CIÊNCIA e NATURA

ISSN 2179-460X
OPEN ACCESS

Ci. e Nat., Santa Maria, 47, spe. 2, e91586, 2025 • https://doi.org/10.5902/2179460X91586
Submitted: 03/31/2024 • Approved: 03/31/2024 • Published: 05/21/2025

Inovações e Soluções Sustentáveis em Engenharia Ambiental

Inverse problem solution for microplastic emission source area estimation in MOHID: the Sepetiba Bay case study

Solução do problema inverso para a estimativa da área de emissão do microplástico: o estudo de caso da Baía de Sepetiba

Nikolas Gomes Silveira de Souza[I], **Jader Lugon Junior**[I], **Alexandre Macedo Fernandes**[II], **Ramiro Joaquim de Jesus Neves**[III], **Antônio José da Silva Neto**[II]

[I] Instituto Federal Fluminense, Campos dos Goytacazes, RJ, Brazil
[II] Universidade do Estado do Rio de Janeiro, Rio de Janeiro, RJ, Brazil
[III] University of Lisbon, Lisbon, Portugal

ABSTRACT

Occasionally, contaminants are found on beaches (oil, plastic, etc.), and determining their origin can be challenging. However, the adaptation of computational tools with the capability of mathematical modelling of the motion of Lagrangian tracers can offer a practical and objective solution. In this study, it is presented a solution for the inverse problem of contaminant emission, with a focus on microplastic. For that matter, the computational platform MOHID was used to simulate the movement of Lagrangian tracers along the estuary connecting Sepetiba and Ilha Grande in Rio de Janeiro/Brazil. Two methods for tracing the origin of the particle were used, traditional backtracking, and a mapping method, both based on box and instantaneous emissions. The outputs were analysed and both methods yielded promising results, though additional criteria-based decision was found to be significantly relevant. In addition, it was observed the complex hydrodynamic ruling the particle motion, with significant longitude and latitude parameter sensitivity for a microplastic search. The mapping method observed the advantage of potentially reducing the time dependence of the model, while backtracking showed faster results. At last, the time and detail of each model output showed important differences, reinforcing the necessity for a criteria-based decision over the use of the model. This work contributes as a support tool for microplastic mitigation and cleansing-related activities and can be extrapolated to address other types of litter.

Keywords: MOHID; Inverse problem; Contaminant

Published by Ciência e Natura under a CC BY-NC-SA 4.0 license.

RESUMO

Frequentemente, contaminantes são identificados em praias (óleo, plástico etc.) e determinar sua origem é um desafio. No entanto, a adaptação de ferramentas computacionais com capacidade de modelagem do movimento de traçadores Lagrangianos pode oferecer uma solução prática e objetiva. Neste estudo, apresentou-se uma solução para o problema inverso da emissão de um contaminante, focado em microplástico. A plataforma computacional MOHID foi utilizada para simular o movimento de traçadores no estuário entre Sepetiba e Ilha Grande no Rio de Janeiro/Brasil. Dois métodos para rastrear a origem da partícula foram utilizados, *backtracking* tradicional e um método de mapeamento, ambos baseados em emissões instantâneas e em caixa. Os resultados foram analisados e os métodos apresentaram resultados promissores, embora critérios adicionais para a tomada de decisões tenham se mostrado relevantes. Ademais, observa-se a complexa hidrodinâmica que orienta o movimento das partículas, com significativa sensibilidade nos parâmetros de longitude e latitude para a busca de microplásticos. O método de mapeamento ofereceu possível vantagem em reduzir a dependência temporal do modelo, enquanto o *backtracking* mostrou resultados mais rápidos. Por fim, o tempo e o detalhe de cada saída do modelo mostraram diferenças importantes, reforçando a necessidade de uma decisão baseada em critérios sobre o uso do modelo. Este trabalho contribui como uma ferramenta de suporte para atividades de mitigação e limpeza relacionadas a microplásticos e pode ser extrapolado para abordar outros tipos de resíduo.

Palavras-chave: MOHID; Problema Inverso; Contaminante

1 INTRODUCTION

Frequently, litter is found in beach regions across the world (Galgani et al., 2021; Tang et al., 2023). Locating the origin of this litter can be essential to apply the legislation and, most importantly, mitigate pollution. Litter, for this matter, can be considered any type of contaminant and may happen as liquid (e.g. oil) or solid (e.g. microplastic), for example (Lugon Jr et al., 2019; Souza, Lugon Junior, et al., 2021; Souza et al., 2023). The use of computational models to recreate systems has been effectively used to trace the forward motion of many types of particles (Dagestad et al., 2018; Souza et al., 2023).

A traditional strategy to move backwards in the models is the backtracking model (Dagestad et al., 2018). This strategy typically reverses the signal of the thorough displacement vector and adapts the timestep to simulate motion in reverse (Breivik et al., 2012; Dagestad et al., 2018; Suneel et al., 2016). Its use is widely present in publications (Abascal et al., 2011; Breivik et al., 2012). It is a potential solution, though weathering and dissolution reverse processes can be limited (Breivik et al., 2012; Lammoglia & Souza Filho, 2015; Suneel et al., 2016). One observation is that the backtracking emission ignites from the observed region (hereby denominated *final location*) where litter was supposedly found. The lack of precision for measuring the final location can alter significantly the backtracking results in sensitive areas (Lugon Jr et al., 2019; Suneel et al., 2016).

The motion of Lagrangian tracers in the publication is generally influenced by the phenomena of hydrodynamic (*water velocity*), the atmosphere (*wind velocity*), the natural *dispersion* characteristics, and finally the unknown motion phenomena (*random walk*) (Rodrigues, 2012).

Another strategy to find the source of an emission is the solution of inverse problems. The objective is to find the best forward problem that recreates the intended system (Barros et al., 2021). With attention to the challenges of non-uniqueness and ill-posedness. The first indicates that there may be multiple possible inputs that can result in the same output, while the second shows potential sensitivity to small changes in the data. These situations happen in the environment and additional criteria are recommended for the decision (Breivik et al., 2012).

Finally, potential parameters, such as the pair of coordinates, obtained by the inverse problem solution are imposed as Lagrangian parameters. The rationale is that the iterative recreation of the emission process will eventually reach the intended final location (Souza, Lugon Jr, et al., 2021).

This study will work with two inverse problem approaches, backtracking and space-time mapping, to estimate the source area of microplastic pollution in Sepetiba Bay. These methods were chosen for their complementary strengths. Backtracking provides a rapid, computationally efficient method for preliminary source estimation. Space-time mapping, on the other hand, offers a more detailed and spatially precise solution by simulating a range of potential emission points simultaneously. Other methods, such as Monte Carlo simulations or neural network models, were not employed in this work. The implementation of these methods would require higher computational cost for pre-processing the parameters.

The objective of this work is to explore solutions provided by backtracking and mapping strategy in the MOHID (Modelagem Hidrodinâmica) platform (Rodrigues, 2012). This platform is an ANSI FORTRAN-95 algorithm that allows the user to simulate particle motion over a pre-computed hydrodynamic basis. In addition to the backtracking code implemented in MOHID, an extra study will be performed producing a space-time mapping of simulated solutions evaluating the statistical distribution. By estimating a hypothetical region where the pollutant was found, the use of the backtracking method and a space-time mapping of the simulation was carried out. This work discusses the efficiency of the models and the limitations observed.

