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The application of Lagrangian particle tracking techniques to modelling of contaminants in water resources

A aplicação de técnicas de rastreamento de partículas Lagrangianas na modelagem de contaminantes em recursos hídricos

L'application des techniques Lagrangiennes de suivi de particules à la modélisation des contaminants dans les ressources en eau

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Abstract: The Lagrangian model is widely used to track particles in water resources. The model, primarily a stochastic deterministic solution, is coupled with virtual passive particles driven by hydrodynamic forces. User methods regarding model parameterization, limitations, and future directions are examined in relevant reviews. The results indicated a logical convergence via a random walk variable and inverse problem methods for the initial parameters. Highlights suggest a limited capacity to replicate a representative tracer trajectory, except for the initial and final pair of coordinates. Future directions combine computational power and algorithm optimization. Future research is recommended to improve understanding of the influence of random walk and how to reduce uncertainties in long-term models. This review aims to contribute to a critical analysis of Lagrangian models and methods. It summarizes methods that can contribute to environmental modeling for the mitigation, control, and cleanup of areas impacted by solids from immiscible passive particles.

Keywords: Lagrangian. Random Walk. Beaching.

Resumo: O modelo Lagrangiano é amplamente utilizado para rastrear partículas em recursos hídricos. O modelo consiste principalmente de uma solução determinística baseada em um elemento estocástico. Partículas passivas virtuais são arrastadas devido a forças hidrodinâmicas. Os métodos utilizados pelos utilizadores de modelos em relação aos critérios de parametrização, limitações do modelo e direções futuras desses modelos são pesquisadas em revisões relevantes. Os resultados indicaram convergência na lógica através de uma variável de *Random Walk* além dos métodos de problema inverso para obter os parâmetros iniciais. Os destaques sugerem capacidade limitada de replicar uma trajetória representativa dos traçadores, exceto pelo par inicial e final de coordenadas. As direções futuras combinam capacidade computacional e otimização de algoritmos. Pesquisas futuras são recomendadas para melhorar a compreensão da influência do *Random Walk* e como reduzir as incertezas em modelos de longo prazo. Esta revisão tem como objetivo colaborar com uma revisão crítica dos modelos e métodos Lagrangianos. Resumindo métodos que podem contribuir para a modelagem ambiental para mitigação, controle e limpeza de zonas impactadas com sólidos de partículas passivas imiscíveis.

Palavras-Chave: Lagrangiano. Movimento aleatório. Beaching.

