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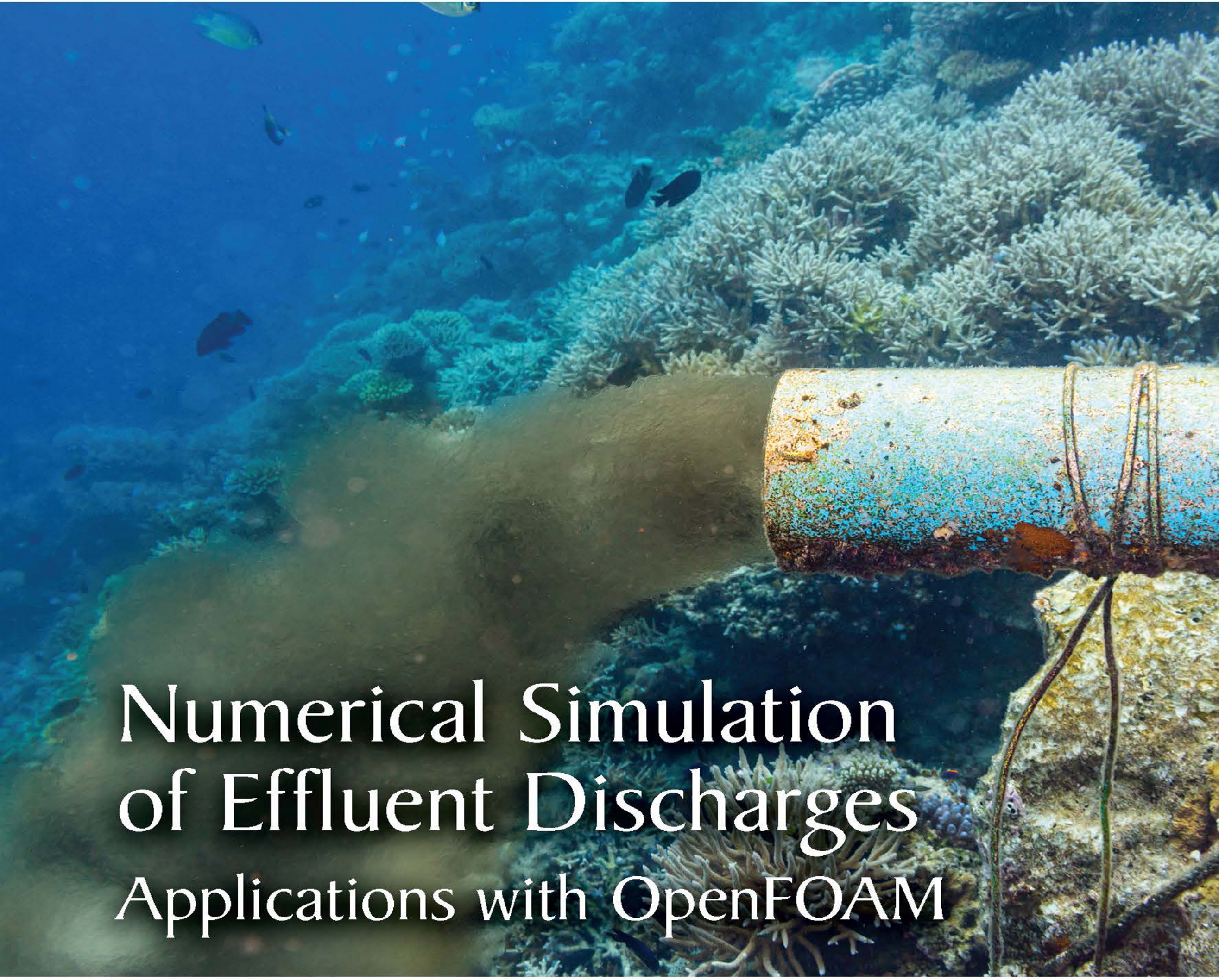

Numerical Simulation of Effluent Discharges

Applications with OpenFOAM

**Abdolmajid Mohammadian,
Hossein Kheirkhah Gildeh,
and Xiaohui Yan**

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Numerical Simulation of Effluent Discharges

Numerical Simulation of Effluent Discharges: Applications with OpenFOAM provides a resource for understanding the effluent discharge mechanisms and the approaches for modeling them. It bridges the gap between academia and industry with a focused approach in CFD modeling and providing practical examples and applications. With a detailed discussion on performing numerical modeling of effluent discharges in various ambient waters and with different discharge configurations, the book covers the application of OpenFOAM in effluent discharge modeling.

