Plastic litter in the ocean

Modeling of the vertical transport of micro plastics in the ocean

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by

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Abstract

Plastic pollution is a big problem all over the world. Every year more plastic is produced, a lot of plastic litter is mismanaged and enters the ocean. It's important to know where these plastics accumulate. With this information the problem can be quantified and the plastic litter can be cleaned up. In this project, the transport of micro plastics will be studied. These are plastic particles with a diameter smaller than 5 mm.

To model micro plastics in an accurate way, it is important to include the physical properties of plastics in a transport model. Plastic particles have an extra upwards buoyancy force in the vertical direction, this force has to be taken into account in the model. Therefore, the two-dimensional vertical behavior of plastic particles is studied in this project. Two common transport models are explored: the advection-diffusion equation and a stochastic random walk model. The properties of plastics are discussed and how the transport models can be adapted to be adequate to model micro plastics.

Micro plastics are assumed as spheres in fluid. With this assumption, the flow regime around a plastic particle is estimated with the Reynolds number. These assumptions make it possible to calculate a terminal buoyancy velocity, due to the floating character of plastic. This velocity is added in the vertical direction to both transport models. To model the turbulence in the ocean, the eddy diffusivity coefficient is defined. This is a variable that states how turbulent the flow is, it can be described as an enhanced diffusion coefficient. The eddy diffusivity coefficient can be estimated with the model Prandlt defined. Here we used a simplified turbulence model for the tests described. In combination with Delft3D-FM the eddy diffusivity from the turbulence model in there can be used.

Both models are implemented in Matlab. The characteristics of the model match with the expected behavior of floating plastics. Plastic particles will perfectly follow the velocity field, except for the extra vertical velocity. When this term is non-zero, the particles will float. Both models have some limitations in efficiency for modeling plastic particles. The advection-diffusion equation is not suitable for high concentration gradients. The random walk model is not suitable for big areas or long timescales. The choice between both models is depending on the sort of case that someone wants to model.

This project has been carried out at Deltares, an independent water research institute. At Deltares there is a two-dimensional horizontal model available to model particles in the ocean. In the future the existing model of Deltares and the model in this project could be combined. This combined model can be tested for real-life situations in the ocean. With this combined model, the physical properties of plastics are included in a three-dimensional particle model.

N. Scheijen
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1

Introduction

Every year more plastic is produced all over the world. Unfortunately, a lot of plastic is mismanaged and enters the ocean. For example, in 2010 the countries around the big oceans in the world produced 275 million metric tons of plastic waste. An estimated 4.8 to 12.7 million metric tons ended up in the ocean. This amount will only increase if no appropriate measures are taken (Jambeck (2015)). Plastic waste has negative influences on many processes and organisms. For example, many animals die due to mistaking plastic for food or get entangled in nets. It takes a lot of money to clean up the waste on shores, and the plastics with toxic chemicals enter the human food chain, shown in figure 1.1. There are two logical measures, the first measure is to reduce the origin of the problem by producing less plastics and manage the plastic waste better. The second measure is cleaning up the current plastics in the ocean.
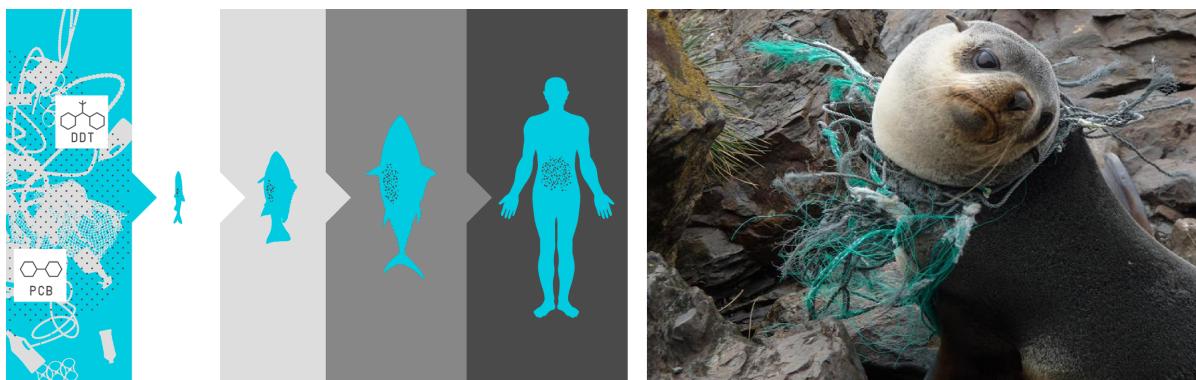

Figure 1.1: Two examples of the negative effect of plastic pollution in the ocean. ©Mendelproject, Pinterest

To collect the plastic litter and clean the ocean, it is important to know the locations of plastic litter. It is possible to determine these locations through observations of the ocean, but also with modeling using the velocity field of the ocean. When plastic litter is assumed as small particles, it can be modeled as particle transport in a fluid. There are two common ways to model particle transport. One way is solving the advection-diffusion equation for mass. This equation is a classical formula often used for describing transport processes. Another way is to derive a stochastic model from the advection-diffusion equation, called a random walk model (Heemink (1990)). With this model a single particle trajectory can be simulated. When a large amount of particles is simulated with this model, the spread of the particles is equal to the concentration function. It can be mathematical derived that the methods are equal for an ideal situation. Unfortunately this ideal situation is impossible to obtain, both models have their own specific advantages and disadvantages for specific cases. They will be further outlined in chapter 2.

Most people think of plastic pollution as bottles, plastic bags and fishing nets. However, a big part of the plastic pollution is not visible. The plastic litter in the ocean is classified in different types. The big plastics such as bottles, fishing nets and plastic bags are classified as macro plastics. Plastic particles smaller than 5 mm, defined by Arthur et al. (2009), are classified as micro plastics. These micro plastics are a big danger to

the marine biota. A lot of plastics have a density lower than the density of the sea water, hence are buoyant. This buoyancy must be taken into account when modeling the plastics. In this project, a vertical velocity term will be included for the floating force of plastics. The characteristics of plastic will be further discussed in subsection 2.3.2.

This project has been carried out at Deltares. Deltares is an independent water research institute located in Delft and Utrecht. One of their areas of expertise is environment, which also includes the plastic pollution in the oceans. A lot of research has been carried out in modeling the three dimensional velocity field in the ocean. This velocity field can be used to simulate the transport of plastics. The velocity field is subject to a lot of different influences, for example wind, bathymetry, salinity and temperature. With help of large satellite datasets on velocities in the ocean, an accurate model for the velocity field can be produced. The model can be produced by use of D-Flow FM, a program of Deltares that is used to simulate all sorts of hydrodynamics, for example in rivers, oceans and coasts. With D-Flow FM we can place particles in a specific reservoir and track these particles.

The particle model is designed in a two-dimensional horizontal way, the vertical fluxes are all set to zero. The model also has not been used for the modeling of plastic particles. Specific structures in the ocean have a vertical velocity force. Plastics also have an important vertical force, they are buoyant. Therefore this research will be about modeling the vertical two-dimensional particle model. This could be useful to improve the D-Flow FM model with a vertical component. With this component the specific characteristics of plastic can be taken into account.

Currently research is performed in the Mediterranean Se area, which has one of the highest amounts of plastic per square kilometer of the world. This is due to very populated coasts surrounding the sea, tourism, 30% of all the maritime traffic passing through and limited exchange with water outside the Mediterranean basin (UNEP/MAP (2015)). Deltares is working on a project for the three dimensional modeling of the velocity field in the Mediterranean. In chapter 3 more will be explained about the Mediterranean sea and the requirement to develop a transport model for plastics in the Mediterranean sea.

Summarizing the above sections, the following research questions are defined:

- Which adjustments and assumptions are needed to adapt the existing transport models in a way that they are adequate for modeling plastic?

- Are the random walk model and the numerical solution of the advection-diffusion equation equally efficient for the modeling of plastics with a vertical velocity term?

- How can the transport model be used to obtain realistic results for an real-life situation, for example the Mediterranean Sea?

<div style="text-align: right; font-size: 4em;">2</div>

<div style="text-align: right; color: #2ba6e0; font-size: 2.5em;">Theory</div>

The transport of plastics in an ocean will be modeled as particles in a fluid. This is the first important assumption that is made in this project. The plastic particles don't influence the flow field and perfectly follow the velocity field. The ultimate goal is to achieve a model for plastic particles for practical use. In this project specific test cases are explored, a two-dimensional reservoir with specific velocities. In this way the methods that can be used for the modeling of the vertical transport of plastics are explored. The flow of the ocean is turbulent, turbulence can also be described as random.The velocity at one point can't predict the velocity just some time later. This has to be included in the test case set-up, to be able to apply it to real-life problems later. The trajectories of plastics in the ocean can be modeled in two different ways. The advection-diffusion equation for mass transport can be solved or a random walk model can be developed. This is an Eulerian and Lagrangian approach to the problem, respectively. The Eulerian approach looks at a quantity as function of time and space. A control volume is defined where the properties of the quantity are measured. The Lagrangian approach looks at the path per particle, by 'tagging' a specific particle and measuring the properties of this particle. In the section below both models are outlined and compared. In this project the goal is to look at the properties of a two-dimensional system, so the equations are also outlined in this dimension.

2.1. Advection-diffusion equation

2.1.1. Concept

The advection-diffusion equation is a partial differential equation (PDE) that is used to describe the transport of physical quantities such as energy, mass or momentum. In this project the physical quantity mass is looked at. The basic advection-diffusion equation in three dimensions is given by:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D_{ij} \nabla c) - \nabla \cdot (\vec{u} c) + R \tag{2.1}$$

With c the concentration of particles at a specific location, $D_{ij} = (D_{x11}, D_{y22}, D_{z33})$ the diffusion coefficient tensor, $\vec{u} = (u_x, u_y, u_z)$ the velocity field of the ocean and R the term of sources or sinks of the particles. The physical explanation of the left term is the change of concentration of particles per time. The first term on the right is the diffusion part, the diffusion is proportional with the concentration gradient. It is the random spread from regions with a high concentration to regions with a low concentration due to molecular motion, modeled as a Fickian process. The second term on the right is the advection term. When someone drops plastic particles in a flow to the south, a high concentration of particles occurs in the south some time later, since the particles follow the flow. The third term on the right is as already said the source or sink term, for example a big city that has a lot of plastic waste could be a source.

In this project turbulent flows are used, therefore it is convenient to decompose the corresponding variables concentration and velocity in two parts, a time-averaged and fluctuating part (from the mean).

$$c = \overline{c} + c' \qquad \vec{u} = \overline{\vec{u}} + \vec{u}' \tag{2.2}$$

<div style="text-align: center;">3</div>

With $^-$ the time-averaged variable and $'$ the fluctuating variable from the mean. This decomposition is called the Reynolds decomposition. The fluctuating term is on average zero, but it can not be neglected because the term is not linear. When both decomposition equations are substituted in equation 2.2, on time average the following equation is found:

$$\frac{\partial \overline{c}}{\partial t} = \nabla \cdot (D_{ij} \nabla \overline{c}) - \overline{\overline{u}} \nabla \overline{c} + R - \nabla(\overline{u'c'}) \tag{2.3}$$

This expression is similar to equation 2.1, with the extra term $\nabla(\overline{u'c'})$ on the right side. This is the advection transport from the fluctuations in the velocity field due to turbulence.

The only term that is still unknown is the term $\nabla(u'c')$. This is called the 'closure problem', because not enough equations are available to solve all unknown variables. Therefore these values will be approximated. A way to approximate these values is to define the eddy diffusivity coefficient:

$$\overline{u'c'} = -\epsilon_{ij} \nabla c \tag{2.4}$$

With $\epsilon_{ij} = (\epsilon_{x11}, \epsilon_{y22}, \epsilon_{z33})$ the tensor for eddy diffusivity.

2.1.2. Eddy diffusivity
Equation 2.4 has the same form as the equation for molecular diffusion. This shows that this turbulent transport also has a diffusive nature. It could be described as an enhanced diffusion coefficient. The form is similar to the equation with the molecular diffusion coefficient D, but since the eddy diffusivity is based on the fluid motion, it is much larger than the diffusion coefficient based on molecular motion. Therefore the term with molecular diffusion D_{ij} can be neglected. Before the model can be implemented, the eddy diffusivity has to be calculated. The turbulent velocities are random, every simulation will give a different result, so the eddy diffusivity is hard to define. A relative simple way to approximate these coefficients is with the Prandlt model. It is based on the idea of mixed length l', the length that a swirl or eddy takes to mix again with the surrounding water. In other words, it displaces the initial concentration a distance equal to the mixing length. In terms of fluxes, as stated in Vallis (2006), the turbulent flux is defined as:

$$F_i = -u'_i l' \partial_j c = -\epsilon_{ij} \partial_j c \tag{2.5}$$

With F_i the turbulent flux in one direction. It is assumed that the fluctuating velocity in one direction and the displacement defined by the mixing length in another direction are not correlated. With this assumption the eddy diffusivity tensor is symmetric, defined as:

$$\epsilon_{ij} = \begin{pmatrix} u'_x l' & 0 \\ 0 & u'_y l' \end{pmatrix} \tag{2.6}$$

The mixing length and the fluctuating velocities are quantities that can be measured during experiments. In this project, mainly test case set up simulations will be simulated. Therefore the eddy diffusivity will be modeled for just two different cases. For one case the eddy diffusivity will be a constant. For the other case, the eddy diffusivity will be modeled as a linear function of the mixing length l'. It is assumed, that near a wall the turbulence will become less. Therefore the eddy diffusivity in the vertical direction will be assumed as a parabolic, as also stated in Stijnen et al. (2006). According to Nencioli et al. (2013), the common horizontal eddy diffusivity is between 0 $m^2 s^{-1}$ and 2 $m^2 s^{-1}$. The vertical eddy diffusivity is much lower, common values are between 10^{-5} $m^2 s^{-1}$ and 10^{-7} $m^2 s^{-1}$, according to Cuypers et al. (2012). Both papers are about the Gulf of Lion in the Mediterranean. These approximate eddy diffusivity coefficients are very rough, but they are sufficient to test the models. The most important characteristic is the difference between the horizontal and vertical eddy diffusivity. This is due to the big difference in length scales between both directions. In the following sections the eddy diffusivity tensor will be denoted as $\epsilon_{ij} = (\epsilon_x, \epsilon_z)$

To obtain the final equation for the simulations, equation 2.4 is substituted in 2.3 to obtain one formula and derive the two-dimensional advection-diffusion equation in turbulent regime. The notation c and u is used instead of $\bar{c}$ and $\bar{u}$ and no sources or sinks are present, so $R = 0$.

$$\frac{\partial c(x,z,t)}{\partial t} = \frac{\partial}{\partial x}(\epsilon_x \frac{\partial c(x,z,t)}{\partial x}) + \frac{\partial}{\partial z}(\epsilon_z \frac{\partial c(x,z,t)}{\partial z}) - \frac{\partial(u_z(x,z)c(x,z,t))}{\partial z} - (\frac{\partial u_x(x,z)c(x,z,t)}{\partial x}) \tag{2.7}$$

Advantages of the method of solving the advection-diffusion equation is that it is accurate at big time scales and large areas. This is very useful for a model of an ocean. The method also has two big disadvantages.

