

Numerical simulation of microplastics transport in a part of Fraser River and detection of accumulation zones based on clustering methods

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Abstract

Microplastics are tiny particles that due to their small size, durability, and widespread usage have become a huge threat to the world and the environment. Aquatic environments like rivers and oceans have faced some irreparable problems such as the extinction of various marine species. Field sampling and numerical modeling are two methods that can help researchers have a better understanding of the situations to come up with the best solutions. Machine learning methods have drawn considerable attention in most engineering fields recently, which can be used in conjunction with field sampling and numerical simulation.

In this study, by generating a fine mesh and using bathymetry, water level, and discharge data, a three-dimensional hydrodynamic modeling of the domain of study was conducted using TELEMAC 3D, which is a model that was used to simulate the behavior of the Fraser River in x, y, and z directions. The results were implemented to track the movements of microplastic particles in the lower part of the Fraser River. CaMPSim-3D, which is a three-dimensional Lagrangian particle tracking model was employed to track microplastic particles. This model, in addition to calculating the horizontal location of particles, computes their vertical movements too. The release locations of microplastic particles were chosen based on the locations of the wastewater treatment plants and combined sewer overflows and in the end, nine scenarios were conducted for this study. An unsupervised branch of machine learning is clustering which helps to cluster points by relying on their different properties. The OPTICS algorithm, which is a density-based clustering algorithm, was used to find the accumulation zones of microplastic particles in the lower part of the Fraser River.

It should be mentioned that in all parts available measured data and information were used for validation. The results of the clustering algorithm indicated that there are eight accumulation zones in the study area and the breakwater in the upper branch of the Fraser River is an ideal place for microplastic particles to accumulate. A reasonable agreement was obtained between the model results and measured data.

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List of Symbols

B_p	Value of any parameter at the location of particle
C_d	Drag coefficient
$N_{Eps}(p)$	Cluster with core point p
Re_p	Particle Reynolds number
T_c	Density of tracer
T_{ref}	Reference temperature
V_{DB}	Davies-Bouldin index
V_s	Settling Velocity
a_i	Distance of the particle from each of the vertices of the prism
p_{atm}	Atmospheric pressure
p_d	Dynamic pressure
u_p	Velocity of a particle in X direction
v_T	Coefficient for tracer diffusion
v_p	Velocity of a particle in Y direction
w_p	Velocity of a particle in Z direction
ρ_0	Reference Density
ρ_p	Density of the particle
σ_k	Turbulent Prandtl number for k
σ_ϵ	Turbulent Prandtl number for ϵ
d	Diameter of particle
Diff.....	Diffusion
Eps.....	Maximum distance of a point from the core of a cluster to be considered in that cluster
g	Gravity
K	Diffusion coefficient
k.....	Turbulent kinetic energy

P		Turbulent energy production
p		Pressure
Q		Tracer sink
S		Salinity
T		Temperature
t		Time
TAF		Tracer accumulation factor
u		Velocity in X direction
v		Velocity in Y direction
w		Velocity in Z direction
C		Concentration of particles
ε		Rate of dissipation of turbulent kinetic energy
ρ		Density
ν		Kinematic viscosity
ψ		Particle shape factor

List of Acronyms

CSO	Combined sewer overflow
WWTP	Wastewater treatment plant
SSO	Sanitary sewer overflow
OPTICS.....	Ordering points to identify the clustering structure
CaMPSim	Canadian microplastic simulation
NRC.....	National research council
DBSCAN	Density-based clustering algorithm
K-Means	Settling Velocity
PTM	Particle tracking modeling
AI	Artificial intelligence
PTM	Particle tracking modeling
MinN	Minimum number of particles
CD	Chart datum
UTM.....	Universal transverse mercator
NAD	North American datum
NumPy.....	Numerical python
SciPy	Scientific python
Esri.....	Environmental systems research institute
GIS	Geographic information system

Chapter 1. Introduction

1.1 Background

There is no doubt that plastics are an integral part of our daily lives. The environment around us is filled with a great deal of plastic, including shopping bags, bottles, and different types of containers. Imagining a world without plastic is currently impossible. There are, however, many harmful effects that these plastic products have on the environment, some of which are irreversible. A direct relationship exists between plastic usage and the number of people and the population. Based on previous research, there is an increase in the number of people per square kilometer each day, which leads to an increase in plastic production and usage (Thompson et al., 2004). Plastic particles persist for a long time in the environment. Therefore, it is not a problem that will go away soon, so governments need to quickly and permanently address this issue. There are several chemical and physical processes that can lead to the creation of microplastics from these large plastic products that will be discussed more in chapter two of the thesis. Plastics can be classified into different categories based on their characteristics such as size, shape, and source. Based on size criteria, plastics can be categorized into four groups, nanoplastics, microplastics, mesoplastics, and macroplastics (Hartmann et al., 2019). Plastics smaller than 5 mm are called microplastics by the U.S. National Oceanic and Atmospheric Administration (Betts, 2008). The shapes of microplastics that affect their settling velocity are normally spheres, granules, films, fibers, pellets, and cylinders (Van Melkebeke et al., 2020). Figure 1.1 displays different microplastics shapes. Microplastics with less than 5 mm in size and spherical shape have been used for this study.



Figure 1.1: Different microplastics shapes (Karimpour et al., 2021)

The density of microplastics can be compared with the density of water. Some of the particles are denser than water and some of them are lighter than water. The ones with low density and small size are a huge danger to the natural world, especially the marine environment (figure 1.2). These particles won't sediment and will remain in the water bodies. Lots of environmental problems that microplastics have caused have made them a global concern (Li et al., 2018). Mainly the density of microplastics is in the range of 0.05 g/cm^3 for polystyrene to 2.3 g/cm^3 for polytetrafluoroethylene (Teflon) (Chubarenko et al., 2016). Common densities of microplastics are mentioned in table 1.1.

Table 1.1: Density of microplastic particles (Andrady, 2011)

Microplastic Particle	Density (kg/m^3)
Polyethylene (PE)	910–950
Polypropylene (PP)	900–920
Poly vinyl chloride (PVC)	1160–1300
Polyamide (PA) or nylon	1130–1150
Polyethylene terephthalate (PET)	1340–1390
Polyester resin + glass fibre	>1350
Cellulose acetate	1220–1240

There are different transformation processes that can affect the density of microplastics such as biofouling, degradation, and fragmentation. Various factors like salinity, temperature, and sunlight can influence the transformation process. In the journey of microplastic particles some microorganisms or algae can accumulate on the particles (biofouling) or some external factors can break them into several parts (Van Utenhove, 2019).

Currently, several studies are in progress about microplastics to understand their behavior in order to manage and reduce their harmful effects. These researches will be discussed more in the following chapter.



Figure 1.2: Microplastics in marine environments (photo from:

<https://www.nasa.gov/feature/esnt2021/scientists-use-nasa-satellite-data-to-track-ocean-microplastics-from-space>)

It is possible for microplastics to enter water bodies in a variety of ways. When we throw plastics away, especially on beaches, we play a major role in this contamination. The use of ships and boats is also widespread all around the globe through rivers and oceans, which are traveled by millions of people every year. They are a source of microplastics. In addition to the aforementioned sources, the combination of sanitary sewer overflows (SSOs), combined sewer overflows (CSOs), and wastewater treatment plant discharges (WWTPs) may be cited as the main source of microplastics in aquatic environments. More details about the sources of microplastics and their pathway through different water bodies are provided in the next chapter. As precipitation and rain increase beyond the design volume of combined sewer systems, extra untreated sewer water enters rivers and oceans (Erikson et al., 2013). Figure 1.3 shows plastic products in combined sewer overflows that are stuck before entering rivers and oceans.

As a result of the low density and durability of microplastics, upon entering the river, they will not be able to settle down easily and will begin to move along. Microplastics are smaller than most of the marine species and therefore one of the most popular targets of them as food. In this way, they will enter the food chain of humans, which is very dangerous and can cause lots of health problems. It is a well-known fact that macroplastics and microplastics accumulate in the middle of oceans to

such an extent that there is always news about their catastrophic consequences, as illustrated in Figure 1.4. Due to the low velocity and sometimes low depth of water in turns and narrow sections of rivers, they settle and this can lead to some changes in the soil's chemical and physical characteristics in those regions. Also other sources of plastics in soils are sewage and waste of agricultural activities. Soil has favorable circumstances for microbes and enzymes. Flow rates in soils are not sufficient to transport plastics and microplastics so that they have adequate time to degrade. One of the consequences is the reduction of soil fertility for agricultural purposes and even some changes in the type of plants that can grow there (Hurley and Nizzetto, 2018).

The effects of microplastics on the surrounding environments and human bodies are discussed in chapter two.



Figure 1.3: Plastics in CSOs (photo from: <https://www.sas.org.uk/news/surfers-against-sewage-calls-on-water-companies-to-investigate-contain-and-control-microplastics-entering-uk-bathing-waters/>)



Figure 1.4: Accumulation of plastics in oceans (photo from: <https://www.ecoredux.com/plastic-pollution-in-ocean>)

As soon as scientists discovered the detrimental effects of plastics on the environment, they began studying and tracking them to understand their behavior, so that they could prevent or at least mitigate the damage they cause. In order to be able to predict the accumulation zones and even the source of plastics, several methods have been explored including field experiments (sampling), modeling, and numerical solutions. Hydrodynamic modeling of rivers is one of the most powerful methods to simulate the behavior of rivers under different conditions. Furthermore, some particle tracking models for tracking plastic particles have been developed, as well as machine learning algorithms for predicting their destinations in the future.

Despite the fact that plastics are an integral part of our daily lives, eliminating them seems impossible in today's world. However, these inseparable objects threaten the environment, wildlife, as well as human health. A replacement for plastics is necessary, but it may take some time to discover something as inexpensive and accessible as plastic. Consequently, it is imperative that we find ways to manage their harmful effects on the environment and our quality of life.

1.2 Study Objectives

A variety of solutions have been developed in order to reduce the negative effects of microplastics on nature. In this study, three of them are used: hydrodynamic modeling, particle tracking modeling, and clustering algorithms. This study aims to simulate the actual condition of the Fraser River by releasing particles virtually in the modeled river, tracking them, and determining their final locations and accumulation zones. As a final step, microplastic accumulation zones were found using the OPTICS algorithm.

Numerical model is one of the most commonly applied approaches in various cases, particularly rivers. Hydrodynamic modeling of rivers can be accomplished with a number of engineering tools. For this study, Bluekenue was used to generate the model's base mesh, and TELEMAC, a sophisticated and well-known hydrodynamic modeling tool, was used to run the simulation.

An integrated particle tracking model was developed by the National Research Council of Canada (NRC) and the University of Ottawa. This tool, by using the results of the hydrodynamic model and solving the equation, predicts the location of each particle at each time step.

The specific objectives of this thesis are:

- Utilize a hydrodynamic model to determine velocity, salinity, and density fields for the Fraser River at a specific period of time
- Track microplastic particles with a particle tracking model and derive their position after releasing in each timestep
- Use OPTICS algorithms to find the accumulation zones of the microplastic particles
- Validate the results of the hydrodynamic model and clustering algorithm

It is worth mentioning that validation was done by using real data and the results of a field campaign.

1.3 Contributions and Novelty

Microplastics have drawn considerable attention in environmental studies in the last few decades. The Fraser River is one of the most important sources of fresh water in Canada. Previously, it was

known as a clean river but now because of the growing cities and industries surrounding it, this river is in danger of microplastic pollution. A few studies have been done about the hydrodynamic modeling of the Fraser River and no numerical model was found for tracking the transport of particles and more specifically microplastic particles in the lower part of the Fraser River. It is appropriate to mention that some samplings have been done in some parts of the Fraser River to count the number of microplastic particles. In the following chapters, more explanations will be provided regarding them.

Several novel elements are proposed and investigated in the current study, as outlined below:

- Three-dimensional hydrodynamic modeling of the lower part of the Fraser River with TELEMAC 3D by considering salinity as a tracer and real water level and discharge data
- Using a three-dimensional Lagrangian particle tracking model to understand the behavior of particles in the Fraser River for the first time
- Implementing CaMPSim-3D for particle tracking which is a newly developed model with well-proven efficiency (Pilechi et al., 2022)
- The characteristics of the microplastic particles are not just assumptions and they are based on the real experiment data
- For the first time, a combination of hydrodynamic modeling, particle tracking modeling, and machine learning algorithms was used to find the accumulation zones of microplastic particles in the lower part of the Fraser River
- Testing the accuracy of the particle tracking model and clustering algorithm using field experiment data for the first time in the lower part of the Fraser River

1.4 Outline

This thesis is divided into 5 chapters as follows:

- Chapter 1: is a brief introduction about the subject of the thesis, why this study should be done, contributions and novelty, and finally the outline
- Chapter 2: provides a comprehensive literature review of the hydrodynamic models, particle tracking models, and different clustering algorithms

- Chapter 3: presents the methodology of creating the base mesh with Bluekenue, essential information for hydrodynamic modeling of the Fraser River with TELEMAC 3D, how to use the result files for tracking the microplastic particles with CaMPSim-3D, and available data about the microplastic source in order to use the OPTICS algorithm
- Chapter 4: provides the results of all three model and compares them with the available measured data to test the accuracy of the models
- Chapter 5: contains the final conclusions of the research along with some suggestions and recommendations for future works

Chapter 2. Literature Review

2.1 Microplastics

Plastics are generally composed of polymers. Humans do not intervene in the natural existence of polymers in the universe. As viewed from a molecular perspective, polymers are made up of many identical or different parts that are linked together. As a matter of fact, plastics are artificial items that have been manufactured by scientists (Geyer, 2020).

The first plastic was made from cellulose nitrate in the middle of the 19th century (Rasmussen, 2021). It should be noted that cellulose serves as the base element in all of them. "Bakelite" was the first plastic product, which was used as a component of radios at that time. However, the widespread use of elastic and tough plastic products began toward the middle of the 20th century following the Second World War (Napper and Thompson, 2020).

There are a number of advantages of plastics, including heat and electricity resistance, longevity, and malleability, which make them a suitable primary material for a large number of products. Plastic components have gradually become part of every industry. Modern society is dependent upon plastics for a wide range of everyday items, including indoor and outdoor clothes, transportation equipment, building and construction, and even medical and technical devices. As a result, the consumption of plastics grew from 0.5 million tons in 1950 to more than 260 million tons in 2009. The degradation of plastics can take hundreds of years. Therefore, their waste has accumulated in different parts of the world, and now people are experiencing the detrimental consequences of that (Thompson et al., 2009).

The term microplastic refers to any plastic that is no larger than 5 mm in diameter (Masura et al., 2015). Generally, microplastics can be divided into two categories: primary microplastics and secondary microplastics. Plastics are sometimes produced in small sizes and their size is not the result of degradation. Plastics in this category are called primary microplastics, such as some small components of technological devices or cosmetics, or even tooth brushes that are used every day. However, some plastics are intended to be something larger than a pointed size, such as shopping bags or water bottles. After their lifetime, they will not simply disappear but will be disintegrated

as a result of reactions caused by nature or artificially induced by humans (Petersen and Hubbart, 2021).

Plastic is a recyclable material, but less than 21% of all plastic products will be reused (Law, 2017), and most of them will remain in the environment. Plastic degradation and breaking is a gradual process that is influenced by the shape, physical, and chemical characteristics of the plastic piece and by the climate and environmental factors in that region (Yuan et al., 2020). Beaches are one of the most popular places for picnics, swimming, and having fun, and people take a great deal of plastic with them when they do so. An experiment done by the National Research Council of Canada (NRC) has shown that beaches are full of plastic packages, shopping bags, and bottles of water. Based on research done by Auta et al, 2017, the creation of microplastics on beaches has one of the highest rates due to numerous factors including Ultraviolet radiation, the impact of the coastal or river waves, the existence of sand or rocks that play the role of sandpaper, and accessible Oxygen based on the elevation.

But in this study, the focus is on the microplastic particles that enter waterbodies. Seafood like fish or lobster is one of the major components of our food chain. Seafood can be divided into two groups, wild and commercial species. Commercial fishes normally grow under the care and in a special environment with a specific diet. Records have indicated that there are less amount of microplastics in the tissue of commercial fishes. But wild fishes feed from whatever they find in marine ecosystems. As it's mentioned previously, microplastics are small and float in waterbodies, so they look like easy prey for them. In this way, these particles enter the marine food chain and finally human food chain (Mercogliano et al., 2020). Figure 2.1 indicates this process.

There are many health risks associated with microplastics. It is believed that they can change DNA and cause genetic mutations, they can stop the normal functions of cells, and since they are toxic, they can cause poisoning (Vethaak and Legler, 2021).

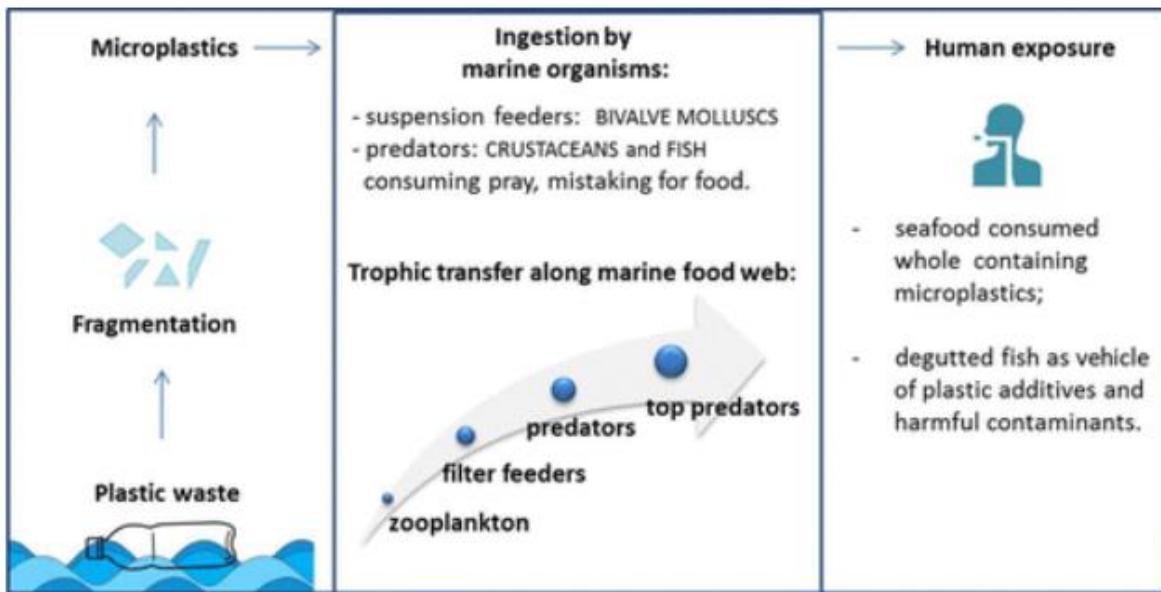


Figure 2.1: Microplastics entrance to human bodies (Mercogliano et al., 2020)

2.2 Different Pathways of Microplastics to Marine Environments

As illustrated previously, the existence of microplastics in marine environments is proven. In this part, various possible ways that microplastics can enter aquatic ecosystems will be discussed. Plastics are not created naturally, and they are man-made parts of this world. So the main sources of microplastics in the rivers and oceans are originally on land. According to previous studies, about 40 percent of microplastics in oceans originate from rivers, 40 percent are from human activities in coastal areas, and the remaining 20 percent come from maritime transportation (Liubartseva et al., 2016). Some of them have more effect than others. There is no doubt that sewer system discharges, urban wastes, and stormwater runoff are some of the most significant contributors to microplastic pollution. Combined sewer systems are designed to collect wastewater from residential and industrial sources as well as runoff from precipitation. Normally, they are disposed of in wastewater treatment plants where they are treated and many manholes are in their way. During storm or rain events, it is possible that the actual amount of wastewater in the system exceeds the design volume. Overflows from combined sewers are intended to divert this extra wastewater into nearby rivers. As a result of the high volume of chemical and biological processes in sewer and combined sewer systems, plastics turn into microplastics (Parizi, 2021). Most

detergents are made of different chains of polymers and they are widely used for cleaning indoor and outdoor spaces and finally, they will find a way to sewer systems (Bergmann et al., 2015). When people are driving on the roads, due to friction, it is possible that small parts of tires separate and remain in that area. Due to their light weight, a gentle wind is able to move them and cause them to enter the manholes (Campanale et al., 2022). Even small and large pieces of plastic that are thrown in the city can get into these systems. Based on previous studies, combined sewer overflows contains a huge amount of microplastic particles which is shown in Table 2.1.

Wastewater treatment plants are one of the most crucial components of water systems. The purpose of this section is to separate toxic and unhealthy substances and pollution through the application of various chemical, physical and biological processes. The aforementioned points regarding microplastics indicate that they are dangerous for human health and can cause a wide range of illnesses. Consequently, microplastics can be removed during two treatment processes, preliminary and primary treatment. In studies, it has been shown that a 35 to 59 percent cleanup of microplastic particles can be achieved through the first treatment and a 50 to 98 percent cleanup can be achieved through the second treatment. The separated particles are typically released into nearby rivers at most wastewater treatment plants. As a result, the discharge of wastewater treatment plants is one of the major sources of microplastics in waterbodies (Sun et al., 2019).

Table 2.1: Annual discharge and number of microplastics in different Combined Sewer Overflows (CSO) and Wastewater Treatment Plants (WWTP) based on previous studies (Parizi, 2021)

Site	MPs/m ³	Mesh size (µm)	Annual Discharge (Million m ³ /year)	Annual Discharge (Billion MPs/year)	Reference
Combined Sewer Overflow					
Vancouver, BC	1,833 - 13,673	50,200	1.43	10.2 - 14.6	Parizi , 2021
Paris, France	1.92 - 2.41 * 10 ⁵	80,300	21	4,027 - 5,051	Dris et al., 2015
Shanghai, China	1.1 - 97 * 10 ⁵	80,300	NR	110 - 22,000	Chen et al., 2020
Wastewater Treatment Plant					
Vancouver, BC	100 - 500	63	183.5	20 - 40	Gies et al, 2018
Paris, France	14,000 - 50,000	65,100	2.3	32.2 - 115	Dris et al., 2015
Shanghai, China	52,000	83,300	NR	143	Chen et al., 2020

2.3 Hydrodynamic Modeling

Identifying the accumulation zones of particles requires first understanding the behavior of rivers and their hydrodynamic parameters. So in this part, hydrodynamic modeling and studies related to that will be discussed.

It is critical to keep in mind that the number of dimensions in hydrodynamic modeling is a function of the situation and the level of detail expected from the model's results. In situations where energy waste is a concern, one-dimensional modeling is often employed. Modeling in two dimensions is used when the flow must be modeled in two perpendicular directions (normally X and Y). Typically, the velocity in the third direction is considered very low in comparison with the other two directions which can be ignored. It is possible to take into account the third dimension when vertical velocity plays a significant role. Compared to the other simulations, this one is a bit more expensive, but it helps to carry out more complicated calculations, such as turbulence intensity (Vouk, 2016).

2.3.1 Governing Equations

There are some simplified assumptions in this study, as well as in other similar studies. Firstly and most importantly, this thesis argues that water is a steady Newtonian liquid that cannot be compacted. As part of the study, Navier-Stokes equations are used to determine the velocity and depth of water at each point of the model based on various factors, including advection, pressure changes, tracers, diffusion, and several other factors (Vouk, 2016).

As a result, some equations are proposed for satisfying continuity control (to ensure that the input fluid matches the output fluid) and momentum control. The number of momentum equations is directly related to the number of spatial dimensions. As a result, in three-dimensional research, there will be one equation for continuity (Equation 1) and three equations for momentum in Cartesian coordinates in the X, Y, and Z directions (Equations 2, 3, and 4) (Gessler et al., 1999).

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (1)$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \quad (2)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) \quad (3)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + \nu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + g_z \left(\frac{\rho - \rho_0}{\rho} \right) \quad (4)$$

$$\frac{\partial p}{\partial z} = -\rho g \quad (5)$$

In these equations, x, y, and z show Cartesian coordinates, and u, v, and w indicate the velocity of the fluid in each X, Y, and Z direction. ρ represents density and ρ_0 is the reference density. Gravity and kinematic viscosity are shown with g and ν .

The pressure component is p which can be separated into two parts, first hydrostatic pressure and second hydrodynamic pressure. Equation 6 indicates the relation for calculating the pressure parameter (telemac3d_user_manual_V7P2).

$$p = p_{atm} + \rho_0 g (Z_s - z) + \rho_0 g \int_z^{Z_s} \frac{\Delta p}{\rho_0} dz + p_d \quad (6)$$

Atmospheric pressure is represented by p_{atm} and Z_s is used for free surface elevation. Δp represents the variation of density around the reference density and p_d shows dynamic pressure.

Density is a parameter that depends on different factors such as salinity and temperature. For instance, when the amount of salt in the fluid increases, the density of the fluid will increase, which will affect the behavior of the fluid and consequently the movement of particles within. Equations 7 and 8 are proposed to calculate the density by considering different tracers. Equation 7 is mostly

used when the tracers are only salinity and temperature and equation 8 is more general (telemac3d_user_manual_V7P2).

$$\rho = \rho_{ref} \left[1 - \left(T(T - T_{ref})^2 - 750S \right) 10^{-6} \right] \quad (7)$$

$$\rho = \rho_{ref} \left[1 - \sum_i \beta_i (T_i - T_i^0)_i \right] \quad (8)$$

T is temperature and T_{ref} is a symbol for reference temperature of the fluid which is 4°C, and reference density (ρ_{ref}) at reference temperature when salinity (S) is zero is equal to 999.972 kg/m³. Volumetric expansion coefficients are represented by β_i and T_i denotes different tracers. It is worthwhile to mention that equation 7 only works when the salinity is between 0 to 42 g/l, and the temperature is between 0 to 40 °C.

2.3.2 $k - \varepsilon$ Model

Calculating and modeling the turbulence with precision is a complex process. There are two proposed computational ways to overcome this. The most common solution is using statistical and experimental analysis in order to find the results of turbulence flow on the characteristics of the model. The second approach solves this complexity based only on the statistical analysis of information gathered from field data (Lane, 1998).

$k - \varepsilon$ model helps by finding the turbulent kinetic energy (k) and rate of dissipation of turbulent kinetic energy (ε) by solving equations 9 and 10.

$$\frac{\partial k}{\partial t} + u \frac{\partial k}{\partial x} + v \frac{\partial k}{\partial y} + w \frac{\partial k}{\partial z} = \frac{\partial}{\partial x} \left(\frac{v_t}{\sigma_k} \frac{\partial k}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{v_t}{\sigma_k} \frac{\partial k}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{v_t}{\sigma_k} \frac{\partial k}{\partial z} \right) + P - G - \varepsilon \quad (9)$$

$$\begin{aligned} \frac{\partial \varepsilon}{\partial t} + u \frac{\partial \varepsilon}{\partial x} + v \frac{\partial \varepsilon}{\partial y} + w \frac{\partial \varepsilon}{\partial z} &= \frac{\partial}{\partial x} \left(\frac{v_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{v_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{v_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial z} \right) \\ &+ C_{1\varepsilon} \frac{\varepsilon}{k} [P + (1 - C_{3\varepsilon})G] - C_{2\varepsilon} \frac{\varepsilon^2}{k} \end{aligned} \quad (10)$$

Where P is turbulent energy production term which can be calculated with equation 11.

$$P = v_t \left(\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i} \right) \frac{\partial \overline{U_i}}{\partial x_j} \quad (11)$$

and G is a source term due to the gravitational forces that can be calculated with equation 12.

$$G = - \frac{v_t}{Pr_t} \frac{g}{\rho} \frac{\partial \rho}{\partial z} \quad (12)$$

$$v_t = C_\mu \frac{k^2}{\varepsilon} \quad (13)$$

In equations 9, 10, 11, 12 and 13, C_μ , Pr_t , $C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{3\varepsilon}$, σ_k and σ_ε are constants which are equal to 0.09, 1, 1.44, 1.92, 0.4, 1 and 1.3 (Launder and Spalding, 1974).

2.3.3 Tracers' Equation

In the rivers, there are different tracers that can affect the characteristics of fluid (water), such as salinity, temperature, and even the effect of sediments, so it is imperative to track them (equation 14).

$$\frac{\partial T_c}{\partial t} + u \frac{\partial T_c}{\partial x} + v \frac{\partial T_c}{\partial y} + w \frac{\partial T_c}{\partial z} = \frac{\partial}{\partial x} \left(v_T \frac{\partial T_c}{\partial x} \right) + \frac{\partial}{\partial y} \left(v_T \frac{\partial T_c}{\partial y} \right) + \frac{\partial}{\partial z} \left(v_T \frac{\partial T_c}{\partial z} \right) + Q \quad (14)$$

Where T_c indicates the density of the tracer, v_T represents the coefficient for tracer diffusion and Q is the tracer sink.

2.3.4 Hydrodynamic models Examples

Solving these equations manually is challenging and in some cases impossible so researchers use different software to overcome this problem. In this part, various examples of hydrodynamic modeling are discussed.

A variety of software packages are available to create one-dimensional models, among which ONE-D which was developed by Environment Canada and MIKE 11 was designed by the Danish Hydraulic Institute are two of the most commonly utilized. Morse et al., 1991, used ONE-D-SED to determine the bed profile and track bed degradation of the Lower Fraser River from 1979 to 1984. Figure 2.2 shows a comparison between observed and model changes in the bed profile of the Fraser River. Mike 11 due to its ability to model runoff, water quality, and other factors, is more widely used. For example, UMA, 2000 used this software to model the flood profile of the Fraser River in order to decrease the risk of flooding in that area (Yusuf, 2001).