This study also aims to contribute by addressing the gap of finding origin from observed litter position, especially for microplastic particles which pose a potential threat to modern society.

1.1 Lagrangian In MOHID

In environmental computational modelling, the use of Lagrangian tracers is an important strategy for understanding the motion of particles over ocean complexities (Ballent et al., 2012; Booth et al., 2017; Cloux et al., 2022). The Lagrangian method aims to retrieve the horizontal and vertical velocities and positions, determined by the time evolution (Rodrigues, 2012). The individual particles are subject to the forces of the water layer, each one at its initial position during a timestep (Mateus & Neves, 2013).

The model uncertainties are calculated by the random walk process (Mateus & Neves, 2013; Souza et al., 2023). In the MOHID platform, the variance and mixing length is decisive for the average velocity, provided the turbulence model adopted in the platform (Rodrigues, 2012; Spagnol et al., 2002).

The vertical motion can be calculated based on a constant or parametrised random walk, based on the shear velocity from the Eulerian model (Souza et al., 2023). The displacement in MOHID is calculated in sequence and is added to the other velocity components such as wind, current, stokes drift to determine the next step of the particle (Rodrigues, 2012).

The computation points are distributed according to the Arakawa C scheme (Mateus & Neves, 2013; Rodrigues, 2012). The horizontal advection of momentum employs a hybrid method, combining upwind and central differences. Similarly, the vertical advection and diffusion of momentum use hybrid schemes (Rodrigues, 2012). The diffusion of momentum is computed using central differences (Mateus & Neves, 2013).

1.2 Inverse Problem Techniques

There are several methods in publications to provide potential candidates for the model parametrization. However, the decision of the method must consider computational efficiency, spatial data, and data availability. Authors suggest that backtracking can provide a faster way to reduce potential source areas before more computationally intensive methods are applied (Cividanes et al., 2024; Courtene-Jones et al., 2021; Liubartseva et al., 2016).

Space-time mapping, by simulating multiple emission points, might offer a higher resolution approach compared to backtracking, which could be limited in its spatial accuracy (Courtene-Jones et al., 2021; Dobler et al., 2019; Souza et al., 2023).

Several sophisticated methods are available in publications; however, it is important to identify their potential drawbacks to this matter. Neural networks (Bennett, 2002; Lugon et al., 2009), for example, while capable of handling complex datasets, needs extensive training data. Additionally, the black box nature could mask the decision-making process, hindering the goal of identifying the pollution source (Bennett, 2002; Richter, 2020). Monte Carlo methods (Balseiro et al., 2003; Richter, 2020), while adept at handling errors and uncertainties, can be computationally expensive, especially for complex models or when a large sample size is needed for accurate estimations. Given that backtracking and space-time mapping were considered sufficient for a preliminary, and subsequently, a more refined analysis of the source area, the added computational burden of Monte Carlo simulations was considered unnecessary.

2 MODEL SETUP

A synthetic hydrodynamic model was designed to be the hydrodynamic background of the Lagrangian model. The hydrodynamic model was implemented as a tidal simulation in shallow waters. For a comprehensive representation of tidal effects, the FES 2014 (Finite Element Solution) was used to capture tidal elevations and currents at the boundaries (Lyard et al., 2006). Implicit calculations in MOHID Water were carried out to provide the internal dynamics driven by the tide-generating forces using the method provided by Kantha and Clayson (Kantha & Clayson, 2000). The Coriolis acceleration force was calculated using the Eq(1):

$$Coriolis\_Aceleration = F_{UV} * VU_{Average} \tag{1}$$

where F_{UV} is the interpolation of Coriolis frequency and $VU_{Average}$ is the average velocity component

The MOHID model was parameterized with wind data from the Global Forecasting System in the National Oceanic and Atmosphere Administration database (NOAA, 2015). The resolution obtained was 0.25º. The random walk parameters were obtained based on turbulence model and mixing length (Allen, 1982; Rodrigues, 2012; Villarreal, 2005). Horizontal and vertical viscosity were recreated at 10 m^2/s and 0.001 m^2/s. Water-air and sediment-water interface rugosity were based on a constant value of 0.0025. These parameters were interpolated in a 250 x 850 computational grid originating from longitude and latitude [-44.7059, -23.3588] in WGS 1984 representation system with cells being a squared 0.00166º representation.

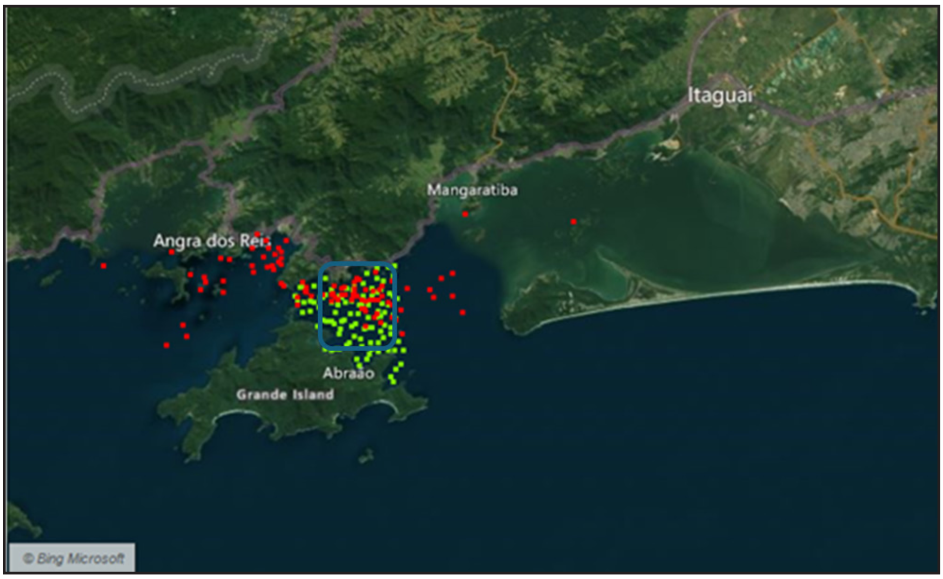
The study site was Sepetiba and Angra dos Reis estuary in the region of Rio de Janeiro/Brazil. This region is relevant due to its dense population, economic and touristic interest, and history of pollution (Rodrigues et al., 2023; Santos et al., 2018). The simulation considered the period of summer (2022-Jan-01 to 2022-Feb-01) for a hypothetical study case. The horizontal discretisation was provided in a bi-dimensional regular grid with approximately 300 metres. The bathymetry was interpolated from the data available at GEBCO for the specific region (Oceans, 2023). To simplify the simulation and reduce the computational cost, the interpolation of bathymetry was calculated on an 800-metre grid and the output was re-interpolated onto a 300-metre grid.

The forward solution started with 100 particles emitted from a box at the central canal between Sepetiba Bay and Ilha Grande Bay (Fig. 1). The box emission will create a virtual three-dimensional box in the domain where particles will be randomly seeded. For this computational experiment, all the emitted particles are buoyant only. The emissions were designed at equidistant grid cell distances, keeping a random position within the grid cell. Providing 100 particles was a solution to reduce bias in the result and amplify the source area likelihood. Hence, the last output of the forward solution will provide the final locations. The reconstruction of the system by backtracking provides that the last position of the particles is known, and the period of travelling is known, but the origin is not known. The backtracking method is then used in the region of observance of the particles to identify their origin.