The method is not always mass conserving and for high concentration gradients, negative concentrations can occur. In a real-life situation with a garbage dump somewhere, it is very likely that this place has a high concentration gradient, so this is not very convenient. Also, plastic particles don't disappear, so the total mass in the system has to stay the same.

2.2. Stochastic random walk model

2.2.1. Concept

To describe the transport of plastic particles, it is also possible to use a stochastic differential equation (SDE) instead of a PDE. First the more well known idea with only an advective term in the model is introduced.

$$\frac{dX_t}{dt} = f(X_t, t) \quad \Longleftrightarrow \quad dX_t = f(X_t, t)dt \tag{2.8}$$

With X_t a stochastic variable for the location of a particle and f a function for the drift velocity. The displacement of the particle is equal to the velocity times the time that the particle feels this velocity. As seen in the advection-diffusion equation, also turbulent diffusivity is important to model plastic particles. In the stochastic model this diffusivity has to be implemented too. Intuitive, this can be defined with a white noise term:

$$\frac{dX_t}{dt} = f(X_t, t) + g(X_t, t)N_t \qquad X_{t0} = X_0 \tag{2.9}$$

With g a function related to the eddy diffusivity coefficient and N_t a stochastic process, white noise, to model the uncertainties in the physical quantity that is described. This kind of model is called a random walk model. The stochastic part of the equation describes the uncertainties of physical quantities in the model. With a random walk model the trajectories of single particles are modeled. When a large amount of particles is simulated, the solution is similar to the solution of the advection-diffusion equation. The probability density function of the particles is equal to the concentration of the particles divided by a constant. Equation 2.9 would be the ideal function to solve, but the white noise term N_t is mathematical not well defined. Because of this, some assumptions must be made. In the following sections is outlined how this basic SDE can be used to model particles. The goal from the sections and definitions below, is to show that the random walk model is equal to the advection-diffusion solution in an ideal situation.

2.2.2. Ito stochastic differential equation

To be able to evaluate the SDE in equation 2.9, the definition of an Ito integral is used, this integral is defined as:

$$\int_{t_0}^{t} G_s dW_s = \lim_{\Delta t \to 0} \sum G_{t_i}(W_{t_{t+i}} - W_{t_i}) \tag{2.10}$$

With G_s and W_s a stochastic process. A lot of different techniques have been developed to define the stochastic integral. The Ito definition is most common and is very convenient for computing. With this definition the given SDE can be evaluated, this will be outlined in a section below.

2.2.3. Wiener process

As already mentioned, the stochastic variable N_t that models the uncertainties has to be defined in a mathematical correct way. In the case of a random walk model, this term models the diffusion of a particle. Therefore the Wiener process is defined, this process is also called the standard Brownian motion. The definition of a standard Wiener process is given by $W_t = [W_t, t > 0]$ on $[0, T]$ with $W_0 = 0$. For any t, s in $0 < s < t < T$, $E[W_t - W_s] = 0$ and $Var[W_t - W_s] = t - s$. This makes dW_t a Gaussian random variable with mean zero and variance dt, which shows that $dW_t = N_t dt$. Equation 2.9 can be transformed into a two-dimensional SDE. This will be useful to show that equation 2.11 is equal to equation 2.7

$$\begin{aligned} dX_t &= f_1(X_t, Z_t, t)dt + g_1(X_t, Z_t, t)dW_t \\ dZ_t &= f_2(X_t, Z_t, t)dt + g_2(X_t, Z_t, t)dW_t \end{aligned} \tag{2.11}$$

These expressions have to be evaluated in the Ito sense. Equation 2.11 is the short notation, the complete mathematical definition in the Ito sense is given by:

$$dX_t = f_1(X_t, Z_t, t)dt + g_1(X_t, Z_t, t)dW_t$$
$$X_t = X_{t_0} + \int_{t_0}^t f_1(X_s, Z_s, s)ds + \int_{t_0}^t g_1(X_s, Z_s, s)dW_s$$

$$dZ_t = f_2(X_t, Z_t, t)dt + g_2(X_t, Z_t, t)dW_t$$
$$Z_t = Z_{t_0} + \int_{t_0}^t f_2(X_s, Z_s, s)ds + \int_{t_0}^t g_2(X_s, Z_s, s)dW_s$$

$$(2.12)$$

2.2.4. Fokker-Planck equation

This equation describes the probability density function (PDF) of the stochastic processes X_t and Z_t of equation 2.11. The PDF for equation 2.10 has the following form in two dimensions, this is already shown by Jazwinski (1970):

$$\frac{\partial P(t,x,z)}{\partial t} = -\frac{\partial}{\partial x}(f_1(t,x,z)P(t,x,z) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(g_1^2(t,x,z)P(t,x,z))$$
$$-\frac{\partial}{\partial z}(f_2(t,x,z)P(t,x,z)) + \frac{1}{2}\frac{\partial^2}{\partial z^2}(g_2^2(t,x,z)P(t,x,z))$$

$$(2.13)$$

With $f_{1,2}, g_{1,2}$ two arbitrary functions and $P(t,x,z)$ the probability density function of one particle. This process is valid in the sense of an Ito differential equation, as defined in equation 2.10. With this equation, it can be shown that a random walk model exists that is equal to the advection-diffusion model, when a large amount of particles is simulated.

2.2.5. Connection with the advection-diffusion equation

To see that the Fokker-Planck equation is equal to the advection-diffusion equation, equation 2.3 is looked at again. As stated before, the concentration of particles and the probability density function is similar, except for a constant. If we divide it by a constant, the mass difference is compensated: $p(t,x,z) = \frac{c(t,x,z)}{C}$ where C is a dimensionless constant. This constant compensates for the difference of the total amount of mass present in the system. When this is substituted in equation 2.13, the following equation is found:

$$\frac{\partial}{\partial t}\frac{c(t,x,z)}{C} = -\frac{\partial}{\partial x}(f(t,x,z)\frac{c(t,x,z)}{C}) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(g^2(t,x,z)\frac{c(t,x,z)}{C})$$
$$-\frac{\partial}{\partial z}(f(t,x,z)\frac{c(t,x,z)}{C}) + \frac{1}{2}\frac{\partial^2}{\partial z^2}(g^2(t,x,z)\frac{c(t,x,z)}{C})$$

$$(2.14)$$

C is dimensionless and with use of the product rule for differentiation, this can be written as:

$$\frac{\partial c(t,x,z)}{\partial t} = -\frac{\partial}{\partial x}(f_1(t,x,z)c(t,x,z)) + \frac{1}{2}\frac{\partial}{\partial x}g_1^2(t,x,z)\frac{\partial}{\partial x}c(t,x,z) + \frac{1}{2}\frac{\partial}{\partial x}c(t,x,z)\frac{\partial}{\partial x}g_1^2(t,x,z)$$
$$-\frac{\partial}{\partial z}(f_2(t,x,z)c(t,x,z)) + \frac{1}{2}\frac{\partial}{\partial z}g_2^2(t,x,z)\frac{\partial}{\partial z}c(t,x,z) + \frac{1}{2}\frac{\partial}{\partial z}c(t,x,z)\frac{\partial}{\partial z}g_2^2(t,x,z)$$

$$(2.15)$$

Equation 2.15 is equal to equation 2.7, if $\bar{f}(t,x,z) = (u_x + \frac{\partial \epsilon_x}{\partial x}, u_z + \frac{\partial \epsilon_z}{\partial z})$ and $\bar{g}(t,x,z) = (\sqrt{2\epsilon_x}, \sqrt{2\epsilon_z})$. The total equation is found by substituting f, g into equation 2.12:

$$dX_t = (u_x + \frac{d\epsilon_x}{dx})dt + \sqrt{2\epsilon_x}dW_t$$
$$dZ_t = (u_z + \frac{d\epsilon_z}{dz})dt + \sqrt{2\epsilon_z}dW_t$$

$$(2.16)$$

These equations have to be evaluated as Ito SDE's. This random walk model is mass conserving, because individual particles are modeled, which is an advantage of this model. This model also has a disadvantage.

A disadvantage is that a really big amount of particles have to be calculated, to find a accurate solution. The bigger the area or the timespan, the more particles have to be simulated. Therefore it is not suitable for large times or big areas.

2.3. Vertical velocity term

2.3.1. Concept

The models defined above are both for particles in fluids, but in both models the particle is assumed as massless. It will perfectly follow the flow defined by the velocity field, with exception of the diffusion. To create a physical accurate model, it is also important to take into account the properties of the particle. In this project, the focus is on the different forces that act on a plastic particle in the vertical direction. The most important forces in the vertical direction are the gravitational force F_g, the buoyancy force F_b and due to these two forces the drag force F_d, as is shown in figure 2.1. This is also mentioned in the book of Morrison (2013).
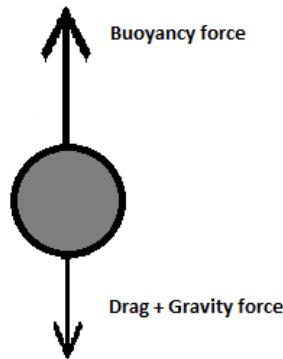

Figure 2.1: Forces on a particle in water

These forces have the following equations:

$$F_d = \frac{1}{2}\rho_w C_d A v^2 \tag{2.17}$$

With F_d the drag force on the particle, ρ_w the density of the water, A the cross section of the particle, C_d the drag coefficient (dimensionless) of the particle and v the velocity of the particle relative to the water.

$$F_b = \rho_w g V_p \tag{2.18}$$

With g the gravitational acceleration (9.81) and V_p the volume of the plastic particle.

$$F_g = V_p \rho_p g \tag{2.19}$$

With ρ_p the density of the plastic particle. To be able to estimate all the above parameters for micro plastics, they are assumed to be spherical. When looking at the three extra vertical forces, the goal is to find a specific velocity due to these forces, called the buoyancy velocity. This is a velocity that is not dependent on the velocity field of the fluid, but on the physical properties of the particle. If the velocity is known, this velocity can easily be substituted in the advection-diffusion equation and the random walk model. The total sum of forces on a particle is defined as:

$$ma = \rho_p V_p \frac{dv}{dt} = F_b - F_d - F_g = \rho_w g V_p - \frac{1}{2}\rho_w C_d A v^2 - V_p \rho_p g \tag{2.20}$$

With $m = \rho_p V_p = \frac{4}{3}\rho_p \pi r^3$ the mass of the plastic particle and a the acceleration of the particle. To find the buoyancy velocity, this equation can be rewritten as:

$$\frac{1}{2g\rho_p V_p(\frac{\rho_w}{\rho_p} - 1) - \rho_w C_d A v^2} dv = \frac{1}{2\rho_w \rho_p} dt \tag{2.21}$$

Then if the constants $a = 2g\rho_p V_p(\frac{\rho_w}{\rho_p} - 1)$ and $b = \rho_w C_d A$ are substituted, the equation is an ordinary differential equation. So integrating both sides gives:

$$\frac{1}{a - b^2} dv = \frac{1}{2\rho_p V_p} dt \quad \Longleftrightarrow \quad \frac{\tanh^{-1}(\frac{\sqrt{b}v}{\sqrt{a}})}{\sqrt{a}\sqrt{b}} = \frac{t}{2\rho_w \rho_p} t + C \tag{2.22}$$

As already stated this buoyancy velocity is defined as a property of the plastic particle and not of the velocity field. This is the terminal constant velocity a particle will obtain when the sum of the forces is zero. The steady-state solution is achieved, when $t \to \infty$. The steady-state solution of 2.22 with the substituted constants a, b is then:

$$v_b = \frac{\sqrt{a}}{\sqrt{b}} \quad \Longleftrightarrow \quad v_b = \sqrt{2g\frac{\rho_p V_p(\frac{\rho_w}{\rho_p} - 1)}{\rho_w C_d A}} \tag{2.23}$$

It's important to notice that this equation only holds for particles that float, because of the term $(\frac{\rho_w}{\rho_p} - 1)$. When the density of a particle is higher than the density of sea water, the solution will become imaginary. This can be solved by altering the equation with $(1 - \frac{\rho_w}{\rho_p})$ when the density of a particle is higher than sea water. Of course, the resulting velocity will be negative then. The buoyancy velocity term is only present when a particle is submerged in water, when a plastic particle is at the surface, $v_b = 0$.

In the above section the steady-state terminal buoyancy velocity has been calculated. Because it is assumed that the velocity and the forces are constant, these are called the 'steady' forces. But these quantities aren't always constant. For a sphere that is moving with an acceleration, a non-constant velocity, in hydrodynamics an extra force is present. These forces are called the 'unsteady' forces. The fluid around the accelerating sphere also has to be accelerated. Therefore the sphere obtains a higher effective inertia, as explained in the article by Pantaleone and Messer (2011). The inertia force is called the added mass. For a sphere the definition for the added mass is:

$$m_{added} = \frac{2}{3}\pi r^3 \rho_w \tag{2.24}$$

With r the radius of the sphere. When this is implemented in equation 2.20, the following equation is found:

$$(m + m_{added})\frac{dv}{dt} = V_p \rho_w g - \frac{1}{2}\rho_w C_d A v^2 - V_p \rho_p g \tag{2.25}$$

The total mass, the mass of the plastic and the added mass together, is referred to as the effective mass. Most plastics have a density that, in order of magnitude, is equal to the density of the water of the sea. Because of this, the effective mass is 1.5 times bigger than the mass of the particle. With equation 2.25 it is possible to calculate the timescale how long it takes before the particle reaches the steady state velocity. If we substitute $c = \frac{V_p \rho_w g - V_p \rho_p g}{m + m_{added}}$ and $d = \frac{\frac{1}{2}\rho_w C_d A}{m + m_{added}}$, equation 2.25 can be written as:

$$\frac{dv}{dt} = c - dv^2 \tag{2.26}$$

This can again be solved for v, which gives the equation:

$$v = \sqrt{c}\frac{\tanh(\sqrt{c}\sqrt{d}c_1 + \sqrt{c}\sqrt{d}t)}{\sqrt{d}} \tag{2.27}$$

The timescale τ is then easily found:

$$\tau = \frac{1}{\sqrt{c}\sqrt{d}} = \frac{m + m_{added}}{\sqrt{\frac{1}{2}\rho_w C_d A(V_p \rho_w g - V_p \rho_p g)}} \tag{2.28}$$

If the timescale is small relative to the changes in the velocity, the term can be neglected. The timescale can be calculated when the characteristics of plastic are known. This will be further outlined in the next section.

The buoyancy velocity term has to be implemented in both models outlined in the previous sections. The velocity is always in the z-direction, therefore the following addition to equation 2.7 is made:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}(\epsilon_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial z}(\epsilon_z \frac{\partial c}{\partial z}) - \frac{\partial((u_z + v_b)c)}{\partial z} - (\frac{\partial u_x c}{\partial x}) \tag{2.29}$$

With an approach similar to equation 2.14-2.16 it can be shown that the random walk model has the following addition:

$$dX_t = (u_x + \frac{d\epsilon_x}{dx})dt + \sqrt{2\epsilon_x}dW_t$$
$$dZ_t = (u_z + \frac{d\epsilon_z}{dz} + v_b)dt + \sqrt{2\epsilon_z}dW_t \tag{2.30}$$

2.3.2. Plastics

In the section above the buoyancy velocity term is implemented in both models. Before these models can be used, the buoyancy velocity has to be calculated. It is important to make a good estimate about the characteristics of plastics in the ocean. As stated in the introduction, this project will focus on the micro plastics in the ocean. These plastics need to be classified to examine the different properties in the models.