Features:

- Discusses effluent discharges into various ambient waters with different discharge configurations.
- Focuses on numerical modeling of effluent discharges.
- Covers the fundamentals in predicting the mixing characteristics of effluents resulting from desalination plants.
- Reviews the past CFD studies on the effluent discharge modeling thoroughly.
- Provides guidance to researchers and engineers on the future steps in modeling of effluent discharges.
- Includes an introduction to OpenFOAM and its application in effluent discharge modeling.

The book will benefit both academics and professional engineers practicing in the area of environmental fluid mechanics and working on the effluent discharge modeling.

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Contents

Preface

This book is an introduction to the numerical modeling of effluent discharges using OpenFOAM. It introduces the relevant background knowledge and modeling techniques of effluents in detail.

With the increase in population, the development of regional economy and the acceleration of industrialization, wastewater effluents are increasing, which puts forward higher requirements for effluent treatment and disposal capacity. The establishment of a water effluent model can play an important role in improving effluent treatment technologies and dealing with environmental pollution. Therefore, effluent modeling is very important. This book introduces computational fluid dynamics (CFD) models of effluent discharges on the basis of understanding the research progress of jets and plumes, analyzes the advantages and disadvantages of different modeling approaches, and puts forward a series of suggestions for future research work.

Although a great deal of research has been done on the mixing properties of wastewater discharges over the past few decades, the simulation of wastewater discharges using modern mathematical and computational techniques is still in its infancy. The basic data problem and the uncertainty of model parameters in the process of model application pose challenges to the reliability of the model. The availability of open-source CFD tools has opened the door to more realistic CFD modeling of effluent discharges. Although the numerical simulation technology has been significantly developed, the turbulence modeling problem of jet or plume has not been completely studied, and further research is needed. This book discusses these gaps in the literatures.

This book is mainly for the undergraduate and graduate students in hydraulics and hydrology, as well as for practitioners. The book begins with an introduction to outfall systems (Chapter 1) and introduces the reader to the application and different configurations of outfalls, various types of effluents, and mixing zones. Chapter 2 introduces the basic principles of numerical modeling. First, it introduces the governing equations, computational domain, boundary conditions, and initial conditions. Then, computational meshing is introduced, including mesh generation and determination of mesh resolution based on mesh sensitivity analysis. Then various methods in turbulence modeling (RANS, LES, DES, DNS) are briefly discussed. The basic concepts are discussed, and the formulations of the selected methods are provided. Finally, the modification of turbulence terms for buoyant discharges is introduced. Chapter 3 is an introduction to OpenFOAM. OpenFOAM is a popular CFD tool for effluent discharge modeling. It mainly introduces the OpenFOAM solvers and mesh generation and post-processing capabilities for effluent discharge modeling. Chapter 4 reviews past numerical studies in this field, points out future research directions, and puts forward suggestions for further improving effluent discharge modeling.

This book builds on past effluent discharge researches with further discussion on CFD modeling approaches and techniques, and it is hoped that these introductions and recommendations will be a useful reference for undergraduate and graduate students in hydraulics and hydrology, as well as the practitioners.

List of symbols

C	concentration of tracers or contaminants
D	diffusivity coefficient
D	diameter of the discharge port
F_r	the densimetric Froude number
g	gravitational acceleration
g_x, g_y, g_z	gravitational acceleration components in the x, y, and z directions
h_0	water depth (m)
k_{eff}	heat transfer coefficient
p	pressure (N/m^2)
pr_t	turbulent Prandtl number
pr	Prandtl number
S	salinity (psu)
t	time (s)
t_0	initial time (s)
T	temperature
T	fluid temperature (°C)
U_j	initial velocity (m/s)
u	instantaneous velocity component (m/s)
u, v, w	velocity components (m/s)
u_x, u_y, u_z	velocity components (m/s)
v	kinematic viscosity
v_t	turbulent viscosity
x, y, z	coordinates
ω	specific dissipation rate
ρ	density
ρ_α	ambient density (g/cm^3)
ρ_j	jet's initial density
τ_{ij}	stress in the *j*-direction exerted on a plane perpendicular to the *i*-axis (N/m^2)