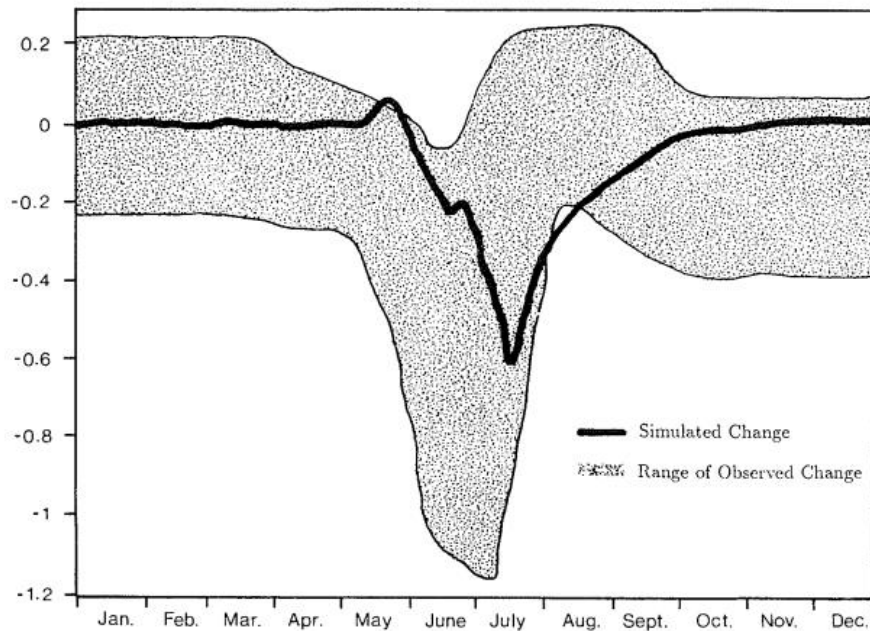


Figure 2.2: A comparison between modeled and field data (Morse et al., 1991)

Although one-dimensional models are good for describing flow in channels and pipes and their results are reliable, two-dimensional models require fewer assumptions and setup time, and it is obvious that the longer running time is more related to the additional details the model generates. Several packages like HEC-RAS 2D, TELEMAC 2D, MIKE 21, and RIVER 2D are used for 2D modeling. Some of them are free and some of them are for commercial purposes (Chen, 2022).

Yusuf, 2001 simulated 13 kilometers of the lower part of the Fraser River with RIVER 2D which was developed by the University of Alberta, in order to find out the advantages and disadvantages of a 2D depth-averaged model. Also, by modeling the gravel reach of the Fraser River calculated the local velocities and erosions in that area.

Chen 2022 used TELEMAC 2D which was designed by Electricity de France, software that allows the user to add hydrologic parameters to the model. This was done to test the software's effectiveness in simulating the runoff result of rain during pluvial flooding in an urban area in the west of Africa. Figure 2.3 shows the results of TELEMAC 2D at different times in this research.

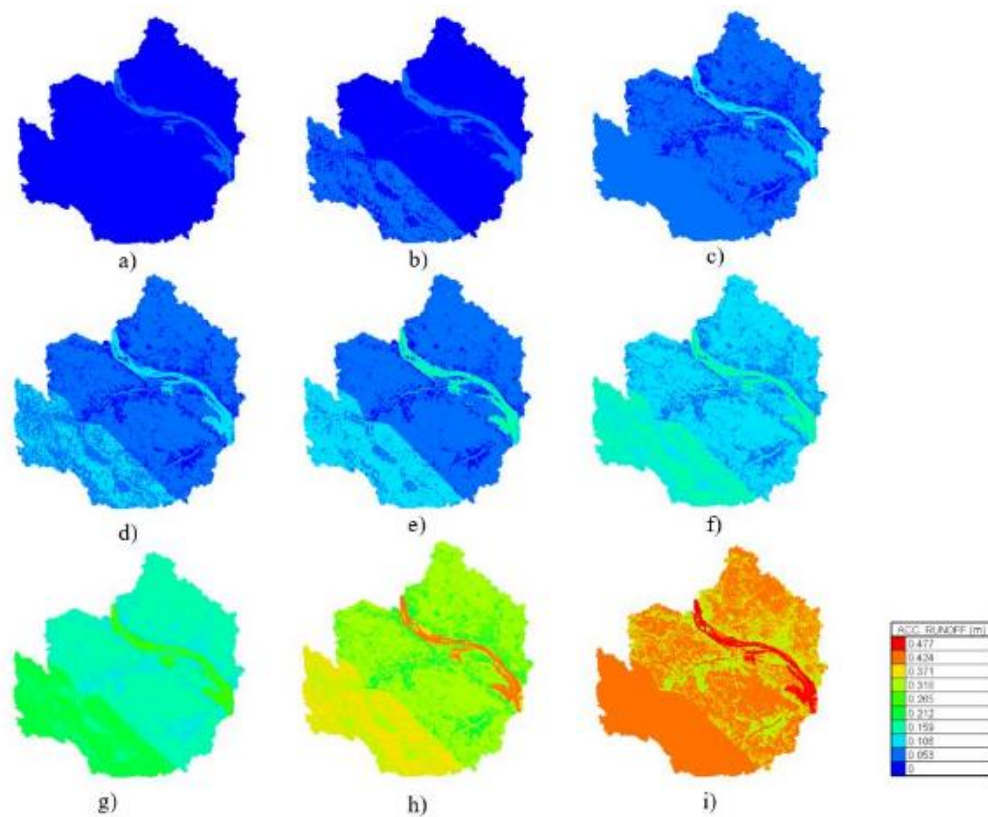


Figure 2.3: Accumulated runoff at a) 7 days, b) 14 days, c) 21 days, d) 28 days, e) 35 days, f) 42 days, g) 49 days, h) 56 days, i) 62 days (Chen 2022)

To predict the flow, salinity, and water level of the Hau River in Vietnam from 2036 to 2065, a combination of one-dimensional and two-dimensional models with MIIKE 11 and MIKE 21 were used. Mike 11 calculated the water level and rainfall as an input for MIKE 22 to estimate the velocity and salinity of the river which is a huge problem in that area (Duong et al., 2018). Figure 2.4 shows the predicted salinity of the Hau River.

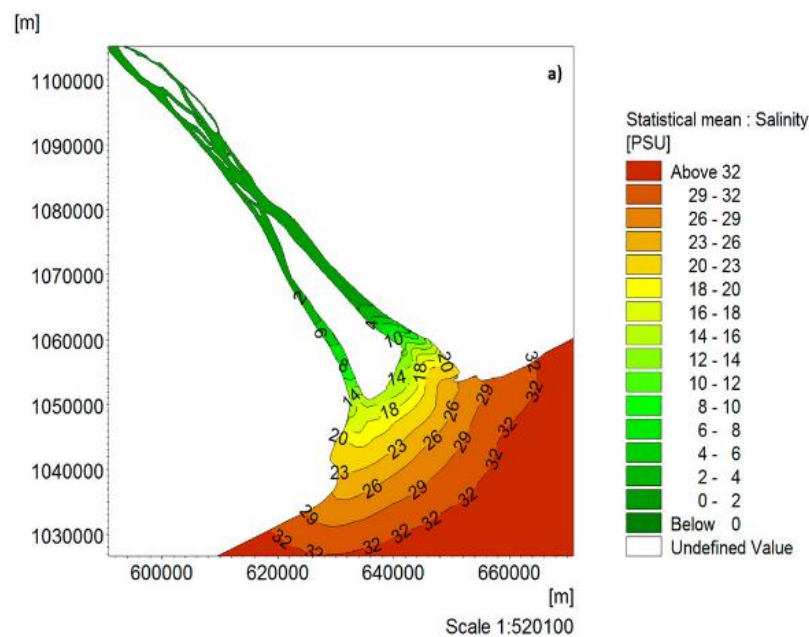


Figure 2.4: The modeled salinity of the Hau River (Duong et al., 2018)

Due to the complexity, computational time, and costs of three-dimensional modeling, there is relatively little research in this area.

Vouk, 2016 compared the results of her three-dimensional model of the Ottawa River with field data. She simulated the mixing and transport of Ammonia discharged to the Ottawa River from wastewater treatment plants with FLOW 3D which was developed by Flow Science Inc, USA. The results of the model and experimental data showed that even though the concentration of Ammonia in the discharge location adhered to regulations, it was still possible that the concentration of Ammonia in downstream was higher than allowed.

The Fraser River is one of the biggest sources of fresh water in Canada, so it is critical to evaluate the quality of water in that area. This river is bordered by several large cities, such as Vancouver,

which can contaminate it with their wastewater treatment plant discharges as well as combined sewer overflows. In a part of the Fraser River, saline water of the ocean is mixed with the freshwater of the river as a result of the tide. Consequently, the density of the water will be affected. MIKE3 FM which was developed by the Danish hydraulic institute was used to understand the results of the aforementioned discharges on the lower part of Fraser river (Masoom and Gu, 2018). Figure 2.5 is a schematic view of a mixture of salty and fresh water. Figure 2.6 displays the predicted salinity in the Fraser River by the three-dimensional model.

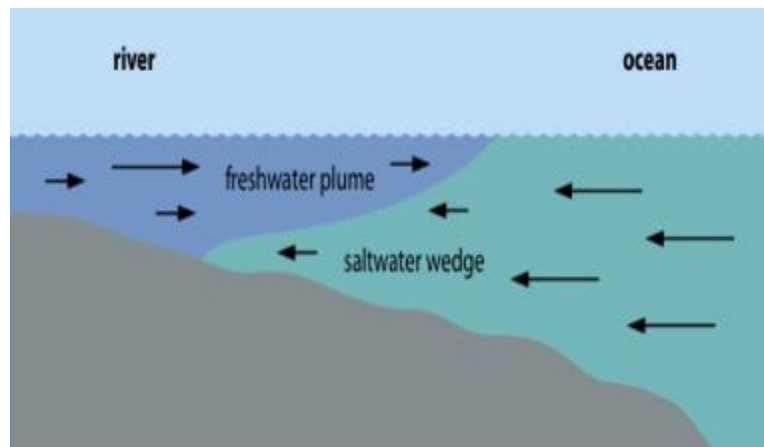


Figure 2.5: Mixture of the water of ocean and river during a rising tide (Masoom and Gu, 2018)

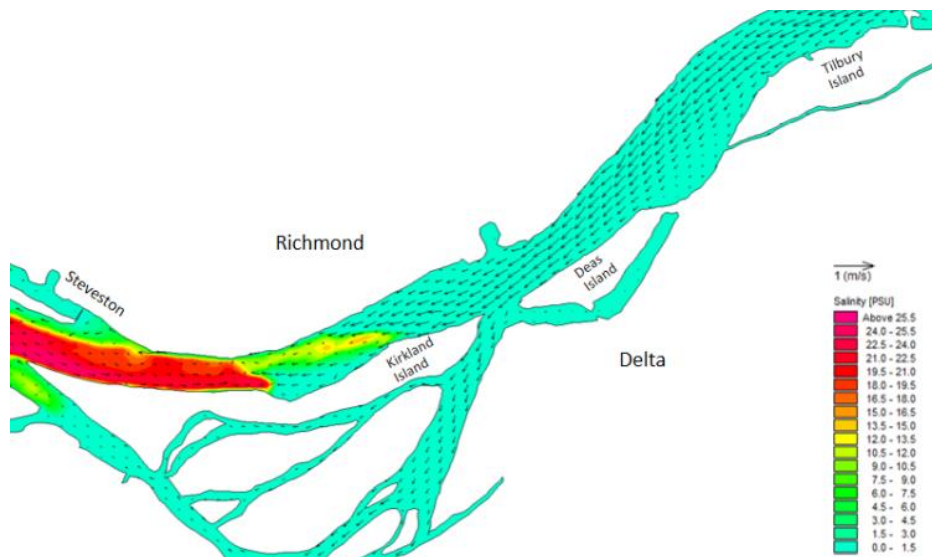


Figure 2.6: Modeled salinity in a part of the Fraser River (Masoom and Gu, 2018)

Different characteristics of water can affect the growth and birth ratio of bacteria, so a three-dimensional model of Swansea Bay which is located in the south-west of the UK was created by TELEMAC 3D to track the movement of bacteria and predict the salinity, temperature, and solar radiation in that location. Now it is possible to calculate all the mentioned ratios based on the biological equations of bacteria (Lam and Ahmadian, 2022).

2.4 Particle Tracking Model

The particle tracking model uses the results of the hydrodynamic model such as velocity, eddy viscosity, and water level at each time step to predict the behavior of released particles and their location. In this part, different studies of particle tracking models will be discussed.

The movement of particles in waterbodies is the result of advection and diffusion. Advection is the movement of particles through the bulk of a fluid due to the velocity of that fluid as predicted by a hydrodynamic model. Kinetic energy is responsible for Brownian movement which causes diffusion. Normally molecules prefer to move from a higher concentration area to a lower concentration area. So the transport of particles can be described by equation 15 which considers advection and diffusion (Pilechi et al., 2022).

$$\frac{\partial C}{\partial t} = \nabla \cdot (CU) + \nabla \cdot (K \nabla C) + \rho(C) \quad (15)$$

Where C represents the concentration at time t, U indicates the velocity of the fluid, K is the diffusion coefficient and the reaction function is shown with $\rho(C)$.

There are two approaches that can be used for tracking microplastic particles in the aquatic environment. The first one is the Eulerian method which evaluates advection and diffusion for each computational node of the model while the second approach, the Lagrangian method, follows the transport of particles individually. Also, it is possible to use a combination of these two methods. On the other hand, based on the aforementioned explanations, the Lagrangian method requires fewer equations (Bigdeli et al, 2022).

It is possible to assume that particles remain on the surface of the water without any vertical movement, and in this situation two-dimensional approaches can be used, but in reality, due to the

density of some of the particles, tidal currents, and vertical mixing processes, there are some vertical movements which three-dimensional approaches can consider (Jalón-Rojas et al., 2019).

The output of the hydrodynamic model has information at each node of the computational mesh. There are, however, times when particles are not located exactly on the nodes, so parameters for their location should be extracted. Equation 16 and figure 2.7 can be used to calculate the value of any parameter at the location of the particle (B_p) by using the Inverse Distance Weighted method. B_i represents the value of that parameter at each of the vertices of the triangular prism and a_i is the distance of that particle from each of those vertices (Chen et al., 2015).

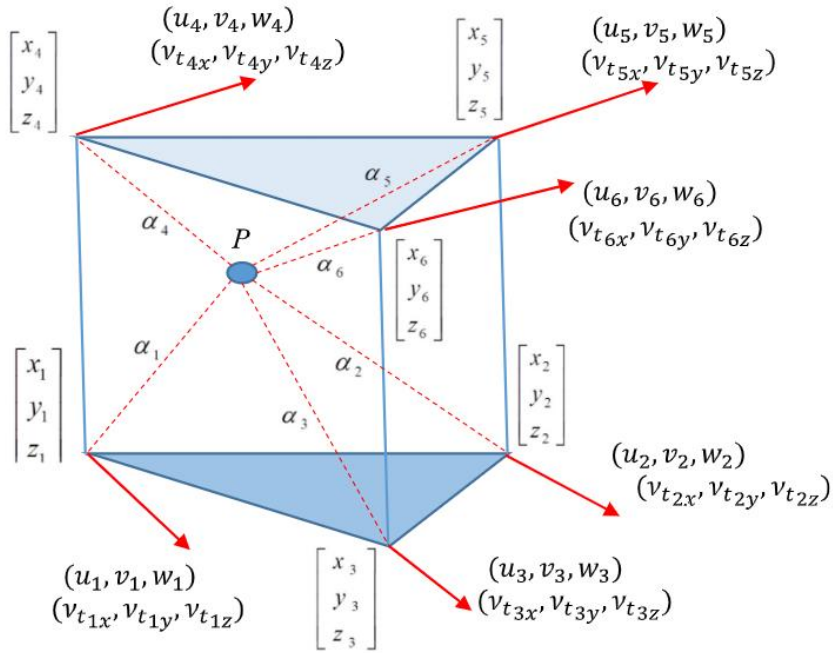


Figure 2.7: Triangular prism element of the base mesh (Pilechi et al., 2022)

$$B_p = \sum_{i=1}^6 \frac{1}{a_i} B_i \bigg/ \sum_{i=1}^6 \frac{1}{a_i} \quad (16)$$

For a particle with a settling velocity of V_s at time step n in the location of x_1 , the particle tracking model by applying advection and diffusion on that will find the location of the particle (x_2) at the next time step $n+1$. A three-dimensional model solves equations 17, 18, and 19 for this purpose (Jalón-Rojas et al., 2019).

$$x_2 = x_1 + u_p \times \Delta t + Diff \quad (17)$$

$$y_2 = y_1 + v_p \times \Delta t + Diff \quad (18)$$

$$z_2 = z_1 + w_p \times \Delta t - V_s \times \Delta t + Diff \quad (19)$$

$$\Delta t = t_2 - t_1 \quad (20)$$

While x_2, y_2 , and z_2 indicate the locations of the particles at time step n+1 in Cartesian directions, x_1, y_1 , and z_1 are the initial locations of them at time step n. u_p, v_p , and w_p represent the velocity of particles in each of the Cartesian directions and V_s is settling velocity which are used for computing the movement caused by advection. By solving equilibrium equations for forces acting on a particle in a fluid environment, Dellino et al., 2005 found equation 21 to calculate settling velocity. t_2 and t_1 are the time values at time steps n+1 and n. Turbulence is responsible for diffusion which is shown by Diff in the above equation. To calculate Diff, Hunter et al., 1993 used a Random Walk Particle Tracking model (equation 22).

$$V_s = \sqrt{\frac{4gd(\rho_p - \rho)}{3C_d\rho}} \quad (21)$$

$$Diff = R\sqrt{2K(t_2 - t_1)} \quad (22)$$

In equation 21, d represents the diameter of the particle, ρ_p is the density of the particle, ρ is the density of the fluid (water), and C_d is the drag coefficient. In this study, spherical microplastic particles are used. Van Melkebeke et al., 2020 offered to use equation 23 for calculating the drag coefficient of spherical particles. In equation 22, K is a diffusion coefficient which is assumed to be constant in time and space, and R is a random number with a normal distribution which is between -1 and 1.

$$C_d = \frac{24}{Re_p} \left(\frac{1 - \psi}{Re_p} + 1 \right)^{0.25} + \frac{24}{Re_p} (0.1806 Re_p^{0.6459}) \psi^{-Re_p^{0.08}} + \frac{0.4251}{1 + \frac{6880.95}{Re_p} \psi^{5.05}} \quad (23)$$

Where ψ is the particle shape factor, which is 1 when the particle is spheres. Re_p is the particle Reynolds number that is between 0.03 and 10^4 (Dioguardi et al., 2018).

2.4.1 Particle Tracking Examples

Particle tracking is about locating thousands of particles at many time steps for a long period of time, so solving the aforementioned equations in this situation is somehow impossible. As a result researchers use different simulation tools to track the movements of particles under different circumstances. In this part, some of them are explained.

PELETS 2D is an offline tool that was developed at the HelmHoltz-Zentrum Geesthacht, and solves the particle tracking equations in a Lagrangian system. This software was used to release various particles into the Southern North Sea from different sources between 2000 and 2008. A time step of 28 hours and hourly wind data were used in this model to understand the effect of wind on the transport of particles. This two-dimensional model tracks the movements of particles on the sea surface which increases the effect of wind. Figure 2.8 shows the results of the model for the entire period of the simulation. The role of wind in the transport of particles is obvious (Neumann et al., 2014).

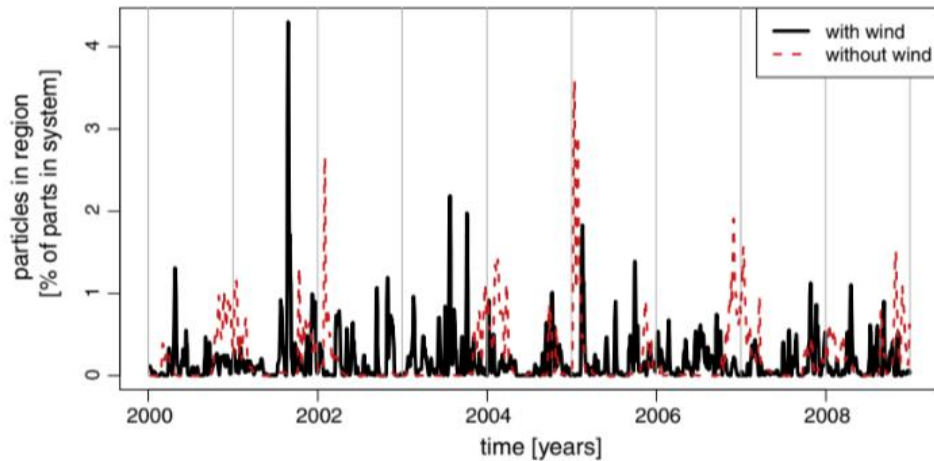


Figure 2.8: The effect of wind on particle transport (Neumann et al., 2014)

Sousa et al 2021, implemented Delft3D-Flow which was developed by Deltares and solves nonlinear shallow water equations to simulate the hydrodynamic model of Ria de Vigo in Spain. Salinity and temperature are two tracers that were considered in this model. The output of Delft3D-Flow was used as input for Delft3D-PART which simulates the transport of particles. Particles were released from 7 locations under four tidal conditions, the beginning of ebb spring and neap tides and the beginning of flood spring and neap tides. Information about different scenarios is indicated in table 2.2. The locations of the release of the particles were chosen based on the locations of wastewater treatment plants in that area, since their discharge contains a large amount of microplastic particles. The peak flow in each of the locations indicates the number of released particles under each scenario. Finally, the concentration of particles in 61 locations which were measured by field experiment, were compared with the results of the model. Figure 2.9 displays the spread of microplastic particles in the study area and figure 2.10 shows a comparison between observed and modeled data (Sousa et al., 2021).

Table 2.2: Scenario's details (Sousa et al., 2021)

Scenario	Release Method	Release Period (days)	Number of particles per release per point ($\times 10^3$)						
			Vigo	Teis	Redondela	Souto Maior	Vilaboa	Moana	cangas
1	Continuous	30	150	6.5	6.25	1	1.27	15	12.5
2	Continuous	30	400	-	-	-	-	-	-
3	Continuous	30	400	6.5	6.25	1	1.27	15	12.5
4	Instantaneous	-	400	-	-	-	-	-	-

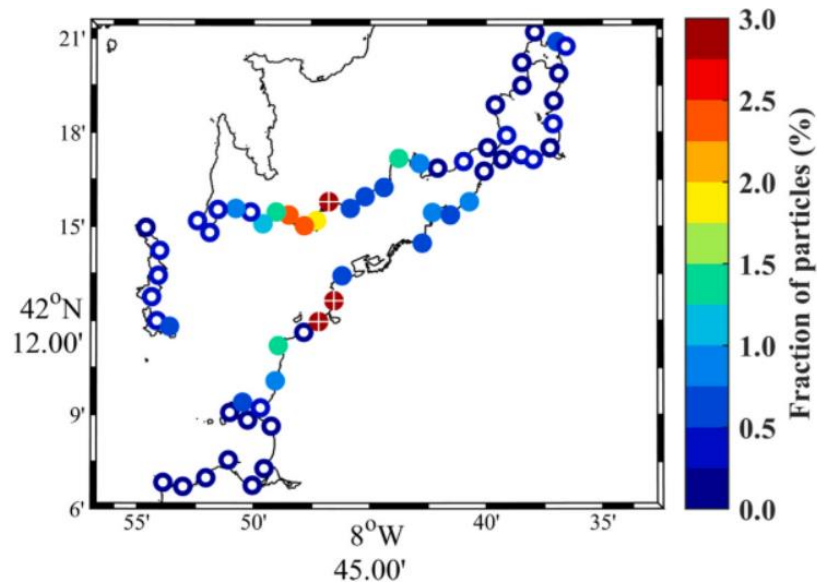


Figure 2.9: Dispersion of microplastics (results of the Delft3D-PART model), empty dots indicate values smaller than 0.5% and crosses in red dots indicate values higher than 2.5% (Sousa et al., 2021)

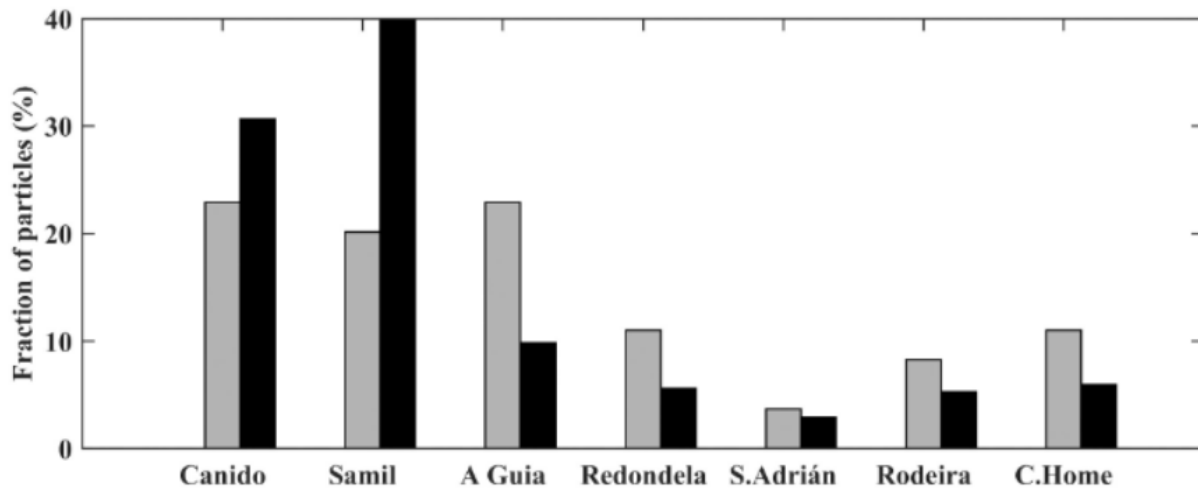


Figure 2.10: Comparison between results of the model and field data at seven locations (Sousa et al., 2021)

Plastic pollution is an increasing concern in South Africa. Due to biofouling caused by temperature, salinity, and radiations from the sun in that area, plastics change to microplastics. As a result, Ichthyop, a Java-based program that was developed by Phillippe Verley from the ROMS

model (Lett et al., 2008), was used to model the fate and transport of microplastic particles in South Africa. Thus, it is possible to find their pathways and accumulation zones, which can help to support the surrounding environment. It is worthwhile to mention that Ichthyop is a free Lagrangian software that initially was used for understanding the dynamic environmental factors on ichthyoplankton, however, it is now being used for tracking the movements of microplastics. In this study, two tracers were considered, salinity and temperature. The density, shape, and size of the particles directly affect the horizontal and vertical velocity of particles. High-density microplastic particles with a density of $\rho = 1.38 \text{ g/cm}^3$ which represent Poly-ethylene terephthalate and Polyvinyl chloride, and low-density microplastic particles with a density of $\rho = 0.92 \text{ g/cm}^3$ which represent Poly-ethylene plastics were used in this study. Considering that the density of water is $\rho = 1.025 \text{ g/cm}^3$, low-density particles will remain on the surface or near the surface, while high-density particles will sink. There are five beaches around the study area that are used for industrial and urban purposes. They considered five release locations. From 2000 to 2010, 10,000 particles were released on the first of January of every year. To find the accumulation zones of microplastic particles equation 24 was used (Collins and Hermes, 2019).

$$TAF(x, y) = c(x, y) \times N/C \quad (24)$$

TAF indicates the tracer accumulation factor, and $c(x, y)$ is the number of particles per grid cell. N represents the number of grid points which is equal to $410 * 365$, and C is the total number of particles that were released (100,000). Figure 2.11 displays the TAF at different locations of the study area for low and high-density particles after one and ten years.

