number of required cells.

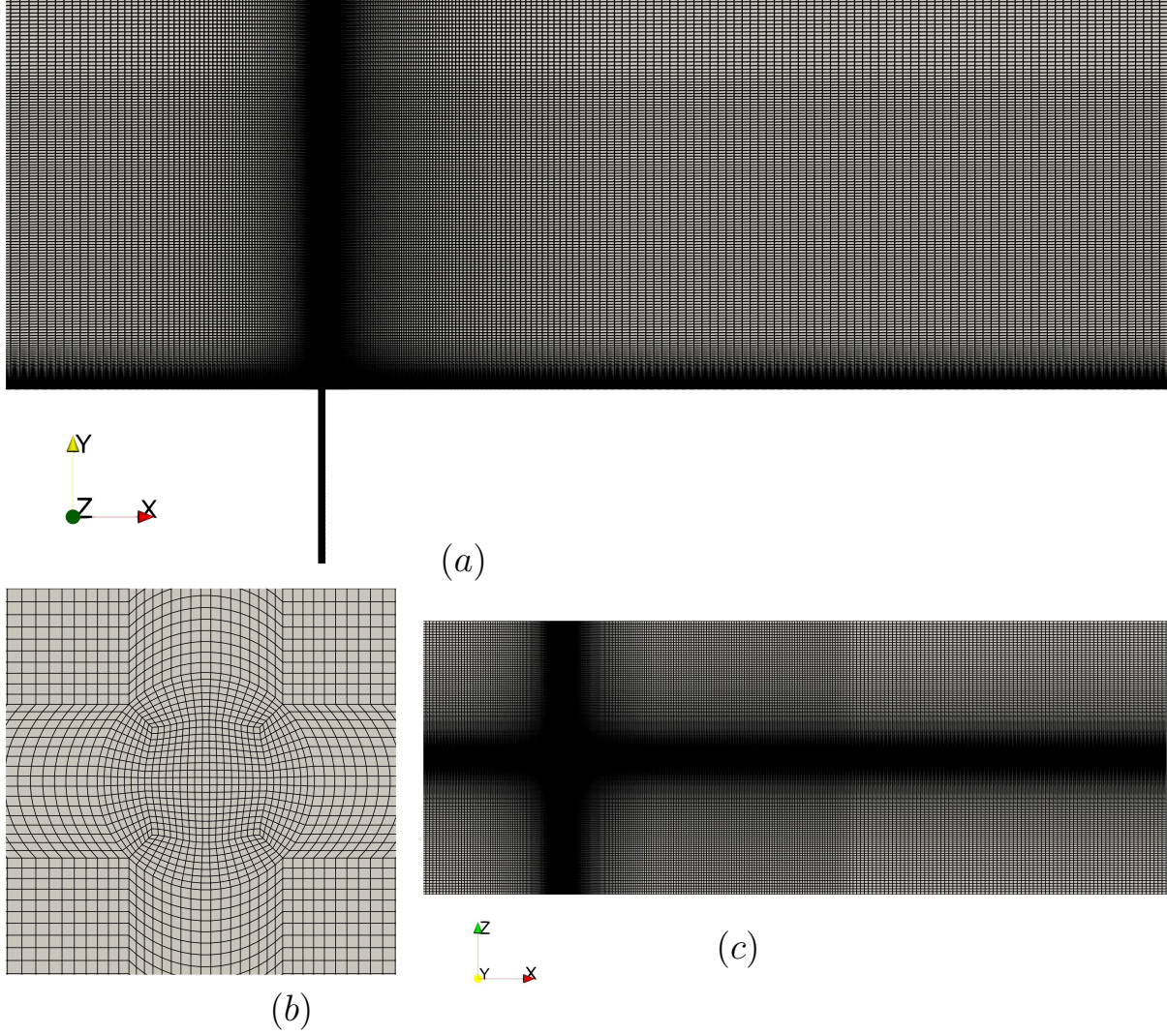


Figure 3.4: The geometry and computational grid with refinements. (a) central slide in the symmetrical $(x - y)$ plane of the mesh, (b) nozzle region, and (c) the bottom view.

To effectively capture the turbulent boundary layer in a wall-resolved LES, a sufficient resolution near the walls is required. The location of the first cell center within the viscous sub-layer ($y^+ < 5$) is commonly expressed in terms of the dimensionless wall distance (y^+), which is a function of the friction velocity and the velocity at the center of the first cell, defined as [41, 188, 189]:

$$y^+ = \frac{u_\tau \Delta y}{\nu} \quad (3.14)$$

where y^+ denotes the dimensionless distance from the wall, u_τ represents the friction velocity, and Δy is the distance from the center of the first cell to the wall [190, 191]. The y^+ values for the final mesh were maintained below five at the nozzle and below one at the channel bed, respectively.

3.2.5 Validation and Simulation Scenarios

To validate the accuracy of the adopted LES approach and computational solver, the simulation results are compared against experimental data from [163], which were also reported and utilized in the study by [3] as cases 2 and 3. Figure 3.5 shows a comparison of the buoyant jet centerline trajectory predicted by our numerical simulations with that reported in [3]. The centerline trajectory refers to the path traced by the maximum scalar concentration along the jet central axis. It is identified by locating the peak concentration values along the vertical plane intersecting the jet axis. The trajectory exhibits a pattern of ascending and descending regions for case 2 and ascending and wavy regions for case 3, separated by a dashed line in the figures. The centerline trajectory of the buoyant plume predicted by our simulations shows slight variations in height, being slightly higher in the ascending region and slightly lower in the descending and fluctuating regions, compared to the data reported by [3]. However, the discrepancy between the simulation results and the data reported by [3] is very small, indicating good agreement between the two. Furthermore, the computational solver and method employed in our study have been widely used and applied in previous studies investigating the effects of density stratification on turbulent mixing [8, 103, 105, 192, 193].

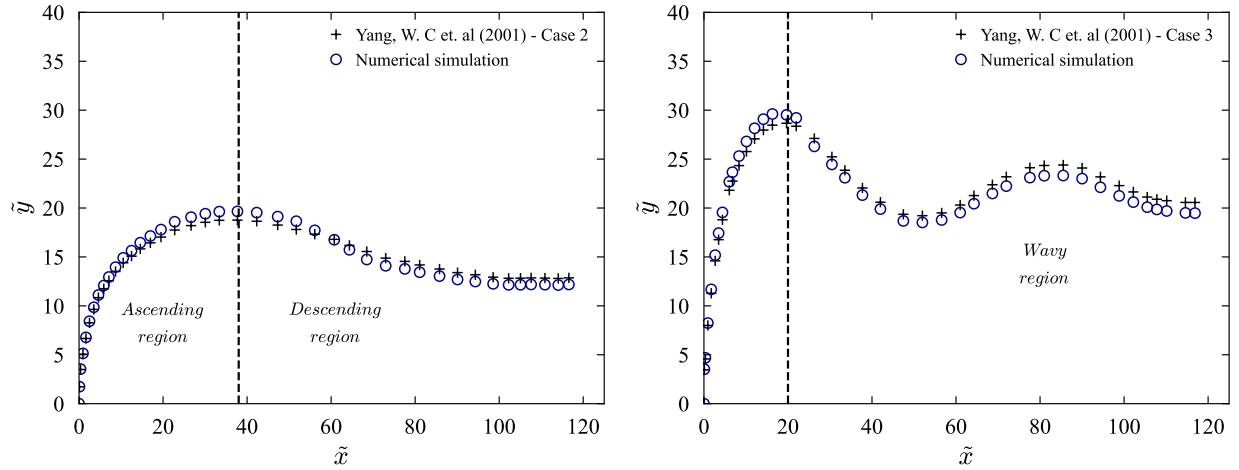


Figure 3.5: Comparison of the results of numerical simulation of buoyant jet plume with centerline of cases 2 and 3 (i.e., mild and strong ambient stratification) reported by [3].

Due to the limited availability of velocity field in the experimental study of buoyant jets in a stratified crossflow, it was not possible to directly compare the simulation velocities with the experimental data. Therefore velocity data of a negatively buoyant jet in uniform crossflow ambient were used to prove the accuracy of the applied code and numerical approach. For this purpose, the normalized velocity of the cases R1 and R2 of the experimental study conducted by [4, 178] were used for comparison with the numerical simulation. The configuration of the experiments is similar to this study except the crossflow is uniform. The buoyant jet is located at the bottom and releases a dense jet flow into the crossflow. In the validation simulations, the ratio of the resolved TKE to total TKE was kept higher than 80% similar to the explained condition. Additionally, the dimensionless distance from the walls was kept below 5 for all the wall boundaries. The comparison showed a good agreement between the

numerical simulation results and the experiments as illustrated in Figure 3.6.

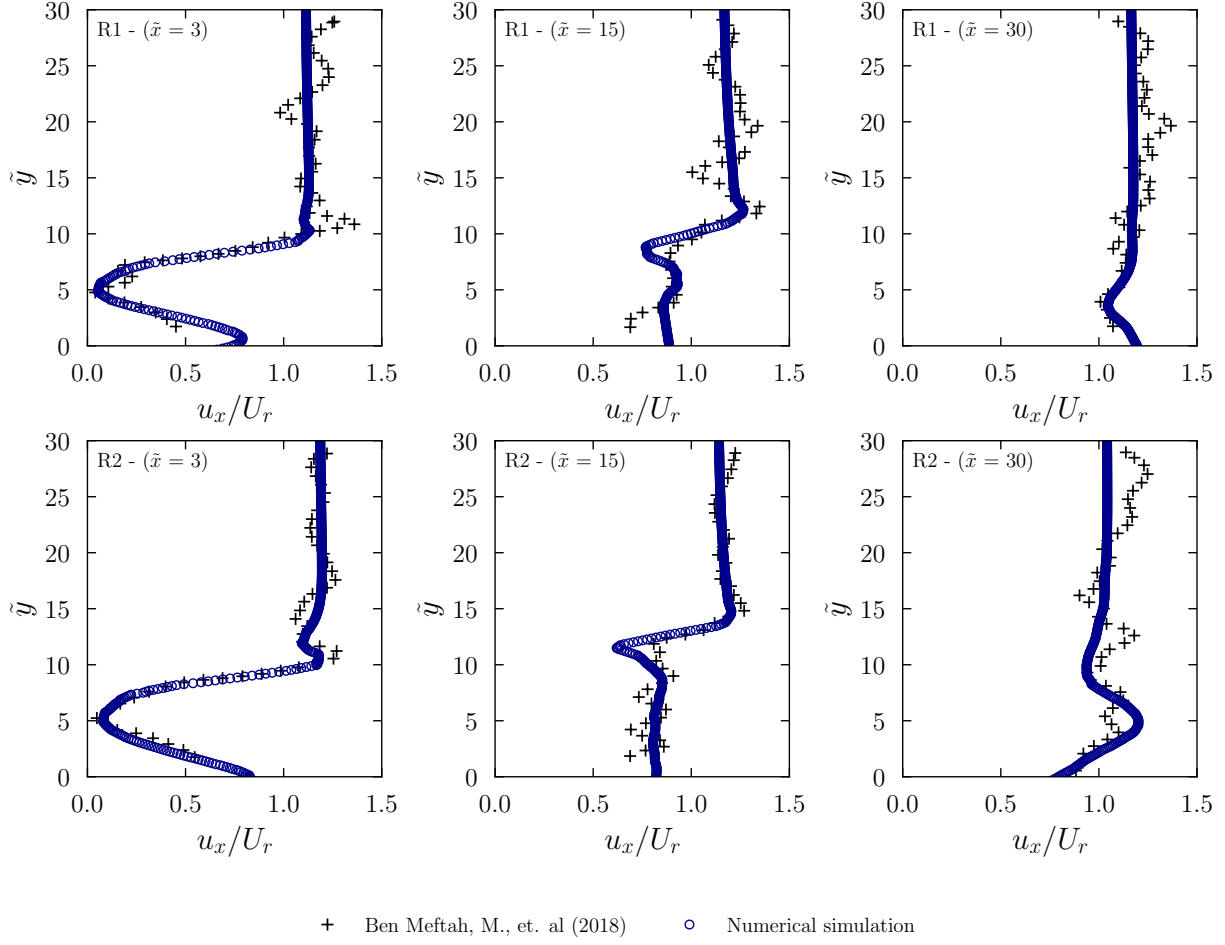


Figure 3.6: Comparison of the normalized velocity in x-direction (u_x/U_r) of numerical simulation with the experimental study by [4].

The 48 numerical simulation cases, as detailed in Tables 3.2 were devised to explore the impacts of varying crossflow scenarios. All simulations were conducted in a nondimensional framework, emphasizing their applicability across various engineering and natural contexts. These cases were defined based on four distinct Re , four stratification intensities and encompassing a spectrum of jet Fr_d values, spanning from 10.82 to 43.26 and ratio of depth averaged crossflow velocity to jet velocity ($R = U_r/U_0$) from 0.042 to 0.250. The ambient stratification intensity is quantified by $\tilde{N}$, which is a measure of the strength of the stratification induced by the concentration difference between the top ($\tilde{c}_t$) and channel bed ($\tilde{c}_b$) of the crossflow. The $\tilde{N}$ is calculated using the following equation [182]:

$$\tilde{N} = \sqrt{\frac{e_i^g}{\tilde{c}_b} \times \frac{d\tilde{c}}{d\tilde{y}}} \quad (3.15)$$

where $\frac{d\tilde{c}}{d\tilde{y}}$ is the vertical gradient of the concentration at the depth of the crossflow.

The defined range of cases, although innovative in its scope, is encompassed by the spectrum of real-world engineering and environmental conditions, as documented in studies such as those by [3, 163–166].

Table 3.2: A summary of the numerical simulation parameters. Columns from left to right are case number, ambient stratification intensity, Reynolds number, the ratio of crossflow to jet velocity, and jet densimetric Froude number (Note: For each group of cases (e.g., 1-4), the parameter values in columns of $\tilde{N}$ and Fr_d are assigned to the respective cases within the group. Specifically, the first value in each column pertains to the first case in the group, the second value to the second case, and so on).

Case	$\tilde{N}$				Re	R	Fr_d				Groups
1-4	0.100	0.086	0.070	0.050	2400	0.083	10.82	12.49	15.30	21.63	$g1$
5-8	0.100	0.086	0.070	0.050	3200	0.063	14.42	16.65	20.39	28.84	$g1$
9-12	0.100	0.086	0.070	0.050	4000	0.050	18.03	20.81	25.49	36.05	$g1$
13-16	0.100	0.086	0.070	0.050	4800	0.042	21.63	24.98	30.59	43.26	$g1$
17-20	0.100	0.086	0.070	0.050	2400	0.167	10.82	12.49	15.30	21.63	$g2$
21-24	0.100	0.086	0.070	0.050	3200	0.125	14.42	16.65	20.39	28.84	$g2$
25-28	0.100	0.086	0.070	0.050	4000	0.100	18.03	20.81	25.49	36.05	$g2$
29-32	0.100	0.086	0.070	0.050	4800	0.083	21.63	24.98	30.59	43.26	$g2$
33-36	0.100	0.086	0.070	0.050	2400	0.250	10.82	12.49	15.30	21.63	$g3$
37-40	0.100	0.086	0.070	0.050	3200	0.188	14.42	16.65	20.39	28.84	$g3$
41-44	0.100	0.086	0.070	0.050	4000	0.150	18.03	20.81	25.49	36.05	$g3$
45-48	0.100	0.086	0.070	0.050	4800	0.125	21.63	24.98	30.59	43.26	$g3$

In this study, simulations were first configured using dimensional input parameters based on characteristic length, velocity, and density scales representative of the physical system. These inputs include jet exit velocity, nozzle diameter, and density differences between the jet and ambient fluids. To generalize the results and facilitate comparison across a range of cases, the governing variables were subsequently nondimensionalized. In the nondimensional simulations, the computational geometry was constructed using the jet diameter as the characteristic length scale. Specifically, the jet diameter was set to one unit length, and all other domain dimensions were defined proportionally, ensuring a fully nondimensionalized spatial framework consistent across all cases. Subsequently, the jet velocity was normalized and set to one unit velocity, while the crossflow velocity was prescribed relative to this reference based on the defined velocity ratio. The flow regime was regulated by specifying the Reynolds number. The jet concentration was also normalized to a value of one, with the ambient concentration and resulting buoyancy effects incorporated through the densimetric Froude number (Fr_d). These nondimensional parameters were implemented in the governing equations (D.6) and (D.8). Further details on the modified solver and simulation configuration are provided in the author’s GitHub repository.¹

¹<https://github.com/HydroCFD>

3.3 Results

A comprehensive set of 48 LES was conducted to investigate the influence of parameters $\tilde{N}$, Fr_d , and R , on the dynamics of a negatively buoyant jet within a stratified crossflow environment. The behavior of a dense jet in a crossflow is influenced by dimensionless parameters of R and Fr_d [194–196]. However, in a stratified ambient environment, the $\tilde{N}$ plays an important role in shaping the mixing and dynamics of the jet. Given the relatively long wavelengths of the jet fluctuations in stratified crossflow, measurements were conducted up to a distance of $187.5d_0$ from the nozzle. The data are analyzed and visualized utilizing open-source Python libraries of Matplotlib², PyVista³, CMasher⁴, and Pandas⁵ [197–200]. All the data presented in the results section are time-averaged values.

3.3.1 General observations

Figure 3.7 presents nondimensional time-averaged concentration contours and streamlines of cases 3, 19, and 35 in the $(x - y)$ plane in the middle of the domain. These cases were deliberately selected to have similar Fr_d and $\tilde{N}$, while varying values of $R = 0.083, 0.167$, and 0.250 to highlight the effects of different R values. In Figure 3.7, the influence of increasing the value of R from 0.083 to 0.250 is apparent in the ascending section of the jet. Case 3 displayed the highest terminal rise, whereas cases 19 and 35 exhibited lower terminal rise heights. For lower values of R , the jet exhibited a nearly vertical trajectory, maintaining its predominantly upward motion. However, with an increase in R , the jet underwent noticeable bending and progressively moved in the direction of the crossflow. The magnitude of the bending amplitude is directly proportional to R . In simple terms, an inverse relationship exists between R and the maximum height reached by the jet. The location of the return points, in both x and y directions, was also affected by the crossflow velocity. It is observed that the return point of the jets with lower values of R is significantly closer to the origin of the jet, while for jets with higher values of R , the return point is moved farther downstream.

²<https://matplotlib.org/>

³<https://pyvista.org/>

⁴<https://cmasher.readthedocs.io>

⁵<https://pandas.pydata.org/>

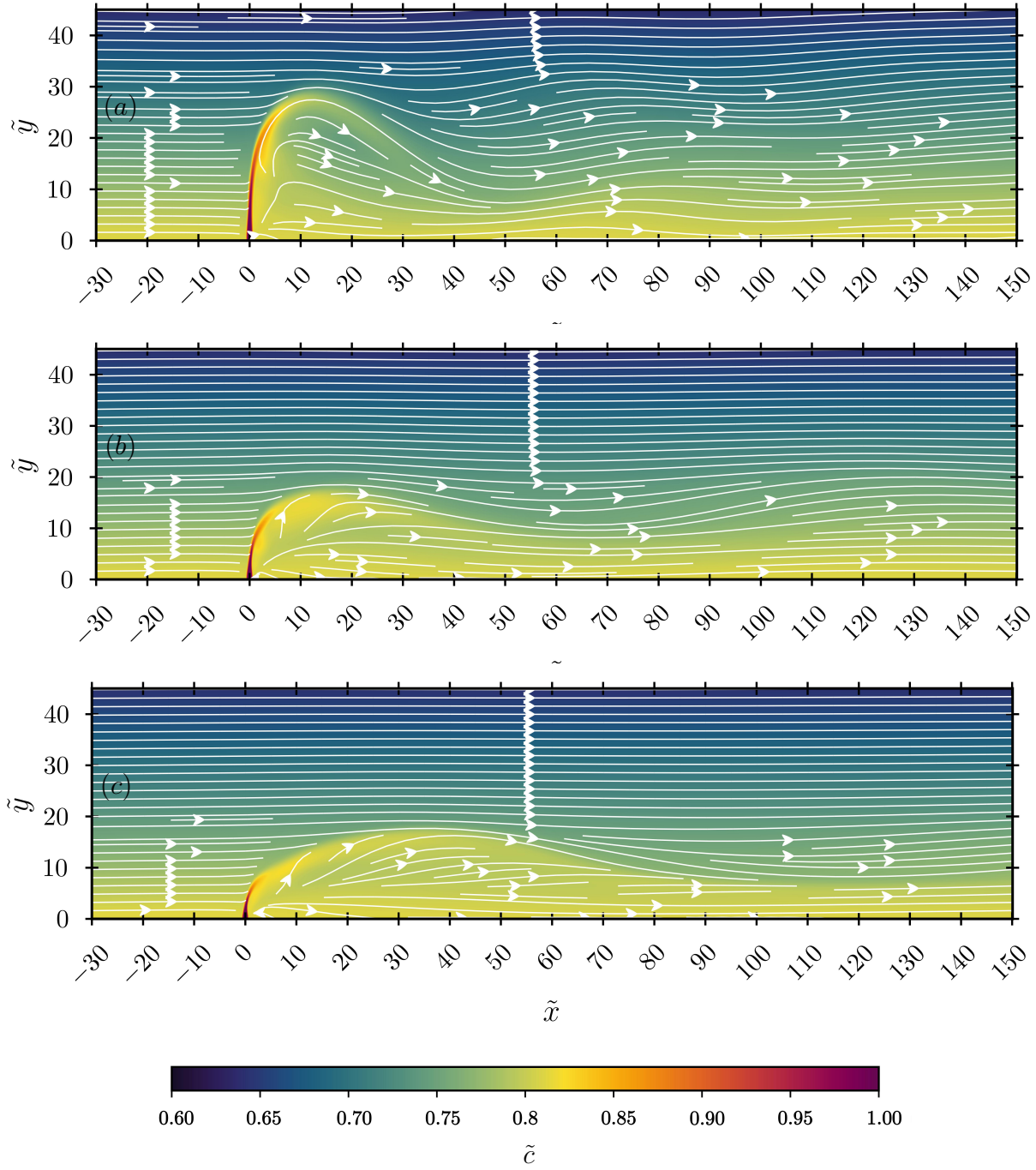


Figure 3.7: Nondimensional time-averaged concentration contours ($\tilde{c}$): (a) case 3 ($R = 0.083$), (b) case 19 ($R = 0.167$), (c) case 35 ($R = 0.250$) with time-averaged flow streamlines in middle of the domain.

One of the features of negatively buoyant jets in stratified crossflow is vertical fluctuations of the jet as it develops downstream. These fluctuations are particularly pronounced in cases with low crossflow velocity ratios (R) under similar stratification intensities ($\tilde{N}$), as observed in case 3 (Figure 3.7 - a). In such conditions, the jet exhibits closer fluctuations with relatively

large upward and downward motion. As R increases, the vertical development of the jet becomes more constrained, and the fluctuations gradually become less distinct. This behavior reflects the influence of crossflow velocity on the balance between the jet's vertical momentum and the stabilizing effect of the stratified ambient. At lower values of R , the jet retains stronger upward motion, reaching higher positions in the domain before starting downward motion due to buoyancy force. The larger vertical displacement leads to more noticeable downward motion, followed by an upward motion due to the interaction of buoyancy forces from the ambient and jet. The shape and extent of the high-concentration core suggest that mixing is more effective in cases with lower R , where the jet shows a larger vertical development before being deflected. In contrast, as R increases, the jet trajectory becomes more horizontal, causing the core to stretch and flatten. This limits vertical entrainment and restricts the mixing to a thinner vertical layer, reducing overall dilution.

3.3.2 Jet trajectory and features

In this section, the influence of crossflow velocity, stratification intensity and jet momentum on the behavior of the jet and plume in a stratified crossflow is investigated through an analysis of the jet trajectory. To mitigate the adverse environmental effects of waste discharges, it is essential to assess key flow parameters of the jet trajectory. These parameters include the location of the maximum rise height (y_t and x_t) along the centerline, and the location of the impact points (y_r , x_r , and y_r^*) depicted in Figure 3.1. The jet trajectory was determined by identifying the center of concentration, defined as the location of maximum concentration ($\tilde{c}$) along lines oriented perpendicular to the local jet direction. Figure 3.8 illustrates the centerline trajectory of the jet for all the cases. To facilitate comparison, the simulation results were categorized into three groups: g_1 (cases 1-16), g_2 (cases 17-32), and g_3 (cases 33-48), defined based on the crossflow Reynolds number (Re_{cr}) (i.e., crossflow velocity is constant). For similar ambient conditions across g_1 , g_2 , and g_3 , an increase in the Fr_d corresponded to a higher terminal rise height of the jet (y_t). For example, comparing Cases 1, 5, 9, and 13, it is evident that as Fr_d increases, the value of y_t also increases. This behavior is attributed to the larger jet momentum at higher Fr_d , which more effectively counteract both the downward buoyancy force of the dense jet and the lateral deflection induced by the crossflow, thereby resulting in a higher terminal rise (y_t). Additionally, an increase in Fr_d leads to a further downstream displacement of the return point in the x -direction. This increased downstream displacement is directly attributed to the jet's larger vertical momentum, which, through its interaction with the crossflow, enhances horizontal displacement; for instance, the downstream shift in x_t and x_r is evident when comparing cases 1, 5, 9, and 13 (also see Table 3.A1). This observed impacts of Fr_d aligns with classical observations of buoyant jets in crossflow without stratification [4, 13, 157, 176, 201].

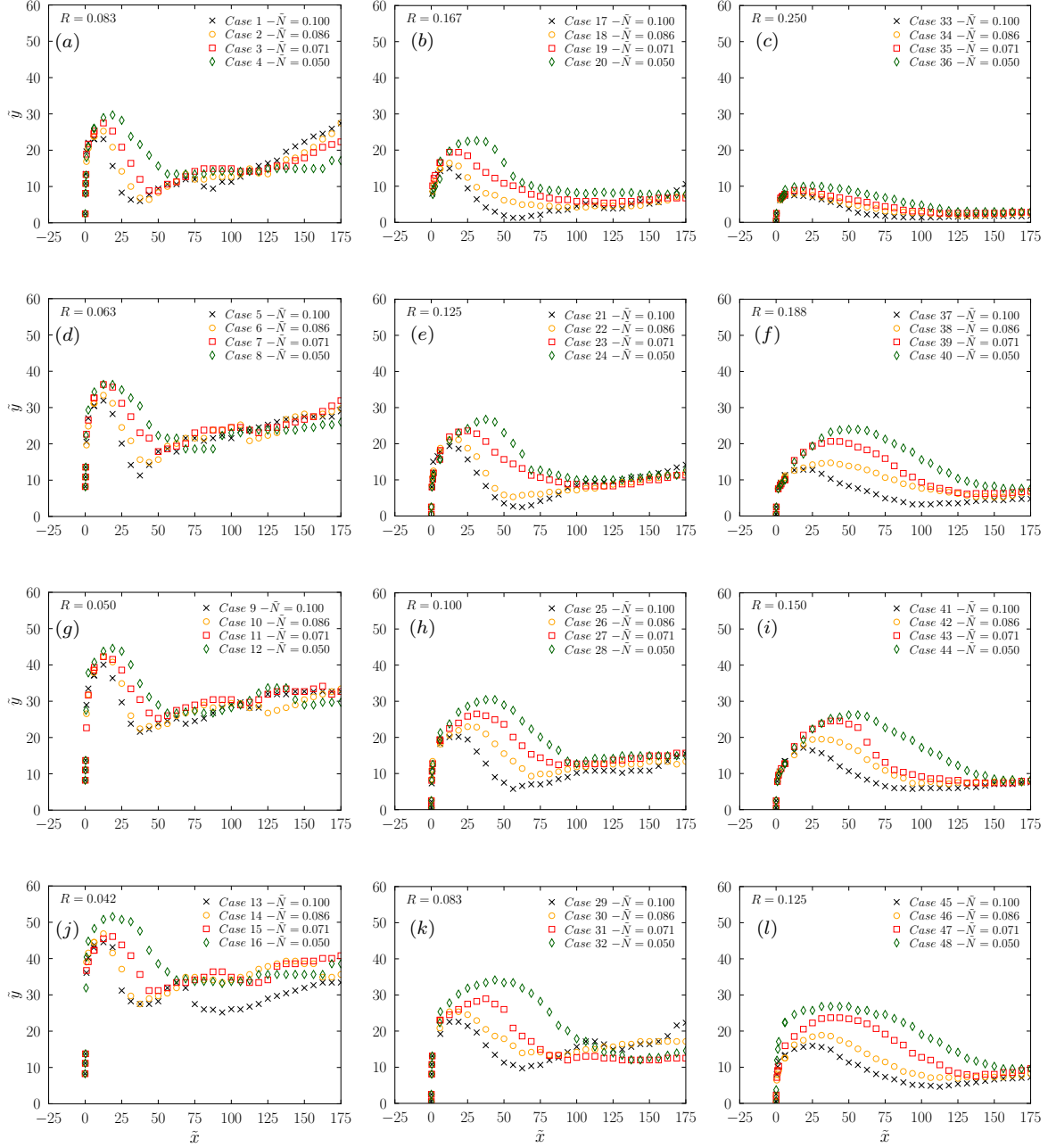


Figure 3.8: Jet trajectory of all the cases in $(x - y)$ plane in middle of stratified crossflow ambient.

In contrast to buoyant jets in non-stratified environments, jets or plumes in stratified ambient conditions do not descend back to the bed. Instead, they reach a level of neutral buoyancy within the stratified ambient, where vertical displacement is limited and governed by the balance between buoyant forces and inertial momentum, resulting in fluctuating motion around that equilibrium layer. This behavior is characterized by continuous upward and downward movement as the jet interacts with the stratified crossflow. The findings indicate an inverse

correlation between the jet fluctuation frequency and the Fr_d , where the frequency of fluctuations decreases as the Fr_d increases. This pattern is evident by comparing cases in Figure 3.8 - a with those in Figure 3.8 - j, where $\tilde{N}$ and crossflow velocity (i.e., Re_{cr}) remain constant. Cases 1-4 exhibit a higher frequency of transitions between fluctuation states compared to cases 13 - 16. A similar reduction in the frequency of upward and downward notions is observed with increasing Fr_d within g_2 (Figure 3.8 - b and k). For g_3 , the horizontal extent of fluctuations is sufficiently large that the a full fluctuation cycle could not be captured within the spatial bounds of the measured area, thereby limiting direct observation in this group. Determining the terminal rise height ($\tilde{y}_t$) and its horizontal distance ($\tilde{x}_t$) is important for evaluating the environmental impact associated with discharges. In this study, the horizontal ($\tilde{x}_t$) and vertical ($\tilde{y}_t$) coordinates of the terminal rise are defined as the locations of the jet centerline where the maximum vertical elevation is attained. Figures 3.9 and 3.10 use distinct markers and colors to differentiate between simulation groups and stratification intensities. The g_1 , g_2 , and g_3 are represented by circles, squares, and diamonds, respectively and the stratification intensities $\tilde{N}$ are distinguished by colors, red for $\tilde{N} = 0.100$, blue for $\tilde{N} = 0.086$, black for $\tilde{N} = 0.070$, and green for $\tilde{N} = 0.050$. The color schemes for the trend lines follow the same convention, reflecting the respective stratification intensities. Figure 3.9 - a presents the variation of $\tilde{x}_t$, as a function of the Fr_d . Overall, Figure 3.9 - a shows a direct relation between $\tilde{x}_t$ and Fr_d , indicating that as the effect of jet momentum increases, the horizontal distance to the jet's terminal rise increases. An increase in crossflow velocity is associated with an increase in $\tilde{x}_t$, as evidenced by the shift in data from g_1 to g_2 and g_3 . For similar stratification conditions, cases in g_3 consistently show higher values of $\tilde{x}_t$ compared to those in g_2 and g_1 , indicating that the jet travels further downstream as reaching its terminal rise. As the crossflow velocity increases, it imposes a stronger bending force on the jet, causing more deflection in the streamwise direction. The downstream movement of the jet is governed by the balance between the jet's momentum, Fr_d , and the bending force imposed by the crossflow, characterized by the velocity ratio R . The trend lines for all stratification intensities exhibit similar slopes, indicating that the sensitivity of $\tilde{x}_t$ to changes in Fr_d remains consistent across the range of ambient stratification intensities. However, the vertical displacement of the trend lines reflects the influence of stratification strength on $\tilde{x}_t$. Specifically, weaker stratification conditions correspond to higher values for $\tilde{x}_t$, suggesting that, for a given Fr_d , the jet develops further downstream reaching the terminal rise. This shift is attributed to the reduced constraining effect of buoyancy under weak stratification of the crossflow, which allows the jet to retain its momentum over a longer horizontal distance. Conversely, in strongly stratified crossflow, the strong stratification limits downstream jet development, leading to consistently lower values of $\tilde{x}_t$ at similar Fr_d . This consistent slope, along with the vertical shift between lines, shows that the relationship between $\tilde{x}_t$ and Fr_d is similar across all cases.

Across all cases, higher values of Fr_d corresponds to an increase in the terminal rise height $\tilde{y}_t$, which consistently observed across g_1 , g_2 , and g_3 , as illustrated in Figure 3.9 - b. For a given Fr_d , cases in g_1 consistently exhibit higher values of $\tilde{y}_t$ compared to those in g_2 and g_3 , highlighting the influence of crossflow velocity on vertical jet development. As the crossflow velocity increases from g_1 to g_3 , the momentum of the ambient flow bends the jet more effectively, limiting its ability to rise vertically. The high crossflow velocity (e.g., g_3) pushes the jet downstream, redirecting its momentum horizontally and reducing the upward

motion. As a result, the jet's development is limited to a lower terminal rise, indicating that increased crossflow velocity constrains vertical motion and enhances lateral deflection. For cases with weaker stratification intensity (i.e., lower $\tilde{N}$), the buoyancy induced constraint of the crossflow is more effective, hindering the jet to reach a higher terminal location. In contrast, in cases with stronger stratification the larger mixing of the jet in domain caused the jet to rise higher. This is due to larger gradient of the concentration at higher levels for the cases with higher $\tilde{N}$. The slopes of the trend lines further show the influence of stratification intensity on the jet's vertical development. Strongly stratified cases (red and blue lines) exhibit steeper slopes, indicating a more rapid increase in $\tilde{y}_t$ with Fr_d . This behavior suggests that stronger stratification increases the sensitivity of the jet trajectory to changes in Fr_d . Conversely, in weakly stratified cases (black and green lines), the slopes are shallower, implying a more gradual response of the terminal rise height to variations in Fr_d .

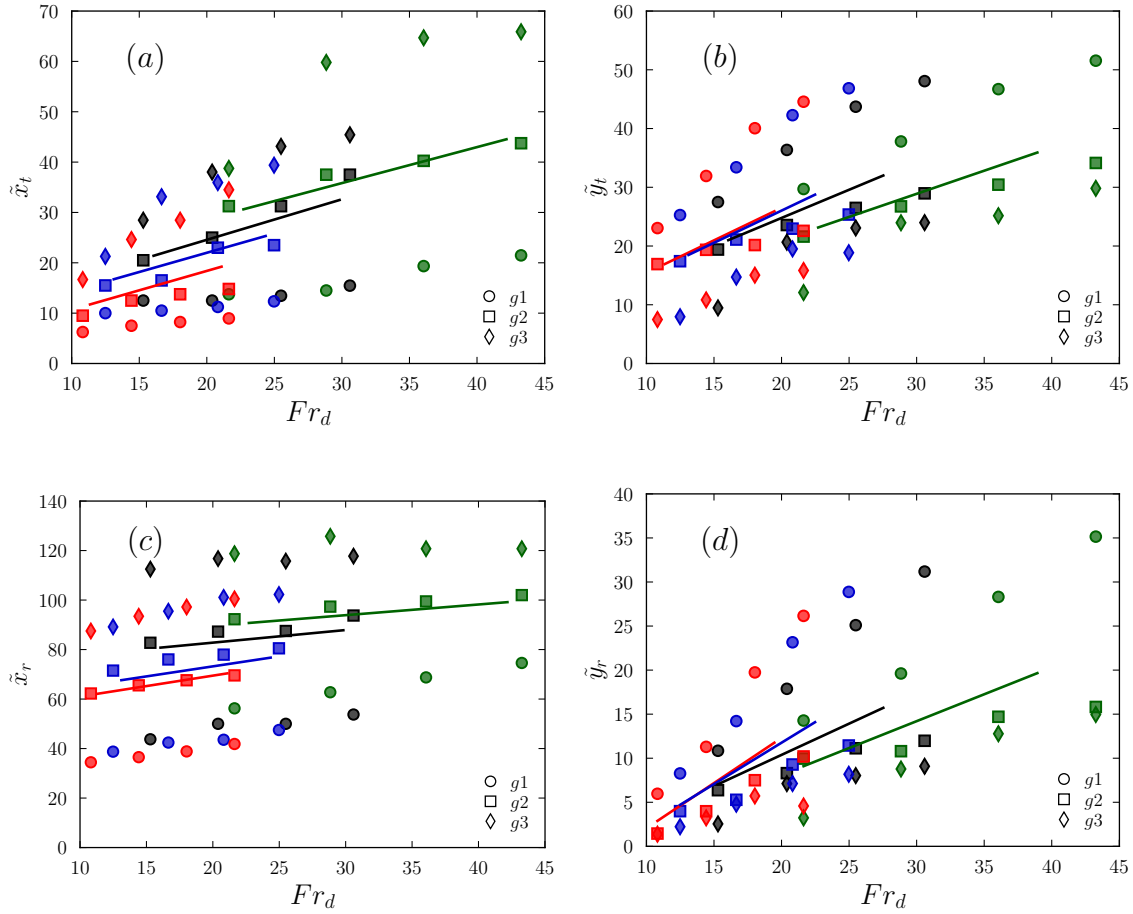


Figure 3.9: Jet trajectory parameters: (a) $\tilde{x}_t$, (b) $\tilde{y}_t$, (c) $\tilde{x}_r$, and (d) $\tilde{y}_r$ as a function of Fr_d . Marker shapes indicate groups (g_1 : circles, g_2 : squares, g_3 : diamonds), and colors represent stratification intensities (red: $\tilde{N} = 0.100$, blue: $\tilde{N} = 0.086$, black: $\tilde{N} = 0.070$, green: $\tilde{N} = 0.050$). Trend lines highlight stratification effects.

The jet, after reaching its terminal rise, enters a descent phase driven by its negative buoyancy

force, causing it to gradually descend towards the bottom. This downward motion continues until the height where the downward buoyancy force diminishes due to mixing with the ambient and the upward (i.e., opposite) ambient buoyancy force becomes dominant. This point is referred as the return point, with its height denoted as $\tilde{y}_r$, and its horizontal distance from the jet represented by $\tilde{x}_r$. The $\tilde{x}_r$ values illustrated in Figure 3.9 - c exhibit an increasing trend with respect to Fr_d , consistent with the behavior observed for $\tilde{x}_t$. As Fr_d increases, the jet penetrates farther into the ambient environment before reversing direction, resulting in a more downstream development of the return point $\tilde{x}_r$. The influence of crossflow velocity is evident when comparing groups g_1 , g_2 , and g_3 . For a given Fr_d , the $\tilde{x}_r$ values in g_1 are consistently lower than those in g_2 and g_3 . The slope of the trend line for $\tilde{x}_r$ decreases from strongly to weakly stratified crossflow, indicating that cases with intense stratification are more sensitive to increases in Fr_d .

Figure 3.9 - d illustrates that the height of the return point, $\tilde{y}_r$, increases with the densimetric Froude number (Fr_d), exhibiting a trend similar to that of the terminal rise height, $\tilde{y}_t$. This upward shift in $\tilde{y}_r$ is associated with the increase in $\tilde{y}_t$. As the jet reaches a higher terminal rise, its concentration decreases due to enhanced dilution, which in turn reduces the jet's negative buoyancy. During the downward motion of the jet, the balance between the downward buoyant force of the jet and the upward buoyant force from the ambient stratification is achieved at higher elevations, resulting in a higher return point. As the crossflow velocity increases from g_1 to g_3 , larger lateral momentum is imposed on descending jet, deflecting its trajectory downstream. This increased horizontal force reduces the vertical descent angle, causing the jet to return closer to the bed and thus lowering $\tilde{y}_r$. Another contributing factor to the reduction in $\tilde{y}_r$ is the diminished terminal rise height $\tilde{y}_t$ observed under higher crossflow velocity conditions. That is, when the jet is unable to ascend to a higher height due to increased horizontal forcing, the subsequent descent also located in a lower elevation, resulting in a reduced $\tilde{y}_r$. The influence of stratification on $\tilde{y}_r$ follows the same pattern observed for $\tilde{y}_t$. Cases with weaker stratification, exhibit lower $\tilde{y}_r$, while cases with stronger stratification, result in higher $\tilde{y}_r$ values. A similar explanation applies to the behavior of $\tilde{y}_r$ as for $\tilde{y}_t$. Higher values of $\tilde{N}$ induce stronger ambient stratification, leading to higher concentration gradients and enhanced dilution of the jet. As a result, the jet's negative buoyancy diminishes more rapidly, causing the return point $\tilde{y}_r$ to occur at a higher elevation.

At the return point, the buoyant jet shifts from downward to upward motion as a balance of ambient upward buoyancy force and jet downward force. This upward movement continues until the jet reaches a level where the upward buoyancy force (i.e., balance of forces) is zero, defined as $\tilde{y}_r^*$. Beyond this point, the plume descends once again due to its higher density relative to the surrounding fluid. These alternating phases of ascent and descent are accompanied by forward advection, producing a fluctuating plume trajectory. Figures 3.10 - a shows the variation of the second terminal rise ($\tilde{y}_r^*$) as functions of Fr_d . The value of $\tilde{y}_r^*$ increases with increasing Fr_d , indicating that larger jet momentum enhances the vertical height development of the jet after return point, consistent with its influence on the first terminal rise height. This outcome is attributed to the enhanced mixing between the jet and the ambient fluid near the terminal rise, which reduces the effective negative buoyancy. As a result, the jet reaches a higher return point elevation ($\tilde{y}_r$), which in turn leads to an increased value of $\tilde{y}_r^*$. Additionally, the effects of stratification intensity and crossflow velocity

on $\tilde{y}_r^*$ exhibit similar trends to those observed for $\tilde{y}_t$. Weaker stratification intensity imposes buoyancy constraints, which hinders vertical development of the jet and hinders the jet to penetrate farther before reversing direction. Additionally, higher crossflow velocities exert larger horizontal momentum on the jet, enhancing streamwise deflection and thereby limiting its vertical propagation.

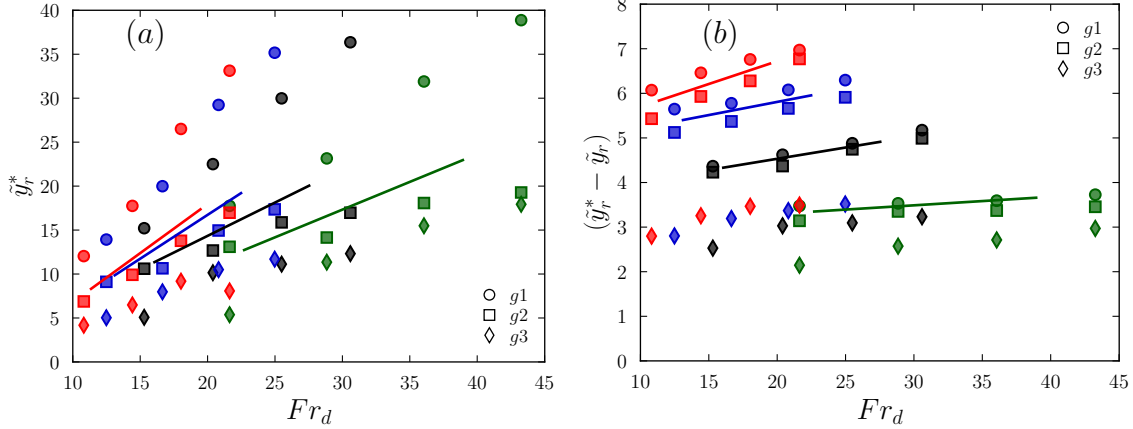


Figure 3.10: Jet trajectory parameters: (a) $\tilde{y}_r^*$, (b) $(\tilde{y}_r^* - \tilde{y}_r)$ as a function of Fr_d . Marker shapes indicate groups (g_1 : circles, g_2 : squares, g_3 : diamonds), and colors represent stratification intensities (red: $\tilde{N} = 0.100$, blue: $\tilde{N} = 0.086$, black: $\tilde{N} = 0.070$, green: $\tilde{N} = 0.050$). Trend lines highlight stratification effects.

Figure 3.10 - b illustrates the variation of the vertical fluctuation magnitude, quantified by the difference $\tilde{y}_r^* - \tilde{y}_r$, as a function of Fr_d , representing the extent of the jet's vertical motion. Across all cases, $\tilde{y}_r^* - \tilde{y}_r$ increases with Fr_d , indicating that higher jet momentum enhances the jet's ability to fluctuate vertically in stratified crossflow. A comparison across crossflow groups shows that this vertical fluctuation amplitude reduces from g_1 to g_3 , suggesting that higher crossflow velocities suppress the jet's vertical instability by redirecting momentum horizontally. The effect of stratification intensity is also evident, cases with stronger stratification (red and blue lines) exhibit steeper slopes and higher values of $\tilde{y}_r^* - \tilde{y}_r$, highlighting enhanced vertical fluctuation due to higher buoyancy induced forcing. In contrast, weaker stratification (green) leads to more confined vertical behavior with reduced fluctuation amplitude.