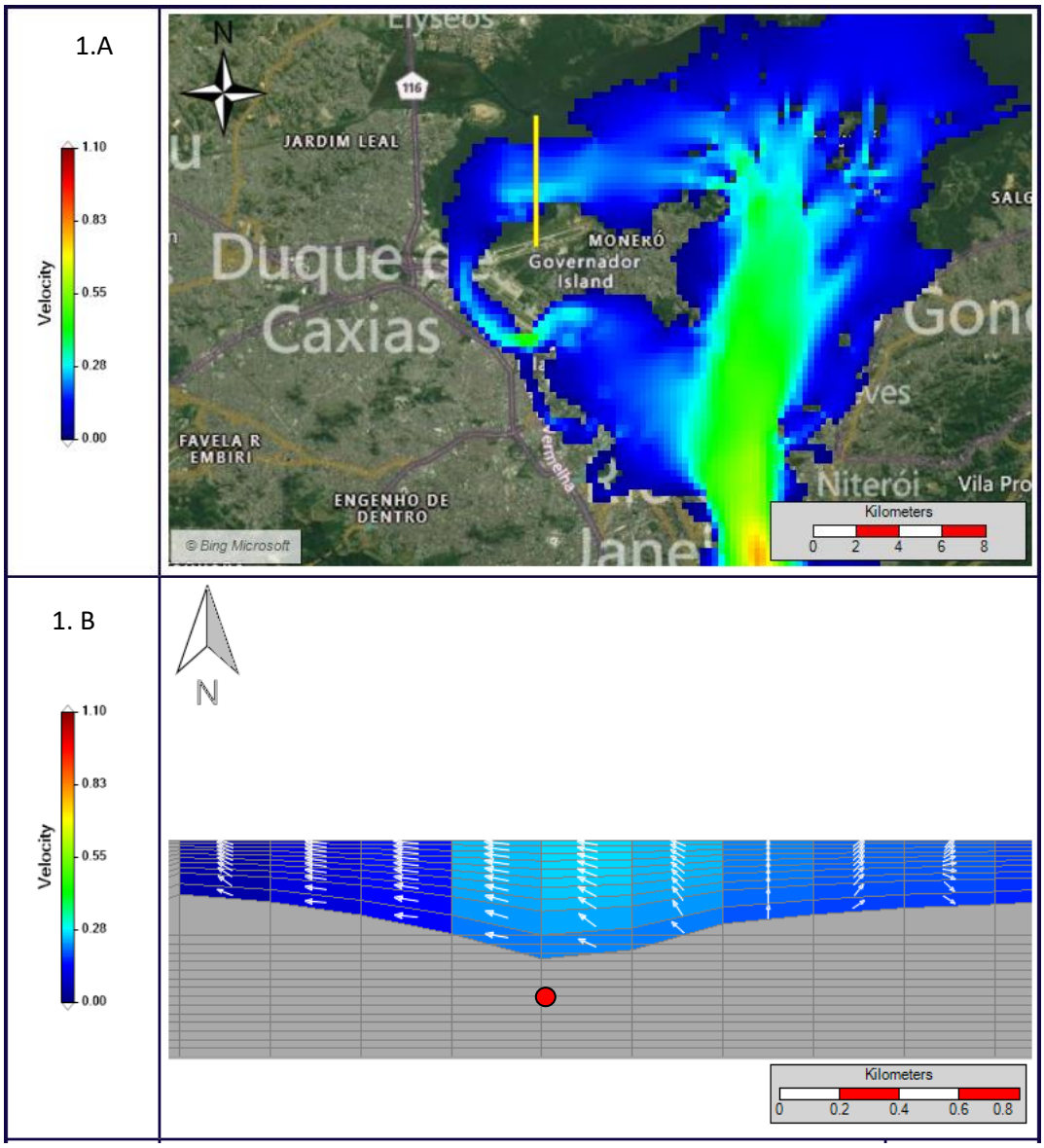
Résumé: Le modèle Lagrangien est largement utilisé pour suivre les particules dans les ressources en eau. Le modèle, principalement une solution déterministe stochastique, est couplé à des particules passives virtuelles entraînées par les forces hydrodynamiques. Les méthodes des utilisateurs concernant la paramétrisation, les limites et orientations futures des modèles sont examinées dans des revues pertinentes. Les résultats ont indiqué une convergence logique via une variable de *Random Walk* et des méthodes de problème inverse pour les paramètres initiaux. Les points saillants suggèrent une capacité limitée à reproduire une trajectoire représentative des traceurs, à l'exception de la paire initiale et finale de coordonnées. Les orientations futures combinent la capacité de calcul et l'optimisation des algorithmes. Des recherches futures sont recommandées pour améliorer la compréhension de l'influence de la *Random Walk* et la manière de réduire les incertitudes dans les modèles à long terme. Cette revue vise à contribuer à une analyse critique des modèles et méthodes Lagrangiens. Elle résume les méthodes qui peuvent contribuer à la modélisation environnementale pour l'atténuation, le contrôle et le nettoyage des zones impactées par des solides de particules passives immiscibles.

Mots-clés: Lagrangien. Mouvement aléatoire. Beaching.