Micro plastics are plastics smaller than 5 mm. These micro plastics can originate as small particles, but also due to fragmenting of bigger plastics. The most used and produced plastics in the world are polyethylene, polypropylene, polyvinyl chloride, polystyrene and polyethylene terephthalate. These plastics are accountable for over 90% of the total production in the world. It can therefore be assumed that these plastics also play the most important role in plastic litter particles in the ocean (do Sul and Costa (2014)). In table 2.1 the specific densities of these materials can be found. Some plastics have a lower density then sea water, which means these plastics will have a floating character. In this project only the micro plastics that have a floating character will be looked at. These plastics are bold in the table.

Name	Density [kg/m^3]
Polyethylene (PE)	920
Polypropylene (PP)	895
Polyvinyl Chloride	1100
Polystyren (PS)	1000
polyethylene terephthalate	1380
Sea Water	1025

Table 2.1: The density and dynamic viscosity of different kind of plastics and sea water at 25 C∘, salinity 35g/kg and 1 atm pressure. ©Wikipedia

In this project, micro plastics are assumed as spheres. To find the flow regime around these particles, the Reynolds number needs to be calculated. The Reynolds number is a dimensionless physical quantity that indicates if the flow regime is laminar or turbulent. For flows around a sphere, the flow is already turbulent at low Reynolds numbers, as shown in figure 2.2. The flow around a sphere is turbulent if the Reynolds number is higher than 10.
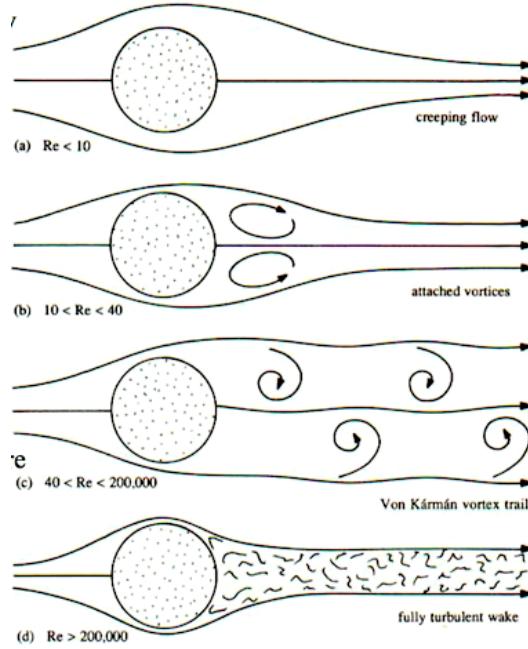
Figure 2.2: A schematic view of the flow regime around a sphere. ©Vogel (1996)

The Reynolds number is defined as:

$$\mathrm{Re} = \frac{\rho_w v_b L}{\mu_w} \tag{2.31}$$

With ρ_w the density of sea water, v_b the velocity of the plastic particle relative to sea water, in this case the buoyancy velocity, L the characteristic length, in the case of a sphere this is the diameter, and μ_w the dynamic viscosity of sea water.

Because not all the parameters are known, the Reynolds number is estimated first. As stated in table 2.1, the density of sea water is 1025 kg/m^3. The dynamic viscosity of sea water is 0.00096 $Pa \cdot s$. The characteristic length is the diameter D, which is not bigger than 5 mm for micro plastics. When these constants are plugged in equations 2.31, the following equation is found for three different sizes micro plastics:

$$
\begin{aligned}
\mathrm{Re} &= 5338.5\, v_b \qquad D = 5.0 mm \\
\mathrm{Re} &= 2669.3\, v_b \qquad D = 2.5 mm \\
\mathrm{Re} &= 1066.7\, v_b \qquad D = 1.0 mm
\end{aligned} \tag{2.32}
$$

From these equations it can be seen that the buoyancy velocity should be respectively 0.0075 m/s, 0.0037 m/s and 0.0094 m/s or smaller for the different sizes to have a laminar flow. Thus the flow around the plastic particles will be modeled as turbulent flows. When the buoyancy velocity is calculated, this assumption will be confirmed again.

At last it is important to have a realistic drag coefficient C_d. With the assumption that a micro plastic is modeled as a sphere, the specific drag coefficient can be found in literature. In figure 2.3, a function based on experimental data for the drag coefficient is plotted versus the Reynolds number.
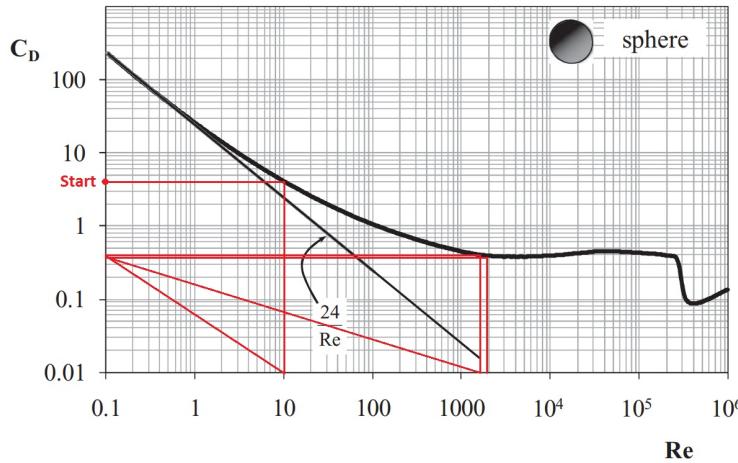
Figure 2.3: A function for the drag coefficient vs the Reynolds number for flows along a sphere (Morrison (2013)). The iterative process to find the buoyancy velocity and the Reynolds number is marked in red.

In the book of Morrison (2013) also a fitted function for the relation between the drag coefficient versus the Reynolds number is defined:

$$C_d = \frac{24}{Re} + \frac{2.6(\frac{Re}{5.0})}{1 + (\frac{Re}{5.0})^{1.52}} + \frac{0.411(\frac{Re}{263000})^{-7.94}}{1 + (\frac{Re}{263000})^{-8.00}} + \frac{0.25(\frac{Re}{10^6})}{1 + (\frac{Re}{10^6})} \qquad (2.33)$$

The final step is to calculate the buoyancy velocity for plastic particles with equation 2.23 and the properties for micro plastics. It is an iterative process, because the drag coefficient C_d and the velocity v_b is depended on one another. The iterative process is shown in figure 2.3. The method is based on picking an estimated drag coefficient C_d and calculate the corresponding velocity and Reynolds number, which will lead to another drag coefficient with 2.33. Table 2.2 shows the found velocities for different sizes of micro plastics.

Diameter [mm]	v_b PE [m/s]	v_b PP [m/s]	v_b PS [m/s]
5	0.20	0.17	0.08
2.5	0.11	0.13	0.05
1	0.05	0.06	0.02

Table 2.2: The diameter of a micro plastic and the corresponding buoyancy velocity for different kind of plastics.

As already assumed the velocity is higher than the velocities mentioned below equation 2.32. This agrees with the assumption to model the flow around the particles as turbulent.

With the assumptions in this section, equation 2.28 can be evaluated to find the velocity timescale of the plastic particle. The timescales are between 0.17 s for 5 mm particles and 0.03 s for 1 mm particles. In both cases this is a very small timescale compared with time scales in the ocean, which are between 30 years and 20 minutes according to Denmon et al. (1996). Therefore it is a valid assumption to use the steady state solution as buoyancy velocity.

2.4. Numerical approach

Both models have to be implemented numerically because it is too hard to solve them analytical. They are solved numerically and are outlined per model. For the advection-diffusion equation the numerical model is first outlined in a one-dimensional case. After that a second dimension is added with the buoyancy velocity. The random walk model is only outlined in two dimensions, because it's easy to derive the one-dimensional scheme from this solution.

2.4.1. Advection-diffusion equation

The advection-diffusion equation will be solved with the finite volume method. The area to be investigated will be divided into a grid with spacing Δx and Δz. Within a cell the physical quantities will be constant. We start with a simple one-dimensional model in the x-direction. Therefore the one-dimensional equation derived from equation 2.29 will be used.

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}(\epsilon_x \frac{\partial c}{\partial x}) - (\frac{\partial u_x c}{\partial x}) \tag{2.34}$$

The spatial component is discretized with the central difference method and the time component with the backward Euler method. These methods are chosen, because they guarantee stability. In the following equations we use the notation c_i^m with i the discretization step in the spatial direction and m the discretization step in time to indicate which grid cell is used. The backward Euler method is defined as:

$$\frac{\partial c_i^m}{\partial t} = \frac{c_i^m - c_i^{m-1}}{\Delta t} \tag{2.35}$$

The central difference method in spatial domain is defined as:

$$\frac{\partial c_i^m}{\partial x} = \frac{c_{i+1}^m - c_{i-1}^m}{2\Delta x} \tag{2.36}$$

$$\frac{\partial^2 c_i^m}{\partial x^2} = \frac{c_{i+1}^m - 2c_i^m + c_{i-1}^m}{(\Delta x)^2} \tag{2.37}$$

If both equations are substituted into equation 2.34 and the terms are rearranged, this gives the following equation:

$$c_i^{m-1} = (-\frac{u_{x,i-\frac{1}{2}}\Delta t}{2\Delta x} - \frac{\epsilon_{x,i-\frac{1}{2}}\Delta t}{\Delta x^2})c_{i-1}^m + (1 + \frac{(\epsilon_{x,i+\frac{1}{2}} + \epsilon_{x,i-\frac{1}{2}})\Delta t}{(\Delta x)^2})c_i^m + (\frac{u_{x,i+\frac{1}{2}}\Delta t}{2\Delta x} - \frac{\epsilon_{x,i+\frac{1}{2}}\Delta t}{\Delta x^2})c_{i+1}^m \tag{2.38}$$

The values of ϵ and u_x in the middle of two concentration points are used, as indicated with $i + \frac{1}{2}, i - \frac{1}{2}$. The used implicit method guarantees stability, but also makes it necessary to solve a system of equations for each time step. This makes it a more time and memory consuming method. With an advection term in the equation, it is important to look at the boundaries of the problem. For the plastic model we expect accumulation of plastics at the boundary at the surface of the ocean. Because the resulting velocity will be up, the velocity term should be implemented with an upwind scheme. This scheme uses the data of the cell before the boundary at the surface and is defined as:

$$\frac{dc_i^m}{dx} = \frac{c_i^m - c_{i-1}^m}{2\Delta x} \tag{2.39}$$

This difference scheme will only work for resulting velocity upwards. When the resulting velocity is downwards, the downwind difference method should be used. In this project, only the upwind difference will be implemented, with upward resulting velocities. This method will be implemented in the two-dimensional scheme. The diffusivity term and the horizontal velocity are discretized with the central difference method. The vertical velocity is modeled with the upwind difference method. In a two-dimensional model the notation becomes $c_{i,j}^m$ with i the discretization step in the spatial z-direction, j the discretization step in the spatial x-direction and m the discretization step in time. This is shown in figure 2.4.

With this discretization and the same approach as the one-dimensional case, the following formula is found:
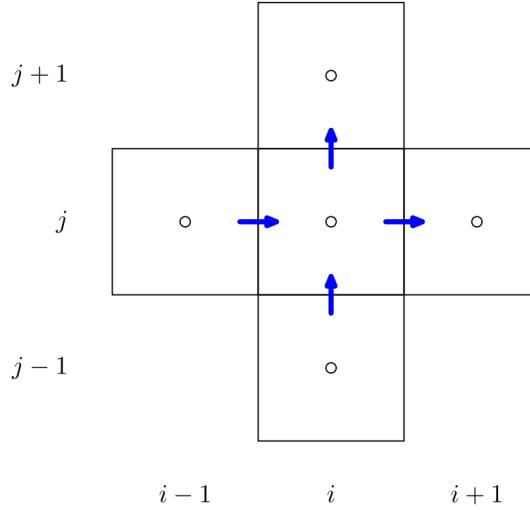
Figure 2.4: Illustration of the discretization. The black open dots represent the concentrations, the blue arrows the fluxes that go into the volume. The letters i and j are used to name the volume cells. ©ten Thije Boonkkamp and Anthonissen (2011)

$$
\begin{aligned}
c_{i,j}^{m-1} = & (\frac{u_{x,i,j+\frac{1}{2}}\Delta t}{2\Delta x} - \frac{\epsilon_{x,i,j+\frac{1}{2}}\Delta t}{\Delta x^2})c_{i,j+1}^m \\
& + (-\frac{u_{x,i,j-\frac{1}{2}}\Delta t}{2\Delta x} - \frac{\epsilon_{x,i,j-\frac{1}{2}}\Delta t}{\Delta x^2})c_{i,j-1}^m \\
& + (1 + \frac{(\epsilon_{x,i,j+\frac{1}{2}} + \epsilon_{x,i,j-\frac{1}{2}})\Delta t}{(\Delta x)^2} + \frac{(\epsilon_{x,i+\frac{1}{2}} + \epsilon_{x,i-\frac{1}{2}})\Delta t}{(\Delta z)^2} + \frac{u_{z,i+\frac{1}{2},j}\Delta t}{2\Delta z})c_{i,j}^m \\
& + (-\frac{\epsilon_{z,i+\frac{1}{2},j}\Delta t}{\Delta z^2})c_{i+1,j}^m \\
& + (-\frac{u_{z,i-\frac{1}{2},j}\Delta t}{2\Delta z} - \frac{\epsilon_{z,i-\frac{1}{2},j}\Delta t}{\Delta z^2})c_{i-1,j}^m
\end{aligned}
\tag{2.40}
$$

2.4.2. Random walk model

Because equation 2.30 has to be interpreted as an Ito differential equation, with a small time step to neglect the limit in equation 2.10, the Euler method can be used:

$$
\begin{aligned}
X_{t+\Delta t} &= X_t + \int_t^{t+\Delta t} f_1(X_s, Z_s, s)ds + \int_t^{t+\Delta t} g_1(X_s, Z_s, s)dW_s \\
&\approx X_t + \int_t^{t+\Delta t} f_1(X_t, Z_t, t)ds + \int_t^{t+\Delta t} g_1(X_t, Z_t, t)dW_s \\
&= X_t + f_1(X_t, Z_t, t)\Delta t + g_1(X_t, Z_t, t)(W_{t+\Delta t} - W_t)
\end{aligned}
\tag{2.41}
$$

$$
\begin{aligned}
Z_{t+\Delta t} &= Z_t + \int_t^{t+\Delta t} f_2(X_s, Z_s, s)ds + \int_t^{t+\Delta t} g_2(X_s, Z_s, s)dW_s \\
&\approx Z_t + \int_t^{t+\Delta t} f_2(X_t, Z_t, t)ds + \int_t^{t+\Delta t} g_2(X_t, Z_t, t)dW_s \\
&= Z_t + f_2(X_t, Z_t, t)\Delta t + g_2(X_t, Z_t, t)(W_{t+\Delta t} - W_t)
\end{aligned}
\tag{2.42}
$$

These formulas can be implemented in Matlab to calculate the solutions.