3.3.3 Jet mixing and dilution

To gain deeper insights into the behavior and mixing characteristics of the buoyant jet, an additional passive scalar, which does not influence the momentum of the jet or crossflow, has been included in the analysis. This passive scalar is modeled by solving an additional advection-diffusion equation similar to Eq. 3.7. The dimensionless concentration of the passive scalar, denoted as $\tilde{s}$, is normalized by the source concentration (S_0), defined as $\tilde{s} = s/S_0$. The passive scalar concentration is initialized at zero concentration within the entire domain. Figures 3.11 and 3.A1 illustrate the evolution of axial concentration profiles

for the dimensionless jet concentration ($\tilde{c}$) and the passive scalar ($\tilde{s}$) obtained from the LES simulations. Each subplot within these figures compares three cases with identical Fr_d and $\tilde{N}$ but varying crossflow velocity (i.e., R), thus isolating the influence of crossflow velocity on the mixing and dilution characteristics. Notably, an increase initial decline in $\tilde{c}$ occurs near the jet source region for all cases, indicating rapid mixing between the jet and the ambient fluid. This initial reduction is especially evident in cases with higher values of Fr_d (e.g., cases 9 and 13), where the jet has larger Fr_d , enhancing vertical entrainment and stronger turbulent mixing. The high initial mixing, i.e., high reduction in $\tilde{c}$, decreases with increasing R , indicating an inverse relationship between mixing intensity and crossflow velocity. This trend is particularly evident in groups g_2 and g_3 , where only a slight decrease in $\tilde{c}$ is observed (e.g., compare initial mixing of cases 13, 29, and 33). In group g_1 , particularly at higher Fr_d , the initial reduction in $\tilde{c}$ is followed by an increase, reflecting the jet's descent into higher concentration ($\tilde{c}$) ambient layers due to its strong downward momentum. This behavior is indicative of enhanced vertical fluctuations and is consistent with the jet trajectory patterns observed in Figure 3.8, where cases with high Fr_d in g_1 exhibit discernible fluctuations. As illustrated in Figure 3.11, stronger stratification enhances jet mixing, resulting in a more noticeable reduction in $\tilde{c}$, as observed in the left graphs. This behavior is attributed to the jet penetrating into ambient layers with substantially lower $\tilde{c}$ values compared to cases with weaker stratification. The observed concentration decay underscores the influence of the buoyancy gradient in promoting vertical confinement and accelerating $\tilde{c}$ dilution under strongly stratified conditions.

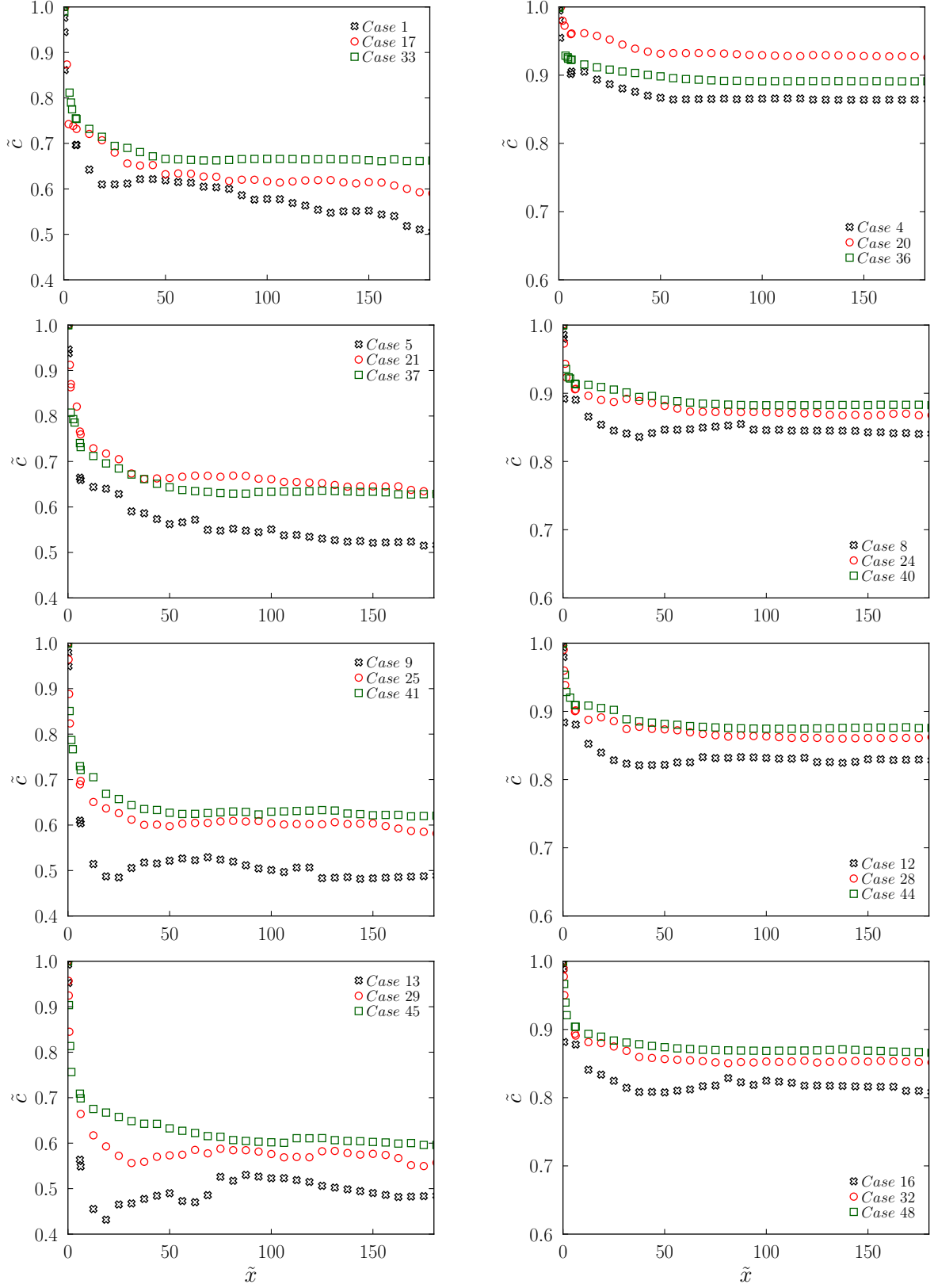


Figure 3.11: Time-averaged normalized concentration $\tilde{c}$ for selected cases with strong stratification (left column $\tilde{N} = 0.100$) and weak stratification (right column $\tilde{N} = 0.050$).

The axial evolution of the passive scalar concentration $\tilde{s}$, presented in Figures 3.A1, exhibits qualitative trends similar to those observed for $\tilde{c}$, including a steep initial decline near the jet source followed by a gradual decay downstream. This behavior reflects the progressive dilution of the scalar with ambient fluid, primarily governed by turbulent mixing and advection downstream by crossflow. The influence of R and $\tilde{N}$ on decay of $\tilde{s}$ aligns with the trends seen in $\tilde{c}$; higher R cases show reduced mixing and slower dilution, while stronger stratification enhances mixing efficiency, resulting in a steeper drop in $\tilde{s}$ near the source. Notably, under strong stratification, the effect of increasing R does not substantially change the decay of $\tilde{s}$, suggesting that enhanced lateral advection does not compensate for the reduced vertical mixing. In contrast, under weak stratification, the increase in R more noticeably suppresses scalar decay, indicating that crossflow momentum becomes the dominant factor in governing mixing dynamics. The effect of Fr_d remains secondary throughout, with only marginal influence on the decay behavior across all stratification levels.

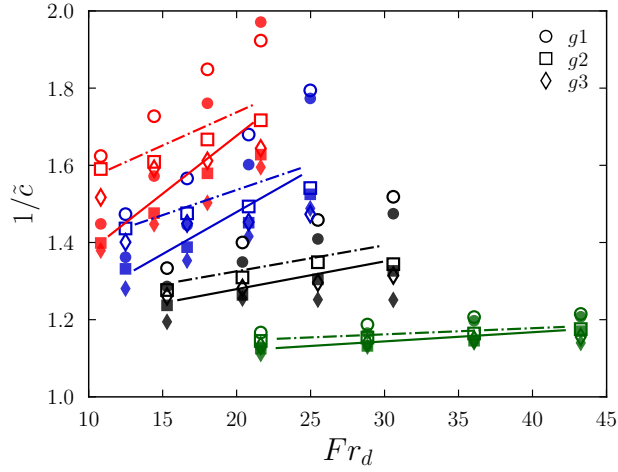


Figure 3.12: Dilution of the jet concentration with respect to bed concentration $1/\tilde{c}$ at y_t (filled markers) and y_r (empty markers). Marker shapes indicate simulation groups (g_1 : circles, g_2 : squares, g_3 : diamonds), and colors correspond to stratification intensities (red: $\tilde{N} = 0.100$, blue: 0.086, black: 0.070, green: 0.050).

Figure 3.12 illustrates the inverse normalized concentration $1/\tilde{c}$, representing the dilution of the jet, plotted against Fr_d . The results show an inverse relationship, as Fr_d increases, dilution increases, indicating that higher jet's momentum results in higher mixing efficiency at both y_t and y_r . This is consistent with the physical expectation that larger Fr_d cause jet to develop more horizontally and increasing entrainment and interaction, which increase dilution. Cases with stronger stratification (red and blue) generally exhibit higher dilution, particularly at high Fr_d , due to increased height that increases mixing early in the jet's path. In contrast, weakly stratified cases show minimal dilution across the Fr_d range, reflecting reduced vertical mixing. Another contributing factor to the elevated $1/\tilde{c}$ observed in strongly stratified cases is the increased concentration gradient between the jet and the ambient fluid at the terminal rise point. The trend lines in the figure represent the overall behavior of dilution, with solid lines corresponding to y_t and dashed lines to y_r . In all stratification intensities, the solid lines lie below the dashed ones, indicating that lower dilution occurs

at y_t . Under strong stratification, the slope of the solid trend line increases with increasing Fr_d , indicating that the reduction in mixing at y_t is more pronounced than y_r as a function of Fr_d . Moreover, the slope of the trend lines across all stratification intensities indicates an overall increase in dilution with rising Fr_d . Notably, the slopes differ among stratification levels, steeper slopes in strongly stratified cases (red and blue) reflect a more sensitivity of dilution to variations in Fr_d , whereas the more gradual slopes observed in weakly stratified groups (black and green) suggest a reduced influence of Fr_d on dilution.

3.3.4 Velocity decay

Figures 3.13 and 3.14 present the time-averaged velocity component $\tilde{v}$ along the jet centerline for cases subjected to strong and weak ambient stratification, respectively. Each subplot compares three cases with constant densimetric Froude numbers (Fr_d), while varying the crossflow velocity. For example, in subplot (a), Cases 1, 17, and 33 have a similar $Fr_d = 10.82$, while the crossflow velocity increases progressively with $R = 0.083, 0.167$, and 0.250 , respectively. Moving from subplot (a) to (d), allowing for the analysis of how vertical velocity evolves under different stratification conditions. For all cases, the $\tilde{v}$ profiles show an initial positive value indicating an upward development of jet from the nozzle, followed by a transition to negative values where transition point to negative value corresponds to the terminal rise point. Generally, higher values of Fr_d lead to larger initial vertical momentum (e.g., Figure 3.13 - d and 3.14 - d), allowing the jet to ascend higher and maintain vertical motion over a longer distance. Conversely, cases with lower Fr_d experience a more rapid decay in vertical velocity due to stronger buoyant suppression (e.g., Figure 3.13 - a and 3.14 - a). An increase in crossflow velocity bends the jet more strongly, shifting the location of the minimum $\tilde{v}$ upstream and decreasing the magnitude of downward motion. This behavior is consistent with the force balance discussed earlier. Higher downward velocities cause stronger fluctuations, leading to the formation of a distinct fluctuating flow region. The vertical velocity experiences substantial decay following the initial and subsequent fluctuations, ultimately diminishing to a negligible level.

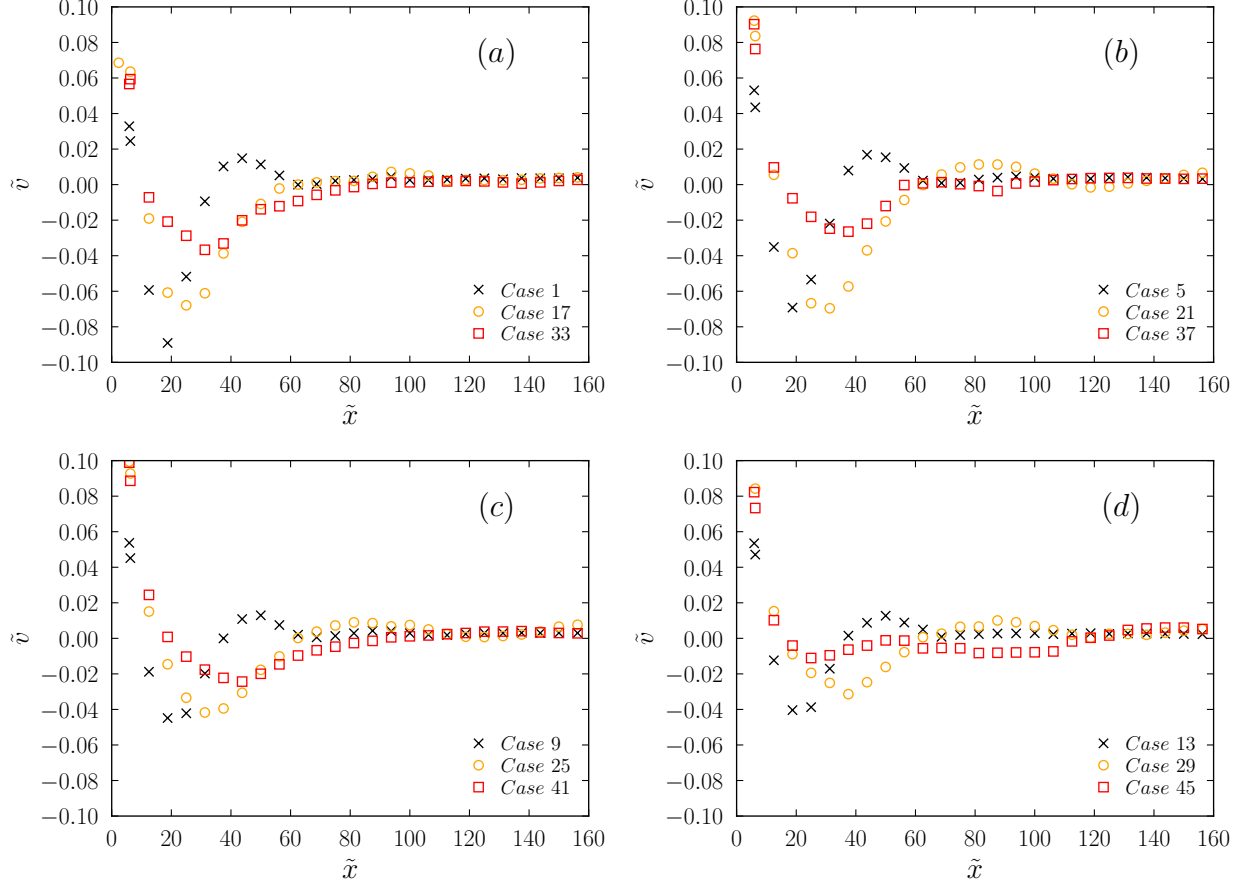


Figure 3.13: Decay of $\tilde{v}$ in the centerline of the jet in an ambient with strong stratification.

It is observed that an increase in R results in a larger decay of the velocity. Specifically, for lower R values (e.g., cases 1, 5, 9 and 13 in Figure 3.13 and cases 4, 8, 12 and 16 in Figure 3.14), the downward velocity of the plume close to the return point is the highest, whereas for higher R values (e.g., cases 33, 37, 41 and 45 in Figure 3.13 and cases 36, 40, 44 and 48 in Figure 3.14), it is the lowest, all while maintaining constant flow conditions of Fr_d and $\tilde{N}$ for each individual subplot. This behavior is primarily governed by the change in the force balance acting on the jet as the crossflow velocity increases. A higher value of R corresponds to stronger crossflow momentum, which exerts a larger horizontal force on the jet and redirects its trajectory more strongly in the streamwise direction. This reorientation reduces the vertical development of the jet by shifting the resultant momentum vector toward the horizontal axis. The comparison of velocities presented in Figures 3.13 and 3.14 reveals that the upward and downward velocities immediately before and after the jet's return point, within the fluctuating region for cases with similar Fr_d and R , are more pronounced under strong stratification conditions (e.g., case 13 and case 4). This is attributed to intensified buoyancy force interactions between the ambient fluid and the jet, i.e., stratification intensity ($\tilde{N}$) is directly correlated with the magnitude of the fluctuating vertical velocity.

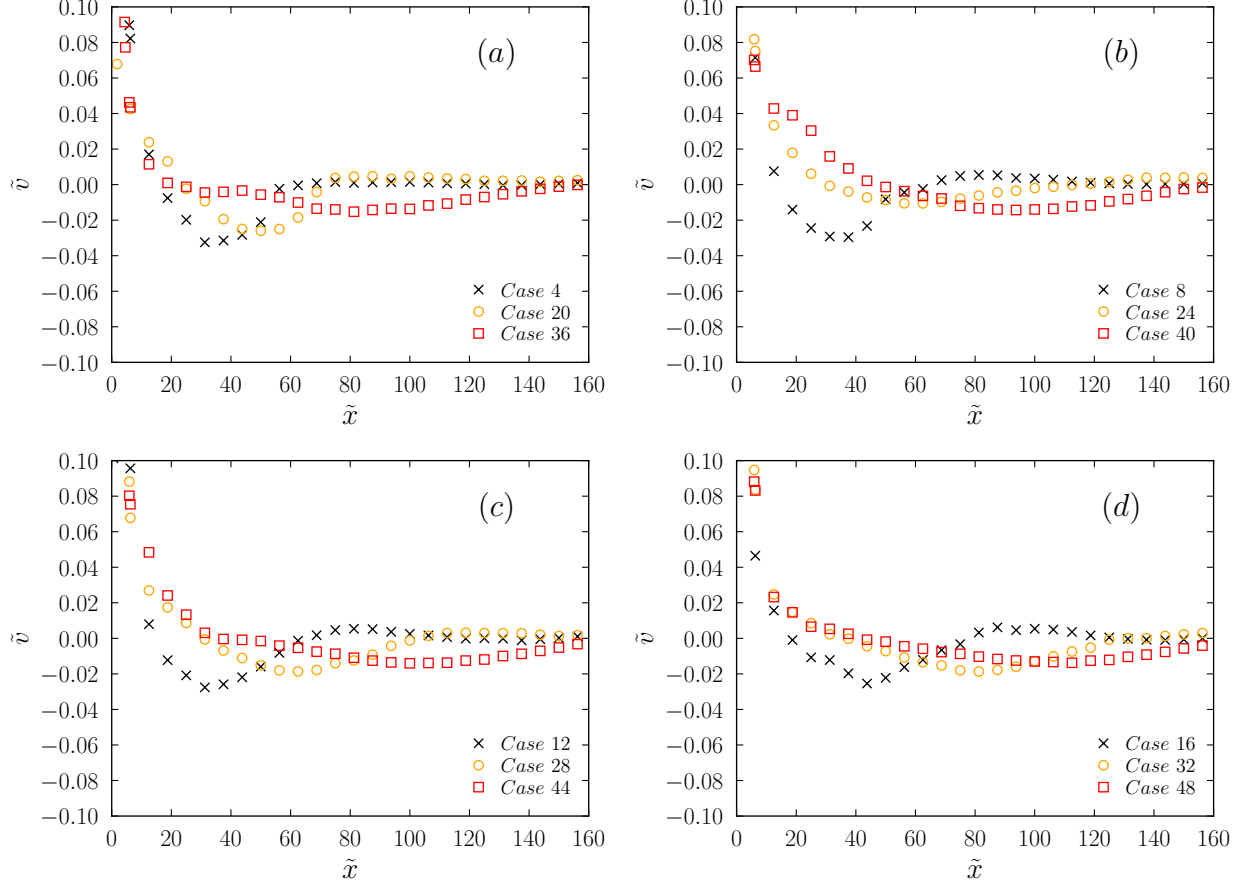


Figure 3.14: Decay of $\tilde{v}$ in the centerline of the jet in an ambient with weak stratification.

3.4 Conclusion

This study employed a high-resolution, nondimensional Large Eddy Simulation (LES) framework to investigate the behavior of negatively buoyant jets discharged into a linearly stratified crossflow. A total of 48 simulation cases were analyzed by varying the densimetric Froude number (Fr_d), crossflow to jet velocity ratio (R), and ambient stratification intensity ($\tilde{N}$). The results elaborate how these parameters influence the jet's trajectory, geometric characteristics, velocity decay, and dilution. An increase in Fr_d enhances the jet's momentum relative to its buoyancy, resulting in a more pronounced vertical rise and extended penetration before reversal. Higher Fr_d cases consistently exhibit greater terminal rise heights ($\tilde{y}_t$) and return point elevations ($\tilde{y}_r$), along with increased values of the vertical rise height after return point ($\tilde{y}_r^*$). This behavior is accompanied by intensified mixing and dilution, leading to reduced jet concentration at the return point. Furthermore, higher Fr_d values promote stronger vertical fluctuations, as evidenced by the increased magnitude of upward and downward motion after the return point. The results indicate that Fr_d plays a dominant role in determining the overall structure, fluctuation intensity, and extent of the jet's upward development and dilution capacity. Variations in R significantly influence the horizontal deflection and vertical

confinement of the jet. Higher R values impose stronger crossflow momentum, bending the jet trajectory in the streamwise direction and thereby reducing its vertical development. This leads to lower terminal rise and return point elevations, as well as decreased vertical velocity magnitudes in the fluctuating region. The data show that increasing R accelerates velocity decay and suppresses vertical fluctuations, ultimately limiting the jet's ability to reach elevated regions and dilute effectively. Additionally, both the terminal rise horizontal distance x_t and the return point horizontal distance x_r extend further downstream with increasing R , reflecting the enhanced horizontal transport imposed by stronger crossflow momentum. The intensity of ambient stratification governs the buoyant interaction between the jet and the surrounding fluid. Weaker stratification (lower $\tilde{N}$) imposes stronger vertical confinement due to limited mixing, hindering the jet's ability to penetrate upward and suppressing vertical fluctuations. In contrast, stronger stratification (higher $\tilde{N}$) provides weaker confinement, enabling the jet to reach higher elevations before reversing direction. This allows for more pronounced vertical development and leads to intensified fluctuation, reflected in elevated values of $\tilde{y}_r^* - \tilde{y}_r$. Future research should focus on exploring the underlying mechanisms of the observed effects and on extending the framework to cover broader parameter ranges, alternative jet configurations (e.g., nozzle angle), and more complex ambient conditions such as non-linear stratification, unsteady crossflows, and wave-induced environments.

Nomenclature

Roman Symbols

d_0	Diameter of nozzle or jet
e_i^g	Direction of the gravitational acceleration
g	Gravitational acceleration
g'	Reduced gravity
k_{Resolved}	Resolved turbulent kinetic energy
k_{sgs}	Unresolved turbulent kinetic energy
u_τ	Friction velocity
u_y	Velocity in y -direction
x_r	Distance of return point in x -direction
x_t	Distance of terminal rise of jet in x -direction
y^+	Non-dimensional wall distance
y_r	Height of return point
y_r^*	Second terminal rise height of jet
y_t	Terminal rise height of jet
y_u	Terminal rise of jet in last measurement location
$\tilde{c}$	Jet dimensionless concentration
$\tilde{c}_b$	Dimensionless concentration at the bottom of channel
$\tilde{c}_t$	Dimensionless concentration at the top of channel
$\tilde{p}$	Filtered dimensionless pressure
$\tilde{s}$	Jet passive scalar concentration
$\tilde{t}$	Dimensionless time
$\tilde{u}_i$	Dimensionless velocity components
$\tilde{x}, \tilde{y}, \tilde{z}$	Dimensionless length in x , y , and z direction
$\tilde{N}$	Stratification intensity
C_s	Smagorinsky coefficient
D	Diffusivity coefficient
Fr_d	Densimetric Froude number
R	Ratio of crossflow velocity to jet velocity
Re	Reynolds number
Re_{cr}	Crossflow Reynolds number
S_{ij}	Strain tensor
Sc	Schmidt number
U_0	Jet velocity
U_r	Crossflow velocity

Greek Symbols

Δ	The filter width
Δ_y	The filter width in the y -direction
ν	Kinematic viscosity
ν_{SGS}	SGS eddy viscosity
ρ_0	Jet density
ρ_a	Ambient density
ρ_b	Channel bed density
ρ_t	Top density
$\tilde{\tau}_{ij}$	Subgrid-scale turbulent stress

Abbreviations

CFL number	Courant Friedrichs Lewy number
FVM	Finite Volume Method
LES	Large Eddy Simulation
LES _{index}	Large Eddy Simulation Index
OpenFOAM	Open Source Field Operation and Manipulation
PIMPLE	Semi-Implicit Method for Pressure-Linked Equations
PISO	Pressure-Implicit of Split-Operations
RANS	Reynolds-Averaged Navier Stokes
SGS	Subgrid-Scale
TKE	Total Kinetic Energy

Appendix - A

Table 3.A1: Summary of LES results for jet trajectory. Columns from left to right are: case number, horizontal distance of terminal rise ($\tilde{x}_t$), vertical distance of terminal rise ($\tilde{y}_t$), horizontal distance of return point ($\tilde{x}_r$), vertical distance of return point ($\tilde{y}_r$), second terminal rise of the jet in the fluctuation region ($\tilde{y}_r^*$), and difference between $\tilde{y}_r^*$ and $\tilde{y}_r$.

Case No.	$\tilde{x}_t$	$\tilde{y}_t$	$\tilde{x}_r$	$\tilde{y}_r$	$\tilde{y}_r^*$	$\tilde{y}_r^* - \tilde{y}_r$
1	6.25	23.05	34.45	5.97	12.04	6.07
2	10.00	25.27	38.75	8.28	13.92	5.65
3	12.50	27.49	43.75	10.85	15.21	4.37
4	13.75	29.71	56.25	14.28	17.75	3.48
5	7.50	31.92	36.52	11.29	17.75	6.46
6	10.50	33.40	42.43	14.21	19.99	5.78
7	12.50	36.36	50.00	17.88	22.50	4.62
8	14.50	37.80	62.75	19.62	23.15	3.53
9	8.23	40.05	38.85	19.74	26.50	6.76
10	11.24	42.27	43.56	23.16	29.23	6.08
11	13.46	43.72	50.00	25.10	29.98	4.88
12	19.35	46.71	68.75	28.31	31.90	3.59
13	8.96	44.56	41.85	26.15	33.12	6.97
14	12.35	46.85	47.50	28.88	35.17	6.30
15	15.46	48.07	53.75	31.18	36.36	5.17
16	21.48	51.55	74.59	35.15	38.88	3.73
17	9.50	16.92	62.25	1.45	6.88	5.43
18	15.50	17.41	71.50	3.99	9.11	5.12
19	20.50	19.40	82.75	6.37	10.60	4.23
20	31.25	21.61	92.25	9.96	13.10	3.14
21	12.50	19.36	65.55	3.98	9.91	5.93
22	16.50	21.10	76.00	5.28	10.65	5.37
23	25.00	23.57	87.25	8.30	12.68	4.37
24	37.50	26.75	97.34	10.80	14.15	3.35
25	13.75	20.16	67.60	7.50	13.78	6.28
26	23.00	22.95	77.95	9.29	14.95	5.66
27	31.25	26.49	87.50	11.13	15.88	4.75
28	40.25	30.44	99.46	14.70	18.08	3.37
29	14.80	22.58	69.56	10.20	16.97	6.77
30	23.50	25.36	80.50	11.44	17.35	5.91
31	37.50	28.97	93.75	11.98	16.97	4.99
32	43.75	34.14	102.00	15.82	19.28	3.46
33	16.67	7.48	87.50	1.38	4.18	2.80
34	21.27	7.96	89.15	2.23	5.03	2.80
35	28.47	9.47	112.50	2.55	5.08	2.53
36	38.75	12.08	118.75	3.23	5.38	2.14
37	24.63	10.83	93.45	3.23	6.48	3.25
38	33.13	14.71	95.50	4.78	7.98	3.19
39	38.03	20.65	116.75	7.12	10.15	3.03
40	59.80	23.96	125.75	8.78	11.35	2.57
41	28.46	15.04	97.20	5.72	9.19	3.47
42	35.94	19.51	101.07	7.13	10.50	3.37
43	43.13	23.08	115.75	8.03	11.13	3.09
44	64.69	25.16	120.75	12.78	15.49	2.71
45	34.50	15.84	100.50	4.58	8.07	3.49
46	39.39	18.86	102.25	8.18	11.69	3.52
47	45.43	23.98	117.75	9.09	12.32	3.23
48	65.89	29.82	120.75	14.96	17.93	2.97

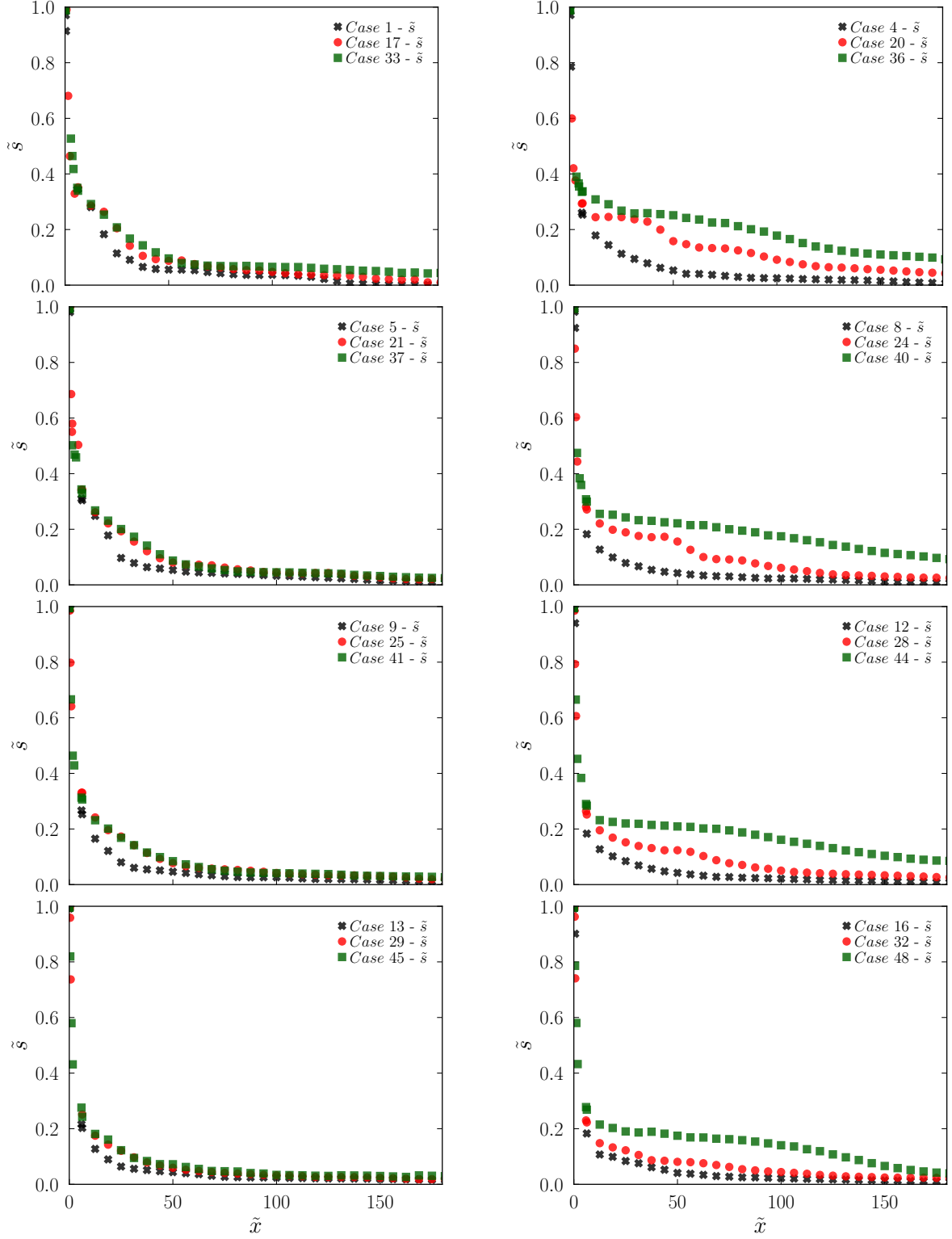


Figure 3.A1: Time-averaged normalized concentration $\tilde{s}$ for selected cases with strong stratification (left column $\tilde{N} = 0.100$) and weak stratification (right column $\tilde{N} = 0.050$).

Chapter 4

Multifidelity Numerical Modeling and Bayesian Hierarchical Prediction of the Desalination Discharges

4.1 Introduction

Desalination plants are essential for supplying potable water in arid and semi-arid regions, where natural freshwater resources are increasingly constrained [202]. These facilities generate effluents with elevated salinity, increased temperature, or a mixture of both (e.g., [6, 203]), which are typically released back into the environment [204]. Wastewater discharged through jets develop negatively or positively buoyant flows, depending on the density difference between the effluent and the receiving ambient water and the jet momentum direction. When the buoyancy force acts in the same direction as the jet momentum, the discharge is classified as positively buoyant, whereas it is considered negatively buoyant when the buoyancy opposes the momentum. In addition to jet characteristics such as the densimetric Froude number (Fr_d , see Eq. 4.1) and the angle of inclination, the interaction between the jet and the ambient environment governs the mixing and dispersion of effluents [25, 26, 39, 46, 46, 205, 206, 206, 207]. A comprehensive understanding of jet behavior is essential for optimizing outfall design in order to enhance dilution efficiency and mitigating adverse environmental impacts.

Research on desalination discharges has traditionally relied on experimental approaches, e.g., laser induced fluorescence (LIF) and particle image velocimetry (PIV), or on computational fluid dynamics (CFD) simulations [2, 13, 14, 39, 208]. While these methods have provided valuable insights, they are also subject to important limitations, experimental investigations are constrained by setup configurations, facility requirements, and measurement uncertainties, whereas numerical simulations demand substantial computational resources and their predictive accuracy is highly dependent on the fidelity of the turbulence models employed. Early numerical studies of buoyant jet simulations predominantly used Reynolds averaged Navier-Stokes (RANS) models, which showed intrinsic limitations in reproducing dilution rates and jet trajectories, leading to discrepancies compared with experimental data e.g., [45, 47, 73]. In contrast, large eddy simulation (LES) resolves the energy containing turbu-

lent structures while modeling the smaller scales with a subgrid-scale modeling, providing a more accurate results of mixing and jet trajectory at Reynolds numbers typical of environmental flows. Applications of LES to desalination jets by Zhang et al. (2015) and Zhang et al. (2016) demonstrated that LES can reproduce jet trajectory and dilution with close agreement to experimental observations, representing a marked improvement over conventional RANS models. Similar conclusions were achieved by Jiang et al. (2019), and by Songa et al. (2020), who reported improved prediction of mean trajectories, while Law et al. (2023) showed that dynamic SGS modeling further enhances consistency with experimental results. These studies establish LES as a more reliable high-fidelity (HF) approach for simulating desalination discharges, offering improved accuracy in trajectory and dilution predictions compared with RANS low-fidelity (LF) while maintaining computational feasibility.

As the number of the parameters under study increases, conducting only HF modeling (both numerical and physical) is impractical due to their high costs. Conversely, LF models like RANS can be conducted more rapidly across a wide range of parameters, but they inevitably introduce inaccuracies. These limitations highlight the need for alternative strategies that can exploit the complementary strengths of different fidelity levels, motivating the development of multifidelity surrogate modeling approaches. The main challenge of developing a surrogate or machine learning (ML) model for predicting desalination jet behavior is their dependence on large datasets to ensure reliable training and validation. The number of experimental or numerical cases required depends on the complexity of the applied model and the physical phenomena under study. Alvir et al. (2023) used a large dataset comprising 500 RANS simulations to investigate and predict the geometrical features of negatively inclined buoyant jets. Similarly, Yan et al. (2023) conducted 100 RANS simulations to model effluent mixing and transport using their proposed parameter based field reconstruction convolutional neural network (PFR-CNN) and Random Forest algorithms. Zhao et al. (2022) utilized a comparatively smaller experimental dataset of 58 runs, resulting in 442 data points for their adaptive neuro fuzzy inference system (ANFIS) model. As HF, e.g., LES, DES or LIF and PIV, simulations are time consuming and expensive, all these studies relied on LF, i.e., RANS, simulations to generate training datasets for their ML models. While using LF data reduces computational costs, it inherently limits the predictive accuracy of the resulting models to the resolution and quality of the LF data. Multi-fidelity (MF) ML models address these challenges by combining less costly LF simulations with more accurate HF results to achieve a better balance between predictive accuracy and computational efficiency [212]. These approaches are particularly advantageous for studying turbulent flows, crucial in numerous engineering applications where the high computational cost of HF methods or lab experiments can be prohibitive.

This study develops a multifidelity (MF) surrogate model based on a Gaussian Process (GP) framework [213, 214] to predict the behavior of desalination discharges. The model combines RANS simulations as low-fidelity (LF) data and LES as high-fidelity (HF) data to achieve an effective balance between computational cost and predictive accuracy, while using TV to correct residual errors and ensure consistency across fidelity levels. The Bayesian formulation connects LF and HF through hierarchical inference, systematically correcting LF bias, calibrating parameters across fidelity levels, and propagating uncertainty through the predictive framework. This approach addresses the limitations of previous machine learning models that relied solely on LF datasets and were therefore constrained by their limited physical

accuracy. By integrating data of different fidelities, the proposed MFGP provides accurate and uncertainty aware predictions of desalination jet behavior while substantially reducing the computational and experimental effort. To assess the performance and generality of the proposed framework, two distinct scenarios were investigated, encompassing a wide range of hydrodynamic conditions and fidelity combinations to evaluate the predictive capability and robustness of the MFGP model. The remainder of this paper is organized as follows: §4.2 describes the numerical and Bayesian machine learning methodologies used to study desalination discharges, §4.3 presents the main results, §4.4 provides the discussion and sensitivity analyses, and §4.5 summarizes the key findings and implications for design and environmental assessment.

4.2 Method

4.2.1 Dimensional analysis

The behavior of dense jets is characterized by the dimensionless Froude number (Fr_d), which represents the balance between inertial and buoyancy forces. This parameter plays a crucial role in analyzing dense jet dynamics, as it indicates whether momentum force or buoyancy force is dominant. The Fr_d is defined as:

$$Fr_d = \frac{U_0}{\sqrt{g'd_0}} \quad (4.1)$$

where U_0 represents the bulk velocity magnitude, d_0 denotes the nozzle diameter, and g' refers to the reduced gravity, defined as:

$$g' = g \frac{\rho_0 - \rho_a}{\rho_a} \quad (4.2)$$

where g represents the gravitational acceleration, ρ_0 denotes the initial jet density, and ρ_a refers to the density of the ambient fluid.

4.2.2 Governing equations for CFD simulations

In the CFD simulations conducted in this study, the transport of momentum and mass is governed by the incompressible Navier-Stokes equations, coupled with an advection-diffusion equation to represent buoyancy effects. LES and RANS turbulence closures are applied using a finite volume method in non-dimensional form as follows [40, 85, 88, 224]:

$$\frac{\partial \tilde{u}_i}{\partial \tilde{x}_i} = 0 \quad (4.3)$$

$$\frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j \partial \tilde{x}_j} - \frac{\partial \tilde{\tau}_{ij}}{\partial \tilde{x}_j} + e_i^g \frac{1}{Fr_d^2} \tilde{c} \quad (4.4)$$

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{c}}{\partial \tilde{x}_i} = \frac{1}{ReSc} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}_i \partial \tilde{x}_i} - \frac{\partial \tilde{\tau}_i^c}{\partial \tilde{x}_i} \quad (4.5)$$

where $i, j = 1, 2, 3$, p represents the pressure, u_i denotes the i -th velocity component, t is time, and τ for LES refers to the subgrid-scale (SGS) stress tensor and for RANS is Reynolds stress tensor. The term e_i^g indicates the direction of gravitational acceleration, given as $(0, -1, 0)$, while c represents the salinity concentration. The Reynolds number (Re) is defined as $Re = U_0 d_0 / \nu$, where ν is the kinematic viscosity [89–92]. In LES, the large turbulent eddies are directly resolved, while the smaller scales are modeled. In contrast, RANS models represent all turbulent fluctuations through statistical averaging over time, providing the mean flow behavior without resolving any instantaneous turbulent structures [104, 192, 215–217]. The Schmidt number (Sc) is given by $Sc = \nu / D$. The constant values of kinematic viscosity and mass diffusivity, ν and D , are set to 1×10^{-6} (m^2/s) and 1.5×10^{-9} (m^2/s), respectively [93, 94]. Dimensionless variables are formulated using characteristic length, velocity, and time scales, as outlined in Table 4.1.

Table 4.1: Definition of non-dimensionalization used in this work.

Parameter	Non-dimensionalization
Spatial coordinates	$\tilde{x}_i = x_i / d_0$
Velocity	$\tilde{u}_i = u_i / U_0$
Time	$\tilde{t} = (U_0 / d_0) t$
Pressure	$\partial \tilde{p} / \partial \tilde{x}_i = (d_0 / \rho_a U_0^2) \partial p / \partial x_i$
Subgrid-scale stress tensor	$\partial \tilde{\tau}_{ij} / \partial \tilde{x}_j = (d_0 / U_0^2) \partial \tau_{ij} / \partial x_j$
Salinity	$\tilde{c} = c / C_0$

To close the equations, the Wall-Adapting Local Eddy-Viscosity (WALE) model is employed for LES due to its capability to accurately capture near-wall turbulence by considering both strain and rotation rates, which are essential in wall-bounded flows and for RANS model, the k - ε RNG model is adopted. Detailed formulations of the closure terms can be found in [40, 88, 96, 184, 218].

4.2.3 Bayesian hierarchical multifidelity model

A three-level Bayesian hierarchical multifidelity Gaussian process (MFGP) model was adopted following the general structure of Goh et al. [213], Kennedy and O’Hagan [219], Qian et al. [220] and the implementation strategy of Rezaeiravesh et al. [212]. The approach hierarchically integrates the information from low-fidelity (LF), high-fidelity (HF), and true-value (TV) datasets in a unified Bayesian framework. In this study, RANS, LES, and experimental measurements (if available) are used as LF, HF, and TV data, respectively. This construction allows the LF simulations to provide broad parametric coverage, while the HF and TV data correct the bias and improve predictive accuracy.

Let $\mathbf{x} \in [0, 1]^d$ denote the design variables normalized to the unit interval across all fidelity levels, while the responses remain in their physical units. The three fidelities are denoted by

L (LF), H (HF), and T (TV). The hierarchy can be written as:

$$Y_L(\mathbf{x}) = f(\mathbf{x}, t_3, t_s) + \varepsilon_L, \quad (4.6)$$

$$Y_H(\mathbf{x}) = f(\mathbf{x}, \theta_3, t_s) + g(\mathbf{x}, t_2, t_s) + \varepsilon_H, \quad (4.7)$$

$$Y_T(\mathbf{x}) = f(\mathbf{x}, \theta_3, \theta_s) + g(\mathbf{x}, \theta_2, \theta_s) + \delta_T(\mathbf{x}) + \varepsilon_T, \quad (4.8)$$

where $f(\cdot)$ and $g(\cdot)$ are two shared latent Gaussian processes (GPs). The first latent process $f(\cdot)$ represents the global trend learned from all fidelities, while $g(\cdot)$ captures additional variations resolved by the HF and TV levels. The top-level discrepancy $\delta_T(\cdot)$ accounts for residual structural bias between the model predictions and the true values. The calibration parameters $(\theta_3, \theta_2, \theta_s)$ are global and inferred during Bayesian training, whereas (t_3, t_2, t_s) represent per-sample calibration inputs for LF and HF data.

Gaussian processes employ covariance kernels to define the correlation structure of the latent functions and discrepancy terms. In this study, each latent component is modeled using an anisotropic Matérn-5/2 kernel with automatic relevance determination (ARD), which assigns distinct length-scales to each input dimension and calibration parameter. The kernel is written as

$$k_j(\mathbf{r}) = \lambda_j^2 \left(1 + \frac{\sqrt{5}r}{\ell_j} + \frac{5r^2}{3\ell_j^2} \right) \exp\left(-\frac{\sqrt{5}r}{\ell_j}\right), \quad j \in \{f, g, \delta_T\}, \quad (4.9)$$

where r is the scaled distance between two feature points, λ_j is the process amplitude, and ℓ_j is the ARD length-scale vector controlling the smoothness of each process. This kernel choice provides flexibility to represent multi-dimensional correlations and varying sensitivities across the input space, consistent with Rezaeiravesh et al. [212]. Independent weakly informative priors are assigned to all model parameters:

$$\mu \sim \mathcal{N}(0, s_\mu^2), \quad \lambda_f, \lambda_g, \lambda_{\delta_T} \sim \text{Half-Cauchy}(0, \beta_\lambda), \quad (4.10)$$

$$\sigma_T, \sigma_H, \sigma_L \sim \text{Half-Cauchy}(0, \beta_\sigma), \quad \ell_j \sim \text{Gamma}(\alpha_\ell, \beta_\ell), \quad \theta_3, \theta_2, \theta_s \sim \mathcal{U}(0, 1). \quad (4.11)$$

Here, μ denotes the constant mean, σ_i are the noise standard deviations for each fidelity, and $\theta_3, \theta_2, \theta_s$ represent the global calibration parameters. The joint posterior distribution combines the likelihood and the priors as

$$\pi(\Theta \mid \mathbf{Y}) \propto \mathcal{N}(\mathbf{Y} - \mu\mathbf{1}; 0, \Sigma(\Theta)) \times \pi_0(\Theta), \quad (4.12)$$

where $\Sigma(\Theta)$ is the hierarchical covariance matrix constructed from the latent Gaussian processes and fidelity-specific noise, and Θ denotes all hyperparameters and calibration parameters.

Because this posterior has no closed form, inference is performed using a Random-Walk Metropolis–Hastings Markov Chain Monte Carlo (MCMC) algorithm. Parameters constrained to be positive, such as amplitudes, kernel length-scales, and noise variances, are sampled on a logarithmic scale, while bounded calibration parameters are sampled through logit transformations.

Predictions for a new input $\mathbf{x}_*$ are obtained from the conditional multivariate normal distribution:

$$Y_T(\mathbf{x}_*) \mid \mathbf{Y}, \Theta \sim \mathcal{N}(\mu_{\text{pred}}, \Sigma_{\text{pred}}), \quad (4.13)$$

with

$$\mu_{\text{pred}} = K_*^\top K^{-1} \mathbf{Y}, \quad \Sigma_{\text{pred}} = K_{**} - K_*^\top K^{-1} K_*. \quad (4.14)$$

Posterior predictions are then averaged over all MCMC samples to yield the Bayesian predictive mean and CIs that quantify both model and parameter uncertainties across fidelity levels.

4.2.4 Case study configurations

To evaluate the performance of the proposed multifidelity model, two representative scenarios were considered. In the first scenario, the model was trained using two fidelity levels, RANS simulations as LF dataset and LES as HF dataset. The true values (TV) obtained from validated LES were not used for model training but rather for independent validation and error quantification. The MFGP was applied to investigate the influence of water depth (H_t) and densimetric Froude number (Fr_d) on the behavior of a 60-degree desalination jet in a shallow water environment. The simulations cover Fr_d values ranging from 10 to 40, chosen to capture the interaction between inertial and buoyant forces, which are essential for determining the jet trajectory and mixing efficiency. Additionally, the water depth (H_t) is varied from 10 to 20 times the jet diameter (d_0), resulting in Fr_d/H_t values ranging from 0.5 to 2.8, representing different flow regimes in shallow ambient conditions. The Reynolds number was set constant at ($Re = 3536$) across all simulations. A total of 24 RANS simulations were performed to serve as LF data, while 11 LES simulations were conducted as the TV reference. Among these, four LES simulations were designated as HF data. For the MF study, a combined dataset consisting of 24 RANS and 4 LES simulations was utilized. The detailed characteristics of the conducted simulations are presented in Table 4.2.