1. Introduction

Predicting contaminant behaviour in water resources is crucial for protecting ecological and public health (Gurgel et al. 2016; Brix, Schlekat, and Garman 2017). Emitted particles in the water resources will be influenced by atmosphere and hydrodynamic conditions. Land boundaries may create a block the transport of particles (*beaching*) temporarily or not (JIMÉNEZ MADRID; GARCÍA-LADONA; BLANCO-MERUELO, 2016). For example, in low tides particles may persist in a shoreland, while high tides may drag these particles back into the water. In addition, the land contour, particularly in islands, may represent important vortexes that will affect the motion of particles by either crossing different flow energy areas, or accumulating in trapping zones. Computational modelling systems address these problems by representing the natural system in computational language using a 2DH or 3D grid cell for representation (Fig 1.A and 1.B). A prominent distinction among models in publications is the Eulerian versus Lagrangian approach.

Figure 1: The region in yellow line in Fig (1.A) is represented by the vertical axis in Fig. (1.B) Grid cell construction in Cartesian (below) and Sigma (above), the red dot indicates the position of a particle at the specific timestep. Both Figures are represented by a colour scheme of velocity fields. Directional vectors represent the influence of hydrodynamic at the timestep. This image was produced from a total of 25 vertical layers. The grey region indicates the floor. This image is based in Guanabara Bay, Rio de Janeiro – Brazil. The bathymetry was imposed by naval measurements.



Eulerian method is commonly used for characterising flow fields (DALLA et al., 2024). Considering a three-dimensional computational grid cell, the concentration volume will move according to the net forces (GUERRINI; MARI; CASAGRANDI, 2021; PÄRN et al., 2023). This approach is commonly used to provide a view of contaminant concentration dispersion and hydrodynamic properties (DE PADOVA et al., 2021).

In contrast, Lagrangian models follow individual particles as they are transported by currents, winds, and other forces providing detailed insights into transport processes by calculating particle positions and velocities (ALOSAIRI; AL-SALEM; AL RAGUM, 2020; LAURENT et al., 2020). Lagrangian models rely on advection velocities pre-calculated by Eulerian hydrodynamic models. (LAURENT et al., 2020; MITCHELL et al., 2023).

The computational platforms are adaptable to various effects and phenomena (HUNTER et al., 2022; JALÓN-ROJAS; WANG; FREDJ, 2019; PÄRT et al., 2023; PILECHI; MOHAMMADIAN; MURPHY, 2022). Despite the commercial computational platforms, several authors offer solutions with a custom-made platform, though the motion rationale remains unchanged (CHEN, 2021; KISNARTI et al., 2024; ZHANG et al., 2020). These models are commonly used in

environmental science for applications such as microplastic accumulation (ALOSAIRI; AL-SALEM; AL RAGUM, 2020; JALÓN-ROJAS; WANG; FREDJ, 2019; MITCHELL et al., 2023; WANG et al., 2023), oil spill (ASCIONE KENOV et al., 2015; CHEN et al., 2015; GONZÁLEZ et al., 2019; JIANG et al., 2021; LAURENT et al., 2020), biological matter transport (ASCIONE KENOV et al., 2015; HUNTER et al., 2022; LAURENT et al., 2020), sediment transport (SIMANTIRIS; AVLONITIS; THEOCHARIS, 2022; WANG et al., 2023), and tracers (particle representation) in general that will represent the contamination particle and properties (ASCIONE KENOV et al., 2015; CAO et al., 2024; GONZÁLEZ et al., 2019; LAURENT et al., 2020). These models are applied to diverse water bodies, including oceans, rivers, estuaries, and coastal waters (MACDONALD; MORTON; JOHANNESSEN, 2003; NEUMANN et al., 2021; STEINER et al., 2015; WU et al., 2019; ZHAO; CHEN; LEE, 2011).

Three important aspects require investigation: (i) model parametrisation, (ii) model limitation, and (iii) future directions of Lagrangian models.

