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Vertical mixing strategies in the Opendrift platform: analytical solution and Random Walk scheme

Estratégias da mistura vertical na Plataforma Opendrift: a solução analítica e esquema Random Walk

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Predicted scenarios for microplastic displacement in the ocean is still a challenging task, where particle trajectory evolution is based on stochastic strategies at each timestep. The Opendrift platform presents a microplastic trajectory evolution solution using two strategies for turbulent vertical mixing. This work simulated microplastic particles emission in the Rio de Janeiro region (Guanabara Bay) and observed its depth over one year. Attentive to subtle differences, a statistical analysis was proposed to observe how particles are affected by the strategies individually. The preliminary observations showed no significant modification on the surface, but the depth had important motion modification. A dispersion was observed in XY coordinates of each particle using statistical analysis. The results demonstrated significant individual movement of microplastic particles. This study encourages the need for a protocol to decide which strategy to be used in computational simulations so that monitoring tasks can have optimum efficiency.
Keywords: microplastic, trajectory, prediction.

A predição de cenários para o deslocamento de microplásticos no oceano ainda é uma tarefa desafiadora, onde a evolução da trajetória das partículas é baseada em estratégias estocásticas a cada evolução temporal. A plataforma Opendrift apresenta uma solução de evolução da trajetória do microplástico usando duas estratégias para mistura vertical turbulenta. Este trabalho simulou a emissão de partículas de microplásticos na região do Rio de Janeiro (Baía de Guanabara) e observou sua profundidade ao longo de um ano. Atento a diferenças sutis, uma análise estatística foi proposta para observar como as partículas são afetadas pelas estratégias individualmente. As observações preliminares não mostraram nenhuma modificação significativa na superfície, mas a profundidade teve importante alteração no movimento. Observou-se uma dispersão das coordenadas XY de cada partícula a partir de análise estatística. Os resultados demonstraram significativa movimentação individual de cada partícula de microplástico Este estudo encoraja a necessidade de um protocolo para decidir qual estratégia a ser usada em simulações computacionais para que as tarefas de monitoramento possam ter maior eficiência.
Palavras-chave: microplástico, trajetória, predição.

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1. INTRODUCTION

There is a growing interest in the presence and movement of smaller parts of plastic (micro-scale) in the ocean [1]. Recent publications present concerning data on how plastic and microplastic are accumulating in the ocean [1-3]. Since the early 1950s, more plastic has been produced and due to transport effects, such as runoff effects, inappropriate litter disposal, and direct emission from vessels, the plastic keeps reaching and accumulating in the ocean [1, 3].

It has been found microplastic presence in food webs in the ocean biota, increasing the concern over the risk of deleterious effects for the biota and consumers of these plants and animals [1, 2].

There are computational platforms aiming to develop solutions to predict microplastic particles movement in the ocean [4, 5]. The traditional Eulerian and Lagrangian approaches are commonly used. However, the computational codes present some alternative solutions for the evolution of the trajectory of microplastics [4-6].

Finding the solution to the microplastic trajectory is complex and involves strategies and natural phenomena understanding and modelling. The reduction of stochasticity in calculations may infer a more robust microplastic tracking. However, there is much to understand about the mechanism of microplastic and how to standardize a procedure to provide more accurate results [4, 6].

The solution of vertical trajectory is commonly based on a random walk strategy or variants. The Opendrift computational platform is an open-source program developed by Norwegian researchers which can incorporate atmospheric and oceanic parameters in order to calculate and deliver the hydrodynamic output [5]. In this platform, the “PlasticDrift” module was developed by MET Norway and presents two solutions for this matter [5, 7].

This work is designed to present two simulations, one for each strategy of the platform so that evaluations can be performed. Understanding the differences between the methods may be useful when deciding which strategy to be taken for an effective monitoring task.

2. PARTICLE TRANSPORT METHODOLOGY

2.1 Opendrift general approach

In observance of the Opendrift code (available on https://github.com/OpenDrift/opendrift/), a numerical solution is based on the stages seen in Figure 1.