Table 4.2: Characteristics of first scenario TV, HF, LF and MF simulations

Case No.	Fr_d	H_t	Fr_d/H_t	TV	HF	LF	MF
1	10	20	0.50	LES	LES	RANS	LES and RANS
2	10	17.5	0.57	LES		RANS	RANS
3	10	15	0.67	LES		RANS	RANS
4	15.0	20	0.75			RANS	RANS
5	10	12.5	0.80	LES		RANS	RANS
6	15.0	17.5	0.86			RANS	RANS
7	10.0	10	1.00	LES	LES	RANS	LES and RANS
8	20	17.5	1.14			RANS	RANS
9	15.0	12.5	1.20			RANS	RANS
10	25.0	20	1.25			RANS	RANS
11	20	15	1.33			RANS	RANS
12	25.0	17.5	1.43			RANS	RANS
13	30	20	1.50	LES		RANS	RANS
14	20	12.5	1.60			RANS	RANS
15	25.0	15	1.67			RANS	RANS
16	30	17.5	1.71			RANS	RANS
17	35.0	20	1.75			RANS	RANS
18	40	20	2.00	LES	LES	RANS	LES and RANS
19	40	17.5	2.29	LES		RANS	RANS
20	35	15	2.33	LES		RANS	RANS
21	30	12.5	2.40			RANS	RANS
22	25.0	10	2.50	LES		RANS	RANS
23	40	15	2.67	LES		RANS	RANS
24	35.0	12.5	2.80	LES	LES	RANS	LES and RANS

In the two-level MFGP model in the first scenario, LF simulations were designed to provide broad coverage across the entire Fr_d/H_t range, taking advantage of their low computational cost, whereas the HF cases were selectively chosen from the TV dataset to ensure representative sampling across all flow regimes while maintaining feasible computational expense. The second scenario focuses on a vertical thermal desalination jet, where LIF experimental data were incorporated alongside RANS and LES simulations to construct a three-level multifidelity framework. In this case, Fr_d ranged from 5 to 30, while the Reynolds number was fixed at $Re = 3100$. The dataset was designed to evaluate the performance of the proposed model in predicting the concentration field of thermal jets under different Fr_d . In this configuration, RANS simulations served as the LF, LES as HF, and the LIF measurements provided the TV reference for calibration and validation. The three levels were hierarchically integrated within MFGP framework, where LF data established the global trend across the parameter space, HF data corrected systematic LF bias, and TV data further refined the predictions and quantified uncertainty at the experimental conditions. Here, the LF simulations covered the entire range of Froude numbers considered in the study, the HF simulations were uniformly distributed across this range, and the TV data from the LIF experiments

were obtained at selected conditions based on experimental feasibility in the laboratory. This configuration allowed the model to achieve high predictive accuracy even with sparse experimental data, demonstrating its capability to efficiently combine numerical and physical observations. The detailed characteristics of the thermal jet cases are summarized in Table 4.3.

Table 4.3: Characteristics of second scenario TV, HF, LF and MF simulations

Case No.	Fr_d	TV	HF	LF	MF
1	5		LES	RANS	LES and RANS
2	6			RANS	RANS
3	7			RANS	RANS
4	8		LES	RANS	LES and RANS
5	9			RANS	RANS
6	10			RANS	RANS
7	11			RANS	RANS
8	12	LIF	LES	RANS	RANS, LES and LIF
9	13			RANS	RANS
10	14			RANS	RANS
11	15	LIF	LES	RANS	RANS, LES and LIF
12	16			RANS	RANS
13	17			RANS	RANS
14	18			RANS	RANS
15	19			RANS	RANS
16	20	LIF	LES	RANS	RANS, LES and LIF
17	21			RANS	RANS
18	22			RANS	RANS
19	23			RANS	RANS
20	24			RANS	RANS
21	25	LIF	LES	RANS	RANS, LES and LIF
22	26			RANS	RANS
23	27			RANS	RANS
24	28			RANS	RANS
25	29			RANS	RANS
26	30			RANS	RANS

4.2.5 Numerical simulation setup for the first scenario

The simulations in this study are conducted by a customized version of the OpenFOAM solver, pimpleFOAM, designed for incompressible flow coupled with an advection-diffusion equation ¹. The governing equations for fluid flow and salinity transport were solved in a non-dimensional form, as detailed in §4.2.2. A hybrid approach known as the PIMPLE algorithm (Pressure Implicit with SIMPLE-PISO, where SIMPLE denotes the Semi-Implicit

¹https://github.com/HydroCFD/buoyant_jet

Method for Pressure-Linked Equations and PISO denotes the Pressure Implicit with Splitting of Operators) is employed to address the pressure-velocity coupling of the Navier-Stokes equations. For further information on the PIMPLE algorithm and its implementation in OpenFOAM, refer to [95–97]. Temporal discretization of the time-derivative terms was carried out using a backward scheme, ensuring second-order accuracy. Gradient terms were discretized employing the Gauss-linear method, while divergence terms were handled using the Gauss limitedLinear scheme to enhance solution stability in regions with steep gradients. Viscous terms were discretized using the Gauss linear scheme, whereas the Laplacian terms were approximated with the Gauss linear uncorrected scheme [99, 100]. To maintain numerical stability and accuracy throughout the simulations, adaptive time-stepping was employed, ensuring that the Courant-Friedrichs-Lewy (CFL) number remained below 0.5 for both RANS and LES cases. For the LES, simulations were continued until a statistically stationary state was reached, defined as the point where the time-averaged flow quantities (e.g., time-averaged of velocity, turbulence kinetic energy) no longer exhibited significant temporal variation. After reaching this state, flow quantities were averaged over a period of 70,000 to 80,000 non-dimensional time units.

Figure 4.A1 presents a schematic illustration of the buoyant jet in a shallow ambient for the first scenario. The nozzle diameter is used as the characteristic length scale ($d_0 = 1$) to generate the geometry in a non-dimensional form. To eliminate any influence of upstream or downstream boundary conditions on jet dynamics, the domain was designed to be sufficiently large, with a length of $l_x = 800d_0$ and a width of $l_z = 600d_0$, while the height varied depending on the specific cases. A circular jet was positioned at coordinates $(0, 0, 0)$, located $5d_0$ above the bed. A quiescent initial condition ($\tilde{u} = 0$, $\tilde{c} = 0$) was imposed throughout the tank before initiating the simulations. The free surface effects were neglected, and the top boundary was modeled with a slip condition to simulate open boundary behavior. A no-slip wall boundary condition was applied at the bottom surface. The side, front, and back boundaries were specified as inlet-outlet conditions, permitting fluid to enter or exit the domain in response to the instantaneous pressure and velocity fields, thereby allowing the flow to adapt dynamically to changing conditions. Distinct meshes were generated for each case, adhering to the criteria specified in [85] to ensure adequate resolution for LES simulations, while a mesh independence study was conducted for RANS simulations. The mesh generation process utilized a multi-level refinement strategy implemented through the open-source software Gmsh, with targeted resolution enhancement in regions of interest [101]. A representative example of the mesh used in this study is presented in Figure 4.1. Hexahedral cells were employed throughout the entire domain, the jet was discretized using an O-grid model, to provide a smooth transition from the circular jet to the square shape of the computational domain. The mesh resolution was designed to capture more than 95% of the total kinetic energy of the jet; however, it is important to note that the Batchelor scales were not resolved in this study. In LES cases, the pipe was extended $7.5d_0$ downward from the jet inlet and the mapped inlet boundary condition explained in [224] is used. This extension was incorporated to accurately resolve the flow development and turbulence structures within the pipe before the jet exits into the tank. Since LES requires capturing detailed turbulence dynamics, the inclusion of the pipe ensures that the inflow conditions are well-developed and realistic, enhancing the accuracy of the simulation. For RANS cases, no pipe extension was included as the RANS models rely on time-averaged equations and turbulence closures, making the detailed resolution of

flow development within the pipe less critical. Instead, the jet inlet was directly defined at the tank boundary, as RANS primarily focuses on predicting mean flow behavior rather than resolving instantaneous turbulent structures.

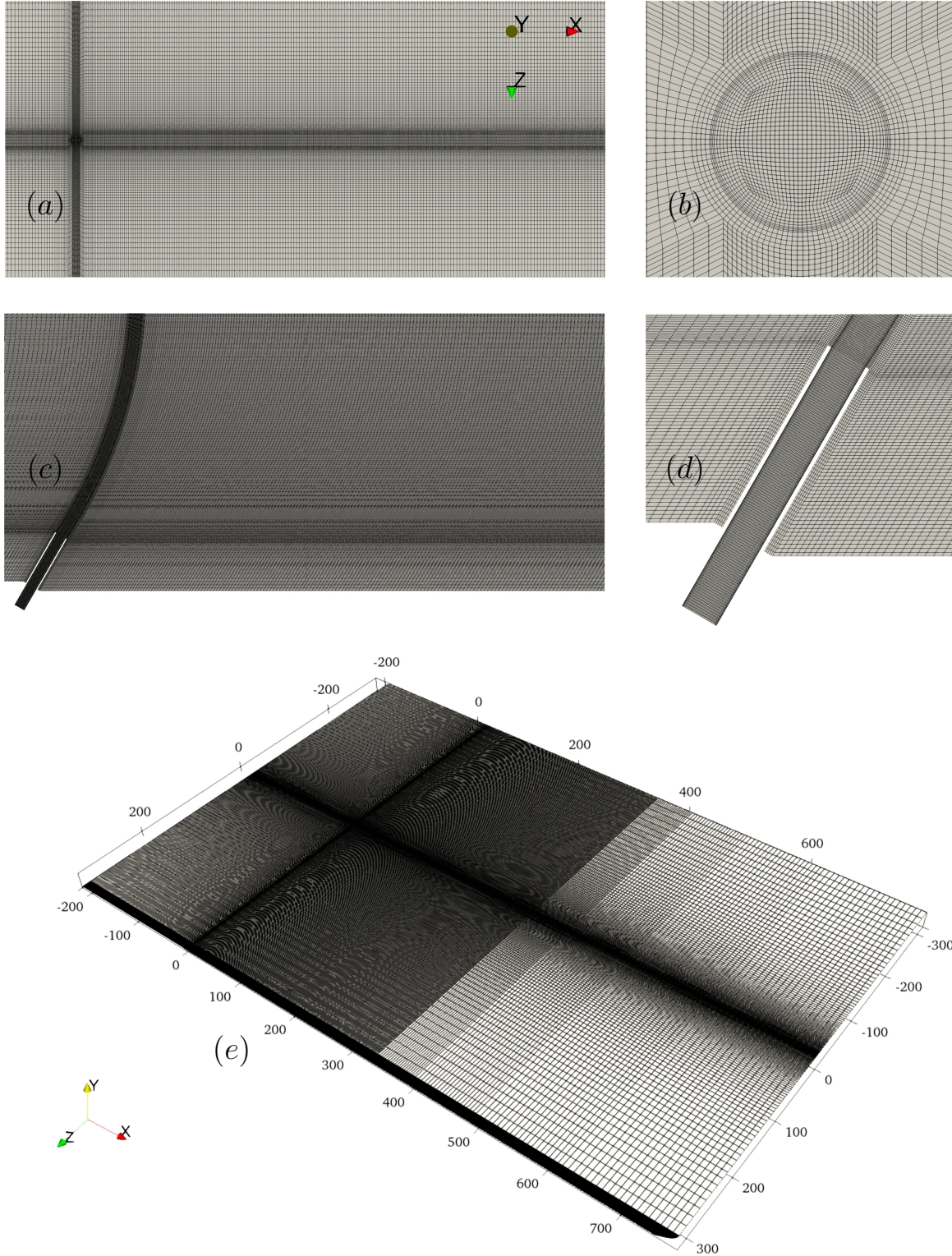


Figure 4.1: A visualization of the computational mesh of the first scenario for LES: (a) top view of domain; (b) top view of the pipe and transition to square mesh; (c) slice in the middle of domain (d) jet slice with wall refinements; (e) full view of domain.

Figure 4.1 illustrates key regions of the mesh employed for LES simulations: (a) shows the expanding horizontal surface (x - z) above the jet, (b) presents the top view of the nozzle pipe, (c) and (d) display a middle slice of the domain, highlighting the refined mesh near the nozzle, and (e) depicts the overall mesh structure. The jet was discretized using 48 cells across its diameter, with near-wall refinements to ensure accurate resolution of boundary layer effects. In the region of interest, the cell size was maintained at less than 2% of the jet diameter to capture the critical flow features effectively.

4.2.6 Validation of LES for first scenario

Figure 4.2 presents a comparison between the LES predicted vertical velocity profiles and the high-resolution PIV measurements at the normalized streamwise location $\tilde{x} = 10$, corresponding to the jet-like region before the jet reaches the free surface. For all investigated Froude numbers ($Fr_d = 15, 25$, and 30), the LES results accurately capture the jet core structure and the decay of velocity across the shear layers. The centerline velocities and the spreading behavior of the jet are in excellent agreement with the experimental measurements, with only minor deviations observed near the peak velocity region. The LES predictions demonstrate a strong ability to resolve the primary momentum transport mechanisms at this early stage of jet development, validating its fidelity in reproducing jet-like turbulent structures under buoyancy-driven conditions.

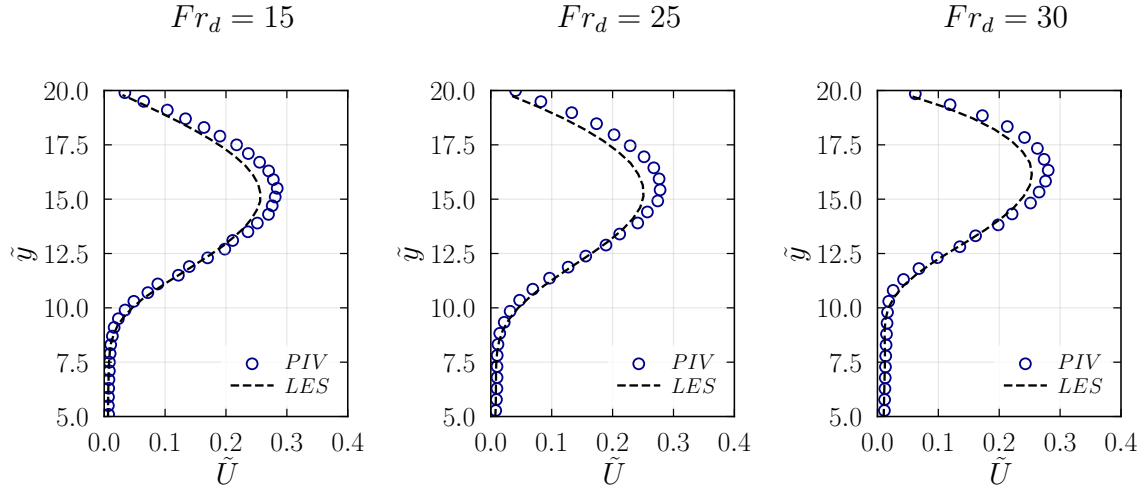


Figure 4.2: Velocity field of the LES and PIV at $\tilde{x} = 10$.

Figure 4.3 illustrates the velocity profiles at $\tilde{x}/Fr_d = 1.5$, where the jet has interacted with the water surface, initiating complex mixing processes. As the jet impinges upon the surface, momentum diffusion becomes more pronounced, leading to a broader velocity distribution and a decrease in the peak centerline velocity. The LES successfully captures these critical transitions, accurately predicting both the extent of lateral spreading and the reduction in velocity magnitude. Compared to the PIV data, the LES exhibits excellent predictive capability, reproducing the effects of surface confinement on the jet dynamics. Minor dis-

crepancies at the peripheries can be associated with three-dimensional effects and surface perturbations, which are challenging to capture through solid boundary in LES. Nonetheless, the LES effectively resolves the large-scale coherent structures and turbulent mixing induced by the surface interaction.

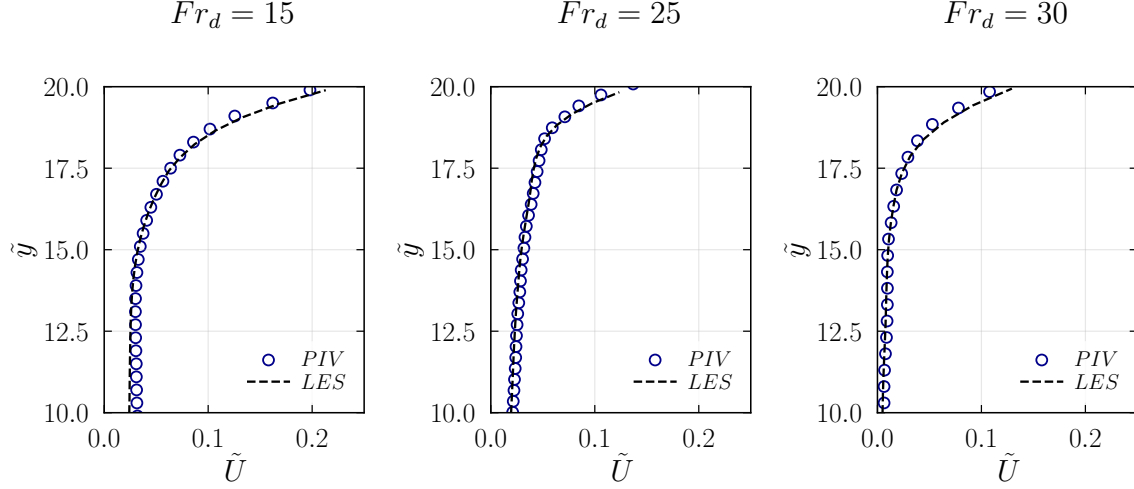


Figure 4.3: Velocity field of the LES and PIV at $\tilde{x}/Fr_d = 1.5$.

In Figure 4.4, the comparison is shown at $\tilde{x}/Fr_d = 3$, representing a more advanced mixing stage where the jet has substantially spread and interacted with the ambient environment. At this location, the velocity profiles exhibit a significant decay in peak velocity and a widened jet cross-section due to enhanced turbulent entrainment and buoyancy-driven dispersion. The LES predictions maintain remarkable agreement with the PIV measurements, accurately capturing the broader spatial distribution and the attenuation of momentum. This strong agreement even at farther downstream locations highlights the robustness of the LES approach in resolving complex turbulence structures and anisotropic mixing phenomena that occur after surface interaction. In contrast to conventional RANS modeling, which often fails to predict detailed turbulent dynamics, LES proves capable of reliably simulating the intricate evolution of dense buoyant jets in shallow ambient environments.

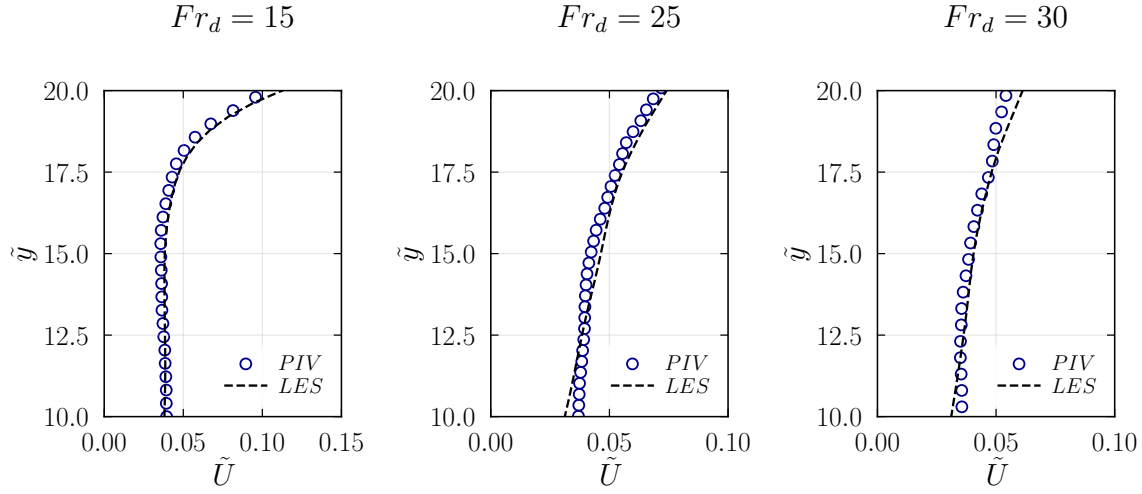


Figure 4.4: Velocity field of the LES and PIV at $\tilde{x}/Fr_d = 3$.

4.2.7 Numerical simulation setup for the second scenario

In the second scenario, RANS simulations were performed using an axisymmetric domain, which significantly reduced the computational cost while retaining the essential jet dynamics. A constant inlet velocity profile was imposed at the nozzle boundary. This profile was not uniform but obtained from a separate fully developed LES pipe simulation, where the velocity distribution was averaged over time to provide realistic inflow conditions. The LES simulations, by contrast, were conducted in a full three-dimensional cylindrical domain, similar to the configuration adopted for the first scenario. Structured hexahedral meshes were used with local refinement in the near-field region around the nozzle and along the jet axis to ensure accurate resolution of turbulent structures. The inflow conditions for LES were also prescribed using the fully developed velocity profile obtained from the precursor pipe simulation. This setup ensured that the LES accurately reproduced turbulent structures and mixing processes from the jet exit, while the axisymmetric RANS configuration enabled efficient coverage of a larger parameter space.

The mesh for the second scenario was generated by Gmsh similar to first scenario. Figures 4.5 a – c correspond to the RANS configuration, where an axisymmetric domain discretized with a structured hexahedral mesh was used. Mesh refinement was applied near the jet and along the jet centerline to resolve steep gradients in momentum and scalar transport. Figure 4.5 - a shows the top view of the axisymmetric domain, Figure 4.5 - b presents a slice through the mid-plane, and Figure 4.5 - c is a zoomed view of the near-field region close to the jet inlet area, showing the local grid refinement. Figures 4.5 d - f show the computational mesh adopted for the LES simulations. The LES domain was constructed as a three dimensional cylindrical geometry discretized with a structured hexahedral mesh. Refinement was applied near the jet outlet and along the jet axis to adequately resolve turbulent structures and scalar gradients. Figure 4.5 - d presents the full three dimensional view of the cylindrical domain, Figure 4.5 - e illustrates a longitudinal slice through the mid-plane parallel to the jet stream direction, and Figure 4.5 - f displays a cross-sectional slice perpendicular to the jet stream direction. This configuration ensured sufficient spatial resolution both in the near-field mixing region and in the far-field development of the jet.

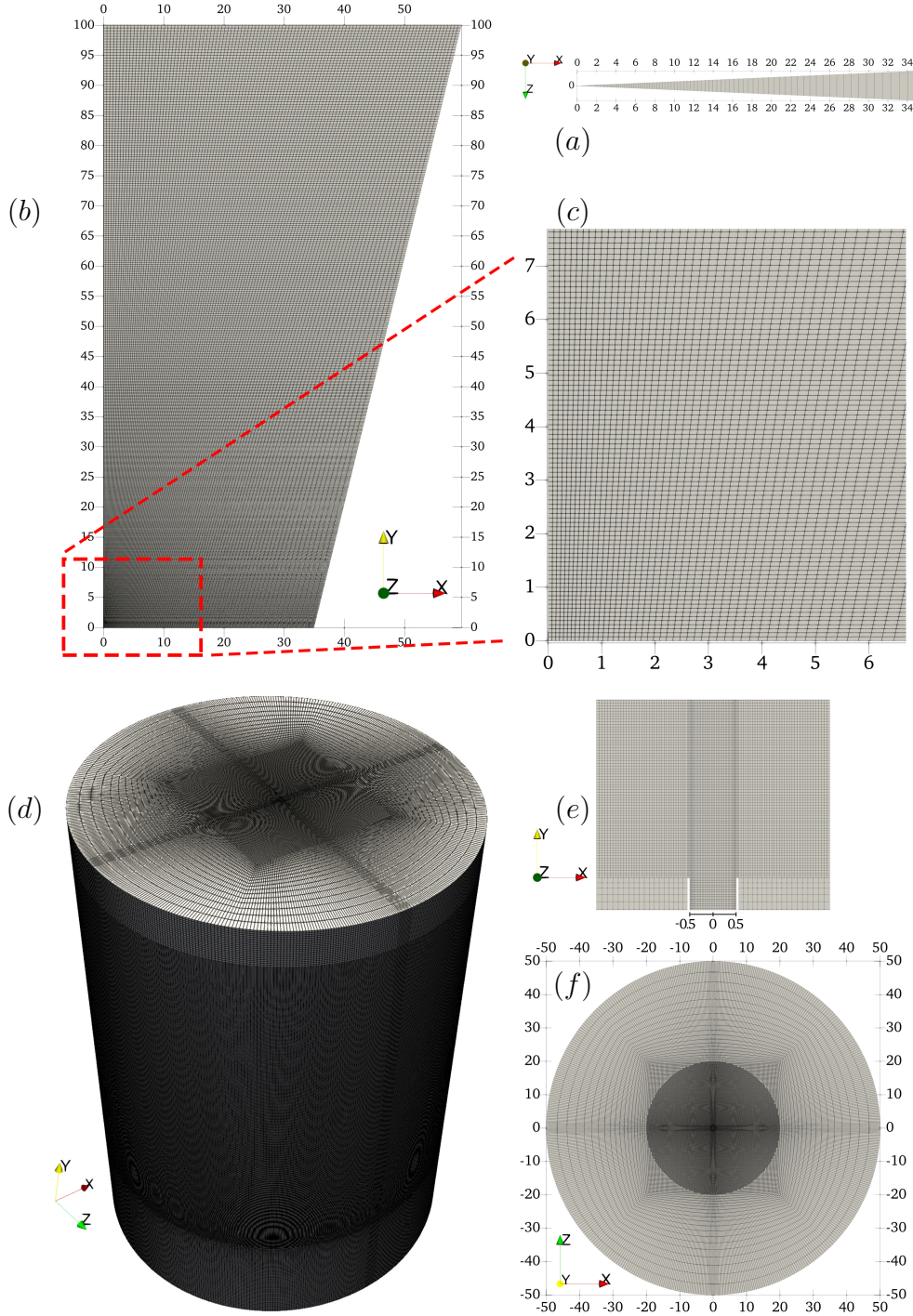


Figure 4.5: A visualization of the computational mesh of second scenario for RANS (a-c) and LES (d-f); (a) top view of axisymmetry domain (RANS); (b) slice in the middle of domain (RANS); (c) zoomed window of the slice (RANS); (d) full view of domain (LES); (e) zoomed slice in the middle of domain parallel to jet stream direction (LES); (f) slice in the domain perpendicular to jet stream direction (LES).

Results of numerical simulation (i.e., OpenFOAM) and LIF experiment data were extracted and processed using open-source Python libraries, including Matplotlib², PyVista³, and Pandas⁴. Machine learning and multifidelity optimization were performed using GPyTorch⁵ and BoTorch⁶ libraries [222, 223].

4.3 Results

The result section of this study is organized into two main parts presenting the first and second scenarios. For each scenario, the overall jet behavior is first reported by comparing the concentration fields obtained from the LF and HF simulations, providing qualitative insight of jet evolution. Next, a quantitative analysis is performed for each scenario, evaluating dilution and horizontal displacement for the first scenario, and centerline dilution for the second, by comparing the LF, HF, and MFGP predictions. Finally, the predictive accuracy is assessed for each fidelity level, and the associated errors are reported.

4.3.1 First scenario

To evaluate the predictive performance of the proposed MFGP framework, the simulation design for scenario 1 was structured to ensure comprehensive representation of the parameter space while maintaining computational efficiency. The LF dataset consisted of 24 RANS simulations uniformly distributed over the range $Fr_d/H_t = 0.5-2.8$, providing broad coverage of jet behavior across shallow ambient regimes. The HF dataset comprised four representative LES cases ($Fr_d/H_t = 0.5, 1.0, 2.0$, and 2.8) selected from the TV ensemble of 11 validated LES simulations. These HF points were chosen based on sensitivity analysis to ensure the inclusion of both near linear and nonlinear regions of the parameter space. Three predictive models were developed for comparison: a low-fidelity Gaussian Process (LFGP) trained on the RANS data, a high-fidelity Gaussian Process model (HFGP) trained on the four LES cases, and a multifidelity Gaussian Process model (MFGP) integrating all datasets as described in the methodology section. This design enables the assessment of predictive accuracy, uncertainty quantification, and computational efficiency of the MFGP framework relative to the single fidelity counterparts.

General observation of CFD simulations

To illustrate the effect of fidelity on the resolved physics, Figure 4.6 compares the concentration field $\tilde{c}$ and velocity streamlines for a single representative shallow ambient case with $Fr_d/H_t = 0.5$, computed once with a LF (RANS) model and once with a HF (LES). The figure shows how the two fidelity levels differ for the same case. Both LF and HF models capture the initial rise of the negatively buoyant jet until it impinges on the surface and subsequently travels attached to it, followed by the development of a downward return flow

²<https://matplotlib.org/>

³<https://pyvista.org/>

⁴<https://pandas.pydata.org/>

⁵<https://gpytorch.ai/>

⁶<https://botorch.org/>

driven by the higher density of the discharge. As the LF model applies a time averaged solution the field appears smoother, with more aligned streamlines. In contrast, the LES reveals intermittent coherent structures, stronger entrainment, and small flow structures (i.e., eddies) that broaden the plume and enhance dilution in the near field.

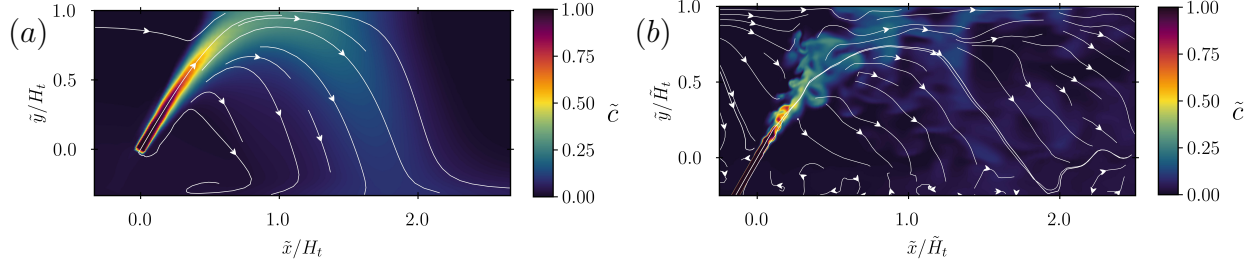


Figure 4.6: Concentration field and velocity streamlines for (a) LF (RANS) simulation and (b) HF (LES) simulation for case $Fr_d/H_t = 0.5$.

Parameterization, settings, and convergence assessment

The two-level multifidelity Gaussian process model was implemented based on the hierarchical structure described in Section 4.2.3. Two shared latent Gaussian processes were used to represent the correlated information across the fidelity levels (LF and HF). Both latent processes were governed by Matérn-5/2 covariance functions with automatic relevance determination across the input feature space, allowing the model to capture variations in the underlying physical relationships. The first latent process was active across both fidelity levels, while the second captured additional HF-specific variation and cross-level correlation between LF and HF. A constant mean and per-fidelity noise variances were applied across the two trained fidelity levels to maintain model identifiability and ensure numerical stability. All input variables were jointly normalized to the interval $[0, 1]$ across the two fidelity levels to ensure consistent kernel scaling and numerical stability, while output quantities were retained in their physical units to preserve dimensional interpretability. The model parameters were assigned weakly informative priors, a small diagonal jitter was added to the covariance matrices to ensure positive definiteness, and posterior inference was performed using a random-walk Metropolis MCMC sampler. Predictive means together with 95% CIs were obtained by marginalizing the Gaussian process conditionals over the posterior samples.

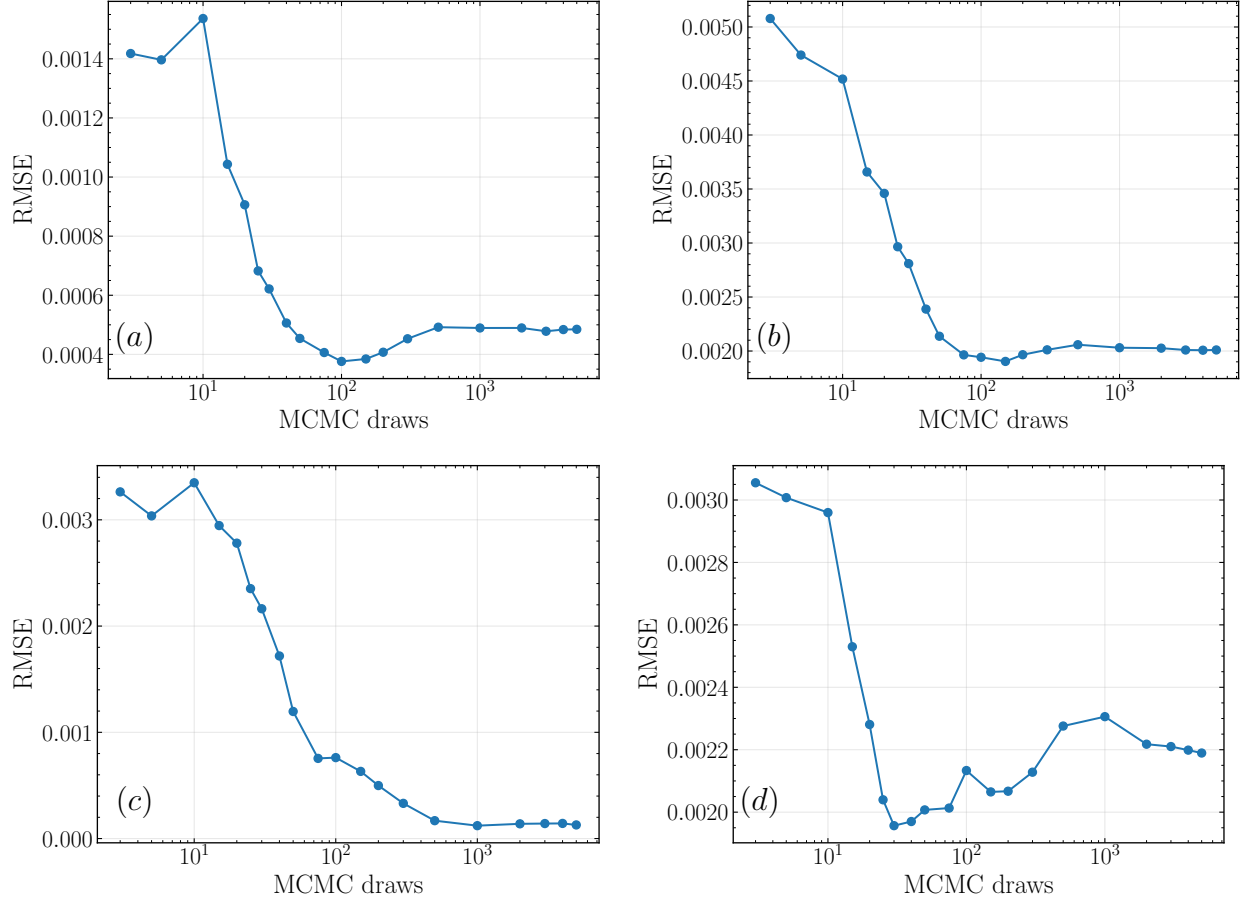


Figure 4.7: The convergence for a: dilution at terminal rise, b: dilution at return point, c: terminal rise and d: return point.

The number of MCMC iterations was determined through a convergence analysis based on the predictive RMSE between the model predictions and the TV, as illustrated in Figure 4.7. For all analyzed quantities, dilution at the terminal rise, dilution at the return point, terminal rise height, and return point location, the RMSE initially decreases sharply during the early iterations, corresponding to the burn-in phase of the Markov chains. After approximately 100-200, the RMSE reaches a stable plateau with negligible fluctuations, indicating that the posterior distributions have converged and additional samples yield no significant improvement in predictive accuracy. Based on this behavior, a total of 5000 draws with 1500 burn-in samples was adopted in the final simulations to ensure statistical robustness while maintaining computational efficiency. This configuration provided consistent posterior means and narrow confidence interval across all investigated flow quantities.

Surface and return point dilution

This section presents the results of different fidelity Gaussian Process (GP) for predicting the jet's surface and return point dilution. Surface and return point dilution are critical parameters in understanding the mixing behavior of dense jets discharged into shallow en-

vironments. Surface dilution s_t represents the concentration at the location where the jet interacts with the water surface, whereas return point dilution refers to the dilution observed when the jet returns to the level of the nozzle center s_r height. These parameters are essential for evaluating the environmental impact of dense jets, as they indicate the effectiveness of dilution and mixing processes in dispersing pollutants or saline effluents into the ambient water. Figure 4.8 - a presents the normalized surface dilution, s_t/Fr_d , as a function of Fr_d/H_t for all scenarios. The scatter points correspond to the available datasets, while the lines represent the predictions of the LF GP, HF GP, and MF GP models and shaded regions denote the 95% CI of the Gaussian Process predictions. Across all models, the slope of the predicted curves is steep for $0.5 \leq Fr_d/H_t \leq 1.1$, indicating a rapid reduction of surface dilution as the confinement effects increase. Beyond this range $1.1 \leq Fr_d/H_t \leq 2$, the relationship becomes nonlinear with a gradually decreasing slope, and at larger Fr_d/H_t values, it transits to an almost linear regime.

The discrepancy between LF and TV is significant across the entire range, although the accuracy of LF slightly improves with increasing (Fr_d/H_t) . This behavior has also been reported in previous studies (e.g., [45]) and is attributed to the limited capability of LF models (i.e., , RANS) in accurately resolving the jet evolution and the associated strong shear regions. The LF GP prediction line aligns closely with the scatter points representing the LF data, as expected. However, due to the restricted accuracy of the LF simulations, it exhibits noticeable discrepancies when compared with the TV results, highlighting the inherent limitations of LF data in capturing detailed flow physics. Consequently, this systematic bias causes the LF GP to underpredict (s_t/Fr_d) across the entire range of (Fr_d/H_t) . A similar limitation was reported by [209], where the analysis was restricted to the geometrical characteristics of the jet without incorporating LF data for dilution prediction. The HF GP prediction aligns closely with the TV for $(Fr_d/H_t) < 1.1$, demonstrating its capability to accurately capture surface dilution in the region where the data follow an approximately linear trend. However, as (Fr_d/H_t) increases to between 1.1 and 2, the dilution behavior becomes noticeably nonlinear, and the accuracy of the HF GP deteriorates. This decline in performance arises because the model has limited HF data within this transition region, resulting in poorer constraint of the covariance structure and a larger prediction uncertainty. Correspondingly, the 95% confidence interval (CI) of the HF GP expands in this range, reflecting the model's reduced confidence and highlighting the sensitivity of the predictions to data scarcity. Beyond $(Fr_d/H_t) = 2$, the discrepancy decreases, but this apparent improvement mainly reflects the more gradual and nearly linear dilution trend in the HF observations, which reduces the variation between successive data points and therefore lowers the measured discrepancy. In this range, the relationship between the input and output becomes more linear, allowing the HF GP to capture the trend more effectively and resulting in improved agreement with the TV data. In contrast, the MF GP prediction line exhibits consistently high accuracy across the entire range of (Fr_d/H_t) , maintaining close agreement with the TV values. This performance arises from the model's hierarchical structure, which effectively combines the broad parametric coverage of the LF simulations with the higher physical fidelity of the HF data. By statistically co-conditioning the two sources of information, the MF GP uses the smooth global trends captured by the LF data while locally refining them using the more accurate HF corrections. This enables the model to reproduce both the linear and the nonlinear mixing trend observed in the low to intermediate range of (Fr_d/H_t) . Even in regions

with sparse HF data, the Bayesian formulation ensures optimal weighting between fidelity levels, preventing overfitting to limited samples while maintaining physical consistency. The narrow CI observed across all (Fr_d/H_t) confirm the stability and reliability of the MFGP predictions, reflecting its ability to reduce epistemic uncertainty and accurately generalize the jet behavior over the entire operating range.

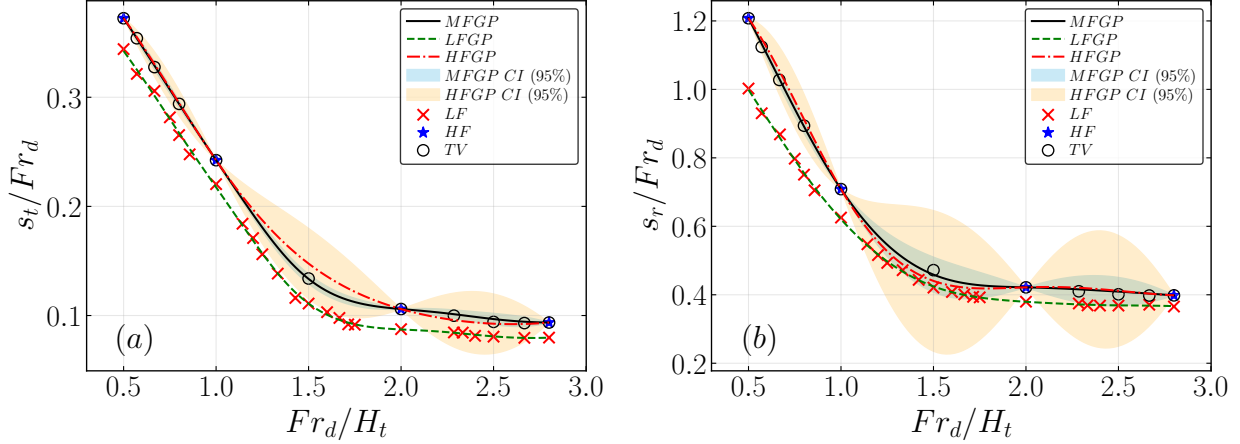


Figure 4.8: The surface and return point dilution for MFGP, HFGP and LFGP.

Figure 4.8 - b illustrates the normalized return point dilution, s_r/Fr_d , as a function of Fr_d/H_t . The normalized return point dilution, (s_r/Fr_d) , decreased sharply with (Fr_d/H_t) in the range of 0.5 to approximately 1.1, reflecting a steep trend. Beyond this point, the decrease became more gradual, with a noticeable reduction in the slope, indicating a transition to a less rapid change as (Fr_d/H_t) continues to increase. For $(Fr_d/H_t) < 1.1$, the slope of the TV curve is noticeably steeper than that of the LF, indicating that the TV data capture a more rapid decrease in (s_r/Fr_d) within this range, whereas the LF results underpredict the rate of change. Beyond $(Fr_d/H_t) \geq 1.5$, the slope of the TV curve becomes more gradual, and the LF curve tends to be nearly parallel to it, although it continues to underestimate the dilution. The limitations of the LFGP are evident, as expected, due to its reliance on LF inputs, similar to the behavior observed in the predictions for s_t . This reflects the inherent shortcomings of LF models, which lack the capability to fully resolve the complex flow structures and mixing dynamics governing jet evolution. Consequently, the LFGP consistently underpredicts s_r/Fr_d across the entire range of (Fr_d/H_t) . The HFGP closely corresponds to the TV for $(Fr_d/H_t) < 1.1$, where the data follow a linear trend. However, for (Fr_d/H_t) in the range of 1.2 to 2, the error increases markedly, highlighting the difficulty in capturing return point dilution. In this range, the scarcity of HF data limits the model's ability to fully constrain the covariance structure, leading to larger predictive deviations and broader 95% CI. Beyond $(Fr_d/H_t) = 2$, the discrepancy further slightly decreases as the dilution trend becomes smoother and approaches a quasi linear, improving the model's alignment with the TV, although the CI of the HFGP remain relatively wide due to limited sampling density. The MFGP demonstrated good performance for the entire range of (Fr_d/H_t) , with its prediction line closely aligning with the TV and exhibiting minimal errors. By combining the wide parametric coverage of the LF data with the higher physical fidelity of the HF simulations, the

MFGP effectively captures both the nonlinear variations at intermediate (Fr_d/H_t) and the more stable, linear behavior at higher values. The hierarchical Bayesian formulation enables optimal weighting between fidelity levels, allowing the model to maintain accuracy even in regions with sparse HF observations. The 95% CI of the MFGP remain narrow throughout the range, reflecting reduced epistemic uncertainty and demonstrating the model’s robustness and accurate predictive capability in reproducing the dilution of the return point.

Horizontal displacement

The horizontal displacement of desalination jets, specifically the terminal rise location ($\tilde{x}_t$) and return point location ($\tilde{x}_r$), is a critical parameter for understanding jet dynamics. These metrics are essential for evaluating jet spreading, mixing efficiency, and interactions with the ambient environment. The horizontal displacement directly reflects the spatial development of momentum and scalar quantities, which are crucial for assessing environmental impacts, optimizing engineering designs, and validating predictive models. Furthermore, analyzing the return point and terminal rise location provides valuable insights into the behavior of buoyancy-driven flows, the effects of ambient constraints such as shallow environments, and the overall effectiveness of dilution processes. The terminal rise horizontal location, $\tilde{x}_t/H_t$, calculated from RANS and LES data exhibits a clear trend of decreasing values with increasing Fr_d/H_t . For both RANS and LES, the slope of this decrease is steeper at lower values of Fr_d/H_t (< 1.0), indicating a more pronounced reduction in the horizontal displacement. As Fr_d/H_t increases beyond 1.5, the slope transits to a more gradual decline, eventually stabilizing into a near linear curve, suggesting reduced sensitivity of the terminal rise horizontal displacement to increases in Fr_d/H_t . A comparison of the RANS and LES results reveals a consistent discrepancy, with RANS predicting slightly larger values than LES across all ranges of Fr_d/H_t .

Figure 4.9 - a illustrates the normalized terminal rise location, $\tilde{x}_t/H_t$, as a function of Fr_d/H_t . The figure compares the predictive performance of three models MFGP, HFGP, and LFGP, against the TV. As the LF model overpredicts $\tilde{x}_t/H_t$ across the entire range of Fr_d/H_t , the LFGP likewise overpredicts $\tilde{x}_t/H_t$ due to its reliance on LF data. The HFGP prediction line aligns closely with the TV for $(Fr_d/H_t) < 1.0$, where the relationship between (Fr_d/H_t) and $\tilde{x}_t/H_t$ is approximately linear. Beyond this range, as the relationship becomes increasingly nonlinear, the discrepancy between the HFGP predictions and the TV grows markedly. This behavior highlights the influence of the limited number of HF data points, which constrains the model’s ability to accurately capture the underlying trends. The widening CI in these regions further indicate the reduced reliability of the HFGP model under sparse data conditions. Unlike the single fidelity counterparts, the MFGP maintains strong agreement with the TV across the full range of Fr_d/H_t . It achieves high predictive accuracy not only in regions exhibiting linear behavior but also in the nonlinear regimes where the availability of HF data is limited. This enhanced performance stems from the model’s hierarchical structure, which leverages the broad parametric coverage of the LF simulations while refining local accuracy through the high-fidelity information. The consistently narrow CI observed for the MFGP further emphasize its stability and reliability, demonstrating the model’s ability to provide accurate and uncertainty aware predictions over the entire parameter space.