3

Implementation in a real ocean

Before the models defined in chapter 2 are implemented, it is important to know some basic ocean characteristics. This information can be used to set up the simulations, in a way the most useful results are found. In this report the models for plastic litter in the ocean will be modeled in a test case. The goal is to have a model for real-life situations. An important point is to be able to estimate where plastics accumulates and to use this information to clean up the ocean. In the sections below, more information is found about components of the ocean circulation, the hydrodynamic model and the validation that can be used to validate results of the models in a real-life situation.

3.1. Ocean circulation components

The circulation of water in the ocean consists of multiple mechanisms. Three main different circulation components are distinguished: Currents, gyres and eddies. Currents are the biggest flows in the ocean. They are mostly horizontal and have a coherent character. They flow over big distances and determine for example the climate. An eddy is a swirling fluid in turbulent flow, they look like a circular motion in the ocean. This can occur on big scales of a couple of kilometers, but also on small scales of one meter. In the oceans two different type of eddies exist. The instantaneous eddies, these don't have a long life time and just originate and disappear. The long life time eddies, they can exist for over years. They can appear due to wind, bathymetry or big ocean currents. The physical properties such as temperature and salinity within an eddy can be very different from the surroundings. A gyre is a big circular current. They are due to wind and the Coriolis effect. Figure 3.1 shows all three components.
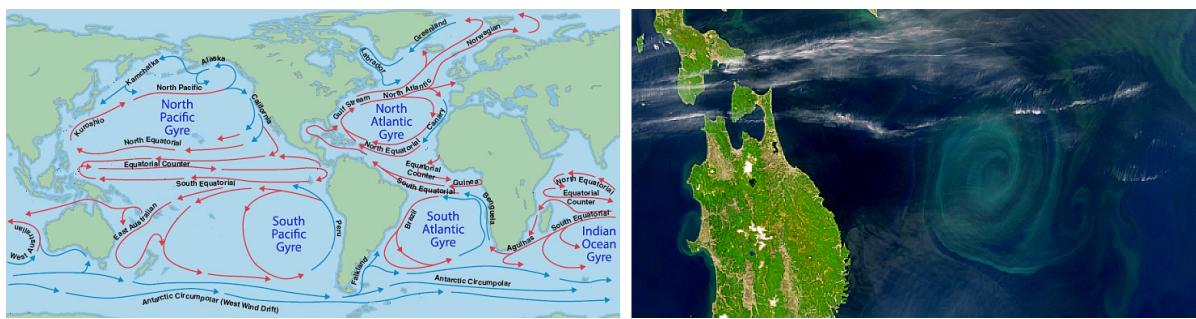
Figure 3.1: The left picture shows the currents in the ocean and the five big gyres in the world, the right picture shows an eddy.
©Recyclingisland, WHO

3.2. Ekman pumping

All circulations components discussed above are important for the transport of plastic litter. To find the accumulation zones, especially the gyres and eddies are interesting. Figure 3.2 shows a picture of the so-called Ekman transport, that originates with eddies and gyres. Water that is diverging or converging at the surface due to wind, causes water to flow vertically. The difference between cyclonic and anti-cyclonic eddies lies in

the hemisphere where the eddy or gyre is formed. In this project especially the converging Ekman transport is very interesting, because floating particles will accumulate here. Typical vertical velocities in an eddy are of magnitude 10^{-5} m/s.
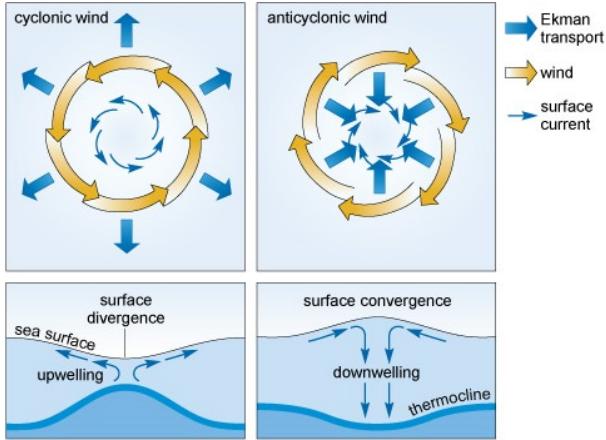

Figure 3.2: Schematic view of Ekman transport in the Northern Hemisphere ©The Open University

To explore the reaction of plastic particles in an eddy or gyre, we need a velocity field that is similar with that of an eddy or gyre. Therefore the following field is defined:

$$\begin{aligned} u_x &= -\sin(dx)\cos(dz) \\ u_z &= \cos(cx)\sin(cz) \end{aligned}$$

(3.1)

With d, c specific constants, chosen such that $u_z = 0$ and $u_x = 0$, on the boundary of the test case set-up. Since water is incompressible, the field needs to be divergence free and the constants are linked. The definition of a divergence free field is:

$$\frac{du_x}{dx} + \frac{du_z}{dz} = 0$$

(3.2)

To obtain a divergence free velocity field, the following constants are chosen: $c = \frac{\pi}{H}$ with H the height of the test case box and $d = \frac{2\pi}{L}$ with L the length of the box. The field is only divergence free if $L = 2H$.

The velocity field is similar to that of an eddy or gyre, shown in figure 3.3. The magnitude of the defined velocity field does not agree with the velocity field of an eddy or gyre in the ocean. To keep the field simple, the vertical velocity term is scaled with the velocity field. This means that in the Matlab model, the buoyancy velocity and the velocity field in an eddy have the same ratio as in real-life. When the model is implemented in DFlow-FM, the real-life velocity field can be used.
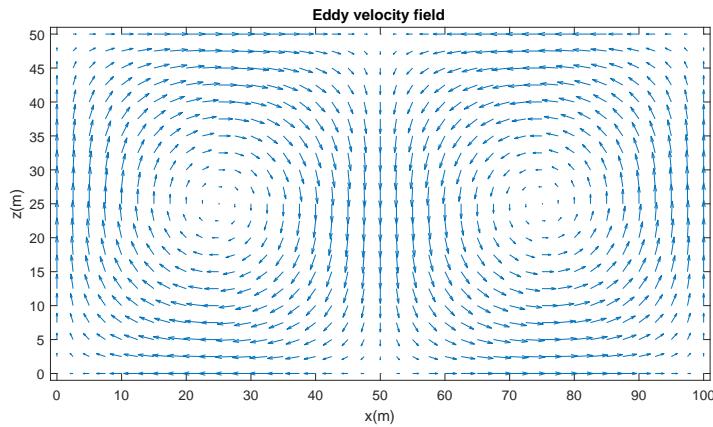
Figure 3.3: Velocity field that is similar to the flows in an eddy or gyre.

3.3. Hydrodynamic model

In the models which are defined, the velocity fields are needed as input. In the test case set-up arbitrary velocities are chosen, but for a realistic ocean model precise velocities are needed. For big regions in the oceans, hydrodynamics models are developed that calculate the velocity fields. For the plastic particle transport model, vertical velocities are important to be included in this model. At Deltares the program Dflow FM is used to calculate these velocity field. It is possible to nudge experimental data to obtain a velocity field that contains all the eddies and specific vertical velocities. With this model the eddy diffusivity is automatically calculated in a way that can be specified, with more accurate equations then defined in this project (Deltares). These values can be used as input for the particle model.

3.4. Validation

After the model is implemented in a real ocean, it is important to check if the model is accurate. In other terms, do the modeled results match with experimental data. A lot of data is available on the accumulation of plastics: surveys by counting the plastic at specific locations, other modeling results in papers, and data of argo floats. Especially argo floats can be useful, if they are placed in an eddy or gyre to track the trajectory in this velocity field. To validate an implemented model properly, it is important to choose an area which has enough data for validation. Figure 3.4 shows an example of multiple trajectories of argo floats in the Mediterranean Sea.
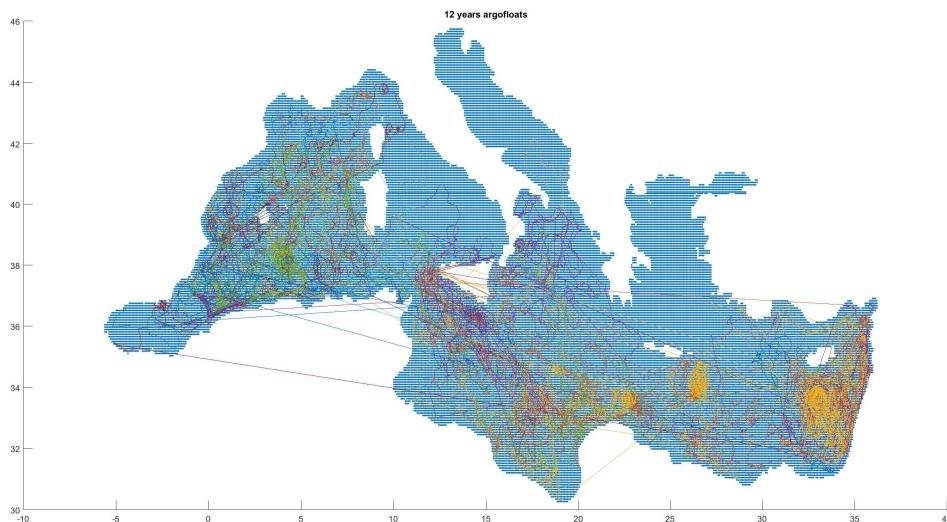
Figure 3.4: Multiple trajectories of argo floats in the Mediterranean Sea from 12 years of data.

3.5. Current situation

Deltares is working on a three-dimensional velocity field model. The new three-dimensional model is called GTSM 3D. This model is developed under the project 'Multi-resolution surface water modeling:From global to local'. With this model, surface velocities can be used to model particle trajectories. This is already done in the Mediterranean Sea, shown in figure 3.5. The vertical fluxes are all zero and the velocity field of the surface flows is used.
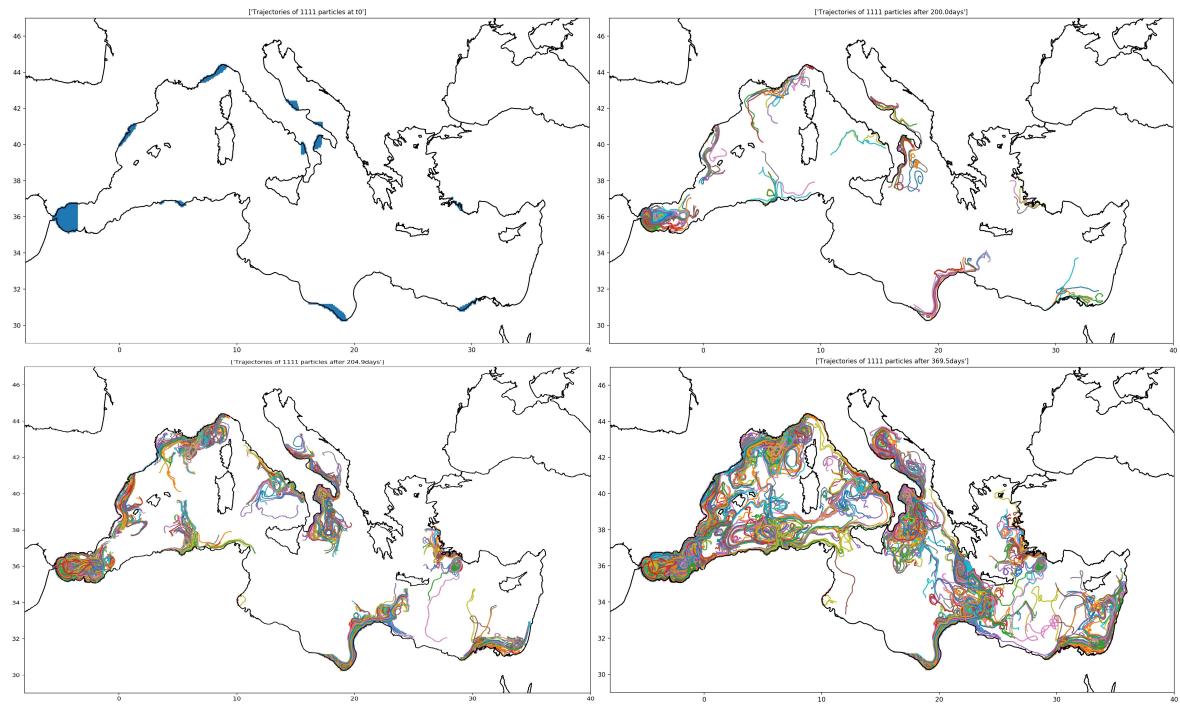
Figure 3.5: Plots of particles trajectories for different times.

Results

This chapter is divided in two parts. The first part is about the one-dimensional simulations and the second part about the two-dimensional simulations. In both cases the results will be showed for varying parameters: variable eddy diffusivity coefficient ($\epsilon_{x11}, \epsilon_{z33}$), velocity field ($u_x, u_z$) and buoyancy velocity v_b.