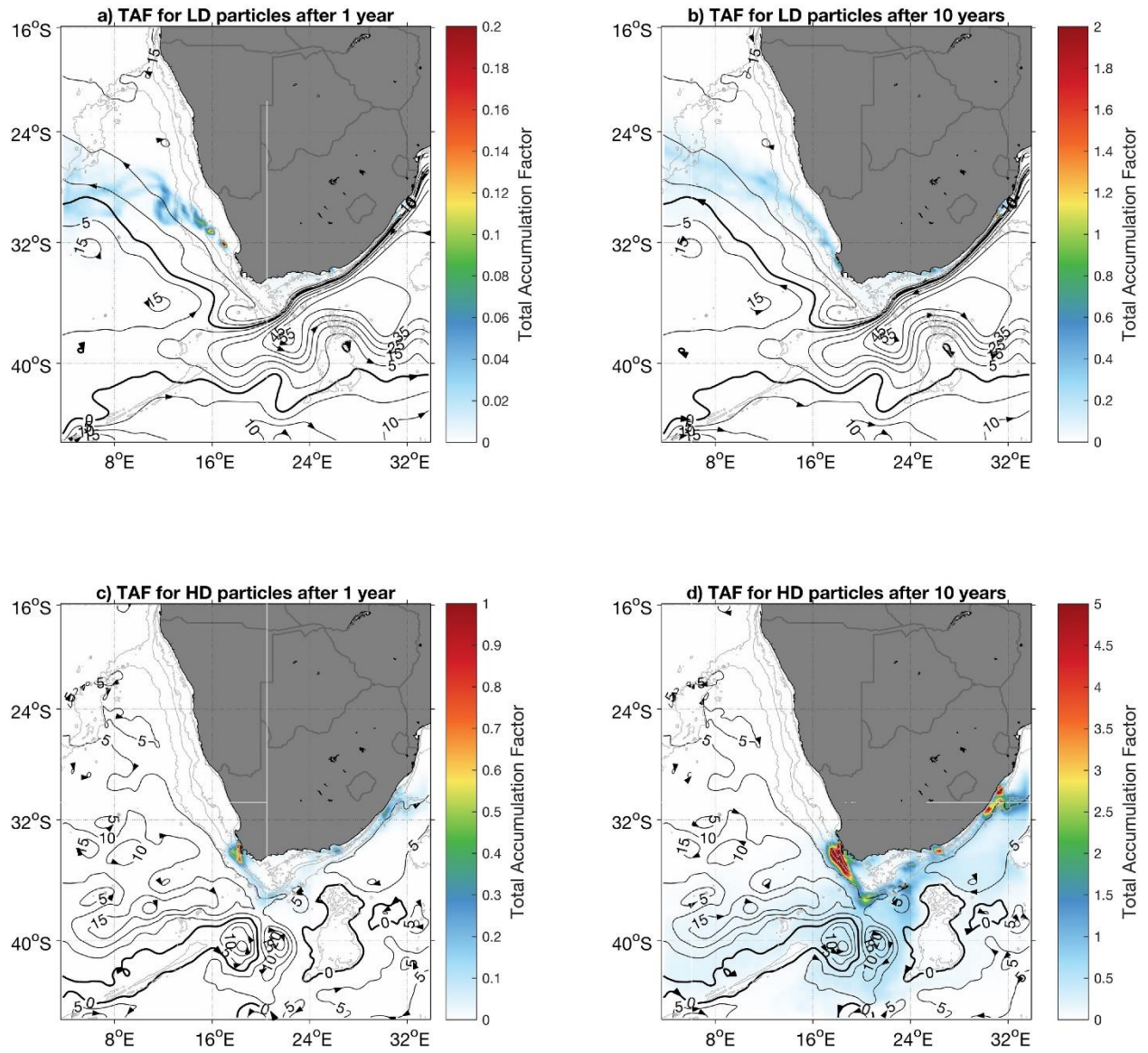


Figure 2.11: TAF in South Africa (Collins and Hermes, 2019)

In previous parts of this chapter, tires of transportation vehicles were discussed as a source of microplastics in roads and urban runoffs. The Gota River in south-west Sweden was chosen for this study since it is the largest river in Sweden and passes through one of the biggest cities in Sweden, Gothenburg. MIKE 3 FM was used to simulate a three-dimensional hydrodynamic model of the Gota River. Salinity, temperature, and wind were considered in this study. The length of the elements of the horizontal mesh varied between 20 to 30 m, and vertical layers were 1 m. To track

the microplastic particles through the river a water quality module, named ECO LAB was implemented. The locations of 21 stormwater discharges into the Gota River were considered as release locations. The particles that are the result of rubbing the tire on asphalt, mostly are cylindrical or spindle-shaped and denser than water. Also in this study, it is assumed that particles do not have any initial velocity and their movements are the result of current and settling velocity and diffusion. One of the study locations had its microplastic discharge measured in another study, and the microplastic discharge of the other study locations was calculated based on their flow and annual average daily traffic. The model was simulated under three scenarios, with settling velocity (1.3×10^{-4} and 2.4×10^{-3} m/s) and without settling velocity. The settling velocity was calculated using equation 25 and all of the particles were released on the surface of the water. Based on the results of the model, it was concluded that particles accumulated mostly on the southern side of the river, which makes sense given the large annual average daily traffic. Also, the transport of smaller particles with less density is easier than bigger particles with higher density (Bondelind et al., 2020).

$$v_s = \frac{gd^2(\rho_p - \rho_w)}{18\nu\rho_w} \quad (25)$$

v_s is settling velocity, g is the acceleration of gravity, d is the diameter of the particle, ρ_p is the density of the particle, ρ_w is the density of water, and ν is the kinematic viscosity of water.

Figure 2.12 and 2.13 shows the concentration of microplastics in the study area based on the results of the model with and without settling velocity.

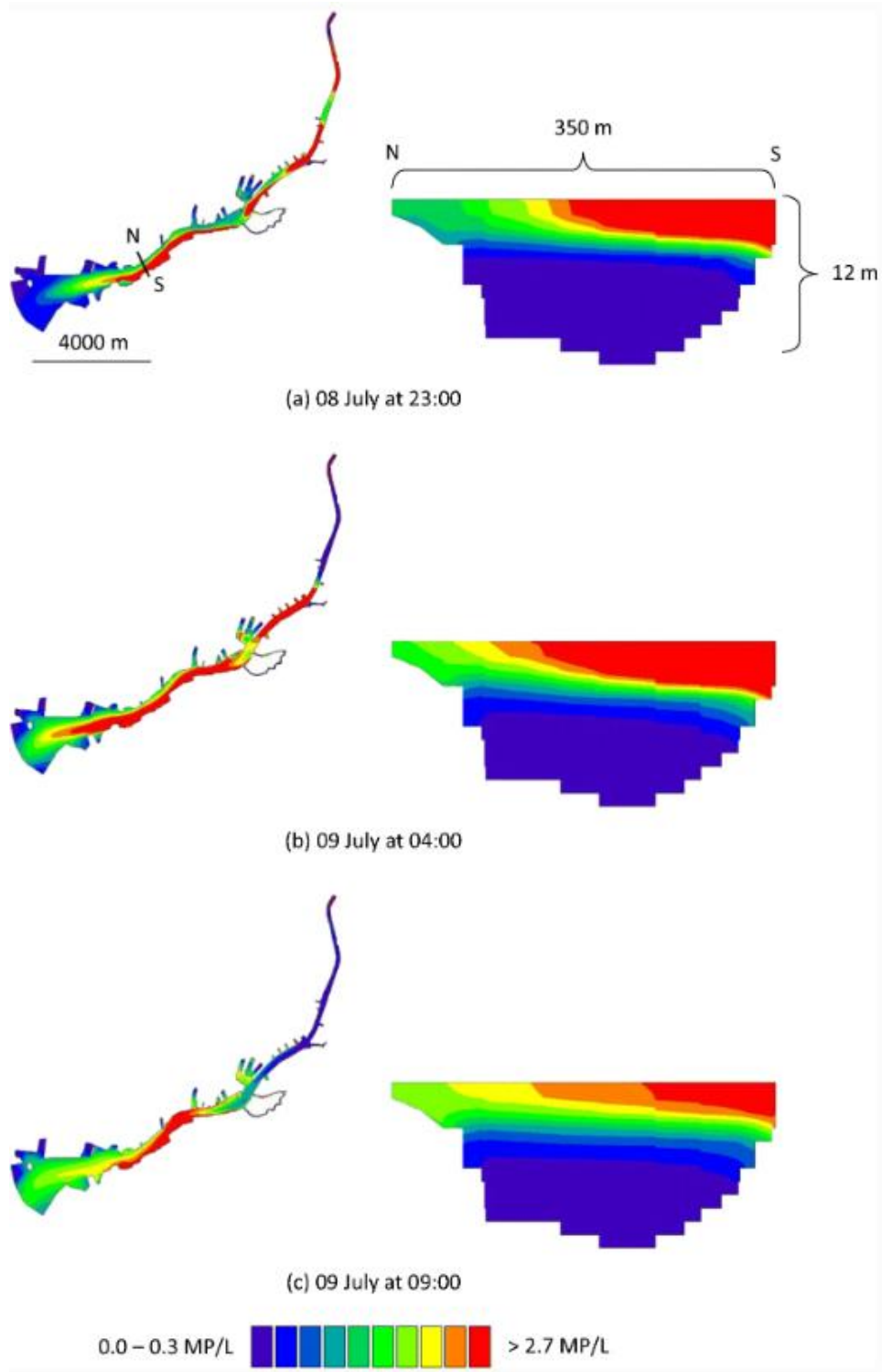


Figure 2.12: The result of the model at three different times without settling velocity (Bondelind et al., 2020)

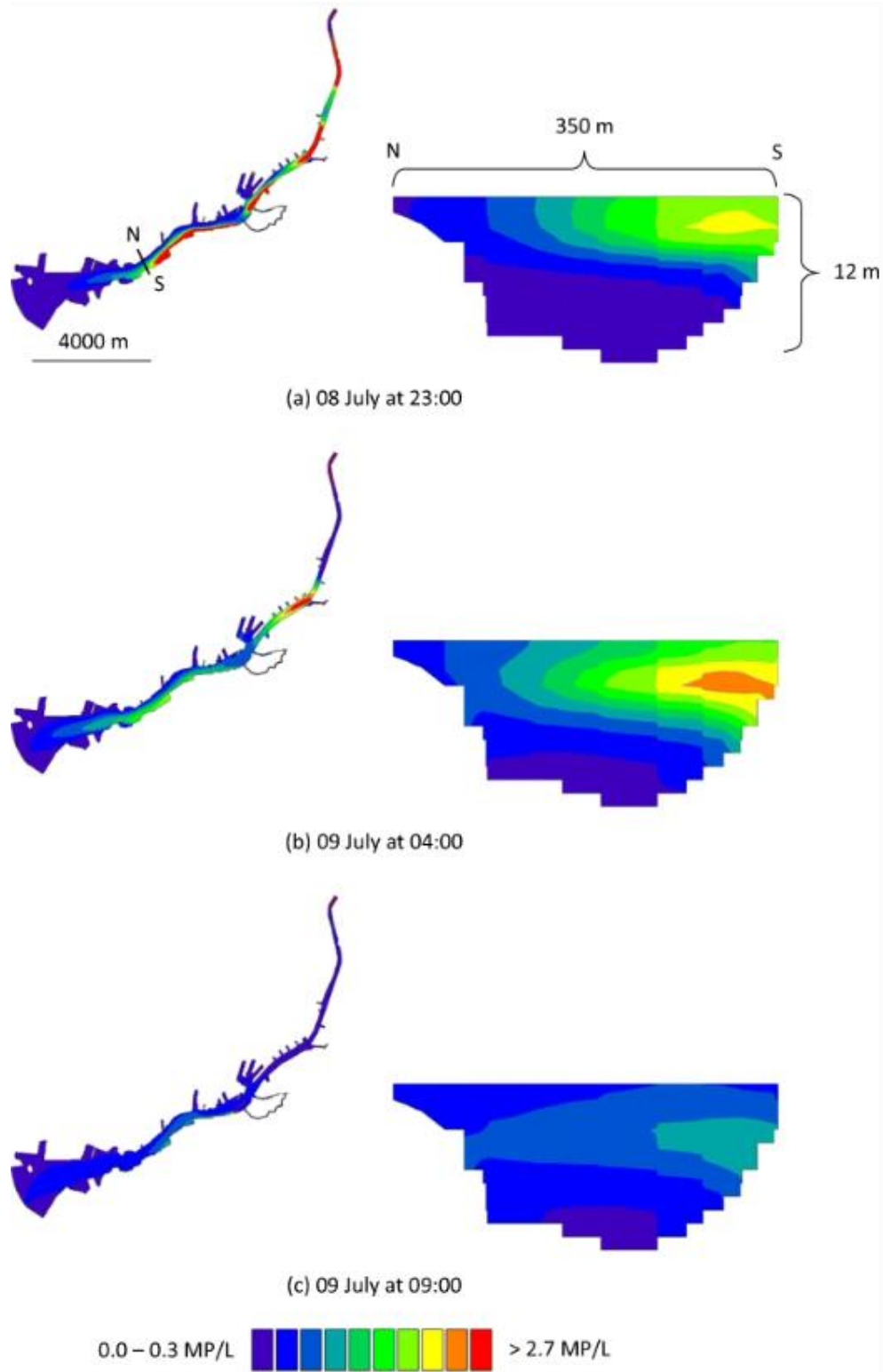


Figure 2.13: The result of the model at three different times with settling velocity ($1.3 \times 10^{-4} \text{ m/s}$) (Bondelind et al., 2020)

Adour Estuary, SW in France is forced by tidal rise, which affects the vertical movement of microplastic particles. Based on previous studies, the most common shapes of microplastic particles in that area are films and fragments. Defontaine et al., 2020 studied the effect of size, density, and river flow conditions in that area. The hydrodynamic part was modeled using TELEMAC 3D. The resolution of the base mesh varied between 30 m in narrow parts to 2000 m in the ocean which was created with Bluekenue which was developed by National Research Council of Canada. The hydrodynamic model consists of 20 vertical layers. Three scenarios were considered based on the type of microplastic particles. Each scenario was simulated twice, once for high flow condition and once for low-flow condition. In table 2.3, three scenarios are presented. Particles were released from a single location for 15 minutes. The results revealed that the physical characteristics of microplastic particles and the tidal situation significantly influence the location of particles vertically and, consequently, horizontally. The velocity near the surface is higher than at the bottom. Therefore, when particles are lighter than water they stay on the surface and move faster but as much as they get denser they move slower and consequently they settle. The concentration of microplastics in the study area based on the results of the model is shown for four control points in figures 2.14 and 2.15. These control points are located at the mouth of the river (C_1), near the source point (C_2), and two points in the upstream of Nive River and Adour River which feed Adour Estuary (C_3 and C_4). C_4 is before C_2 and C_3 is after C_2 . Based on these two figures, particle movement during the high-flow period is greater than during the low-flow period, therefore particles have less time to accumulate. Figs 14 and 15 S2 show that particles settle faster when the settling velocity is higher, and even these particles do not reach the mouth of the river. When the density is higher than water but the settling velocity is low particles exist in all vertical layers of the river and as a result, they spread better just like S1 in figures 14 and 15.

Table 2.3: Different scenarios (Defontaine et al., 2020)

Name of Scenario	Mean Diameter (mm)	Density (g/cm^3)	Settling Velocity (mm/s)	Representative of
S1	0.5	1.05	4	Polystyrene
S2	4.9	1.13	127	Polycaprolactone
S3	3	1	0	Ideal Particle

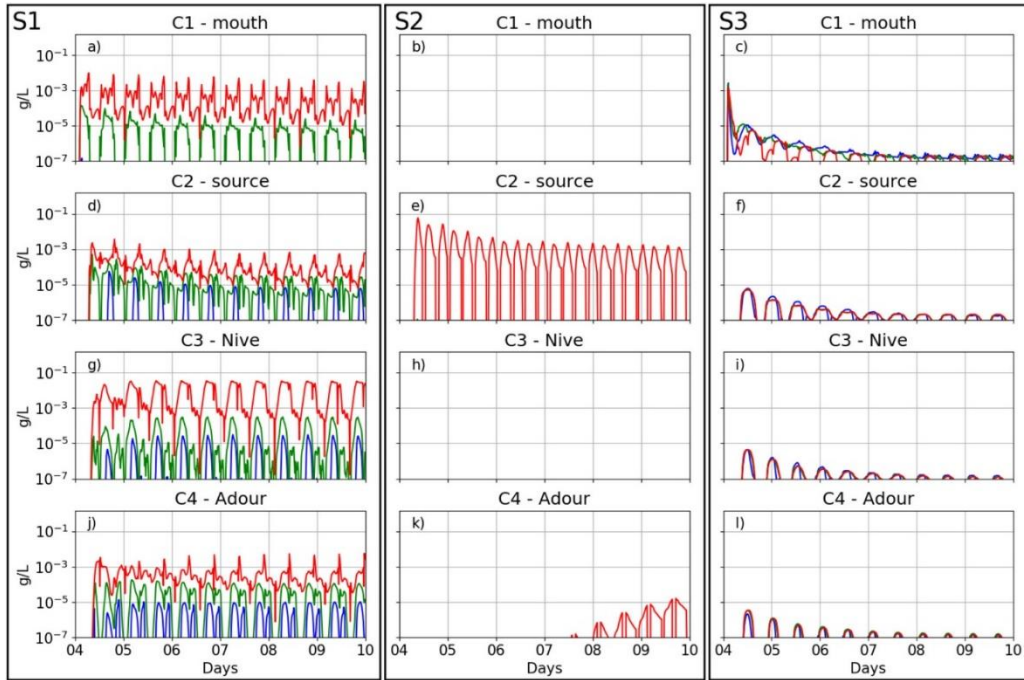


Figure 2.14: Results of the model at four control points during low-flow condition (blue lines indicate surface, green lines indicate middle and red lines indicate bottom, the vertical axis shows the concentration of microplastics) (Defontaine et al., 2020)

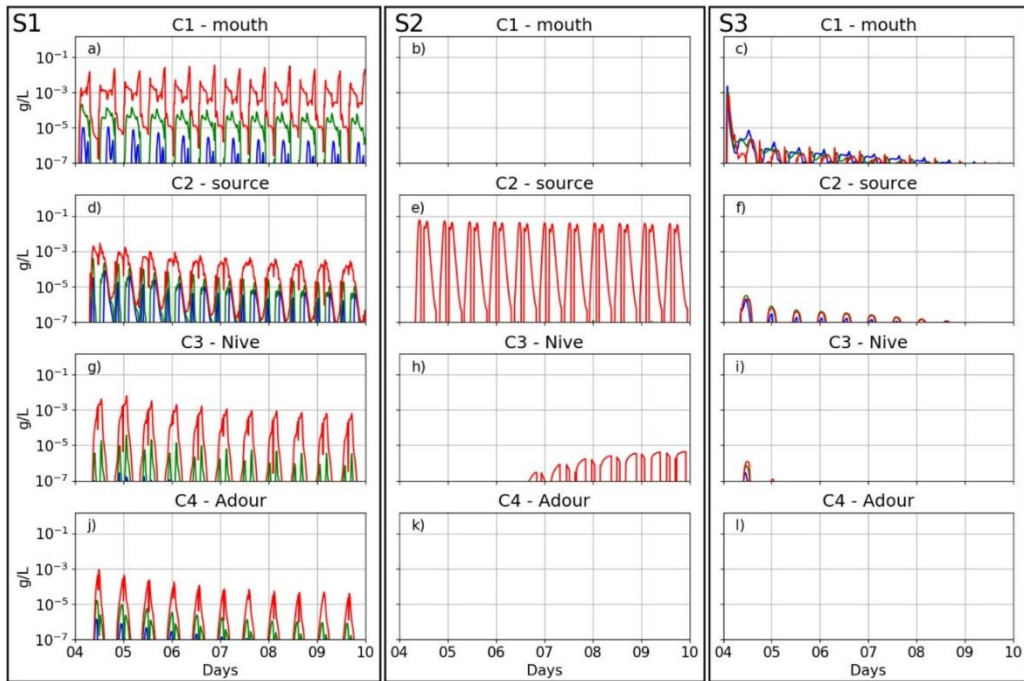


Figure 2.15: Results of the model at four control points during high-flow condition (blue lines indicate surface, green lines indicate middle and red lines indicate bottom, the vertical axis shows the concentration of microplastics) (Defontaine et al., 2020)

Canadian Microplastic Simulation (CaMPSim-3D) was developed by the National Research Council of Canada in collaboration with the University of Ottawa. CaMPSim-3D is a three-dimensional model that tracks the transport of particles in an Eulerian-Lagrangian system. There are different parameters that affect the movement of particles in this model such as density, size, shape, positive or negative buoyancy, and biofouling. This model follows 4 steps to find the final location of particles: 1) Point location, 2) Interpolation, 3) Advection and dispersion, and 4) Transformation (Pilechi et al., 2022). The equations of this model are mentioned in the first part of the Particle Tracking Model, in this study. This model is the particle tracking model that was used in this study.

2.5 Artificial Intelligence

Intelligence determines how to achieve goals and targets. Intelligence is a benefit to humans, animals, and even machines. The science that helps machines move through this intelligence process is called Artificial Intelligence (McCarthy, 2007). The ability of a machine to learn from input data with computational methods and produce an algorithm to find a relation between input and output data is called machine learning (Zhou, 2021).

The first attempt at machine learning techniques in a modern way was done by a psychologist named Frank Rosenblatt from Cornell University. He was working on the nervous system of humans. He designed a machine that worked very similar to the nervous system of humans to understand letters from the alphabet Rosenblatt (Fradkov, 2020).

Machine learning is currently used in different parts of our daily lives like playing games, speech recognition, understanding natural language, computer vision, expert systems, and heuristic classification (McCarthy, 2007).

Machines learn algorithms from input data. However, depending on the label and type of data, the algorithm used can be different. Machine learning algorithms can be divided into various categories such as supervised learning, unsupervised learning, semi-supervised learning, reinforcement learning, multi-task learning, ensemble learning, neural networks, and instance-based learning. In all the groups except unsupervised learning data have labels and algorithms try to find a relation between input data and their labels and predict the labels for new input data. But

in unsupervised learning models are implemented to produce labels for input data (Mahesh, 2019). For further information about each algorithm, please refer to Mahesh, 2019.

In learning algorithms (except unsupervised learning), training datasets are used to train the model. Data sets for training are part of the input data so that the machine can find the rules. The input data can be split into a training dataset and a test dataset. The common ratio for this division is 66 percent. Test datasets are used for evaluating the accuracy of the model (Berry and Mohamed, 2020). Figure 2.16 displays how learning algorithms work.

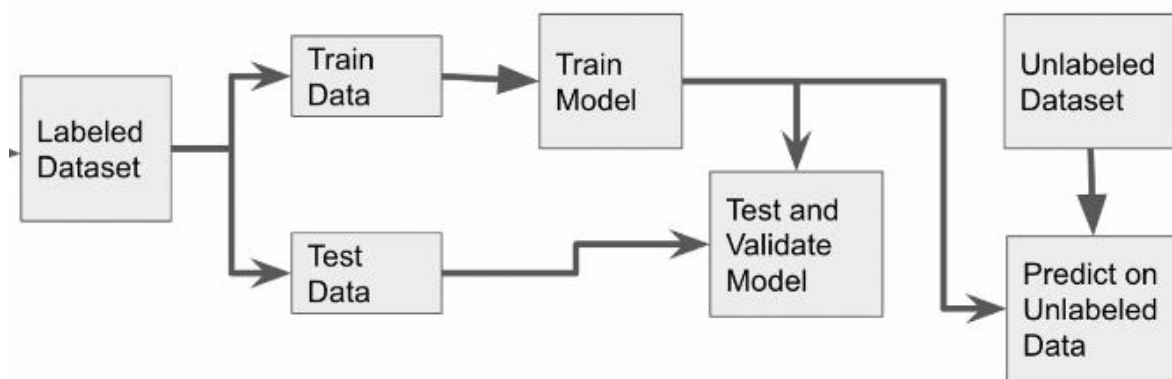


Figure 2.16: Learning algorithms process (<https://arshren.medium.com/supervised-unsupervised-and-reinforcement-learning-245b59709f68>)

The majority of unsupervised algorithms are clustering algorithms. In clustering algorithms, different methods are used for labeling input data by relying on distance factors. Different parameters such as the number of input data and the clustering method can indicate which algorithm should be used. The main clustering algorithms are hierarchical algorithms, centroid-based algorithms, and density-based algorithms. Two other minor groups of clustering algorithms are distribution-based algorithms and grid-based algorithms (Vanesschi and Silva, 2023).

In the rest parts, the three most common clustering algorithms will be discussed.

2.5.1 K-Means Clustering Algorithm

This algorithm is one of the easiest to use and has solved many problems. In the K-Means algorithm, all input data will be assigned to one of the n clusters. Initially, the user should enter the number of clusters (n), and then n random center points will be chosen. The bisector line between the center points will indicate the initial clusters. This time based on the locations of the

points in each cluster, the center point will be indicated and the process will be repeated until the main center points and clusters are found (Vanesschi and Silva, 2023). Figure 2.17 shows a schematic view of the K-Means clustering algorithm.

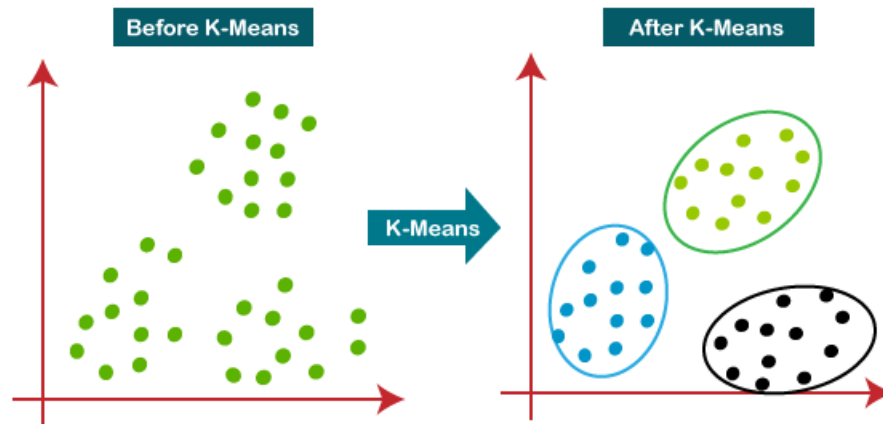


Figure 2.17: A schematic view of the K-Means clustering algorithm

(<https://www.javatpoint.com/k-means-clustering-algorithm-in-machine-learning>)

K-Means algorithms are mostly used in vector quantization, cluster analysis, and feature learning (Ikotun et al., 2023). One weakness of this algorithm is that it clusters all the points.

Banjarmasin is the capital city of one of the biggest provinces in Indonesia. There are various urban and industrial activities near the Banjarmasin River. Based on previous studies the water quality in this river has deteriorated significantly. Machine learning technique and more specifically K-Means algorithm was used to classify 40 control points in this river based on different parameters such as Biological Oxygen Demand (BOD), Chemical Oxygen Demand (COD), Total Suspended Solid (TSS), and Dissolved Oxygen (DO). Depending on the intensity of pollution in those control points they were labeled as heavily polluted, moderately polluted, lightly polluted, and not polluted (Zubaidah et al., 2018).

The Heihe River Basin in Northwest China has a key role in the ecological situation and climate change of the surrounding area. There are harmful winds, water shortages, and soil erosion in this region, so how water is distributed and managed is vital. Chen et al., 2016 clustered the Heihe River and its watershed into 3 main groups based on their resistance to mentioned annihilator factors I for the wind resistance group, II for water conservation areas, and III for soil conservation

areas, and 8 secondary groups I1, I2, I3, and I4 based on desert distribution, II1 and II2 based on soil texture and landform type and III1 and III2 based on land use type. To achieve this goal K-Means algorithm was used. The results are shown in figure 2.18.

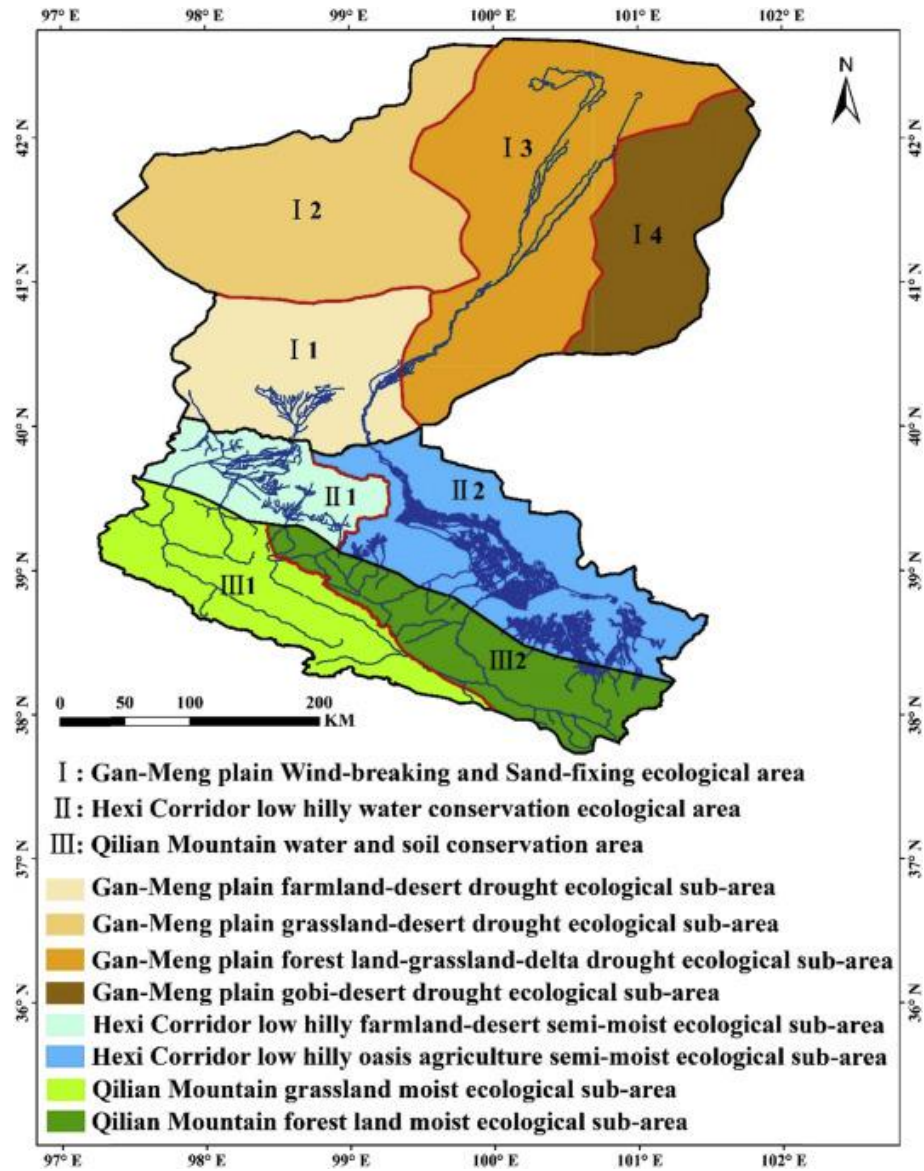


Figure 2.18: Primary and secondary clustering of Heihe River (Chen et al., 2016)

2.5.2 DBSCAN Clustering Algorithm

Density-Based Spatial Clustering of Applications with Noise or DBSCAN is the first density-based clustering algorithm that was developed by Ester in 1996. This algorithm recognizes the denser areas based on the distance of points. DBSCAN requires that the user indicate the minimum number of points in each cluster (MinN) and the maximum distance of a point from the core of a cluster to be considered in that cluster (Eps). The core point in DBSCAN is a point that has at least MinN points within the distance of Eps. Equations 26 and 27 are the conditions for the core point (p) and its border points (q) to be considered as a cluster. Finally, clusters with a distance less than Eps will merge (Khan et al., 2014).

$$N_{Eps}(p) = \{q \in D | dis(p, q) < Eps\} \quad (26)$$

$$N_{Eps}(p) > MinN \quad (27)$$

$N_{Eps}(p)$ indicates a cluster with core point (p), D is the set of points, and dis is the distance between two points. Figure 2.19 is a schematic view of the DBSCAN clustering algorithm.