List of abbreviations

CFD	computational fluid dynamics
CORMIX	Cornell mixing zone expert system
DES	detached eddy simulation
DIC	diagonal incomplete Cholesky
DILU	diagonal incomplete lower upper
DNS	direct numerical simulation
EPA	environment Protection Agency
EU	European Union
FDIC	faster diagonal incomplete-Cholesky
FV	finite volume
FVC	finite volume calculus
FVM	finite volume method
FDM	finite difference method
GAMG	geometric-algebraic multi-grid
GGDH	general gradient diffusion hypothesis
LES	large eddy simulation
MSF	multistage flash
NS	Navier-Stokes equations
OSS	open source software
ODE	ordinary differential equations
PBiCG	preconditioned bioconjugate gradient
PCG	preconditioned conjugate gradient
PDE	partial differential equation
PDR	partial differential equation
PML	Prandtl mixing length
RANS	Reynolds-averaged Navier-Stokes
RNG	renormalization group
RO	reverse osmosis
RSM	Reynolds Stress Model
RWPT	random walk particle tracking
SGDH	simple gradient diffusion hypothesis
VTK	visualization toolkit
WSL	windows subsystem for Linux

Chapter 1

Introduction

1.1 Identifying the problem

Discharges of industrial effluents into coastal and estuarine waters and the emissions of incinerated urban waste into the atmosphere provide two examples of environmental flows in which water and air quality, respectively, are determined by the behavior and structure of the particle-laden, turbulent, dense/buoyant jets, or plumes generated by discharges. Industrial power plants discharge residual byproducts into water bodies (Lattemann and Höpner, 2008), mostly as submerged jets due to their higher effectiveness.

Moreover, rising populations, shortages of clean and potable water, and advancements in desalination plant technology have increased rapidly in recent decades. In arid and semi-arid countries, desalination plants are actively considered as the best alternative to respond to the high demand for drinkable water. Desalination plants remove the dissolved minerals from coastal water bodies and produce effluents with a high-salt concentration, called brines, that may also have an elevated temperature, especially for multistage flash (MSF) desalination plants. Disposal of these brines, which have higher density than the receiving water, causes many environmental impacts, especially in the near field of outfall systems, which is the natural habitat of marine species and fish cultures (Hashim and Hajjaj, 2005; Lattemann and Höpner, 2008). Some areas such as the Red Sea, Persian Gulf, and generally low energy areas with shallow waters are very sensitive to effluent discharges.

The effluent discharge systems of industrial power plants have to be designed properly in order to minimize environmental impacts and financial costs. They also must satisfy the environmental criteria and standards (e.g., US-EPA and EU regulations). Nevertheless, ocean outfall systems are mostly not optimized, either regarding environmental impacts or practical needs. In some cases, regulations also lack clear guidelines for ambient water or effluent standards (Jirka, 2004).

The density differences between the effluent and ambient water, represented by the buoyancy flux, result in various flow and mixing characteristics of the discharge. In the case of dense jets, especially brine from reverse osmosis (RO) desalination plants, the flow has the tendency to fall as negatively buoyant plumes. On the other hand, buoyant jets (e.g., effluents from MSF desalination plants) have lower density than ambient water which causes the plumes to rise.

Besides being designed to minimize environmental impacts and financial costs, discharge outfalls must be in compliance with regulatory criteria. The first step before working on the discharge outfall design is to decrease the concentrations of the waste

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source within the industrial plant (e.g., decreasing the additive usage, enhancing plant efficiency, pretreatment technologies, etc.). The second step is the application of improved mixing technologies, like submerged diffusers, and to discharge in less sensitive regions (offshore, deep waters).

Although experimental studies on scaled physical models have been primarily used to study the mixing problems in jets and plumes, this book only focuses on the numerical aspects of such problems. Therefore, the problem at hand is clear: how numerical modeling can be of help to design effluent discharges in open waters more efficiently. This requires an understanding of the problem and knowledge of the tools needed to address the questions surrounding it.

The term “numerical modeling” is still a general term and vague to some extents. There are different numerical modeling techniques that try to solve the equations of transport for effluent discharges. These models may use either simplified or complex sets of partial differential equations (PDEs) such as mass conservation, momentum conservation, and transport equations. There are two main methods available in solving effluent discharge problems numerically that are briefly summarized below.

1.1.1 Integral models

Jet integral models, according to Robinson et al. (2015), solve mass and momentum conservation equations based on the assumptions that the velocity profiles of jets have no radial variation, and that the jet profile is axisymmetric and Gaussian. In other words, complex governing equations of flow hydrodynamics are integrated over the cross section, assuming a Gaussian cross-sectional distribution. These models simplify the PDEs to ordinary differential equations (ODEs) that can be easily solved using numerical integration of differential equations such as explicit and implicit numerical methods. Explicit methods calculate the state of a system at a later time using the state of the system at the current time ($S(t + \Delta t) = F(S(t))$, while implicit methods use both current and future states of the system to find a solution ($F(S(t), S(t + \Delta t)) = 0$). In the 1950s and 1960s, first-order jet integral models were proposed by Morton et al. (1956) and Fan (1967) based on the jet entrainment closure approach and by Abraham (1963) and Turner (1969) based on the jet diffusion approach. Wang and Law (2002), Yannopoulos (2006), and Jirka (2004) developed second-order jet integral models. Since the turbulent mixing of effluent discharges are complex, as are their numerical solutions, integral models rely on experiments to derive the coefficients for their simplified analytical methods.