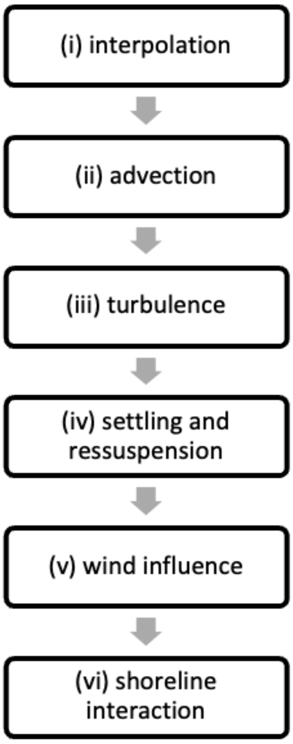


Figure 1: Scheme of the major processes involved in Opendrift computational code for modelling ocean drift and settling.

i) Interpolating the available data with time and space. This stage is crucial for the model as data must be accurate. Even small noises (or lack of data) can affect the complexity of the model significantly. The microplastic particles are expected to initiate the trajectory from a specific coordinate in the grid so that the dragging effect incurring is the result of this interpolation with water properties (salinity, temperature, diffusivities, tide, etc.) and atmosphere (x-wind, y-wind, wind direction, humidity, etc.).

For microplastic dynamics, the vertical motion will be considered, and each layer will be calculated in the model. A simple 3 layers geometry, equally divided, was imposed.

ii) The 2D movement is influenced by advection. The solution is reached using the Runge-Kutta method. At each timestep, the new velocities (x and y) are calculated for each particle.

iii) The turbulence in the water is also a key factor to be considered. For the Opendrift platform, the Plasticdrift module governs the motion of the lagrangian particles. The turbulent vertical mixing can be performed using two different schemes named (i) *analytical* (ii) and *random walk.*

iv) Settling and resuspension are complex, though important factors. In the Opendrift platform the solution is observed in a random motion solutions.

v) The wind affects the particles drift on the ocean surface. Particles with lower density than the water will keep floating, and thus be dragged by the wind.

vi) The shoreline interaction (*beaching*) is a computational strategy that relates the position of the particle at each timestep to the region of the coastline.

2.2 Opendrift approach for microplastic vertical movement

The Opendrift platform presents a module that can track the vertical movement of plastic particles throughout the ocean (PlasticDrift), based on ocean currents, stokes drift effect and wind drag [5]. A traditional Eulerian and Lagrangian element approach is conducted to simulate particles drifting through the ocean. This module is prepared to calculate the particle vertical motion under the effect of the vertical mixing phenomenon, which is oriented by the terminal velocity [5, 7].

There are two vertical motion schemes available in the Opendrift module, named: (i) the random walk strategy; and (ii) the analytical solution. The first method is based on Visser model [5, 7] for a random walk mixing strategy. The code ruling the vertical motion is:

```
(1) >>>      if self.get_config('vertical_mixing:mixingmodel') == 'randomwalk':
(2)>>>                 self.elements.z = self.elements.z* - self.elements.moving*(
(3)>>>                 dKdz*dt_mix - R*np.sqrt((Kz*dt_mix*2/r)))
```

The platform follows the user-input approach outlined in line(1) and executes the computation described in lines (2) and (3). In this process, the goal is to determine the updated vertical position of the particles, denoted as (*self.elements.z*). The result is based on the effects of turbulence and random walk perturbation.

Based on the code implemented in the Opendrift platform, the turbulence is represented by *dKdz* within a specific time (*dt_mix*). Concurrently, the random walk component encompasses two key elements. The parameter *R* represents the turbulent length scale of the mixed layer, influencing the scale of turbulent-induced movement. The variable *r* denotates a random number sourced from a uniform distribution within the interval (0,1).