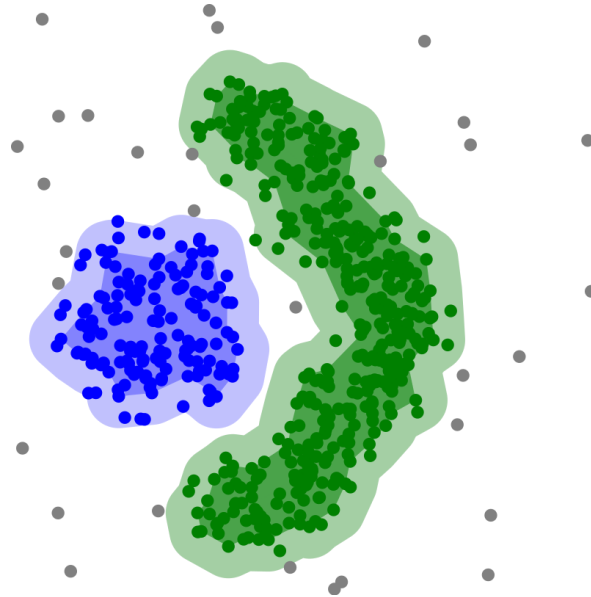


Figure 2.19: DBSCAN clustering algorithm (green and blue colors indicate two clusters, darker green and blue areas are the locations of merged core points, and gray points do not belong to any cluster) (<https://en.wikipedia.org/wiki/DBSCAN>)

Flooding is one of the most detrimental natural disasters in the world. Tangerang in Indonesia in 2016 experienced a devastating flood that destroyed lots of houses and disappeared lots of people. This city is surrounded by four rivers, Serpong River, Batubeulah River, Pamulang River, and Sawangan River. To understand the high-risk times for floods during the year, the water level data of these four rivers from 2013 to 2017 were collected. The data consists of big and small numbers so preprocessing is needed to convert the raw data into usable data. To find the flood period and location K-Medoids, DBSCAN, and X-Means algorithms were used. Results showed that at a water level of more than 1.35, flood risk is high (Natalia et al., 2019).

DBSCAN can also be used to identify blind spots. There are lots of people who die because of a car accident in India. Several factors can lead to a car accident, including drowsiness and inadequate vision. Accidents caused by drowsiness don't have specific locations, but those that occur in blind spots have specific locations. The car accident data was collected between 2014 and 2019. It was reported that more than 248,000 accidents happened in just one year. Data consist of X and Y coordinates of the car accident locations. By using the DBSCAN algorithm, the high-risk areas were recognized as blind spots (Kumar et al., 2021).

2.5.3 OPTICS Clustering Algorithm

OPTICS is the updated version of DBSCAN. In OPTICS indicating the maximum distance between the core point and border points is not mandatory. Instead, two supplementary definitions are added, core distance and reachability distance. Core distance is the minimum distance from the core point to satisfy the minimum number of points in each cluster. Reachability distance is the distance between point r and core point p . The reachability plot for each point from the nearest core point should be depicted. Points with a low reachability distance can be considered clusters. As it is shown in figure 2.20 the valleys in the plot display the clusters (https://en.wikipedia.org/wiki/OPTICS_algorithm). Also, the difference between the DBSCAN algorithm and the OPTICS algorithm is indicated in figure 2.21. Clusters in the DBSCAN algorithm have the same density but in OPTICS their density can be different.

OPTICS has some advantages in comparison with the two aforementioned algorithms. It doesn't need to indicate the number of clusters and Eps which are very valuable for this study (<https://towardsdatascience.com/understanding-optics-and-implementation-with-python-143572abdfb6>).

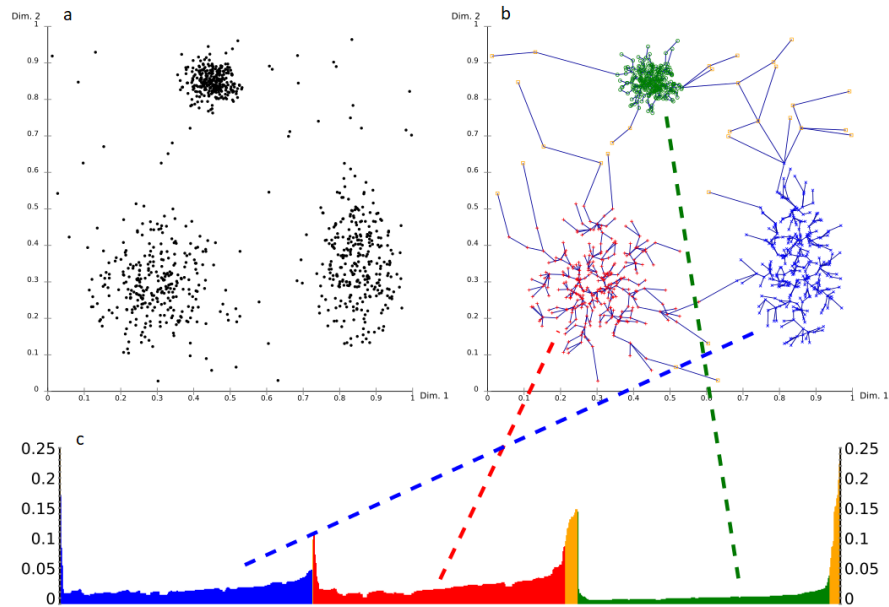


Figure 2.20: Optics algorithm: a) Locations of points, b) green, red, and blue points indicate three clusters, c) reachability plot based on the reachability distance

(https://en.wikipedia.org/wiki/OPTICS_algorithm)

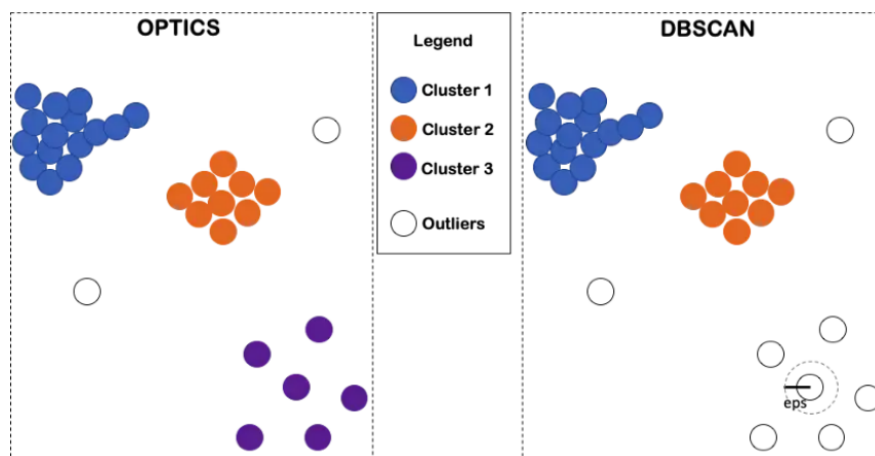


Figure 2.21: Comparison between OPTICS and DBSCAN algorithms

(<https://towardsdatascience.com/understanding-optics-and-implementation-with-python-143572abdfb6>)

Islam et al., 2021 made a comparison between four clustering algorithms by finding high-risk locations for car accidents in Virginia, USA. In this study, DBSCAN, OPTICS, K-Means, and Mini-Batch K-Means were applied to the data. For comparison, two factors were used, the Silhouette Coefficient and the Davies-Bouldin index. Silhouette Coefficient evaluates the performance of the algorithm using equation 28. As much as this coefficient is higher the performance is better.

$$s = \frac{b - a}{\max(a, b)} \quad (28)$$

Where s is the Silhouette Coefficient, b is distance between two clusters and a is the maximum distance of a point in a cluster from the core point.

The Davies-Bouldin index shows the similarity in each cluster and the difference with other clusters, As much as this index is less the performance is better. Equation 29 is used for calculating the Davies-Bouldin index.

$$V_{DB} = 0.5 \times \sum_{i=1}^k \max D_{ij} \quad (29)$$

$$D_{ij} = \frac{(\bar{d}_i + \bar{d}_j)}{d_{ij}} \quad (30)$$

Where V_{DB} is the Davies-Bouldin index, k is the number of clusters, between cluster i and j $\bar{d}$ is the average distance of points in a cluster and d_{ij} is the distance between core points of two clusters. Figure 2.22 displays the performance of algorithms based on these factors. DBSCAN has the highest Silhouette Coefficient and the least Davies-Bouldin index which means the performance of DBSCAN was better in comparison with three other algorithms in finding the high-risk zones. But in this study, since there is no information about the maximum distance between two particles in a cluster, we decided to continue with OPTICS which doesn't need any value for ϵ .

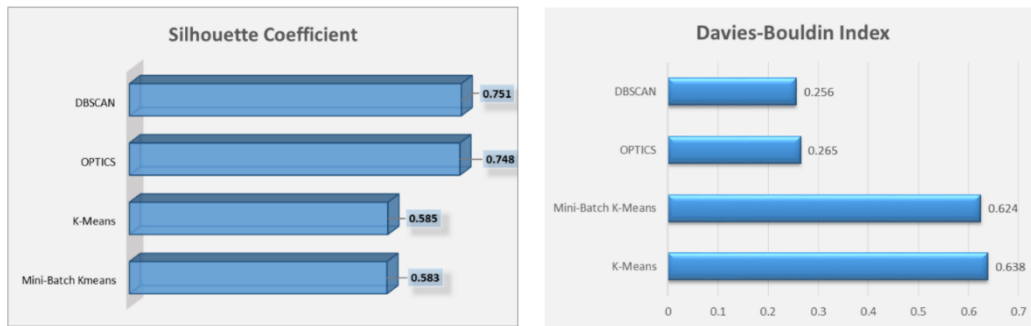


Figure 2.22: Comparison between four clustering algorithms (Islam et al., 2021)

In this study, the goal is to find the accumulation zones of microplastics in the Fraser River, which can help in future water resources management programs. Bluekenue and TELEMAC 3D will be used to create the hydrodynamic model, then CaMPSim-3D particle tracking model will be used to find the final location of microplastic particles. In last step, OPTICS algorithm will be applied to find the accumulation zones of microplastics in the lower part of the Fraser River.

Chapter 3. Numerical Models and Clustering Algorithm

3.1 Hydrodynamic Model

The hydrodynamic model of the Fraser River was created using TELEAC 3D. TELEMAC is one of the most powerful tools in this field. To build the model some input files are required that in the rest of this part they will be discussed. It is good to mention that all data are vertically referenced to Chart Datum (CD).

3.1.1 Study Area

The Fraser River is one of the largest rivers in Canada and the longest river in British Columbia. It runs from Fraser Pass located in the neighboring Rocky Mountains to its mouth at the Strait of Georgia, which flows into the Pacific Ocean. It passes through many big and influential cities such as Vancouver for more than 1370 kilometers (Thomson, 1981). The Fraser River is the major source of fresh water in British Columbia, Canada, which provides water for various activities in that area like agriculture. Due to higher temperatures in summer and late spring, the snows in the mountains start melting and the discharge during these periods is higher, but in autumn, winter, and early spring, the Fraser River experiences lower discharge values (Kostaschuk and Atwood, 1990).

This study focuses on the lower Fraser River, from Douglas Island to its mouth at the Strait of Georgia, as well as a part of the ocean. So about a 35 km stretch of the Fraser River is modeled in this thesis. As it was mentioned, the Fraser River is a source of fresh water, but in recent years it has become more polluted. It can have various reasons, such as developing cities around it, more surrounding industrialized areas, and more population. But the most critical thing is understanding and predicting the behavior of these particles in order to make the most appropriate decisions for saving that region. This area is under tidal currents and as a result, saline water comes up and mixes with fresh water which causes some changes in the density of water. So it is imperative to

choose the location of the upstream boundary in a place that always has fresh water. Tsz Yeung Leung et al., 2018, did an experiment to find the salinity of the different parts of the lower part of the Fraser River. This experiment was done at different times of the year. Based on the results, the salinity at the zero salinity point which is indicated in figure 3.1 is almost zero in all the experiments, so the intrusion of ocean water near Douglas Island is negligible. Also, the downstream boundary, due to the stability of the model is chosen in the ocean.

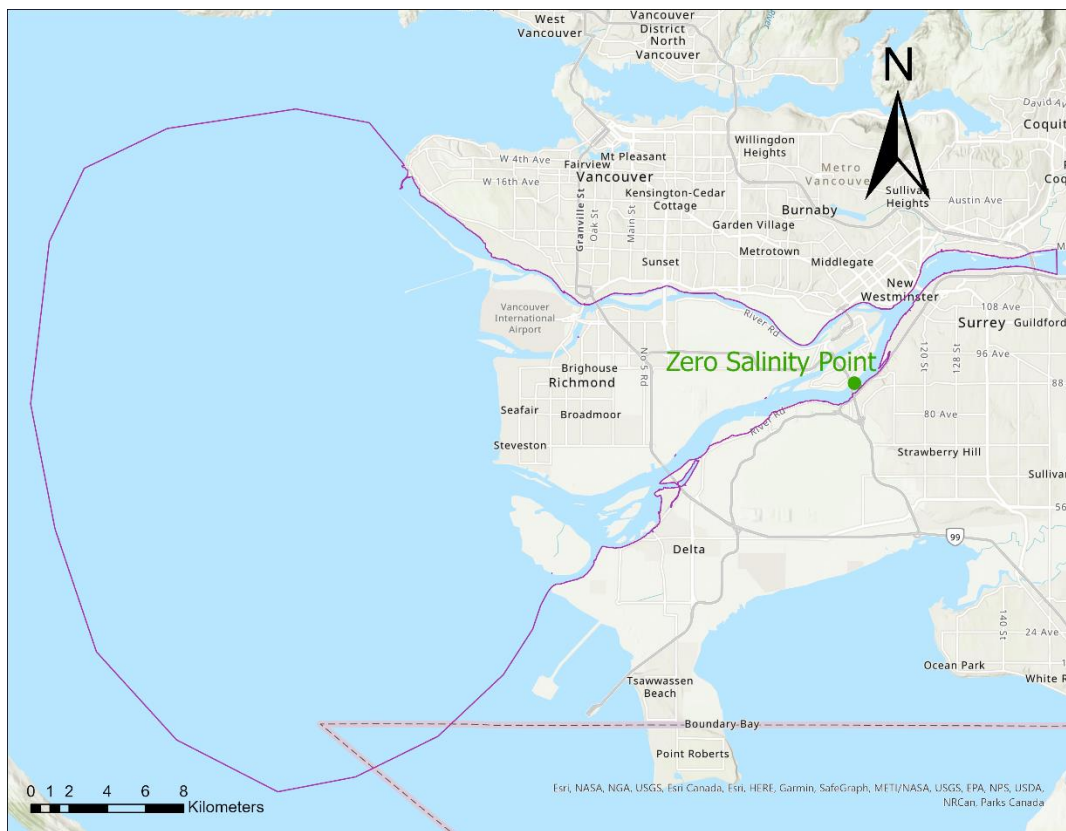


Figure 3.1: Study area (purple line) and location of zero salinity point (green circle)

3.1.2 Study Period

The location and movements of the earth, moon, and sun have a significant effect on the situation and water level in rivers. Due to the locations of the earth, moon, and sun and their angle, every 14.76 days a full spring-neap tidal cycle will be completed (Kvale, 2006). For the main modeling

period, two full spring-neap tidal cycles or 30 days were considered in this study. Furthermore, the model was initially run for 11 days as a spin-up.

As it was mentioned previously, during autumn and winter the flow values are lower which means microplastic pollution is more severe in this period and these particles have more time to settle and accumulate in vulnerable areas. After checking available data from various discharge and water level stations, and experiment data for validation the period of October 21, 2019 up to November 30, 2019 (total 41 days) was chosen.

3.1.3 Computational Mesh

As it was mentioned in the previous chapter the base mesh was created using Bluekenue 3.3.4. To create the base mesh the outlines of the lower part of the Fraser River and its islands are needed. These files were downloaded from the official website of the government of British Columbia in the format of shapefile and their coordinate system was converted to NAD 1983 UTM zone 10N. The base mesh consists of 55,423 triangular elements and 31,065 nodes in one horizontal plane. Considering 15 layers, the total number of nodes is 465,975. It was tried that every part of the Fraser River, even the narrow sections, would possess at least 5 triangular elements, so the length of these triangular elements varies between 10 m in narrow parts to 600 m in the ocean.

3.1.4 Steering File

The first and most important file is the steering file which is an ASCII file that contains all information about all computational parameters. TELEMAC is designed in a way that if a parameter is not specified in the steering file it will use its default values. The time step of the hydrodynamic model is 10 seconds but the time step for printing the results in the result files is 450 seconds. This model prints u, v, w, and tracer 1 in the 3D result file. The bottom friction follows Manning's law and the friction coefficient is 0.07. This number is chosen based on the bedrock type file which was downloaded from the official website of the government of British Columbia in the format of a shapefile. In figure 3.2 the bedrock type map is shown. Zones with different colors indicate the bedrock type in that area and the brown line indicates the outline of

our study area. Based on this file the bedrock all along the lower Fraser River is undivided sedimentary rock with the mentioned friction coefficient.

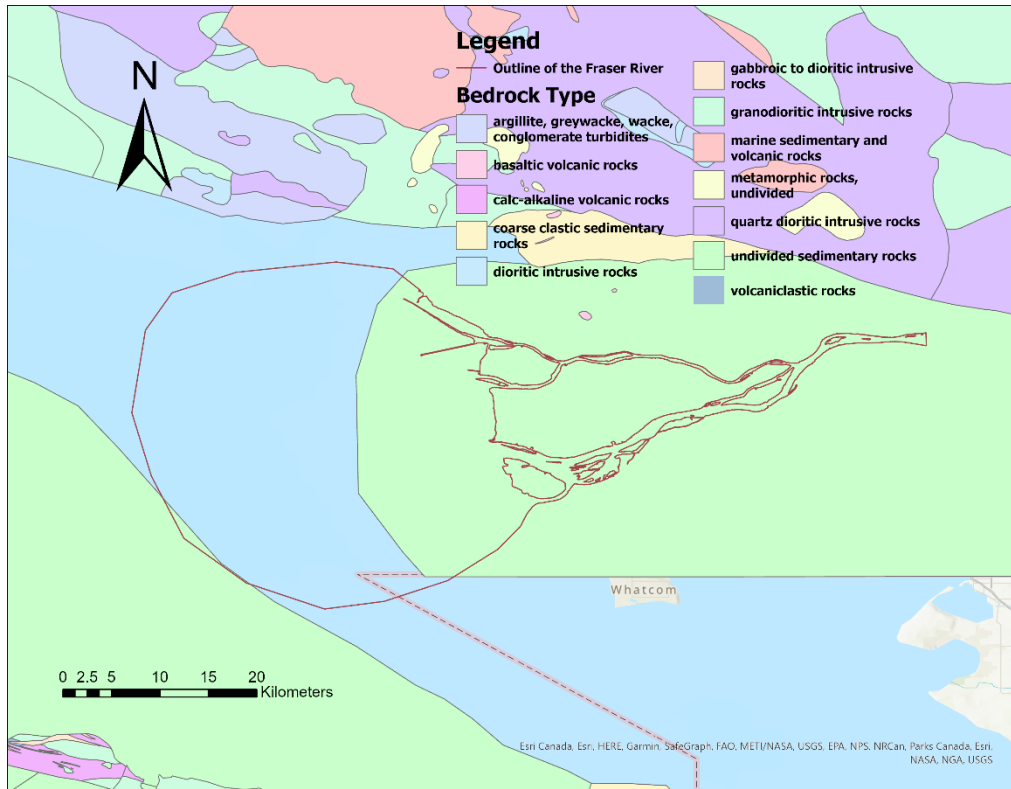


Figure 3.2: Bedrock type map

The vertical and horizontal turbulence model are set to be constant and the value is equal to 10^{-4} which is a typical value. The vertical velocity profile is constant in both of the boundaries and the horizontal velocity profile is normal and homogeneous along the boundaries. This model has 15 Sigma layers (Phillips, 1957) in the vertical direction. The model has only one tracer which is salinity. Salinity in the downstream boundary which is in the ocean is equal to 30 ppt and the upstream boundary is assumed to be fresh water, these values are chosen based on a study done by Tsz Yeung Leung et al., 2018 and they are constant throughout modeling period.

3.1.5 Geometry File

To create the geometry file the base mesh and bathymetry data are necessary. The bathymetry data were derived from the website of Open Government. To find the elevation at the locations of the nodes of the base mesh a 2D interpolator tool in Bluekenue was used. This tool uses Inverse

Distance Weighted Method for interpolation. Finally, the interpolated mesh is saved as a SERAFIN file which is readable for TELEMAC. The interpolated mesh is displayed in figure 3.3.

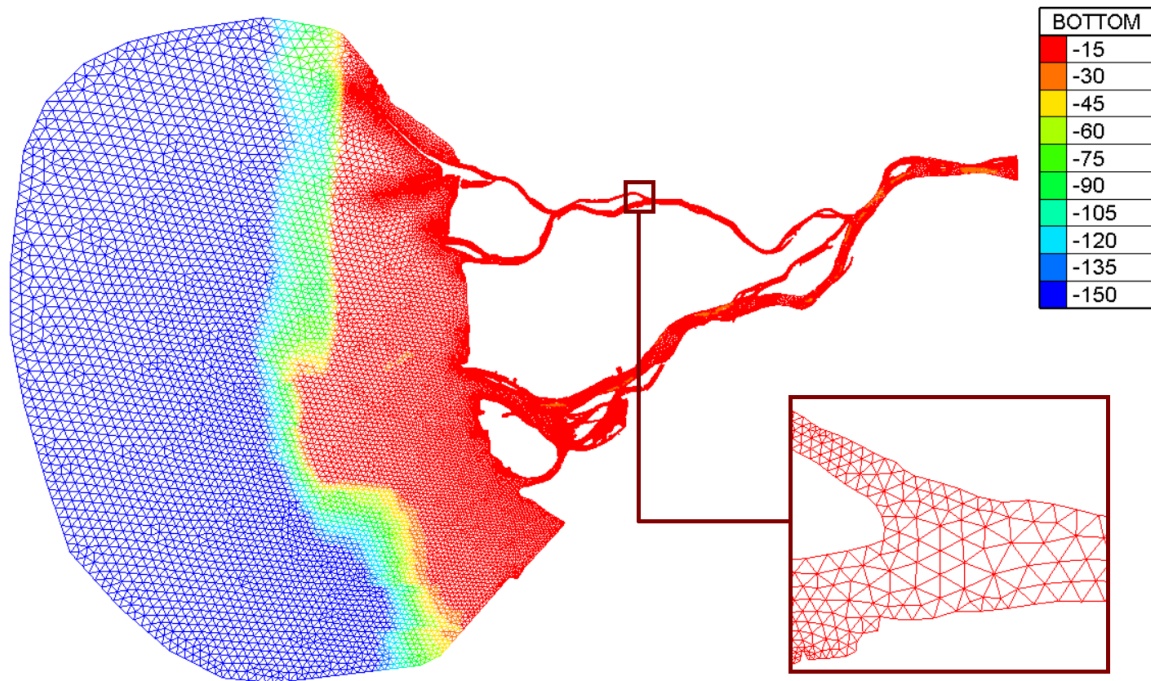


Figure 3.3: Base mesh and bottom elevation of the lower part of the Fraser River

3.1.6 Boundaries Conditions File

This model consists of two boundaries. The upstream boundary is located near Douglas Island which was prescribed by freshwater. The downstream boundary is located near the mouth of the river in the Strait of Georgia. Some parts of the ocean were included in the model to satisfy the stability requirement. This boundary is forced by tidal elevation.

The boundary conditions file contains information about the nodes that are located in the outlines of the mesh in the counterclockwise direction and nodes located in the outlines of islands in the clockwise direction, and finally their types. This file was created using Bluekenue and both boundaries are open boundaries. The format of the Boundary condition file is cli and each line of that refers to a node in the mesh includes the identification number of boundary nodes and their type.

3.1.7. The Liquid Boundaries File

To indicate the situation in each of these two boundaries, the liquid boundaries file is used. As it was mentioned in the previous part, one of the boundaries is prescribed by discharge and the other one is prescribed by water level. The hourly water level data was derived from the website of Fisheries and Oceans Canada. Sand Heads station (07594) was the nearest station to the downstream boundary. Port Mann Pumping Station (08MH126) is the closest station to the upstream boundary that has discharge data. Information about this station was downloaded from the website of the Government of Canada (water office). The outline of the study area and the locations of these two stations are displayed in figure 3.4.

The liquid boundaries file is an ASCII file that has three columns one for time, one for the flow rate, and the last one for water depth.

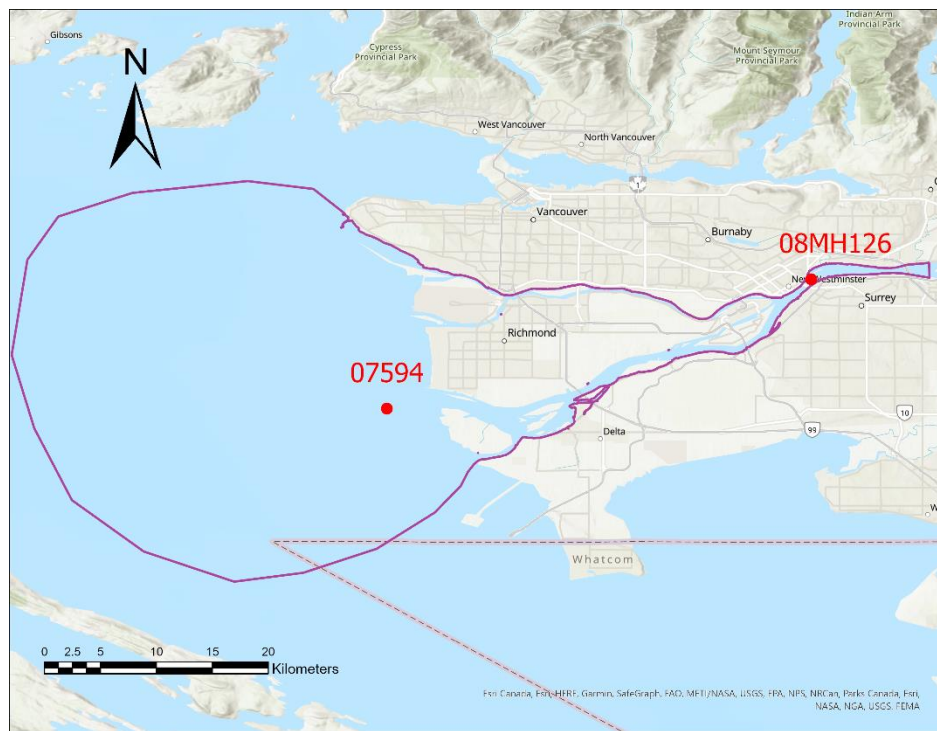


Figure 3.4: Water level and discharge stations

3.2 Microplastics Pollution

The lower part of the Fraser River is located in the south of Vancouver, British Columbia which is a big and populated city. Since there is higher amount of rain in the surrounding area, combined sewer systems overflow and discharge into the Fraser River. Also, wastewater treatment plants are designed to remove harmful and external particles from wastewater but the point is that both combine sewer overflows (CSO) and discharge of wastewater treatment plants (WWTP) contain lots of microplastic particles. In this study the locations for releasing microplastic particles are chosen based on the location of combined sewer overflows and wastewater treatment plants.

A report published by MetroVancouver, indicated the locations and situation of CSOs and WWTPs in 2019. Based on this report there are 7 CSOs (Glenbrook, New Westminster, Borden, South Hill, Manitoba, Angus, and MacDonald) and 2 WWTPs (Annacis Island WWTP and Lulu Island WWTP) from Douglas Island up to the Strait of Georgia. Figure 3.5 shows the location of CSOs and WWTPs in the study area.

A report released on the official website of the Government of British Columbia specified the average seasonal discharge overflow in each of these CSOs. Based on this report, a year is divided into two measuring seasons, spring and winter. Also, the average annual amounts of the discharge of those two WWTPs have been mentioned in the aforementioned report. Table 3.1 shows the values for CSOs discharges. And table 3.2 shows the discharges from WWTPs.

Table 3.1: Discharge values for CSOs

CSO's Name	Seasonal Discharge Million m^3 /season (winter)	Frequency Time/season (winter)
Glenbrook	4.8	6
New Westminster	3.5	6
Borden	4.8	6
South Hill	2.9	6
Manitoba	2.9	6
Angus	1	6
MacDonald	0.5	6

Table 3.2: Discharge values for WWTPs

WWTP's Name	Average Annual Discharge (Million m^3)
Annacis Island WWTP	182,556
Lulu Island WWTP	55,508



Figure 3.5: Locations of combined sewer overflows (orange circles) and wastewater treatment plants (red circles)

Parizi, 2021 did an experiment on the lower part of the Fraser River in order to find the amount and different characteristics of microplastic particles in that region. The two sampling sites measured in this study are useful for the current study. Information about these two sites can be found in table 3.3.

Table 3.3: Amount of microplastic particles and their characteristics (Parizi, 2021)

Site	MP/ m^3	Annual Discharge (Billion MP/year)	Fibers (%)	Fragments (%)
Angus CSO	1,833 - 13,673	10.2 - 14.6	66 - 78	25 - 31
Annacis Island WWTP	100 - 500	20 - 40	66	28.1

But there is no information about other release locations. So in this study, the number of particles that were released from each CSO was calculated by comparing the discharge flow of that site with the discharge flow of Angus CSO discharge flow and for WWTPs the total number of microplastics was calculated based on the ratio of discharge flow of WWTP to discharge flow of Annacis Island WWTP.

Also, there is another feature of microplastic particles that needs to be specified in the model. The density of particles is an important characteristic that influences the settling velocity of particles and their accumulation in narrow and shallow parts of the river. Parizi, 2021 had 8 sampling sites in the lower part of the Fraser River and counted the number of microplastic particles, and indicated their primary ingredient. The results show that Polyester is the major constituent and it is mostly found in textiles, ropes, and even insulation. After Polyester, Polyethylene is the most common material used in freezer bags, water pipes, and cables. The number of microplastic particles and their type is indicated in figure 3.6.

According to the aforementioned points, the studied type of microplastic particles is Polyester. This is because it is the major ingredient found in almost all sampling locations, and its density is

assumed to be 1.37.