According to Robinson et al. (2015), the integral models are less reliable when there is any of the following: (i) the discharge’s initial momentum and buoyancy acting in opposite directions, resulting in instabilities on the edge, as observed in the inner half (lower half) of inclined dense jets; (ii) noticeable interaction between the mean flow and the jet, (iii) an unsteady mean ambient flow; (iv) a significant effect due to horizontal or lateral boundaries; (v) an unstable near-field area, with a re-entrainment of concentrated effluent into the jet; or, (vi) a large re-entrainment of concentrated effluent from mid- and far-fields into the near-field jet due to tidal cycles.

The most popular integral models in effluent discharge modeling are: CORMIX, VISUAL PLUMES, and VISJET. These models have been reviewed by Palomar et al. (2012) in detail, and the following provides a summary of that study.

CORMIX (Cornell Mixing Zone Expert System) software (Doneker and Jirka, 2001) is a commercial model that was developed in the 1980s at Cornell University (USA) as a project funded by the Environmental Protection Agency (EPA). Supported by the EPA, it became one of the most popular programs for discharge modeling. CORMIX is an expert system for predicting the discharge trajectory and dilution into water bodies in steady-state without considering time series data. CORMIX can simulate the disposal of effluents with positive, negative, and neutral buoyancy under different discharge and ambient conditions. The subsystems CORMIX 1, 2, and 3 are based on dimensional analysis of the processes, while the CORJET model is based on the integration of differential equations.

VISUAL PLUMES by Frick (2004) is a free access software developed by the EPA, which includes several models to simulate positively, negatively, and neutrally buoyant effluents discharged into receiving water bodies. VISUAL PLUMES considers the effluent properties, the discharge configuration, and the ambient conditions (temperature, salinity, and currents whose intensity and direction can be variable through the water column). It is limited to near-field region modeling and does not simulate the interaction of the flow with boundaries. It can consider time series data, simulating discharges in scenarios which change over time.

VISJET (Innovative Modeling and Visualization Technology for Environmental Impact Assessment) software (Cheung et al., 2000) is a commercial model developed by the University of Hong Kong, which can simulate positively and negatively buoyant discharges. VISJET considers the effluent properties, the discharge configuration, and the ambient conditions (temperature, salinity, and currents whose intensity and direction can be variable through the water column). It is limited to near-field region modeling and does not simulate the interaction of the flow with boundaries.

1.1.2 Computational fluid dynamics (CFD) models

Effluent discharge modeling by CFD tools is not perfect, but it is an improvement over the parameter-based jet integral models. Issues that remain with CFD tools include the following: (i) accuracy, (ii) stability, (iii) computational time, (iv) complicated codes that require expert knowledge to use them efficiently and accurately, and (v) simulations that need calibrating and validating.

Turbulent flow models are often resolved with a turbulence model to parameterize unresolved mixing and dispersion scales. One should apply turbulence models with caution, as they sometimes provide stable but unrealistic solutions, such as when they are applied to physical scenarios for which they have not been validated for.

When using a CFD model, it can be a challenge to create and resolve the mesh and to define appropriate boundary conditions (e.g., intensity and turbulence dissipation rate). A high-mesh resolution is often needed for a stable solution, even when the turbulence model is a good match. This means that CFD modeling is computationally expensive. Even with current computing systems, accurate CFD models for near-field dispersion and mixing might need simulation times of several days or weeks. This is much more expensive compared to the integral models that can produce results on the order of minutes and seconds. There is a balance between model stability, numerical diffusion, mass and momentum conservation, boundedness, and computational cost. These choices can significantly influence the estimation of modeled concentration.

However, once built, calibrated, and validated, CFD models can produce high-resolution three-dimensional images of jet mixing and dynamics. CFD models are free from some of the assumptions that restrict integral models. Since CFD models do not require the assumption of a steady-state condition or self-similarity in the jet profile, they can include a variety of external effects such as the presence of surface waves and encompass a wide range of boundary conditions to allow users to directly simulate the boundary interaction.