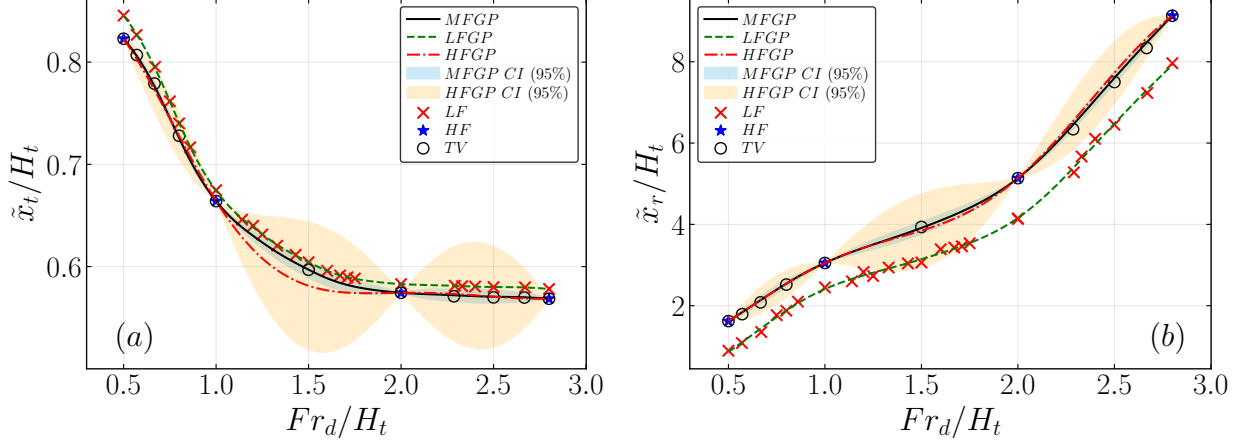


Figure 4.9: The Horizontal displacement location for MFGP, HFGP and LFGP.

The CFD results, obtained from LF and HF simulations, exhibit a similar increasing trend in the horizontal displacement of the return point, $\tilde{x}_r/H_t$, as Fr_d/H_t increases. The rate of increase is characterized by a steeper slope for $Fr_d/H_t < 1.0$ and $Fr_d/H_t > 2.0$, while the slope becomes less pronounced within the intermediate range of $1.0 < Fr_d/H_t < 2.0$. Figure 4.9 - b illustrates the normalized return point location, $\tilde{x}_r/H_t$, as a function of Fr_d/H_t , comparing the predictive performance of the applied models against the TV data. Similar to previous observations, the LF data consistently exhibit discrepancies with the TV across the entire range of Fr_d/H_t , highlighting the limitations of LF model in accurately predicting jet dynamics. In contrast, the HFGP prediction line closely aligns with the TV for $(Fr_d/H_t) < 1.0$. However, beyond the of $(1.0 < Fr_d/H_t)$ the discrepancy increased and widening CI for the HFGP in these regions further indicate reduced predictive reliability. The MFGP prediction demonstrates more accurate agreement with the TV across the entire range of Fr_d/H_t . Unlike the single fidelity models, the MFGP effectively captures both linear and nonlinear trends in $\tilde{x}_r/H_t$, maintaining minimal error even in regions with sparse HF data. The narrow CI associated with the MFGP predictions reflects a high level of confidence in its results, further underscoring the robustness and reliability of the multifidelity approach.

Error analysis of prediction

The predictive accuracy of each model presented in Table 4.4 were calculated by comparing the predictions of the respective models against the TV data. The Mean Absolute Error (MAE) was used to quantify the difference between the predicted values and the reference TV data. The MAE is defined as follows:

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |y_i^{\text{pred}} - y_i^{\text{ref}}|, \quad (4.15)$$

where y_i^{pred} is the predicted value, y_i^{ref} is TV data, and N is the total number of data points. Table 4.4 summarizes the prediction errors for s_t , s_r , $\tilde{x}_t$, and $\tilde{x}_r$ across the three models. Among the models, MFGP consistently achieves the lowest errors, demonstrating its robustness and enhanced predictive accuracy. For instance, in predicting $\tilde{x}_t$, the MAE of the MFGP

is approximately one order of magnitude lower than that of the HFGP and more than two orders lower than that of the LFGP. These reductions in error reflect the MFGP’s ability to efficiently integrate the extensive parametric coverage of the LF with the higher precision of the HF data through its hierarchical Bayesian formulation. This multifidelity coupling enables the model to reproduce both the global trends and the local nonlinearities of the jet dilution and trajectory behavior.

Table 4.4: Mean Absolute Error (MAE) for s_t , s_r , $\tilde{x}_t$, and $\tilde{x}_r$ across the LFGP, HFGP, and MFGP models.

Model	s_t	s_r	$\tilde{x}_t$	$\tilde{x}_r$
LFGP	0.0209	0.0686	0.0100	0.8459
HFGP	0.0039	0.0163	0.0054	0.0935
MFGP	0.0014	0.0070	0.0010	0.0470

The prediction error associated with each model was quantified through the root mean square error (RMSE), defined as:

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i^{\text{pred}} - y_i^{\text{ref}})^2} \quad (4.16)$$

where y_i^{pred} denotes the model prediction, y_i^{ref} the corresponding TV, and N the number of test cases. Equation (4.16) was evaluated for all four response quantities surface dilution s_t , return point dilution s_r , terminal rise x_t , and return point x_r , over the range of nondimensional governing parameters.

Table 4.5 reports the global (domain averaged) RMSE values, while Figures 4.10 and 4.11 present local absolute error distributions as functions of Fr_d/H_t . As seen in Table 4.5, the MFGP consistently achieves the lowest RMSE values across all four quantities, indicating higher accuracy in predictions relative to both single fidelity models. For example, the MFGP reduces the RMSE of $\tilde{x}_t$ from 0.0106 in the LFGP and 0.0077 in the HFGP to only 0.0013, representing improvements of roughly one order of magnitude. Similar reductions are observed for s_t and s_r , where the MFGP achieves average RMSE values of 1.8×10^{-3} and 8.4×10^{-3} , respectively, compared to 2.15×10^{-2} and 8.32×10^{-2} in the LFGP.

Table 4.5: Root Mean Square Errors (RMSE) s_t , s_r , $\tilde{x}_t$, and $\tilde{x}_r$ across the LFGP, HFGP, and MFGP models.

Model	s_t	s_r	$\tilde{x}_t$	$\tilde{x}_r$
LFGP	0.0215	0.0832	0.0106	0.8612
HFGP	0.0058	0.0195	0.0077	0.1249
MFGP	0.0018	0.0084	0.0013	0.0625

Figures 4.10 and 4.11 further reveal the local absolute error distributions, providing insight into the fidelity specific behavior of each model. For surface dilution (s_t) and return point

dilution (s_r) (Figure 4.10), the LFGP exhibits the largest local errors across all Fr_d/H_t , exceeding 3×10^{-2} for s_t and 2×10^{-1} for s_r . The HFGP provides improved accuracy, with typical errors remaining below 1.5×10^{-2} and 1.0×10^{-1} , respectively. The MFGP achieves the best performance, maintaining nearly uniform absolute errors below 1×10^{-2} across the full range of Fr_d/H_t , demonstrating its ability to capture both global and local dilution trends with high precision.

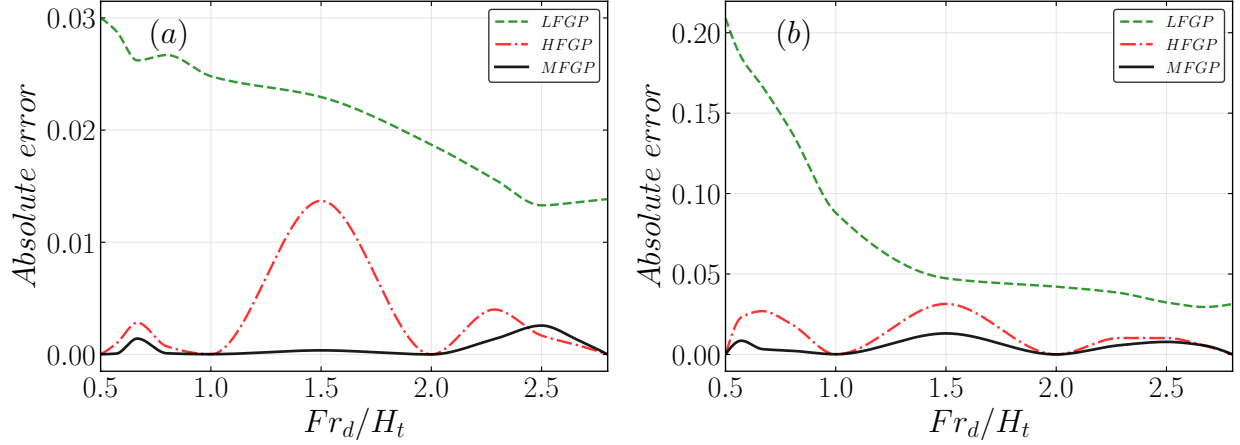


Figure 4.10: Absolute error of (a) surface dilution location s_t and (b) return point dilution s_r .

A similar hierarchy is observed in the geometrical quantities (Figure 4.11). For the terminal rise location ($\tilde{x}_t$), the LFGP shows the highest errors, reaching up to 2×10^{-2} , while the HFGP improves this to approximately 1×10^{-2} . The MFGP again performs best, keeping the local error consistently below 2×10^{-3} . For the return point location ($\tilde{x}_r$), the differences between models are more pronounced: the LFGP error grows steadily with Fr_d/H_t and exceeds unity, the HFGP limits this to about 1.2×10^{-1} , and the MFGP further reduces the error to below 7×10^{-2} .

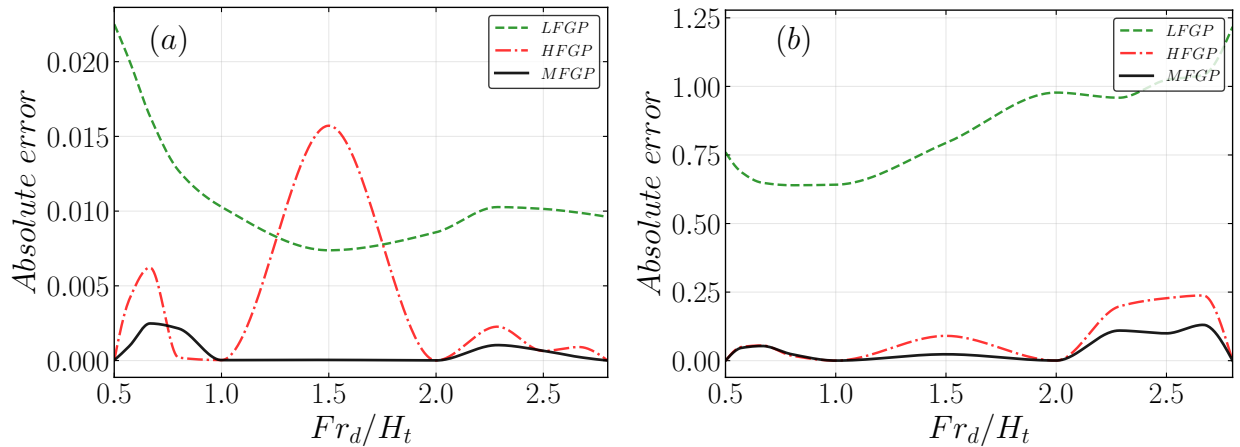


Figure 4.11: Absolute error of (a) terminal rise location $\tilde{x}_t$ and (b) return point location $\tilde{x}_r$.

4.3.2 Second scenario

The second scenario focuses on the vertical thermal discharge, representing a fundamental configuration in thermal desalination systems where heated effluents are released into the ambient receiving waters. Such discharges are of particular importance due to the strong interaction between momentum and buoyancy, which gives rise to complex flow behaviors including rapid entrainment, axisymmetric expansion, and nonlinear dilution patterns. Accurately capturing these processes is essential for assessing the dispersion efficiency of the discharge, ensuring compliance with thermal discharge regulations, and mitigating potential environmental impacts in coastal environments. In this section, the proposed MFGP framework is evaluated for its capability to predict the behavior of desalination discharges using three datasets of LIF experiments, LES, and RANS simulations. The LIF experiments, described in detail in appendix (LIF configuration), provide high-resolution concentration fields and serve as the TV for this scenario. The LES data represent the HF data, capturing the dominant turbulent structures and detailed flow physics with high spatial and temporal resolution and RANS simulations constitute the LF data, offering computationally efficient yet less accurate approximations of the discharge dynamics.

General observation of CFD simulations

Figure 4.12 shows the concentration fields of the vertical thermal jet at $Fr_d = 15$, obtained from LIF measurements, LES, and RANS simulations. The LIF data reveal fine scale turbulent structures and strong entrainment of ambient fluid, clearly illustrating the progressive dilution of the jet with height. Small scale vortical motions are captured in the near field, reflecting the high level of turbulent mixing captured in LIF. The LES results reproduce the overall jet behavior and capture large coherent structures with good agreement to the experimental observations. Although the smallest scales are not fully resolved due to grid constraints, LES still represents the main turbulent eddies and entrainment mechanisms, providing a realistic description of plume development. In contrast, the RANS does not capture any scales, as the time-averaged turbulence modeling suppresses the unsteady structures seen in LIF and LES.

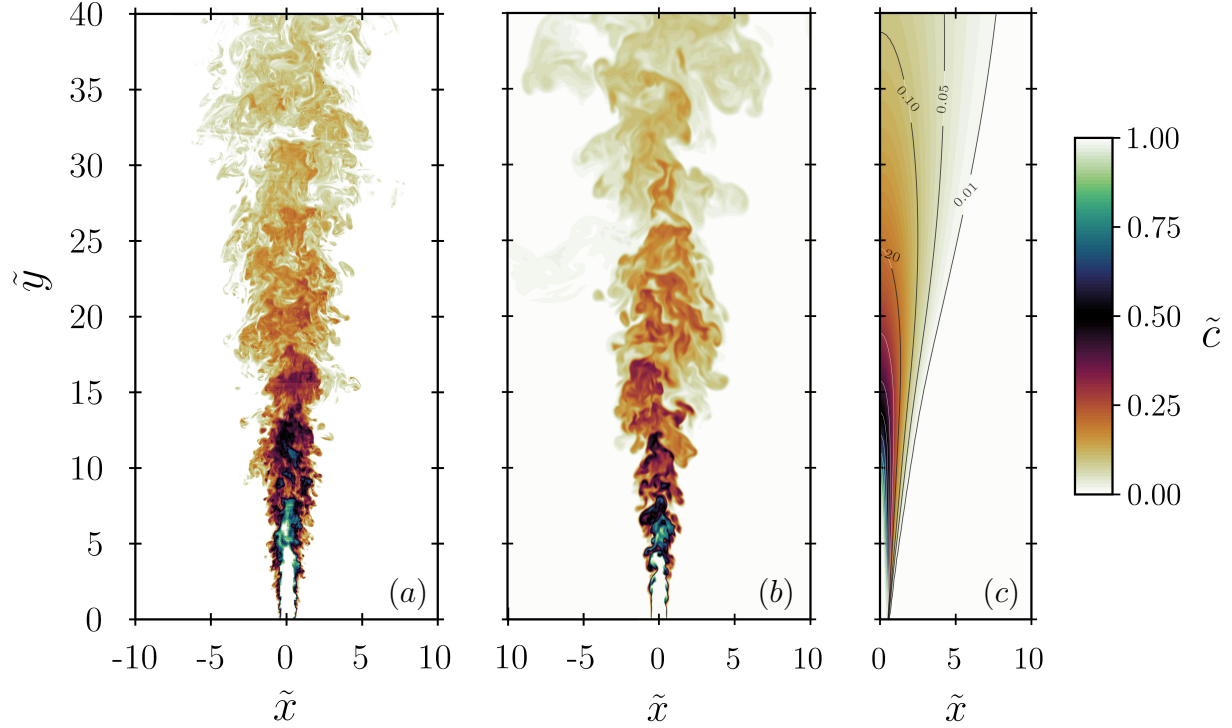


Figure 4.12: Comparison of concentration fields for the vertical thermal jet: (a) LIF measurements, (b) LES, and (c) RANS. (Please note: The RANS contour is displayed only on one side of the jet since the simulation is axisymmetric.)

Centerline concentration

Figure 4.13 presents the concentration field ($\tilde{c}$) with respect to (Fr_d) at five downstream locations ($\tilde{y} = 10 - 40$). At near-field ($\tilde{y} = 10$), the LF results exhibit an almost constant $\tilde{c}$ across all Fr_d . This behaviour reflects an unrealistically long core region, in which centreline concentration remains nearly unchanged and turbulent entrainment is weak. As a result, dilution and mixing are substantially underpredicted in this zone. The plot reflects the limitations of LF modeling, in which the exclusion of instantaneous turbulent fluctuations leads to an overestimation of the centerline concentration and an inaccurate linear trend of dilution. Both HF and TV data capture reduction in $\tilde{c}$ with higher Fr_d , where lower buoyancy forces resulted in lower dilution of jet concentration. The HF data slightly underpredict $\tilde{c}$ relative to the TV results at low and intermediate Fr_d , which is consistent with the stronger entrainment and enhanced dilution produced by the resolved large-scale turbulent structures in the LES. At intermediate and far-field locations ($\tilde{y} = 15-40$), the concentration field ($\tilde{c}$) decreases with downstream distance, reflecting the enhanced entrainment and mixing with the ambient fluid that progressively dilute the jet. Across all downstream locations, dilution of $\tilde{c}$ reduces with increase in Fr_d , indicating that momentum driven discharges remain more coherent and sustaining higher centerline concentrations. At low Fr_d , the stronger buoyancy accelerates the jet to plume transition, enhancing turbulent entrainment and mixing. This intensified buoyancy driven entrainment causes faster dilution, leading to lower centerline concentrations ($\tilde{c}$) compared to higher Fr_d cases. The differences between low and high Fr_d

diminish with downstream distance, and the slope of $\tilde{c}$ with respect to Fr_d becomes less pronounced beyond $\tilde{y} = 30$, indicating that the influence of buoyancy progressively weakens as the flow approaches a quasi-self-similar regime.

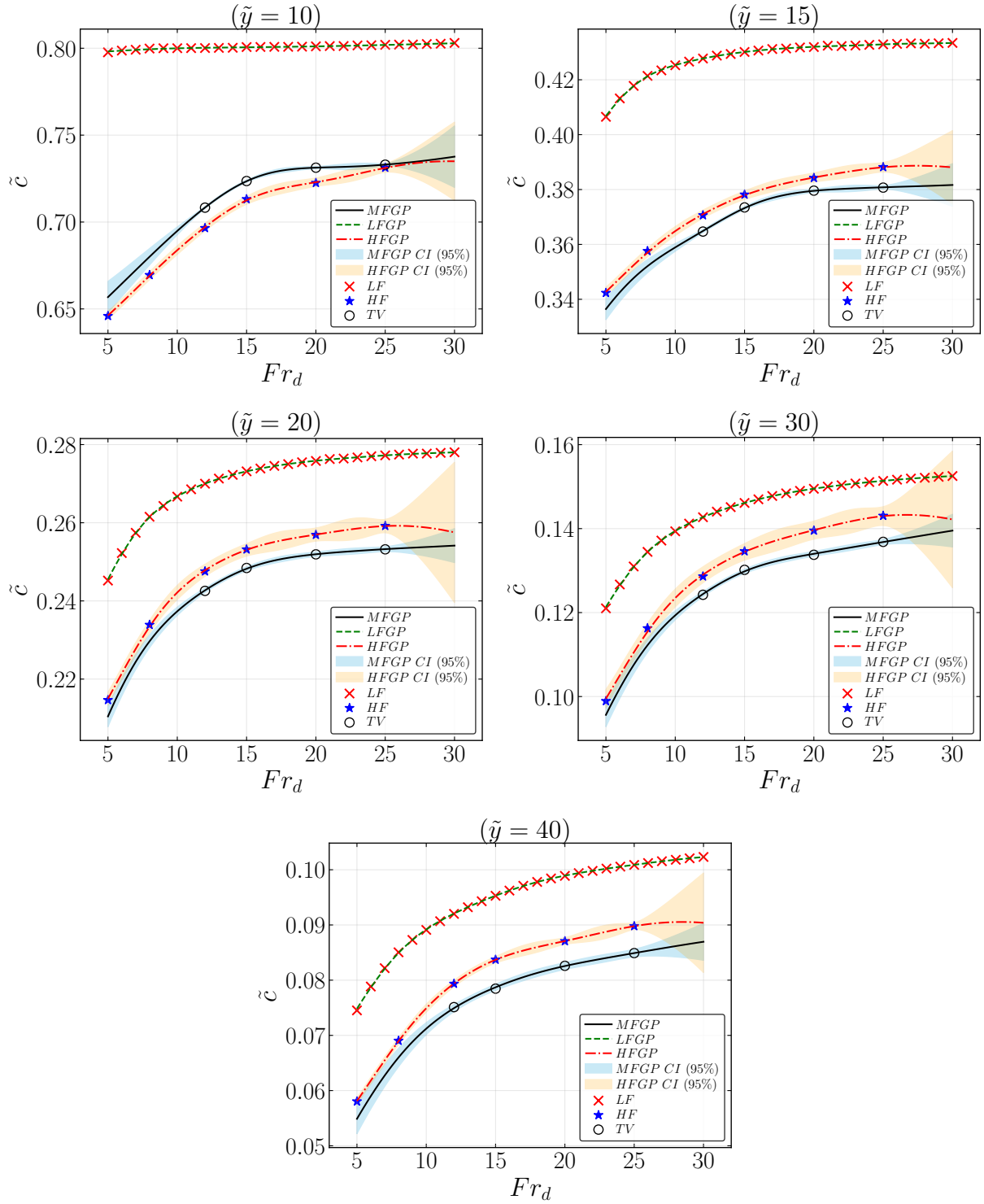


Figure 4.13: Centerline concentration ($\tilde{c}$) as a function of densimetric Froude number (Fr_d) at $\tilde{y} = 10$, $\tilde{y} = 15$, $\tilde{y} = 20$, $\tilde{y} = 30$, $\tilde{y} = 40$.

The predictive behavior of the GP models underscores the value of multifidelity coupling across the examined downstream locations. The LFGP captures the overall trend but sys-

tematically overestimates the concentration, especially in the near field (at $\tilde{y} = 10$), owing to its limited representation of turbulent mixing in the LF training data. The HFGP improves both trend and magnitude by using HF data, yet its predictive variance grows between sparsely sampled HF points, most visibly for $Fr_d \gtrsim 25$, a typical outcome for single fidelity GPs under low sampling density and nonlinear trends. In contrast, MFGP delivers robust and consistent predictions that reconcile the broad parametric guidance of LF with the local accuracy of HF. Its confidence intervals remain narrow where the posterior is well constrained by HF data ($12 \leq Fr_d \leq 25$) and widen toward extrapolated regions ($Fr_d < 12$ and $Fr_d > 25$), reflecting realistic epistemic uncertainty. The larger CI at low Fr_d arises from stronger nonlinearity in buoyancy dominated regimes, where small changes in Fr_d markedly affect entrainment and dilution; at high Fr_d , the widening is tied to momentum dominated conditions with limited HF coverage and weaker sensitivity of $\tilde{c}$ to Fr_d . The reduced CI of MFGP relative to HFGP within the data supported range highlights how LF information effectively regularizes the posterior, while the controlled CI growth outside that range indicates appropriate uncertainty quantification.

Error analysis of prediction

Table 4.6 summarizes the predictive accuracy of single fidelity and MFGP models at five downstream locations in terms of RMSE and MAE relative to the reference TV data (only in region where TV is available ($12 \leq Fr_d \leq 25$)). MFGP achieves the highest predictive accuracy, with errors reduced by one to two orders of magnitude compared to both single fidelity models. At the near-field position ($\tilde{y} = 10$), where buoyancy effects are dominant and strong concentration gradients prevail, the LF model exhibits the largest deviations (RMSE = 0.0747, MAE = 0.0744) due to reliance of LF on LF data. The HFGP model improves the accuracy substantially (RMSE = 0.0082, MAE = 0.0078), while the MFGP further reduces the error to (RMSE = 0.0010, MAE = 0.0007) by hierarchically combining the global trend information from LF with the local accuracy of the TV data. As the discharge evolves downstream, both RMSE and MAE systematically decrease for all models, reflecting the gradual attenuation of concentration gradients and the transition toward a self-similar flow regime. At intermediate and far-field locations ($\tilde{y} = 20$ -40), the MFGP maintains high accuracy with RMSE values below 3×10^{-4} and MAE values below 2×10^{-4} , whereas the HF model remains approximately an order of magnitude higher.

Table 4.6: Root Mean Square Error (RMSE) and Mean Absolute Error (MAE) for the centerline concentration ($\tilde{c}$) at different downstream locations.

$\tilde{y}$	LFGP		HFGP		MFGP	
	RMSE	MAE	RMSE	MAE	RMSE	MAE
10	0.0747	0.0744	0.0082	0.0078	0.0010	0.0007
15	0.0551	0.0550	0.0057	0.0056	0.0005	0.0003
20	0.0248	0.0247	0.0054	0.0054	0.0003	0.0002
30	0.0160	0.0160	0.0056	0.0055	0.0002	0.0002
40	0.0166	0.0166	0.0049	0.0049	0.0002	0.0002

The spatial trend in Table 4.6 (evaluated over the validation window $12 \leq Fr_d \leq 25$)

is consistent with the physics of the flow and with the model uncertainty quantification. In the near field ($\tilde{y} = 10$), where the relation of Fr_d and $\tilde{c}$ is nonlinear and buoyancy momentum interactions are most intense, errors are largest for all models, with LFGP notably overpredicting $\tilde{c}$. Moving downstream, both RMSE and MAE decline as the jet approaches a quasi-self-similar regime and concentration gradients reduces; correspondingly, the predictive intervals tighten in the data supported range.

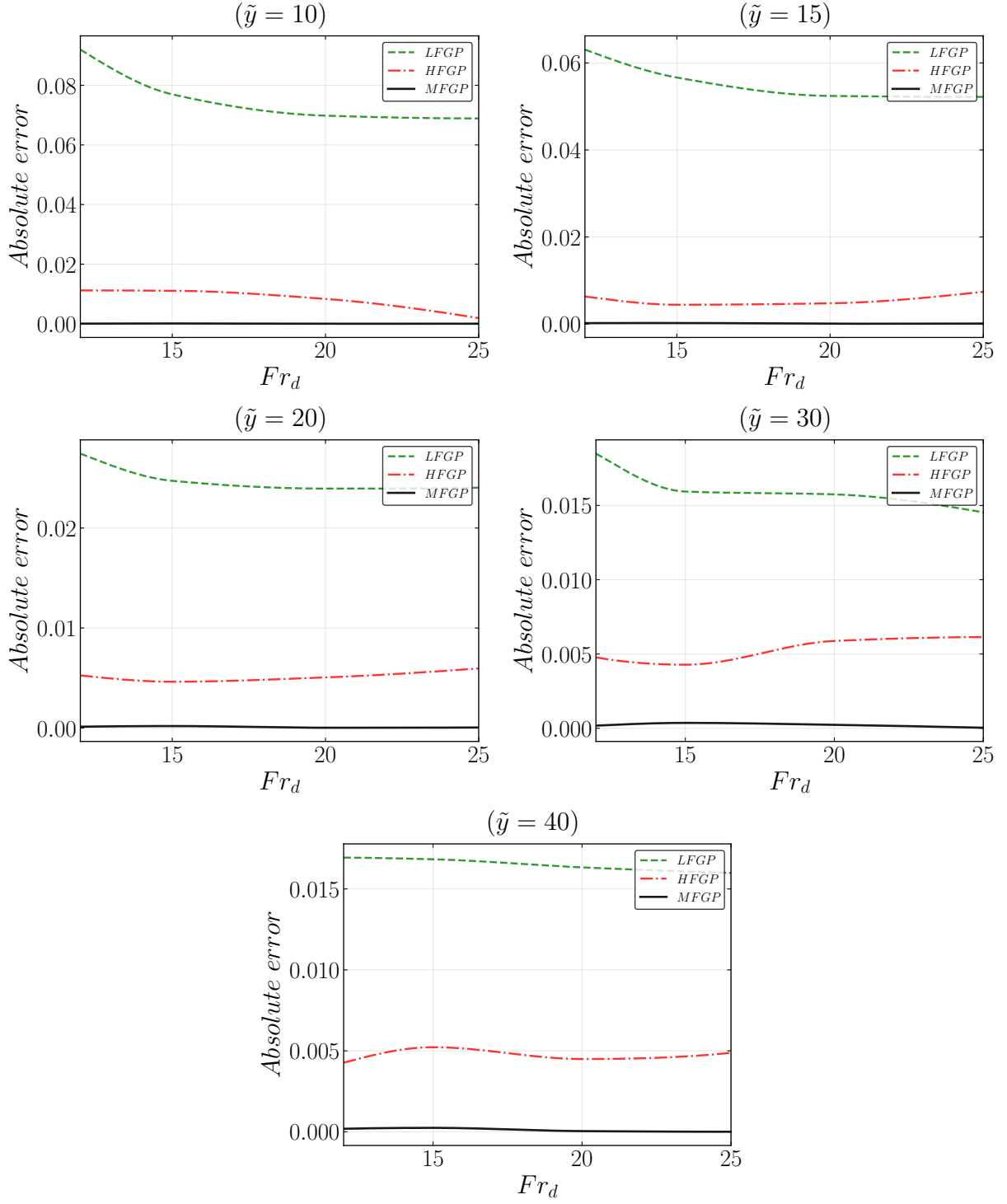


Figure 4.14: Absolute error of $\tilde{c}$ as a function of Fr_d at $\tilde{y} = 10$, $\tilde{y} = 15$, $\tilde{y} = 20$, $\tilde{y} = 30$, $\tilde{y} = 40$.

Figure 4.14 presents the absolute prediction errors of the LFGP, HFGP, and MFGP models at five downstream locations ($\tilde{y} = 10$ -40). Across all cases, the MFGP consistently yields the lowest absolute errors over the range of densimetric Froude numbers (Fr_d), demonstrating its

accuracy to reconcile low- and high-fidelity trends. At the near-field location ($\tilde{y} = 10$), where buoyancy and strong mixing dominate, the LF GP shows large deviations due to limited turbulence representation, while the HF GP improves the accuracy but still exhibits localized bias. The MF GP, by integrating both global and local information hierarchically, substantially reduces the error and provides smoother predictions over Fr_d . As the flow develops downstream ($\tilde{y} = 15$ -30), the overall errors for all models decrease, reflecting the gradual attenuation of buoyancy effects and stabilization of the jet structure. The MF GP maintains a clear advantage, particularly near the transition between the rising and spreading regions, where it captures the nonlinear variations of dilution more accurately than either single fidelity model. At the far-field position ($\tilde{y} = 40$), the differences between models become smaller as the concentration gradients weaken; however, the MF GP still provides the lowest residuals and the most consistent trend with the reference data.

4.4 Discussion

The limitations of LF only machine learning approaches for desalination discharges are well documented, LF datasets (e.g., RANS) can propagate systematic bias into surrogates, whereas costly HF modeling (e.g., LES) over the full design space is not practical. Prior studies illustrate this trade off Alvir et al. used 500 RANS runs to reconstruct only the inclined dense jet geometry as the LF mixing had large error; Yan et al. trained PFR-CNN and Random Forest models on ~ 100 RANS cases; Zhao et al. used 58 laboratory runs (442 points) for an ANFIS model [211], yet each faces either LF bias or limited parametric coverage. The proposed framework is developed for predictive modeling and performance assessment of desalination discharge mixing, where computationally inexpensive LF simulations are used to capture global parametric trends, and a limited number of HF and TV evaluations are employed to correct systematic bias and quantify predictive uncertainty in critical regions. In such applications, LF models can significantly misrepresent mixing and dilution processes, with deviations reaching up to $\sim 20\%$ in key jet characteristics [47]. The results of this study illustrate the magnitude of improvement in prediction of the desalination jet behavior. Across both scenarios, MF GP consistently outperform LF GP and HF GP, achieving higher predictive accuracy. In scenario 1 improvements in prediction accuracy of geometric metrics are significant as MAE for s_t decreases from LF GP 0.0209 and HF GP 0.0039 to MF GP 0.0014, while for $\tilde{x}_r$ improves from 0.8459 and 0.0935 to 0.0470. A similar hierarchy is observed in RMSE, where s_t drops from 0.0215 and 0.0058 to 0.0018, and $\tilde{x}_r$ from 0.8612 and 0.1249 to 0.0625, proving the capability of the hierarchical coupling in reducing both systematic and random errors in prediction of behavior of desalination jet. In scenario 2, the centerline concentration prediction by MF GP achieves highest level of agreement with the reference data. For instance, the RMSE at $\tilde{y} = 10$ decreases from 0.0747 (LF GP) and 0.0082 (HF GP) to 0.0010 (MF GP), while at $\tilde{y} = 30$ it reduces from 0.0160 and 0.0056 to 0.0002. At $\tilde{y} = 40$, the MAE declines from 0.0166 and 0.0049 to 0.0002. The applied MF GP demonstrates the highest predictive fidelity, effectively integrating the global trends captured by LF GP with the localized accuracy of HF GP.

In this study, the fidelity hierarchy is organized based on the to the order of resolved physics and computational expense. LF data are obtained from RANS, which provide broad coverage

of the desalination discharge design parameter (e.g., Fr_d) at low cost, although with the inherent bias of turbulence modeling. HF data are generated from LES, which resolve the dominant eddies governing mixing and therefore yield higher physical accuracy. The reference dataset for the MFGP is taken from LES validated by PIV in scenario 1 (two levels of fidelity) and from LIF experiments in scenario 2 (three levels of fidelity). Computational demands differ by several orders of magnitude, with each LES requiring $\mathcal{O}(10^5 - 10^6)$ CPU hours compared to $\mathcal{O}(10^2 - 10^3)$ for RANS in scenario 1 and less than 10^1 in scenario 2. The MFGP effectively exploits this asymmetry, the low-cost RANS ensemble spans the parameter domain and captures the global Fr_d - $\tilde{c}$ trend, while a limited number of LES and, where available, LIF data at selected conditions correct systematic LF bias and quantify predictive uncertainty. Within data supported regions, posterior means closely follow the HF and TV trends, and the 95% CI contract where data are dense and widen smoothly under extrapolation, maintaining accuracy comparable to TV at significantly reduced cost. From a design and operational perspective, the MFGP surrogate offers a practical and efficient framework for desalination discharge studies. LF (RANS) simulations are first employed to explore the full design space (e.g., Fr_d , nozzle angle, submergence, port spacing, bed slope, ambient depth) and establish the global trend, while a smaller set of higher-cost HF (LES) and, where feasible, TV (LIF) measurements are incorporated at locations of high LF discrepancy or posterior variance to correct bias and calibrate uncertainty.

Extending the analysis of MFGP accuracy and improvement, this study further examines the sensitivity of model performance and predictive uncertainty to both the number and spatial distribution of training samples. The sensitivity analysis systematically explores all possible arrangements of available data subsets to ensure unbiased evaluation of sampling effects. For example, when a number of training points are considered, every unique combination of that number of data locations is exhaustively tested, and the resulting predictive means and associated 95% CIs are averaged over all realizations to derive representative trends for each configuration. For scenario 1 (two levels), Figures 4.C1-4.C4 vary only the LF sample count while holding the HF level fixed. Across all quantities (s_t , s_r , $\tilde{x}_t$, $\tilde{x}_r$), the 95% CI widths decrease rapidly as the number of LF increases from small sets to moderate coverage, after which further additions provide only marginal improvement. This behaviour indicates that a moderate number of LF samples is sufficient to capture the dominant global trend, and that expanding the LF ensemble beyond this point adds little new information. The predictive means remain stable under random resampling of the LF subsets, confirming that the model performance is robust to the specific allocation of training points. For scenario 2 (three levels), Figures 4.C5-4.C7 assess the separate effects of number of LF and HF data at $\tilde{y} = 10, 20$, and 40. Two consistent patterns emerge. First, increasing number of LF primarily reduces global uncertainty by narrowing CIs in regions with sparse coverage, with limited benefit beyond moderate sizes. Second, increasing number of HF has a stronger per-sample influence; adding a small number of HF cases produces a marked CI contraction and aligns the predictive mean with the reference data, particularly in the near field where gradients are steep. Beyond a few HF points, improvements become minor. Taken together, these results support a data efficient strategy in which near HF/TV accuracy can be achieved using only a limited number of HF samples compared to the available LF data. Additional HF or TV acquisitions should be selectively concentrated in regions exhibiting high posterior variance or pronounced LF-HF discrepancies, where they provide the greatest improvement in predictive

performance.

In scenario 1, the posterior CIs are largest in parameter regions with sparse coverage or strong nonlinearity, and they shrink once a moderate LF set stabilizes the global trend. In scenario 2, CIs are widest in the near field close to the nozzle and narrow downstream. LF data first span the admissible parameter space and establish global Fr_d , response trends, and a small targeted set of HF and, where available, TV (LIF) measurements is then added where the surrogate indicates high uncertainty or pronounced LF-HF discrepancy. Data acquisition can conclude once the 95% CIs widths and validation errors stabilize, since additional HF or TV measurements provide only marginal gains. As with ARD Matérn GP surrogates, the kernel is stationary and extrapolation beyond the data supported domain increases uncertainty, which is explicitly reflected by widening CIs. Within the design envelope, the proposed MFGP achieves high predictive fidelity with quantified uncertainty while requiring far fewer HF evaluations than dense sampling.

4.5 Conclusion

This study presented a Multifidelity Gaussian Process (MFGP) framework for the predicting the behavior of desalination discharge under varying configurations. Two representative scenarios were investigated: (i) a 60-degree inclined dense jet in shallow ambient conditions using RANS and LES simulations validated against PIV measurements, and (ii) a vertical thermal desalination jet combining RANS and LES simulations with LIF experimental data. The results demonstrated that RANS consistently overpredicted concentration and underestimated dilution due to its inability to resolve turbulence and entrainment. LES reproduced the jet dynamics with much higher fidelity, showing close agreement with LIF experimental data. The integration of these fidelity levels within the MFGP framework enabled accurate predictions of key jet characteristics, including surface and return point dilution, horizontal displacement, and centerline concentration. Compared with single fidelity Gaussian process models, the MFGP consistently achieved lower errors, while maintaining better confidence intervals across the range of parameters of study. By combining the broad parametric coverage of LF (e.g., RANS) simulations with the accuracy of HF (e.g., LES) and experimental data, the proposed MFGP framework offers a computationally efficient and reliable surrogate modeling approach. This enables rapid design exploration, uncertainty quantification, and performance evaluation of desalination discharges, which would otherwise be expensive using full LES or experiments alone.

Future work should extend the framework to include different desalination discharge configurations (e.g., varying jet angles, port geometries, and submergence depths), incorporate experimental measurements, and explore active learning strategies for adaptive high-fidelity data selection, thereby further enhancing predictive capability and reducing computational costs in complex environmental flow applications.

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Data Availability

The solver, Gmsh mesh generation script, and a simple example of the non-dimensional modeling approach developed in this study are publicly available at the following link: https://github.com/HydroCFD/buoyant_jet/tree/main/MF_Dense_jet. This repository provides the necessary tools to reproduce the simulation setup and facilitates the application of the proposed methodology in related studies.

Nomenclature

Abbreviations

ANFIS	Adaptive Neuro Fuzzy Inference System
ARD	Automatic Relevance Determination
CFD	Computational Fluid Dynamics
CI	Confidence Interval
CNN	Convolutional Neural Network
GP	Gaussian Process
GPR	Gaussian Process Regression
HF	High-fidelity
LES	Large eddy Simulation
LIF	Laser Induced Fluorescence
LF	Low-fidelity
LFGP	Low-fidelity Gaussian Process
MCMC	Markov Chain Monte Carlo
MF	Multifidelity
MFGP	Multifidelity Gaussian Process
PFR-CNN	Parameter-based Field Reconstruction Convolutional Neural Network
PISO	Pressure Implicit with Splitting of Operators
PIMPLE	Pressure Implicit with SIMPLE–PISO
PIV	Particle Image Velocimetry
RANS	Reynolds averaged Navier-Stokes
RF	Random Forest
RMSE	Root mean-squared error
SIMPLE	Semi Implicit Method for Pressure Linked Equations
SGS	Subgrid-scale
TV	True values (experimental/reference)
WALE	Wall-Adapting Local Eddy Viscosity model

Symbols

C_0	Reference salinity concentration
D	Molecular diffusivity
Fr_d	Densimetric Froude number
H_t	Ambient water depth (normalizing length in Fr_d/H_t)
K, K_*, K_{**}	Covariance matrices for train, cross, and test sets
L	Cholesky factor of a covariance matrix
$\mathcal{N}$	Gaussian (normal) distribution
Re	Reynolds number
Sc	Schmidt number
U_0	Bulk exit velocity magnitude
Y	Vector of observations (training outputs)
Y_L, Y_H, Y_T	Low-, high-, and top-fidelity (TV) outputs
c	Salinity concentration
$\tilde{c}$	Normalized salinity concentration
d_0	Nozzle diameter
e_i^g	Unit vector in direction of gravity $(0, -1, 0)$
$f(\mathbf{x}, \cdot)$	Shared latent GP for global trend
g	Gravitational acceleration
$g(\mathbf{x}, \cdot)$	Shared latent GP for intermediate-scale variation
g'	Reduced gravity
$k_j(\mathbf{r})$	Anisotropic Matérn-5/2 kernel with ARD ($j \in \{f, g, \delta_T\}$)
ℓ_j	ARD length-scale vector of kernel $k_j(\cdot)$
p	Pressure
s_r	Return point dilution
s_t	Surface dilution
t	Time
u_i	i -th component of velocity
$\mathbf{x}$	Vector of normalized design variables in $[0, 1]^d$
$\tilde{x}_i, \tilde{y}_i, \tilde{z}_i$	Spatial coordinates in the x, y and z direction
$\tilde{x}_r$	Return point horizontal distance
$\tilde{x}_t$	Terminal rise horizontal distance

Greek symbols

α_ℓ	Shape hyperparameter used in priors for length-scales
$\beta_\ell, \beta_\lambda, \beta_\sigma$	Rate/scale hyperparameters in prior distributions
$\Gamma(\cdot)$	Gamma function (in prior definitions)
δ	Discrepancy term between fidelity levels
$\delta_T(\mathbf{x})$	Top-level discrepancy capturing residual structural bias
ε	Observation noise (Gaussian)
$\boldsymbol{\theta} = (\theta_2, \theta_3, \theta_s)$	Inter-fidelity coupling/calibration parameters
$\boldsymbol{\Theta}$	Collection of all model (hyper)parameters
$\lambda_f, \lambda_g, \lambda_{\delta_T}$	Signal standard deviations of latent GPs and δ_T
μ	GP mean (assumed constant)
μ_{pred}	Posterior predictive mean at top fidelity
ν	Kinematic viscosity
$\pi(\cdot)$	Prior/posterior density
ρ	GP correlation (kernel) parameter
ρ_0, ρ_a	Jet initial density; ambient fluid density
σ	Observation-noise standard deviation (shared across fidelities)
σ_μ^2	Prior variance of the GP mean
$\Sigma_\mu(\boldsymbol{\Theta})$	Hierarchical block covariance matrix
Σ_{pred}	Posterior predictive covariance at top fidelity
τ_{ij}	SGS stress tensor (LES) / Reynolds stress tensor (RANS)

Appendix - A: Experimental setup

PIV configuration

Since the velocity field is a critical parameter for validating the applied numerical code, discretization schemes, and mesh quality, three high-resolution PIV experiments were conducted, and the accuracy of the LES predictions was evaluated by comparing them with the experimental results. A series of high-resolution PIV experiments [116] were performed to evaluate and validate the results of implemented LES. The experiments were carried out in a glass wall water tank with dimensions of 3 m in length, 1.2 m in width, and 1 m in depth. An aluminum apparatus was installed within the tank to produce a 60-degree jet, achieved using two adjustable sliding components. The jet was created using a solid polymer pipe with a diameter of 6 mm and a straight length equivalent to $40d$. In these experiments, the saline jet density was maintained in order to generate 0.75, 1.25, and 1.50 $d_0 Fr_d / H_t$ and a fixed Reynolds number of 3536 for the experimental modeling (summarized in Table 4.A1). The flow rate was supplied through a head tank located above the test tank, which was continuously pumped with homogeneous saline water from a large storage tank. To ensure the density uniformity of the saline water, two mixing pumps were constantly operated within the storage tank. A schematic of experimental configuration is shown in Figure 4.A1. The density and temperature of both saline and freshwater were measured using a portable density meter (DMA 35, Anton Paar) with an accuracy of 0.001 g/cm³.

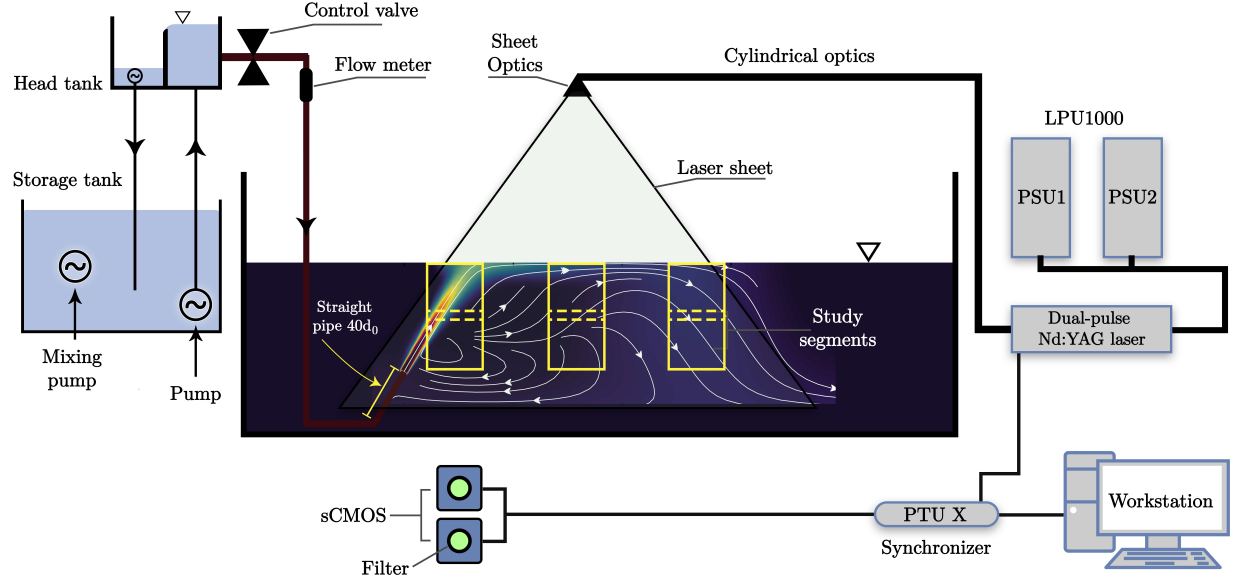


Figure 4.A1: A schematic representation of the experimental setup, including the saline reservoir, piping system, nozzle, and PIV equipment.