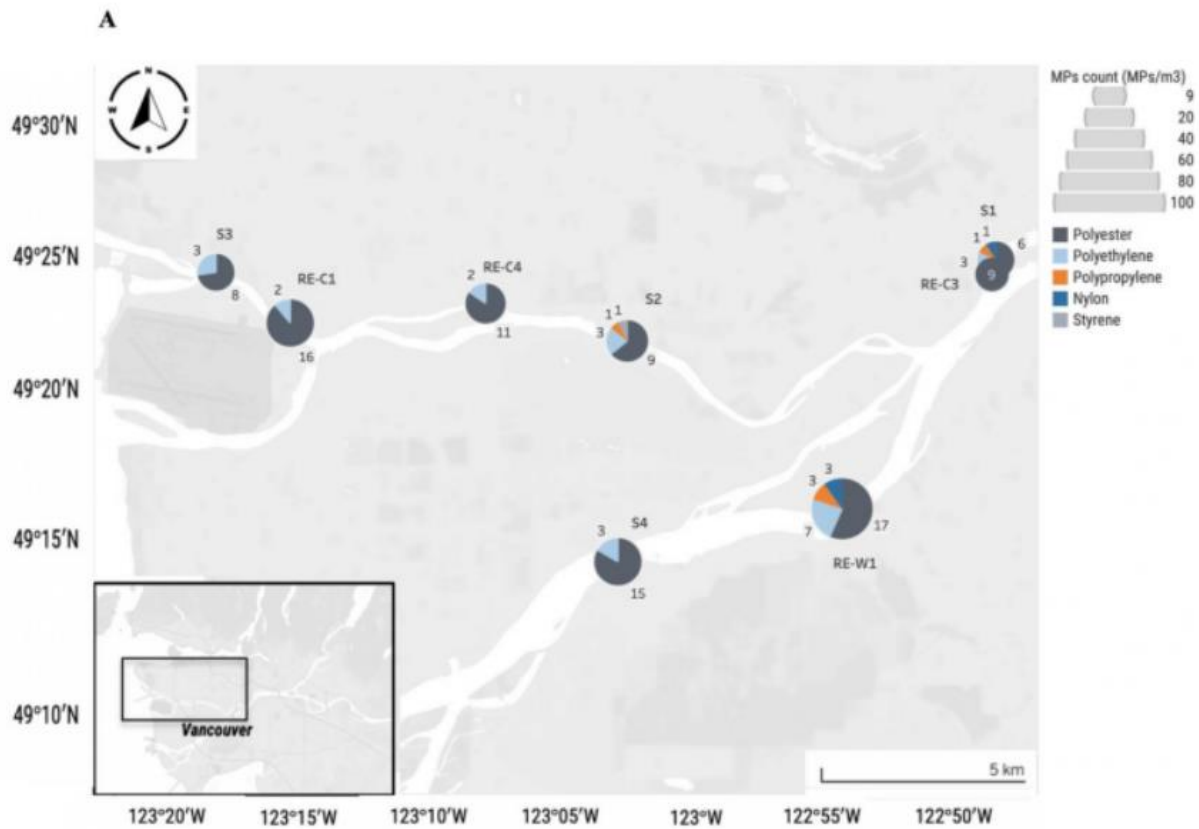


Table 3.4: Different scenarios for particle tracking model

Scenario	CSO or WWTP Name	Number of Microplastic Particles	Type	Density	Shape
S1	Glenbrook CSO	60,000	Polyester	1.37	Spherical
S2	New Westminster CSO	40,000	Polyester	1.37	Spherical
S3	Borden CSO	60,000	Polyester	1.37	Spherical
S4	South Hill CSO	40,000	Polyester	1.37	Spherical
S5	Manitoba CSO	40,000	Polyester	1.37	Spherical
S6	Angus CSO	15,000	Polyester	1.37	Spherical
S7	MacDonald CSO	10,000	Polyester	1.37	Spherical
S8	Annacis Island WWTP	40,000	Polyester	1.37	Spherical
S9	Lulu Island WWTP	10,000	Polyester	1.37	Spherical

As it was mentioned in the previous chapter this model uses the results of the hydrodynamic model. Some of these files can be used directly in the model and some of them need preprocessing. In the following parts, the input files for the particle tracking model will be discussed.

3.3.1 The 3D Result File

This file is directly used from the results of the hydrodynamic model. This is a SERAFIN file that contains mesh geometry as well as a few variables like velocity in every three directions and the concentration of tracers in each node of the base mesh for each graphic printout.

3.3.2 Mesh File

Mesh file is a text file that contains all the geometry information about the base mesh. In the first row, it contains information about the total number of nodes in the mesh which is equal to 31,065, the smallest and largest values for X and Y in Cartesian directions, and maximum free surface elevation through all the nodes. After that it includes some columns that indicate the identification number for nodes, their location in Cartesian directions, water depth, and free surface elevation. Each row is representative of a node in the base mesh.

3.3.3 2D Element File

This text file has information about all 2D elements in the model. The information is about the total number of 2D elements in the base mesh (55423), the total number of nodes in one 2D layer (31065), the identification number of the elements, and the constituent nodes of that element.

3.3.4 Boundary Nodes File

This file contains information about the total number of nodes in the two boundaries of the model and the identification number of them. The format of the boundary nodes file is a text file.

3.4 Clustering Algorithm

Based on the explanations in the literature review, the OPTICS algorithm was selected for clustering particles and finding their accumulation zones in the Fraser River. Prior to that, every machine learning algorithms requires data preprocessing. It helps to improve the accuracy, reduce the time and resources required to train the model, prevent overfitting, and improve the interpretability of the model. The Standard Scaler method was used in this study. This method removes the mean and scales to unit variance. New values are calculated using equation 31.

$$z_i = \frac{x_i - \mu}{\sigma} \quad (31)$$

$$\mu = \frac{1}{N} \sum_{i=1}^N x_i \quad (32)$$

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \mu)^2} \quad (33)$$

Where z indicates new values after preprocessing, x represents the input values before preprocessing and N is the total number of input data. In this way, the results of the model are more accurate and reliable. Figure 3.7 displays the effect of data preprocessing. Before preprocessing red point has more similarity with the blue point than the yellow point, but after preprocessing all the features have same scale and now it is obvious that red point has more similarity with yellow point.

It is better that the input data follow normal distribution. Figure 3.8 shows the distribution of particles in scenario 1 which is close to normal distribution. Other scenarios are very close to normal distribution but due to limitation in space they are not included in the text.

For preprocessing, Python 3.8.8 which is a free and one of the most common programming languages was used. Python contains different libraries that one of them is Scikit-Learn. Scikit-Learn is an open-source library that was built on NumPy, SciPy, and matplotlib. This library is mostly used for classification, regression, clustering, preprocessing, dimensionality reduction, and model selection. One of the packages of Scikit-Learn is preprocessing which has a module named StandardScaler. This module was used in this study for normalizing the input data.

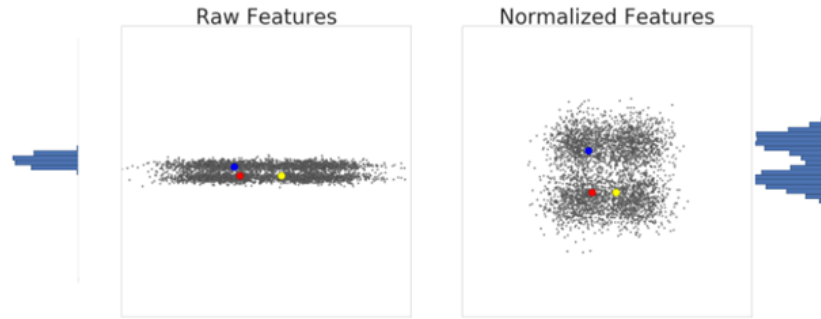


Figure 3.7: The effect of data preprocessing, red, yellow, and blue points are representatives of three points in the input data (<https://developers.google.com/machine-learning/clustering/prepare-data>)

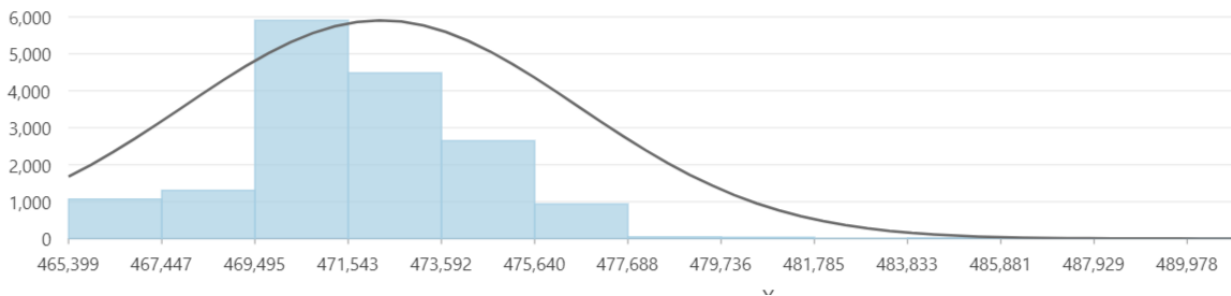


Figure 3.8: Normal distribution of particles in scenario 1

After preprocessing data is ready for clustering. In order to apply OPTICS algorithm on the final location of particles to find their accumulation zones, the cluster package of Scikit-Learn was implemented. OPTICS module was used for clustering in this study. The minimum number of microplastic particles in each cluster is indicated based on the suggestion by Collins and Hermes,

2019. Wherever more than 0.5 percent of particles accumulate, there is an accumulation zone. This minimum number for each scenario is displayed in table 3.5.

Table 3.5: Minimum number of microplastic particles in each cluster for each scenario

Scenario	Minimum Number of Particles
S1	300
S2	200
S3	300
S4	200
S5	200
S6	80
S7	60
S8	200
S9	60

In order to visualize the results better and make them more useful for future studies, the shapefile of the locations of microplastics in each cluster was created. Python Shapefile Library makes it possible to read data of shapefiles and also create files in the format of Esri shapefile. Using this library it is possible to define different fields for each particle that can be the number of their cluster. Figure 3.9 is a flowchart of what is done in Python.

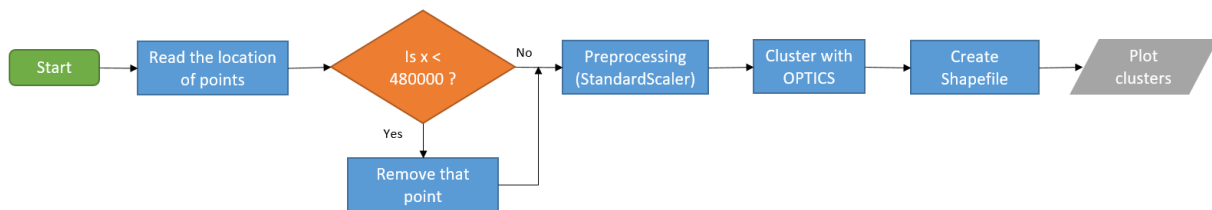


Figure 3.9: Flowchart of the clustering algorithm

Chapter 4. Results and Discussion

4.1 Sensitivity Analysis

Hydrodynamic models work based on some equations and relations, so there is no certainty about their results. Different parameters can have significant influences on the accuracy of the results. Some of them are more critical than others. Hydrodynamic modeling can be very time and cost consuming so it is a necessity to choose the most appropriate values. Therefore, it is essential to ensure that the most critical ones have optimal values, because overly cautious values might not provide better results while they cost more.

The most common factors to be examined are the smallest size of the base mesh, roughness, and the turbulent vertical diffusion coefficient.

4.1.1 Base Mesh Size

As it was mentioned in the previous chapter, the smallest length of a triangle in the base mesh is 10 m. So for testing the sensitivity of these computations to mesh size, only the smallest length in the base mesh was changed to 9 m and other lengths and computational parameters were exactly the same. Due to the high computational time for this model, it was only run for the first 10 days. The changes in the results were insignificant and could be ignored. So the optimal smallest length of the base mesh is 10 m in this study and smaller values do not cause better results. Figure 4.1 compares the result of the model in node number 456700 for 10 days in both cases.

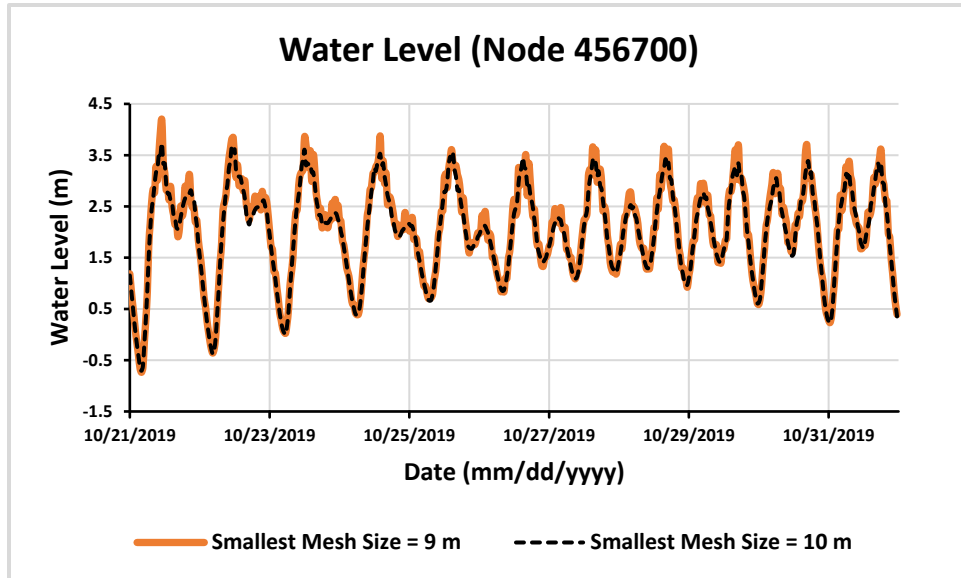


Figure 4.1: Water level comparison between meshes with two different sizes

4.1.2 Roughness

Roughness is an influential factor that impacts both the water depth and velocity of water, especially in the lower layers. As demonstrated in the previous chapter, all the study area is covered by the same type of bedrock, so the roughness coefficient should be the same throughout the lower part of the Fraser River. Additionally, a value for this coefficient was determined on the mentioned shapefile. As a result, the model was run using only one roughness coefficient, and other values were not taken into consideration in order to simulate real conditions.

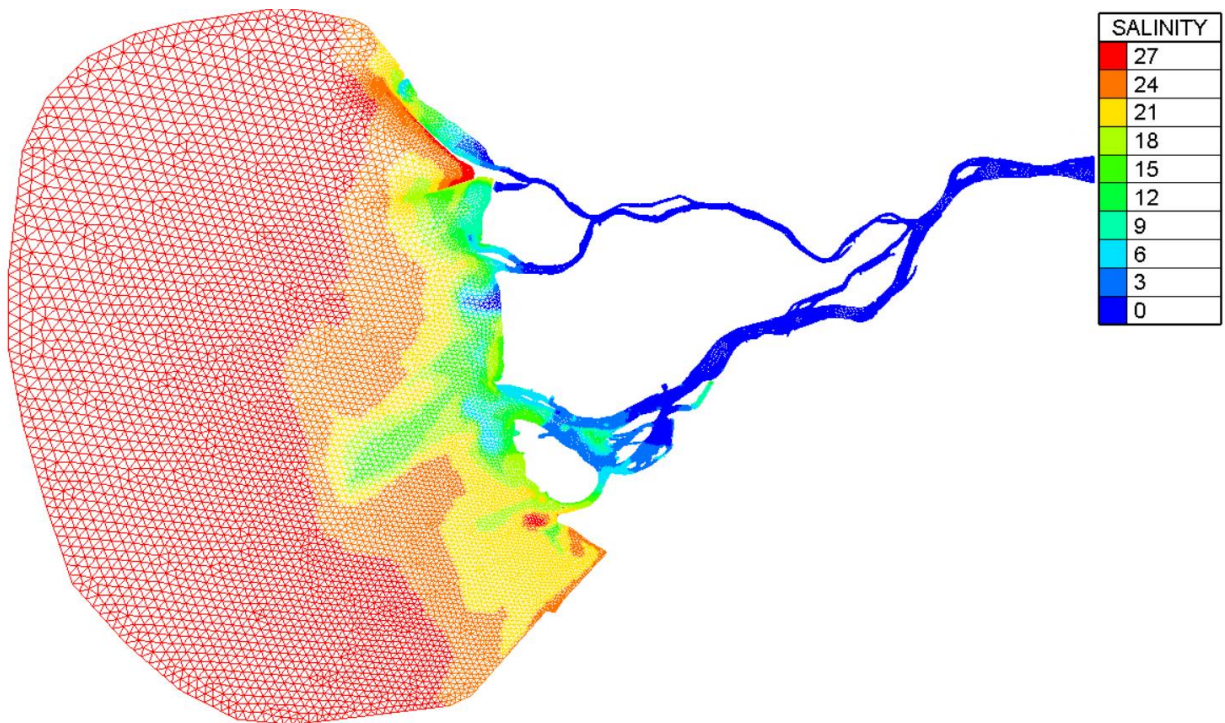
4.1.3 Turbulent Vertical Diffusion Coefficient

Saline water due to the salt that is dissolved inside it has a higher density in comparison with normal water. It flows into the lower layers and fresh water moves through the upper layers. Due to tidal forces in this area and vertical turbulence, fresh and saline water mix together. The amount of dissolved salt in different water layers varies according to these factors. One of the most reliable ways to find the appropriate value for the turbulent vertical diffusion coefficient is field measurement, but in this study, this option was not possible so typical values were tested.

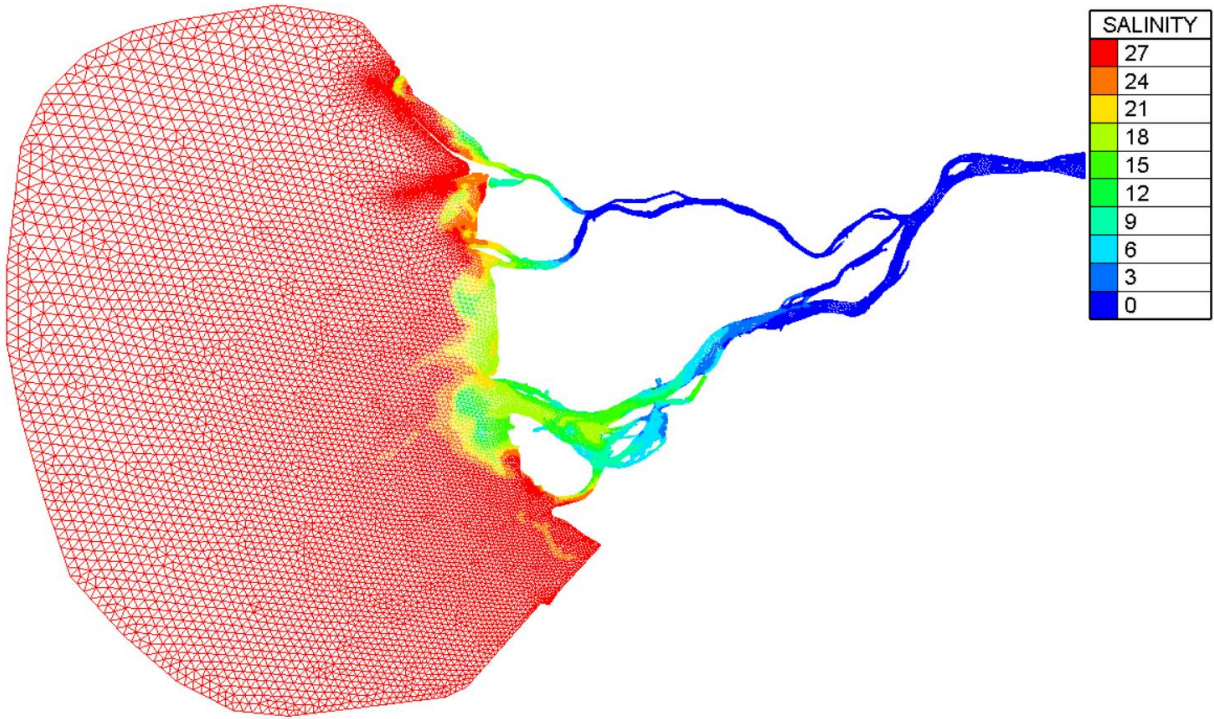
The higher turbulent vertical diffusion coefficient will result in faster mixing. For this part, two models were tested, one with a turbulent vertical diffusion coefficient equal to 10^{-4} and the other one with a turbulent vertical diffusion coefficient equal to 10^{-5} . The results of these simulations are displayed in figures 4.2 and 4.3. Each of the figures contains three pictures. The hydrodynamic model has 15 layers and each of these pictures displays the salinity of water in layers 15, 8, and 1. It is worthwhile to mention that in this part all other values were constant and only the turbulent vertical diffusion coefficient was different between these two simulations.

The results of the model in these two figures are expectable and it is obvious that in the first figure, the saline water mixed with fresh water faster and salinity of water in some parts of the Fraser River is not around zero anymore. Based on the discussion in the numerical models chapter, saline water sometimes comes up and mixes with fresh water along the river. Consequently, the results of the simulation with a turbulent vertical diffusion coefficient equal to 10^{-4} , are more similar to reality.

a)



b)



c)

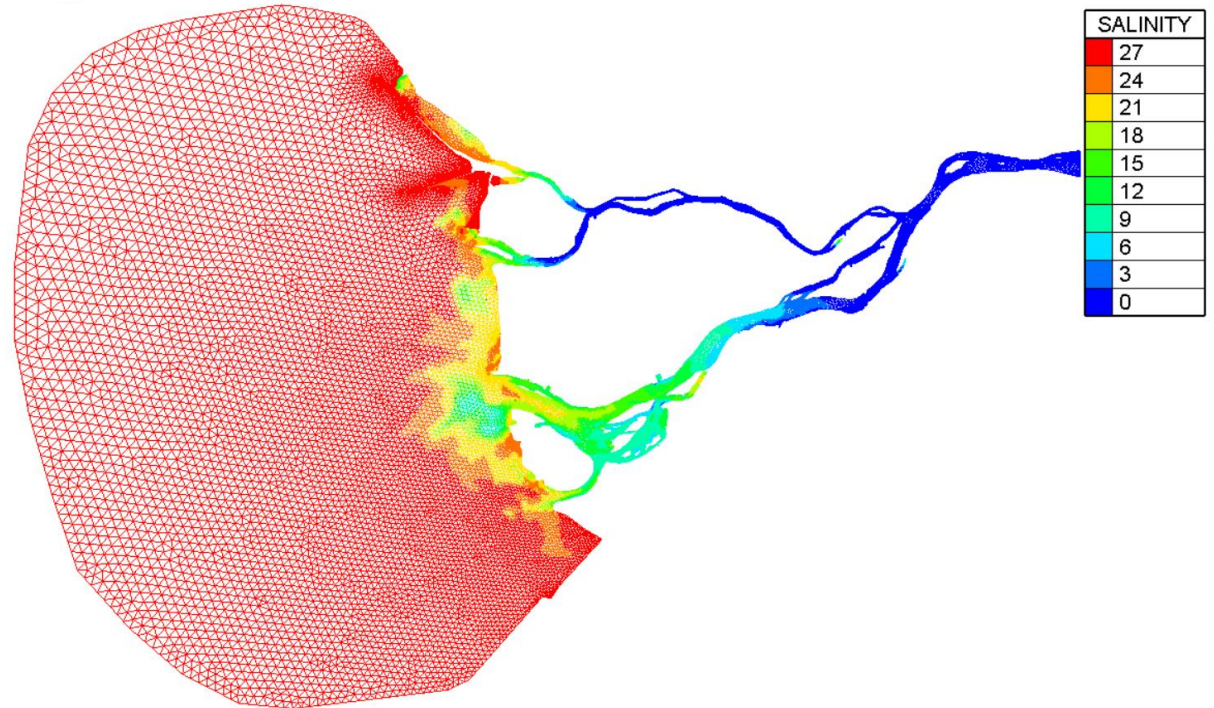
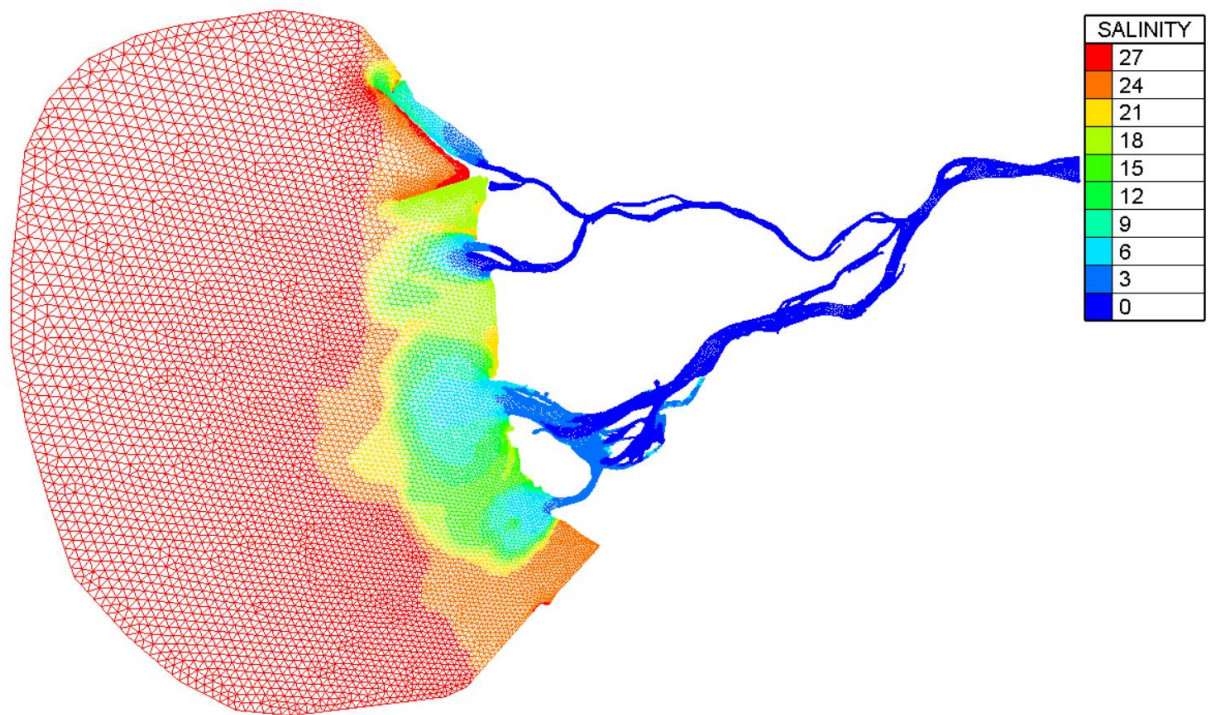
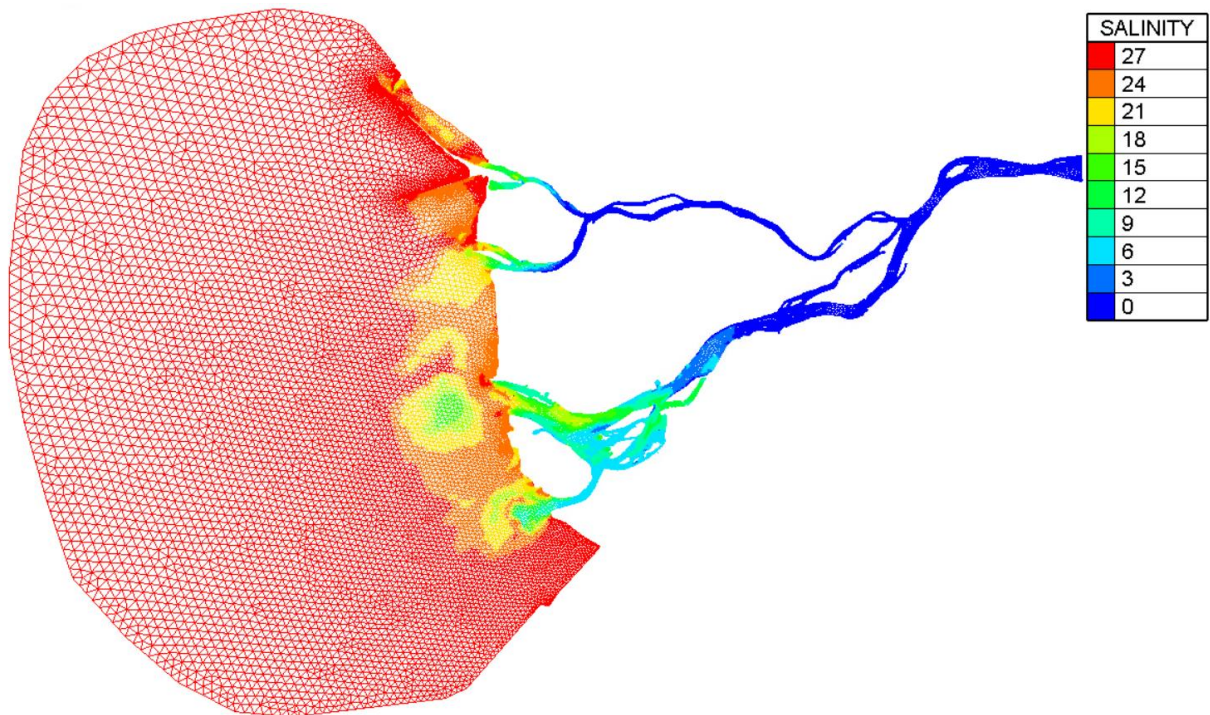


Figure 4.2: Results of the model with a turbulent vertical diffusion coefficient equal to 10^{-4} , showing salinity (ppt) in the study area on 10/26/2019: a) Layer 15, b) Layer 8, c) Layer 1

a)



b)



c)

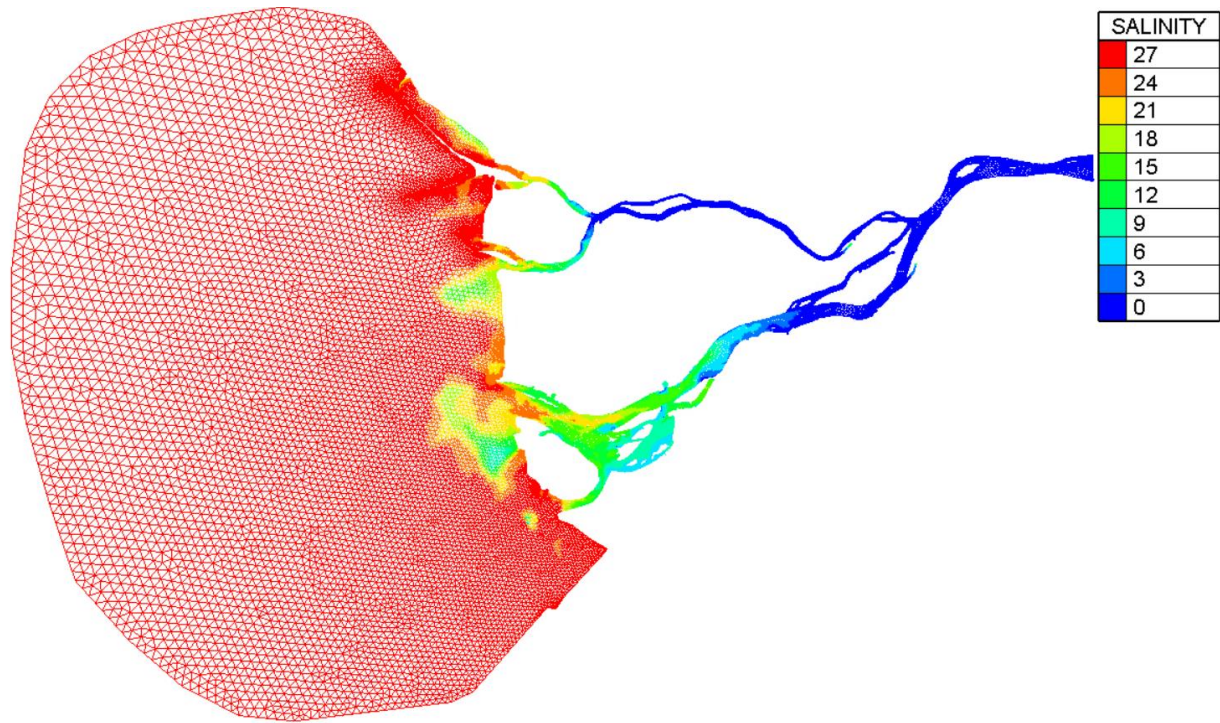


Figure 4.3: Results of the model with a turbulent vertical diffusion coefficient equal to 10^{-5} , showing salinity (ppt) in the study area on 10/26/2019: a) Layer 15, b) Layer 8, c) Layer 1

4.2 Results of the Hydrodynamic Model

Based on the previous chapter, the model was run in two parts, first part: 11 days as spin-up, second part: 30 days as the main simulation. In this part the results of the hydrodynamic model for the main 30 days will be discussed.