The backtracking simulation used the same parameters as the forward simulation, except for the emission coordinates. The backtracking process in MOHID follows a standard by opposing motion/time vectors of the forward problem models, tailored to the reverse particle motion. Thus, reconstructing their past trajectories while accounting for the physical processes.

Provided a hypothetical emission occurring in a region of the bay, after 30 days, the particles will reach the final location to be backtracked (Fig. 1). A box was developed for the forward solution to account for the emission area and the target final location. The target final location was considered as the area in blue in Fig. 1. The backtracking solution box is created based on the target final location.

Figure 1 – Representation of emissions. It is seen the final location of the forward model (red dots), and the source area (in green). In the blue square, the area is used as the target final location



Source: Authors (2024)

2.1 Space-time mapping design

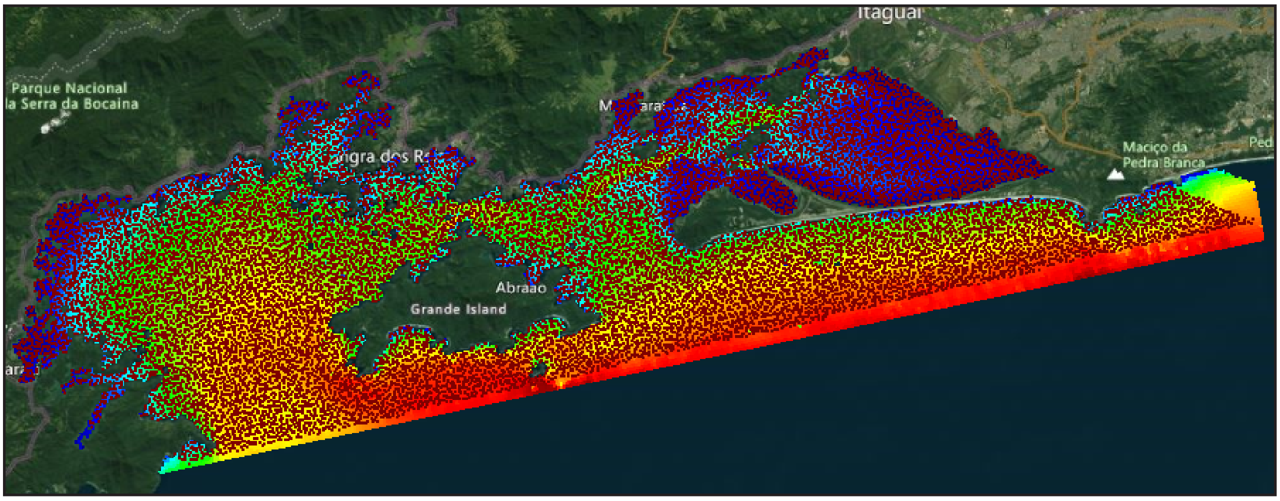
The mapping strategy involved seeding 19,750 particles within a defined box encompassing all grid cells within the study area. The Lagrangian box emission was created based on the computational grid, with reduction in the lower corners. The left corner was positioned at longitude and latitude [-44.5401, -23.3165], while the right corner was positioned [-43.3886, -23.0757]. This horizon representation was made considering the southerly island of Angra dos Reis (Jorge Grego Island).

Inspired by Souza et al. (2023), this design aimed to explore all potential source points within the simulated environment, with the presumption that at least one particle from a source region would reach the designated target location. The particle movement was solely driven by the hydrodynamic forcing, and the threshold for particle inclusion in the analysis was based on whether the particles reached the target area at the end of the simulation. This design ensured a comprehensive exploration of the solution space.

To examine sensitivity to small changes in emission locations, seven tracers were seeded within the same source region, but distributed across different grid cells. This allowed the observation whether emissions from specific cells, separated by the grid resolution of the model, would result in noticeably different trajectories.

As the forward solution is widely validated and accepted in publications (Lugon Jr et al., 2019; Mateus & Neves, 2013; Pablo et al., 2019), it is reasonable that recreating a series of forward emissions would reach the target final location (Breivik et al., 2012; Souza, Lugon Junior, et al., 2021; Souza et al., 2023). For this work, 19,750 particles were seeded in a box (Fig. 2). The particles are moved due to the hydrodynamic forcing only, exploring the solution space. The threshold was considered within the bathymetric layer limits, as seen in Fig. 2.

Figure 2 – Emission region with 19750 lagrangian tracers seeded at initial conditions overlaying the bathymetric layer background

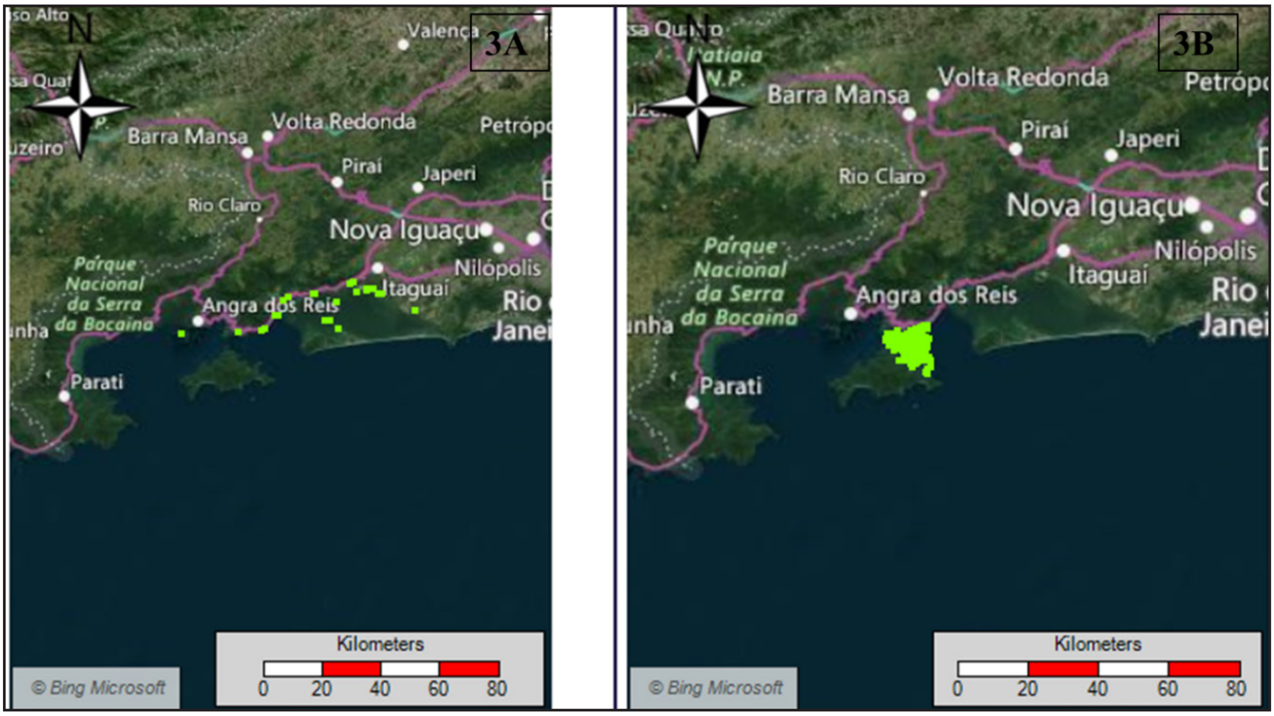


Source: Authors (2024)

3 RESULTS AND DISCUSSION

The backtracking model duration was significantly faster than the mapping strategy. The first timeframe of the model estimates that the particles must have originated from the sources in green (Fig 3A) while the last timeframe reunites the particle as defined by the model construction (Fig 3B).