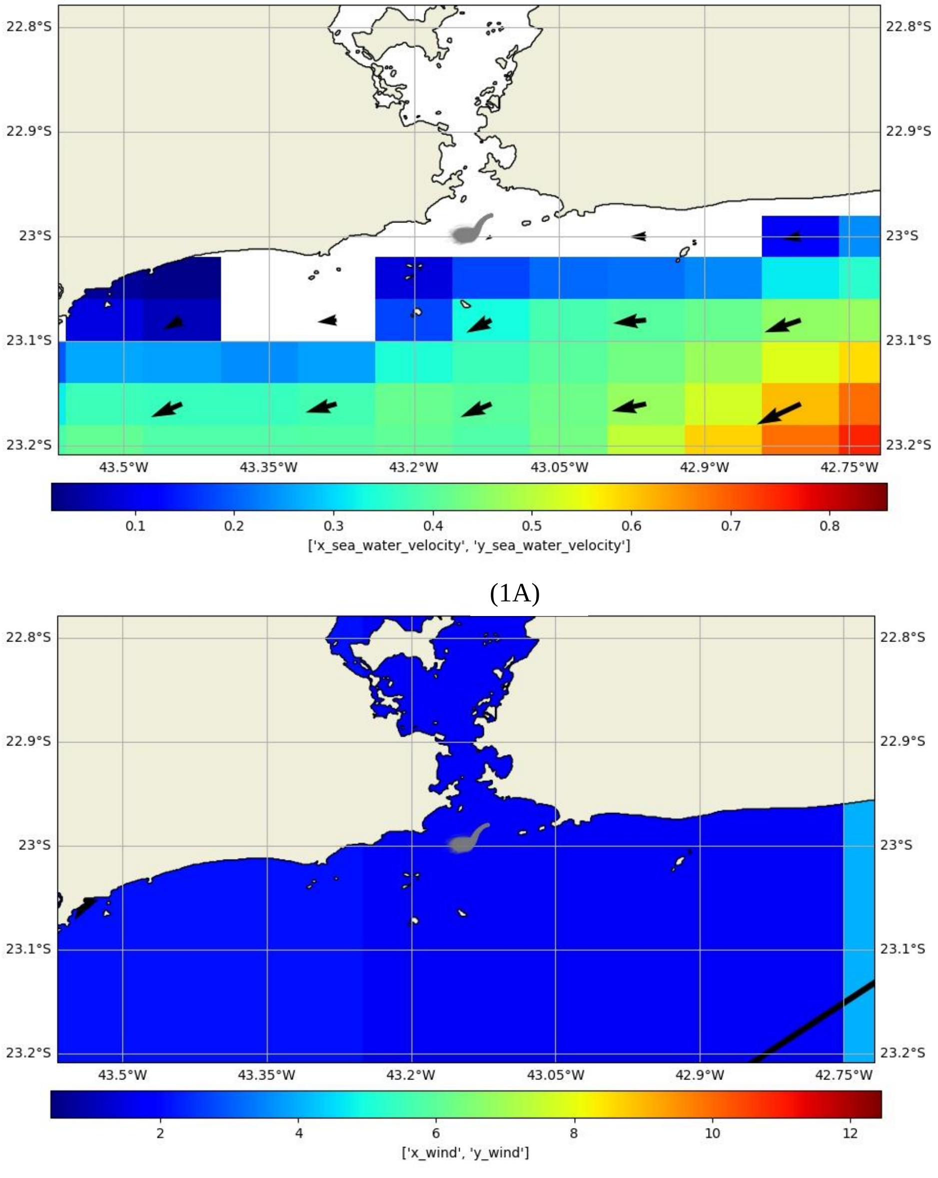
The second method is based on diffusivity and terminal velocity ratio, which provides the position in (z) of a group of elements in the ocean simulation as seen in the following codes:

```
(1)>>>     self.elements.z = -np.random.exponential(
(2)>>>           scale=self.environment.ocean_vertical_diffusivity/
(3)>>>                 self.elements.terminal_velocity,
```

where line (1) sets the vertical position of the elements in the model, based on a random number from an exponential distribution, provided negative (settling) otherwise buoying, and lines (2-3) provide the core part of the function based on the ratio between the ocean's diffusivity profile and the terminal velocity of the plastic particles, and thus how quickly the exponential function decays into zero.