4.1. One-dimensional

For the one-dimensional case, two settings are explored. The first setting has no velocity field and a constant eddy diffusivity: $\vec{u} = (u_x, u_z) = (0,0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0.05, 0)$. The second setting has a constant velocity in the x-direction and a constant eddy diffusivity: $\vec{u} = (u_x, u_z) = (4,0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0.05, 0)$. In the x-dimension there is no buoyancy velocity, so $v_b = 0$ for all one-dimensional cases. The following equations, derived from the two-dimensional case in 2.29 and 2.30, are used:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}(\epsilon_x \frac{\partial c}{\partial x}) - (\frac{\partial u_x c}{\partial x}) \tag{4.1}$$

$$dX_t = (u_x + \frac{d\epsilon_x}{dx})dt + \sqrt{2\epsilon_x}dW_t \tag{4.2}$$

To show the different particle trajectories, a finite amount of particles is simulated with 4.2. Figure 4.1 shows that this is a Brownian motion, as expected if we look at equation 4.2 with the defined constants.
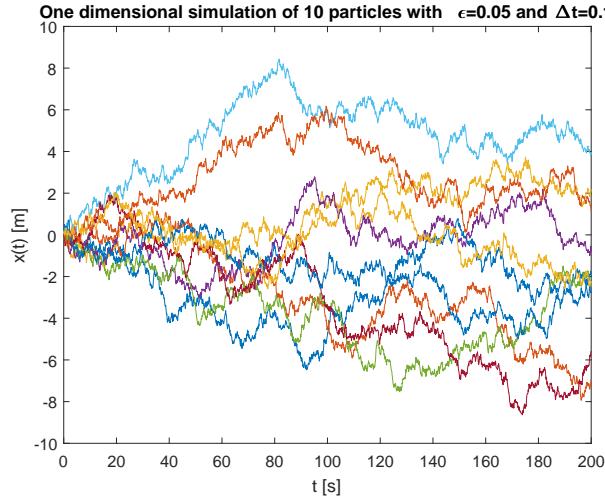
Figure 4.1: Simulation of 10 particles with the random walk model with $\Delta t = 0.1$, $\vec{u} = (u_x, u_z) = (0,0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0.05, 0)$

When a large amount of particles is simulated with the one-dimensional equation, we should find the probability density function of a particle. This is equal to the concentration profile calculated from the

advection-diffusion equation. To be able to compare the two methods, the particles of the random walk are counted per box of length Δx. First the one-dimensional advection-diffusion equation will be solved numerically. To avoid numerical problems for a high concentration gradient, an exponential function $C(t = 0) = 10e^{x^2}$ is chosen as initial condition of the concentration. This initial condition is implemented in both models to check their similarity in one dimension. Figure 4.2 shows the solution of the one-dimensional advection-diffusion equation. As expected has the initial condition the highest peak, the peak gradually spreads out over time due to turbulent diffusion.
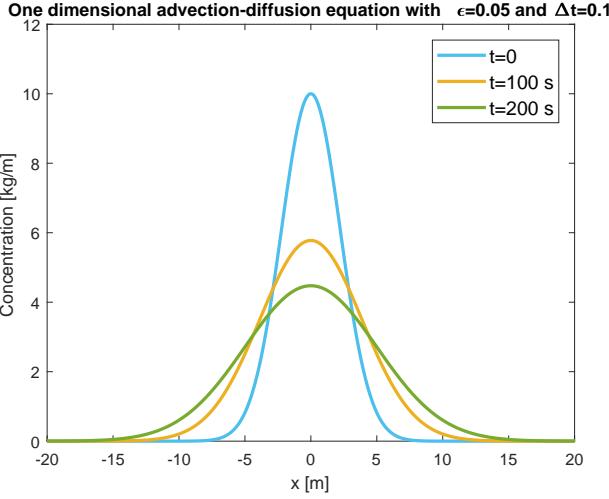
Figure 4.2: Numerical solution of the advection-diffusion equation with initial condition $C(t = 0) = 10e^{x^2}$, $\Delta t = 0.1$, $\vec{u} = (u_x, u_z) = (0,0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0.05, 0)$

Figure 4.3 shows the solution of the advection-diffusion equation and the random walk model in one figure. The figure shows that the two models are very similar.
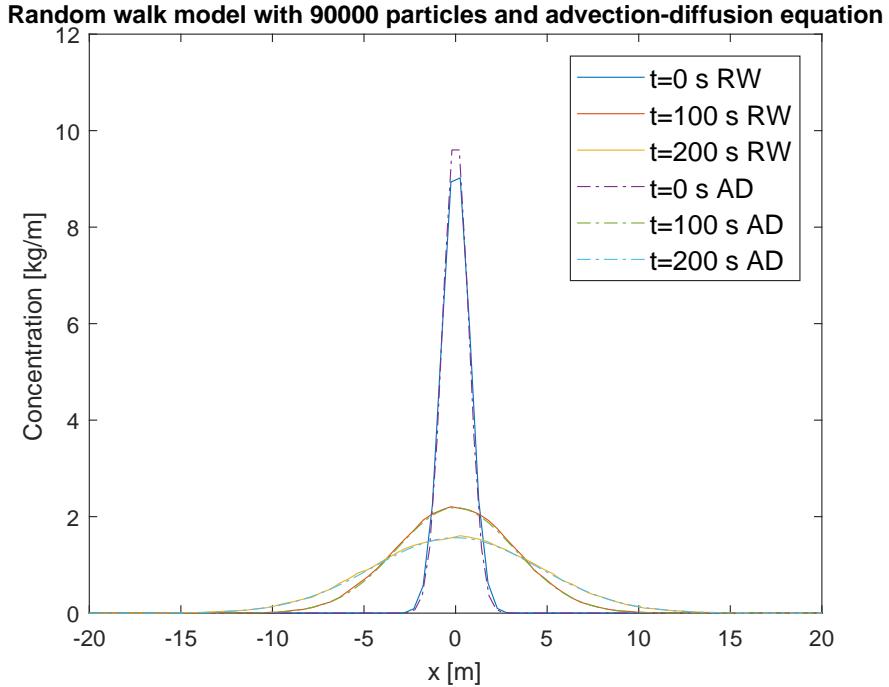
Figure 4.3: Simulation of 90000 particles with the random walk model (RW) and the solution of the advection-diffusion equation (AD) with initial condition $C(t = 0) = 10e^{x^2}$, $\Delta t = 0.1$, $\vec{u} = (u_x, u_z) = (0,0)$ and $\epsilon_{ij} = (\epsilon_{x11}, \epsilon_{z33}) = (0.05, 0)$

Now setting two will be explored, a velocity field is added. Figure 4.4 shows the trajectories of 10 plastic particles.
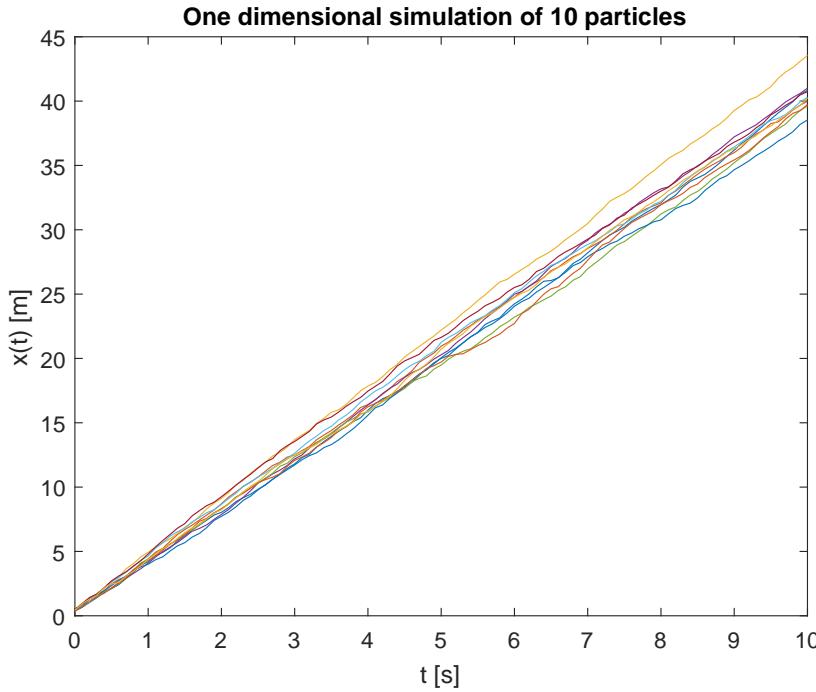

Figure 4.4: Simulation of 10 particles with the random walk model with $\Delta t = 0.1$, $\vec{u} = (u_x, u_z) = (4, 0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0.05, 0)$

Figure 4.5 shows the solution of the advection-diffusion equation and the random walk model in one figure.
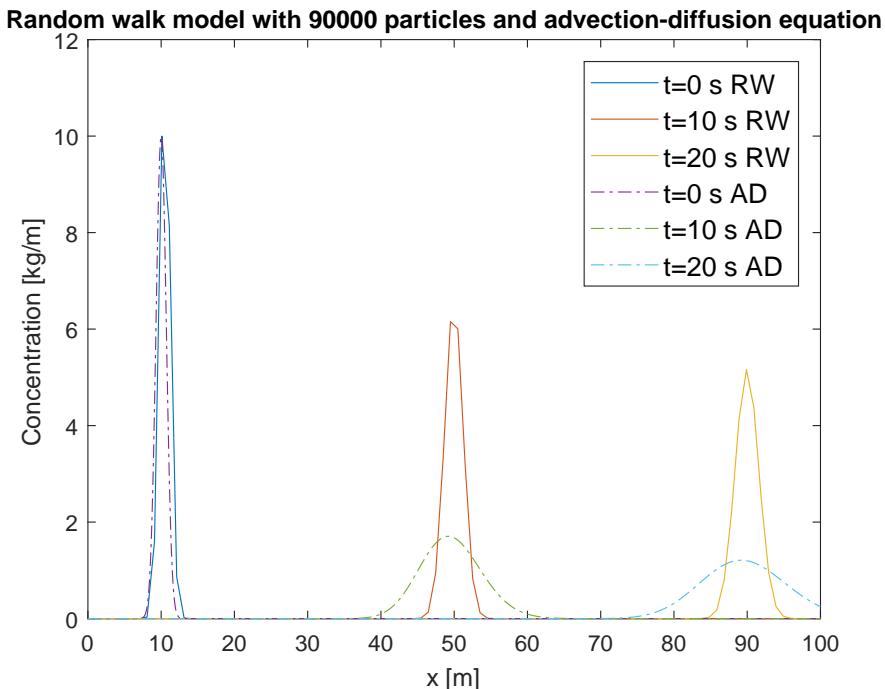
Figure 4.5: Simulation of 90000 particles with the random walk model (RW) and the solution of the advection-diffusion equation (AD) with initial condition $10e^{x^2}$, $\Delta t = 0.1$, $\vec{u} = (u_x, u_z) = (0, 0)$, $\Delta t = 0.1$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0.05, 0)$

The two models are not similar for this test case, see figure 4.5. It seems like the advection-diffusion equation is much more diffusive than the random walk model for the same parameters. This is due to numerical diffusion. This is not an error in the model, but in the numerical method or resolution. To show this, in figure 4.6 the time step in the numerical method is 0.001 s instead of 0.1 s. With this adjustment the two methods are very similar again.
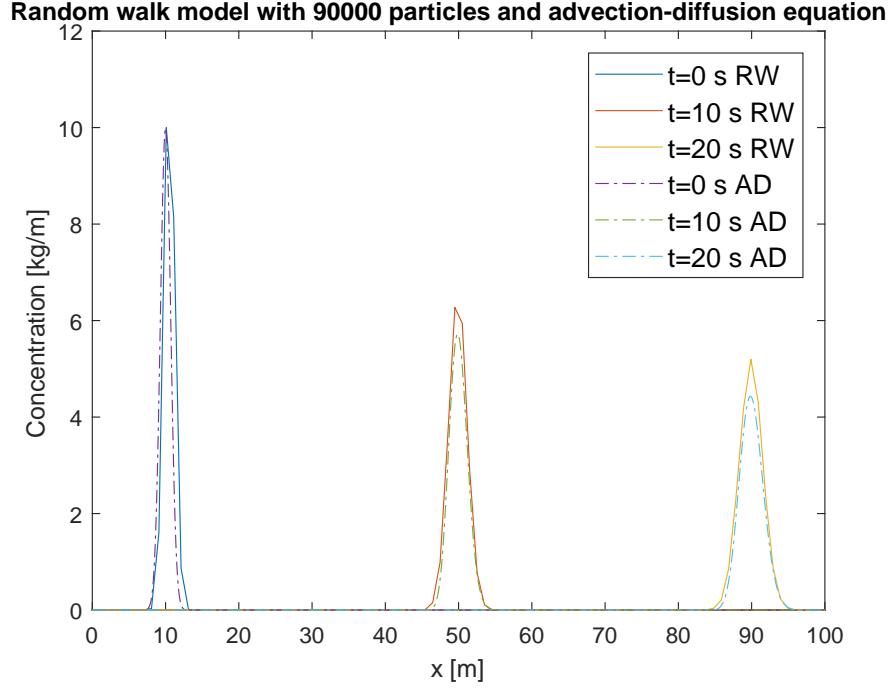
Figure 4.6: Simulation of 90000 particles with the random walk model (RW) with $\Delta t = 0.1$ and the solution of the advection-diffusion equation (AD) with $\Delta t = 0.001$. Both models with initial condition $C(t = 0) = 10e^{x^2}$, $\vec{u} = (u_x, u_z) = (0, 0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0.05, 0)$

4.2. Two-dimensional

For the two-dimensional case also different settings are explored, with varying velocity field, eddy diffusivity, buoyancy velocity and initial condition. Equation 2.29 and 4.4 are used to simulate the results:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}(\epsilon_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial z}(\epsilon_z \frac{\partial c}{\partial z}) - \frac{\partial((u_z + v_b)c)}{\partial z} - (\frac{\partial u_x c}{\partial x}) \tag{4.3}$$

$$dX_t = (u_x + \frac{d\epsilon_x}{dx})dt + \sqrt{2\epsilon_x}dW_t$$
$$dZ_t = (u_z + \frac{d\epsilon_z}{dz} + v_b)dt + \sqrt{2\epsilon_z}dW_t \tag{4.4}$$

To compare the random walk model with the advection-diffusion solution, the particles are counted in the same box area as the spatial discretization Δx and Δz of the advection-diffusion equation. Just like the one-dimensional case, the following initial condition is used:

$$C(t=0) = 10e^{-0.05((x-k_x)^2 + (z-k_z)^2)} \tag{4.5}$$

With k_x and k_z constants to specify the center of the peak. The values of these constants will be specified per test case. The two-dimensional results are divided in four different parts: the diffusion, the asymmetric diffusivity, the advection and the eddy velocity field. In the following sections the titles of the figures with the random walk model will be abbreviated with RW and the advection-diffusion equation with AD.