Figure 3 – (A) Backtracking solution: possible regions of source and (B) backtracking particles final location



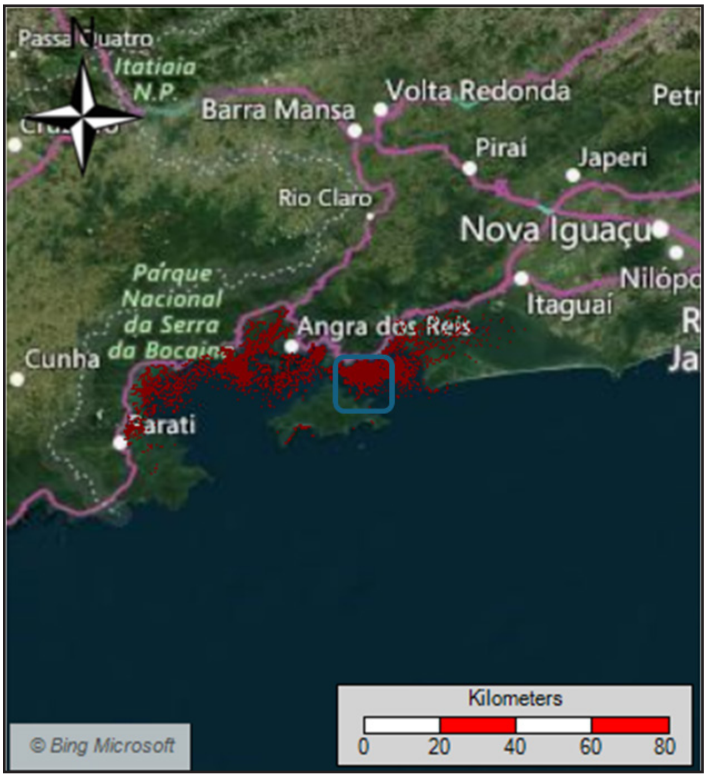
Source: Authors (2024)

The backtracking system provides a fast and reasonable solution, however, minor imprecisions in model design may affect overall accuracy (Breivik et al., 2012).

The space-time mapping strategy was designed to cover the entire region of study and simulate several pairs of coordinates emission at once (Barros et al., 2021; Souza et al., 2023).

A number of 8,992 tracers were still present in the domain at the last timeframe (Fig 4).

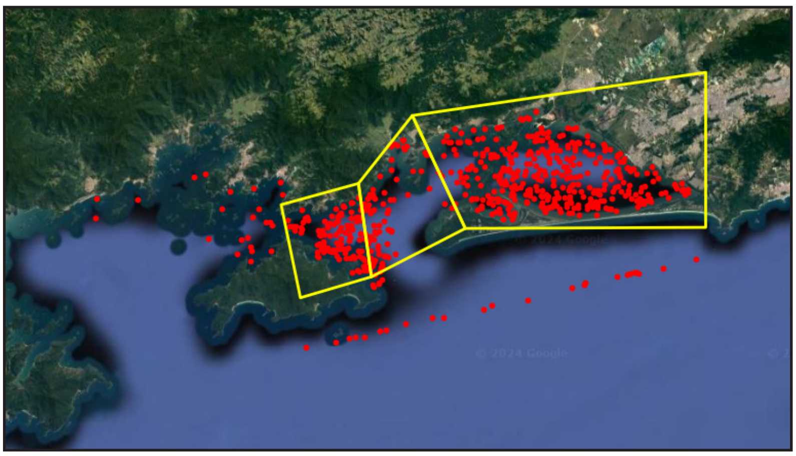
Figure 4 – Last timeframe of emissions and region of synthetic emission; in blue box the target



Source: Authors (2024)

In Fig. 5 the initial timestep is reconstructed exclusively with the particles that reach the target in Fig. 4B in the initial condition. The particles were counted in each polygon as seen in Table 1.

Figure 5 – Representation of the initial timestep with particles that reach the target area. From the left to the right, the polygons will be represented as P1 = polygon 1, P2 = polygon 2 and P3 = polygon 3



Source: Authors (2024)

Table 1 – Number of particles emitted from the polygons 1, 2, and 3 in the initial timestep that enter the search area of the last timestep of the forward model

Polygon ID:	Particle Counts
Polygon 1	106
Polygon 2	76
Polygon 3	357
Outer area	52

Source: Organized by the Authors (2024)

Both predictors can be considered effective as they reach the hypothetical source within their probable solutions. Nevertheless, as the simulation time increases, there might be significant numerical dispersion observed in the process. It should be highlighted that finding the likely source of an emission is too complex for a deterministic solution (Richter, 2020). The backtracking model in the MOHID platform was primarily prepared to work with oil, in which advection and diffusive processes are calculatable, though weathering processes of the Lagrangian tracers are not reversible (Rodrigues, 2012). For items such as microplastic, the non-weathering feature does not represent an actual limitation (Ballent et al., 2012; Booth et al., 2017; Tang et al., 2023), as it is observed that microplastic particles take a significant time to weather and a group of plastic composition is based on buoyant plastic (El-Sherif et al., 2022; Galgani et al., 2021; Tang et al., 2023). This is of special importance to consider this method as a feasible operation.

For immediate needs, the authors acknowledge that the backtracking solution is effective. The reason for this consideration takes into account time, computational cost and complexity. However, merging methods is a potential solution to reduce the initial search area and potentially reduce the complexity of identifying the pollutant's likely source (Richter, 2020).