4.2.1 Water Level

As discussed in the previous chapter, this model was run for 30 days which contains two full spring-neap tidal cycles. It is important that these two cycles be displayed in the water level graph at all points in this simulation. For testing this theory, a point from the base mesh was chosen and a time series of water levels for that point was extracted. Figure 4.4 indicates the location of this point on the map. Figure 4.5 shows the water level time series for point 464369. Two full spring-neap tidal cycles are visible in this figure.



Figure 4.4: Location of point 464369 in the study area (Blue line indicate the study area)

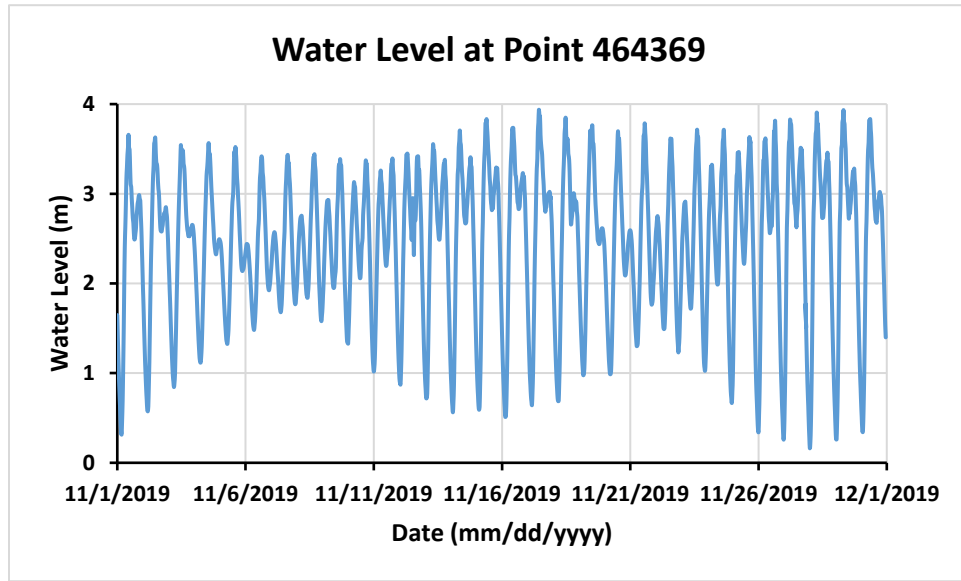


Figure 4.5: Water level at point 464369 for 30 days based on the results of the hydrodynamic model

4.2.2 Velocity

The velocity of water changes during a month and even during different times of the day. It's a result of temperature that causes ice melting in the mountains, rain events that increase the discharge of the river, and even tidal forces. These changes can affect the value of the velocity or the direction of the velocity. Sometimes the flow is from the river to the ocean and sometimes it is reversed, and water moves from the ocean to the river. To show these changes point 447873 from the base mesh is chosen. Figure 4.6 indicates the location of this point in the study area. The vertical and horizontal velocity and the direction of the horizontal velocity vector with the horizontal direction of the Cartesian coordinate system are shown in figures 4.7, 4.8, and 4.9. It is pertinent to mention that the two full spring-neap tidal cycles are visible in the pictures. Definitely, the vertical velocity is much lower than the horizontal velocity that can be seen in the pictures. It is good to mention that positive vertical velocity means the water level moves up and negative

vertical velocity means the water level comes down. The minimum horizontal velocity in the river part of the model is almost zero m/s and the maximum velocity in that part is near 1.8 m/s.



Figure 4.6: Location of point 447873 in the study area (Brown line indicates the study area)

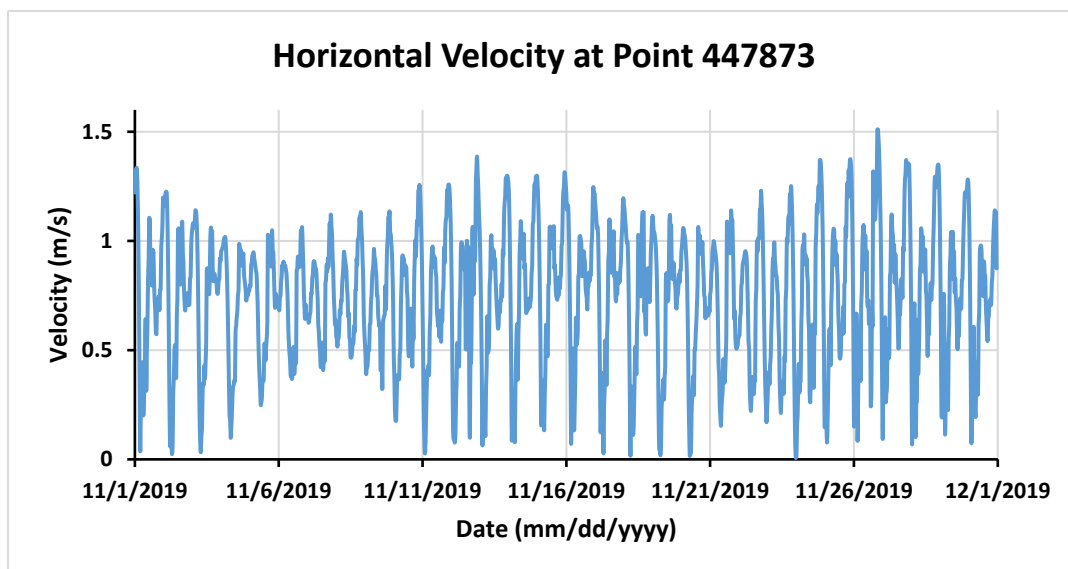


Figure 4.7: Horizontal velocity at point 447873 for 30 days based on the results of the model

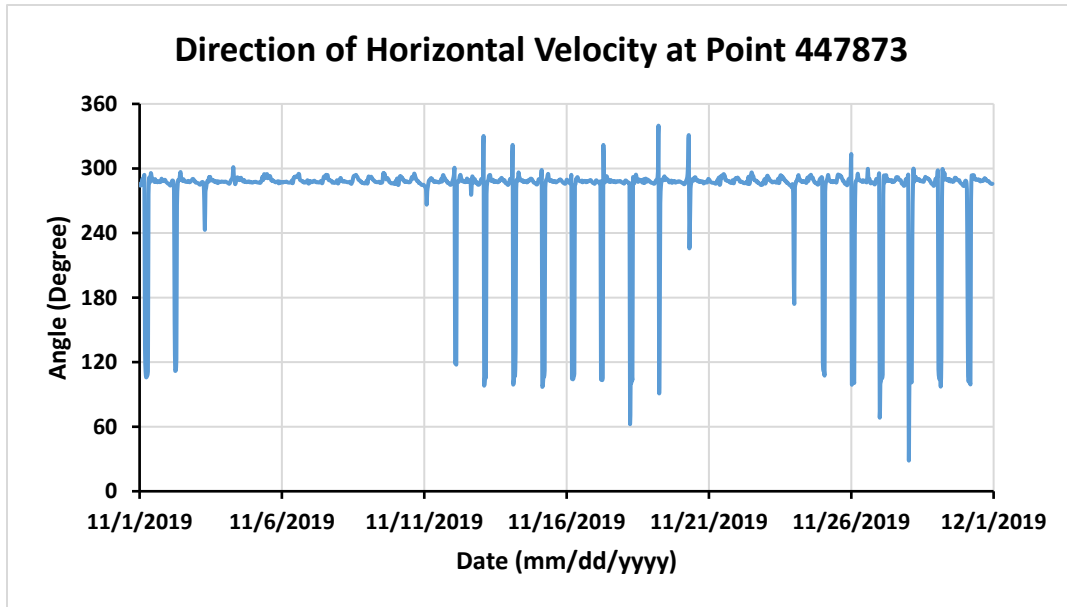


Figure 4.8: Direction of the horizontal velocity vector at point 447873 for 30 days based on the results of the model

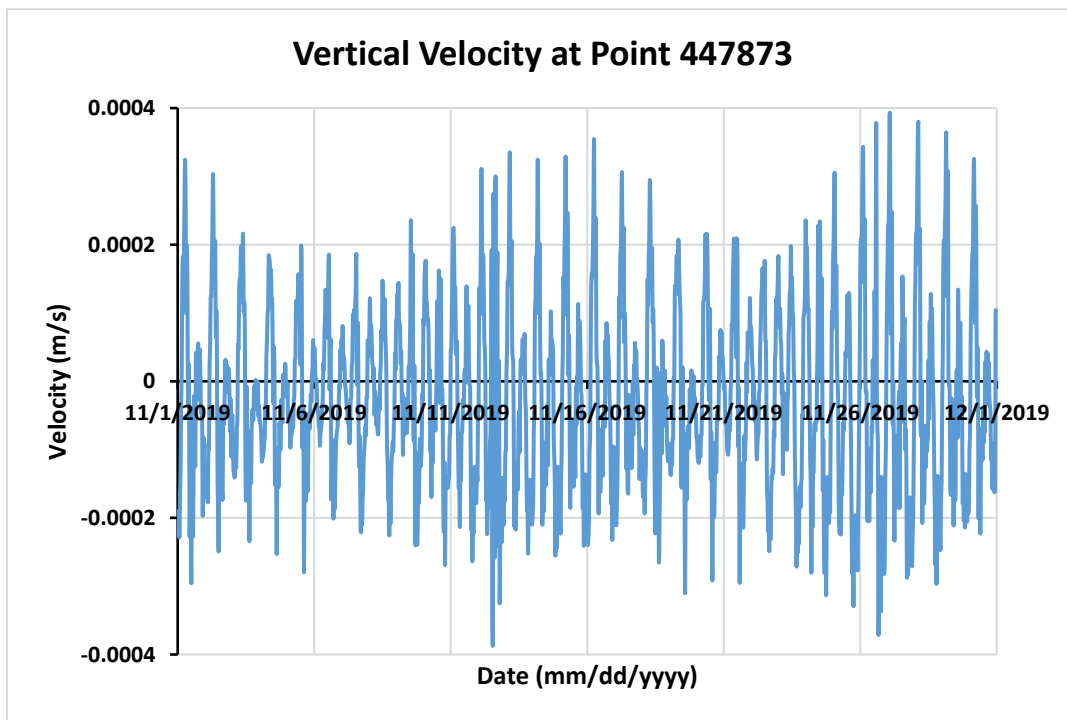


Figure 4.9: Vertical velocity at point 447873 for 30 days based on the results of the model

4.2.3 Salinity

Salinity is an important factor that changes during time based on the flow and affects the density of water and the movement of microplastic particles in the river. Salinity changes through various layers due to differences in the density of saline and fresh water. Figure 4.10 shows the location of point 453348. The salinity profile of layers 15, 8, and 1 at this point are displayed in figure 4.11. Based on this figure, stratification is captured between different layers.



Figure 4.10: Location of point 453348 in the study area (Brown line indicates the study area)

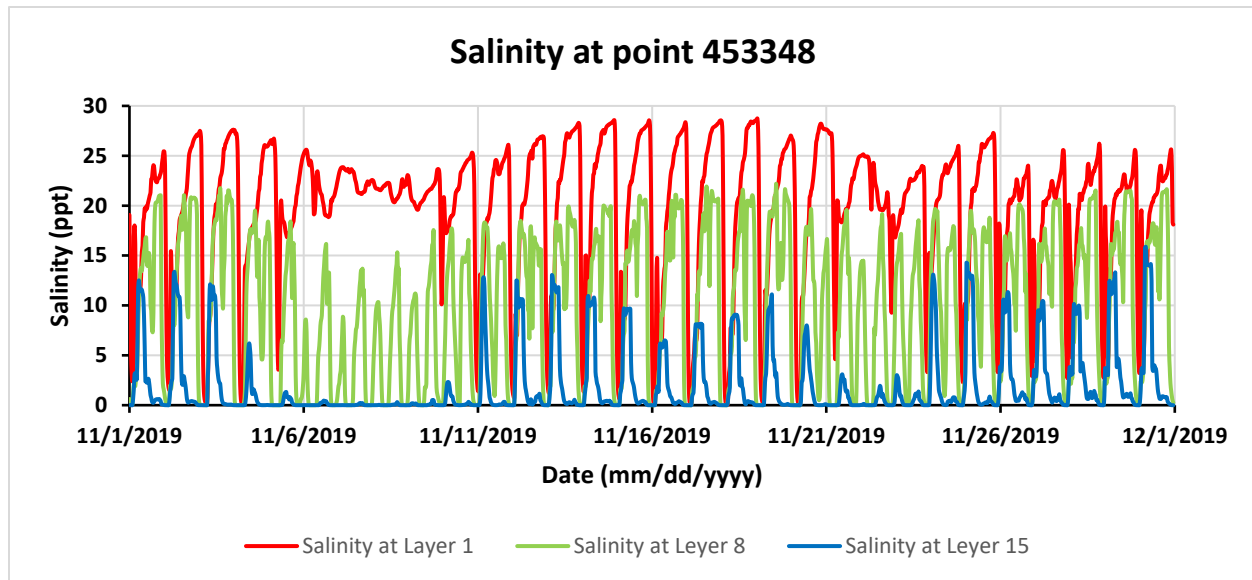


Figure 4.11: Comparison between salinity in layers 15, 8, and 1 at point 453348 for 30 days based on the results of the hydrodynamic model

As Point 453348 is located very close to the ocean, most of the water in the lower layers is very salty. The salinity of water in higher layers due to vertical turbulence and mixing increases at special times of the month and day. The graph of the velocity of water and as a result salinity in different layers doesn't follow a line due to flow from upstream and water level from downstream. Sometimes this graph gets close to a line, a logarithmic graph, or a power graph. This is the reason differences in salinity between different layers in all these 30 days are not the same.

Also, the salinity for all points in the base mesh for two days, 11/02/2019 at 18:00 and 11/28/2019 at 17:30 in figures 4.12 and 4.13. It was tried two times with the highest amount of saline water in the river being shown. Since saline water moves through lower layers these figures display the salinity of water through the lower part of the Fraser River in the first layer. The results of the hydrodynamic model match reasonably with the result of the field experiment done by Tsz Yeung Leung et al., 2018, which were discussed in the previous chapter.

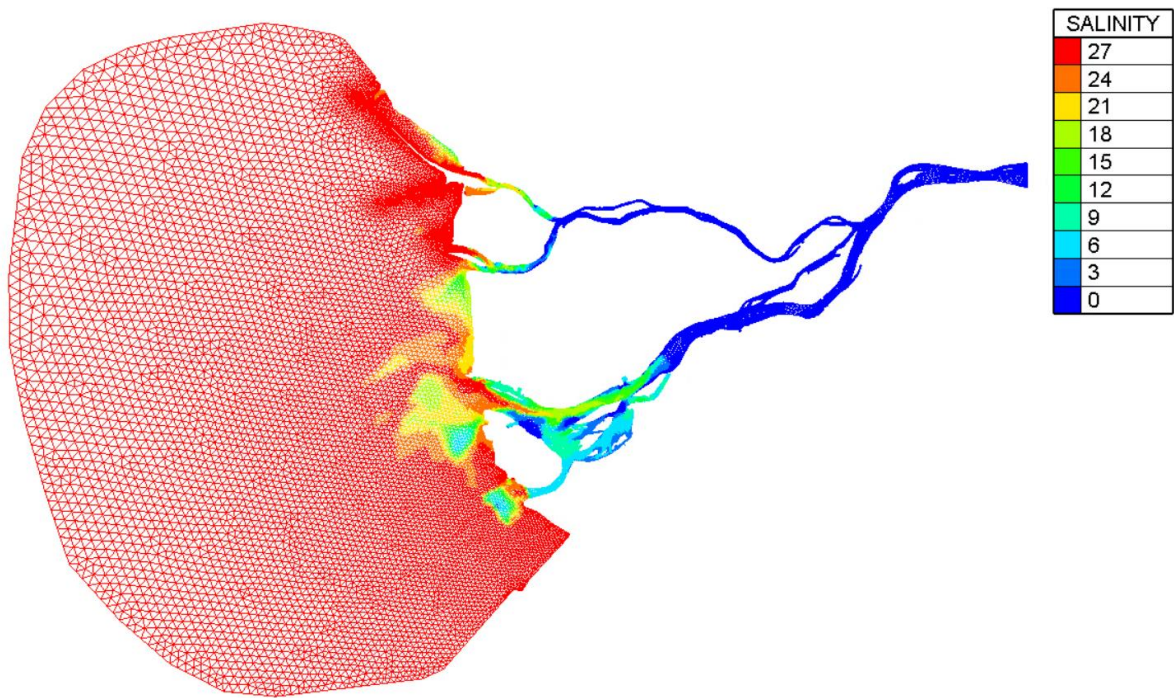


Figure 4.12: Salinity (ppt) of water based on the results of the model at 11/02/2019, 18:00

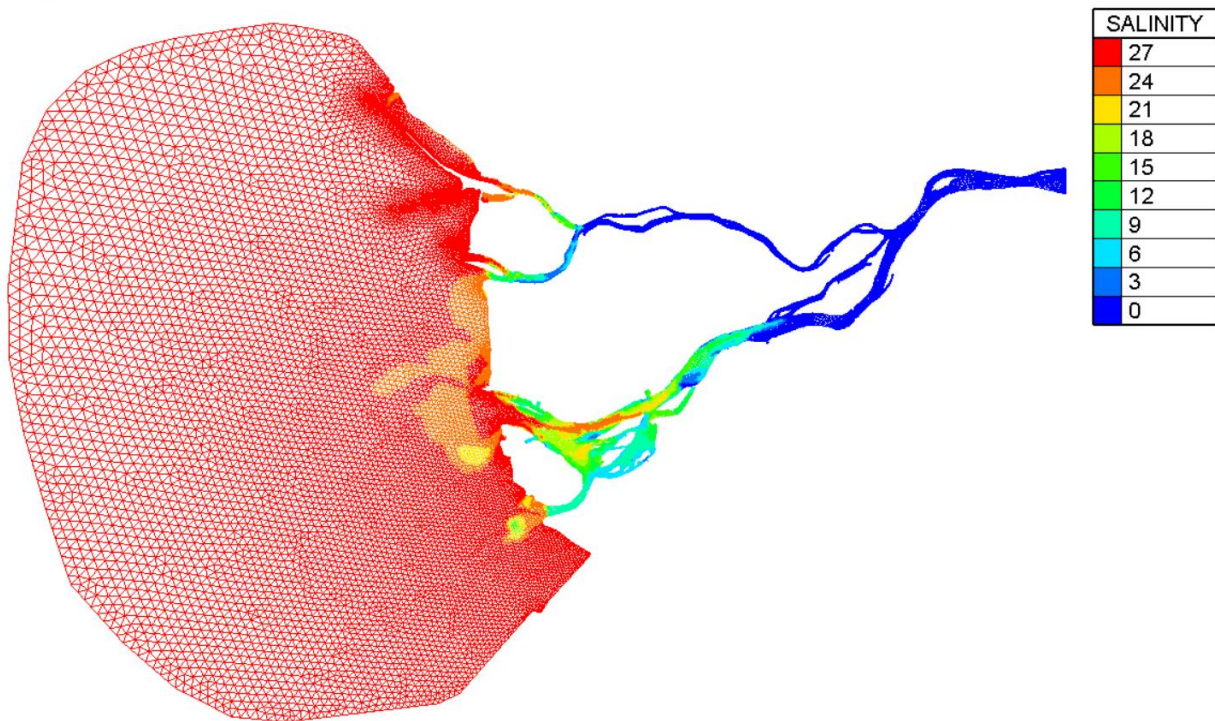


Figure 4.13: Salinity (ppt) of water based on the results of the model at 11/28/2019, 17:30

4.2.4 Validation

Validation is required for every hydrodynamic model. Since it can help to have more confidence in the computed results. The only flow measurement station in this part of the Fraser River was used in the boundary conditions section. The most detailed information about salinity in the study area was discussed previously. The only parameter that is left for validation is water level. In this region, there is another water level station very close to the upstream boundary that was used for results validation. The location of station New Westminster (07654) is displayed in figure 4.14. The resolution of water level data at this station between 11/1/2019 and 11/30/2019 is hourly. The nearest point in the base mesh to the location of this station is point 439467. A comparison between the real data and modeled data about the water level at this point is displayed in figure 4.15.



Figure 4.14: Location of station New Westminster (07654) for water level data

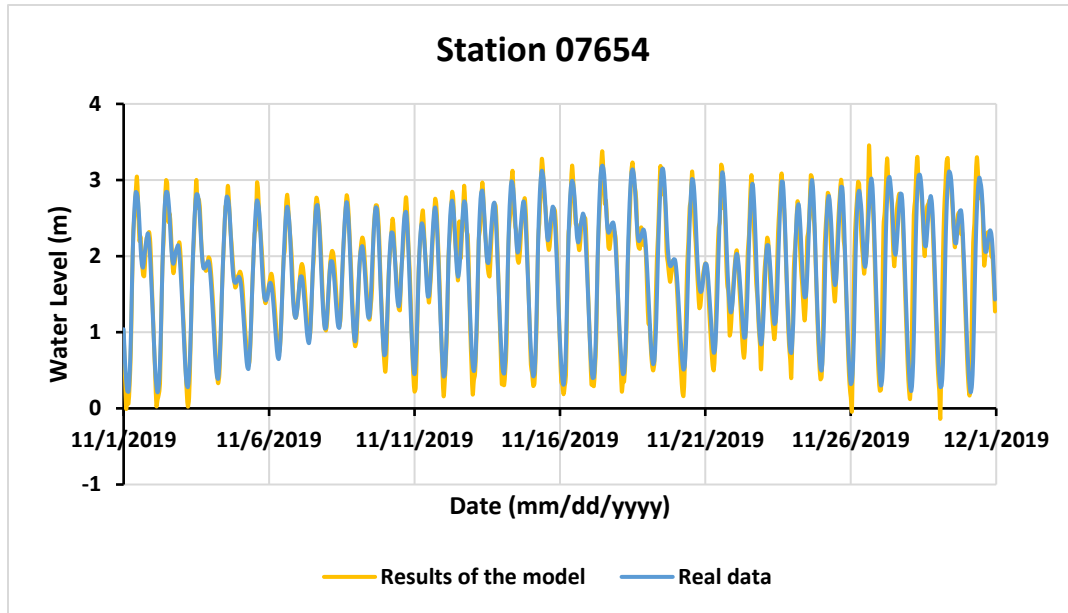


Figure 4.15: A comparison between the real data and modeled data about the water level at station 07654

In this photo, the modeled data follows the pattern of the real data. In some parts, the differences are lower, and in some parts this difference increases. A number of reasons may account for this such as the resolution and error of the input data, the location of the water level measurement station for indicating the boundary conditions was not very close to the downstream boundary, inaccuracies in the estimation of roughness coefficient and vertical diffusion coefficient, and the distance between the upstream boundary and discharge measurement station. The maximum value for real data is equal to 3.23 m and the minimum value for real data is 0.12 m. The results of the simulation show that the maximum water level for this period is 3.41 m and the minimum water level is equal to -0.09 m. The maximum difference between measured and simulated data is about 12 % which is acceptable in this study.

4.3 Results of the Particle Tracking Model

In this section, the results of the CaMPSim-3D model will be discussed for all nine scenarios. A point worth mentioning about all the pictures in this part of the chapter, some particles have the

same locations, so the photos only show the areas of the Fraser River with microplastic particles and not the total amount.

Each scenario in the particle tracking model has 2876 time steps. The results of the model for the first scenario are discussed with details in the next part to explain more about the process and after that, all other eight scenarios will be discussed briefly.

4.3.1 Scenario 1

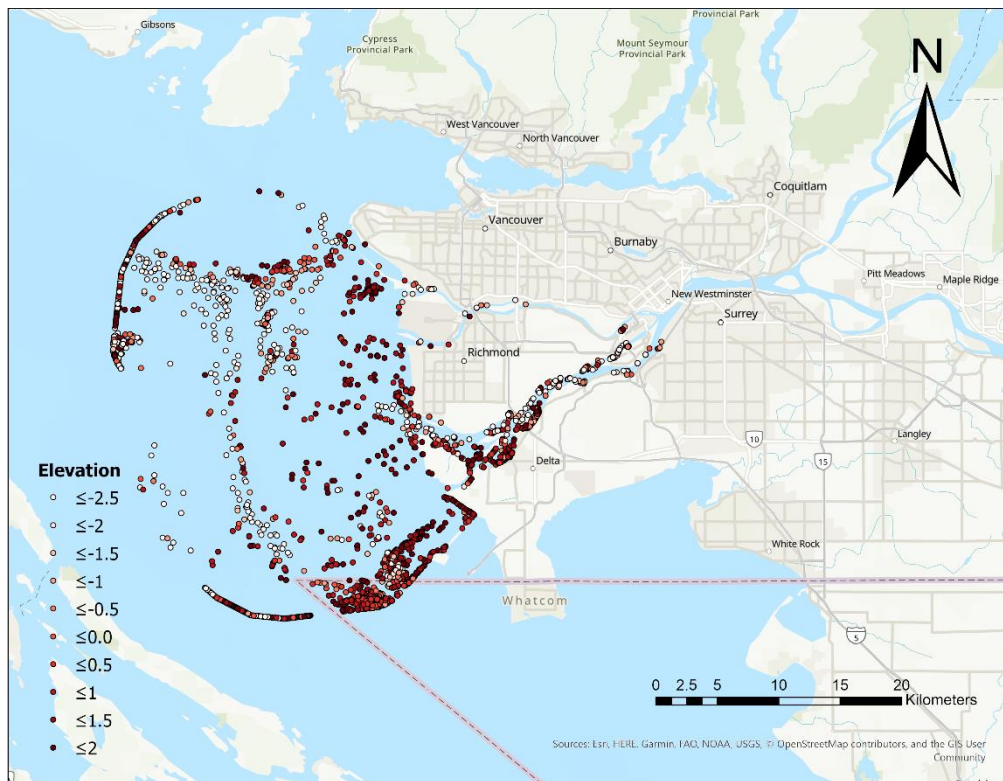
In this scenario 60,000 microplastic particles were released immediately from Glenbrook CSO. Tenkilometers after Douglas Island, the lower part of the Fraser River splits into two branches. This combined sewer overflow is located about 6.5 kilometers from Douglas Island. The lower branch is wider, and the elevation of the ground is lower there, so it has more flow than the upper branch. It is reasonable that most of the particles flow from CSO to the ocean through this branch. Results showed that only 6 percent of all released particles from this CSO remained in the river after 30 days and others entered the ocean. It is important to mention that vertical circulations in this area affect the vertical positions of the particles. Figure 4.16 shows the location of particles and their elevation on 11/02/2019 at 00:00 am, 11/16/2019 at 00:00 am, and 12/01/2019 at 00:00 am.