To conduct the experiments, both the saline tank and fresh water were homogeneously seeded with hollow, non-porous glass microspheres with a diameter of $9\text{ }\mu\text{m}$ and a specific gravity of 1.1 g/cm^3 . Laser light, generated by a dual-pulse Nd:YAG laser with a 532 nm wavelength, was delivered through an articulated light arm and shaped into an approximately 1 mm thick laser sheet using optics. Images were captured by two dual-frame sCMOS cameras (2D2C) located vertically, each with a resolution of 2560×2160 pixels and a total of 3000 images at a frame rate of 10 Hz , were captured to have a uniform time averaged data. The cameras, covering an area of 105 mm in the x -direction and 180 mm in the y -direction with 10% overlap, provided a spatial resolution of slightly more than 24 pixels per millimeter. Each camera is equipped with a 50 mm focal length lens, an aperture of $f/1.8$, and a bandpass filter centered at 532 nm with a 10 nm bandwidth to block ambient light. The time delay between the two laser pulses was adjusted from $250\text{ }\mu\text{s}$ to $1000\text{ }\mu\text{s}$, depending on the average flow velocity within the sampling region, ensuring particle displacement remained within $1/4$ of the interrogation window size. Two-dimensional velocity distributions were calculated using cross-correlation algorithms within 32×32 pixel interrogation windows. Due to the high spatial resolution of the imaging system and the limited measurement area, it was not possible to capture the entire jet development in a single recording session. Therefore, the experiment was conducted in three to five sequential recording sessions, each covering a different portion of the jet from the nozzle to the return point. After completing each recording section, the tank was drained, refilled with fresh water, and reseeded to eliminate any residual salinity and to allow camera repositioning and recalibration for the next measurement section. Data acquisition and processing were carried out using the LaVision system and DaVis 10.2.1 software on a workstation equipped with an Intel(R) Xeon(R) W-3235 CPU @ 3.30 GHz and 128 GB of RAM, ensuring high-resolution and reliable results. To minimize errors and uncertainties (less than 5%) calculated by the Davis software, the experiments were repeated at each recording session. Additionally, all PIV measurements were conducted

following the standardized procedures outlined by LaVision⁷, thereby ensuring the reliability and consistency of the data acquisition process.

Table 4.A1: Characteristics of PIV experiments

PIV cases	Fr_d/H_t	Flow rate (L/hr)	ρ_j (kg/m^3)	ρ_a (kg/m^3)	g' (m/s^2)	Fr_d
1	0.75	60	1024.18	998	0.257	15
2	1.25	60	1007.43	998	0.093	25
3	1.50	60	1004.55	998	0.064	30

It should be noted that behavior of jets in shallow environments is significantly influenced by the proximity of the water surface, which confines the development of the jet and prevents it from reaching its terminal height. While previous studies addressed the impact of shallow conditions, one crucial parameter that remains underexplored is the distance between the nozzle tip and the bed. This bottom boundary distance is critical, as it directly affects the jet's dynamics and interaction of the jet with its surroundings. Ramakanth et al. have highlighted the influence of bottom boundary distance on jet behavior in deep ambient, but the implications of this parameter in shallow environments have not been systematically addressed. This study did not examine the effect of bed distance and instead employed a fixed distance across all scenarios.

LIF configuration

The experiments were conducted in a transparent large tank supplied by a storage tank and a constant head tank, with a pipe with diameter of $d_0 = 0.008m$ and length of approximately $20d_0$ ensuring fully developed flow prior to discharge into the tank, as illustrated in Figure 4.A2. The hot water was prepared in the storage tank with mixing pumps to maintain uniformity and was subsequently supplied to the head tank to deliver a steady flow rate, monitored by a flowmeter and regulated by a control valve. LIF was employed to measure the concentration field along the vertical centerline of the jet using a continuous Nd:YAG laser generated a thin vertical light sheet in the jet center plane, and Rhodamine 6G dye was introduced at low concentrations to preserve a linear intensity-concentration relationship. The emitted fluorescence was recorded using an Imperx C2420 camera with a resolution of 2464×2056 pixels operating at frame rates of 97 frames per second. The camera with a 50mm lens was located orthogonally to the laser sheet. In Each run 5000 images were recorded, providing statistically converged measurements of both mean and fluctuating scalar fields. Details of the post-processing procedure are provided in [208].

⁷<https://www.lavision.de/en/downloads/manuals/>

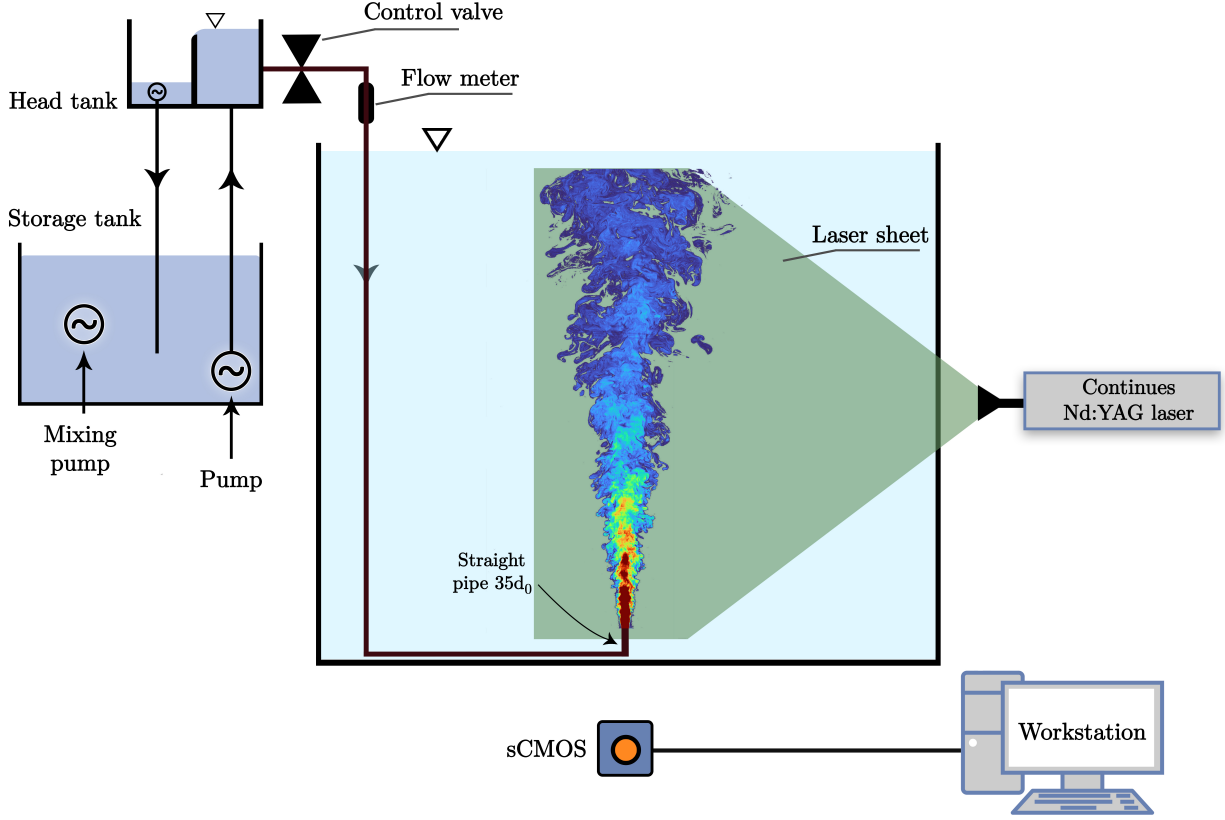


Figure 4.A2: A schematic representation of the experimental setup, including the hot water reservoir, piping system, nozzle, and LIF equipment.

A total of four LIF experiments were conducted to investigate the vertical thermal jet under varying buoyancy conditions. In all cases, the flow rate was kept constant at 70 L/hr resulting $Re = 3100$, and the jet density ρ_j was adjusted to obtain different Fr_d values. The characteristics of the experiments are summarized in Table 4.A2.

Table 4.A2: Characteristics of LIF experiments

LIF cases	Flow rate (L/hr)	ρ_j (kg/m^3)	ρ_a (kg/m^3)	Fr_d
1	70	984.88	998	12
2	70	989.64	998	15
3	70	994.83	998	20
4	70	995.06	998	25

Appendix - B: Gaussian process setup and parameters

As scenario 2 involves a three-level fidelity configuration (low-, high-, and TV-fidelity), presenting all posterior results at every location would be excessive. Therefore, only the representative case at $\tilde{y} = 10$ is reported here to illustrate the key hyperparameter behaviors

and the hierarchical coupling characteristics of the GP model, as the other locations exhibit similar posterior trends with only marginal variations.

Calibration posteriors for Scenario 2 at $y = 10$

Figure 4.B1 and Figure 4.B2 present the posterior probability density functions (PDFs) of the key GP hyperparameters obtained from the three-level hierarchical multifidelity model for scenario 2 at $\tilde{y} = 10$. These parameters describe the smoothness, precision, and inter-fidelity coupling across the latent processes f , g , and δ_T , which respectively represent the low-, high-, and TV-fidelity components of the hierarchical structure. All parameters were inferred through MCMC sampling, and their posterior distributions characterize the uncertainty of the calibration at this $y = 10$.

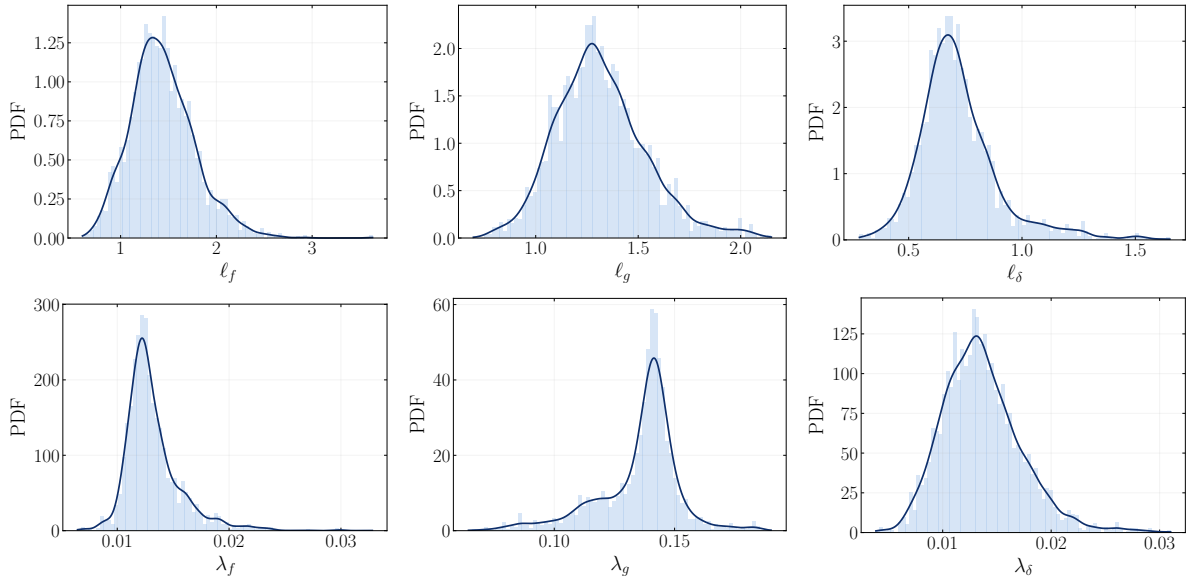


Figure 4.B1: Posterior distributions of GP length-scale (ℓ) and precision (λ) parameters for the latent processes for scenario 2 at $\tilde{y} = 10$.

The first group of parameters, ℓ_f , ℓ_g , and ℓ_δ , define the characteristic correlation lengths of the latent processes. Narrow peaks at moderate values of ℓ_f and ℓ_g indicate that both the LF and HF-fidelity functions exhibit smooth, spatially correlated behavior over the Fr_d range, whereas the shorter ℓ_δ suggests that the TV-fidelity correction δ_T captures finer local variability unresolved by the lower levels. This behavior is consistent with the expected flow regime transition around $Fr_d \approx 12-15$, where the experimental data exhibit strong buoyancy effects and enhanced small-scale variability. The second group, λ_f , λ_g , and λ_δ , quantify the marginal amplitude of each process. The higher posterior modes of λ_g and λ_δ relative to λ_f indicate that the HF contribute more strongly to the predictive variance reduction, reflecting the model's confidence in the LES and experimental (TV) data. This precision hierarchy aligns with the observed order of magnitude error reduction in Table 4.6.

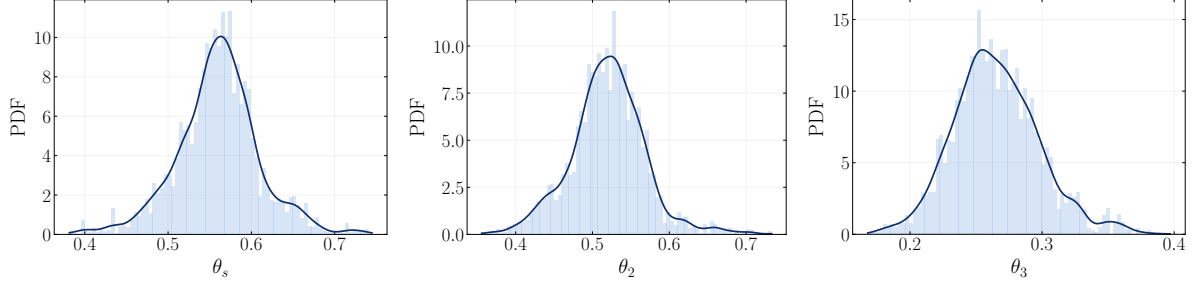


Figure 4.B2: Posterior distributions of inter-fidelity coupling parameters θ_s , θ_2 , and θ_3 for scenario 2 at $\tilde{y} = 10$.

The coupling parameters θ_s , θ_2 , and θ_3 describe the structural correlation among the three fidelity levels. The sharply peaked unimodal posteriors centered around 0.4-0.7 indicate strong and stable inter-fidelity coupling, ensuring efficient information transfer from the LF (RANS data) to the HF (LES data) and true-value (TV) observations. Among them, θ_3 shows a slightly narrower distribution, implying tighter dependence between the high- and TV-fidelity layers. This result supports the model's ability to refine the LES prediction near the TV-fidelity domain without overfitting. These posterior behaviors confirm that the MFGP effectively balances global smoothness inherited from lower fidelities with local adaptability governed by the TV correction, which is essential for accurately reconstructing concentration profiles.

Appendix - C: Sensitivity and uncertainty analysis

This appendix presents the sensitivity analyses for both scenario 1 and scenario 2, including the effects of LF and HF sample sizes and the corresponding 95% CI widths along the densimetric Fr_d range. Sensitivity analysis of MFGP to the number of LF sample for scenario 1 is shown in Figures 4.C1, 4.C2, 4.C3, and 4.C4.

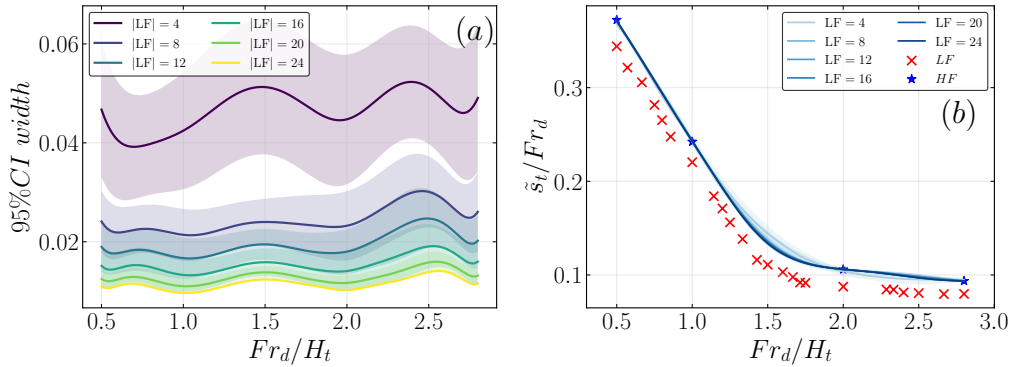


Figure 4.C1: Scenario 1 sensitivity of MFGP predictions of s_t/Fr_d to the number of LF samples and corresponding 95% CI.

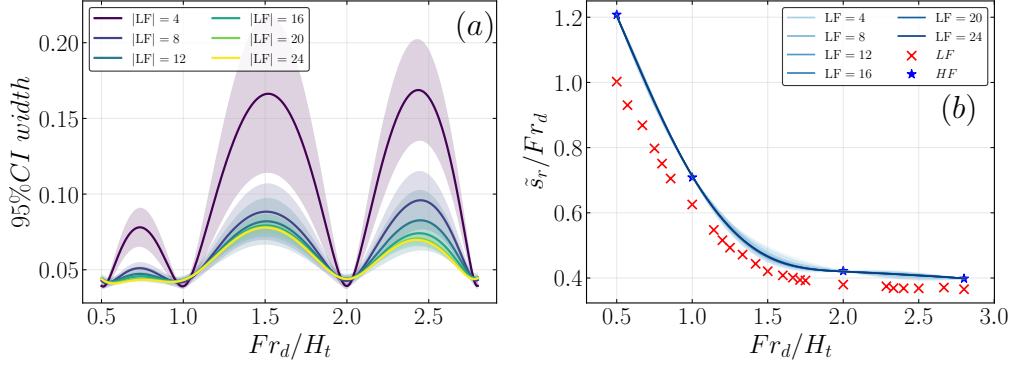


Figure 4.C2: Scenario 1 sensitivity of MFGP predictions of s_r/Fr_d to the number of LF samples and corresponding 95% CI.

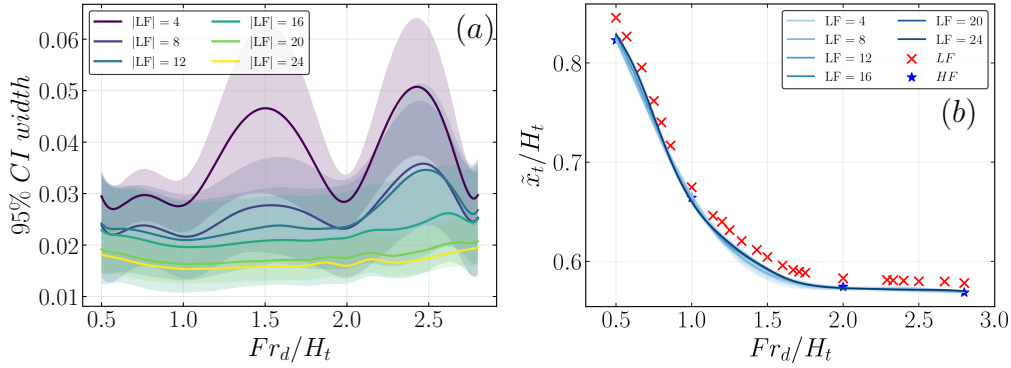


Figure 4.C3: Scenario 1 sensitivity of MFGP predictions of $\tilde{x}_t/H_t$ to the number of LF samples and corresponding 95% CI.

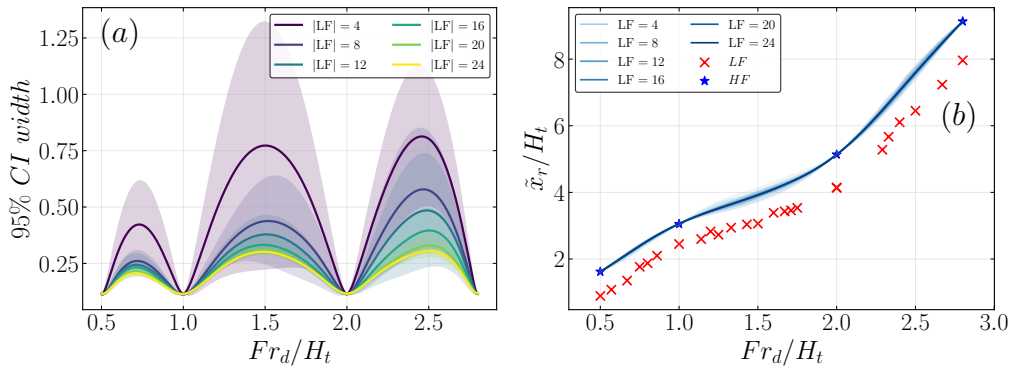
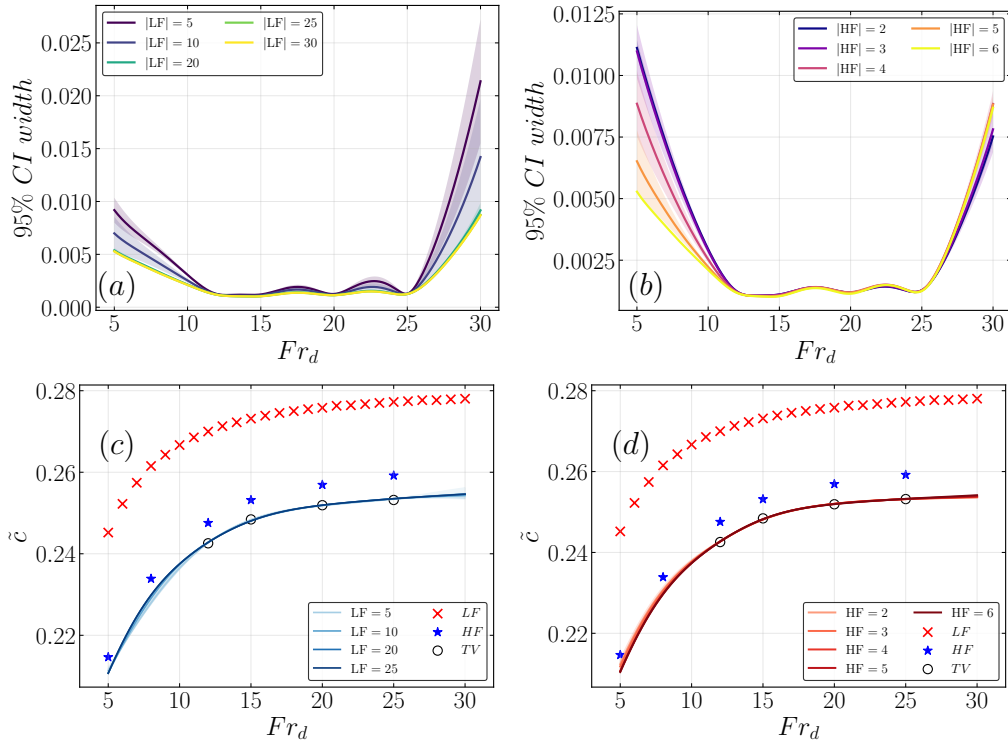
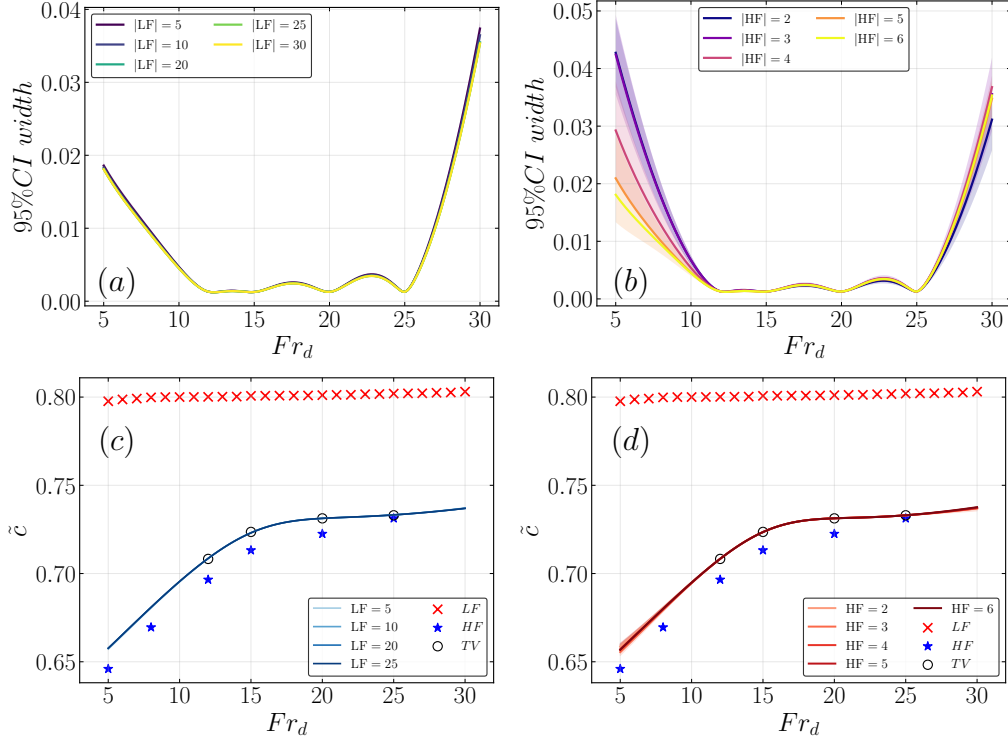


Figure 4.C4: Scenario 1 sensitivity of MFGP predictions of x_r/H_t to the number of LF samples and corresponding 95% CI.

Sensitivity analysis for scenario 2 for prediction of centerline concentration and representative locations of $\tilde{y} = 10, 20, 40$; the remaining distances display similar trends with only marginal variations and are therefore omitted for brevity.



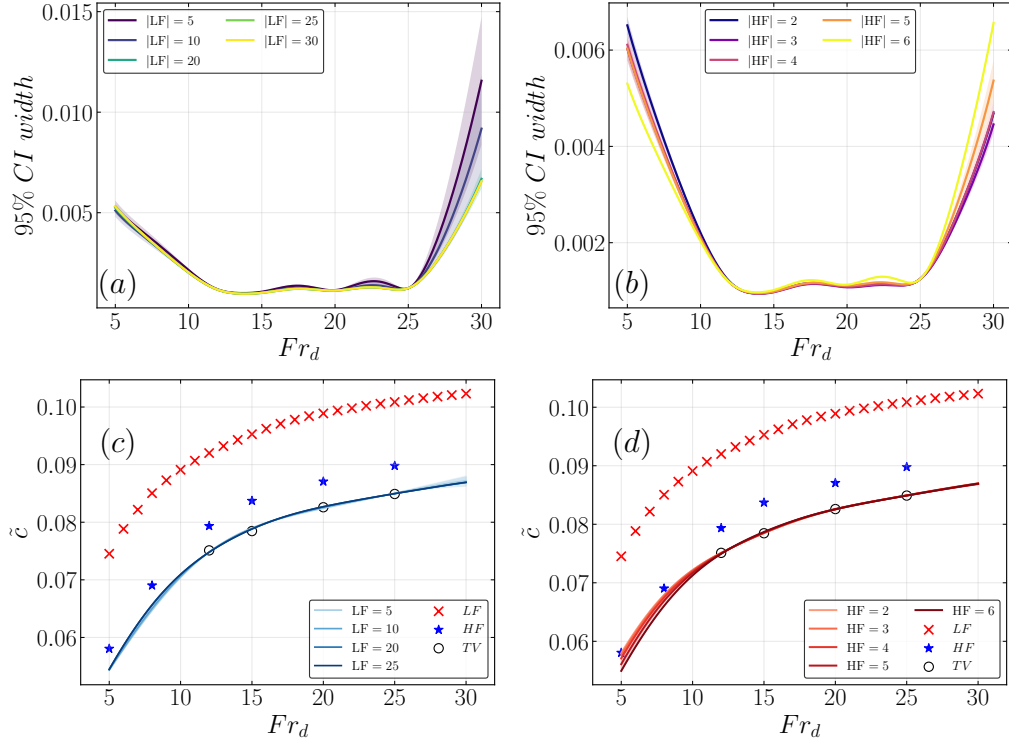


Figure 4.C7: Scenario 2 at $\tilde{y} = 40$: sensitivity of MFGP predictions to the number of LF and HF samples, and corresponding 95% CI.

Chapter 5

Conclusions and Future Perspectives

5.1 Summary of Findings

This thesis has undertaken a comprehensive investigation of jet dynamics from desalination discharges, combining advanced experimental measurement with high-fidelity numerical simulations. The research addressed critical gaps in the understanding of turbulent mixing, buoyancy driven entrainment, and multifidelity modeling of saline and thermal jets.

Four main contributions have been achieved:

1. **Large Eddy Simulation (LES) inlet impacts.** A systematic evaluation of inlet boundary conditions for LES of desalination jets was carried out. The study demonstrated that the choice of inflow turbulence treatment exerts a decisive influence on near-field turbulence generation and consequently on the prediction of jet dilution. The mapped and turbulent flow inflow conditions produced the closest agreement with high-resolution Particle Image Velocimetry (PIV), highlighting the importance of physically consistent boundary specification.
2. **LES of dense jets in stratified crossflow.** Through large-scale simulations, the impact of density stratification on the trajectory and dilution of dense jets was quantified. Results showed strong asymmetry in entrainment and enhanced suppression of vertical penetration under stable stratification.
3. **Multi-fidelity Gaussian Process (MFGP) modeling.** A Bayesian hierarchical framework was developed to integrate low- and high-fidelity numerical data for uncertainty aware prediction of jet evolution. The approach successfully reduced computational cost while retaining predictive accuracy, demonstrating the potential of MFGP models as surrogates for prediction of desalination outfalls behavior.
4. **Direct Numerical Simulation (DNS) of buoyant thermal jets.** A high-resolution DNS case was established as a benchmark to study scalar transport and thermal mixing in positively buoyant jets. The results provided insights into the interplay between coherent structures, Reynolds number effects, and buoyancy, offering reference data.

5.2 Scientific Contributions

This thesis advances the state of knowledge in several respects:

- It clarifies the role of inlet turbulence specification in LES, a recurring source of discrepancy in numerical predictions of dense jet mixing. By systematically comparing uniform, synthetic, mapped, turbulent velocity, and fully developed inflow conditions, the study demonstrates that realistic inflow turbulence significantly improves agreement with experimental velocity and scalar fields.
- It delivers the first integrated LIF-LES-RANS modeling framework for desalination jets, bridging fundamental and applied perspectives. This multi-scale approach enables rigorous validation of turbulence-resolving simulations against laboratory measurements, while also providing insight into the capabilities and limitations of lower-order RANS models for engineering applications.
- It quantifies, for the first time, the influence of crossflow stratification intensity on dense jet behavior using high-resolution LES. The results reveal that stronger stratification suppresses vertical jet penetration, enhances lateral spreading, and alters entrainment dynamics, ultimately reducing dilution efficiency. These findings provide new physical understanding and benchmark data for the design of waste discharges in stratified coastal environments.
- It establishes, for the first time, a Direct Numerical Simulation (DNS) of a positively buoyant thermal jet. This high-fidelity dataset provides detailed information on scalar transport, turbulence buoyancy interactions, and coherent structures, serving as a benchmark for LES validation and future reduced-order modeling.
- It contributes novel benchmark datasets (PIV, LIF, DNS) and open-source image-processing and data-analysis workflows that may serve as validation material and methodological reference for the wider research community.
- It develops and validates, for the first time, a nondimensionalized OpenFOAM solver for buoyant jet simulations. This solver allows simulations to be performed in a generalized framework, significantly reducing the number of dimensional parameters and enabling direct comparison across different jet configurations and experimental scales.

5.3 Limitations

While the thesis has addressed several challenges, certain limitations remain:

- Laboratory-scale experiments, while highly resolved, cannot fully reproduce the variability of field-scale outfalls subject to waves, currents, and bathymetry.
- LES and DNS simulations were conducted for canonical geometries; practical diffuser configurations with multiport interactions require further investigation.

- The MF-GP framework was demonstrated on point data; extending it to multi-dimensional parameter spaces (e.g., salinity, temperature, ambient turbulence, stratification) remains computationally demanding.

5.4 Future Perspectives

Building on the present findings, future research directions include:

1. **Extension to other configurations:** Applying the validated LES models to more complex jet configurations, such as multiport diffuser systems, different jet angles, and outfalls interacting with coastal bathymetry. This will enable the assessment of mixing efficiency and environmental impact under different conditions.
2. **Coupled multiphase and microplastic transport:** Integrating CFD-DEM models to examine the co-dispersion of brine, heat, and microplastics, a pressing concern in coastal environments.
3. **Advanced UQ frameworks:** Extending multi-fidelity Gaussian Process modeling toward active learning strategies and Bayesian optimization, enabling robust design under uncertainty.
4. **Data-driven reduced-order models:** Exploiting Proper Orthogonal Decomposition (POD) and machine learning surrogates to accelerate simulations and enable real-time environmental assessments.

APPENDICES

Appendix A

Comment on Venturi nozzles for desalination brine discharges

A.1 Introduction

The management of saline wastewater requires environmental consideration. Outfalls are recognized as a method for discharging saline wastewater into the environment [16, 225]. Therefore, understanding the dynamics of saline outfalls from desalination plants is essential for minimizing their adverse environmental impacts. The paper, titled “Venturi Nozzles for Desalination Brine Discharges” examined the effects of Venturi nozzles on saline discharges through numerical and experimental modeling [84]. They conducted a series of LID (LIF) experiments and LESs to study the dynamics of saline discharge within a Venturi nozzle. Their experimental LIF results demonstrated that the Venturi nozzle restricted the jet development and reduced dilution. The comparison of experimental and numerical simulation results exhibited certain limitations in numerical results. Notably, they found an underestimation of the jet’s geometrical characteristics and its mixing efficiencies.

The LES model directly resolves the large eddies while models the smaller scales [40]. As mentioned in the method section of [84], a *fixedValue* boundary condition was employed for velocity (see [84], §2.2. - page 5). The *fixedValue* boundary condition in OpenFOAM applies a uniform velocity profile that remains constant both spatially across the entire patch and temporally throughout the simulation, as described [84]:

$$U_x = U_0 \cos(\theta), \quad U_y = U_0 \sin(\theta), \quad U_z = 0, \quad C = C_0 \quad (\text{A.1})$$

here U_0 is jet velocity and U_x , U_y and U_z are velocity in x , y and z direction, C_0 and C are jet concentration and concentration respectively.

The accuracy and applicability of LES in any computational fluid dynamics (CFD) study significantly depend on how precisely the physical flow field is replicated [59, 110, 226]. The fidelity of LES relies on accurately resolving the large-scale turbulent structures while modeling the smaller scales through subgrid-scale models. In contrast to the Reynolds-averaged Navier–Stokes (RANS) model, the LES model is both spatially and temporally dependent, making it more effective in capturing the dynamics of turbulent flows. This requires not only high-resolution meshes but also appropriate boundary conditions that can

generate realistic inflow turbulence characteristics. For LES, an appropriate inlet boundary condition should form three-dimensional eddies and should also accurately generate both the mean flow field and the turbulence statistics of the flow at the inlet [59, 110, 226–228].

This comment focuses on the numerical method aspects of [84], including the improper implementation of the inlet boundary condition, the ratio of resolved total kinetic energy to total total kinetic energy presented in Figure 2 of [84], the mesh resolution, and the overall results of the numerical section of the study under discussion. The *fixedValue* boundary condition is not able to generate eddies or turbulent fluctuations within the inflow, nor is it able to form a fully developed flow velocity profile. As the *fixedValue* condition does not generate TKE, any estimation for mesh resolution based on the LES index of Resolution Quality (shown by M as the proportion of resolved total kinetic energy to total total kinetic energy ($M = \frac{TKE_{resolved}}{TKE_{sgs} + TKE_{resolved}}$ [40, 186]), as mentioned in [84], is not accurate. To address these issues, two simulations were conducted using *fixedValue* and *mapped* inlet conditions.

A.2 Numerical method

To examine the effect of inlet boundary conditions on the dynamics of the buoyant jet, two simulations with a densimetric Froude number (Fr) of 7.5 and Reynolds number (Re) of 3500 similar to those in [84] with a simple nozzle (without a Venturi nozzle) are conducted. The dynamics of the buoyant jet are computed using the incompressible filtered Navier-Stokes equations (Equations A.2 and A.3), coupled with a mass transport equation (Equation A.4), and are expressed in nondimensional form as follows [40, 43]:

$$\frac{\partial \tilde{u}_i}{\partial \tilde{x}_i} = 0 \quad (\text{A.2})$$

$$\frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j \partial \tilde{x}_j} - \frac{\partial \tilde{\tau}_{ij}}{\partial \tilde{x}_j} + e_i^g \frac{1}{Fr^2} \tilde{c} \quad (\text{A.3})$$

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{c}}{\partial \tilde{x}_i} = \frac{1}{ReSc} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}_i \partial \tilde{x}_i} - \frac{\partial \tilde{\tau}_i^c}{\partial \tilde{x}_i} \quad (\text{A.4})$$

where $\tilde{p}$ represents the pressure, $\tilde{u}_i$ is the velocity component, $\tilde{t}$ is time and $\tilde{\tau}_{ij}$ represents the subgrid stresses, Sc is Schmidt number, $\tilde{c}$ is concentration and e_i^g is direction of the gravitational acceleration $(0, -1, 0)$. Here Tilde symbol ($\sim$) is used to represent dimensionless filtered quantities. The Reynolds number and densimetric Froude number are Reynolds number and densimetric Froude number, respectively, and are calculated as follows:

$$Re = \frac{U_0 d_0}{\nu} \quad (\text{A.5})$$

$$Fr = \frac{U_0}{\sqrt{g' d_0}} \quad (\text{A.6})$$

where U_0 is jet velocity (characteristic velocity scale), d_0 is diameter of jet (characteristic length scale), ν is kinematic viscosity and g' is reduced gravity defined as:

$$g' = g \frac{\rho_0 - \rho_a}{\rho_a} \quad (\text{A.7})$$

where g denotes the gravitational acceleration (0, -9.81, 0), ρ_0 and ρ_a are the jet and ambient densities. Dimensionless variables are established with respect to characteristic length, velocity, and time scales, as defined in Table A.1:

Table A.1: Definition of non-dimensionalization used in this work.

Parameter	Non-dimensionalization
Spatial coordinates	$\tilde{x}_i = x_i/d_0$
Velocity	$\tilde{u}_i = u_i/U_0$
Time	$\tilde{t} = (U_0/d_0)t$
Pressure	$\partial\tilde{p}/\partial\tilde{x}_i = (d_0/\rho_a U_0^2) \partial p/\partial x_i$
Subgrid-scale stress tensor	$\partial\tilde{\tau}_{ij}/\partial\tilde{x}_j = (d_0/U_0^2) \partial\tau_{ij}/\partial x_j$
Salinity	$\tilde{c} = c/C_0$

The constant values for momentum diffusivity (ν) and salt diffusivity (D) are considered to 1×10^{-6} and 1.5×10^{-9} , respectively based on [93, 94].

In this study, the Wall-Adapting Local Eddy-viscosity (WALE) model is utilized as the subgrid-scale model. For more detailed information, readers are referred to [88]. The simulations were conducted in nondimensional mode by the open-source OpenFOAM for over 20,000 nondimensional time units and the flow characteristics were averaged across more than 10,000 nondimensional time units [229]. A modified version of pimpleFoam, coupled with an advection-diffusion equation, is used to conduct the simulations, with the Boussinesq approximation employed to account for the effects of buoyancy on the fluid dynamics. To ensure second-order accuracy, the time derivative terms were discretized using the backward scheme, the gradient terms were handled with the Gauss linear method, divergence terms were discretized using the Gauss limitedLinear scheme, viscous terms with the Gauss linear scheme, and Laplacian terms with the Gauss linear uncorrected scheme [98–100]. To improve stability and accuracy during the simulations, the maximum Courant Friedrichs Lewy number (CFL number) was maintained below 0.5. For further details on OpenFOAM, readers are referred to Holzmann, Moukalled et al..

Among the applicable inlet conditions for LES as outlined in [59, 110, 226], in this study *mapped* inlet condition is utilized within OpenFOAM to generate a fully developed turbulent inflow for the jet. The *mapped* inlet is a three-dimensional turbulent inflow method that depends on both spatial and temporal variations, based on the technique proposed by Lund, Wu, and Squires [107]. This method involves extracting flow characteristics from a comparable cross-section within the interior at a specific downstream location and reapplying them to the inlet [108]. The *mapped* inlet technique is a type of precursor simulation method integrated directly into the solution domain, allowing the turbulent flow to be generated by the primary flow mechanisms within the main computational domain.

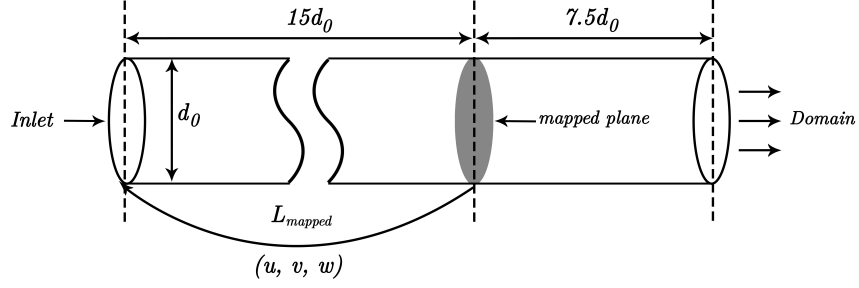


Figure A.1: Schematic representation of the *mapped* inlet configuration (not to scale).

The interior cross-section, or mapped plane, is positioned within the domain to allow sufficient length for eddy formation while being far enough from the downstream region to avoid additional perturbations from that area [59]. In this study, the *mapped* inlet is created using a pipe connected to the domain. The mapped length (L_{mapped}) within the pipe is set to $15d_0$, and the distance from the mapped plane to the main domain is $7.5d_0$ as illustrated in Figure A.1.

A fully hexahedral mesh comprising 11 million cells was generated using the Gmsh open-source mesh generator [230], as illustrated in Figure A.2. The mesh was created using a multi-level refinement method, with enhanced resolution near the nozzle, pipe, and plume development zone, ensuring the capture of over 90% of the total total kinetic energy. (It should be noted that this study does not resolve the Batchelor scales.)

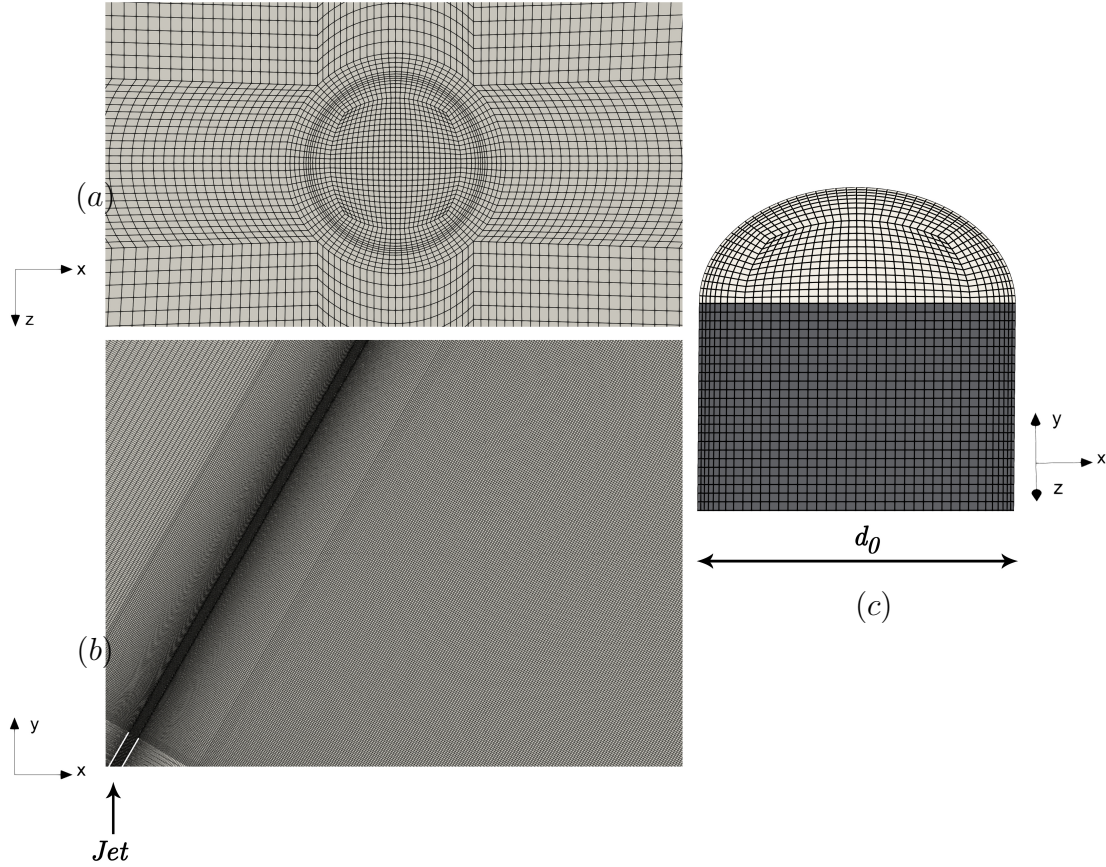


Figure A.2: Visualization of the computational mesh; (a) surface over jet, (b) a surface in middle of the domain near the jet area, and (c) pipe (or nozzle).

Due to the lack of available experimental data on time-averaged velocity and fluctuations, a direct comparison of the jet and pipe results is not possible. However, the applicability and effectiveness of the *mapped* inlet have been thoroughly examined in various studies, such as [109, 110, 226].

A.3 Discussion of the effects of inlet boundary condition

The results were post-processed using open-source Python libraries, including Matplotlib¹, PyVista², and Pandas³. As the simulations were conducted in nondimensional mode, all reported quantities are nondimensional, and the overline symbol ($\bar{}$) represents the time-averaged quantities.