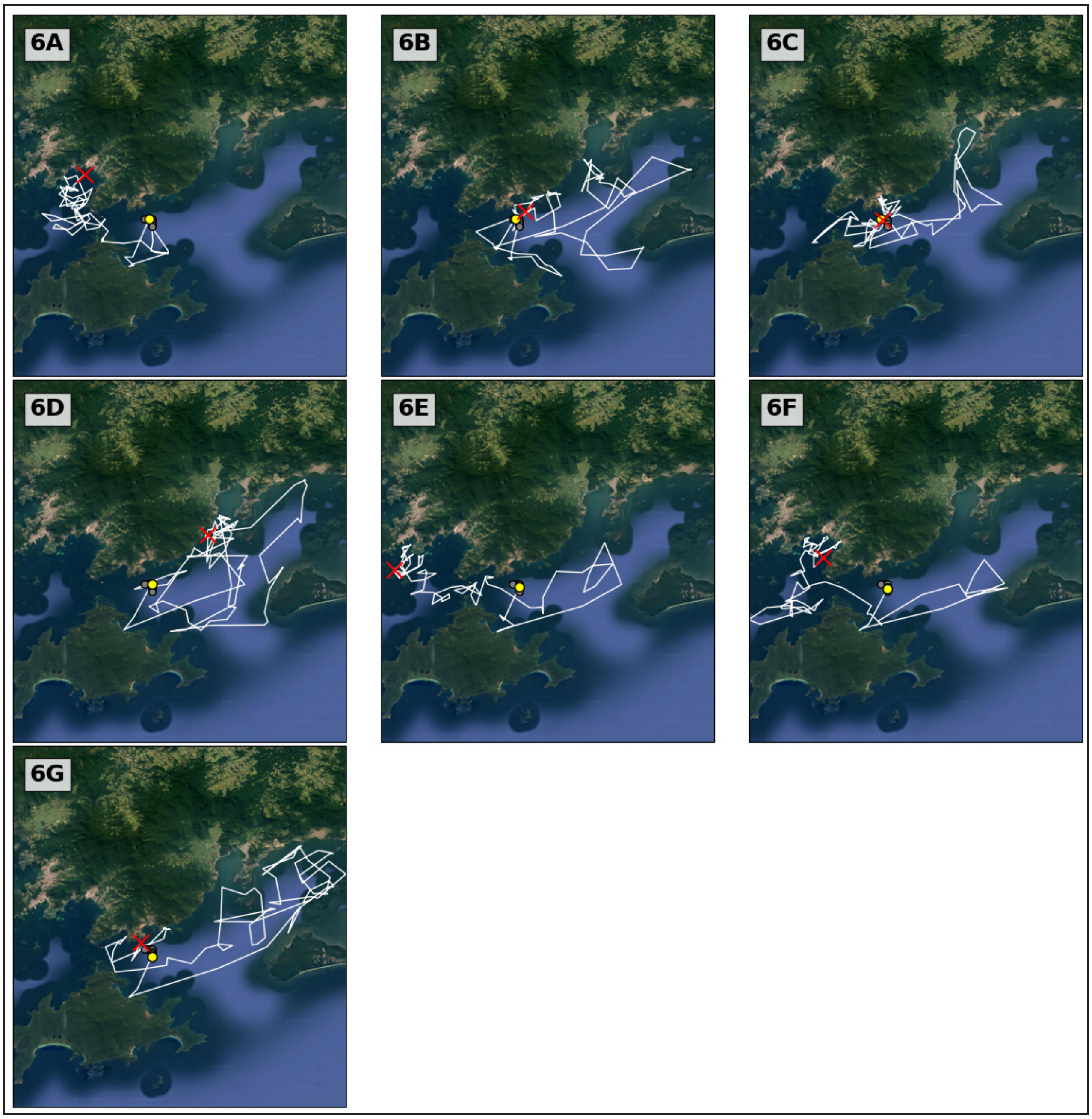
The mapping strategy, however, provides a more detailed way to locate the origin and a promising solution using heuristics. For both cases, the proper calibration of the hydrodynamic is thus essential as Lagrangian tracers will move along the water and atmospheric influence.

Another important remark is that the mapping strategy does not bypass the influence of the model sensitivity. This means that a small deviation in the initial condition may alter the output significantly.

Although the mapping strategy (Fig 5) offered more detailed results when compared to backtracking (Fig 1), the results did not approach the expected emission site. In this simulation, the realism of the interplay among the hydrodynamic forces and random walk on the passive tracers yielded in the concentration pattern of Fig. 5. Small deviations in the emission parameter yielded significant imprecisions in prediction, as observed in Fig. 6.

Figure 6 explores the sensitivity of Lagrangian trajectories to initial position variations, demonstrating the influence of grid resolution on particle dispersion. Seven emission sites (6A-6G) are analysed, each representing a distinct location within the study area. The central emission (6D) occurs at -44.1634° longitude and -23.0622° latitude. For each emission site, seven tracers were released with initial longitudinal or latitudinal offsets of 0.003°, corresponding to the grid resolution of the model. Three particles were emitted to the West (6A-6C) and three particles to the South (6E-6G), respectively. This spatial variation aims to capture the potential variability of Lagrangian motion within neighbouring grid cell. The observed dispersion patterns across the seven sites highlight the significant impact of seemingly minor initial location changes on particle trajectories, emphasising the role of subgrid-scale processes and initial location within a grid cell in determining particle fate.

Figure 6 – Dispersion of Lagrangian tracers from seven emission sites (6A-6G), highlighting the sensitivity of particle trajectories to initial location variations. The initial seeding point is marked with a yellow circle, other points are shown in grey, and the final point is marked in a red cross



Source: Authors (2024)

It is important to reinforce that this mapping strategy considers that the emission area is not known, thus a large hypothetical area (the entire domain) was considered a likely solution for emission. Determining searching criteria or reducing the area of search are potential solutions for computational expense and accuracy.

The mapping strategy can be considered an inverse problem method, in which several inputs are proposed to obtain the best output (Lugon Jr et al., 2019; Richter, 2020). Strategies to decide the best match include the cost function concept (Barros et al., 2021). This concept aims to quantify how well the particle-based model matches the observations, followed by an optimisation process. In this context, the number of particles within the target box due to hydrodynamic model can be considered the product of iterative seeding that seeks to minimise the cost function. A heuristic approach of moving particles to areas where they better match observations is the output of optimization (Barros et al., 2021; Mansour & El-Fakih, 1999). The key to this study was to seed multiple particles at once and optimising them simultaneously rather than sorted seeding (Barros et al., 2021; Lugon Jr et al., 2019; Souza, Lugon Junior, et al., 2021).

There are methods that can be used in order to apply the inverse problem solution such as the GRIPP platform (Barros et al., 2021; Lugon Jr et al., 2019; Souza, Lugon Junior, et al., 2021). The implementation simplicity and readily differentiability are highlights while sensitivity to outliers due to hydrodynamic complexity can be a potential limitation.

3.1 Limitations and Mitigation

Backtracking was highly sensitive to small errors in the assumed final location of the tracers. One hypothesis is due to the chaotic nature of the ocean currents and its stochastic representation. Thus, recreating the system would require a small-scale precision in the initial parameters. Otherwise, accumulated errors could lead to a large-scale imprecision (Wichmann et al., 2019). In addition, few model limitations range from factors such as grid resolution, numerical schemes, and incomplete representation of the physical processes. This represents a challenge to obtain an accurate deterministic representation. Finally, the backtracking process may also depend on more data on weathering, buoyancy and degradation processes for an appropriate recreation of the system (Breivik et al., 2012).

Obtaining field data is also another important factor. A study in microplastics discussed the need and gaps of drifter data to estimate dispersion parameters and validate trajectories (Jalón-Rojas et al., 2019). In addition, other authors discuss the need of accurate in-situ measurement and simplifications to provide Stokes Drift (Dobler et al., 2019), amount of particle input (Taghavy et al., 2015), aggregations and settling velocity parameters (Jalón-Rojas et al., 2019; Souza et al., 2023; Zhu et al., 2018), and model sensitivity to small inaccuracies (Alosairi et al., 2020).

While effective for floating tracers, backtracking may present challenges when applied to non-buoyant tracers or tracers that over time lose its buoyancy capability. Typically, backtracking models neglect dynamic changes of the particle (Breivik et al., 2012; Dagestad et al., 2018).