As can be seen in the images, at first the particles are close to the surface, but eventually, they sink due to their settling velocity and vertical circulation. In the last step, particles are mostly located at specific locations, so many of them have the same x and y coordinates. In figure 4.16.c the color of each circle shows the highest elevation of particles at that point. The results of the model show that the particles distribute in different elevation levels and based on the ArcGIS Pro the mean value for the elevation of particles after 30 days of simulation is approximately -38 m, which is reasonable since most of them enter the ocean and do not stay on the surface.

a)



b)



c)

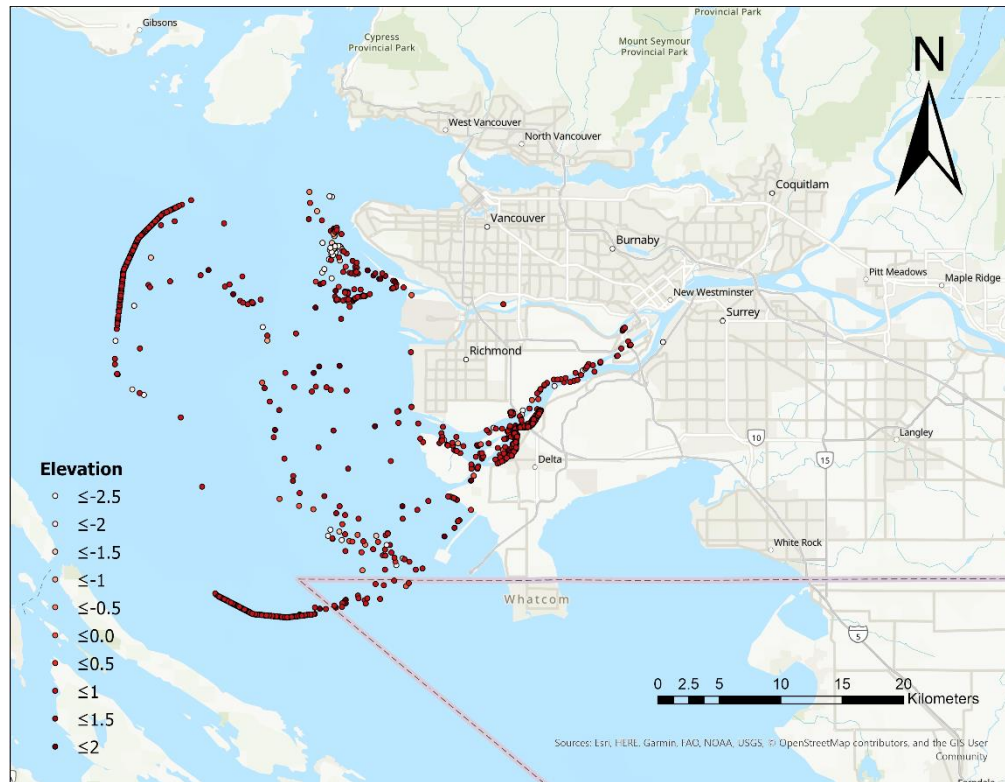


Figure 4.16: Location and elevation (m) of microplastic particles after a) 1 day, b) 15 days, and c) 30 days based on the results of the model

4.3.2 Other Scenarios

In this part, the final location of particles in the last time step for 8 other scenarios will be shown in figures 4.17-24. Also, more details about the results of each scenario are discussed in table 4.1.

Due to the higher number of tight turns with low depths of water in the lower branch of the Fraser River, if a particle enters the lower branch it has a greater chance of remaining in the river. But at the end of the upper branch, there are two breakwaters. In the area between these two, the velocity of water is very low (this is the reason for building breakwaters) and also the depth is low too. These are the reasons that in most of the scenarios, this region is full of particles.

It is worthwhile to mention that, similar to figure 4.16, when the particles have the same x and y coordinates, the particle with the highest elevation is shown in the pictures, but the mean elevation values for each of the scenarios are indicated in table 4.1.

In this study, points with x less than 480,000 are considered in the ocean.

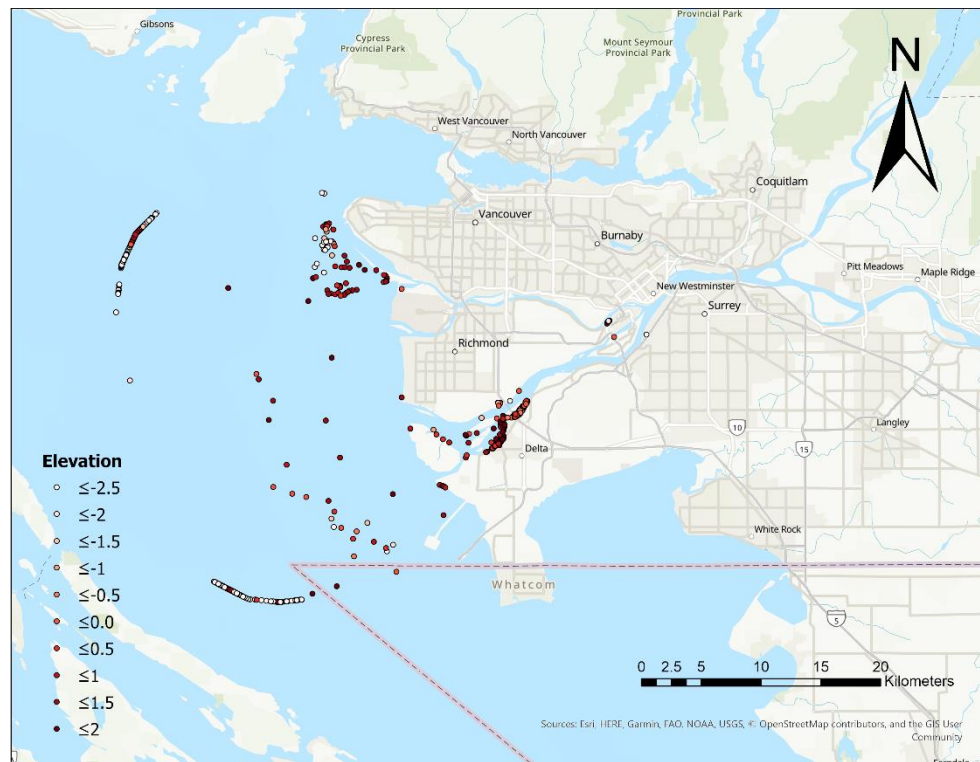


Figure 4.17: Final location and elevation (m) of particles S2, release location: New Westminster CSO, 12/01/2019 00:00 am

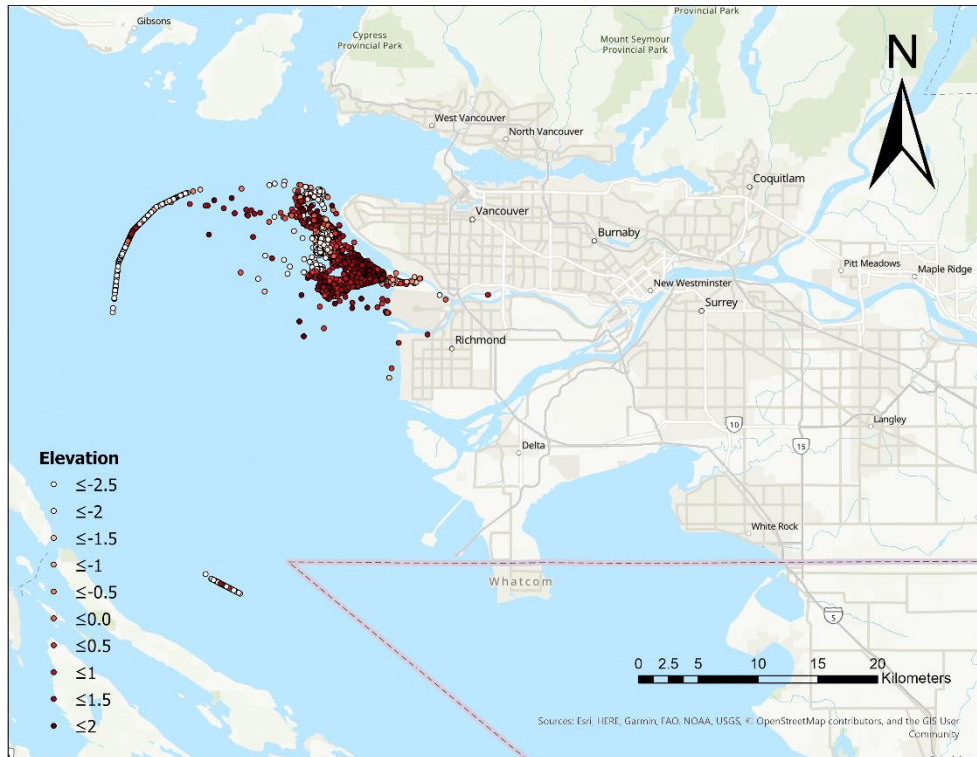


Figure 4.18: Final location and elevation (m) of particles S3, release location: Borden CSO, 12/01/2019 00:00 am

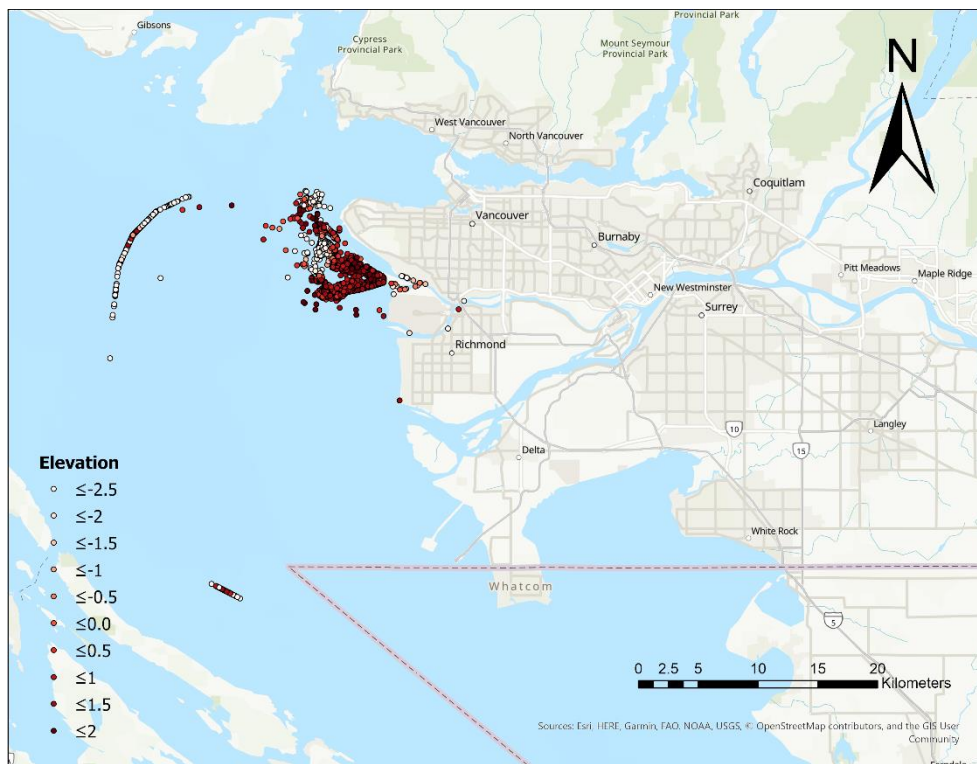


Figure 4.19: Final location and elevation (m) of particles S4, release location: South Hill CSO, 12/01/2019 00:00 am

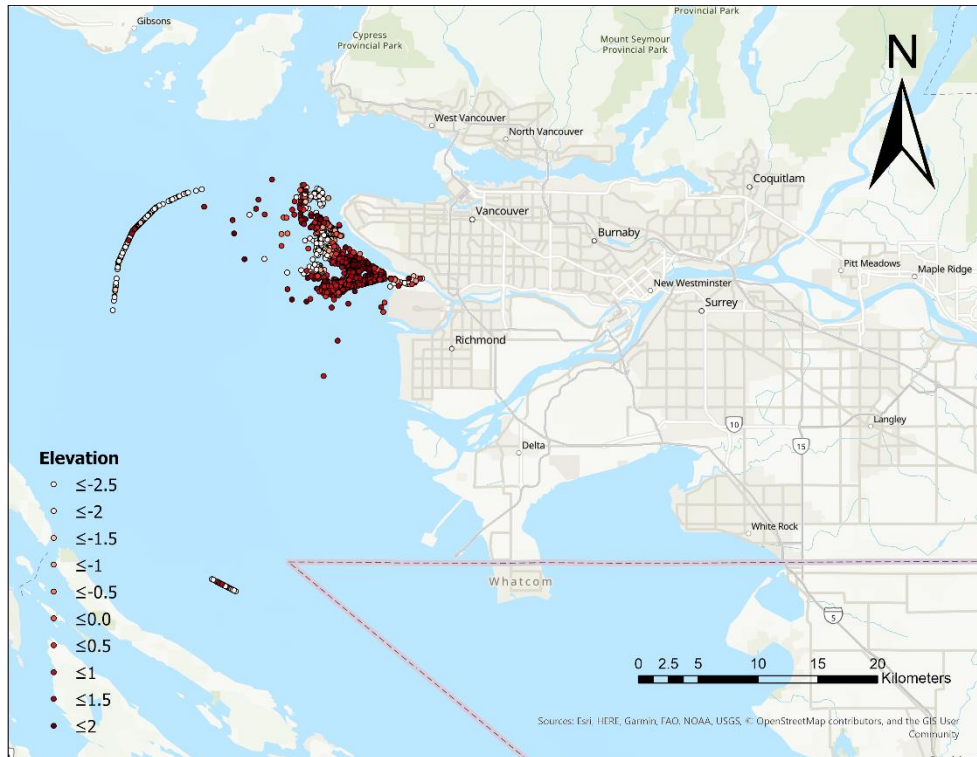


Figure 4.20: Final location and elevation (m) of particles S5, release location: Manitoba CSO, 12/01/2019 00:00 am

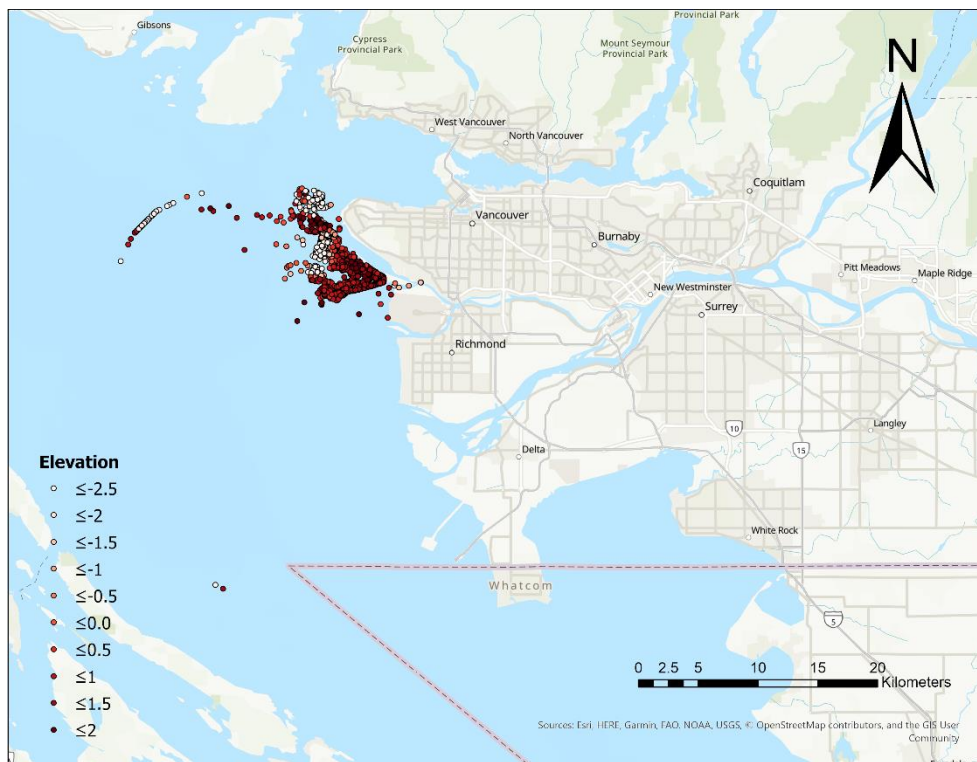


Figure 4.21: Final location and elevation (m) of particles S6, release location: Angus CSO, 12/01/2019 00:00 am

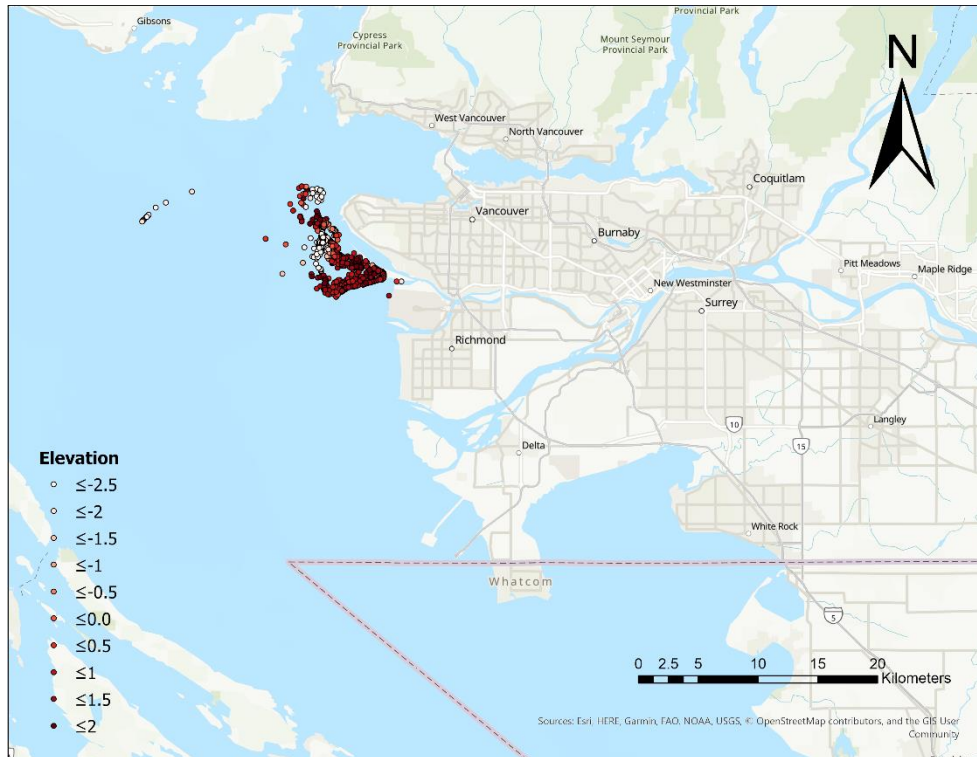


Figure 4.22: Final location and elevation (m) of particles S7, release location: MacDonald CSO, 12/01/2019 00:00 am

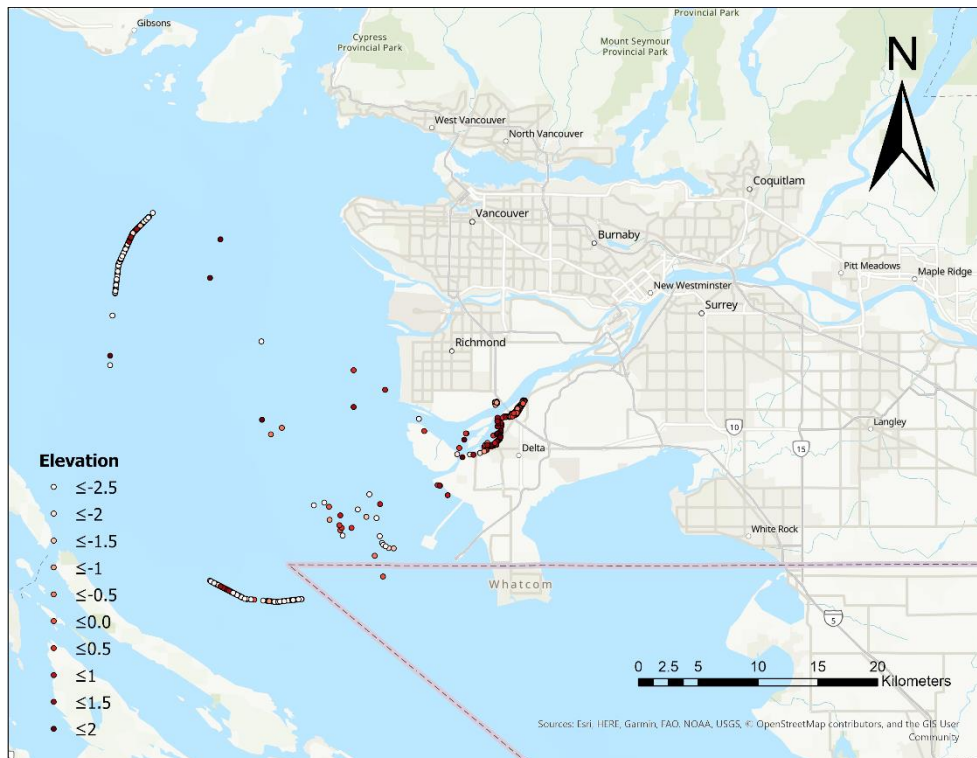


Figure 4.23: Final location and elevation (m) of particles S8, release location: Annacis Island WWTP, 12/01/2019 00:00 am



Figure 4.24: Final location and elevation (m) of particles S9, release location: Lulu Island WWTP, 12/01/2019 00:00 am

In the next section, table 4.1 is shown. In this table, details about the results of the particle tracking model for all nine scenarios will be indicated, such as the number of particles that will remain in the river after 30 days of simulation and their percentage, and also the average values of the elevation of the microplastic particles both in the Fraser River and in the ocean.

Table 4.1: Results of the particle tracking model for all nine scenarios

Scenario	Release Location	Number of Particles Remained in the River	Percentage	Mean Elevation (m)
S1	Glenbrook CSO	3673	6	-38
S2	New Westminster CSO	1998	5	-50
S3	Borden CSO	6051	10	-130
S4	South Hill CSO	4104	11	-130
S5	Manitoba CSO	3978	10	-134
S6	Angus CSO	3136	21	-156
S7	MacDonald CSO	1907	19	-161
S8	Annacis Island WWTP	2002	5	-38
S9	Lulu Island WWTP	49	<0.5	-43

4.4 Results of the Clustering Algorithm

In this part the OPTICS algorithm is used for the final location of microplastic particles in the last time step of each scenario, to find the accumulation zones of microplastics. The particles in each scenario are released immediately. Based on the results of the hydrodynamic model, it is reasonable to assume that the mean velocity in the lower part of the Fraser River is approximately 1 m/s or 3.6 km/h. The length of the study area is about 36 km, which means that only 10 hours is enough for a particle to enter the ocean. In light of the lower velocities in narrow areas, backwaters, and tidal forces during the day, it may be reasonable to consider that 24 hours or a day is enough time for a particle to release and enter the ocean. As a result, it is possible to say that particles that are still in the river will remain in the river for a longer time and the areas with a high amount of particles are permanent accumulation zones of microplastic particles.

In this section, first, the accumulation zones based on the release locations are indicated for each scenario, and then by putting the results of the particle tracking model for all scenarios together the main accumulation zones of microplastic particles in the Fraser River will be found. In this way, more details about the final locations of particles and their accumulation zones are provided for each scenario which can be used for future source-receptor studies. Also, the main accumulation zones correspond more closely to the real situation and can be used to manage the lower part of the Fraser River, and the City of Vancouver or other nearby cities can find the most polluted locations and make the best decisions based on that information.

Figures 4.25, 4.26, and 4.27 display the accumulation zones for scenarios 1, 2, and 3. From scenario 4 up to scenario 7 the accumulation zones are the same as scenario 3 and only the size of the accumulation zone and the number of particles in those zones are different which is not visible and doesn't make big differences in the pictures. So the results of scenarios 4 to 7 are not shown but are the same as in figure 4.27. Figure 4.28 displays the results of scenario 8.

Also based on table 4.1 in the previous part, since the Lulu Island WWTP is very close to the ocean most of the particles are evacuated to the ocean. As a result, there is no accumulation zone in the river in scenario 9. Figure 4.29 shows the results of all nine scenarios together which is the main location and quantity of particles that we were looking for. It is good to mention that in CaMPSim-

3D particles do not leave the study area, as a result they stick to the boundaries. Figure 4.30 illustrates the accumulation zones for all scenarios together.

It is good to mention that this algorithm is only used for particles that are in the river and not in the ocean. This is the reason that there is no accumulation zone in the ocean, regardless of the microplastic particles are in the ocean.

The locations of accumulation zones that are predicted by the OPTICS algorithm are reasonable and predictable. Most of these locations are in the narrow parts, turns, breakwaters, and dead ends of the river, where the velocity and depth of water are lower there.