CFD modeling of jet discharges has been approached in a variety of ways, including both hydrostatic and nonhydrostatic approaches to the Reynolds-averaged Navier-Stokes (RANS) and the Large Eddy Simulations (LES) models. Both models have functioned well over the past decade to simulate effluent discharges. RANS models are based on a time-averaging method and result in a time-averaged mean velocity field, which is averaged over a longer time period than the time constant of the velocity fluctuations, and results in a constant mean velocity without fluctuation for time-dependent variations. LES is based on filtering instead of averaging. A filter size is identified, and flow scales equal to or larger than this size are calculated exactly, and scales smaller than the filter size are modeled. The smaller the filter size, the more concise is the calculated time variation resolution of the velocity vectors. RANS models are more numerically efficient than LES models, while providing enough detail for engineering applications. Thus, they have become the most prevalent CFD models used for the design of outfall systems.

The Direct Numerical Simulation (DNS) method is less applicable to engineering problems, functioning more as a research tool. It is CPU-intensive, as it attempts to resolve Navier-Stokes equations with no approximation of the turbulence and requires a very fine numerical resolution to capture all the turbulence details. It basically resolves entire turbulence scales temporally and spatially. Mesh systems should be very fine to resolve all the spatial scales (Kolmogorov, 1941).

Table 1.1 (after Zhao, Chen and Lee, 2011) summarizes the existing modeling packages (commonly used in the academia and industry) for the simulation of jet and plume mixing.

1.2 Application of outfalls

Outfalls have been used for many years. Initially, they have been used as a means of transporting the effluents to the discharge point, in the absence of environmental regulations. In the modern era, outfalls are used in both inland and coastal waters more carefully, and as a system that increases the dilution of discharged effluents to meet the environmental regulations in both near-field and far-field mixing zones. In other words, outfalls are not simply a method of transport, they represent a sustainable technology to preserve the environment while meeting its main objectives. More restrictive regulations have been developed throughout the years and the design of outfall systems has become more complex.

It is noteworthy that stormwater outfalls that discharge non-impacted waters into river or marine environments are not part of what is discussed here. In this book, we primarily refer to the outfalls that transport and discharge effluents with elevated temperature, salinity, and other chemicals. For instance, outfalls used in desalination plants, nuclear power plants, and wastewater treatment plants are among those mostly studied with respect to mixing problems.

Table 1.1 Existing modeling packages for simulation of jet and plume mixing

Models	*Mathematical approaches for jet/plume mixing*	*Availability*	*Major functionalities and capabilities*
CORMIX	Empirical solutions; Eulerian jet integral method	Commercial package	Prediction of jet and (or) plume geometry and dilution in the near field; single or multiple jets
VISJET	Lagrangian jet integral method	Commercial package	
Visual PLUMES	Empirical solutions; Eulerian and Lagrangian jet integral methods	Free package	
NRFIELD	Empirical solutions	Free package	Prediction of jet and (or) plume geometry and dilution in the near field of multiport diffusers
Sophisticated Multidisciplinary Models			
OpenFOAM	FVM; RWPT method	Free package	Predictions of ocean hydrodynamics; pollutant fate and transport in the near and far fields; water quality; sediment processes
MIKE21/3	FVM; RWPT method	Commercial package	
Delft3D	FDM; RWPT method	Free package	
ANSYS CFX	FVM; RWPT method	Commercial package	
ANSYS Fluent	FVM; RWPT method	Commercial package	
FLOW-3D	FDM; RWPT method	Commercial package	
TELEMAC-2D/3D	FEM; RWPT method	Free package	
EFDC	FDM; RWPT method	Commercial package	Predictions of ocean hydrodynamics; Pollutant dispersion in the far field; Suspended sediment transport
HydroQual–ECOMSED	FDM; RWPT method	Free package	Predictions of ocean hydrodynamics; Pollutant fate and transport in the far field; Sediment processes

Note: FVM: Finite Volume Method, FDM: Finite Difference Method, RWPT: Random Walk Particle Tracking.

Although outfalls are essential to human needs, they impact the environment they discharge into. The direct discharge of wastewater into lakes, rivers, and seas can increase turbidity and change the ambient temperature. Salinity is also a major public and scientific concern. Coastal waters receive concentrated salt brine as discharges from seawater desalination plants, chemical wastes from biofouling (e.g., chlorine), and fertilizers. The water bodies that receive the industrial discharges are often very sensitive environments, and designing outfalls to disperse effluent and reduce the concentration of effluents is essential in helping to protect the receiving water bodies.

Hopner and Windelberg (1996) noted that certain coastal ecological zones are particularly vulnerable to effluent discharges, including salt marshes, mangrove forests, coral reefs, and other low-energy intertidal areas. The Persian Gulf and the Red Sea are particularly sensitive to effluent due to their low hydro-dynamism. Local fisheries, tourism industries, and other economic concerns are affected by the health of coastal environments (Figure 1.1).