4.2.1. Diffusion

This section is used to show the similarity between both models in the eddy diffusivity component. The following variables are used $\vec{u} = (u_x, u_z) = (0,0)$, $v_b = 0$, $\Delta t = 0.05$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, 10^{-5})$. Figure 4.7 shows the random walk model for a finite number of particles. The transport of the particles is only due to the eddy diffusivity. This is as expected a two-dimensional Brownian motion. The big difference in the horizontal and vertical eddy diffusivity is very clear at the axes of the figure.
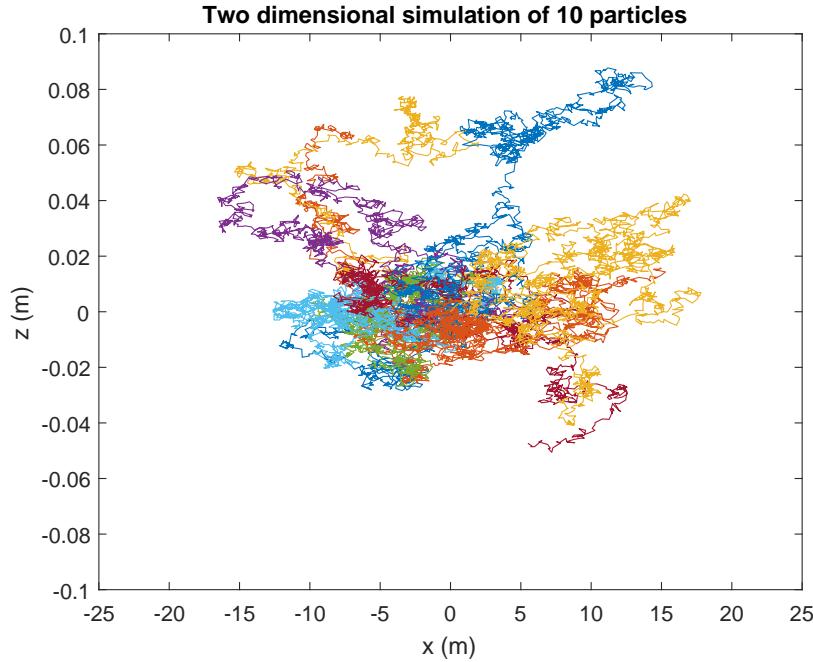

Figure 4.7: Simulation of 10 particles with the random walk model with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = (0,0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, 10^{-5})$

Figures 4.8-4.10 show respectively the random walk model simulation, the solution of the advection-diffusion equation and the difference between the two models. The figure clearly shows that the horizontal

diffusivity is much higher than the vertical diffusivity. The random walk model and the advection-diffusion equation show very similar behavior. The difference figure shows the relative difference in respect to the current concentration of the models. The differences are all below 5%. This indicates, that with ideal circumstances (infinite particles, no numerical errors), the solution will be equal. The biggest relative differences are at the outside of the diffusion cloud. This occurs because only a finite amount of particles is available. As expected the random walk model becomes less accurate when the timescale and area is larger.
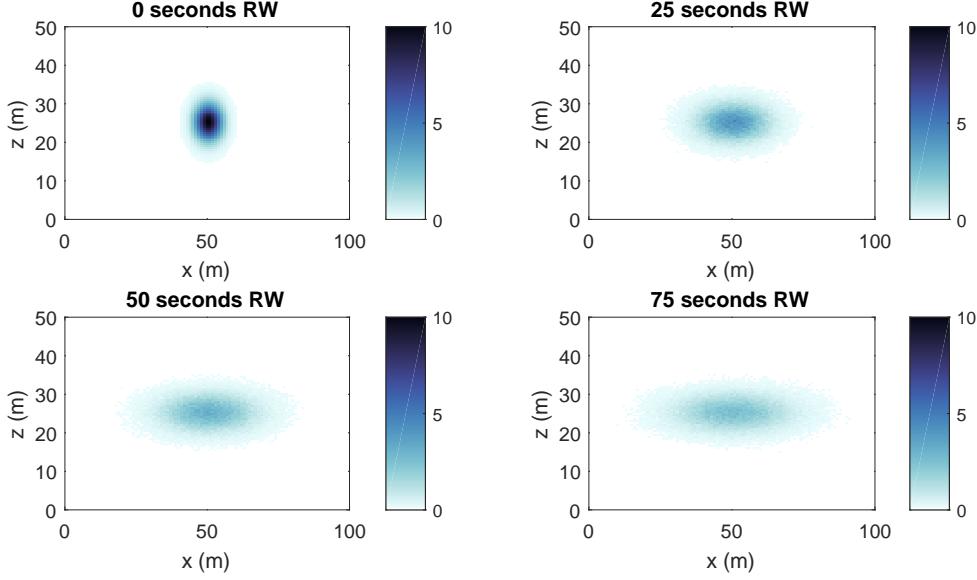
Figure 4.8: Simulation of 100000 particles with the random walk model (RW) with $\Delta t = 0.05$, $k_x = 50$, $k_z = 25$, $\vec{u} = (u_x, u_z) = (0,0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, 10^{-5})$
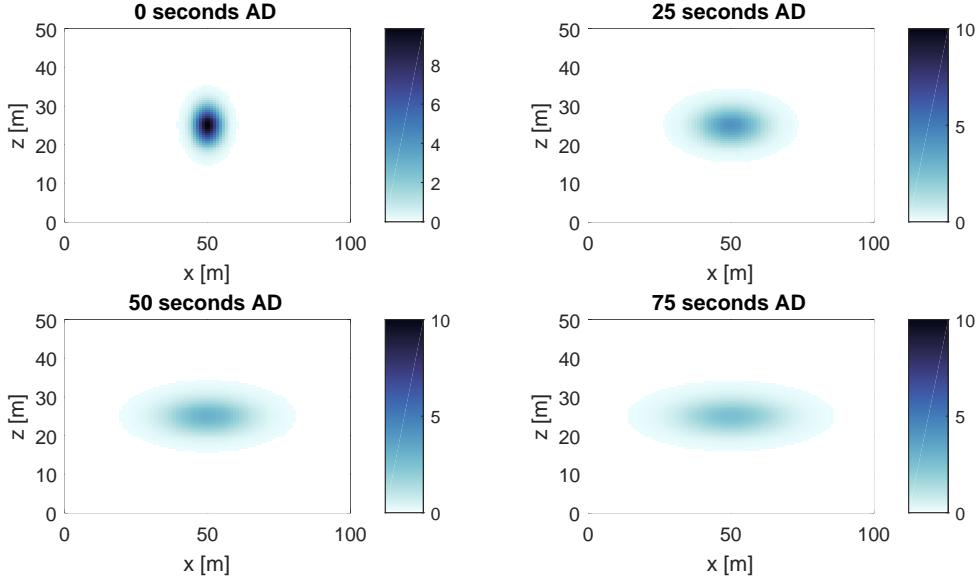
Figure 4.9: The solution of the advection-diffusion equation (AD) with $\Delta t = 0.05$, $k_x = 50$, $k_z = 25$, $\vec{u} = (u_x, u_z) = (0,0)$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, 10^{-5})$
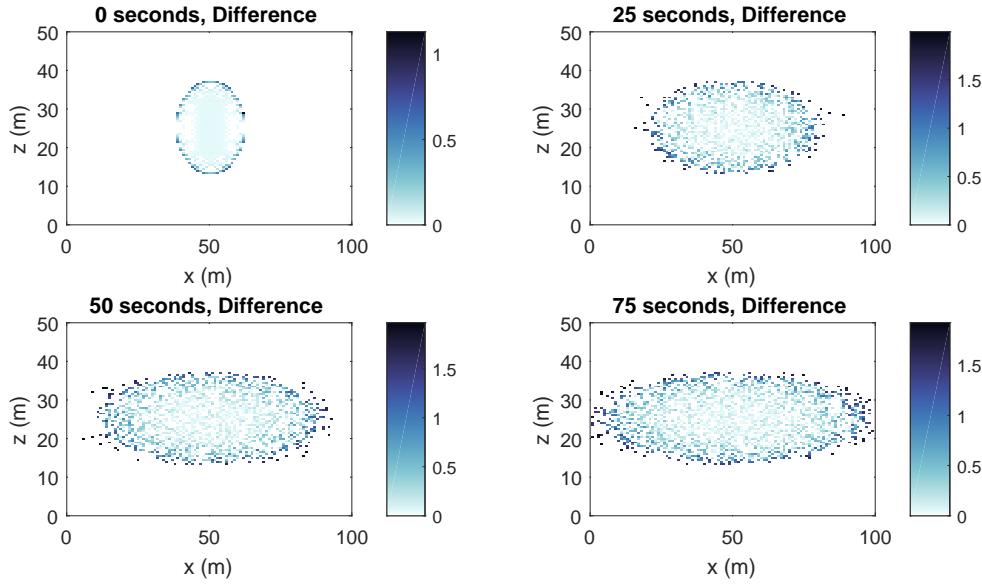
Figure 4.10: The difference between the random walk model and the solution of the advection diffusion equation.

4.2.2. Asymmetric diffusivity

This test case is used to look at the influence of the less intuitive terms $\frac{d\epsilon_z}{\partial z}$ and $\frac{d\epsilon_x}{\partial z}$. Only the vertical term $\frac{d\epsilon_z}{\partial z}$ will be explored, this term has more impact because of the smaller spatial range. The eddy diffusivity in the vertical direction will be defined with the following function:

$$f(z) = \epsilon_z = (\frac{2}{H})^2 (H - z)z \tag{4.6}$$

With H the height of water in the test case. The magnitude of the parabola is not a value that can occur in real-life, but the differences between the two simulations will be more clearly with this value. Figure 4.11 shows the plot of equation 4.6:
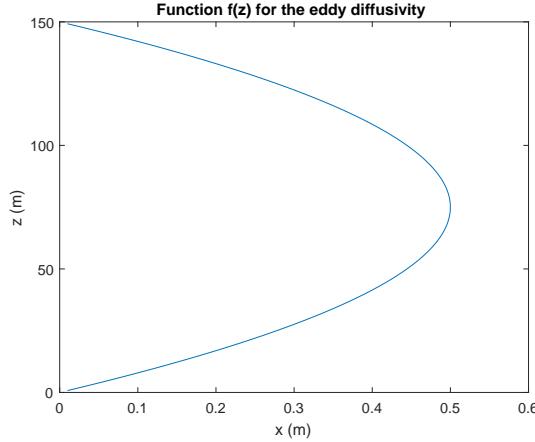
Figure 4.11: Function $\epsilon_z = (\frac{2}{H})^2 (H - z)z$.

The test case is very similar to the diffusion test case, but the placement of the initial condition is very important is this case. In the center of the test case the derivative of the eddy diffusivity term is zero. If the initial condition is placed here, no difference will appear. Therefore the initial condition is chosen in the lower part of the test case, with $k_x = 50$ and $k_z = 40$. The first two figures are respectively the simulations of the random walk model with and without implementation of the term $\frac{d\epsilon_z}{\partial z}$. The following variables are used $\vec{u} = (u_x, u_z) = (0,0)$, $v_b = 0$, $\Delta t = 0.05$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, f(z))$.
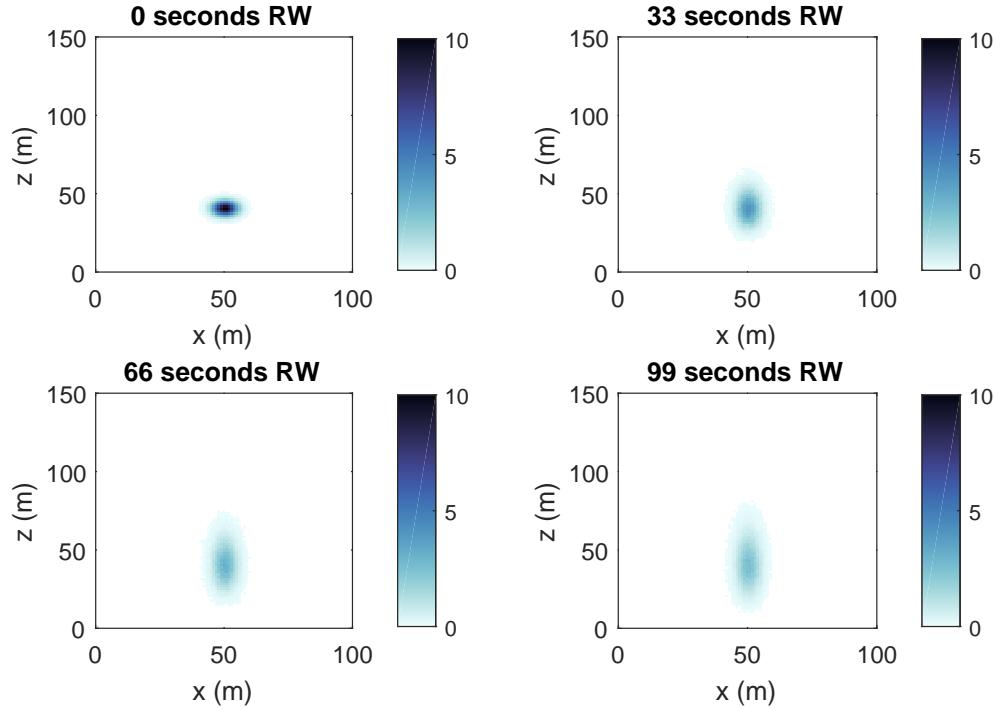
Figure 4.12: Simulation of 100000 particles with the random walk model (RW) with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = (0,0)$, $k_x = 50$, $k_z = 40$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, f(z))$, with the term $\frac{d\epsilon_z}{\partial z}$ implemented.
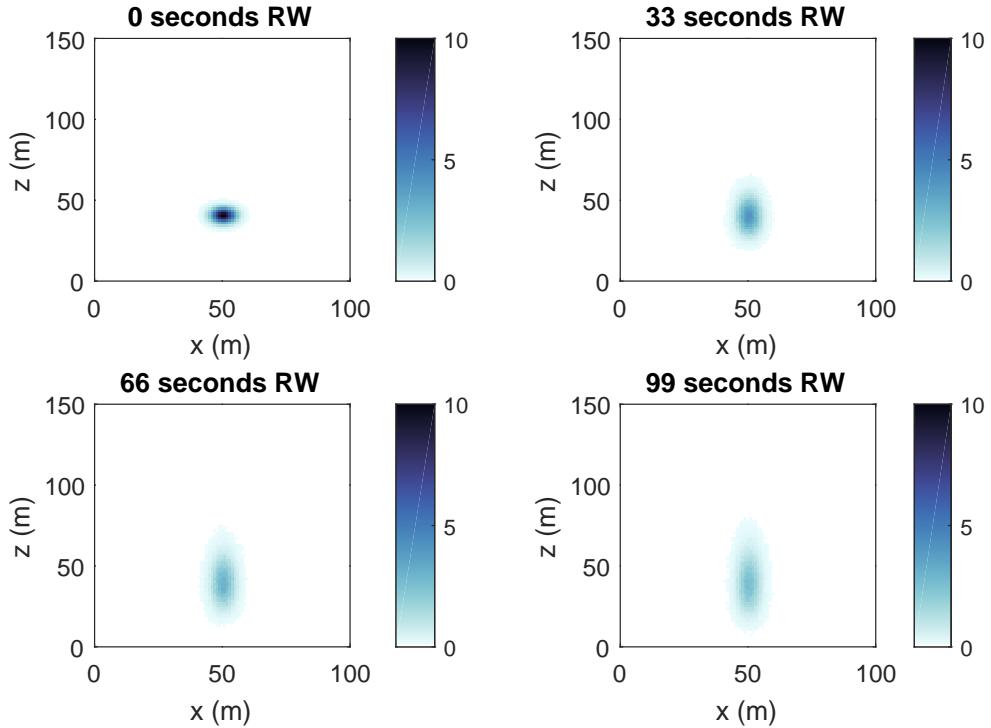
Figure 4.13: Simulation of 100000 particles with the random walk model (RW) with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = (0,0)$, $k_x = 50$, $k_z = 40$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, f(z))$, without the term $\frac{d\epsilon_z}{\partial z}$ implemented.