A hypothesis is that advancements in computational power and data availability have led to increased sophistication of Lagrangian models for contaminant transport (ANGUIANO-GARCÍA et al., 2019). However representing horizontal and vertical mixing processes and parameterising particle behaviour in complex environments remain ongoing challenges (KOOI et al., 2017; KUKULKA et al., 2012; SOUZA; LUGON JR; SILVA NETO, 2023; VISSER, 1997). A solution for parametrisation could be in the inverse problems methods (ARGOUL, 2012; BARROS et al., 2021; JULIANO et al., 2012; LUGON; SILVA NETO; RODRIGUES, 2008a). The inverse problem in this context aims to identify the initial parameters that will provide as a last output the observed natural system. For example, a particle is found at a certain position in the waterbody. The inverse problem will compute several attempts to identify the parameters that will represent better the observed system.

This review critically examined recent advancements in Lagrangian modelling techniques for contaminant particle tracking. Addressing (i) how are Lagrangian models used to study contaminant transport, (ii) parameter and input data determination for diverse settings, (iii) the utility of inverse problem methods for parameterizing input data, (iv) horizontal and vertical particle motion modelling, (v) beaching conditions (particle retention on shorelines), and (vi) limitations and uncertainties of Lagrangian models, and potential mitigation strategies.

The objective of this review is to identify potential gaps in the Lagrangian modelling of contaminant dispersion and identify potential solutions available in publications. This work contributes to researchers that work with Lagrangian simulations to enhance the capacity of the computational platform. Thus, contributing to pollution control, pollutant transport management, in water resources, which affects the society in various spheres.

2. Method

In order to compile a database for the Lagrangian approaches for particle motion in water resources, it was conducted targeted publication search in the platforms *Web of Science*, *Scopus*, and *Google Scholar* using the keywords "*Lagrang* model**", "*particle tracking*", "*lagrang* contaminant transport*", "*inverse problem contaminant*". The use of Web of Science and Scopus is due to its relevance of important publications. The Google Scholar was used to collect relevant publications that were available in the other two platforms. Then a manual screening process identified in titles and abstracts the compatibility of the publication within the scope of this review.

Based on the compiled database, a third step was to identify how researchers determine model input, represent motion, and address model limitations within publications.

Given the challenges in parametrisation widely mentioned in a preliminary reading, it was added to the scope an examination of the strategies employed. Horizontal and vertical modelling frameworks were analysed to identify gaps and robust approaches. As the deterministic discussion is not innovative for this scope, the random walk implementation method was scrutinised. Finally, it was explored strategies for addressing inherent model uncertainties stemming from input parameters, unknown or simplified phenomena, and stochastic processes. For parametrisation uncertainty, it was discussed whether the inverse problem methods could be a potential solution.

This review will not focus on computational solutions, such as high-order advection and programming details. The main focus of this review is to collect data, identify if there are standard protocols, and discuss the Lagrangian models and address uncertainties. In addition, future directions of Lagrangian models toward challenges. This methodological approach was used to provide a compilation of relevant, convergent and divergent insights to provide sufficient background for discussion for this qualitative literature review.