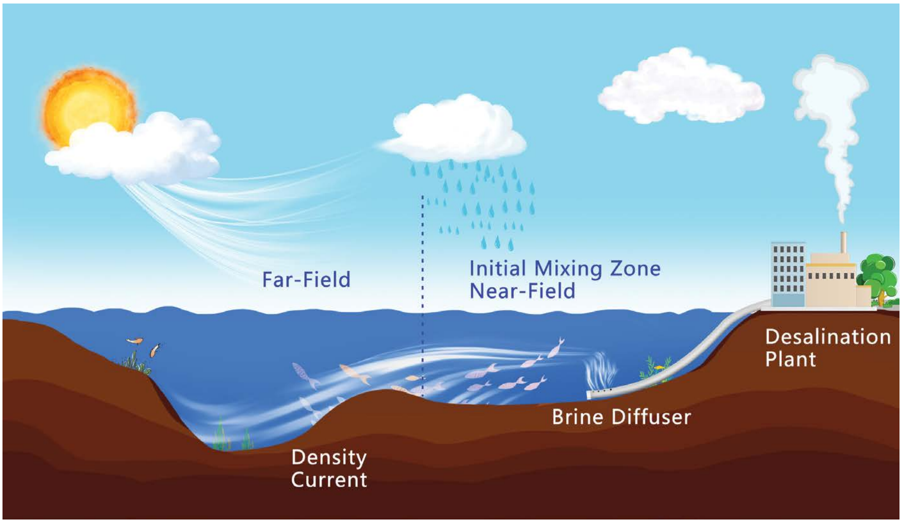


Figure 1.1 An overview of the effluent discharge in a water balance concept.

Based on the above paragraphs, it is clear that outfalls are not only a technical and economic concern. It goes beyond that as it affects the socio-environmental aspects of our lives. It is important that both designers and regulators pay attentions to each single outfall system being designed and constructed, as each outfall has its own challenges and unique characteristics.

A key item to note when reviewing the applications of outfalls for effluent discharges is the discharge objectives that would be the basis for the process leading to the water quality regulations, discharge limits, and design criteria. Figure 1.2 shows the general flowchart of environmental evaluations when designing the proper outfall system for a specific site.

The performance of an ocean or inland effluent discharge outfall is dependent on several factors such as the outfall configuration, topographic and bathymetric conditions of the discharge area, receiving water hydrodynamics, etc. This is the main reason that each outfall should be looked at as a unique design with unique characteristics. The following sections summarize key characteristics of effluent discharges.

1.3 Different outfall configurations

The effluents produced by industrial plants (e.g., brine produced by a desalination plant) can be disposed of in several ways such as discharge in inland open waters, injection into ground wells, discharge into a large evaporation pond, or discharge into coastal waters. There are two general methods of discharging effluents: surface discharge through open channels and submerged discharges through pipes extending into ambient waters. These two methods are illustrated in Figure 1.3. Both these types of discharges intend to increase the dilution and mitigate the environmental impacts.

The selection of the type of outfall is site specific and depends on several parameters such as desalination technology, plant operation and production rate, costs, and environmental considerations. Moreover, the characteristics of discharge (such as density)