Inaccurate or incomplete hydrodynamic data can introduce significant biases in the model results. When the temporal resolution of hydrodynamic data is insufficient to capture the actual variability of ocean currents, it can lead to aliasing. Studies often highlight the importance of accurate data for precise simulation (Al-Salem et al., 2017; Wekerle et al., 2018). Solutions provided by authors suggest employing hydrodynamic datasets with finer temporal resolution to capture short-term variability and transient events more effectively (Wang & Hood, 2021). Other groups suggest data assimilation techniques and ensembled models to validate the system recreation (Bennett, 2002; Cedarholm et al., 2019; Dagestad et al., 2018). The interpolation used in the models will create a continuous field for modelling. Backtracking may be susceptible to interpolation bias (Al-Salem et al., 2017). Thus, controlling the interpolation results may anticipate erroneous data points, which will minimise the impact of the error (Aral et al., 2001; Bennett, 2002). Number of particles and its distribution pattern should be carefully considered, as they can improve predictions by a not significant computational cost (Al-Salem et al., 2017).

Another limitation that is common is the duration of the simulation (Atiwesh et al., 2021; Chubarenko et al., 2016; Tang et al., 2023). It is not possible to anticipate the duration of the event on the water surface. In backtracking, this data is crucial to obtain outputs, while in the mapping strategy, the result may be reasonably interpreted as solutions in a partial time. Provided that the event actually started on December 20th, for example, but particles only entered the domain on January 1st, this strategy would be potentially effective to find the partial trajectory with higher efficiency (as seen in Fig 5 – the lower edge particles) while backtracking is limited in this operation. Applying these methods to real-world microplastic pollution scenarios is crucial to validate their effectiveness and identify practical challenges.

These limitations highlight the need for further research into more robust methods for microplastic source identification. Future studies should focus on addressing the dynamics of the tracers. For microplastic, for example, the dynamic on a buoyant particle that will submerge after biofilm development (Jalón-Rojas et al., 2022; Semcesen & Wells, 2021; Shang et al., 2014).

4 CONCLUSIONS

The conclusion of this work reinforces that there is no global solution. The methods provided results which contained the approximated solution of the hypothetical problem. However, additional search criteria were observed as crucial to offering better solutions in both cases.

The backtracking model suggested several probable places of origin without converging into a single area. On the other hand, the mapping showed a more detailed behaviour of the likely emission area. On the other hand, the mapping showed a potential detailed area of emission. The backtracking model showed a higher velocity of output than the mapping, which is expected since a simplified solution is being performed. The decision of the dates for the simulation is a challenge in modelling the inverse problem and the mapping strategy may be of important solution to address this gap.

This study did not provide any additional criteria for the mapping strategy or backtracking as it understands that each area of study is of particular interests and criteria. The establishment of criteria can be effective to locate the origin of persistent tracers such as microplastic, oil slick, and other contaminants.

Revealing the contaminants' source may provide a significant contribution to society. More studies on strategies and criteria should be developed to ensure contamination mitigation and cleanse capabilities.

ACKNOWLEDGEMENTS

The authors acknowledge the financial support provided by FAPERJ-Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro, CNPQ-Conselho Nacional de Desenvolvimento Científico e Tecnológico and CAPES - Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Finance Code 001 and program CAPES/FCT, Process Number 88881.467784/2019-01.

REFERENCES

Abascal, A. J., Castanedo, S., Fernandez, V., Ferrer, M. I., & Medina, R. (2011). Oil spill trajectory forecasting and backtracking using surface currents from high-frequency (HF) radar technology. *OCEANS 2011 IEEE - Spain*, 1–8. https://doi.org/10.1109/Oceans-Spain.2011.6003575

Allen, C. M. (1982). Numerical simulation of contaminant dispersion in estuary flows. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, *381*(1780), 179–194. https://doi.org/10.1098/rspa.1982.0064

Alosairi, Y., Al-Salem, S. M., & Al Ragum, A. (2020). Three-dimensional numerical modelling of transport, fate and distribution of microplastics in the northwestern Arabian/Persian Gulf. *Marine Pollution Bulletin*, *161*, 111723. https://doi.org/10.1016/j.marpolbul.2020.111723

Al-Salem, K., Alosairi, Y. Y., & Al-Rashed, A. A. (2017). Development of a Backtracking Numerical Model for Offshore Oil Spills. *Journal of Engineering Research*, *5*(1), Article 1. https://kuwaitjournals.org/jer/index.php/JER/article/view/1447

Aral, M. M., Guan, J., & Maslia, M. L. (2001). Identification of Contaminant Source Location and Release History in Aquifers. *Journal of Hydrologic Engineering*, *6*(3), 225–234. https://doi.org/10.1061/(ASCE)1084-0699(2001)6:3(225)

Atiwesh, G., Mikhael, A., Parrish, C. C., Banoub, J., & Le, T.-A. T. (2021). Environmental impact of bioplastic use: A review. *Heliyon*, *7*(9), e07918. https://doi.org/10.1016/j.heliyon.2021.e07918

Ballent, A., Thomsen, L., Ballent, A., Purser, A., De, P., Mendes, J., Pando, S., & Thomsen, L. (2012). Physical transport properties of marine microplastic pollution Robotic Exploration of Extreme Environments (ROBEX) View project Marine cabled observatory networks for the large-scale ecosystem monitoring View project Physical transport properties of marine microplastic pollution. *Biogeosciences Discuss*, *9*, 18755–18798. https://doi.org/10.5194/bgd-9-18755-2012

Balseiro, C. F., Carracedo, P., Goīmez, B., Leitao, P. C., Montero, P., Naranjo, L., Penabad, E., & Peīrez-Munuzuri, V. (2003). Tracking the Prestige oil spill: An operational experience in simulation at. *Weather*, *58*.

Barros, Y. T. de, Lugon Jr, J., Kalas, F. A., Rodrigues, P. P. G. W., & Silva Neto, A. da. (2021, December 20). *Identificação de Trajetórias com Uso das Plataformas MoHid e GRIPP para Aplicações Ambientais*. https://doi.org/10.5540/03.2021.008.01.0423

Bennett, A. F. (2002). *Inverse Modeling of the Ocean and Atmosphere* (1st ed.). Cambridge University Press. https://doi.org/10.1017/CBO9780511535895

Booth, A. M., Kubowicz, S., Beegle-Krause, C. J., Skancke, J., Nordam, T., Landsem, E., Throne-Holst, M., & Jahren, S. (2017). *Microplastic in global and Norwegian marine environments: Distributions, degradation mechanisms and transport*. Report. Available on: https://www.miljodirektoratet.no/globalassets/publikasjoner/m918/m918.pdf

Breivik, Ø., Bekkvik, T. C., Wettre, C., & Ommundsen, A. (2012). BAKTRAK: backtracking drifting objects using an iterative algorithm with a forward trajectory model. *Ocean Dynamics*, *62*(2), 239–252. https://doi.org/10.1007/s10236-011-0496-2

Cedarholm, E. R., Rypina, I. I., Macdonald, A. M., & Yoshida, S. (2019). Investigating Subsurface Pathways of Fukushima Cesium in the Northwest Pacific. *Geophysical Research Letters*, *46*(12), 6821–6829. https://doi.org/10.1029/2019GL082500

Chubarenko, I., Bagaev, A., Zobkov, M., & Esiukova, E. (2016). On some physical and dynamical properties of microplastic particles in marine environment. *Marine Pollution Bulletin*, *108*(1–2), 105–112. https://doi.org/10.1016/j.marpolbul.2016.04.048