2.3 Hydrodynamic model

The parameters for this model were incorporated from Hycom and NCEP Global Forecast System numerical weather prediction model for 8-day, 3-hourly at approximately 50-km resolution as can be seen in Figure 2.



(1A)

(1B)

Figure 2: Hycom sea water velocity (2A) and wind conditions (2B).

2.4 Model setup

Three thousand particles were seeded at longitude [-43.12] and latitude [-22.98] in WGS 1984 coordinates (Figure 3), the region is in Guanabara Bay tidal inlet region, in Rio de Janeiro, Brazil. This is a region with a strong economy and large population, whereas the highly wealthy regions are connected to more plastic consumption and social features provide inappropriate litter discard. Scientific papers are available supporting the existence and threats of this contaminant in Guanabara Bay [8, 9].

Simulation datetime is based on an instantaneous emission occurring on February 3rd, 2021 and simulated along the following 365 days.

The bathymetry was prepared using the *global_landmask* function provided by Opendrift reader. The database used was the Global Self-Consistent, Hierarchical, High-resolution Geography Database (GSHHG) available at https://www.ngdc.noaa.gov/mgg/shorelines/.

The two models were considered: (1) analytical mixing model and (2) random walk scheme.

The visual results and statistical evaluation were conducted to observe how the two vertical mixing schemes can influence the particle trajectory evolution implemented in Opendrift. For the statistical evaluation, the Python packages - *scipy* and *statistics* - were used.

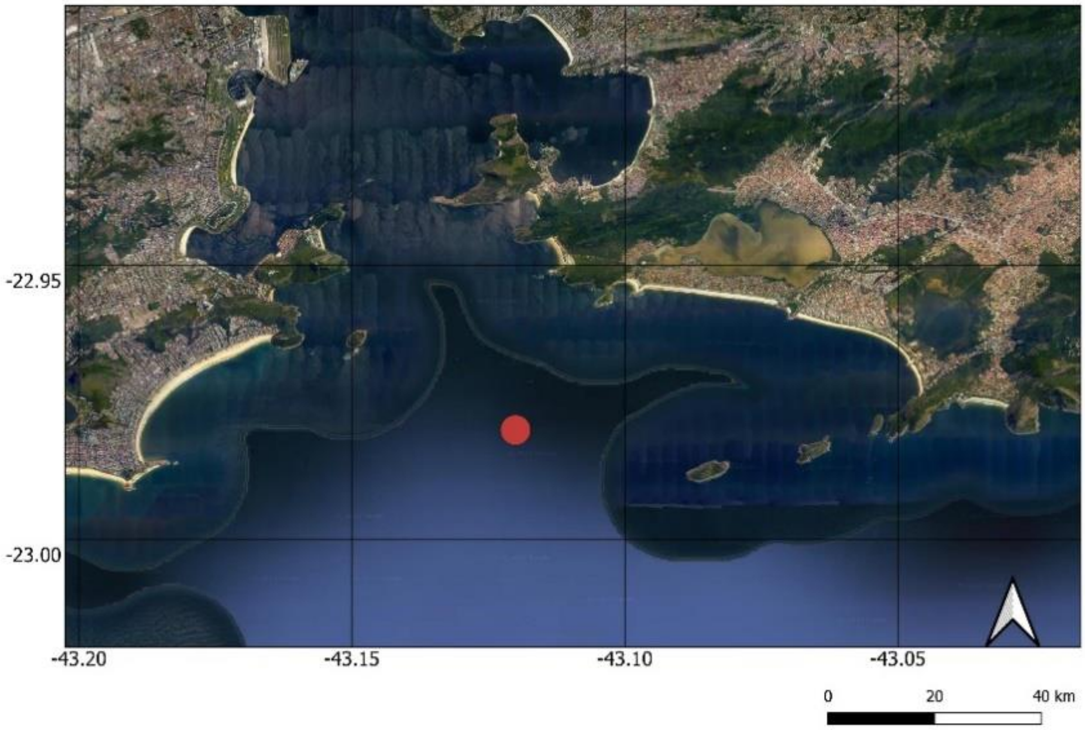


Figure 3: Georeferenced point of emission coordinates represented by the red dot.