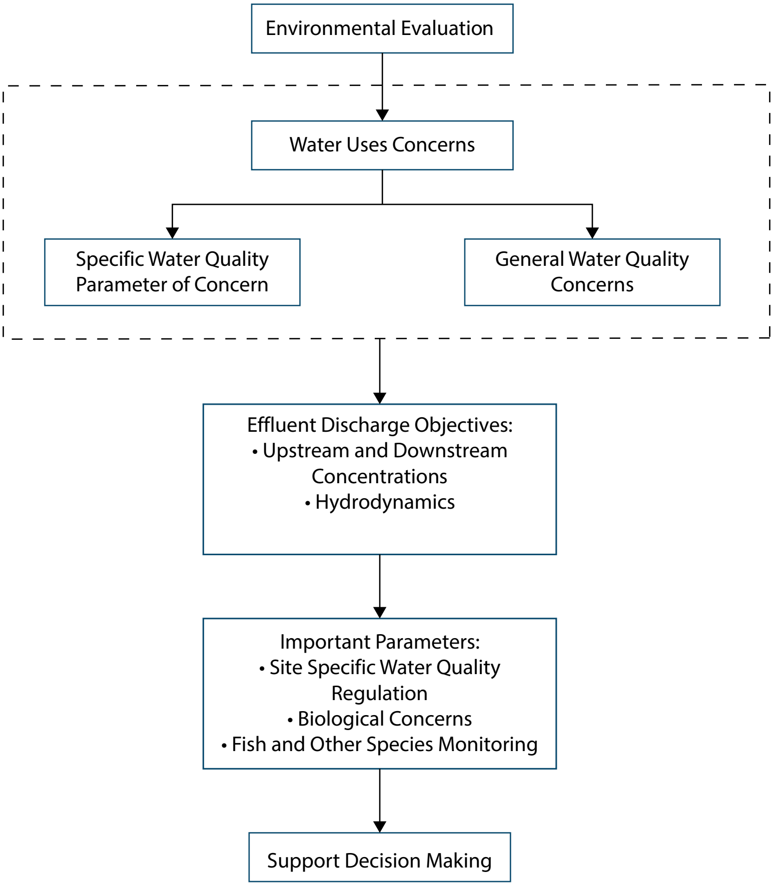


Figure 1.2 Environmental evaluations to preserve aquatic environments from effluent discharge.

and receiving ambient waters (such as density, ambient currents, and buoyancy) influence the type of outfall to be selected.

Surface discharges through open channels are often the most economic options available due to easier construction and maintenance. They are still constructed and used, despite the fact that their efficiency is lower than submerged discharge outfalls in terms of mixing and entrainment (dilution). Surface discharges are excellent options for plants that discharge effluents at a high flow rate, where conveyance through long pipes is extremely difficult due to pipe size and head losses associated with the conduits. Figure 1.4 illustrates the various surface discharge configurations.

On the other hand, submerged discharges are very popular due to their higher efficiency in reaching the required dilution. Therefore, many industrial plants (e.g., mining) will consider the discharge requirements at the very initial stages of the design, and will thus use submerged outfalls in order to meet the regulatory requirements for their permitting purposes. Submerged outfalls often use a pipe near the seabed to discharge effluents. The submerged discharges have been well studied both experimentally and numerically in past decades and our understanding of their mechanisms is relatively well established. It is noteworthy that outfall often refers to the pipe that transports the effluents from

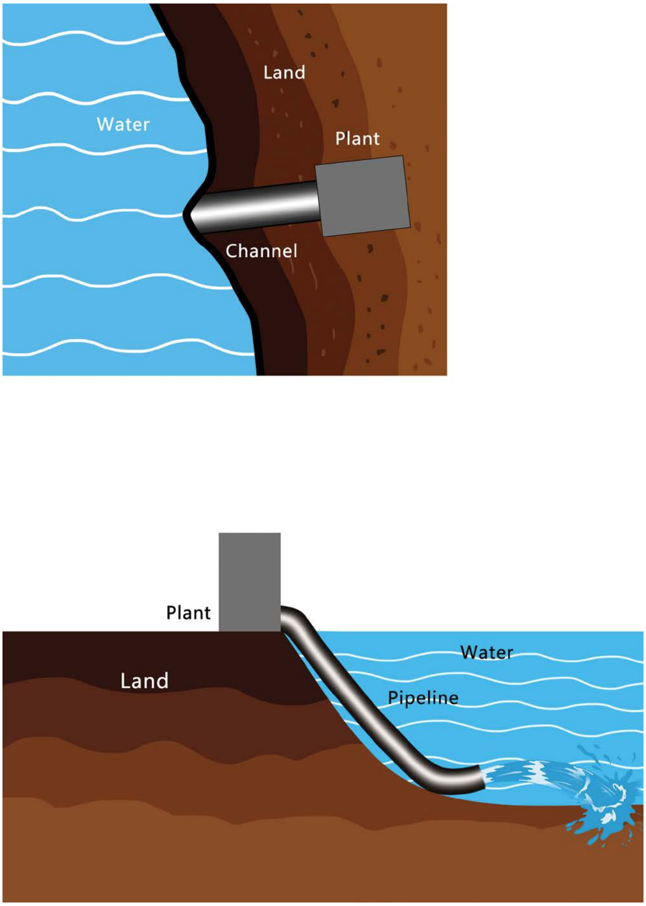
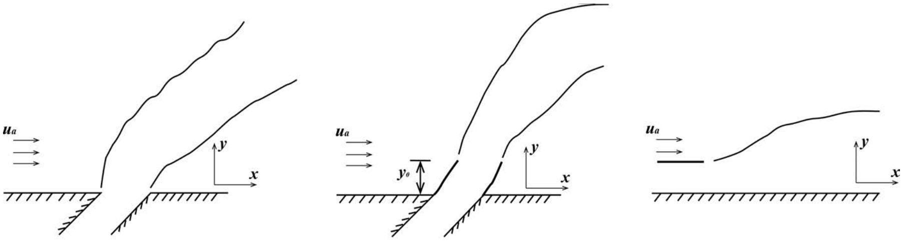