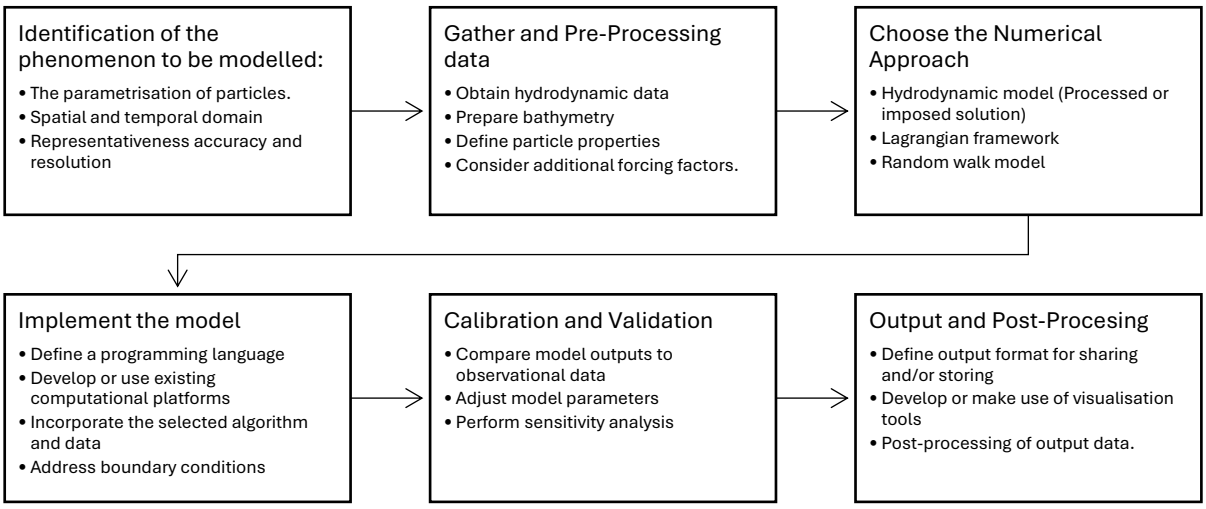
3. Input parameter

The Lagrangian models will represent the motion of particles in the natural system. It comprehends a series of steps to parametrise the particle, define the boundary conditions, and input data. It is a usual habit to obtain atmosphere and hydrodynamic models from accredited platforms (CHEN et al., 2015; COPERNICUS MARINE, 2020; JALÓN-ROJAS; WANG; FREDJ, 2019), as well as bathymetry (OCEANS, 2023). The numerical approach may be used to model hydrodynamic models (Eulerian approach) as well as Lagrangian models (Silva et al. 2013; Souza, Lugon Jr, and Silva Neto 2023; Jalón-Rojas, Wang, and Fredj 2019). The random walk is an implicit factor that will be further discussed in this review. As the model is implemented in important programming languages such as FORTRAN, C++, and interpreters such as Python, execution depends on the platform protocol (DAGESTAD et al., 2018; JALÓN-ROJAS; WANG; FREDJ, 2019; RODRIGUES, 2012).

The following step will compare the model to the real system, observing whether initial or boundary should be calibrated to a better representation of the system. Often, a sensitivity analysis is recommended by authors to identify important parameters (BEVEN, 2009). Finally, the output is commonly stored in a file with large database capacity extension (e.g HDF5, NC), which will be useful for further processing and analysis (DAGESTAD et al., 2018; DE DOMINICIS et al., 2013; RODRIGUES, 2012). These analyses can be handled by platforms such as *Python*, *Mathlab* or *R statistics* depending on the necessity of the researcher.

A summary of model construction is depicted in Fig. 2.