In these two figures it is difficult to see difference between the two simulations. Figure 4.14 shows the solution of the advection-diffusion equation for this test case.
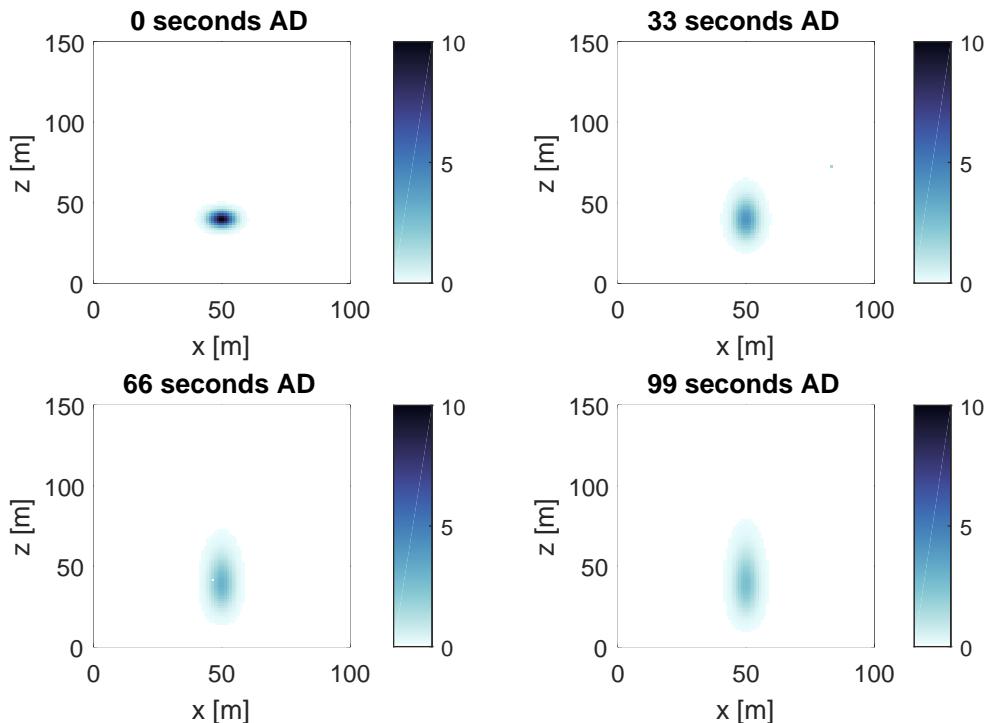

Figure 4.14: The solution of the advection-diffusion equation (AD) with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = (0,0)$, $k_x = 50$, $k_z = 40$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, f(z))$

Figures 4.15 and 4.16 show the two difference figures of the advection-diffusion equation solution with the random walk model. In figure 4.16 the difference has a shift in the lower part. It becomes larger, because the solution of the advection-diffusion equation has shifted in an advective way. This indicates that the random walk model with the term $\frac{d\epsilon_z}{\partial z}$ included is better in accordance with the advection-diffusion equation solution. This is in corresponds with the mathematical derivation.
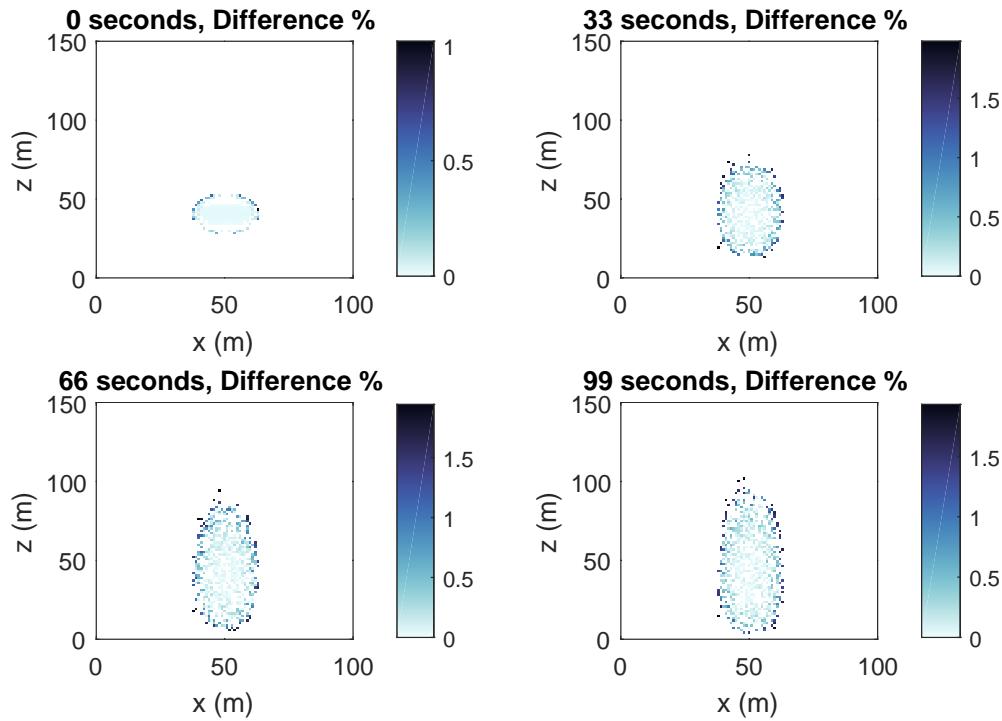
Figure 4.15: The difference between the random walk model and the solution of the advection diffusion equation, with the term $\frac{d\epsilon_z}{\partial z}$ implemented.
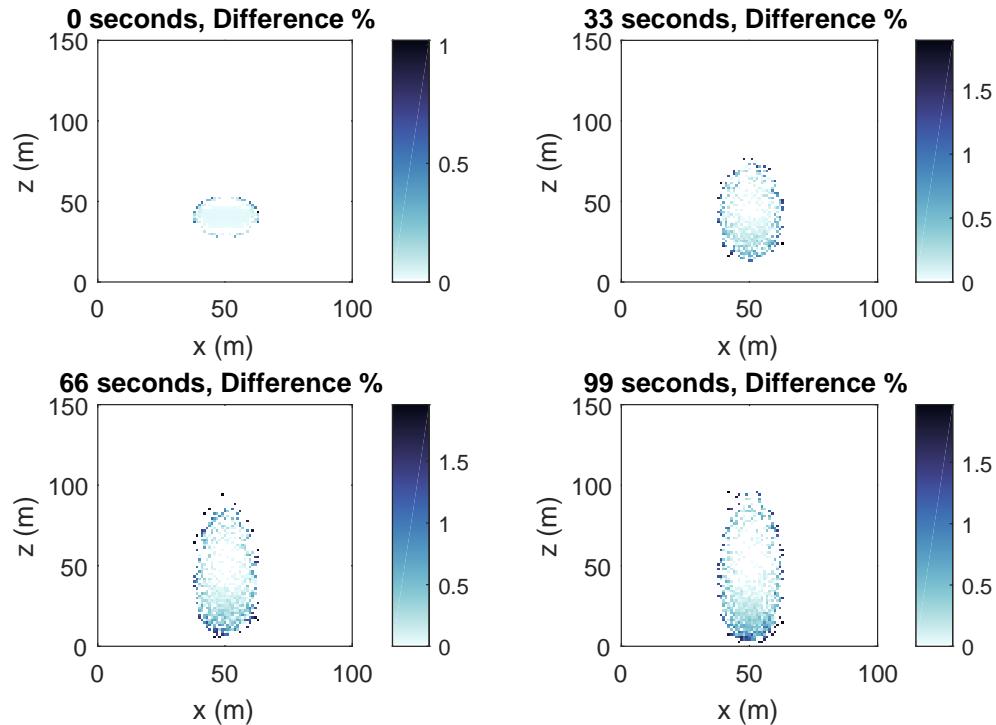

Figure 4.16: The difference between the random walk model and the solution of the advection diffusion equation, without the term $\frac{d\epsilon_z}{\partial z}$ implemented.

4.2.3. Advection

In this section the similarity between both models in the advection component is explored. A velocity field with a x-component and a buoyancy velocity is implemented. The following variables are used: $\vec{u} = (u_x, u_z) = (1.5, 0)$, $v_b = 1.1$, the initial condition with $k_x = 15$, $k_z = 15$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0, 0)$. Figure 4.17 shows the random walk model for a finite number of particles.
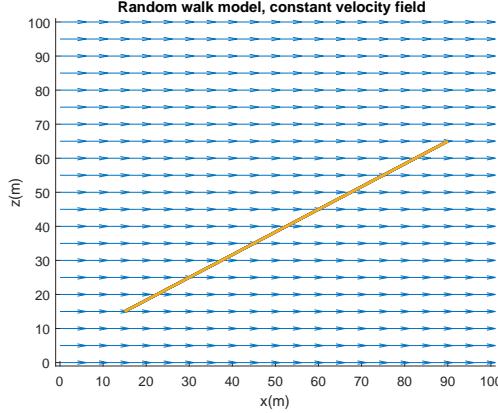

Figure 4.17: Simulation of 10 particles with the random walk model with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = (1.5, 0)$, $v_b = 1$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0, 0)$

The transport of the particles is only due to the horizontal velocity and the vertical buoyancy velocity. Therefore the displacement is completely straight, with no diffusivity. Figures 4.18-4.20 show respectively the random walk model simulation, the solution of the advection-diffusion equation and the difference between the two models. The solution of advection-diffusion reaches the top of the test case. At the boundaries of the test case, the perpendicular velocities are set zero. Therefore an accumulation will occur at the boundary. It is clearly visible that the two models do not have similar solutions. Similar to the one-dimensional test case, this is due to numerical diffusion. This could be solved with choosing a smaller time step, but with the implicit numerical scheme this is very time-consuming. The characteristics will be similar for an ideal situation with no numerical error and infinite particles.
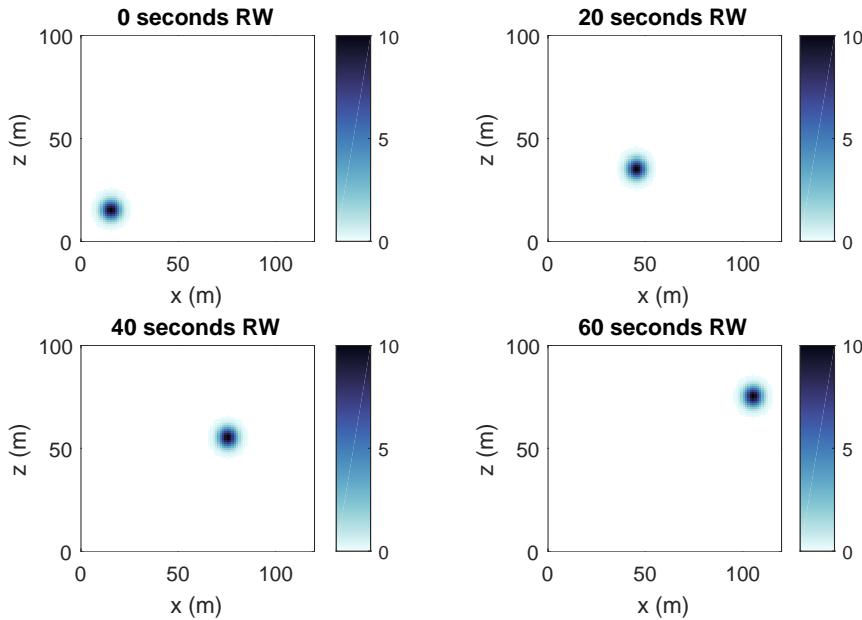

Figure 4.18: Simulation of 100000 particles with the random walk model (RW) with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = (1.5, 0)$, $v_b = 1$, $k_x = 20$, $k_z = 20$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0, 0)$
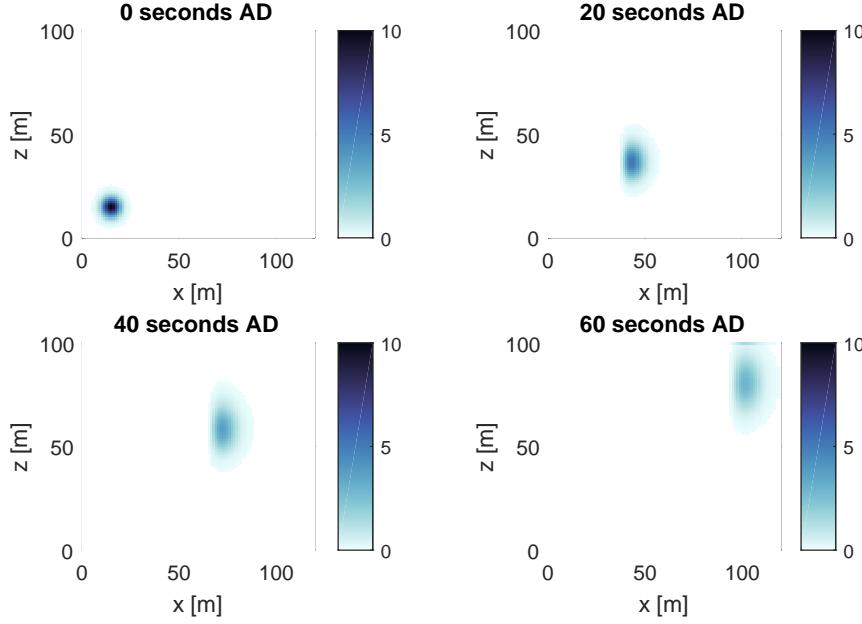
Figure 4.19: The solution of the advection-diffusion equation (AD) with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = (1.5, 0)$, $v_b = 1$, $k_x = 20$, $k_z = 20$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (0, 0)$
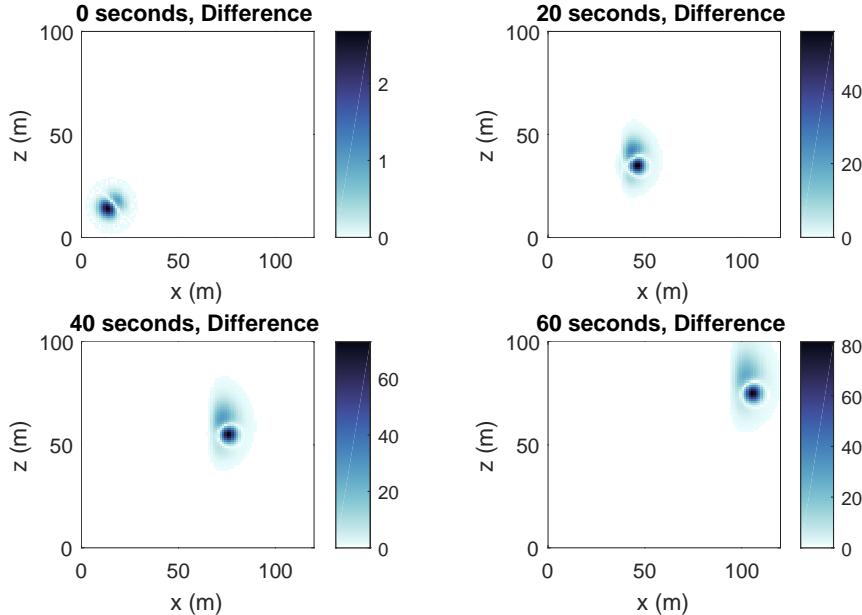

Figure 4.20: The difference between the random walk model and the solution of the advection diffusion equation.