Cividanes, M., Aguiar-González, B., Gómez, M., Herrera, A., Martínez, I., Pham, C. K., Pérez, L., & Machín, F. (2024). Lagrangian tracking of long-lasting plastic tags: From lobster fisheries in the USA and Canada to Macaronesia. *Marine Pollution Bulletin*, *198*, 115908. https://doi.org/10.1016/j.marpolbul.2023.115908

Cloux, S., Allen-Perkins, S., de Pablo, H., Garaboa-Paz, D., Montero, P., & Pérez Muñuzuri, V. (2022). Validation of a Lagrangian model for large-scale macroplastic tracer transport using mussel-peg in NW Spain (Ría de Arousa). *Science of the Total Environment*, *822*. https://doi.org/10.1016/j.scitotenv.2022.153338

Courtene-Jones, W., Maddalene, T., James, M. K., Smith, N. S., Youngblood, K., Jambeck, J. R., Earthrowl, S., Delvalle-Borrero, D., Penn, E., & Thompson, R. C. (2021). Source, sea and sink—A holistic approach to understanding plastic pollution in the Southern Caribbean. *Science of The Total Environment*, *797*, 149098. https://doi.org/10.1016/j.scitotenv.2021.149098

Dagestad, K.-F., Röhrs, J., Breivik, Ø., & Ådlandsvik, B. (2018). OpenDrift v1.0: A generic framework for trajectory modelling. *Geoscientific Model Development*, *11*(4), 1405–1420. https://doi.org/10.5194/gmd-11-1405-2018

Dobler, D., Huck, T., Maes, C., Grima, N., Blanke, B., Martinez, E., & Ardhuin, F. (2019). Large impact of Stokes drift on the fate of surface floating debris in the South Indian Basin. *Marine Pollution Bulletin*, *148*, 202–209. https://doi.org/10.1016/j.marpolbul.2019.07.057

El-Sherif, D. M., Eloffy, M. G., Elmesery, A., Abouzid, M., Gad, M., El-Seedi, H. R., Brinkmann, M., Wang, K., & Al Naggar, Y. (2022). Environmental risk, toxicity, and biodegradation of polyethylene: A review. *Environmental Science and Pollution Research*, *29*(54), 81166–81182. https://doi.org/10.1007/S11356-022-23382-1/TABLES/6

Galgani, F., Brien, A. S., Weis, J., Ioakeimidis, C., Schuyler, Q., Makarenko, I., Griffiths, H., Bondareff, J., Vethaak, D., Deidun, A., Sobral, P., Topouzelis, K., Vlahos, P., Lana, F., Hassellov, M., Gerigny, O., Arsonina, B., Ambulkar, A., Azzaro, M., & Bebianno, M. J. (2021). Are litter, plastic and microplastic quantities increasing in the ocean? *Microplastics and Nanoplastics*, *1*(1), 2. https://doi.org/10.1186/s43591-020-00002-8

Jalón-Rojas, I., Romero-Ramírez, A., Fauquembergue, K., Rossignol, L., Cachot, J., Sous, D., & Morin, B. (2022). Effects of Biofilms and Particle Physical Properties on the Rising and Settling Velocities of Microplastic Fibers and Sheets. *Environmental Science & Technology*, *56*(12), 8114–8123. https://doi.org/10.1021/acs.est.2c01302

Jalón-Rojas, I., Wang, X. H., & Fredj, E. (2019). A 3D numerical model to Track Marine Plastic Debris (TrackMPD): Sensitivity of microplastic trajectories and fates to particle dynamical properties and physical processes. *Marine Pollution Bulletin*, *141*, 256–272. https://doi.org/10.1016/j.marpolbul.2019.02.052

Kantha, L. H., & Clayson, C. A. (2000). *Numerical Models of Oceans and Oceanic Processes* (1st ed.). Academic Press.

Lammoglia, T., & Souza Filho, C. R. de. (2015). Chronology and backtracking of oil slick trajectory to source in offshore environments using ultraspectral to multispectral remotely sensed data. *C*, *39*, 113–119. https://doi.org/10.1016/j.jag.2015.03.007

Liubartseva, S., Coppini, G., Lecci, R., & Creti, S. (2016). Regional approach to modeling the transport of floating plastic debris in the Adriatic Sea. *Marine Pollution Bulletin*, *103*(1–2), 115–127. https://doi.org/10.1016/j.marpolbul.2015.12.031

Lugon, J., Silva Neto, A. J., & Santana, C. C. (2009). A hybrid approach with artificial neural networks, Levenberg–Marquardt and simulated annealing methods for the solution of gas–liquid adsorption inverse problems. *Inverse Problems in Science and Engineering*, *17*(1), 85–96. https://doi.org/10.1080/17415970802082922

Lugon Jr, J., Kalas, F. de A., Rodrigues, P. P. G. W., Jeveaux, J. L., Neto, H. G., Juliano, M. M., & da Silva Neto, A. J. (2019). Lagrangian Trajectory Simulation of Floating Objects in the State of São Paulo Coastal Region. *Defect and Diffusion Forum*, *396*, 42–49. https://doi.org/10.4028/www.scientific.net/DDF.396.42

Lyard, F., Lefevre, F., Letellier, T., & Francis, O. (2006). Modelling the global ocean tides: Modern insights from {FES2004}. *Ocean Dynamics*, *56*(5), 394–415. https://doi.org/10.1007/s10236-006-0086-x

Mansour, N., & El-Fakih, K. (1999). Simulated {Annealing} and {Genetic} {Algorithms} for {Optimal} {Regression} {Testing}. *Journal of Software Maintenance: Research and Practice*, *11*(1), 19–34. https://doi.org/10.1002/(SICI)1096-908X(199901/02)11:1<19::AID-SMR182>3.0.CO;2-M

Mateus, M., & Neves, R. (2013). Ocean modelling for coastal management–Case Studies with MOHID. *IST Press Http://Www. Mohid. Com/Books/2013OceanModellingMOHID. Pd*.

National Centers For Environmental Prediction/National Weather Service/NOAA. (2015). *NCEP GFS 0.25 Degree Global Forecast Grids Historical Archive* (p. 109.074 TB) [WMO_GRIB2,WMO_GRIB2]. UCAR/NCAR - Research Data Archive. https://doi.org/10.5065/D65D8PWK

Oceans, G. B. C. of the. (2023). *GEBCO_2023 Grid*. GEBCO. https://www.gebco.net/data_and_products/gridded_bathymetry_data/GEBCO_2023/

Pablo, H., Sobrinho, J., Garcia, M., Campuzano, F., Juliano, M., & Neves, R. (2019). Validation of the 3D-MOHID Hydrodynamic Model for the Tagus Coastal Area. *Water*, *11*(8), 1713. https://doi.org/10.3390/w11081713

Richter, M. (2020). *Inverse Problems*. Springer International Publishing. https://doi.org/10.1007/978-3-030-59317-9

Rodrigues, P. P. G. W. (2012). *Descrição do MOHID / MARETEC* (1st ed.). Essentia Editora. http://essentiaeditora.iff.edu.br/index.php/livros/article/view/2174