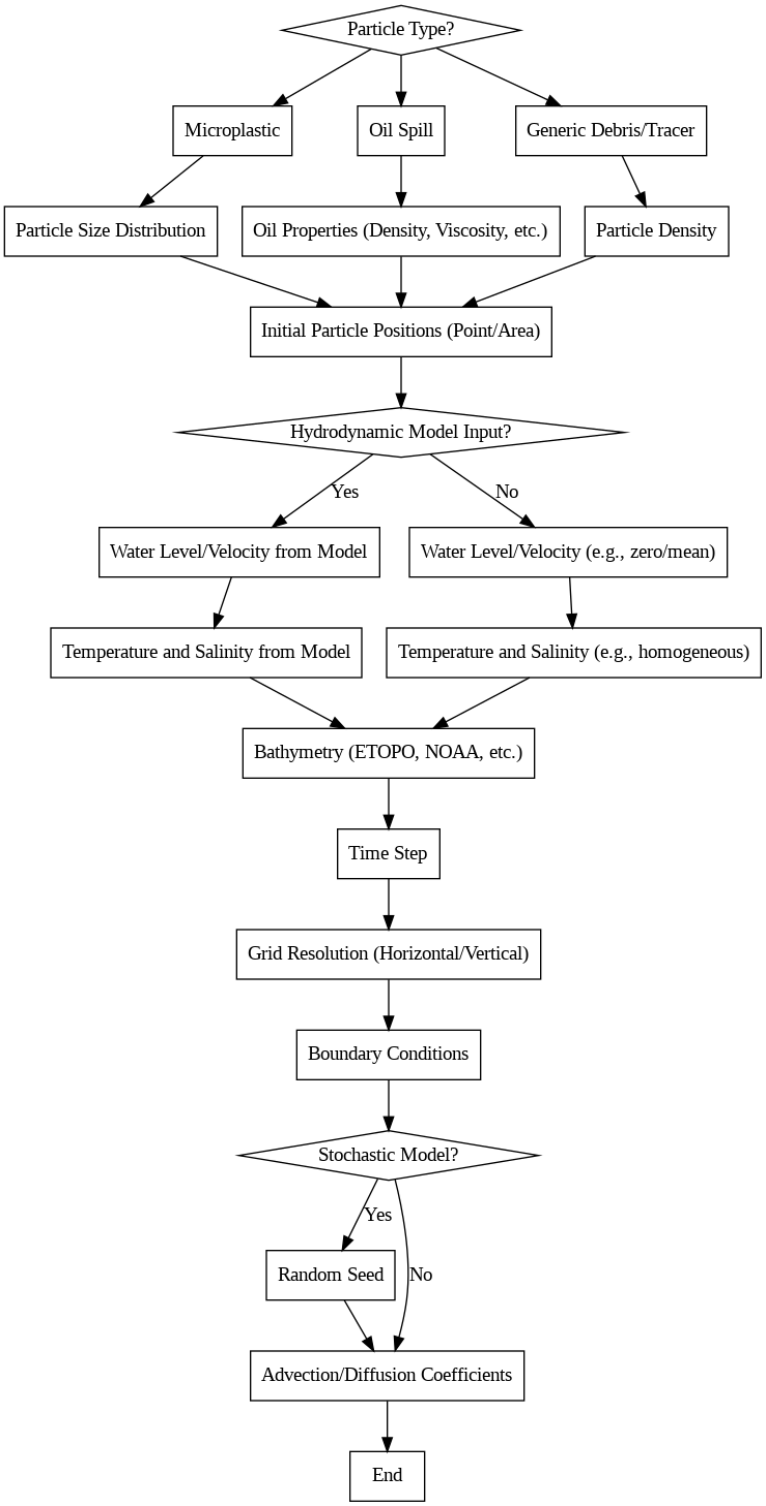
Figure 2: Basic Workflow for Developing and Implementing a Lagrangian Particle Model.



The design of the model algorithm and numerical model will allow the use of tracer properties such as microplastic and oil (DE DOMINICIS et al., 2013; JALÓN-ROJAS; WANG; FREDJ, 2019). Fig. 3 presents a flowchart outlining the initial conditions observed in publications for Lagrangian particle tracking models. The process begins with specifying the particle type, which dictates subsequent parameter choices. For microplastics, the size distribution is crucial due to its influence on settling behaviour (ALOSAIRI; AL-SALEM; AL RAGUM, 2020; KOOI et al., 2017), while oil spill simulations require defining oil properties such as density and viscosity (CHEN et al., 2015; DE DOMINICIS et al.,

2013; FENG et al., 2019). Generic tracer particles typically need information on particle density to represent floating or sinking processes (DALLA et al., 2024; GU et al., 2024). All particle types share common parameters: initial positions (defined as point sources or distributed areas) and the number of particles released. The number of particles is a relevant topic as tracers are probabilistic solutions. This information will be discussed ahead of this review. The next stage involves incorporating environmental conditions. If a hydrodynamic model is used, it provides the initial water level, velocity field, temperature, and salinity (RHOMAD et al., 2022). Otherwise, these parameters are initialised using simplified assumptions (e.g., zero velocity, mean water level, homogeneous temperature and salinity). Hydrodynamic models can also be exported and exchanged between algorithms and imposed for the need of Lagrangian models. Bathymetry data, mostly sourced from databases such as ETOPO or NOAA, defined the model domain. Model configuration follows, encompassing the time step, horizontal and vertical grid resolutions, and boundary conditions. Finally, stochastic models, employing random walk for diffusion, require a random seed for reproducibility, while more deterministic models require specification of advection and diffusion coefficients. These coefficients often require calibration, and the simulation always requires validation against observational data.