Figure 1.3 Schematic representation of brine discharge systems.

upland into the water. At the discharge location, it can be discharged through the same pipe (i.e., one discharge nozzle) or through a series of nozzles (diffusers). If a single nozzle is used to discharge the effluent into the receiving water, it is called a "single-port diffuser." However, in many cases, the series of nozzles are attached to the discharge point of the outfall, which is called a multiport diffuser (referring to several ports/nozzles to discharge effluents). In this case, the total discharge head



discharge flush with bank

protruding discharge

coflowing along bank

Figure 1.4 Discharge configurations of surface channel relative to bank/shoreline.

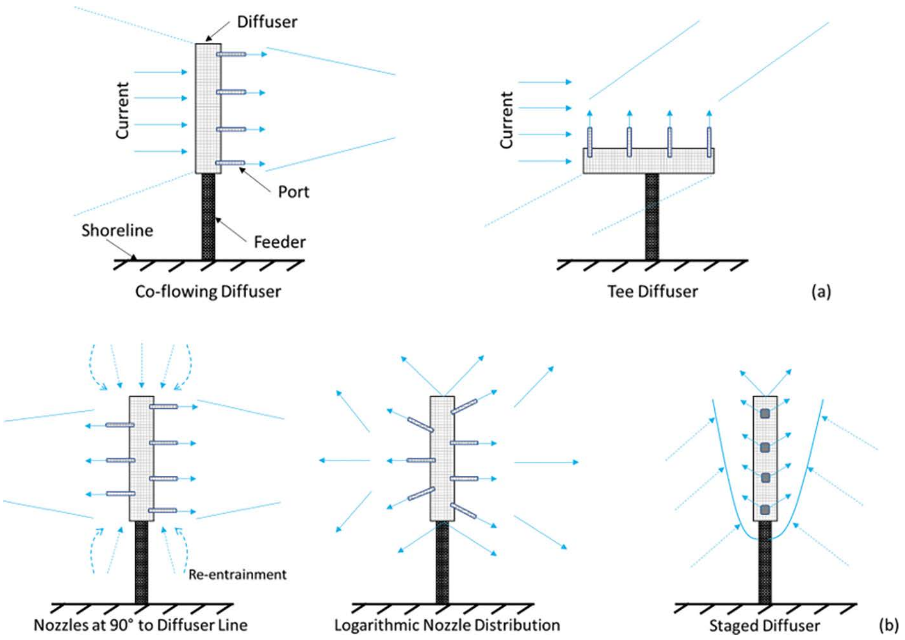


Figure 1.5 Multiport diffusers: (a) Unidirectional diffusers with cross-flow; (b) Alternating diffuser.

is distributed between the number of ports. The configuration of nozzles can vary depending on the ambient condition and design considerations. Figure 1.5 shows five different configurations of multiport diffusers that are commonly used. Another emerging multiport diffuser configuration is the rosette outfall configuration, as shown in Figure 1.6. Unlike the single-port discharges, multiport effluent discharges have been less studied, both experimentally and numerically.

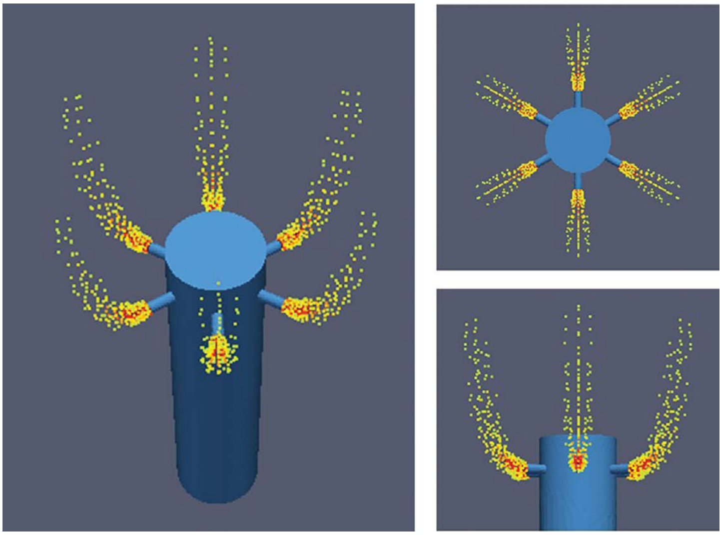


Figure 1.6 Rosette jet, top view.

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