3. RESULTS AND DISCUSSION

The results obtained from both the analytical model and random walk model by the Opendrift platform support suggest that the emissions from Guanabara Bay will route South as can be seen in Figure 4. The model demonstrated accumulation of particles in the Argentinean region, with potential concern in the Rio de la Plata (La Plata estuary mouth) region. This region has been studied by Pazos et al. (2017) [10] where microplastic accumulation was found in the region of the estuary mouth.

The random walk output showed a higher concentration of particles near the mouth of the estuary compared to the analytical solution. However, the actual scenario presents a continuous emission problem leading to increased particle amounts, shapes, and physicochemical properties, that can impact settling properties.

The microplastic movement is currently a challenging task to be tackled. Platforms are mostly based on advection, diffusive, and empirical sedimentation displacement for the prediction of the 3D movement of the particles [11], while other phenomena which might alter the prediction are not fully understood and covered. One example is that the presence of moving biota is not considered. It may alter the motion of the particles, through consumption or adherence to their bodies [10].

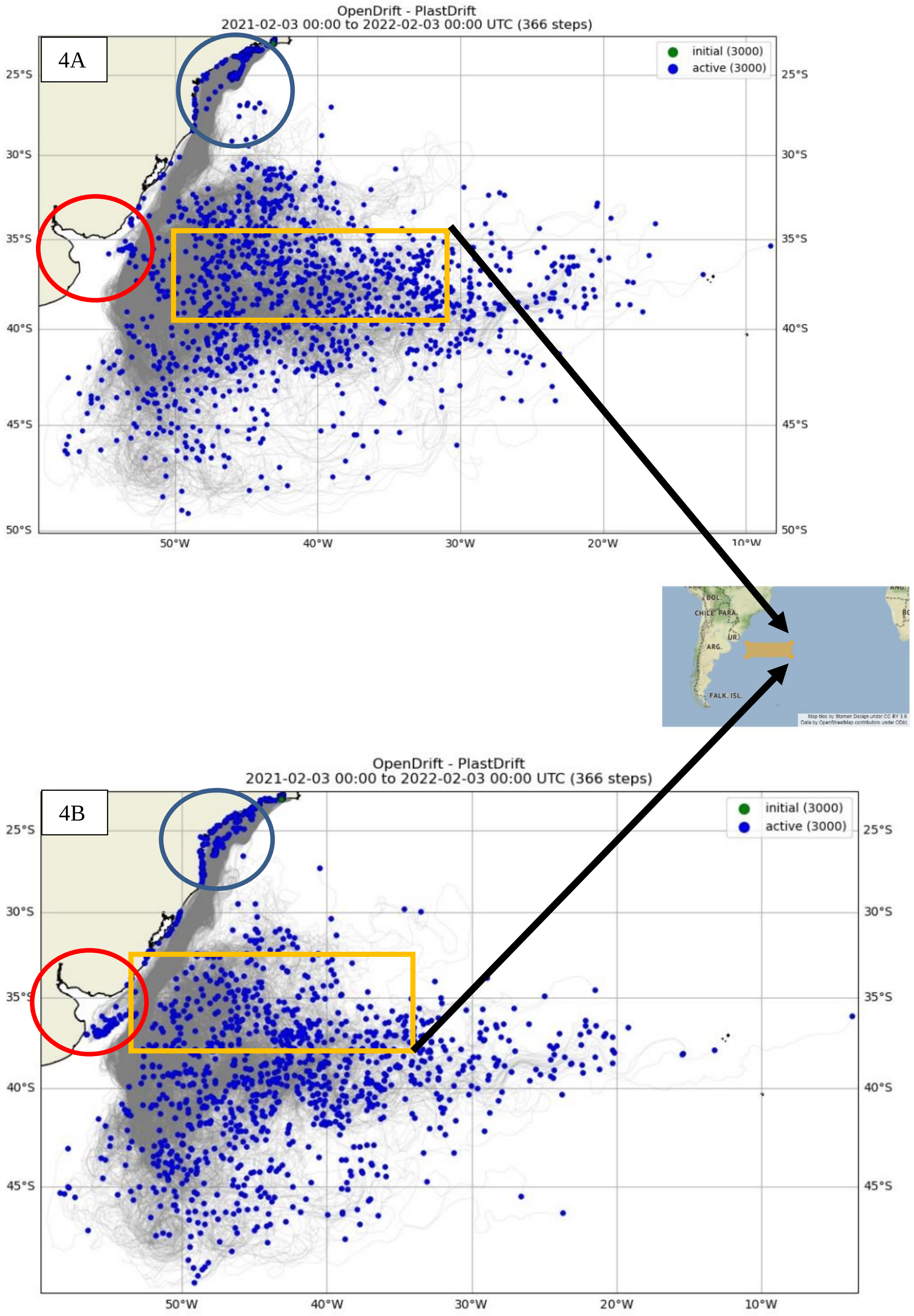
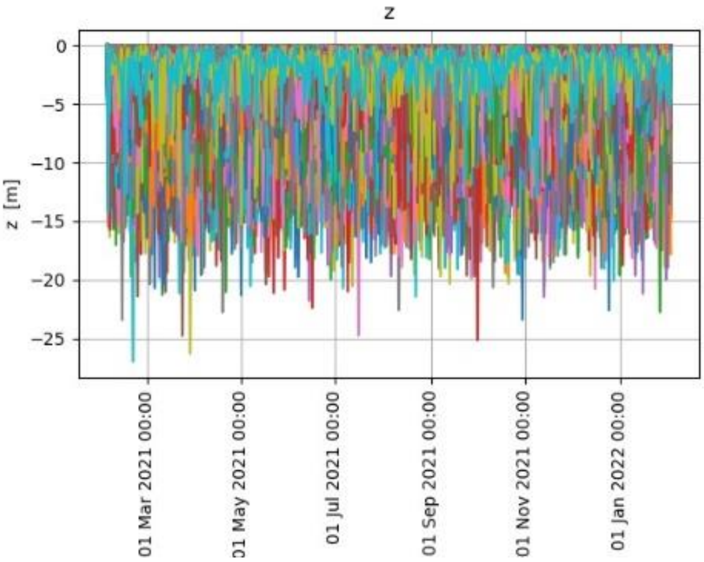
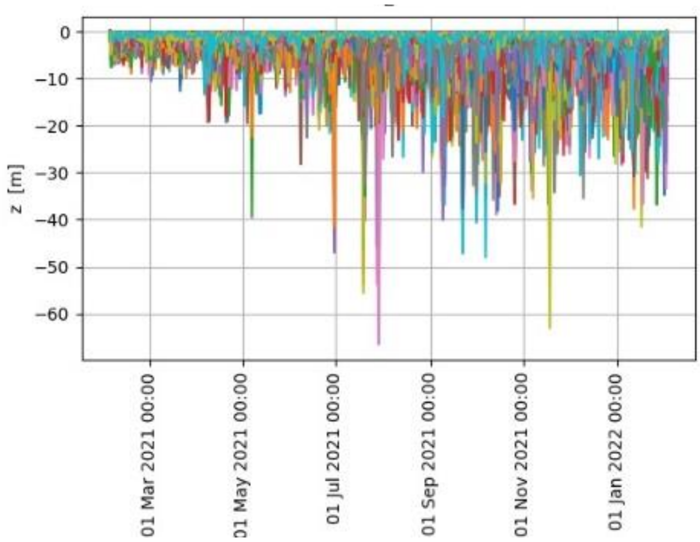


Figure 4: The analytical model (4A) and random-walk scheme (4B) results, in which the red circle indicates the microplastic accumulation and the blue circle the potential beaching effect.