Figure A.3 illustrates the evolution of both the time-averaged ($\bar{c}$) and instantaneous concentration ($\tilde{c}$) of the jet under the *mapped* and *fixedValue* inlet conditions. It is evident

¹<https://matplotlib.org/>

²<https://pyvista.org/>

³<https://pandas.pydata.org/>

that the *fixedValue* condition under-estimates the development of the buoyant jet, confirming the observations made by [84]. The contours of the concentration clearly indicates that the growth of the jet, under the *fixedValue* boundary condition, fails to reach higher level in the y-direction and, consequently, does not extend in the x-direction as *mapped* inlet condition. The under-estimation noted in jet trajectory for *fixedValue* inlet conditions is similarly evident in Figure 9 of [84], where the simple nozzle, indicated by a dashed line, clearly under-estimates the trajectory of the buoyant jet.

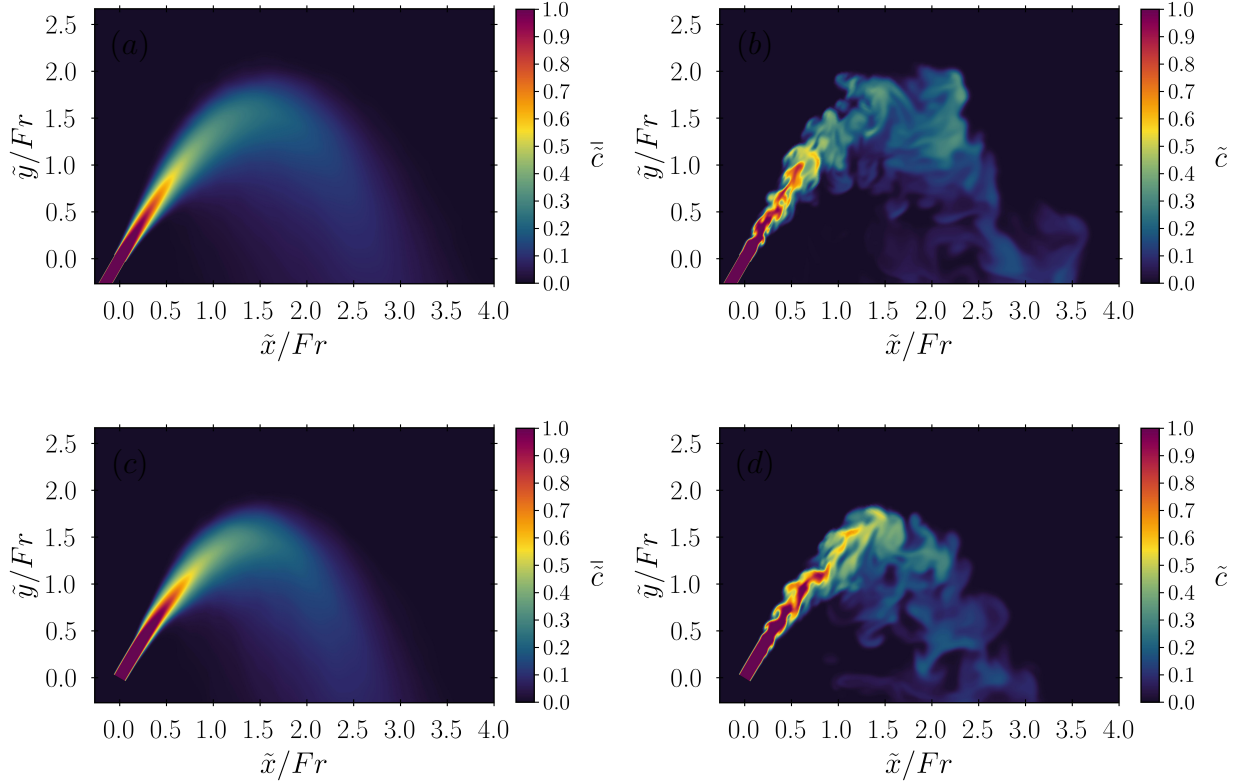


Figure A.3: Contours of time-averaged and instantaneous concentration contours of saline jet for *mapped* inlet condition (a and b) and *fixedValue* condition (c and d)

Figure A.4 shows the time-averaged Reynolds flux $(\overline{u'u'})$, $(\overline{v'v'})$, and $(\overline{u'v'})$ for the *mapped* inlet condition (left column) and the *fixedValue* inlet condition (right column). It is apparent that the simulation with the *fixedValue* inlet boundary condition consistently under-predicts the Reynolds flux across all components when compared to the *mapped* simulation. This under-prediction is indicative of a less dynamic interaction in the flow field, which is due to the inability of the *fixedValue* condition to generate the eddies and turbulent structures that are characteristic of buoyant jet flow. The under-prediction of Reynolds flux by the *fixedValue* inlet significantly impacts the dynamics of the buoyant jet and its mixing. The *fixedValue* condition's limitation in capturing these aspects leads to an inaccurate representation of the flow, affecting the reliability of outcomes.

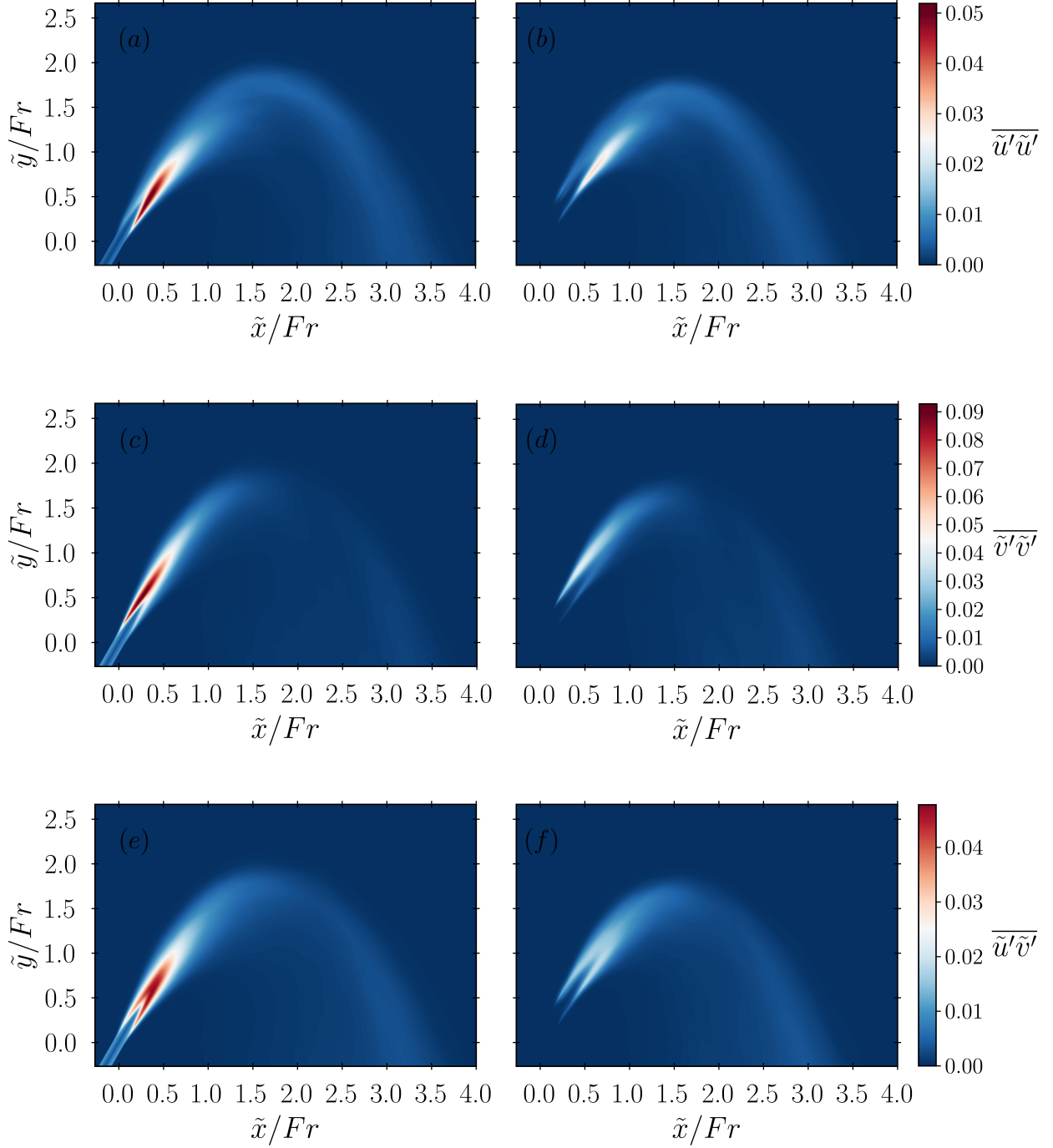


Figure A.4: Contours of time-averaged Reynolds flux $\overline{u'u'}$, $\overline{v'v'}$, and $\overline{u'v'}$. The left column (a, c, e) represents the results for the *mapped* inlet condition, and the right column (b, d, f) corresponds to the *fixedValue* inlet condition. Sub-figures of (a) and (b) represent $\overline{u'u'}$, (c) and (d) represent $\overline{v'v'}$, and (e) and (f) represent $\overline{u'v'}$.

Besides the under-estimation associated with the *fixedValue* boundary condition, another issue is the location of the peak fluctuations formed in the domain as illustrated in Figures

A.4 and A.5. The constant and uniform value imposed by the *fixedValue* condition leads to delayed fluctuation development, observed at a distance of $5d_0$ from the inlet. In contrast, under the *mapped* condition, fluctuations emerge in the pipe and near to the nozzle, where the flow is both fully turbulent and developed. Figure A.5 shows three components of the time-averaged turbulent concentration flux on cross-sections perpendicular to the concentration centerline at four distances from the source (from $(0, 0, 0)$). The scatter plots show that the *fixedValue* inlet condition consistently under-estimates fluxes compared to the *mapped* across all measured distances. Specifically, close to nozzle at $2d_0$ and $3d_0$ from the nozzle, the turbulent concentration flux for the *fixedValue* condition are nearly zero, whereas for the *mapped* inlet, exhibits two peaks at these distances in shear layer of the jet. The *mapped* inlet exhibits two peaks near the nozzle, where the velocity gradient is steep, and by $5d_0$, these peaks converge, a behavior which is observed by Shao and Law [19]. In contrast, under the *fixedValue* condition, an increase in peaks is not observed until reaching $5d_0$. The discrepancies in turbulent concentration flux are a direct indicator that the mixing processes are under-estimated when the *fixedValue* condition is applied. This condition imposes an overly simplistic representation of the complex mixing dynamics, failing to capture the essential turbulence characteristics necessary for accurate simulation of the physical phenomena.

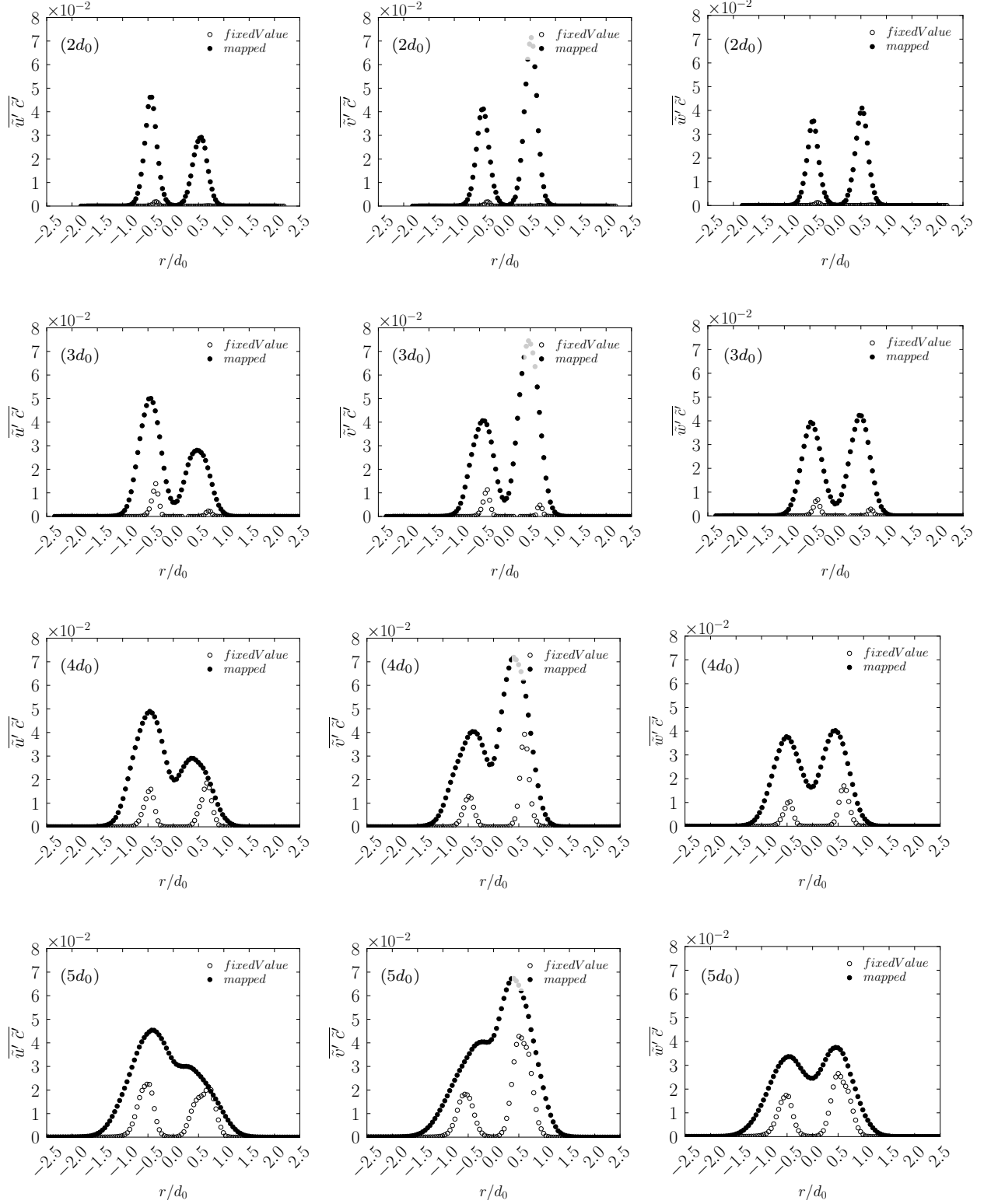


Figure A.5: Scatter plots of three components of time-averaged concentration fluxes in three directions at distances of $2d_0$, $3d_0$, $4d_0$ and $5d_0$ on cross-sections perpendicular to concentration centerline for both *fixedValue* and *mapped* inlet conditions. Here, negative r/d_0 refers to the part of the cross-section below the centerline while positive represents the above the centerline.

Figure A.6 represents a similar trend in the time-averaged concentration fluctuations ($\overline{\tilde{c}\tilde{c}'}$) for both *mapped* and *fixedValue* inlet conditions. For the *mapped* inlet condition, concentration fluctuations were initiated at the nozzle's entrance, consistent with the findings reported by [231]. Conversely, with the *fixedValue* inlet condition, the initiation of concentration fluctuations occurs farther from the nozzle. This delay is attributed to the late formation of the shear layer, and as a result, the downward buoyancy force causes the jet to bend downward.

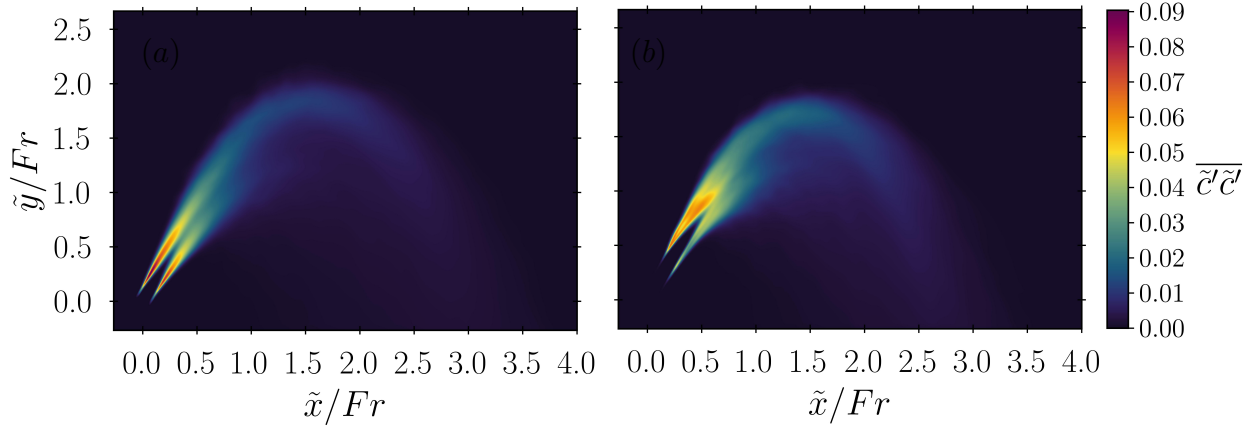


Figure A.6: Contours of time-averaged concentration fluctuations ($\overline{\tilde{c}\tilde{c}'}$). The sub-figure (a) corresponds to the results of *mapped* inlet condition, and the sub-figure (b) corresponds to the *fixedValue* inlet condition.

Figure A.7 illustrates the influence of the inlet boundary condition on the time-averaged total TKE of the buoyant jets. The *mapped* inlet condition generates a developed turbulent flow, leading to a higher TKE compared to the case with the *fixedValue* inlet condition. This observation aligns with the velocity fluctuations depicted in Figure A.4.

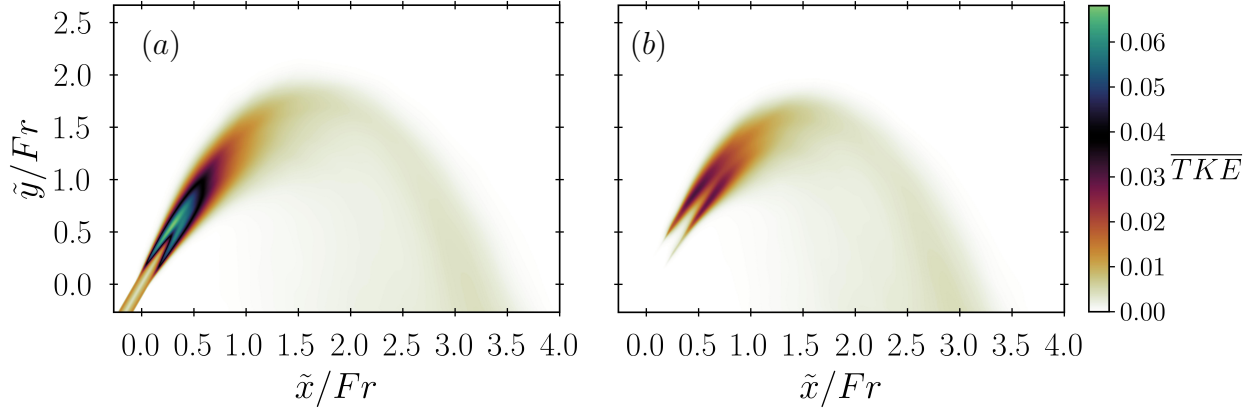


Figure A.7: Contours of time-averaged total TKE for *mapped* and *fixedValue* inlet conditions. The sub-figure (a) corresponds to the results of *mapped* inlet condition, and the sub-figure (b) corresponds to the *fixedValue* inlet condition.

The most important issue in [84] is the number of grids and consequently the grid size utilized for the LES. It is claimed that grids, comprising of 1,461,769 cells generated by snappyHexMesh, is capable of directly resolving over 75% of the total TKE and Figure 2 page 5 of [84] shows the proportion of resolved TKE to total TKE ($M > 75\%$). It is proven that the total TKE generated by the *fixedValue* boundary condition is significantly underestimated, as illustrated in Figure A.7, compared to the *mapped* boundary condition. This indicates that the total TKE generated by the *fixedValue* boundary condition is not physical and fails to accurately represent real-world conditions. Therefore, the grid applied in [84] for a jet with Reynolds number = 3500 is insufficient to satisfy the M criterion.

As the *fixedValue* boundary condition does not generate any TKE, in the nozzle velocity fluctuations should form due to the velocity gradient caused by the no-slip boundary condition at the walls. Considering the applied grid, as shown in Figure 1 of [84], which features a uniform size mesh without refinement near the walls, the increased TKE near the walls should result in a decrease in the M value, given the uniformity of the mesh. In other words, a higher velocity gradient and higher TKE should be generated near the walls, resulting in a lower M on a uniform, fixed-size grid. However, Figure 2 in [84] presents the opposite scenario. Despite mentioning the use of a no-slip boundary condition at the walls, the discrepancy may arise from the application of an inappropriate boundary condition near the Venturi nozzle walls.

Table A.2: Summary of geometrical characteristics of numerical results compared with previous experimental data.

BJIBC	$\tilde{y}_m/Fr$	$\tilde{y}_t/Fr$	$\tilde{x}_r/Fr$	$\tilde{s}_r/Fr$
<i>fixedValue</i> - Simple Nozzle LES	1.44	1.91	2.41	1.36
<i>mapped</i> - Simple Nozzle LES	1.65	2.25	2.79	1.57
Amiri, Abessi, and Roberts [128] - Simple Nozzle LES	1.35	1.89	2.56	1.18
Crowe [2]	1.62	2.12	2.81	—
Oliver, Davidson, and Nokes [14]	1.61	2.21	2.76	1.55
Papakonstantis, Christodoulou, and Papanicolaou [21]	1.68	2.15	2.75	1.68

Table A.2 compares the geometrical characteristics and dilution of numerical results with previous experimental data. Although the previous experiments reported a wide range of desalination jet characteristics, the data for the *fixedValue* condition are consistently under-predicted. This underestimation highlights the limitations of the *fixedValue* boundary condition in accurately capturing the jet dynamics. In contrast, the results from the *mapped* inlet condition show better alignment with the experimental data.

A.4 Conclusion

For accurate simulations of buoyant jets using LES, selecting appropriate boundary conditions is crucial. Our comparison of *mapped* versus *fixedValue* inlet conditions underscores the importance of boundary conditions in achieving precise LES results. The significant discrepancy between experimental and numerical findings, as noted in [84], may in part be explained by the improper implementation of the inlet boundary condition and grid resolution. Future LES research should emphasize choosing proper boundary condition (a physical boundary condition) at the inlet to ensure accurate and reliable results.

Future studies could focus on refining the inlet flow generator to enhance simulation results through more physically accurate inflow conditions, such as synthetic methods. Additionally, examining the effects of inflow grid resolution on simulation outcomes could provide further insights into optimizing model accuracy and reliability. Furthermore, the effects of Re and Fr_d can be studied to better understand their impact on simulation results under different boundary conditions or simulation parameters.

Appendix B

Direct Numerical Simulation of thermal jet

B.1 Introduction

Turbulent jets are free shear flows of fundamental importance in turbulence research and of wide relevance in applied fluid mechanics. They occur in diverse contexts, ranging from propulsion and combustion systems to environmental discharges such as cooling water effluents, thermal plumes, and desalination brine outfalls. The scientific interest in jets arises from their role as model problems for turbulence research and from their practical relevance, since entrainment, mixing, and dilution processes control efficiency in engineering systems and impact assessments in environmental applications [232–234]. In non-buoyant round jets, extensive experimental and numerical studies have established the existence of self-similar behavior in the far field, with velocity and scalar profiles collapsing under appropriate scaling [235–237]. A defining property of jets is their statistical self-similarity in the far field, where normalized velocity and scalar profiles collapse to universal forms [235, 238]. However, the onset and characteristics of this self-similarity have been shown to depend on initial and boundary conditions, including inlet turbulence and nozzle configuration [236]. In buoyant jets, the self-similar state is further modified by buoyancy forces, which alter entrainment rates, decay laws, and turbulence structures. The densimetric Froude number, $Fr_d = u_0/\sqrt{g'd_0}$, provides a central parameter distinguishing momentum dominated ($Fr_d \gg 1$) from buoyancy dominated ($Fr_d \sim \mathcal{O}(1)$) regimes. Lower values of Fr_d lead to rapid jet deflection and enhanced spreading, whereas higher values recover behaviors closer to non-buoyant jets [239, 240].

Alongside laboratory studies, numerical simulations have provided essential insights into jet development and turbulence structure. Large Eddy Simulations (LES) have been used to explore scalar transport and entrainment in thermal jets at moderate to high Reynolds numbers, while direct numerical simulations (DNS) have been applied to spatially developing round jets at lower Reynolds numbers, offering fully resolved turbulence statistics [241–243]. Early DNS demonstrated the sensitivity of jet development to inlet conditions, and more recent simulations with extended computational domains and long sampling duration have yielded highly converged statistics, documenting self-similar behavior of velocity and scalar fields, as well as detailed turbulence budgets. A recent DNS study of a non-buoyant round jet at $Re = 3500$ reported a domain length of $75d_0$, long sampling over $75,000 d_0/U_0$, and

the use of a turbulent pipe inflow to ensure a rapid approach to self-similarity [243]. That work, conducted with the high-order spectral element code **Nek5000**, produced high-quality statistics of velocity moments, Reynolds stress budgets, and probability density functions, thereby setting a new standard for DNS of turbulent jets. The methodological advances of this study, including inlet generation, domain design, and convergence strategy, are directly transferable to buoyant thermal jets, where systematic DNS data remain scarce.

Motivated by these gaps, the present work performs DNS of a positively buoyant thermal round jet at $Re = 5300$ for two densimetric Froude numbers, $Fr_d = 5$ and $Fr_d = 15$. By varying Fr_d at fixed Reynolds number, the study isolates buoyancy effects on jet development, mean decay and spread, turbulence statistics, and scalar transport. The simulations aim to extend DNS quality evidence into the buoyant jet regime, providing new insights into how buoyancy intensity reorganizes entrainment and the transition toward self-similar behavior.

B.2 Methodology

B.2.1 Governing equations

The governing equations are the incompressible Navier-Stokes equations coupled with the transport of a buoyancy-active scalar (temperature), under the Boussinesq approximation. In dimensionless form, they read

$$\frac{\partial \tilde{u}_i}{\partial \tilde{x}_i} = 0, \quad (\text{B.1})$$

$$\frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j \partial \tilde{x}_j} + e_i^g \frac{1}{Fr^2} \tilde{c}, \quad (\text{B.2})$$

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{c}}{\partial \tilde{x}_i} = \frac{1}{ReSc} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}_i \partial \tilde{x}_i}, \quad (\text{B.3})$$

Here, $\tilde{u}_i$ denotes the nondimensional velocity components, $\tilde{p}$ the nondimensional pressure, and $\tilde{c}$ the buoyancy-active scalar (temperature fluctuation in the present case). The Reynolds number is defined as

$$Re = \frac{U_0 d_0}{\nu},$$

where U_b is the bulk jet velocity at the nozzle exit, D the jet diameter, and ν the kinematic viscosity. Buoyancy forcing enters through the densimetric Froude number

$$Fr_d = \frac{U_0}{\sqrt{g' d_0}},$$

with $g' = g \Delta\rho/\rho_0$ the reduced gravity based on the density difference $\Delta\rho$ between the jet and the ambient fluid.

B.3 Direct numerical simulation details

The governing equations are solved using the spectral element solver **Nek5000** [244], which is based on the high-order spectral element method originally introduced by Patera [245]. For

spatial discretization, a polynomial order of $N = 9$ is employed, and time integration is carried out with a third-order backward differentiation formula (BDF3). The present simulations are performed for a turbulent thermal round jet at $Re = 5300$, with a computational domain extending to $z/D = 40$. A fully developed turbulent velocity profile, generated from a precursor simulation of a cyclic pipe flow, is imposed at the jet inlet to provide physically consistent inflow turbulence. The pipe flow simulation is conducted using the same spectral element framework, and the instantaneous velocity fields extracted at the outlet of the pipe domain are interpolated onto the jet inlet plane through the `neknek` coupling procedure. This approach ensures seamless data transfer between the precursor and main domains, while preserving spatial and temporal coherence of the inflow turbulence. Buoyancy is introduced through a scalar difference between the jet and the ambient fluid under the Boussinesq approximation. The scalar transport equation is solved for a passive thermal scalar. At the inlet, the jet scalar concentration is prescribed as unity inside the nozzle and zero outside. To prevent unphysical reflections, an open boundary condition for the scalar field is applied at the side walls and outlet boundaries.

B.4 Results

Figure B.1 shows instantaneous contours of the temperature field $\tilde{c}$ for the two simulated buoyant thermal jets. Figure B.1 - a corresponds to the case with $Fr_d = 5$, and Figure B.1 - b depicts the case with $Fr_d = 15$. For $Fr_d = 5$, buoyancy forcing is stronger and accelerates the core vertically, yielding a more columnar, plume like structure with reduced cross-stream distribution in the near and intermediate fields. At comparable downstream locations the scalar envelope remains comparatively narrow, and large coherent billows are predominantly aligned with the jet axis. In contrast, the $Fr_d = 15$ case is more momentum dominated. The shear layers roll up and pair earlier, lateral distribution is more pronounced, and the instantaneous scalar field occupies a wider cross-stream extent over much of the domain. The envelope of elevated $\tilde{c}$ is broader, with intermittent eddies convecting outward from the shear layers, indicative of enhanced lateral dispersion by momentum driven turbulence.

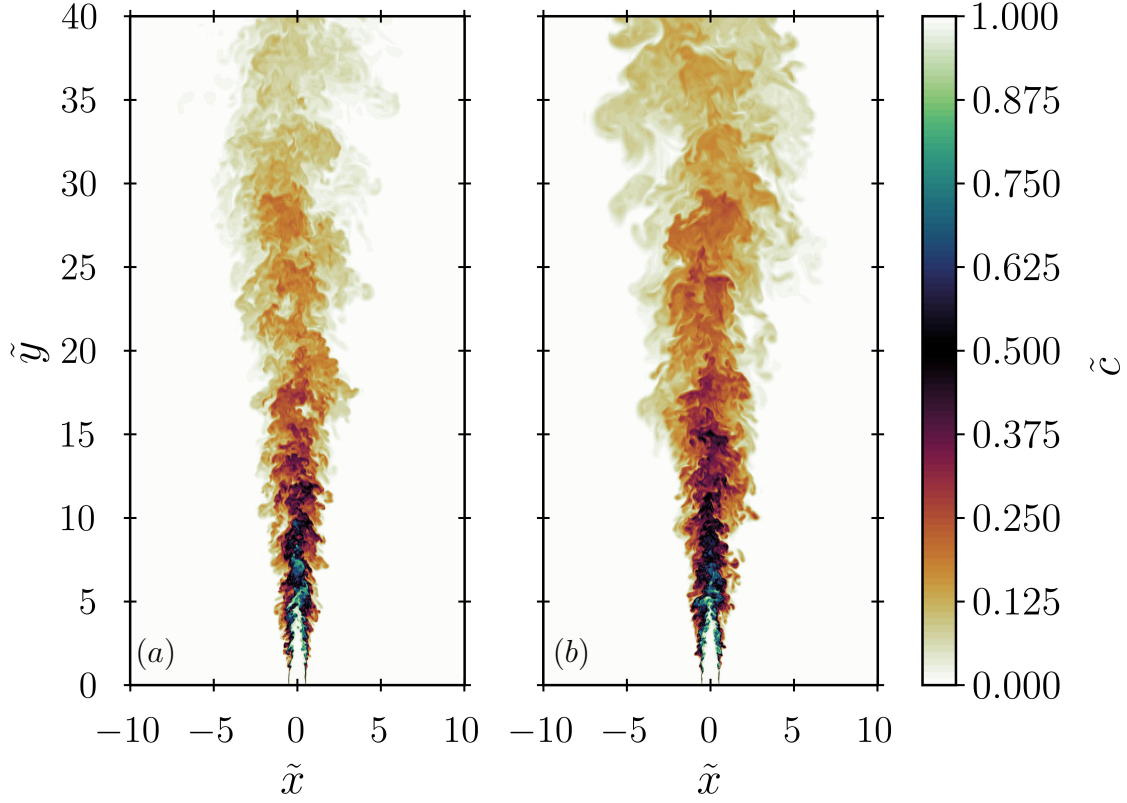


Figure B.1: Instantaneous temperature fields $\tilde{c}$; (a) $Fr_d = 5$ and (b) $Fr_d = 15$.

Figure B.2 illustrates the instantaneous velocity $\tilde{U}$ for the buoyant thermal jets. The flow issues with a narrow, high momentum core that decays downstream through turbulent entrainment and shear layer roll up, which generate vortical structures responsible for momentum transfer from the jet to the ambient. Relative to the scalar field, the velocity field displays more intense small scale fluctuations superposed on the large coherent motions, especially in the intermediate region where the potential core collapses. The comparison between the two cases shows a faster centerline velocity decay for the $Fr_d = 15$ case. The higher Fr_d jet is more momentum dominated at the exit, yet the shear layers thicken more rapidly and produce stronger turbulent mixing, which shortens the potential core length and accelerates the reduction of $\tilde{U}$ along the axis. In contrast, the $Fr_d = 5$ jet maintains a more vertically stretched, plume like core with a slower axial decay of velocity.

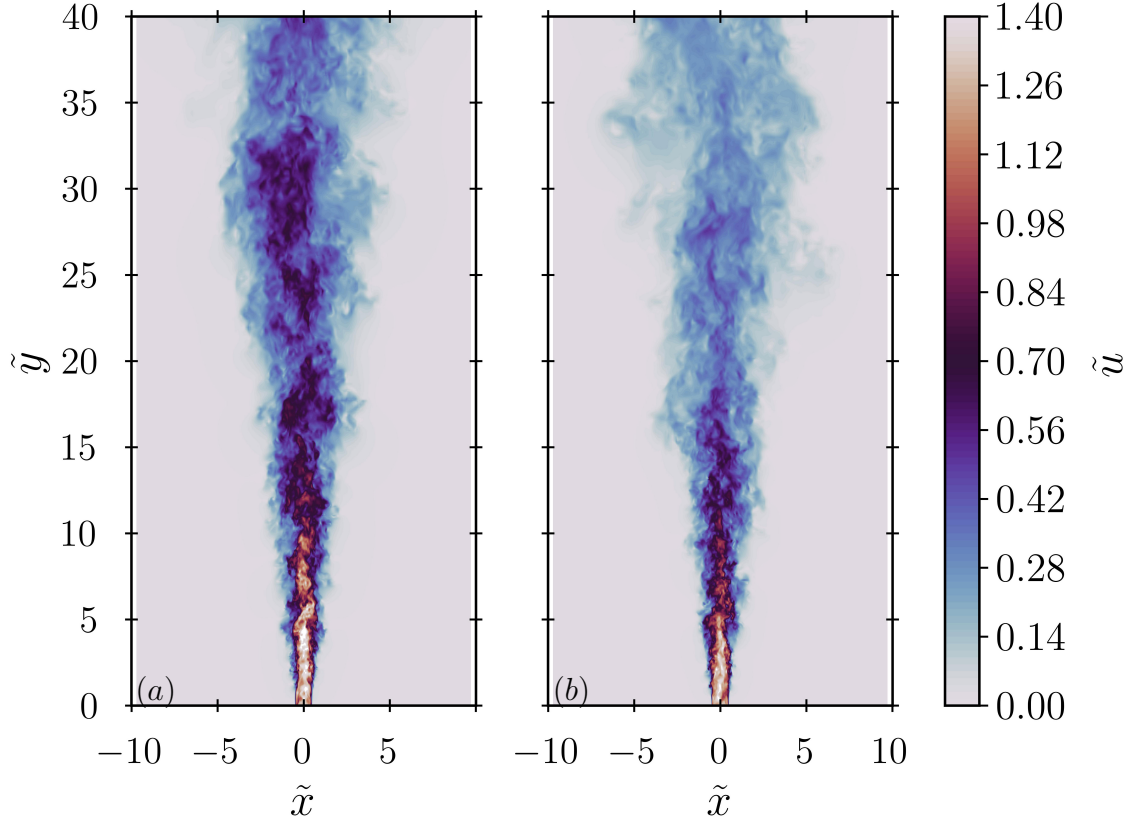


Figure B.2: Instantaneous velocity fields $\tilde{u}$; (a) $Fr_d = 5$ and (b) $Fr_d = 15$.

B.4.1 Mean statistics

Figure B.3 shows the inverse of the normalized mean centerline velocity, U_0/U_c , as a function of downstream distance for the two simulated cases, $Fr_d = 5$ and $Fr_d = 15$. The results are compared with previous DNS data from Nguyen and Oberlack and Babu and Mahesh. The influence of buoyancy intensity on velocity decay is evident. For the strongly buoyant case ($Fr_d = 5$), the axial momentum is sustained over a longer distance, resulting in a slower centerline decay relative to both the momentum dominated case and the reference non-buoyant DNS. In contrast, at higher Froude number ($Fr_d = 15$), buoyancy plays a weaker role and the jet behaves more like a classical momentum driven round jet. The enhanced shear layer development in this regime promotes entrainment and mixing, which accelerates the decay of the mean centerline velocity. The $Fr_d = 15$ case aligns more closely with the decay rates reported for non-buoyant round jets, while the $Fr_d = 5$ case departs significantly, reflecting plume-like behavior with a reduced decay constant. These findings are consistent with the established role of Fr_d in governing the balance between inertia and buoyancy, and demonstrate that stronger buoyancy (lower Fr_d) retards velocity decay, while weaker buoyancy (higher Fr_d) enhances it.

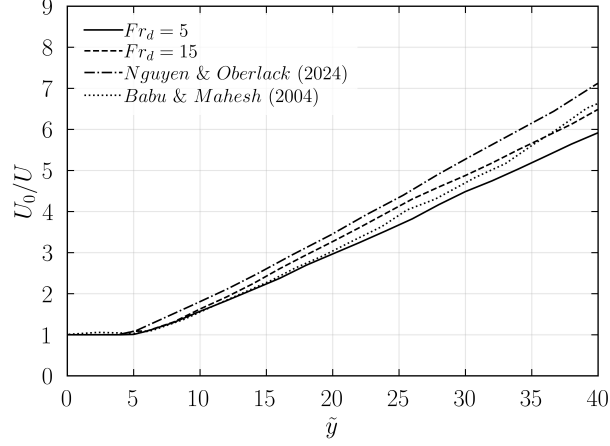


Figure B.3: Inverse of the normalized mean centerline velocity U_0/U_c as a function of downstream distance $\tilde{y}$ for $Fr_d = 5$ and $Fr_d = 15$.

Figure B.4 plots the inverse of the mean centerline scalar $\tilde{c}_0/\tilde{c}_c$ as a function of downstream distance. The present results for $Fr_d = 5$ and $Fr_d = 15$ are compared with DNS data from Nguyen and Oberlack, Nguyen and Oberlack, Lubbers et al., and Babu and Mahesh. The effect of the densimetric Froude number on scalar decay is evident. For the lower Froude number ($Fr_d = 5$), buoyancy accelerates vertical transport and enhances entrainment of ambient fluid, which leads to a more rapid dilution of the jet scalar and thus a faster decay of the centerline concentration. In contrast, the higher Froude number case ($Fr_d = 15$) is more momentum-dominated, and the scalar anomaly persists over a longer distance, yielding a slower decay rate that is closer to the behavior observed in non-buoyant DNS. The $Fr_d = 15$ case aligns well with the passive scalar decay constants reported in non-buoyant round jets [237, 247], while the $Fr_d = 5$ case departs significantly, reflecting plume-like behavior with strong buoyancy forcing and enhanced mixing. These results confirm that buoyancy intensity, as quantified by Fr_d , directly modulates scalar dilution: lower Fr_d accelerates scalar decay, whereas higher Fr_d sustains the core concentration over longer distances.

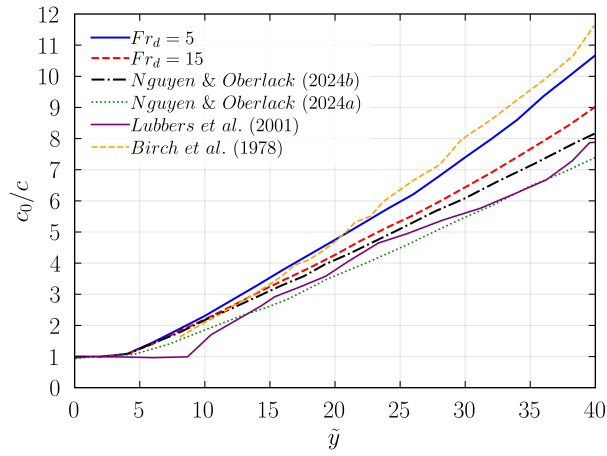


Figure B.4: Inverse of the normalized mean centerline scalar c_0/c_c as a function of downstream distance $\tilde{y}$ for $Fr_d = 5$ and $Fr_d = 15$.

Figure B.5 shows the radial distributions of the normalized mean axial velocity U/U_c at several downstream stations, scaled by the jet half-width $r_{1/2}$. Results are presented for both $Fr_d = 5$ and $Fr_d = 15$.

Near the nozzle exit ($y/D = 1$ and $y/D = 2$), the two cases exhibit nearly identical profiles, characterized by a narrow high-momentum core and a steep shear-layer gradient. This similarity indicates that the imposed turbulent pipe inflow provides consistent initial conditions, and that buoyancy has not yet significantly influenced the near-field velocity distribution.

With increasing downstream distance ($y/D = 5$ to $y/D = 10$), the differences between the two Froude numbers become more pronounced. For $Fr_d = 15$, the profiles show a faster reduction of centerline velocity and a broader distribution across the radial direction, reflecting enhanced shear-layer growth and stronger entrainment of ambient fluid. In contrast, the $Fr_d = 5$ case retains a more peaked distribution with slower decay of the core velocity, consistent with the plume-like behavior induced by stronger buoyancy.

Farther downstream ($y/D = 12.5$ and $y/D = 15$), the divergence between the two regimes is clear. The $Fr_d = 15$ jet exhibits a significantly flatter profile with reduced centerline magnitude and extended radial spread, whereas the $Fr_d = 5$ jet still maintains a more concentrated velocity core. This trend confirms that higher Froude numbers promote momentum-driven spreading and rapid dilution, while lower Froude numbers sustain vertical acceleration and delay lateral dispersion.

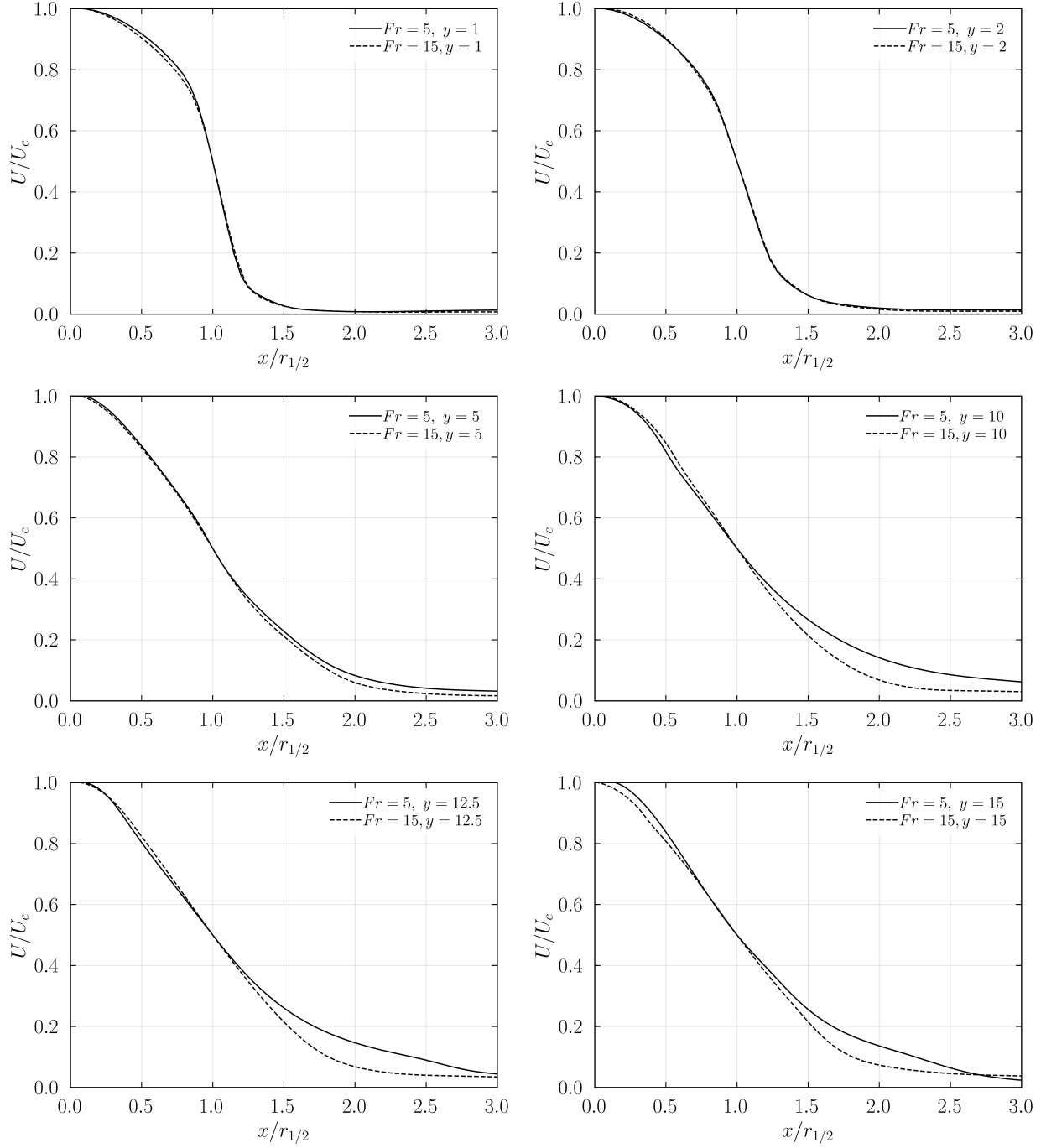


Figure B.5: Radial distributions of normalized mean axial velocity U/U_c at $y/D = 12.5$ and $y/D = 15$, scaled with the half-width $r_{1/2}$, for $Fr_d = 5$ and $Fr_d = 15$.

Figures B.6 plots the radial distributions of the normalized scalar concentration c/c_c at $y/D = 5$ and $y/D = 10$, scaled with the local half-width $r_{1/2}$. Results are shown for both $Fr_d = 5$ and $Fr_d = 15$. At $y/D = 5$, the two cases are still relatively similar, with a sharp gradient across the shear layer and comparable profile shapes. However, a small difference can already be observed: the $Fr_d = 5$ jet exhibits slightly faster scalar decay away

from the centerline, reflecting the stronger entrainment associated with buoyancy-driven acceleration. In contrast, the $Fr_d = 15$ jet retains a somewhat broader distribution of scalar, consistent with the slower decay of centerline concentration reported earlier. By $y/D = 10$, the distinction between the two regimes becomes more pronounced. The $Fr_d = 5$ case shows steeper radial gradients and lower concentrations at the edge of the jet, indicative of enhanced mixing and plume-like behavior. Conversely, the $Fr_d = 15$ jet maintains higher scalar values farther from the centerline, which reflects its momentum-dominated character and reduced dilution relative to the low- Fr_d case.