4.2.4. Eddy velocity field

This test case is used to implement both models with a real-life velocity field of an eddy. The velocity field showed in figure 3.3 and defined in equation 3.1 is applied for this test case. The following variables are used: $\vec{u} = (u_x, u_z) =$ (eq.3.1), $v_b = 1.1$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, 10^{-5})$. Similar to the section about the advection component, at the boundaries of the test case the perpendicular velocities are set zero. Also the perpendicular eddy diffusivity coefficients at the boundaries are set to zero. In this way no particles can cross a boundary and vanish out of the test case. The buoyancy velocity is stronger than all vertical velocities of the velocity field. Therefore an accumulation will occur at the top boundary. To model a case with plastics distributed

in the ocean, an initial condition is chosen with three different peaks for $k_x = 15, 50, 85$ and $k_z = 15, 25, 35$. Figure 4.21 shows the test case with a finite amount of particles.
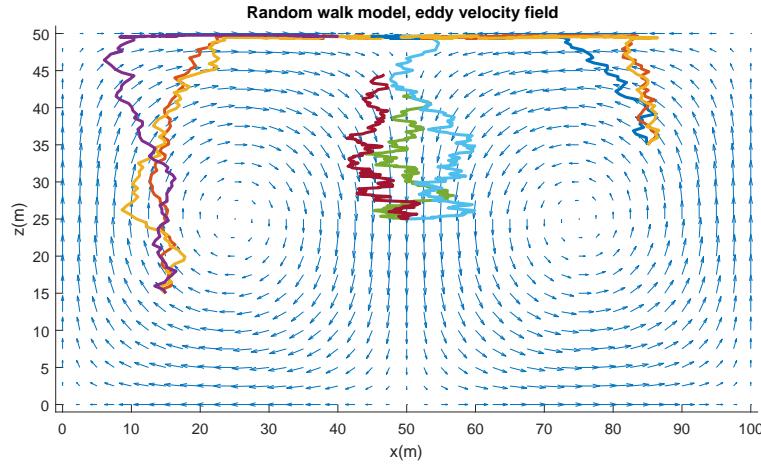

Figure 4.21: Simulation of 9 particles with the random walk model with $\Delta t = 0.1$, $\vec{u} = (u_x, u_z) = $ (eq.3.1), $v_b = 1.1$ and $\vec{\epsilon} = (\epsilon_x, \epsilon_z) = (1, 10^{-5})$

Figures 4.22-4.24 show respectively the random walk model simulation, the solution of the advection-diffusion equation and the difference between the two models. Both models behave similar and as expected; the plastic particles accumulate at the surface of the water in an eddy. The boundary conditions are properly implemented, the particles don't cross the boundary of the test case. They accumulate for the converging ekman transport. The differences become again larger with a larger timescale.
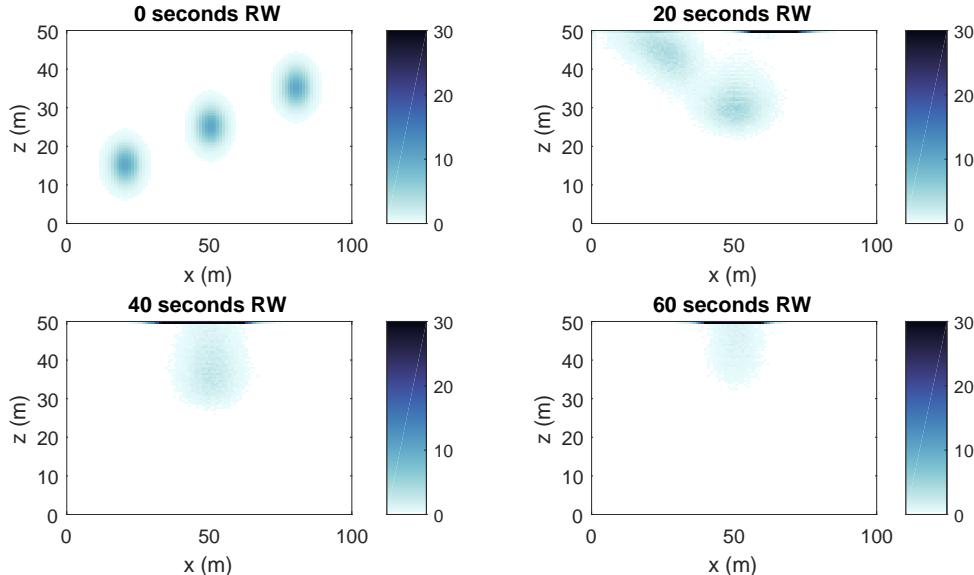

Figure 4.22: Simulation of 100000 particles with the random walk model (RW) with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = $ (eq.3.1), $v_b = 1.1$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, 10^{-5})$
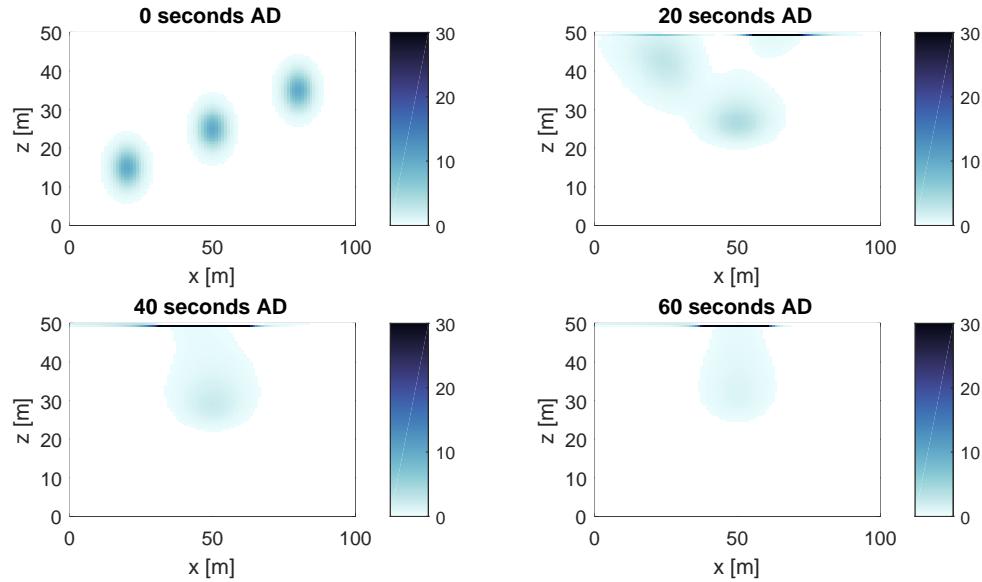
Figure 4.23: The solution of the advection-diffusion equation (AD) with $\Delta t = 0.05$, $\vec{u} = (u_x, u_z) = $ (eq.3.1), $v_b = 1.1$ and $\epsilon_{ij} = (\epsilon_x, \epsilon_z) = (1, 10^{-5})$
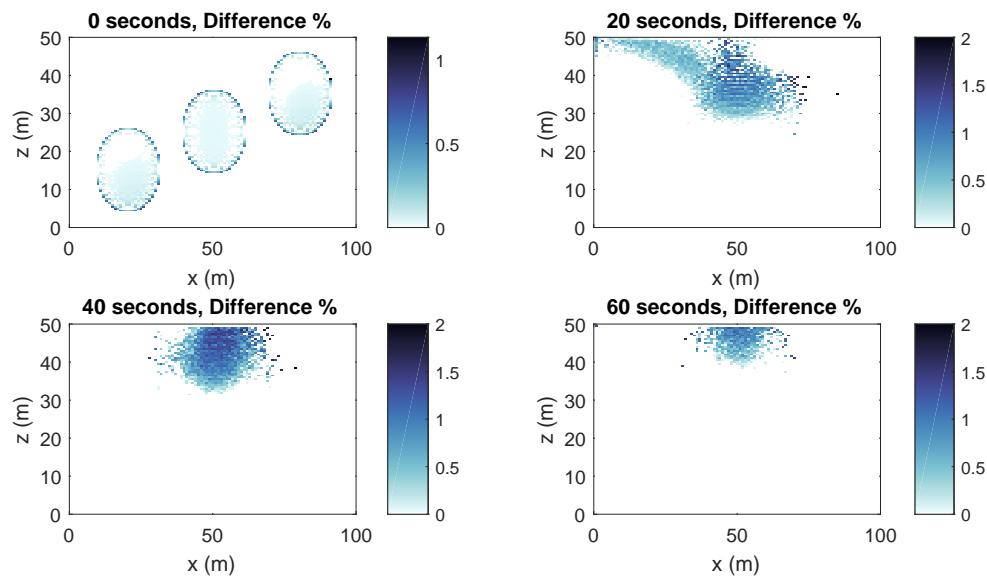

Figure 4.24: The difference between the random walk model and the solution of the advection diffusion equation.

5

Conclusion and recommendations

In the following sections the conclusions and recommendations are presented. First the research questions will be answered individually. Secondly, some general points that can be improved are discussed. At the end the recommendations for further research are presented.

5.1. Conclusion

In the first part of the conclusion, the three research questions are answered:

- Which adjustments and assumptions are needed to adapt the existing transport models in a way that they are adequate for modeling plastic?

The most important adjustment is including the vertical forces for a plastic particle. With this adjustment, the plastic particles will be buoyant, which is in accordance with the physical properties of plastics. Secondly it is important to have a right estimation of the turbulent eddy diffusivity, to model the small turbulence motions in the ocean which influence plastics. At last, it is important to take into account the time scale of plastics to adjust to the velocity field. When this time scale is small, the steady state buoyancy velocity is assumed.

- Are the random walk model and the numerical solution of the advection-diffusion equation equally efficient for the modeling of plastics with a vertical velocity term?

Both models have some limitations in efficiency. The advection-diffusion equation is not suitable for high concentration gradients. The random walk model is not suitable for big areas or long timescales. For example a dumping of plastics from a ship, can be modeled better with the random walk model. Since this is only a small area or small time, but a large concentration gradient. To discover a permanent accumulation zone, the advection-diffusion equation is a better approach. Since a large area and timescale is needed to find permanent zones. Both approaches can be implemented as a combination, to take full advantage of the good features of both models and bypass the bad ones. This idea is already mentioned by Stijnen et al. (2006).

- How can the transport model be used to obtain realistic results for an real life situation, for example the Mediterranean Sea?

Deltares has a two-dimensional horizontal model for the tracking of particles in the ocean. To be able to model plastic particles with a buoyancy force, the two-dimensional vertical model defined in this project should be combined with the already existing model from Deltares. With such a model, the vertical and horizontal forces are both included, which will give accurate results. This can be verified with surveys, other modeling data and argo float data.

Besides the conclusions to the research questions, there are also some other general points that can be discussed.

The stratification in the ocean has not been taken into account. In real-life the ocean is stratified with different characteristics in different layers, for example salinity and temperature levels. It is very unlikely that a plastic particle will move from one layer to another layer. This has to be implemented in the model, this is possible with a variable eddy diffusivity coefficient. This value should decrease near boundaries between layers, the surface of the ocean and the ocean floor, as defined in the paper of Stijnen et al. (2006).

The applied model for the eddy diffusivity coefficient is not very accurate. It is a simple approximation, but not always accurate for the complex turbulence field in the ocean. D-Flow FM could be used to calculate a real-life velocity field with corresponding eddy diffusivity. In this program more complex approximations are used.

Several improvements are possible for the numerical approach. A higher order numerical method can be implemented to solve the advection-diffusion equation. This would reduce the numerical diffusion, which is visible in some of the results. The numerical discretization could be changed to better match with the x and z dimension. In oceans, the x-direction is a much larger field than the z-direction. Smaller time steps in the vertical direction can be used to be more accurate. Too large time steps can result in a particle that crosses a physical boundary. Larger time steps in the horizontal direction can be used to keep the calculations fast.

The chosen velocity field is at first sight similar to the velocity fields within an eddy. But this is a cosine function, so there is no proof that this velocity field really matches with the properties of an eddy. This could be solved when the velocity field of a hydrodynamic model in D-Flow FM is implemented.

5.2. Recommendations

For further research the existing model of Deltares and the model in this project could be combined. The result will be a three-dimensional model that includes the physical properties of plastics. This model can be used with real-life data from for example the Mediterranean with D-Flow FM. The accuracy of this model can be tested with real-life data from surveys, other modeling programs and argo float data.

The difference between a future three-dimensional model and the two-dimensional horizontal model from Deltares could be explored. The differences between the two models can be quantified to determine which model will be useful in which specific situation. The three-dimensional model will have longer calculation times, but more accurate solutions.

Bibliography

Courtney Arthur, Joel Baker, and Holly Bamford. Proceedings of the international research workshop on the occurrence, effects and fate of microplastic marine debris. 01 2009.

Yannis Cuypers, Pascale Bouruet-Aubertot, Claudie Marec, and Jean-Luc Fuda. Turbulence in the mediterranean sea during boum experiment and perspectives. 2012.

Deltares. Technical reference manual dflow fm.

K Denmon, E Hofmann, H Marchant, M R Abbott, T S Bates, Stephen Calvert, M J Fasham, R Jahnke, S Kempe, R J Lara, C S Laws, P Liss, Anthony Michaels, Thomas Pedersen, M A Pena, T Platt, JH Sharp, David Thomas, K A van Scoy, and Andrew Watson. Chapter 10: Marine biotic responses to environmental change and feedbacks to climate, 01 1996.

Juliana A. Ivar do Sul and Monica F. Costa. The present and future of microplastic pollution in the marine environment. *Environmental Pollution*, 185(Supplement C):352 – 364, 2014. ISSN 0269-7491. doi: https://doi.org/10.1016/j.envpol.2013.10.036. URL http://www.sciencedirect.com/science/article/pii/S0269749113005642.

A. W. Heemink. Stochastic modelling of dispersion in shallow water. *Stochastic Hydrology and Hydraulics*, 4(2):161–174, Jun 1990. ISSN 1435-151X. doi: 10.1007/BF01543289. URL https://doi.org/10.1007/BF01543289.

Jenna Jambeck. Plastic waste inputs from land into the ocean. *Science Magazine*, 347:786–771, 2015.

A.H. Jazwinski. *Stochastic Processes and Filtering Theory*. Mathematics in Science and Engineering. Elsevier Science, 1970. ISBN 9780080960906. URL https://books.google.nl/books?id=nGlSNvKyY2MC.

F. Morrison. *An Introduction to Fluid Mechanics*. Cambridge University Press, 2013. ISBN 9781139615594.

Francesco Nencioli, Francesco D'Ovidio, Andrea Doglioli, and A A. Petrenko. In situ estimates of submesoscale horizontal eddy diffusivity across an ocean front: In situ horizontal eddy diffusivity. 118, 12 2013.

J. Pantaleone and J. Messer. The added mass of a spherical projectile. *American Journal of Physics*, 79:1202–1210, December 2011. doi: 10.1119/1.3644334.

J. W. Stijnen, A. W. Heemink, and H. X. Lin. An efficient 3d particle transport model for use in stratified flow. *International Journal for Numerical Methods in Fluids*, 51(3):331–350, 2006. URL www.scopus.com. Cited By :15.

J. H. M. ten Thije Boonkkamp and M. J. H. Anthonissen. The finite volume-complete flux scheme for advection-diffusion-reaction equations. *Journal of Scientific Computing*, 46(1):47–70, Jan 2011. ISSN 1573-7691. doi: 10.1007/s10915-010-9388-8. URL https://doi.org/10.1007/s10915-010-9388-8.

UNEP/MAP. Marine litter assessment in the mediterranean. 2015. URL https://wedocs.unep.org/rest/bitstreams/9739/retrieve.

G. K. Vallis. *Atmospheric and Oceanic Fluid Dynamics*. Cambridge University Press, Cambridge, U.K., 2006.

S. Vogel. *Life in Moving Fluids, The Physical Biology of Flow*. 1996.