Rodrigues, S. K., Machado, W., Barreira, J., & Vinzón, S. (2023). *Historical Trends of Trace Metals in the Sepetiba Bay Sediments: Pollution Indexes, Fluxes and Inventories*. https://doi.org/10.21203/rs.3.rs-3393671/v1

Santos, A. L. F. dos, Pontes, L., Peixoto, R. dos S., Rosman, P. A., & Rosman, P. C. C. (2018). *Projeto Baías do Brasil—Baías de Ilha Grande e Sepetiba, Rio de Janeiro. Relatório Descritivo.* Universidade Federal do Rio de Janeiro (UFRJ). http://www.baiasdobrasil.coppe.ufrj.br/assets/relatorios/rel_ilhagrande_sepetiba.html

Semcesen, P. O., & Wells, M. G. (2021). Biofilm growth on buoyant microplastics leads to changes in settling rates: Implications for microplastic retention in the Great Lakes. *Marine Pollution Bulletin*, *170*, 112573. https://doi.org/10.1016/j.marpolbul.2021.112573

Shang, Q., Fang, H., Zhao, H., He, G., & Cui, Z. (2014). Biofilm effects on size gradation, drag coefficient and settling velocity of sediment particles. *International Journal of Sediment Research*, *29*(4), 471–480. https://doi.org/10.1016/S1001-6279(14)60060-3

Souza, N. G. S. de, Lugon Jr, J., Yamasaki, E., Kyriakides, I., & Silva Neto, A. J. da. (2021). OTIMIZAÇÃO DO RASTREAMENTO DE DERRAMAMENTO DE ÓLEO E REDUÇÃO SISTEMÁTICA DA ÁREA DA REGIÃO DE PESQUISA: A PLATAFORMA GRIPP. In Universidade do Estado do Rio de Janeiro (Ed.), *X Congresso sobre Planeamento e Gestão das Zonas Costeiras dos Países de Expressão Portuguesa*. Universidade do Estado do Rio de Janeiro.

Souza, N. G. S. de, Lugon Jr., J., Yamasaki, E. N., Kyriakides, I., & Neto, A. J. S. (2023). An assessment of relative potential impacts to Cyprus' shoreline due to oil spills in the Eastern Mediterranean Sea. *Revista de Gestão Costeira Integrada*, *23*(1), 29–42. https://doi.org/10.5894/rgci-n499

Souza, N. G. S. de, Lugon Junior, J., Yamasaki, E., Kyriakides, I., & da Silva Neto, A. J. (2021). Parameter sensitivity study and water property influence: An evaluation of the determining factors on oil drifting effect. *Revista Cereus*, *13*(1), 1595–1604. https://doi.org/10.18605/2175-7275/cereus.v13n1p186-198

Souza, N., Lugon Jr, J., & Silva Neto, A. J. D. (2023). Vertical mixing strategies in the Opendrift platform: Analytical solution and Random Walk scheme. *Scientia Plena*, *19*(11). https://doi.org/10.14808/sci.plena.2023.119904

Spagnol, S., Wolanski, E., Deleersnijder, E., Brinkman, R., McAllister, F., Cushman-Roisin, B., & Hanert, E. (2002). An error frequently made in the evaluation of advective transport in two-dimensional Lagrangian models of advection-diffusion in coral reef waters. *Marine Ecology Progress Series*, *235*, 299–302. https://doi.org/10.3354/meps235299

Suneel, V., Ciappa, A., & Vethamony, P. (2016). Backtrack modeling to locate the origin of tar balls depositing along the west coast of India. *Science of The Total Environment*, *569–570*, 31–39. https://doi.org/10.1016/j.scitotenv.2016.06.101

Taghavy, A., Pennell, K. D., & Abriola, L. M. (2015). Modeling coupled nanoparticle aggregation and transport in porous media: A Lagrangian approach. *Journal of Contaminant Hydrology*, *172*, 48–60. https://doi.org/10.1016/j.jconhyd.2014.10.012

Tang, L., Feng, J.-C., Li, C., Liang, J., Zhang, S., & Yang, Z. (2023). Global occurrence, drivers, and environmental risks of microplastics in marine environments. *Journal of Environmental Management*, *329*, 116961. https://doi.org/10.1016/j.jenvman.2022.116961

Villarreal, M. R. (2005). *Marine Turbulence: Theories, Observations and Models: Coupling of the GOTM turbulence module to some three-dimensional ocean models*. Cambridge University Press.

Wang, J., & Hood, R. R. (2021). Modeling the Origin of the Particulate Organic Matter Flux to the Hypoxic Zone of Chesapeake Bay in Early Summer. *Estuaries and Coasts*, *44*(3), 672–688. https://doi.org/10.1007/s12237-020-00806-0

Wekerle, C., Krumpen, T., Dinter, T., Von Appen, W.-J., Iversen, M. H., & Salter, I. (2018). Properties of Sediment Trap Catchment Areas in Fram Strait: Results From Lagrangian Modeling and Remote Sensing. *Frontiers in Marine Science*, *5*, 407. https://doi.org/10.3389/fmars.2018.00407

Wichmann, D., Delandmeter, P., Dijkstra, H. A., & Van Sebille, E. (2019). Mixing of passive tracers at the ocean surface and its implications for plastic transport modelling. *Environmental Research Communications*, *1*(11), 115001. https://doi.org/10.1088/2515-7620/ab4e77

Zhu, Z., Waterman, D. M., & Garcia, M. H. (2018). Modeling the transport of oil–particle aggregates resulting from an oil spill in a freshwater environment. *Environmental Fluid Mechanics*, *18*(4), 967–984. https://doi.org/10.1007/s10652-018-9581-0

Authorship contributions

1 – Nikolas Gomes Silveira de Souza

Master's degree in environmental engineering.
https://orcid.org/0000-0002-5724-2911 • nichsouz@msn.com
Contribution: Investigation; formal analysis; methodology; visualization; software; data curation; writing – original

2 – Jader Lugon Junior

PhD in Computer Computational Modelling.
https://orcid.org/0000-0001-8030-0713 • jlugonjr@gmail.com
Contribution: software; formal analysis; data curation; writing – review and editing.

3 – Alexandre Macedo Fernandes

PhD in Physical Oceanography.
https://orcid.org/0000-0001-6884-0303 • alxmfr@gmail.com
Contribution: Investigation; formal analysis; methodology; data curation; writing – review and editing; funding acquisition; resources.

4 – Ramiro Joaquim de Jesus Neves

PhD in Physical Oceanography.
https://orcid.org/0000-0003-4577-5443 • ramiro.neves@tecnico.ulisboa.pt
Contribution: Investigation; formal analysis; methodology; data curation; writing – review and editing; funding acquisition; resources.

5 – Antônio José da Silva Neto

PhD in Mechanical Engineering.
https://orcid.org/0000-0002-9616-6093 • ajs_neto@uol.com.br
Contribution: Investigation; formal analysis; methodology; data curation; writing – review and editing; funding acquisition; resources.

How to quote this article

Souza, N. G. S., Lugon Junior, J., Fernandes, A. M., Neves, R. J. J., & Silva Neto, A. J. (2025). Inverse problem solution for microplastic emission source area estimation in MOHID: the Sepetiba Bay case study. *Ciencia e Natura*, Santa Maria, 47, spe. 2, e91586. DOI: https://doi.org/10.5902/2179460X91586. Available in: https://doi.org/10.5902/2179460X91586