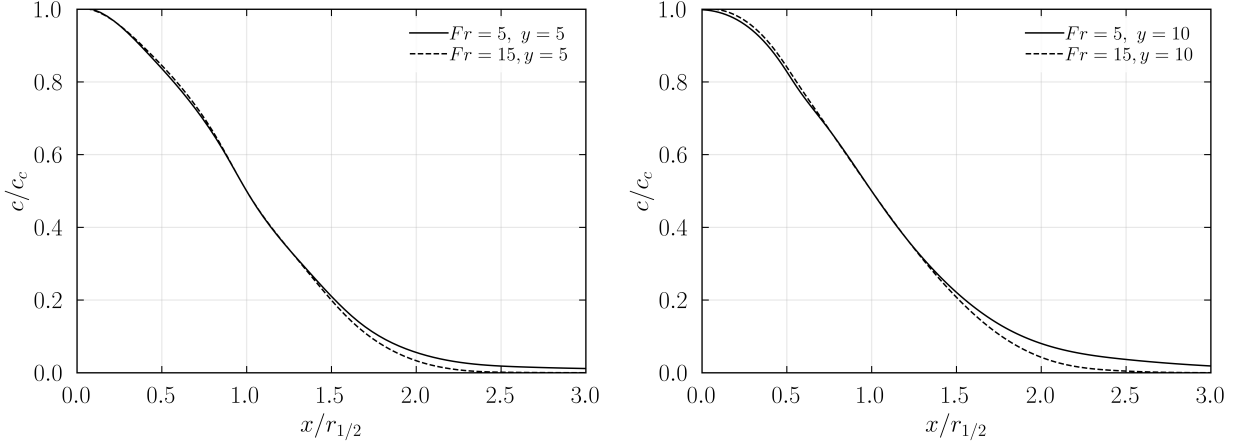


Figure B.6: Radial distributions of normalized scalar concentration c/c_c at $y/D = 5$ and $y/D = 10$, scaled with the half-width $r_{1/2}$, for $Fr_d = 5$ and $Fr_d = 15$.

B.5 Conclusions

Direct numerical simulations of positively buoyant thermal round jets at $Re = 5300$ were conducted for two densimetric Froude numbers, $Fr_d = 5$ and $Fr_d = 15$. The results highlight the governing influence of buoyancy intensity on jet development and mixing. Instantaneous fields revealed that the lower Froude number case produces a more columnar, plume-like structure with rapid scalar dilution, while the higher Froude number jet exhibits broader lateral spread and faster decay of axial velocity. Mean statistics confirmed these trends: velocity decay was retarded at low Fr_d , whereas scalar concentration decayed more rapidly due to buoyancy-driven entrainment. Radial profiles further demonstrated that high- Fr_d jets evolve more quickly toward self-similar momentum-driven behavior, while low- Fr_d jets retain plume-like features over a longer distance. Overall, the study provides DNS-quality evidence of how the Froude number controls the balance between inertia and buoyancy in thermal jets, offering new benchmarks for turbulence modeling and validation of buoyant jet predictions.

Appendix C

Numerical scheme impact on convection term

C.1 Convection schemes analysis

To systematically investigate the effects of numerical schemes and grid resolution on convection (without diffusion), a two-dimensional mass transport model is conducted. A computational domain of 1×1 unit length is discretized using five different mesh resolutions, generated with *blockMesh*, consisting of 10×10 , 20×20 , 40×40 , 80×80 , and 160×160 hexahedral cells (see Figure C.1). The left and bottom boundaries are defined as inlets, where both non-dimensional velocity $\tilde{U}$ and non-dimensional scalar $\tilde{c}$ are imposed using the *fixedValue* condition. The right and top boundaries are specified as outlets with a *zeroGradient* condition. Since the velocity field is not computed and remains fixed throughout the simulation, an initial non-dimensional velocity of $(0.70711, 0.70711, 0)$ is prescribed across the domain. The non-dimensional scalar $\tilde{c}$ is initially set to zero throughout the domain. To replicate a similar scenario to that in [79], where a jet enters the domain discretized with hexahedral cells at a 45-degree angle, a constant non-dimensional scalar value of 1 is prescribed at the left boundary (see Figure C.1). The simulations are performed by solving the mass transport equation (D.8), without the diffusion term ($\frac{1}{ReSc} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}_i \partial \tilde{x}_i} = 0$) and SGS term ($\frac{\partial \tilde{\tau}_i^c}{\partial \tilde{x}_i} = 0$), to exclusively assess the influence of numerical schemes and grid resolution on convection.

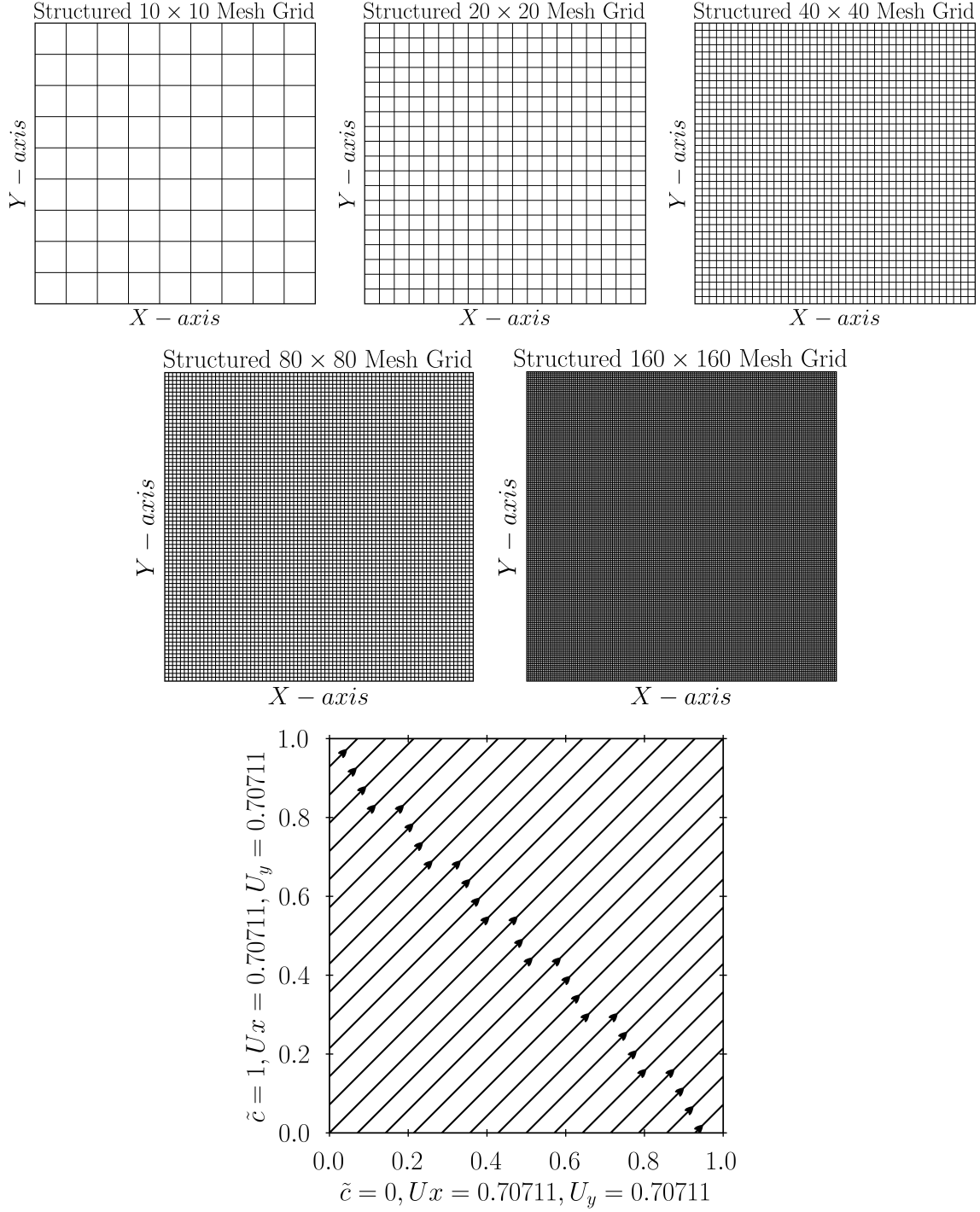


Figure C.1: Generated meshes and boundary conditions; streamlines show the flow direction.

Fifteen simulations are performed, including three numerical schemes of *cubic*, *limitedLinear*, and *limitedUpwind*, as applied in [79], across five different mesh resolutions. Figure C.2 presents the scalar concentration field $\tilde{c}$ computed using the *cubic* scheme (the contour plots are generated using linear interpolation implemented through the Matplotlib library). As the mesh resolution increases, the numerical diffusion effects associated with the convection term

progressively diminish. In the coarsest resolution (10×10), significant numerical diffusion is observed, resulting in a smoothed and artificially broadened scalar profile along the diagonal convection path. With a moderate increase in resolution (20×20 and 40×40), the scalar gradient becomes more defined; however, some numerical diffusion persists, leading to slight artificial spreading perpendicular to the primary transport direction. At finer resolutions (80×80 and 160×160), the scalar transport exhibits a sharper and more well-defined interface. The numerical diffusion is significantly reduced, and the concentration field maintains a distinct boundary with minimal artificial broadening. The highest resolution (160×160) yields the most accurate representation of convection-dominated transport, preserving the sharp interface with minimal numerical errors.

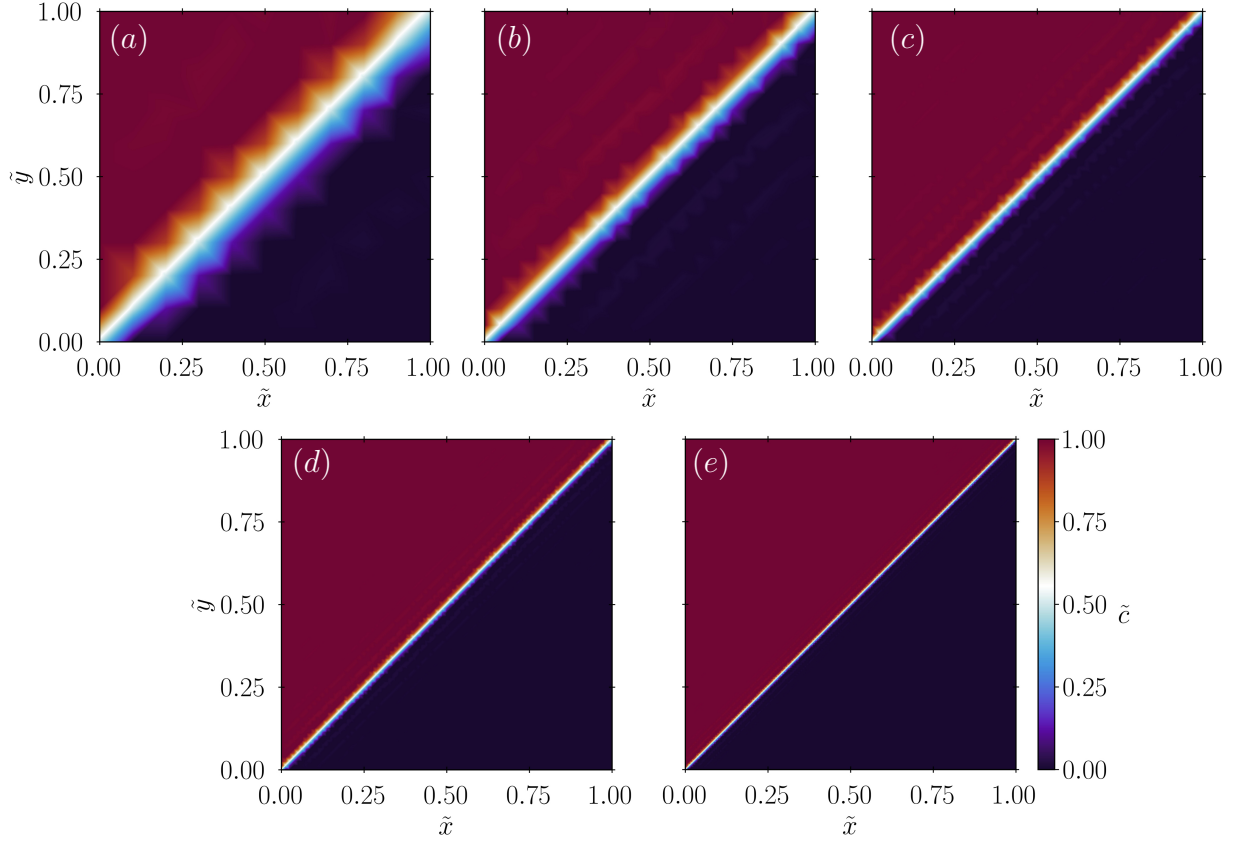


Figure C.2: Scalar concentration ($\tilde{c}$) computed using the *cubic* scheme; a: (10×10), b: (20×20), c: (40×40), d: (80×80) and e: (160×160).

The scalar concentration fields $\tilde{c}$ computed using the *limitedLinear* and the *linearUpwind* schemes are plotted in Figures C.3 and C.4 respectively. Both schemes exhibit similar trends in terms of reducing numerical diffusion with increasing mesh resolution. At lower resolutions (10×10 and 20×20), both schemes show significant numerical diffusion, resulting in a broadening of the scalar transport profile along the diagonal convection path. As the resolution increases to 40×40 , the scalar gradient becomes sharper for both schemes, though *limitedLinear* provides a slightly better-defined interface compared to *linearUpwind*. At higher

resolutions (80×80 and 160×160), both schemes achieve well-defined scalar transport with minimal artificial diffusion. The diagonal interface remains sharper, and numerical dissipation effects are significantly reduced.

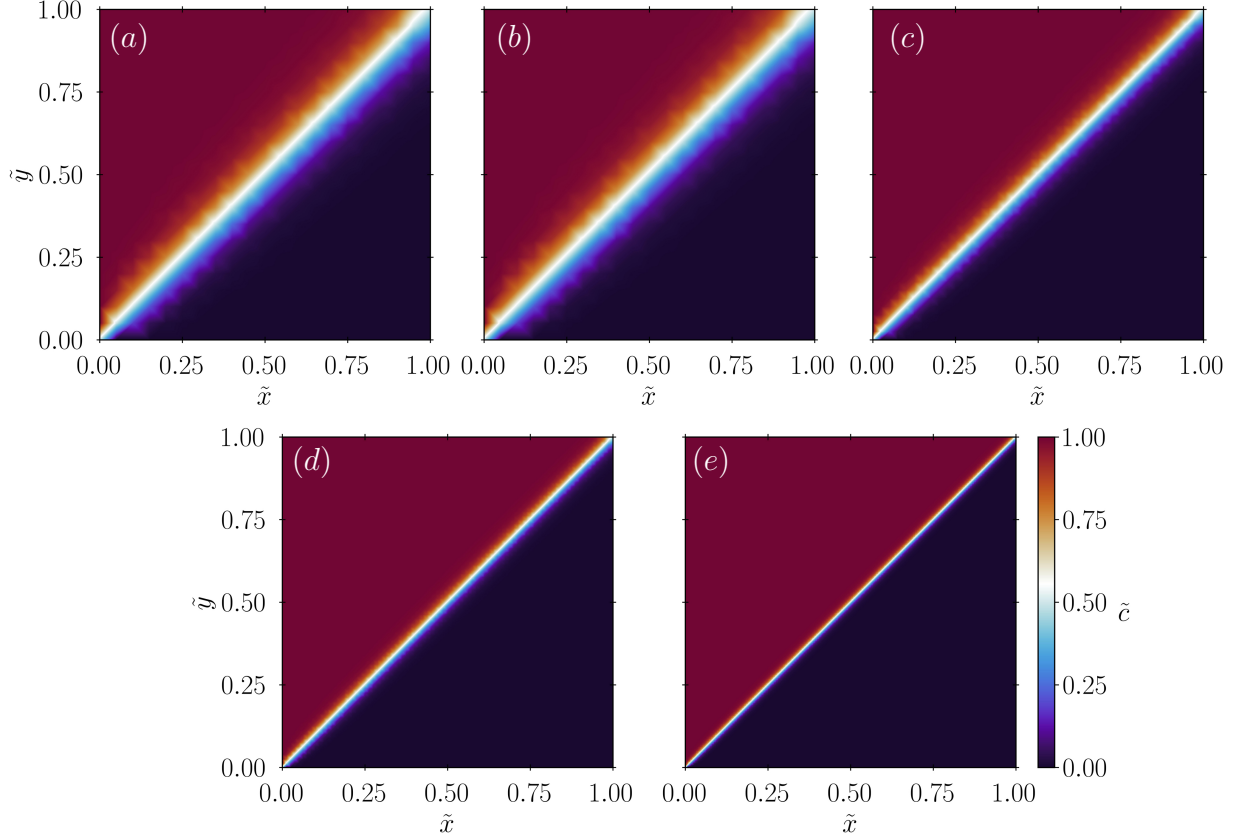


Figure C.3: Scalar concentration ($\tilde{c}$) computed using the *limitedLinear* scheme for mesh resolutions; a: (10×10), b: (20×20), c: (40×40), d: (80×80) and e: (160×160).

At lower resolutions, both *limitedLinear* and *linearUpwind* exhibit a more uniform scalar distribution compared to the *cubic* scheme, which tends to introduce oscillations at coarser resolutions due to its high-order nature. However, at higher resolutions, the *cubic* scheme captures sharper gradients compared to the *limitedLinear* and *linearUpwind* schemes, which exhibit slightly more numerical diffusion.

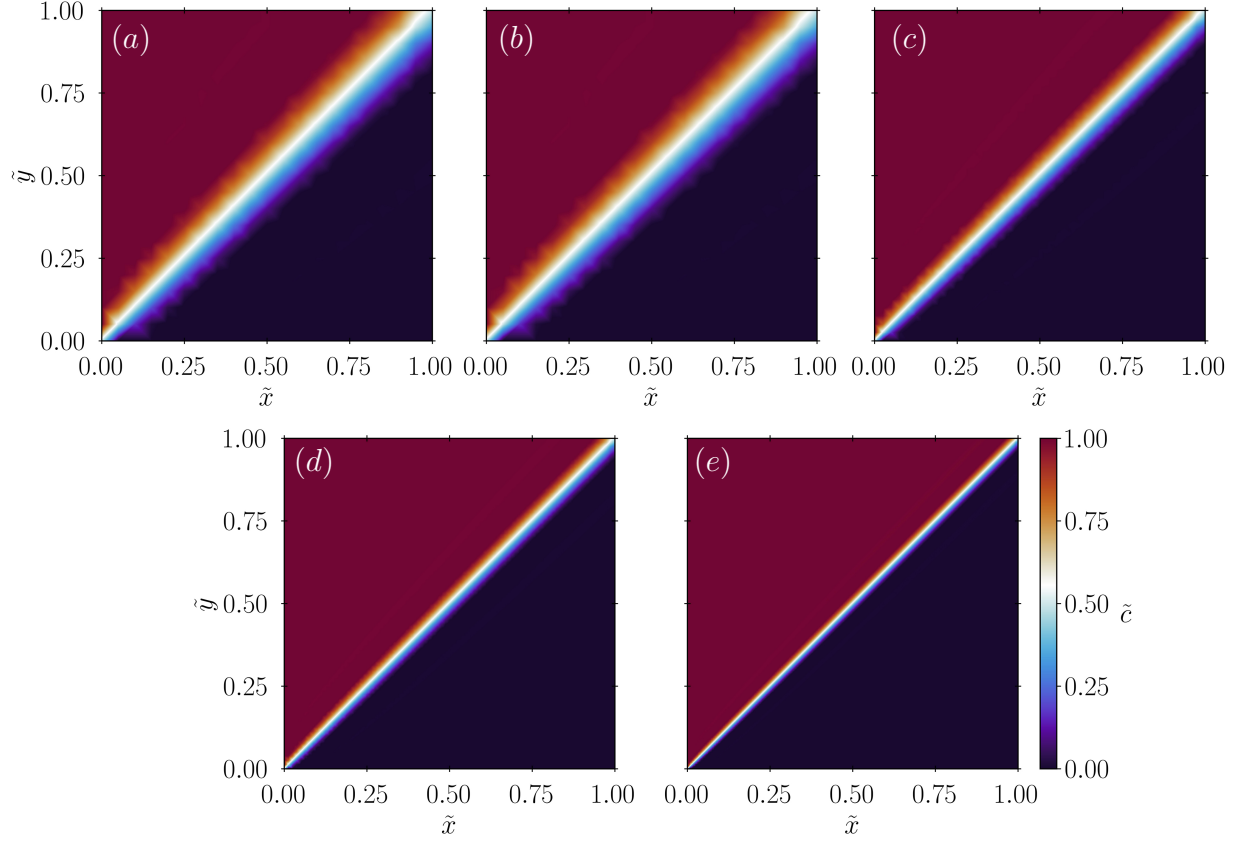


Figure C.4: Scalar concentration ($\tilde{c}$) computed using the *linearUpwind* scheme for mesh resolutions; a: (10×10) , b: (20×20) , c: (40×40) , d: (80×80) and e: (160×160) .

To provide a more detailed comparison of the effects of different schemes, non-dimensional scalar data are extracted along a horizontal line from $(0, 0.5, 0)$ to $(1, 0.5, 0)$ and presented in Figure C.5. At the coarsest resolution (10×10) , significant numerical diffusion is observed in all three schemes, leading to a smoothed concentration gradient. The *cubic* scheme exhibits the highest numerical diffusion among the three, resulting in larger deviation. As the resolution increases to 20×20 and 40×40 , the scalar gradient becomes sharper, and numerical diffusion is reduced for all the schemes. The *cubic* scheme exhibits more oscillations at the interface but provides higher accuracy, whereas *limitedLinear* and *linearUpwind* produce smoother transitions with an increased numerical diffusion. At higher resolutions (80×80) and (160×160) , the numerical diffusion is significantly minimized, and the scalar profile exhibits a sharper gradient. The *cubic* scheme maintains the most distinct gradient but continues to display slight oscillatory behavior. The *limitedLinear* and *linearUpwind* achieve smoother yet slightly more diffusive profiles compared to exact solution.

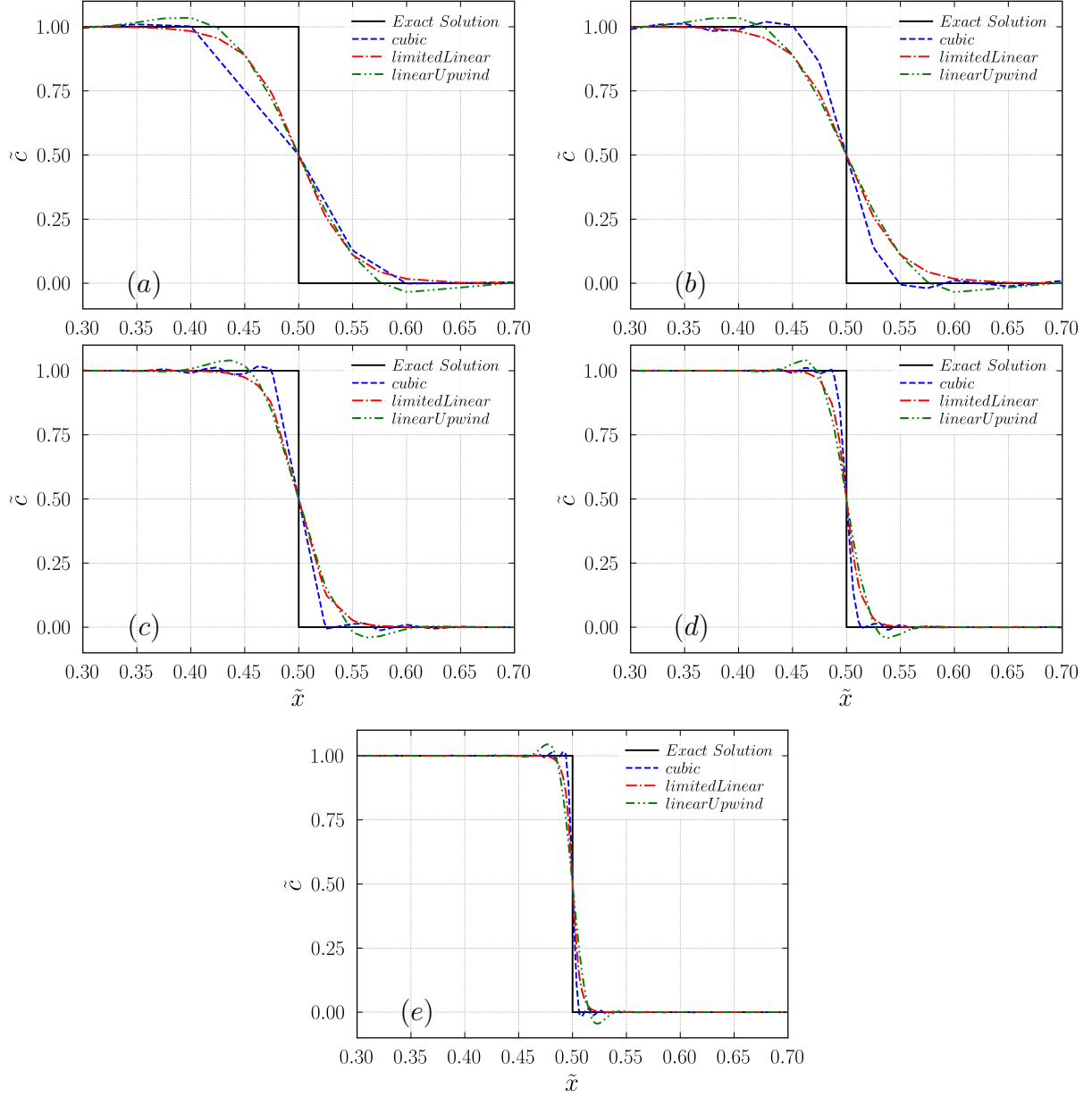


Figure C.5: Scalar concentration $\tilde{c}$ profiles along the line $(0, 0.5, 0)$ to $(1, 0.5, 0)$ for different mesh resolutions (a: 10×10 , b: 20×20 , c: 40×40 , d: 80×80 , and e: 160×160) for the *cubic*, *limitedLinear*, and *linearUpwind* schemes.

The high numerical diffusion observed in the *cubic* scheme, as reported in [79], is a consequence of improper mesh refinement for LES. In their study, mesh adequacy was assessed at the terminal rise location rather than in regions with higher turbulence intensity leading to insufficient resolution in critical areas. As noted in conclusion of [79], “*In regions close to the discharge point, due to the dominance of momentum force, all of the considered discretization schemes except for the cubic scheme predicted the jet centerline trajectory with good agreement relative to the experimental results, and differences between discretization schemes started to*

appear from the second region where effects of buoyancy force emerge.” This finding aligns with the results of the convection simulation, which demonstrated that insufficient grid resolution intensifies numerical diffusion, particularly for higher-order schemes like *cubic*. Similar trends have been reported in [249], where high-order schemes exhibited increased numerical diffusion under insufficient mesh refinement. As stated in [79], *“The cubic scheme imposed a high numerical diffusion in the results due to the order of truncation error in Taylor’s expansion and dissatisfaction of the boundedness feature. This scheme predicted the geometric and mixing characteristics lower and higher than experimental results, respectively.”* While this observation suggests that the *cubic* scheme introduces excessive numerical diffusion, it is important to recognize that high-order schemes are generally expected to yield more accurate results, provided that the mesh resolution is sufficiently refined. High-order schemes inherently reduce truncation error and improve solution accuracy, but their effectiveness is contingent on an adequately refined computational grid to resolve the underlying flow structures accurately. Concluding that the cubic scheme performs poorly based on simulations conducted on a coarse mesh may lead to misleading or incomplete assessments. Instead, a proper evaluation should consider whether the grid resolution meets the requirements not only for LES framework but also for the scheme requirement [250], ensuring that the high-order scheme’s advantages are not undermined by insufficient refinement.

As stated in [79], *“In contrast to the cubic scheme, the second-order upwind scheme could not capture buoyancy-induced instabilities and, therefore, predicted a higher jet trajectory.”* The instability observed in the *cubic* scheme can be attributed to numerical instability caused by the use of a coarse mesh, which fails to sufficiently resolve the flow structures required for accurate LES predictions. Conversely, the inability of the second-order upwind scheme to capture buoyancy-induced instabilities is a consequence of an improper inlet condition, as highlighted in [85]. The use of an inappropriate inlet does not introduce three-dimensional eddies into the domain, thereby limiting the capability of LES as an eddy-resolving turbulence model. This omission compromises the representation of turbulence dynamics, particularly in buoyancy-driven flows, leading to inaccuracies in the predicted jet trajectory.

C.2 Conclusion

A convection study was conducted to systematically investigate the influence of numerical schemes and grid resolution on scalar transport. The results indicate that higher-order schemes, such as *cubic*, require finer grid resolutions to avoid numerical instabilities and diffusion, while *limitedLinear* and *linearUpwind* schemes introduce more numerical diffusion but provide stable solutions across a broader range of grid resolutions. The findings emphasize that grid resolution plays a crucial role in the performance of numerical schemes, and evaluations of numerical accuracy should account for the interplay between the chosen scheme and the grid refinement level.

To enhance the accuracy and reliability of LES in future studies of dense jets, it is essential to adopt proper inflow boundary conditions that generate fully developed turbulent inflow, thereby avoiding the artificial laminarization observed with the *fixedValue* condition. Additionally, symmetry boundary conditions should be avoided in LES as it imposes artificial constraints on turbulence evolution. Grid refinement studies should be conducted in regions

with high turbulence intensity (close to nozzle and inside the pipe for full domain) to ensure that the mesh adequately resolves the large and intermediate turbulent scales while minimizing numerical dissipation.

Furthermore, a systematic investigation into the combined effects of numerical schemes and mesh resolution on both convective and diffusive terms in the Navier-Stokes equations is essential. Key LES parameters, such as the ratio of resolved to total TKE, should be examined for both low- and high-order schemes across different mesh resolutions to enable a quantitative assessment of their impact on jet characteristics.

Appendix D

Non-dimensionalization method in OpenFOAM and mesh generation

D.1 Introduction

Non-dimensionalization is a fundamental procedure in computational fluid dynamics (CFD) that allows the governing equations and numerical results to be expressed in a dimensionless form. This facilitates generalization, enables comparison across different flow regimes, and reduces the number of governing parameters. In the present study, all numerical simulations were performed using the open-source CFD toolbox **OpenFOAM**, and the solver settings were adapted to a non-dimensional framework suitable for buoyant jets. The source code and case files developed for this purpose are openly available on GitHub at:

https://github.com/HydroCFD/buoyant_jet/tree/main/OpenFOAM

This appendix provides a detailed explanation of the procedure followed for non-dimensionalization, the characteristic scales used, and the implications for interpreting simulation results.

D.2 Governing Equations in Dimensional Form

The incompressible Navier–Stokes equations with buoyancy coupling (via the Boussinesq approximation) can be written in dimensional form as:

$$\frac{\partial u_i}{\partial x_i} = 0, \quad (\text{D.1})$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + g_i \frac{\Delta \rho}{\rho_0}, \quad (\text{D.2})$$

where u_i is the velocity vector, p is the pressure, ρ_0 is the reference density, $\Delta \rho = \rho - \rho_0$ is the density difference, ν is the kinematic viscosity, and g_i represents the gravitational acceleration vector.

The density field is typically linked to a transported scalar c (temperature or concentration), allowing buoyancy to be expressed as:

$$g' = g \frac{\Delta\rho}{\rho_0}, \quad (\text{D.3})$$

where β is the expansion coefficient (thermal or solutal).

D.3 Choice of Characteristic Scales

To obtain dimensionless equations, reference scales are defined. For buoyant jets, the nozzle exit properties provide the most natural scaling:

- **Length scale:** jet diameter d_0 ,
- **Velocity scale:** jet velocity U_0 ,
- **Scalar scale:** jet concentration C_0 ,

With these definitions, the relevant dimensionless groups emerge:

$$Re = \frac{U_0 d_0}{\nu}, \quad Fr_d = \frac{U_0}{\sqrt{g' d_0}}, \quad Ri = \frac{1}{Fr_d^2}, \quad Sc = \frac{\nu}{D}, \quad (\text{D.4})$$

where Re is the Reynolds number, Fr_d is the densimetric Froude number, Ri is the Richardson number, and Sc is the Schmidt number, defined as the ratio of kinematic viscosity ν to scalar diffusivity D .

D.4 Non-dimensional Form of the Equations

Introducing the dimensionless variables

$$\tilde{x}_i = \frac{x_i}{d_0}, \quad \tilde{u}_i = \frac{u_i}{U_0}, \quad \tilde{c} = \frac{c}{C_0}, \quad (\text{D.5})$$

the governing equations become:

$$\frac{\partial \tilde{u}_i}{\partial \tilde{x}_i} = 0, \quad (\text{D.6})$$

$$\frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j \partial \tilde{x}_j} + e_i^g \frac{1}{Fr^2} \tilde{c}, \quad (\text{D.7})$$

where δ_{i3} represents the vertical buoyancy forcing direction.

The scalar transport equation reads:

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{\partial \tilde{u}_i \tilde{c}}{\partial \tilde{x}_i} = \frac{1}{Re Sc} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}_i \partial \tilde{x}_i}, \quad (\text{D.8})$$

D.5 Implementation in OpenFOAM

In OpenFOAM, dimensional consistency is ensured through the use of SI units specified in the `dimensions` entries of field files. To adapt OpenFOAM to a non-dimensional framework, all quantities are scaled by their reference values. Specifically:

- The velocity field is initialized in terms of $\tilde{u}$.
- The scalar field is prescribed in normalized form $\tilde{c}$.
- Transport properties such as ν and D are redefined in terms of Re and Sc , ensuring that the solver internally operates on dimensionless groups rather than dimensional quantities.
- Boundary conditions at the inlet and outlet are expressed in dimensionless terms, ensuring that changes in Re or Fr_d can be applied without redefining all physical parameters.

For practical implementation, case dictionaries were constructed to directly input non-dimensional variables. For example, the kinematic viscosity is not set as ν in m^2/s , but instead computed as:

$$\nu^* = \frac{U_0 d_0}{Re}, \quad (\text{D.9})$$

where ν^* is the dimensionless viscosity.

The complete set of OpenFOAM case files with detailed configuration can be accessed at:

https://github.com/HydroCFD/buoyant_jet/tree/main/OpenFOAM

D.6 Advantages of the Non-dimensional Framework

Adopting a non-dimensional framework offers multiple benefits:

1. **Generality:** Results can be applied to a broad range of physical conditions without re-running simulations for each case.
2. **Parameter reduction:** Governing equations depend only on dimensionless groups (Re , Fr_d , Sc), simplifying parametric studies.
3. **Scalability:** Results can be scaled to laboratory or field conditions by appropriate choice of d_0 and U_0 .
4. **Validation:** Facilitates direct comparison with theoretical similarity laws and experimental data expressed in dimensionless form.

D.7 Concluding Remarks

The non-dimensionalization method employed in this work provides a robust and generalizable approach for simulating buoyant jets in **OpenFOAM**. By expressing all governing equations and input parameters in terms of dimensionless quantities, the methodology enhances comparability, reduces parameter dependence, and ensures that results can be interpreted in the broader context of environmental fluid mechanics. This framework forms the basis for the high-fidelity simulations reported in the main chapters of this thesis.

Listing D.1: Momentum equation in **OpenFOAM** with non-dimensional buoyancy term.

```
1 // Solve the Momentum equation
2
3 MRF.correctBoundaryVelocity(U);
4
5 tmp<fvVectorMatrix> tUEqn
6 (
7   fvm::ddt(U)
8   + fvm::div(phi, U)
9   + MRF.DDt(U)
10  + turbulence->divDevReff(U)
11  - g*T*pow(Fr, -2.0)
12  ==
13  fvOptions(U)
14 );
15
16 fvVectorMatrix& UEqn = tUEqn.ref();
17
18 UEqn.relax();
19
20 fvOptions.constrain(UEqn);
21
22 if (pimple.momentumPredictor())
23 {
24     solve(UEqn == -fvc::grad(p));
25
26     fvOptions.correct(U);
27 }
28
```

Note. The momentum equation in **OpenFOAM** is revised in the solver as shown in Listing D.1, where the non-dimensional buoyancy term $e_i^g \frac{1}{Fr^2} \tilde{c}$ has been introduced explicitly.

Non-dimensional computational domain and mesh generation

All geometry and mesh coordinates are constructed in *non-dimensional* units such that the characteristic length scale equals unity. In this study, the characteristic length is the nozzle diameter, hence:

$$d_0 = 1, \quad \tilde{\mathbf{x}} = \frac{\mathbf{x}}{d_0}.$$

With this choice, distances measured in the mesh (**Gmsh**/**OpenFOAM**) are already in multiples of d_0 ; for example, a downstream distance of 50 in the mesh corresponds to $50 d_0$

physically. This convention eliminates a unit-conversion layer and ensures consistency with the non-dimensional governing equations.

A template for the jet domain is provided for convenience:

https://github.com/HydroCFD/buoyant_jet/tree/main/Gmsh/inlcined_jet

Please note: This mesh is for training purposes and should be adjusted to global sizes, near-nozzle refinements, grading, and far-field extents to suit your specific Re , Fr_d , and resolution targets.

Mesh generation for jet simulations

When building a mesh for jet simulations, the geometry should be scaled in non-dimensional units with the nozzle diameter set to $d_0 = 1$. The inlet is represented as a circular patch of diameter one, and the domain must extend sufficiently in the streamwise, lateral, and vertical directions to avoid boundary effects (typically tens of diameters in each direction). Finer resolution is required near the nozzle exit and in the shear layer, while gradual coarsening is acceptable further downstream. The mesh should also be structured or semi-structured in the near field to capture the core dynamics and scalar mixing.

Gmsh follows a bottom-up workflow:

1. **Points** define coordinates in space and serve as the seeds of the geometry.
2. **Curves (lines or arcs)** connect points to form the edges of the geometry.
3. **Surfaces** are constructed by combining closed loops of curves, creating two-dimensional faces of the domain.
4. **Volumes** are obtained by *extruding* surfaces or enclosing them to form three-dimensional regions.
5. **Discretization** is applied by assigning element sizes, transfinite constraints, and mesh recombination (to obtain quadrilateral or hexahedral cells).
6. **Physical groups** assign names to boundaries and volumes so that solvers such as OpenFOAM can recognize them as inlets, outlets, walls, or flow domains.

Geometry construction: A script usually begins by defining constants such as characteristic scales, angles, and lengths. Then, *points* are created to locate critical features (e.g., inlet center, walls, corners). These points are connected by *curves* to define edges, and closed loops of curves are used to create *surfaces*.

Extrusions. Two-dimensional surfaces are extruded in different directions to build the three-dimensional domain.

- Upward extrusions form the main flow region above the base plane.
- Downward extrusions extend the inlet or nozzle section.

- Streamwise extrusions enlarge the computational box along the jet trajectory.
- Layering during extrusion allows local mesh refinement, especially in the near field of the jet.

Mesh definition: Mesh resolution is controlled by prescribing the number of divisions along curves and applying transfinite constraints to enforce structured patterns. Surfaces and volumes can be recombined to generate quadrilateral (2D) or hexahedral (3D) elements, which are often preferred in CFD applications.

Physical groups: Surfaces and volumes are grouped into meaningful labels such as `inlet`, `outlet`, `top`, `walls`, or `flowDomain`. These labels are essential for exporting the mesh into CFD solvers, since they define boundary conditions and the computational region.

Non-dimensional usage: All geometrical quantities are expressed in units of the nozzle diameter ($d_0 = 1$). Thus, a coordinate of 50 in the mesh corresponds to a physical distance of $50 d_0$, ensuring consistency with the non-dimensional governing equations.

References

- [1] Xiaohua Wu and Parviz Moin. A direct numerical simulation study on the mean velocity characteristics in turbulent pipe flow. *Journal of Fluid Mechanics*, 608:81–112, 2008.
- [2] Adam Timothy Crowe. *Inclined negatively buoyant jets and boundary interaction*. University of Canterbury. Civil and Natural Resources Engineering, 2013.
- [3] Wen-Chang Yang and Robert R Hwang. Vertical buoyant jets in a linearly stratified ambient cross-stream. *Environmental Fluid Mechanics*, 1:235–256, 2001.
- [4] M Ben Meftah, D Malcangio, F De Serio, and M Mossa. Vertical dense jet in flowing current. *Environmental Fluid Mechanics*, 18:75–96, 2018.
- [5] Edward Jones, Manzoor Qadir, Michelle TH van Vliet, Vladimir Smakhtin, and Seongmu Kang. The state of desalination and brine production: A global outlook. *Science of the Total Environment*, 657:1343–1356, 2019.
- [6] Tobias Bleninger, GH Jirka, and S Lattemann. Environmental planning, prediction and management of brine discharges from desalination plants. *Middle East Desalination Research Center (MEDRC): Muscat, Sultanate of Oman*, 5, 2010.
- [7] Mitchell J Baum and Badin Gibbes. Field-scale numerical modeling of a dense multiport diffuser outfall in crossflow. *Journal of Hydraulic Engineering*, 146(1):05019006, 2020.
- [8] Danial Goodarzi, Abdolmajid Mohammadian, and Saleh Rezaeiravesh. Numerical simulation of desalination brine discharges: Effects of inlet boundary conditions. Manuscript under review at *Desalination*, 2025.
- [9] P Palomar, JL Lara, and IJ Losada. Near field brine discharge modeling part 2: Validation of commercial tools. *Desalination*, 290:28–42, 2012.
- [10] SAR Saeidi Hosseini, Mostafa Taherian, Abdolmajid Mohammadian, Simone Ferrari, and Philip JW Roberts. Mixing behavior of multiport diffusers with non-uniform port orientation. *Desalination*, 567:116962, 2023.
- [11] Anton Purnama. Analytical model for brine discharges from a sea outfall with multiport diffusers. *International Journal of Mathematical, Computational, Physical, Electrical and Computer Engineering*, 56:57, 2011.
- [12] Gustaaf A Kikkert, MJ Davidson, and RI Nokes. Inclined negatively buoyant discharges. *Journal of Hydraulic Engineering*, 133(5):545–554, 2007.

- [13] Chris CK Lai and Joseph HW Lee. Initial mixing of inclined dense jet in perpendicular crossflow. *Environmental Fluid Mechanics*, 14:25–49, 2014.
- [14] CJ Oliver, MJ Davidson, and RI Nokes. Removing the boundary influence on negatively buoyant jets. *Environmental Fluid Mechanics*, 13:625–648, 2013.
- [15] Ilias G Papakonstantis, George C Christodoulou, and Panos N Papanicolaou. Inclined negatively buoyant jets 2: concentration measurements. *Journal of Hydraulic Research*, 49(1):13–22, 2011.
- [16] AT Crowe, MJ Davidson, and RI Nokes. Velocity measurements in inclined negatively buoyant jets. *Environmental Fluid Mechanics*, 16(3):503–520, 2016.
- [17] Hossein Kheirkhah Gildeh, Abdolmajid Mohammadian, Ioan Nistor, and Hazim Qiblawey. Numerical modeling of 30° and 45° inclined dense turbulent jets in stationary ambient. *Environmental Fluid Mechanics*, 15:537–562, 2015.
- [18] Ioan Nistor Hazim Qiblawey Hossein Kheirkhah Gildeh, Abdolmajid Mohammadian and Xiaohui Yan. Cfd modeling and analysis of the behavior of 30° and 45° inclined dense jets – new numerical insights. *Journal of Applied Water Engineering and Research*, 4(2):112–127, 2016. doi: 10.1080/23249676.2015.1090351.
- [19] Dongdong Shao and Adrian Wing-Keung Law. Turbulent mass and momentum transport of a circular offset dense jet. *Journal of Turbulence*, (10):N40, 2009.
- [20] Dongdong Shao and Adrian Wing-Keung Law. Mixing and boundary interactions of 30 and 45 inclined dense jets. *Environmental fluid mechanics*, 10:521–553, 2010.
- [21] Ilias G Papakonstantis, George C Christodoulou, and Panos N Papanicolaou. Inclined negatively buoyant jets 1: geometrical characteristics. *Journal of Hydraulic Research*, 49(1):3–12, 2011.
- [22] Sina Tahmooresi, Danial Goodarzi, Abdolmajid Mohammadian, and Ioan Nistor. Lif measurement of turbulent horizontal dense jets in stagnant ambient. *International Journal of Heat and Mass Transfer*, 244:126867, 2025.
- [23] Shuai Zhang, Adrian Wing-Keung Law, and Bing Zhao. Large eddy simulations of turbulent circular wall jets. *International Journal of Heat and Mass Transfer*, 80: 72–84, 2015.
- [24] Shuai Zhang, Baoxin Jiang, Adrian Wing-Keung Law, and Bing Zhao. Large eddy simulations of 45 inclined dense jets. *Environmental Fluid Mechanics*, 16:101–121, 2016.
- [25] Shuai Zhang, Adrian Wing-Keung Law, and Mingtao Jiang. Large eddy simulations of 45 and 60 inclined dense jets with bottom impact. *Journal of hydro-environment research*, 15:54–66, 2017.