The sedimentation and resuspension processes were observed in simulations performed with the platform as particles rose and sank throughout the simulation. For the analytical scheme, the particles tended to keep a regular depth of approximately 25m, and no significant difference was observed throughout the representations (Figure 5A). However, when the random walk scheme results were plotted regarding the vertical mixing, the particles were found at more profound and uneven levels (Figure 5B). It is expected that different properties in the particle (size, shape, etc) will affect the settling properties.



(5A)



(5B)

Figure 5: Vertical particle distribution calculated with the analytical solution (5A) and the random walk scheme (5B).

The results from the simulations showed a large group of buoyant particles regardless of the approach used (Figure 6). The submerged particles respected each layer's dynamic (wave, current, etc) and moved accordingly.

Several particles reached the shoreline. The platform demonstrated that a group of particles beached (Figure 3). The circulation of the ocean and the wind conditions will provide the necessary conditions for the buoyant microplastic to consequently beach [11]. The regions near the river are shallower than the ocean, which facilitates the microplastic to rapidly settle and interact with the soil. Observations on Guanabara Bay and La Plata region may suggest that the particles were moved by hydrodynamic and wind conditions or an unbalanced microplastic inlet [1, 2, 7, 9].

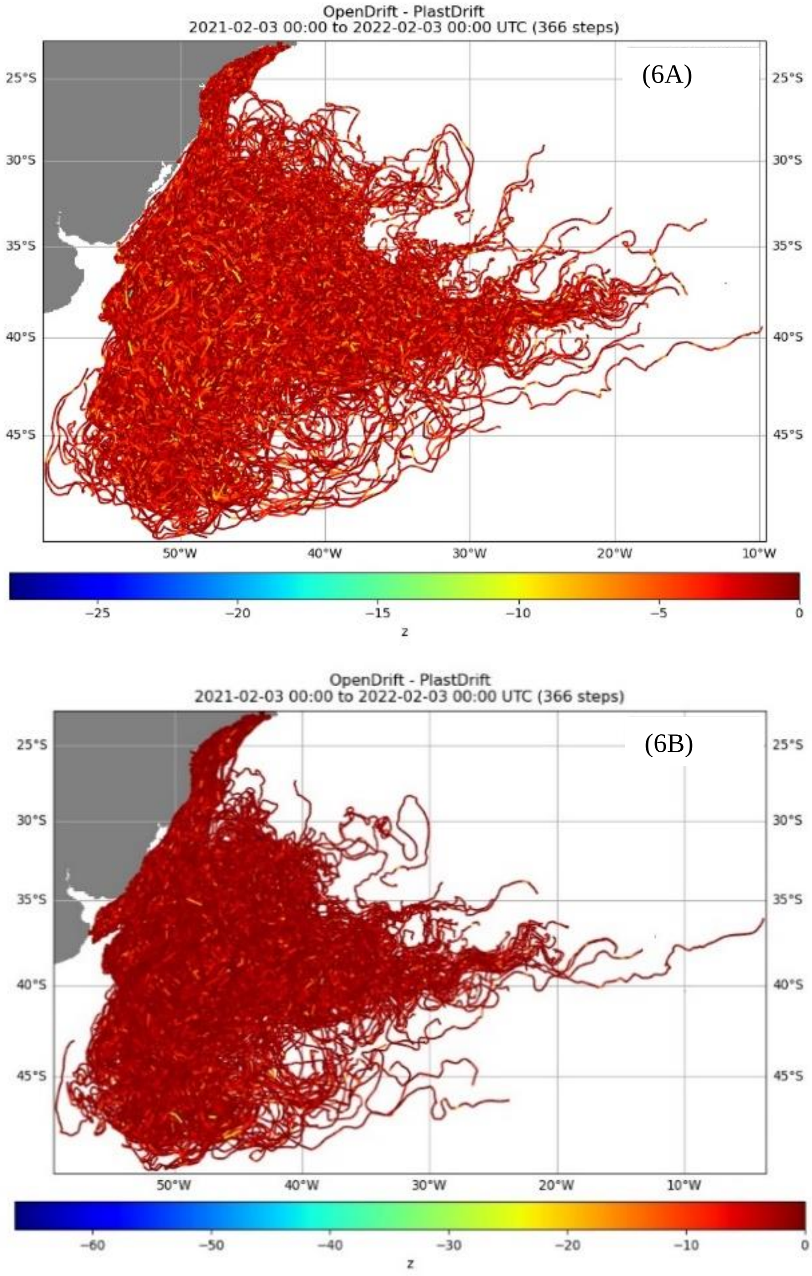


Figure 6: Calculated microplastic trajectory with a vertical colour scale representation using the analytical scheme (6A) and the random walk scheme (6B).

The computational platforms commonly use a regular spherical shape [4, 5, 11]. However, the reality of microplastic shapes is vast and hard to predict. Another factor to be considered is the possibility of the microplastic adhering to other surfaces and being transported by moving bodies (such as fish, a boat, etc.). Though it is reasonable to believe that a small group of particles should not be of concern, frequent transportation of microplastic can be of potential ecological harm and difficult to be predicted [11]. It is relevant to provide more studies in migratory fish and frequent vessel motion in order to qualify and quantify the potential impacts of adhered microplastic.

4. STATISTICAL EVALUATION

The statistical values for the differences between the random method coordinates and analytical method coordinates are presented in Table 1. In terms of the range, both longitude and latitude differences exhibit significant variability, spanning from negative to positive values. The average longitude difference is slightly positive, suggesting a systematic tendency towards higher longitudes in the observations. Similarly, the average latitude difference is also positive, indicating a systematic tendency toward higher latitudes. However, the latitude differences exhibit lower kurtosis and skewness, suggesting a more symmetric distribution with fewer extreme deviations compared to longitude differences. Longitude differences, on the other hand, show higher kurtosis and skewness, indicating the presence of pronounced outliers and extreme deviations. The pronounced outliers between the models indicate a sensitivity to the method.