Figure 3: The general sequence of processes used in publications to model the Lagrangian tracers.

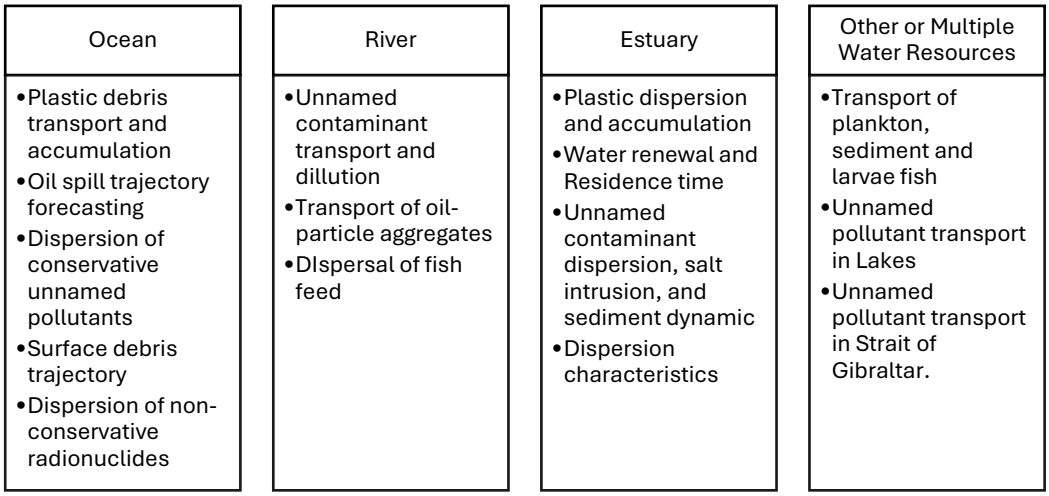


Sensitivity analysis is often employed to identify influential parameters, ensuring robustness (ALOSAIRI; AL-SALEM; AL RAGUM, 2020; TAGHAVY; PENNELL; ABRIOLA, 2015). For instance, Alosairi et al. (2020) suggested windage is most significant for offshore microplastic transport in the Arabian-Persian Gulf in comparison to diffusivity, number of particles released, beaching probability, and particle density. Taghavy et al.(2015) highlighted the importance of aggregation efficiency and primary particle diameter for nanoparticle transport in porous media. The work used varied parameters such as pore water velocity, influent particle concentration, aggregation efficiency, and primary particle diameter. Jalón-Rojas et al.(2019) demonstrated the dominant role of sinking in marine plastic debris fate using parameters related to physical processes (horizontal and vertical dispersion, washing-off, and sinking) and particle behaviours (physical properties, biofouling, and degradation). Finally, Liang et al.(2021) emphasised the influence of

ice drift and biofouling on microplastics in the Arctic Ocean. Existing publications are also relevant for justifying parameter choices in similar environments or model setups.

It was observed in publications that parametrisations may occur based on a general contaminant and passive particle, otherwise a named contaminant with more specifications. A summary of the uses of Lagrangian model and parametrisation focus is observed for each water resource as in Fig. 4.

Figure 4: Use of Lagrangian models in publications referenced in this review, the tracer identification categorised by water resource classification.