- [26] Sina Tahmooresi, Abdolmajid Mohammadian, Ioan Nistor, and Hossein Kheirkhah Gildeh. Reynolds flux modeling; new numerical insights into inclined dense jets. *Environmental Fluid Mechanics*, pages 1–27, 2023.
- [27] Jun Sakakibara, Koichi Hishida, and Masanobu Maeda. Measurements of thermally stratified pipe flow using image-processing techniques. *Experiments in Fluids*, 16(2): 82–96, 1993.
- [28] Amirsaman Eghtesad, Mohamad Ali Bijarchi, Mohammad Behshad Shafii, and Hossein Afshin. A state-of-the-art review on laser-induced fluorescence (lif) method with application in temperature measurement. *International Journal of Thermal Sciences*, 196:108686, 2024.
- [29] F Lemoine, Y Antoine, M Wolff, and M Lebouche. Simultaneous temperature and 2d velocity measurements in a turbulent heated jet using combined laser-induced fluorescence and lida. *Experiments in fluids*, 26(4):315–323, 1999.
- [30] MCJ Coolen, RN Kieft, CCM Rindt, and AA Van Steenhoven. Application of 2-d lif temperature measurements in water using a nd: Yag laser. *Experiments in Fluids*, 27(5):420–426, 1999.
- [31] Sven Scharnowski and Christian J Kähler. Particle image velocimetry-classical operating rules from today’s perspective. *Optics and Lasers in Engineering*, 135:106185, 2020.
- [32] Mohammed Raad Abdulwahab, Yasir H Ali, Fatima J Habeeb, Abdoulhadi A Borhana, Ahmed M Abdelrhman, and Salah M Ali Al-Obaidi. A review in particle image velocimetry techniques (developments and applications). *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences*, 65(2):213–229, 2020.
- [33] MA Zeitoun and William Franklin McIlhenny. Conceptual designs of outfall systems for desalination plants. In *Offshore technology conference*, pages OTC–1370. OTC, 1971.
- [34] WR Lindberg. Experiments on negatively buoyant jets, with and without cross-flow. *Recent research advances in the fluid mechanics of turbulent jets and plumes*, pages 131–145, 1994.
- [35] Philip JW Roberts, Adrian Ferrier, and Greg Daviero. Mixing in inclined dense jets. *Journal of Hydraulic Engineering*, 123(8):693–699, 1997.
- [36] S Nemlioglu and PJW Roberts. Experiments on dense jets using three-dimensional laser-induced fluorescence (3dlif). In *4th International conference on marine waste water disposal and marine environment*, pages 1–10, 2006.
- [37] CJ Oliver, MJ Davidson, and RI Nokes. Predicting the near-field mixing of desalination discharges in a stationary environment. *Desalination*, 309:148–155, 2013.
- [38] Ilias G Papakonstantis, George C Christodoulou, and Panos N Papanicolaou. Inclined negatively buoyant jets 1: geometrical characteristics. *Journal of Hydraulic Research*, 49(1):3–12, 2011.

- [39] Chris CK Lai and Joseph HW Lee. Mixing of inclined dense jets in stationary ambient. *Journal of hydro-environment research*, 6(1):9–28, 2012.
- [40] Stephen B. Pope. *Turbulent Flows*. Cambridge University Press, 2000.
- [41] Joel H Ferziger, Milovan Perić, and Robert L Street. *Computational methods for fluid dynamics*, volume 3. Springer, 2002.
- [42] Brian Edward Launder and Dudley Brian Spalding. The numerical computation of turbulent flows. In *Numerical prediction of flow, heat transfer, turbulence and combustion*, pages 96–116. Elsevier, 1983.
- [43] Pierre Sagaut. *Large eddy simulation for incompressible flows: an introduction*. Springer Science & Business Media, 2006.
- [44] Parviz Moin and Krishnan Mahesh. Direct numerical simulation: a tool in turbulence research. *Annual review of fluid mechanics*, 30(1):539–578, 1998.
- [45] Sina Tahmooreesi and Davoud Ahmadyar. Effects of turbulent schmidt number on cfd simulation of 45° inclined negatively buoyant jets. *Environmental Fluid Mechanics*, 21(1):39–62, 2021.
- [46] Hossein Kheirkhah Gildeh, Abdolmajid Mohammadian, and Ioan Nistor. Inclined dense effluent discharge modelling in shallow waters. *Environmental Fluid Mechanics*, 21: 955–987, 2021.
- [47] Sina Tahmooreesi and Davoud Ahmadyar. Application of reynolds flux modeling in cfd simulation of 45° inclined negatively buoyant jets. *Environmental Fluid Mechanics*, 22(1):55–86, 2022.
- [48] Shuen Law, Mark J Davidson, Craig McConnochie, and Daniel Lagrava. Improved numerical predictions of inclined negatively buoyant jet behaviour. *Environmental Fluid Mechanics*, 23(4):879–906, 2023.
- [49] Mingtao Jiang, Adrian Wing-Keung Law, and Adrian CH Lai. Turbulence characteristics of 45° inclined dense jets. *Environmental Fluid Mechanics*, 19:27–54, 2019.
- [50] Carlo Cintolesi, Andrea Petronio, and Vincenzo Armenio. Turbulent structures of buoyant jet in cross-flow studied through large-eddy simulation. *Environmental Fluid Mechanics*, 19(2):401–433, 2019.
- [51] Shahriar Ghahremanian and Bahram Moshfegh. Evaluation of rans models in predicting low reynolds, free, turbulent round jet. *Journal of Fluids Engineering*, 136(1):011201, 2014.
- [52] EJ Smith, J Mi, GJ Nathan, and BB Dally. Preliminary examination of a” round jet initial condition anomaly” for the k- ϵ turbulence model. In *15th Australasian Fluid Mechanics Conference*, pages 1–4. The University of Sydney, Sydney, Australia, 2004.

- [53] Trushar B Gohil, Arun K Saha, and K Muralidhar. Numerical study of instability mechanisms in a circular jet at low reynolds numbers. *Computers & fluids*, 64:1–18, 2012.
- [54] Saleh Rezaeiravesh, Ricardo Vinuesa, and Philipp Schlatter. On numerical uncertainties in scale-resolving simulations of canonical wall turbulence. *Computers & Fluids*, 227: 105024, 2021.
- [55] H Kanchi, K Sengupta, and F Mashayek. Effect of turbulent inflow boundary condition in les of flow over a backward-facing step using spectral element method. *International Journal of Heat and Mass Transfer*, 62:782–793, 2013.
- [56] Xiaohua Wu, Parviz Moin, and Jean-Pierre Hickey. Boundary layer bypass transition. *Physics of Fluids*, 26(9), 2014.
- [57] Ning Li, Elias Balaras, and Ugo Piomelli. Inflow conditions for large-eddy simulations of mixing layers. *Physics of Fluids*, 12(4):935–938, 2000.
- [58] Xiaohua Wu, Parviz Moin, Ronald J Adrian, and Jon R Baltzer. Osborne reynolds pipe flow: Direct simulation from laminar through gradual transition to fully developed turbulence. *Proceedings of the National Academy of Sciences*, 112(26):7920–7924, 2015.
- [59] Nitin S Dhamankar, Gregory A Blaisdell, and Anastasios S Lyrantzis. Overview of turbulent inflow boundary conditions for large-eddy simulations. *Aiaa Journal*, 56(4): 1317–1334, 2018.
- [60] G Carazzo, E Kaminski, and S Tait. On the rise of turbulent plumes: Quantitative effects of variable entrainment for submarine hydrothermal vents, terrestrial and extra terrestrial explosive volcanism. *Journal of Geophysical Research: Solid Earth*, 113(B9), 2008.
- [61] Pierfrancesco Dellino, Fabio Dioguardi, Daniela Mele, M D’Addabbo, Bernd Zimmanowski, Ralf Buettner, Domenico M Doronzo, Ingo Sonder, Roberto Sulpizio, Tobias Duerig, et al. Volcanic jets, plumes, and collapsing fountains: evidence from large-scale experiments, with particular emphasis on the entrainment rate. *Bulletin of Volcanology*, 76:1–18, 2014.
- [62] Spyros N Michas and Panos N Papanicolaou. Horizontal round heated jets into calm uniform ambient. *Desalination*, 248(1-3):803–815, 2009.
- [63] GR Hunt and HC Burridge. Fountains in industry and nature. *Annual Review of Fluid Mechanics*, 47:195–220, 2015.
- [64] Andrea Cipollina, Angelo Bonfiglio, Giorgio Micale, and Alberto Brucato. Dense jet modelling applied to the design of dense effluent diffusers. *Desalination*, 167:459–468, 2004.
- [65] WD Baines, JS Turner, and IH Campbell. Turbulent fountains in an open chamber. *Journal of Fluid Mechanics*, 212:557–592, 1990.

- [66] EJ List. Turbulent jets and plumes. *Annual review of fluid mechanics*, 14(1):189–212, 1982.
- [67] FA Berson and G Baird. A numerical model of cumulonimbus convection generating a protected core. *Quarterly Journal of the Royal Meteorological Society*, 101(430): 911–928, 1975.
- [68] G Carazzo, E Kaminski, and S Tait. On the dynamics of volcanic columns: A comparison of field data with a new model of negatively buoyant jets. *Journal of Volcanology and Geothermal Research*, 178(1):94–103, 2008.
- [69] Albert B Pincince and E John List. Disposal of brine into an estuary. *Journal (Water Pollution Control Federation)*, pages 2335–2344, 1973.
- [70] I Alameddine and M El-Fadel. Brine discharge from desalination plants: a modeling approach to an optimized outfall design. *Desalination*, 214(1-3):241–260, 2007.
- [71] Shuen Law, Mark J Davidson, Craig McConnochie, and Pedro J Lee. Turbulent fluxes, integral model coefficients, and desalination discharge predictions. *Desalination*, page 119137, 2025.
- [72] Mostafa Taherian, Seyed Ahmad Reza Saeidi Hosseini, Abdolmajid Mohammadian, Simone Ferrari, and Philip JW Roberts. Laboratory study on inclined desalination discharges in perpendicular cross-flow. *Desalination*, 583:117719, 2024.
- [73] Ali Galeshi, Ozeair Abessi, Mahdi Yousefifard, and Ali Rahmani Firoozjaee. Inclined dense discharge in stagnant and wave environments: An experimental and numerical study. *Ocean Engineering*, 278:114045, 2023.
- [74] Xiaohui Yan, Abdolmajid Mohammadian, and Xin Chen. Numerical modeling of inclined plane jets in a linearly stratified environment. *Alexandria Engineering Journal*, 59(3):1857–1867, 2020.
- [75] David Robinson, Matthew Wood, Matthew Piggott, and Gerard Gorman. Cfd modelling of marine discharge mixing and dispersion. *Journal of Applied Water Engineering and Research*, 4(2):152–162, 2016.
- [76] CJ Oliver, MJ Davidson, and RI Nokes. $k-\varepsilon$ predictions of the initial mixing of desalination discharges. *Environmental Fluid Mechanics*, 8:617–625, 2008.
- [77] Mohammadmehdi Ramezani, Ozeair Abessi, and Ali Rahmani Firoozjaee. Effect of proximity to bed on 30° and 45° inclined dense jets: a numerical study. *Environmental Processes*, 8:1141–1164, 2021.
- [78] Jie Songa, Mingtao Jiangd, Myung Eun Lee, and Adrian Wing-Keung Lawd. Study on horizontal jets with buoyancy in shallow waters. *Desalination and Water Treatment*, 185:111–123, 2020.

- [79] Narges Vafa, Amin Azadi, and Bahar Firoozabadi. Effect of numerical schemes on advection terms for large eddy simulation of inclined dense jets. *Environmental Fluid Mechanics*, 21:1227–1252, 2021.
- [80] Amin Azadi and Bahar Firoozabadi. New criterion for characterization of thermal-saline jets discharged from thermal desalination plants. *International Journal of Heat and Mass Transfer*, 195:123142, 2022.
- [81] S Habibi, A Azadi, and B Firoozabadi. Large eddy simulation of inclined negatively buoyant jets with sloped beds. *Journal of Hydraulic Engineering*, 148(11):04022023, 2022.
- [82] Hessam Tofighian, Abdolreza Aghajanpour, Ozeair Abessi, and Mohammadmehdi Ramezani. Simulation of inclined dense jets in stagnant environments: an les and experimental study. *Environmental Fluid Mechanics*, 22(5):1161–1185, 2022.
- [83] Shayan Habibi, Amin Azadi, and Bahar Firoozabadi. Identification of turbulent structures of inclined negatively buoyant jets with bed effects. *International Journal of Heat and Mass Transfer*, 208:124040, 2023.
- [84] Niki Soleimani Amiri, Ozeair Abessi, and Philip JW Roberts. Venturi nozzles for desalination brine discharges. *Desalination*, page 117193, 2023.
- [85] Danial Goodarzi. Comment on “venturi nozzles for desalination brine discharges” [amiri, ns, abessi, o., & roberts, pj, desalination volume 573, 2024, 117193]. *Desalination*, 592: 118105, 2024.
- [86] Kai Zeng, Zhuoneng Li, Zeeshan A Rana, and Karl W Jenkins. Implicit large eddy simulations of turbulent flow around a square cylinder at $re = 22,000$. *Computers & Fluids*, 226:105000, 2021.
- [87] David J Tritton. *Physical fluid dynamics*. Springer Science & Business Media, 2012.
- [88] Franck Nicoud and Frédéric Ducros. Subgrid-scale stress modelling based on the square of the velocity gradient tensor. *Flow, turbulence and Combustion*, 62(3):183–200, 1999.
- [89] N Williamson, N Srinarayana, SW Armfield, GD McBain, and W Lin. Low-reynolds-number fountain behaviour. *Journal of Fluid Mechanics*, 608:297–317, 2008.
- [90] NB Kaye and GR Hunt. Weak fountains. *Journal of Fluid Mechanics*, 558:319–328, 2006.
- [91] HC Burridge and GR Hunt. The rise heights of low-and high-froude-number turbulent axisymmetric fountains. *Journal of fluid mechanics*, 691:392–416, 2012.
- [92] James S Turner. Jets and plumes with negative or reversing buoyancy. *Journal of Fluid Mechanics*, 26(4):779–792, 1966.

- [93] Maksim Dadonau, JL Partridge, and PF Linden. The effect of double diffusion on the dynamics of horizontal turbulent thermohaline jets. *Journal of Fluid Mechanics*, 905: A23, 2020.
- [94] TGL Shirtcliffe. Transport and profile measurements of the diffusive interface in double diffusive convection with similar diffusivities. *Journal of Fluid Mechanics*, 57(1):27–43, 1973.
- [95] Tobias Holzmann. Mathematics, numerics, derivations and openfoam®. *Loeben, Germany: Holzmann CFD*, 2016.
- [96] Fadl Moukalled, Luca Mangani, and Marwan Darwish. The finite volume method. In *The finite volume method in computational fluid dynamics*, pages 103–135. Springer, 2016.
- [97] Hrvoje Jasak. Openfoam: Open source cfd in research and industry. *International Journal of Naval Architecture and Ocean Engineering*, 1(2):89–94, 2009. ISSN 2092-6782. doi: <https://doi.org/10.2478/IJNAOE-2013-0011>. URL <https://www.sciencedirect.com/science/article/pii/S2092678216303879>.
- [98] Hrvoje Jasak. Error analysis and estimation for the finite volume method with applications to fluid flows. 1996.
- [99] J Martínez, Federico Piscaglia, Andrea Montorfano, Angelo Onorati, and SM Aithal. Influence of spatial discretization schemes on accuracy of explicit les: Canonical problems to engine-like geometries. *Computers & Fluids*, 117:62–78, 2015.
- [100] Andrei Sergeevich Epikhin. Numerical schemes and hybrid approach for the simulation of unsteady turbulent flows. *Mathematical Models and Computer Simulations*, 11(6): 1019–1031, 2019.
- [101] Christophe Geuzaine and Jean-François Remacle. Gmsh: A 3-d finite element mesh generator with built-in pre- and post-processing facilities. *International Journal for Numerical Methods in Engineering*, 79(11):1309–1331, 2009. doi: <https://doi.org/10.1002/nme.2579>. URL <https://onlinelibrary.wiley.com/doi/abs/10.1002/nme.2579>.
- [102] Markus Klein. An attempt to assess the quality of large eddy simulations in the context of implicit filtering. *Flow, Turbulence and Combustion*, 75:131–147, 2005.
- [103] Danial Goodarzi, Kaveh Sookhak Lari, and Farshid Mossaiby. Thermal effects on the hydraulic performance of sedimentation ponds. *Journal of Water Process Engineering*, 33:101100, 2020.
- [104] Abolghasem Alighardashi and Danial Goodarzi. Simulation of depth and wind effects on the hydraulic efficiency of sedimentation tanks. *Water and Environment Journal*, 34(3):432–440, 2020.

- [105] Danial Goodarzi, Abdolmajid Mohammadian, Jonathan Pearson, and Soroush Abolfathi. Numerical modelling of hydraulic efficiency and pollution transport in waste stabilization ponds. *Ecological Engineering*, 182:106702, 2022.
- [106] Mingqi Guo, Danial Goodarzi, Jonathan Pearson, Abdolmajid Mohammadian, and Soroush Abolfathi. The effects of permeable baffles on hydraulic and treatment performance in retention ponds. *Journal of Water Process Engineering*, 69:106593, 2025.
- [107] Thomas S Lund, Xiaohua Wu, and Kyle D Squires. Generation of turbulent inflow data for spatially-developing boundary layer simulations. *Journal of computational physics*, 140(2):233–258, 1998.
- [108] Eugene De Villiers. The potential of large eddy simulation for the modeling of wall bounded flows. *Imperial College of Science, Technology and Medicine*, 2006.
- [109] Zhixin Wang, Ramis Örlü, Philipp Schlatter, and Yongmann M Chung. Direct numerical simulation of a turbulent 90 bend pipe flow. *International Journal of Heat and Fluid Flow*, 73:199–208, 2018.
- [110] MH Baba-Ahmadi and Gavin Tabor. Inlet conditions for les using mapping and feedback control. *Computers & Fluids*, 38(6):1299–1311, 2009.
- [111] R Poletto, T Craft, and A Revell. A new divergence free synthetic eddy method for the reproduction of inlet flow conditions for les. *Flow, turbulence and combustion*, 91: 519–539, 2013.
- [112] Ruggero Poletto. *Divergence free development of the synthetic eddy method in order to improve synthetic turbulence for embedded les simulations*. The University of Manchester (United Kingdom), 2015.
- [113] N Jarrin, R Prosser, J-C Uribe, S Benhamadouche, and D Laurence. Reconstruction of turbulent fluctuations for hybrid rans/les simulations using a synthetic-eddy method. *International Journal of Heat and Fluid Flow*, 30(3):435–442, 2009.
- [114] Nina Gall Jørgensen and HÅKAN Nilsson. Implementation of a turbulent inflow boundary condition for les based on a vortex method. *A course at Chalmers University of Technology*, 2012.
- [115] OpenFOAM Foundation. *Turbulent Inlet Boundary Condition*, 2023. URL <https://doc.openfoam.com/2306/tools/processing/boundary-conditions/rtm/derived/inlet/turbulentInlet/>. Accessed: December 2, 2024.
- [116] Markus Raffel, Christian E Willert, Fulvio Scarano, Christian J Kähler, Steve T Wereley, and Jürgen Kompenhans. *Particle image velocimetry: a practical guide*. springer, 2018.
- [117] Lawrence Sirovich. Turbulence and the dynamics of coherent structures. i. coherent structures. *Quarterly of applied mathematics*, 45(3):561–571, 1987.

- [118] John Leask Lumley. The structure of inhomogeneous turbulent flows. *Atmospheric turbulence and radio wave propagation*, pages 166–178, 1967.
- [119] Zhao Wu, Dominique Laurence, Sergey Utyuzhnikov, and Imran Afgan. Proper orthogonal decomposition and dynamic mode decomposition of jet in channel crossflow. *Nuclear Engineering and Design*, 344:54–68, 2019.
- [120] Gal Berkooz, Philip Holmes, and John L Lumley. The proper orthogonal decomposition in the analysis of turbulent flows. *Annual review of fluid mechanics*, 25(1):539–575, 1993.
- [121] Chuangxin He and Yingzheng Liu. Proper orthogonal decomposition of time-resolved lif visualization: scalar mixing in a round jet. *Journal of Visualization*, 20:789–815, 2017.
- [122] Dalibor Cavar and Knud Erik Meyer. Les of turbulent jet in cross flow: Part 2–pod analysis and identification of coherent structures. *International Journal of Heat and Fluid Flow*, 36:35–46, 2012.
- [123] Julien Weiss. A tutorial on the proper orthogonal decomposition. In *AIAA aviation 2019 forum*, page 3333, 2019.
- [124] Kit Ming Lam. Application of pod analysis to concentration field of a jet flow. *Journal of Hydro-environment Research*, 7(3):174–181, 2013.
- [125] SV Gordeyev and Flint O Thomas. Coherent structure in the turbulent planar jet. part 2. structural topology via pod eigenmode projection. *Journal of Fluid Mechanics*, 460: 349–380, 2002.
- [126] M Ben Chiekh, Marc Michard, MS Guellouz, and JC Béra. Pod analysis of momentumless trailing edge wake using synthetic jet actuation. *Experimental thermal and fluid science*, 46:89–102, 2013.
- [127] Khaled J Hammad and Ivana M Milanovic. A pod study of an impinging jet flowfield. In *Fluids Engineering Division Summer Meeting*, volume 43727, pages 1477–1485, 2009.
- [128] Simone Ferrari and Giorgio Querzoli. Mixing and re-entrainment in a negatively buoyant jet. *Journal of Hydraulic Research*, 48(5):632–640, 2010.
- [129] Gustaaf Adriaan Kikkert. Buoyant jets with two and three-dimensional trajectories. 2006.
- [130] Marcie Stuber, K Todd Lowe, and Wing F Ng. Synthesis of convection velocity and turbulence measurements in three-stream jets. *Experiments in Fluids*, 60(5):83, 2019.
- [131] Claudio Alanis Ruiz, Twan van Hooff, Bert Blocken, and GertJan van Heijst. Piv measurements and validation of rans solutions for plane turbulent impinging co-flowing and angled jets at moderate reynolds numbers. *Flow, Turbulence and Combustion*, pages 1–35, 2025.

- [132] Jie Yao, Saleh Rezaeiravesh, Philipp Schlatter, and Fazle Hussain. Direct numerical simulations of turbulent pipe flow up to. *Journal of Fluid Mechanics*, 956:A18, 2023.
- [133] Yi Wang, Giulio Vita, Bruno Fraga, Jianchun Wang, and Hassan Hemida. Effect of the inlet boundary conditions on the flow over complex terrain using large eddy simulation. *Designs*, 5(2):34, 2021.
- [134] Donnatella Xavier, Saleh Rezaeiravesh, and Philipp Schlatter. Autoregressive models for quantification of time-averaging uncertainties in turbulent flows. *Physics of fluids*, 36(10), 2024.
- [135] Saleh Rezaeiravesh, Christian Gscheidle, Adam Peplinski, Jochen Garcke, and Philipp Schlatter. In-situ estimation of time-averaging uncertainties in turbulent flow simulations. *Computer Methods in Applied Mechanics and Engineering*, 433:117511, 2025.
- [136] Saleh Rezaeiravesh, Ricardo Vinuesa, Mattias Liefvendahl, and Philipp Schlatter. Assessment of uncertainties in hot-wire anemometry and oil-film interferometry measurements for wall-bounded turbulent flows. *European Journal of Mechanics-B/Fluids*, 72: 57–73, 2018.
- [137] Bernhard Wieneke. Piv uncertainty quantification from correlation statistics. *Measurement Science and Technology*, 26(7):074002, 2015.
- [138] Bernhard Wieneke. Piv uncertainty quantification and beyond, phd thesis. 2017.
- [139] Andrea Sciacchitano and Bernhard Wieneke. Piv uncertainty propagation. *Measurement Science and Technology*, 27(8):084006, 2016.
- [140] M Ben Meftah, D Malcangio, F De Serio, and M Mossa. Vertical dense jet in flowing current. *Environmental Fluid Mechanics*, 18(1):75–96, 2018.
- [141] Wesley P James, Ignacio Vergara, and Ken Kim. Dilution of a dense vertical jet. *Journal of environmental engineering*, 109(6):1273–1283, 1983. doi: [https://doi.org/10.1061/\(ASCE\)0733-9372\(1983\)109:6\(127](https://doi.org/10.1061/(ASCE)0733-9372(1983)109:6(127).
- [142] Hugo B Fischer, John E List, C Robert Koh, Jorg Imberger, and Norman H Brooks. *Mixing in inland and coastal waters*. Academic press, 1979.
- [143] Niranjana S Ghaisas, Dinesh A Shetty, and Steven H Frankel. Large eddy simulation of turbulent horizontal buoyant jets. *Journal of Turbulence*, 16(8):772–808, 2015.
- [144] HC Burridge, A Mistry, and GR Hunt. The effect of source reynolds number on the rise height of a fountain. *Physics of Fluids*, 27(4):047101, 2015.
- [145] Joseph K Ansong, Patrick J Kyba, and Bruce R Sutherland. Fountains impinging on a density interface. *Journal of Fluid Mechanics*, 595:115–139, 2008.
- [146] Yen-Lung Chen and Shih-Chun Hsiao. Numerical modeling of a buoyant round jet under regular waves. *Ocean Engineering*, 161:154–167, 2018.

- [147] Zhiguo He, Han Zhang, Yanan Chen, Samuel Ukpang Okon, and Yingzhong Lou. Hydrodynamics of horizontal heated buoyant jet in linearly stratified fluids. *Physics of Fluids*, 34(2):025108, 2022.
- [148] Yanan Chen, Zhiguo He, Yingzhong Lou, Han Zhang, Rui Zhu, and Samuel Ukpang Okon. Experimental study of horizontal heated buoyant jets in a linearly stratified ambience. *Physics of Fluids*, 33(4), 2021. doi: <https://doi.org/10.1063/5.0045906>.
- [149] Yizhou Xiao, Wenxin Huai, Bin Ji, and Zhonghua Yang. Verification and validation of urans simulations of the round buoyant jet in counterflow. *Water*, 10(11):1509, 2018.
- [150] Chetankumar Anghan, Mukund H Bade, and Jyotirmay Banerjee. A review on fundamental properties of the jet in the wave environment. *Ocean Engineering*, 250:110914, 2022.
- [151] Mouldi Ben Meftah, Francesca De Serio, Daniela Malcangio, Michele Mossa, and Antonio Felice Petrillo. Experimental study of a vertical jet in a vegetated crossflow. *Journal of Environmental Management*, 164:19–31, 2015. doi: <https://doi.org/10.1016/j.jenvman.2015.08.035>.
- [152] Lynyrd de Wit, Cees van Rhee, and Geert Keetels. Turbulent interaction of a buoyant jet with cross-flow. *Journal of Hydraulic Engineering*, 140(12):04014060, 2014.
- [153] Lester L Yuan and Robert L Street. Trajectory and entrainment of a round jet in crossflow. *Physics of fluids*, 10(9):2323–2335, 1998.
- [154] Joseph HW Lee and Peter Neville-Jones. Initial dilution of horizontal jet in crossflow. *Journal of hydraulic Engineering*, 113(5):615–629, 1987.
- [155] Steven J Wright. Mean behavior of buoyant jets in a crossflow. *Journal of the Hydraulics Division*, 103(5):499–513, 1977.
- [156] Gerhard H Jirka and Henry LM Fong. Vortex dynamics and bifurcation of buoyant jets in crossflow. *Journal of the Engineering Mechanics Division*, 107(3):479–499, 1981.
- [157] Amir Gharavi, Abdolmajid Mohammadian, Ioan Nistor, Enrique Peña, and José Anta. Experimental study of surface buoyant jets in crossflow. *Environmental Fluid Mechanics*, 20(4):1007–1030, 2020.
- [158] Ruoyao Ou. *Numerical Modeling of Horizontal Buoyant Jet Entering Shallow Water with a Crossflow*. PhD thesis, Université d’Ottawa/University of Ottawa, 2020.
- [159] Wen-Chang Yang and Robert R Hwang. Vertical buoyant jets in a linearly stratified ambient cross-stream. *Environmental Fluid Mechanics*, 1(2):235–256, 2001.
- [160] Heinz G Stefan and Ruochuan Gu. Efficiency of jet mixing of temperature-stratified water. *Journal of Environmental Engineering*, 118(3):363–379, 1992. doi: [https://doi.org/10.1061/\(ASCE\)0733-9372\(1992\)118:3\(363\)](https://doi.org/10.1061/(ASCE)0733-9372(1992)118:3(363)).

- [161] Ruochuan Gu and Heinz G Stefan. Analysis of turbulent buoyant jet in density-stratified water. *Journal of Environmental Engineering*, 114(4):878–897, 1988. doi: [https://doi.org/10.1061/\(ASCE\)0733-9372\(1988\)114:4\(878\)](https://doi.org/10.1061/(ASCE)0733-9372(1988)114:4(878)).
- [162] Robert R Hwang, TP Chiang, and WC Yang. Effect of ambient stratification on buoyant jets in cross-flow. *Journal of engineering mechanics*, 121(8):865–872, 1995.
- [163] Robert R. Hwang and T.P. Chiang. Buoyant jets in a crossflow of stably stratified fluid. *Atmospheric Environment*, 20(10):1887–1890, 1986. ISSN 0004-6981. First International Conference on Atmospheric Sciences and Applications to Air Quality Part II.
- [164] Robert R Hwang, TP Chiang, and WC Yang. Effect of ambient stratification on buoyant jets in cross-flow. *Journal of engineering mechanics*, 121(8):865–872, 1995.
- [165] GA Bemporad. Simulation of round buoyant jet in stratified flowing environment. *Journal of hydraulic Engineering*, 120(5):529–543, 1994.
- [166] Robert R Hwang, Yin-Fan Pon, and Wen-Chang Yang. Multiple-port buoyant jets in density stratified cross flow. *Journal of the Chinese Institute of Engineers*, 13(5): 543–553, 1990.
- [167] Robert R Hwang and TP Chiang. Numerical simulation of vertical forced plume in a crossflow of stably stratified fluid. 1995.
- [168] A Ramakanth, MJ Davidson, and RI Nokes. Laboratory study to quantify lower boundary influences on desalination discharges. *Desalination*, 529:115641, 2022.
- [169] Loh-Nien Fan and Norman H. Brooks. *Numerical solutions of turbulent buoyant jet problems*. Apr 2004. Funding by U.S. Public Health Service (USPHS).
- [170] GA Bemporad. Simulation of round buoyant jet in stratified flowing environment. *Journal of hydraulic Engineering*, 120(5):529–543, 1994.
- [171] Michael Schatzmann. An integral model of plume rise. *Atmospheric Environment (1967)*, 13(5):721–731, 1979.
- [172] Gerhard H Jirka. Integral model for turbulent buoyant jets in unbounded stratified flows. part i: Single round jet. *Environmental Fluid Mechanics*, 4(1):1–56, 2004.
- [173] Panos N Papanicolaou, Ilias G Papakonstantis, and George C Christodoulou. On the entrainment coefficient in negatively buoyant jets. *Journal of Fluid Mechanics*, 614: 447–470, 2008.
- [174] Rabah Mehaddi, Olivier Vauquelin, and Fabien Candelier. Analytical solutions for turbulent boussinesq fountains in a linearly stratified environment. *Journal of fluid mechanics*, 691:487–497, 2012.

- [175] LG Sarasua, D Freire, C Cabeza, and Arturo C Marti. Spreading height and critical conditions for the collapse of turbulent fountains in stratified media. *Physics of Fluids*, 33(1):015106, 2021.
- [176] Endam Gungor and Philip JW Roberts. Experimental studies on vertical dense jets in a flowing current. *Journal of Hydraulic Engineering*, 135(11):935–948, 2009.
- [177] M Ben Meftah, D Malcangio, F De Serio, and M Mossa. Vertical dense jet in flowing current. *Environmental Fluid Mechanics*, 18(1):75–96, 2018.
- [178] Mouldi Ben Meftah and Michele Mossa. Turbulence measurement of vertical dense jets in crossflow. *Water*, 10(3):286, 2018.
- [179] Steven J Wright. Buoyant jets in density-stratified crossflow. *Journal of Hydraulic Engineering*, 110(5):643–656, 1984.
- [180] JW Roberts and PR Matthews. Behavior of low buoyancy jets in a linearly stratified fluid. *Journal of Hydraulic Research*, 25(4):503–519, 1987.
- [181] R Byron Bird. Transport phenomena. *Appl. Mech. Rev.*, 55(1):R1–R4, 2002.
- [182] Geoffrey K. Vallis. *Atmospheric and Oceanic Fluid Dynamics: Fundamentals and Large-Scale Circulation*. Cambridge University Press, 2 edition, 2017.
- [183] Joseph Smagorinsky. General circulation experiments with the primitive equations: I. the basic experiment. *Monthly weather review*, 91(3):99–164, 1963.
- [184] David C Wilcox et al. *Turbulence modeling for CFD*, volume 2. DCW industries La Canada, CA, 1998.
- [185] Parviz Moin and John Kim. Numerical investigation of turbulent channel flow. *Journal of fluid mechanics*, 118:341–377, 1982.
- [186] I. B. Celik, Z. N. Cehreli, and I. Yavuz. Index of Resolution Quality for Large Eddy Simulations. *Journal of Fluids Engineering*, 127(5):949–958, 09 2005. ISSN 0098-2202.
- [187] Lynyrd de Wit and Cees van Rhee. Testing an improved artificial viscosity advection scheme to minimise wiggles in large eddy simulation of buoyant jet in crossflow. *Flow, turbulence and combustion*, 92:699–730, 2014.
- [188] Haecheon Choi and Parviz Moin. Grid-point requirements for large eddy simulation: Chapman’s estimates revisited. *Physics of fluids*, 24(1):011702, 2012.
- [189] Hermann Schlichting, Klaus Gersten, Hermann Schlichting, and Klaus Gersten. Boundary-layer equations in plane flow; plate boundary layer. *Boundary-layer theory*, pages 145–164, 2017.
- [190] Dean R Chapman. Computational aerodynamics development and outlook. *AIAA journal*, 17(12):1293–1313, 1979.

- [191] Saleh Rezaeiravesh and Mattias Liefvendahl. Effect of grid resolution on large eddy simulation of wall-bounded turbulence. *Physics of Fluids*, 30(5):055106, 2018.
- [192] Danial Goodarzi, Kaveh Sookhak Lari, Ehsan Khavasi, and Soroush Abolfathi. Large eddy simulation of turbidity currents in a narrow channel with different obstacle configurations. *Scientific Reports*, 10(1):12814, 2020.
- [193] Danial Goodarzi, Soroush Abolfathi, and Sina Borzooei. Modelling solute transport in water disinfection systems: effects of temperature gradient on the hydraulic and disinfection efficiency of serpentine chlorine contact tanks. *Journal of Water Process Engineering*, 37:101411, 2020.
- [194] Mingtao Jiang, Wei Chen, and Adrian Wing-Keung Law. Mixing characteristics of 45° inclined duckbill dense jets in co-flowing currents. *Journal of Hydro-environment Research*, 36:77–86, 2021.
- [195] Mingtao Jiang, Adrian Wing-Keung Law, and Shuai Zhang. Mixing behavior of 45 inclined dense jets in currents. *Journal of hydro-environment research*, 18:37–48, 2018.
- [196] Paul CK Chu, Joseph H Lee, and Vincent H Chu. Spreading of turbulent round jet in coflow. *Journal of Hydraulic Engineering*, 125(2):193–204, 1999.
- [197] Ellert van der Velden. CMasher: Scientific colormaps for making accessible, informative and 'cmashing' plots. *The Journal of Open Source Software*, 5(46):2004, February 2020. doi: 10.21105/joss.02004.
- [198] J. D. Hunter. Matplotlib: A 2d graphics environment. *Computing in Science & Engineering*, 9(3):90–95, 2007. doi: 10.1109/MCSE.2007.55.
- [199] C. Bane Sullivan and Alexander Kaszynski. PyVista: 3d plotting and mesh analysis through a streamlined interface for the visualization toolkit (VTK). *Journal of Open Source Software*, 4(37):1450, may 2019. doi: 10.21105/joss.01450. URL <https://doi.org/10.21105/joss.01450>.
- [200] Jeff Reback, Wes McKinney, Joris Van Den Bossche, Tom Augspurger, Phillip Cloud, Adam Klein, Simon Hawkins, Matthew Roeschke, Jeff Tratner, Chang She, et al. pandas-dev/pandas: Pandas 1.0. 5. *Zenodo*, 2020. URL <https://doi.org/10.5281/zenodo.3509134>.
- [201] Philip JW Roberts and G Toms. Inclined dense jets in flowing current. *Journal of Hydraulic Engineering*, 113(3):323–340, 1987.
- [202] J Ayoub and R Alward. Water requirements and remote arid areas: the need for small-scale desalination. *Desalination*, 107(2):131–147, 1996.
- [203] Dror Drami, Yosef Z Yacobi, Noga Stambler, and Nurit Kress. Seawater quality and microbial communities at a desalination plant marine outfall. a field study at the israeli mediterranean coast. *Water research*, 45(17):5449–5462, 2011.

- [204] GC Christodoulou, IG Papakonstantis, and IK Nikiforakis. Desalination brine disposal by means of negatively buoyant jets. *Desalination and Water Treatment*, 53(12):3208–3213, 2015.
- [205] Matthew T Flavin, Jenifer Fernandes, Rawan AlQabandi, Eric Adams, Jongyoon Han, and Bader Al-Anzi. Numerical modeling of plunging jets of brine: Mass transport and implications for desalination plant outfalls. *Desalination*, 568:116996, 2023.
- [206] Baoxin Jiang, Adrian Wing-Keung Law, and Joseph Hun-Wei Lee. Mixing of 30° and 45° inclined dense jets in shallow coastal waters. *Journal of Hydraulic Engineering*, 140(3):241–253, 2014. doi: 10.1061/(ASCE)HY.1943-7900.0000819.
- [207] Hossein Kheirkhah Kheirkhah Gildeh, Abdolmajid Mohammadian, and Ioan Nistor. Vertical dense effluent discharge modelling in shallow waters. *Water*, 14(15):2312, 2022.
- [208] Sina Tahmooresi, Danial Goodarzi, Abdolmajid Mohammadian, and Ioan Nistor. Lif measurement of turbulent horizontal dense jets in stagnant ambient. *International Journal of Heat and Mass Transfer*, 244:126867, 2025. ISSN 0017-9310. doi: <https://doi.org/10.1016/j.ijheatmasstransfer.2025.126867>. URL <https://www.sciencedirect.com/science/article/pii/S001793102500208X>.
- [209] Marta Alvir, Luka Grbčić, Ante Sikirica, and Lado Kranjčević. Reconstruction and analysis of negatively buoyant jets with interpretable machine learning. *Marine pollution bulletin*, 190:114881, 2023.
- [210] Xiaohui Yan, Huade Cao, Penghai Yin, Jianwei Liu, and Zuhao Zhu. Concentration field estimation on effluent mixing and transport with a parameter-based field reconstruction convolutional neural network and random forests. *Water Resources Research*, 59(5):e2022WR033375, 2023.
- [211] Yufeng Zhao, Junshi He, Xiaohui Yan, and Jianwei Liu. Using an adaptive neuro-fuzzy inference system to predict dilution characteristics of vertical buoyant jets subjected to lateral confinement. *Journal of Marine Science and Engineering*, 10(3):439, 2022.
- [212] Saleh Rezaeiravesh, Timofey Mukha, and Philipp Schlatter. Efficient prediction of turbulent flow quantities using a bayesian hierarchical multifidelity model. *Journal of Fluid Mechanics*, 964:A13, 2023.
- [213] Joslin Goh, Derek Bingham, James Paul Holloway, Michael J Grosskopf, Carolyn C Kuranz, and Erica Rutter. Prediction and computer model calibration using outputs from multifidelity simulators. *Technometrics*, 55(4):501–512, 2013.
- [214] Dave Higdon, Marc Kennedy, James C Cavendish, John A Cafeo, and Robert D Ryne. Combining field data and computer simulations for calibration and prediction. *SIAM Journal on Scientific Computing*, 26(2):448–466, 2004.

- [215] Volker John. *Large eddy simulation of turbulent incompressible flows: analytical and numerical results for a class of LES models*, volume 34. Springer Science & Business Media, 2003.
- [216] Danial Goodarzi, Kaveh Sookhak Lari, and Abolghasem Alighardashi. A large eddy simulation study to assess low-speed wind and baffle orientation effects in a water treatment sedimentation basin. *Water Science and Technology*, 2017(2):412–421, 2018.
- [217] Giancarlo Alfonsi. Reynolds-averaged navier–stokes equations for turbulence modeling. *Applied Mechanics Reviews*, 62(4):040802, 06 2009. ISSN 0003-6900. doi: 10.1115/1.3124648. URL <https://doi.org/10.1115/1.3124648>.
- [218] Pierre Sagaut. *Large eddy simulation for incompressible flows: an introduction*. Springer Science & Business Media, 2005.
- [219] Marc C Kennedy and Anthony O’Hagan. Predicting the output from a complex computer code when fast approximations are available. *Biometrika*, 87(1):1–13, 2000.
- [220] Zhiguang Qian, Carolyn Conner Seepersad, V. Roshan Joseph, Janet K. Allen, and C. F. Jeff Wu. Building surrogate models based on detailed and approximate simulations. *Journal of Mechanical Design*, 128(4):668–677, 06 2005. ISSN 1050-0472. doi: 10.1115/1.2179459. URL <https://doi.org/10.1115/1.2179459>.
- [221] Christopher KI Williams and Carl Edward Rasmussen. *Gaussian processes for machine learning*, volume 2. MIT press Cambridge, MA, 2006.
- [222] Jacob Gardner, Geoff Pleiss, Kilian Q Weinberger, David Bindel, and Andrew G Wilson. Gpytorch: Blackbox matrix-matrix gaussian process inference with gpu acceleration. *Advances in neural information processing systems*, 31, 2018.
- [223] Maximilian Balandat, Brian Karrer, Daniel R. Jiang, Samuel Daulton, Benjamin Letham, Andrew Gordon Wilson, and Eytan Bakshy. BoTorch: A Framework for Efficient Monte-Carlo Bayesian Optimization. In *Advances in Neural Information Processing Systems 33*, 2020. URL <http://arxiv.org/abs/1910.06403>.
- [224] Danial Goodarzi, Abdolmajid Mohammadian, and Saleh Rezaeiravesh. Numerical simulation of desalination brine discharges: Effects of inlet boundary conditions. *Desalination*, page 119389, 2025. ISSN 0011-9164. doi: <https://doi.org/10.1016/j.desal.2025.119389>. URL <https://www.sciencedirect.com/science/article/pii/S0011916425008653>.
- [225] Xiaohui Yan and Abdolmajid Mohammadian. Numerical modeling of vertical buoyant jets subjected to lateral confinement. *Journal of Hydraulic Engineering*, 143(7): 04017016, 2017.
- [226] Gavin R Tabor and MH Baba-Ahmadi. Inlet conditions for large eddy simulation: A review. *Computers & Fluids*, 39(4):553–567, 2010.

- [227] Alex W Abboud and Sean T Smith. Large eddy simulation of a coaxial jet with a synthetic turbulent inlet. *International journal of heat and fluid flow*, 50:240–253, 2014.
- [228] Andrea Montorfano, Federico Piscaglia, and Giancarlo Ferrari. Inlet boundary conditions for incompressible les: A comparative study. *Mathematical and Computer Modelling*, 57(7-8):1640–1647, 2013.
- [229] Hrvoje Jasak, Aleksandar Jemcov, Zeljko Tukovic, et al. Openfoam: A c++ library for complex physics simulations. In *International workshop on coupled methods in numerical dynamics*, volume 1000, pages 1–20, 2007.
- [230] Christophe Geuzaine and Jean-François Remacle. A three-dimensional finite element mesh generator with built-in pre-and post-processing facilities. *Int. J. Numer. Methods Eng*, 11:79, 2020.
- [231] Dongdong Shao and Adrian Wing-Keung Law. Boundary impingement and attachment of horizontal offset dense jets. *Journal of Hydro-environment Research*, 5(1):15–24, 2011.
- [232] Israel Wygnanski and Ho Fiedler. Some measurements in the self-preserving jet. *Journal of Fluid Mechanics*, 38(3):577–612, 1969.
- [233] Nagangudy R Panchapakesan and John L Lumley. Turbulence measurements in axisymmetric jets of air and helium. part 1. air jet. *Journal of Fluid Mechanics*, 246:197–223, 1993.
- [234] Hussein J Hussein, Steven P Capp, and William K George. Velocity measurements in a high-reynolds-number, momentum-conserving, axisymmetric, turbulent jet. *Journal of Fluid Mechanics*, 258:31–75, 1994.
- [235] William K George. The self-preservation of turbulent flows and its relation to initial conditions and coherent structures. *Advances in turbulence*, 3973, 1989.
- [236] E Ferdman, MV Otugen, and S Kim. Effect of initial velocity profile on the development of round jets. *Journal of Propulsion and Power*, 16(4):676–686, 2000.
- [237] Cat Tuong Nguyen and Martin Oberlack. Comparative study of turbulent round jet flows through direct numerical simulation at medium–high reynolds numbers. *Physics of Fluids*, 36(11), 2024.
- [238] AAR Townsend. *The structure of turbulent shear flow*. Cambridge university press, 1976.
- [239] RA Antonia and J Mi. Temperature dissipation in a turbulent round jet. *Journal of Fluid Mechanics*, 250:531–551, 1993.
- [240] Alexis Darisse, Jean Lemay, and Azemi Benaïssa. Budgets of turbulent kinetic energy, reynolds stresses, variance of temperature fluctuations and turbulent heat fluxes in a round jet. *Journal of Fluid Mechanics*, 774:95–142, 2015.

- [241] Bendiks J Boersma, Geert Brethouwer, and Frans TM Nieuwstadt. A numerical investigation on the effect of the inflow conditions on the self-similar region of a round jet. *Physics of fluids*, 10(4):899–909, 1998.
- [242] GN Taub, Hyungoo Lee, S Balachandar, and SA Sherif. A direct numerical simulation study of higher order statistics in a turbulent round jet. *Physics of Fluids*, 25(11), 2013.
- [243] Cat Tuong Nguyen and Martin Oberlack. Analysis of a turbulent round jet based on direct numerical simulation data at large box and high reynolds number. *Physical Review Fluids*, 9(7):074608, 2024.
- [244] Paul F Fischer, James W Lottes, and Stefan G Kerkemeier. nek5000 web page, 2008.
- [245] Anthony T Patera. A spectral element method for fluid dynamics: laminar flow in a channel expansion. *Journal of computational Physics*, 54(3):468–488, 1984.
- [246] Pradeep C Babu and Krishnan Mahesh. Upstream entrainment in numerical simulations of spatially evolving round jets. *Physics of Fluids*, 16(10):3699–3705, 2004.
- [247] CL Lubbers, Geert Brethouwer, and BJ Boersma. Simulation of the mixing of a passive scalar in a round turbulent jet. *Fluid Dynamics Research*, 28(3):189, 2001.
- [248] Pradeep Babu and Krishnan Mahesh. Direct numerical simulation of passive scalar mixing in spatially evolving turbulent round jets. In *43rd AIAA Aerospace Sciences Meeting and Exhibit*, page 1121, 2005.
- [249] Georgios Maragkos, S Verma, A Trouvé, and Bart Merci. Evaluation of openfoam’s discretization schemes used for the convective terms in the context of fire simulations. *Computers & Fluids*, 232:105208, 2022.
- [250] Takayuki Utsumi, Tomoaki Kunugi, and Takayuki Aoki. Stability and accuracy of the cubic interpolated propagation scheme. *Computer physics communications*, 101(1-2): 9–20, 1997.