Table 1: Statistical values for random and analytical method coordinates difference metrics, Eqs. (1) and (2).

	Coordinate parameters	
Statistical parameter	Longitude	Latitude
Min/Max points	-34.96 / + 42.11	-26.73 / + 27.02
Average	0.26	0.71
Variance	16.31	43.11
Skewness	-0.91	0.006
Kurtosis	7.20	2.70

The analytical scheme produced a wider range of particle depths, resulting in some particles being found at deeper levels in the water column. In contrast, the random walk scheme led to a narrower range of particle depths, with particles distributed more closely around the mean. While the *analytical* method may allow for a more diverse and uneven distribution of particles, the *random walk* model provided a more consistent and clustered distribution of particles. Therefore, the choice of method for simulating vertical mixing should be carefully considered, considering the significant impact that both models presented on horizontal transport due to the vertical mixing strategy.

5. CONCLUSION

According to the results obtained in this study, microplastics were able to travel long distances, starting from Guanabara Bay in Rio de Janeiro, Brazil, and reaching as far as the Argentinean shoreline. The result of the model allowed the identification of potential areas of accumulation at the mouth of the La Plata river.

It is important to highlight that this work designed a simulation representing an instantaneous emission of limited particles. Actual scenarios are more likely to provide continuous emissions through a larger period. The vertical motion was provided by probabilistic methods and provided depth values that are insignificant to reach the seabed. The advection influenced the motion of the particles on the surface, which was obtained by wind and hydrodynamic.

The results showed a discreet statistical discrepancy in the horizontal position of the particles which indicates that even subject to the same velocity field imposed by the hydrodynamic, the particles had different trajectories.

In addition, methods using mechanical laws may provide more realistic models for the dynamic of microplastics. Contributions from chemical aggregation and biofilm formation must be explored in order to observe how they may influence settling.

More experiments must be conducted in order to find better and more realistic solutions for the microplastic trajectory dynamics. The consideration of other phenomena is important, such as particle density, non-spherical shapes, and physicochemical modifications that might affect the behavior of microplastic in the aquatic environment.

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