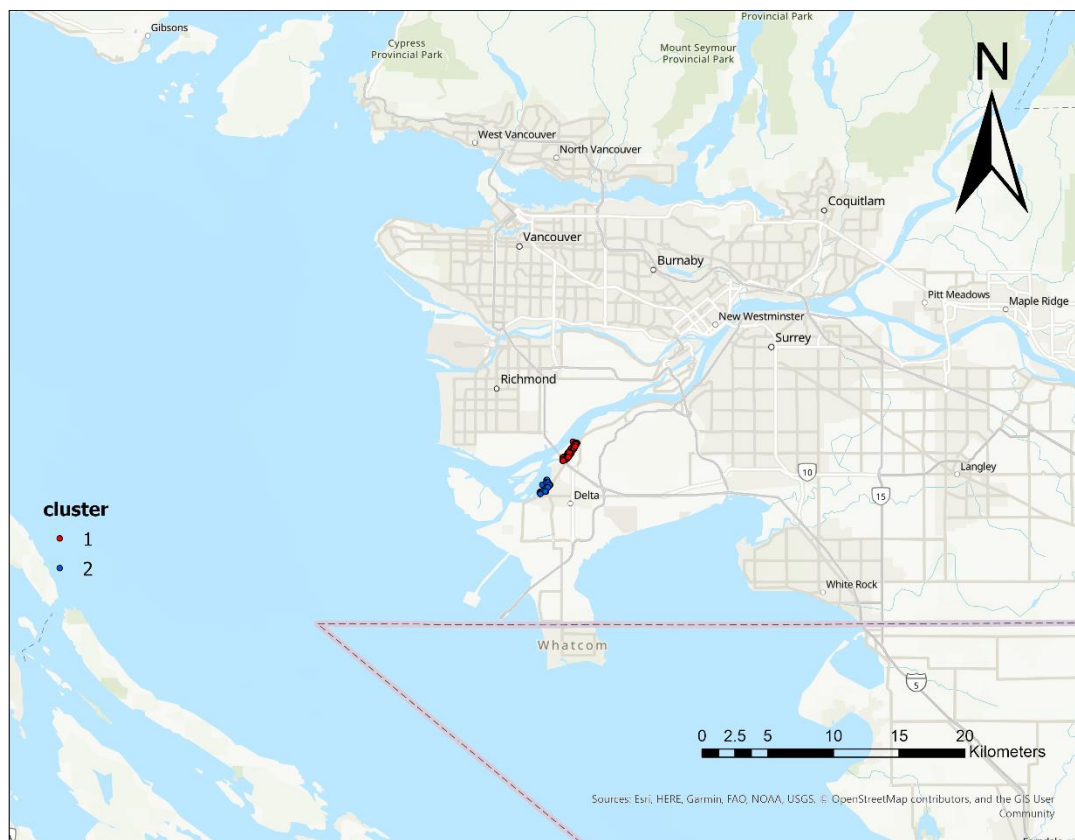


Figure 4.25: Accumulation zones in scenario 1

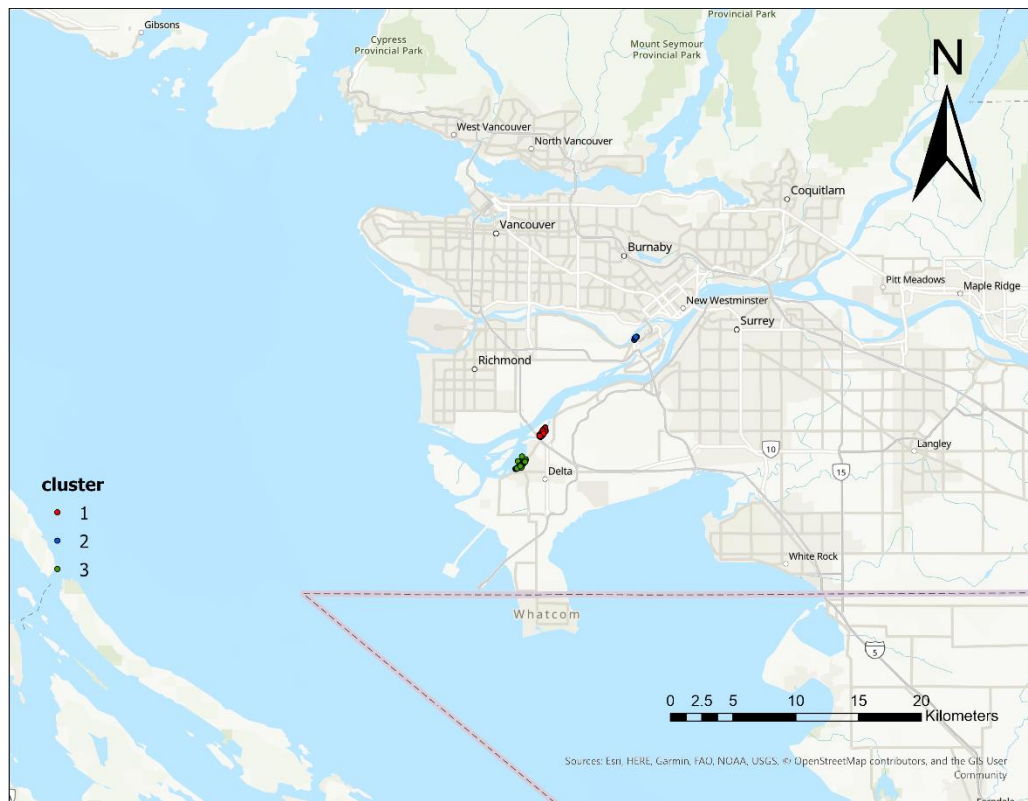


Figure 4.26: Accumulation zones in scenario 2

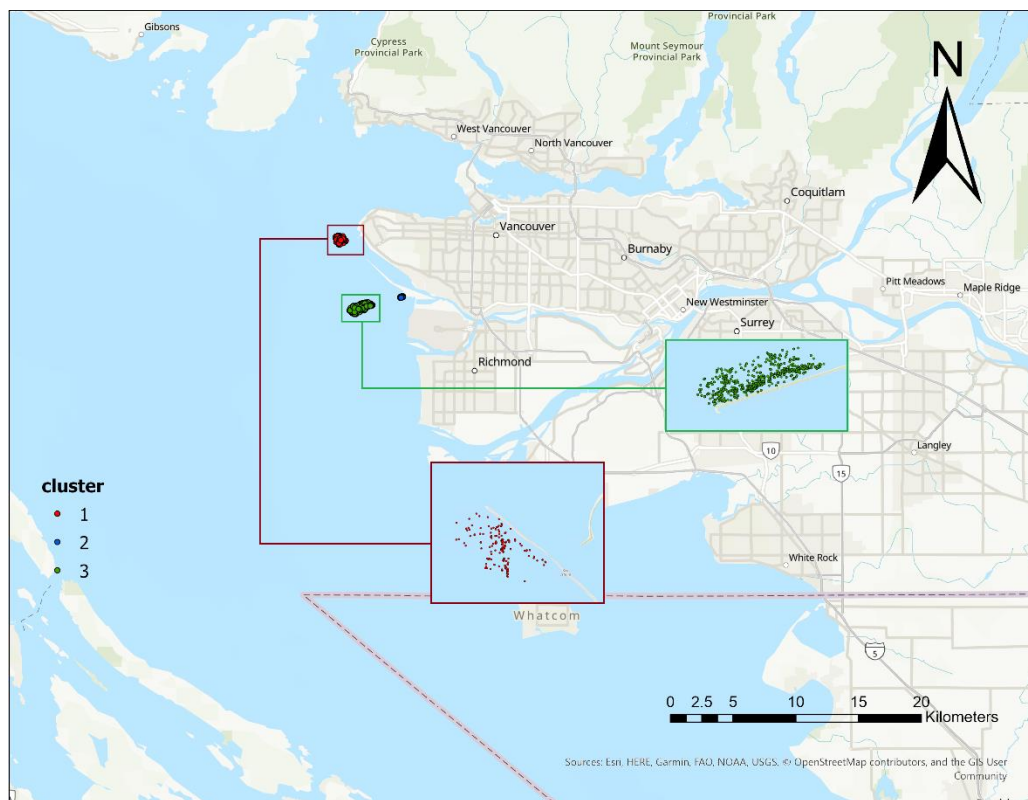


Figure 4.27: Accumulation zones in scenario 3

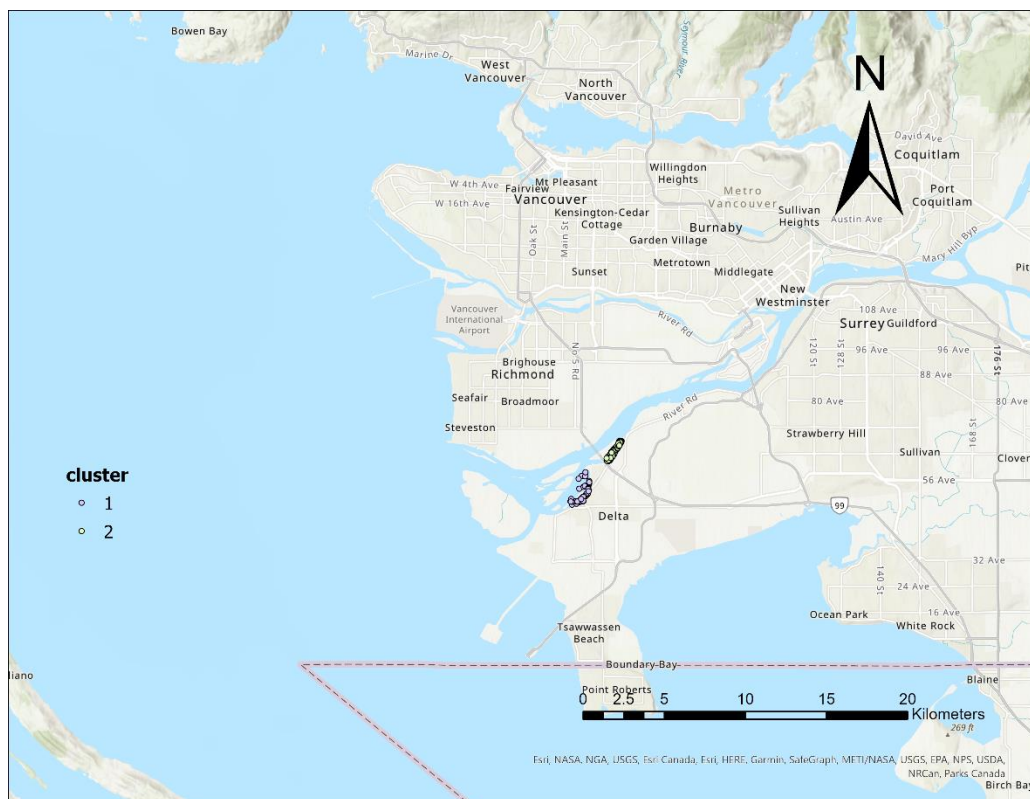


Figure 4.28: Accumulation zones in scenario 8

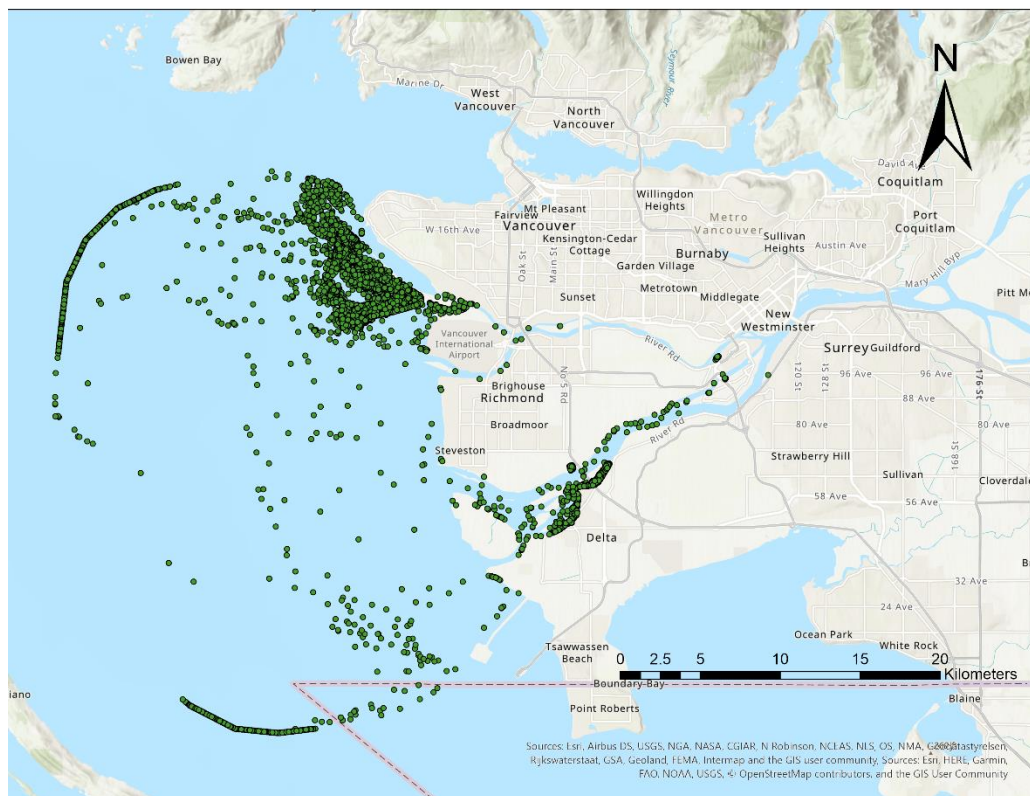
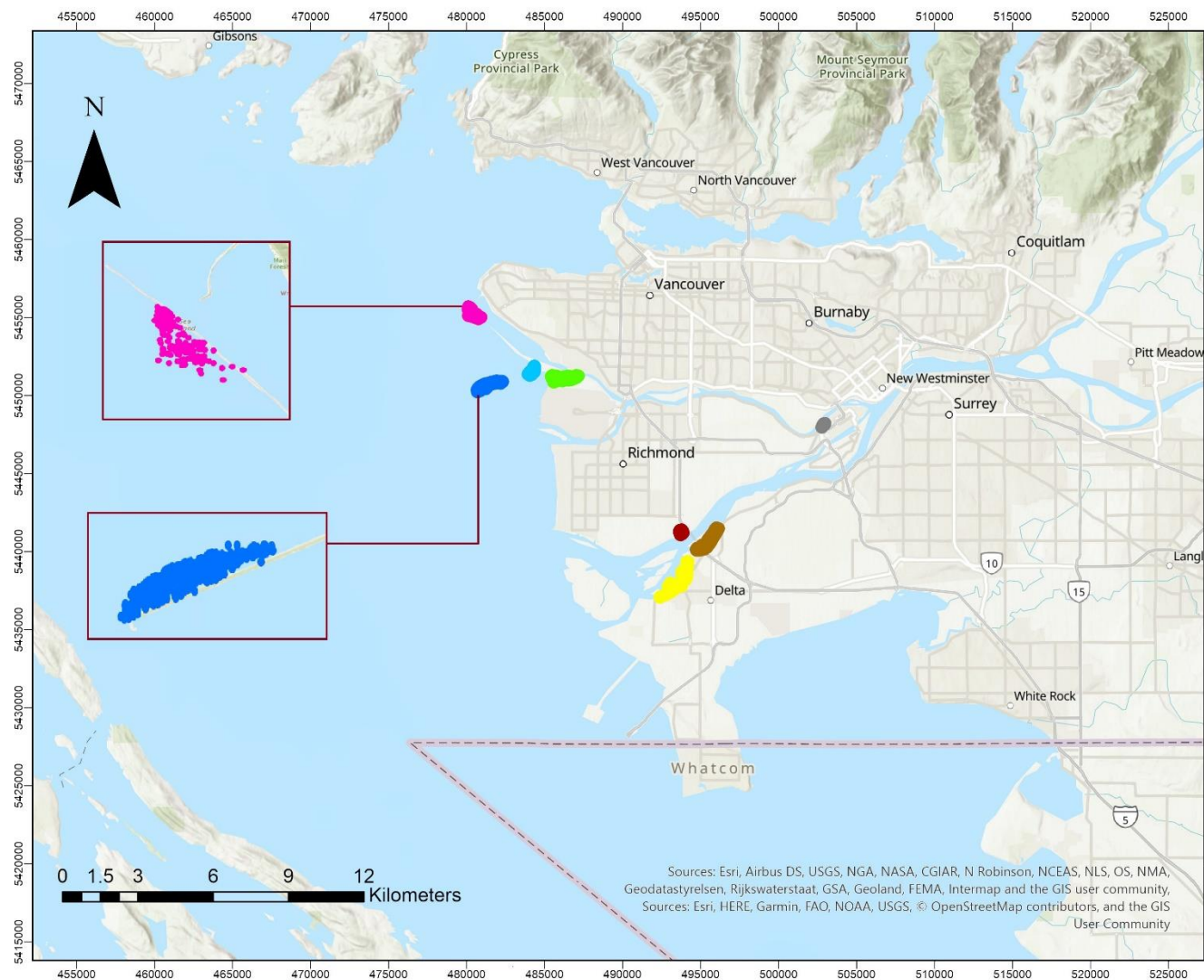


Figure 4.29: Final location of all particles



Location of predicted accumulation zones of microplastics in the lower part of the Fraser River

Figure 4.30: Main accumulation zones

To validate the results of the clustering algorithm and check the accuracy of accumulation zones, two experiments were chosen. One was done by the National Research Council of Canada (NRC), and the other one was done by Brunner, 2021. In the NRC field experiment, sampling was done during times when combined sewer overflows were actively discharging. The sampling locations were chosen based on the CSOs locations at different depths. So they possibly have the highest numbers of microplastic particles in the Fraser River. The research done by Brunner, 2021, is a continuation to Bourdages et al., 2017. In these studies sampling from different parts of the Fraser River was done based on the population, surrounding industries, water depth, and water velocity. Finally 5 locations with the highest number of microplastic particles were chosen for further research, and in total 65 samples during different times of the year were collected from these five locations. Three of them were in the study area of this thesis.

Figure 4.31 displays the locations of sampling in these two studies. Table 4.2 provides more information about each of the sampling sites.

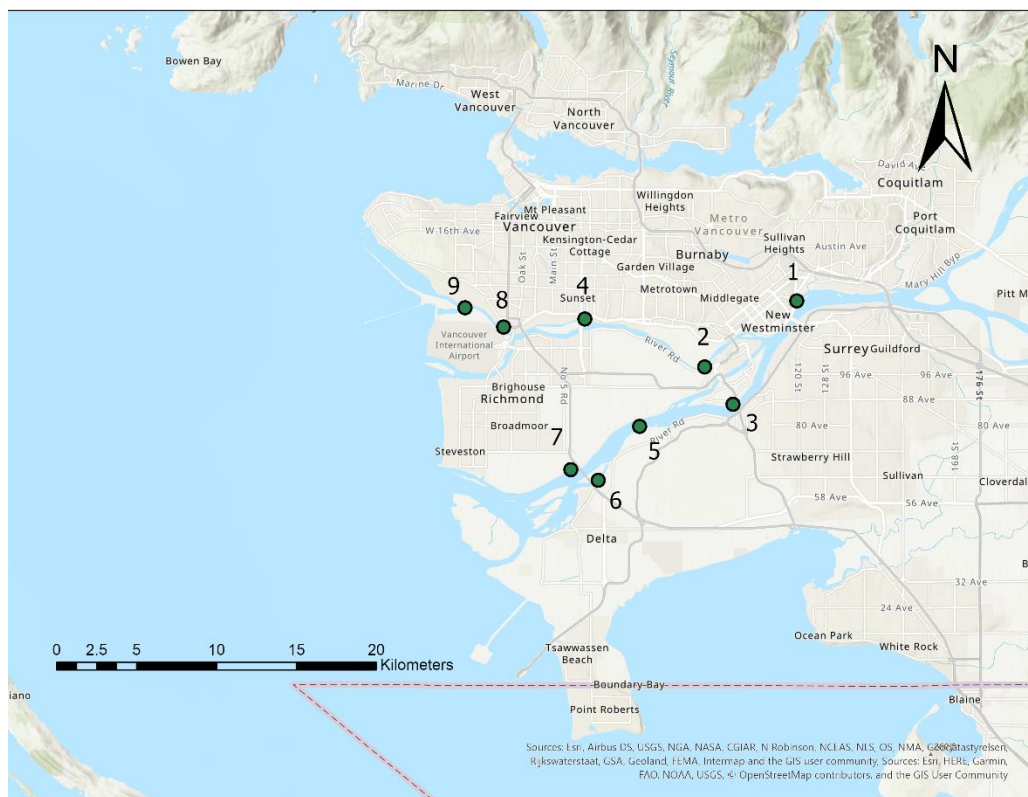


Figure 4.31: Sampling locations in the lower part of the Fraser River

Four of the predicted accumulation zones by the OPTICS algorithm are very close to some of these suspicious locations which are considered to have the highest number of microplastic particles.

There are various reasons for some differences between the sampling results and the results of the model. The most important reason to note is that these samples were collected during CSO discharges, which means during sampling times, those locations experienced the most particles, which was temporary, but in this study, the goal was to determine the permanent locations of accumulation zones. This period has also seen some microplastic particles entering the study area from the upstream boundary, which due to lack of information are not taken into account in this study. It is noteworthy that in this study three models are used and they depend on each other. Each of them has errors. Also, sampling is done by humans, which means there are possible human errors.

Also, the breakwater in the upper branch is not considered as part of the river in the sampling studies so there is no measurement for that location but because of low water velocity and depth, logically it is one of the most vulnerable places.

Table 4.2: Sampling details

ID	Site Name	Water Depth (m)	Sampling Depth (m)	Number of Microplastics (MPs/m ³)	Reference
1	Sepperton	15.5	6	10	Parizi, 2019
2	Boundary	9.2	5	12	Parizi, 2019
3	Annacis Island	15.5	6	1955	Brunner, 2021
4	Glenbrook	7	3	10	Parizi, 2019
5	Tilbury	14.1	6	14	Parizi, 2019
6	Deas Island	-	-	12.2	Brunner, 2021
7	Deas Pacific Marine	-	-	14	Brunner, 2021
8	Angus	4.4	2	10111	Parizi, 2019
9	Macdonald	6.2	3	12	Parizi, 2019

In this table, Angus and Annacis Island sampling points are located in the discharge area of combined sewer overflow and wastewater treatment plant and their results are used in this study for computing the number of released particles. As explained above this fact affects the number of microplastics and the results of the samplings in those locations and this is the reason for two highest numbers in the table 4.2 which are far from other numbers. The other way that can help us to make sure about the correctness of the results of the OPTICS algorithms is that the average of microplastic particles in these locations is $12 \text{ MPs}/m^3$ (without considering those two samplings), and the number of microplastic particles in all those four locations is above the average.

Chapter 5. Conclusions and Recommendations for Future Studies

5.1 Conclusion

The objective of this study was to identify the accumulation zones of microplastic particles with the help of numerical models, as well as machine learning algorithms, in order to address one of the world's growing concerns. Initially, the base mesh was created, and then by using available bathymetry, water level, and discharge data, the hydrodynamic model was created using TELEMAC 3D. It is worth mentioning that there was only one tracer in this model which is salinity and its values in the two boundaries were derived from the literature. To validate the results of the model a comparison between the measured water level and the simulated water level at a point in the study area was done. Particle tracking was performed using a new model called CaMPSim-3D. Nine scenarios were considered based on the release locations of microplastics studied by previous researchers. The results of these scenarios were studied separately and together. In the final step, OPTICS algorithms which is a branch of unsupervised learning and more specifically clustering, indicated the accumulation zones of microplastic particles. The results of the OPTICS algorithm were compared with the results of some field experiments. There were some similarities and some differences that were discussed in the previous chapter.

A summary of the most important points in this thesis is provided below:

- The Hydrodynamic model was able to simulate the water level in the study area with an acceptable accuracy
- There were no detailed data about the salinity of the lower part of the Fraser River but the results match with the limited available measured data
- Stratification consequent of mixing fresh water and saline water was captured in the hydrodynamic model

- The effect of tidal forces and vertical circulations is visible on the elevation of microplastic particles
- The particle tracking model shows that the final location of particles depends on their release location but in all of the scenarios almost 80 percent of particles entered the ocean, but definitely the remaining particles are harmful to the surrounding environment and need to be treated in the right way
- The predicted accumulation zones are reasonable due to the water level, velocity, and shape of the river in those regions and also have a good match with the measured accumulation zones
- The OPTICS algorithm predicted eight accumulation zones in the study area and based on the results the breakwater in the upper branch is a threat to its surrounding environment, also two beaches in the lower branch should be cleaned regularly since they are famous places that people go in their free time and microplastic pollution there can be dangerous

5.2 Recommendations for Future Studies

Based on the results obtained from this study, the following recommendations are proposed for future studies:

- Some field measurements about the salinity, water level, and flow in the boundaries, since the available stations are close to the boundaries, but they are not located exactly on the boundaries
- In this study, due to a lack of knowledge about the microplastic particles entering the study area from the upstream boundary, they were not considered but their number is significant so in future studies, it is better to consider them
- Microplastics have different shapes, sizes, and densities which affect their settling velocity and definitely their accumulation zones so in future research it is better to study the transport of other types of microplastic particles
- Collecting more precise data about the discharge of microplastic particles from combined sewer overflows and wastewater treatment plants

- Using different clustering algorithms for finding accumulation zones and comparing their results together to find the best one
- Field sampling from the predicted accumulation zones and the rest of the Fraser River to have a better tool for validating the results of the clustering algorithms
- Performing source-receptor studies

Chapter 6. References

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Appendix

Steering File

```
/-----  
/ TELEMAC3D Version v8p2  
/ nom inconnu  
/-----  
/-----  
/ INPUT-OUTPUT, FILES  
/-----  
LIQUID BOUNDARIES FILE  ='LQD.lqd'  
3D RESULT FILE          ='test_3D.slf'  
GEOMETRY FILE           ='final2.slf'  
2D RESULT FILE          ='test_2D.slf'  
/STEERING FILE          ='BerreLagoon.cas'  
BOUNDARY CONDITIONS FILE ='final.cli'  
FORTRAN FILE = 't3d_tidal_flats.f'  
COMPUTATION CONTINUED = NO  
/PREVIOUS COMPUTATION FILE='lastStep.slf'  
INITIAL TIME SET TO ZERO = YES  
/-----  
/ INPUT-OUTPUT, GRAPHICS AND LISTING  
/-----  
VARIABLES FOR 3D GRAPHIC PRINTOUTS =Z,U,V,W,TA1  
GRAPHIC PRINTOUT PERIOD      =450  
LISTING PRINTOUT PERIOD      : 450  
VARIABLES FOR 2D GRAPHIC PRINTOUTS =U,V,S,B  
/NUMBER OF FIRST TIME STEP FOR GRAPHIC PRINTOUTS: 241920
```

```

MASS-BALANCE                      =true
/-----
/ EQUATIONS
/-----
/MAXIMUM NUMBER OF ITERATIONS FOR PROPAGATION    =600
NUMBER OF BOTTOM SMOOTHINGS                =2
ACCURACY FOR DIFFUSION OF VELOCITIES          =1.E-8
ACCURACY FOR DIFFUSION OF TRACERS              =1.E-8
LAW OF BOTTOM FRICTION                      =4
FRICTION COEFFICIENT FOR THE BOTTOM            =0.07
SOLVER FOR PROPAGATION                      =2
NON-HYDROSTATIC VERSION                     =NO
VERTICAL TURBULENCE MODEL                   =2
COEFFICIENT FOR VERTICAL DIFFUSION OF VELOCITIES : 1.0E-4
COEFFICIENT FOR VERTICAL DIFFUSION OF TRACERS: 0.0
COEFFICIENT FOR HORIZONTAL DIFFUSION OF TRACERS: 0.0
HORIZONTAL TURBULENCE MODEL                  : 1    /1:constant 2:Mixing Length
Model 3:k-eps 4:smagorinsky
COEFFICIENT FOR HORIZONTAL DIFFUSION OF VELOCITIES : 1.0E-4
/HORIZONTAL TURBULENCE MODEL
/MIXING LENGTH MODEL                        : 1
MIXING LENGTH MODEL                        : 3
DAMPING FUNCTION                            : 3
/MAXIMUM NUMBER OF ITERATIONS FOR VERTICAL VELOCITY =500
/-----
/ EQUATIONS, BOUNDARY CONDITIONS
/-----
VELOCITY VERTICAL PROFILES                =1;1
VELOCITY PROFILES                        =1;1
OPTION FOR LIQUID BOUNDARIES              =1;2

```

```

TREATMENT OF FLUXES AT THE BOUNDARIES =1;2
/-----
/ EQUATIONS, DIFFUSION
/-----
/MAXIMUM NUMBER OF ITERATIONS FOR PROJECTION           =600
/MAXIMUM NUMBER OF ITERATIONS FOR DIFFUSION OF VELOCITIES =600
PRECONDITIONING FOR PPE                                =34
/MAXIMUM NUMBER OF ITERATIONS FOR PPE                    =500
PRECONDITIONING FOR DIFFUSION OF VELOCITIES      : 34
PRECONDITIONING FOR DIFFUSION OF TRACERS        : 34
/-----
/ EQUATIONS, INITIAL CONDITIONS
/-----
INITIAL ELEVATION =5.0
/-----
/ INPUT-OUTPUT, INFORMATION
/-----
/TELEMAC-2D RELEASE ='V7P01'
/-----
/ NUMERIC PARAMETERS
/-----
ORIGINAL DATE OF TIME = 2019;10;21
ORIGINAL HOUR OF TIME = 00;00;00
TIME STEP = 10. /previously 5 for 10 layers
DURATION = 950400 / max = 11 days (950400s)
NUMBER OF HORIZONTAL LEVELS =15 /15
MESH TRANSFORMATION                                :
/-----
/ NUMERICAL PARAMETERS
/-----

```

TREATMENT OF NEGATIVE DEPTHS =2
BYPASS VOID VOLUMES =true
FREE SURFACE GRADIENT COMPATIBILITY =0.9
PRESCRIBED FLOWRATES =0.0;0.0
MATRIX STORAGE =3
SCHEME FOR ADVECTION OF VELOCITIES : 14
SCHEME FOR ADVECTION OF DEPTH : 5
SCHEME FOR ADVECTION OF TRACERS : 14
SCHEME FOR ADVECTION OF K-EPSILON : 14
SUPG OPTION =0;0
PRESCRIBED ELEVATIONS =0.0;0.0
MASS-LUMPING FOR DIFFUSION =1.
VERTICAL VELOCITY DERIVATIVES =1
HYDROSTATIC INCONSISTENCY FILTER =true
/-----
/ TRACERS
/-----
NUMBER OF TRACERS : 1
NAMES OF TRACERS : 'SALINITY '
INITIAL VALUES OF TRACERS : 0.0
TRACERS VERTICAL PROFILES : 1;1
PRESCRIBED TRACERS VALUES : 30.0;0.0
TREATMENT OF FLUXES AT THE BOUNDARIES = 2;1 / 2 is dirichlet not obeyed but
fluxes correct
DENSITY LAW : 2 / 0=Nothing,1=Temp, 2=Salinity,3=Temp and Salinity,4=Beta Coefficient
/COEFFICIENT DE DILATATION BETA POUR LES TRACEURS : -1.65
/VALEUR DE REFERENCE DES TRACEURS : 0.
/-----
/ NUMERICAL PARAMETERS, K-EPSILON MODEL
/-----

/MAXIMUM NUMBER OF ITERATIONS FOR DIFFUSION OF K-EPSILON =600

/-----

/ NUMERICAL PARAMETERS, VELOCITY-CELERITY-DEPTH

/-----

IMPLICITATION FOR DEPTH =1.

MASS-LUMPING FOR VELOCITIES =1.

MASS-LUMPING FOR DEPTH =1.

/-----

/ PHYSICAL CONSTANTS

/-----

/CORIOLIS COEFFICIENT =7.6E-5

Liquid Boundaries File (First two days)

DEBIT A L'ENTREE ET SURFACE LIBRE A LA SORTIE

#

T Q(2) SL(1)

s m³/s m

0 1110 3.12

3600 1140.416667 2.69

7200 1170.833333 2.18

10800 1201.25 1.71

14400 1231.666667 1.36

18000 1262.083333 1.2

21600 1292.5 1.3

25200 1322.916667 1.64

28800 1353.333333 2.17

32400 1383.75 2.77

36000 1414.166667 3.38

39600 1444.583333 3.9
43200 1475 4
46800 1505.416667 4.37
50400 1535.833333 4.33
54000 1566.25 4.17
57600 1596.666667 3.92
61200 1627.083333 3.66
64800 1657.5 3.47
68400 1687.916667 3.37
72000 1718.333333 3.36
75600 1748.75 3.4
79200 1779.166667 3.46
82800 1809.583333 3.45
86400 1840 3.33
90000 1843.333333 3.08
93600 1846.666667 2.72
97200 1850 2.28
100800 1853.333333 1.84
104400 1856.666667 1.5
108000 1860 1.31
111600 1863.333333 1.36
115200 1866.666667 1.64
118800 1870 2.12
122400 1873.333333 2.69
126000 1876.666667 3.3
129600 1880 3.8
133200 1883.333333 4.16
136800 1886.666667 4.31
140400 1890 4.24
144000 1893.333333 4.02

```
147600 1896.666667 3.71
151200 1900 3.39
154800 1903.333333 3.1
158400 1906.666667 2.94
162000 1910 2.91
165600 1913.333333 2.98
169200 1916.666667 3.09
172800 1920 3.17
```

Clustering Python Code

```
import pandas as pd
import numpy as np
import sklearn
from sklearn.cluster import OPTICS
from sklearn.preprocessing import StandardScaler
from matplotlib import pyplot as plt
from random import randint
import shapefile

data = pd.read_excel('result.xlsx')

delete = []

for i in range(0,len(data.index)):
    value = data._get_value(i,'X')
    if value < 480000:
        delete.append(i)

print(len(delete))
```

```

Percent = len(data.index)/len(delete)
print(Percent)

new_data = data.drop(delete,0)
final_data = data.drop(delete,0)

scaler = StandardScaler()
scaler.fit(new_data[['X']])
new_data[['X']] = scaler.transform(new_data[['X']])

scaler.fit(new_data[['Y']])
new_data[['Y']] = scaler.transform(new_data[['Y']])

optics = OPTICS(min_samples = 200)
predicted_label = optics.fit_predict(new_data[['X', 'Y']])

final_data['cluster'] = predicted_label
num_cluster = max(final_data.cluster)

color = []

for i in range(0,num_cluster+1):
    color.append('#%06X' % randint(0, 0xFFFFFFFF))

for i in range(0,num_cluster+1):
    plt.scatter(final_data.loc[final_data['cluster'] == i]['X'], final_data.loc[final_data['cluster'] == i]['Y'], color = color[i])

plt.show()

```

```
final_data.to_csv('optics.csv')
```

```
sf = shapefile.Writer('points', shapeType = shapefile.POINT)
sf.field('cluster')
```

```
a = []
```

```
X = []
```

```
Y = []
```

```
points = []
```

```
for i in range(0,len(final_data.index)):
```

```
    a.append(final_data.index[i])
```

```
cluster = []
```

```
for i in a:
```

```
    cluster.append(final_data._get_value(i,'cluster'))
```

```
for i in a:
```

```
    x = final_data._get_value(i, 'X')
```

```
    X.append(x)
```

```
    y = final_data._get_value(i,'Y')
```

```
    Y.append(y)
```

```
for i in range(0, len(X)):
```

```
    points.append([X[i], Y[i]])
```

```
for i in range(0,len(X)):
```

```
    sf.point(X[i], Y[i])
```

```
    sf.record(cluster[i])
```

`sf.close()`