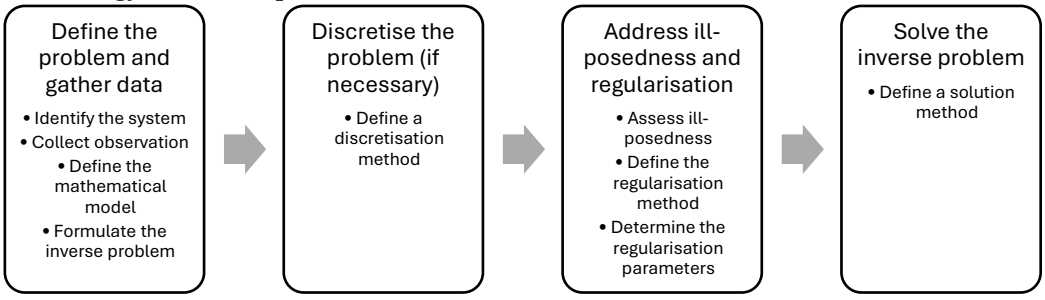
4. Inverse Problem Method to Solve Initial Parameters

Forward problems use known parameters to simulate system behaviour (BREIVIK et al., 2012; LUGON; SILVA NETO; RODRIGUES, 2008b). Inverse problems seek to identify parameters based on the observed effects (BREIVIK et al., 2012; SUNEEL; CIAPPA; VETHAMONY, 2016). Although challenges arise from potential non-uniqueness, non-existence of solutions, and sensitivity to input data changes (HASANOV HASANOĞLU; ROMANOV, 2017; LUGON JUNIOR; SILVA NETO, 2011; ROUCHIER, 2018).

Regularization techniques and cost functions (e.g., least squares estimation, maximum likelihood estimation, Bayesian inference) address these challenges (LUGON JUNIOR; SILVA NETO, 2011; ZHAO; SUN; MEI, 2019). Optimization techniques (e.g., Genetic Simulated Annealing, Genetic Algorithm, Luus Jaakola) aid in parameter retrieval (LOBATO; STEFFEN JR., 2008; MANSOUR; EL-FAKIH, 1999; XIANG et al., 2013).

The methodology for the inverse problem is summarised in Fig. 5.

Figure 5: Basic methodology for inverse problem solution.



There are R and Python language programming platform packages with varied optimisation techniques to retrieve the potential values of the parameters (LOBATO; STEFFEN JR., 2008; SCRUCCA, 2013; XIANG et al., 2013). The

Genetic Algorithm is a population-based optimization technique inspired by the principles of natural selection and evolution from biology sciences (MANSOUR; EL-FAKIH, 1999). The model depends on the initial population of candidate solutions (potential parameters) and advances these parameters over generations using genetic operators such as *selection* (choosing the fittest individuals), *crossover* (recombining solutions to generate new ones), and *mutation* (introducing small random changes) (SCRUCCA, 2013).

The Genetic Simulated Annealing is based on annealing in metallurgy (MANSOUR; EL-FAKIH, 1999). This process originated from the process of refinement by heating and gradually cooling materials. This method is commonly employed when the system has many local solutions (XIANG et al., 2013). The objective of this method is to retrieve the global solution or nearby. The *temperature* parameter indicates the criteria for accepting the worst solutions.

Finally, the Luus Jakola method is a straightforward, derivative-free optimisation algorithm designed for solving bounded problems (LOBATO; STEFFEN JR., 2008). This method works by iteratively reducing the search space around the best solution in time and randomly sampling new candidate solutions within the region. If a better solution is found, the algorithm updates the centre of the search space; otherwise, it will continue reducing the region size.

These methods are presented in Table 1, describing the search type, structure, parameter control, problem suitability, strength and weakness. There are several in publications, but not the scope of this work.

Table 1: Description and interpretation of Genetic Simulated Annealing (GSA), Genetic Algorithm (GA), and Luus-Jakola (LJ) to resolve inverse problems.

Feature	*GSA*	*GA*	*LJ*
Search Type	Hybrid (global & probabilistic)	Population-based global search	Local search (random)
Structure	The population of Solutions with Simulated Annealing	Population evolution via GA rules	Single-solution iteration
Parameter Control	Temperature from Simulated Annealing	GA parameters (e.g., mutation)	Shrinking region
Problem Suitability	Complex, mixed-mode problems	Global optimization problems	Bounded, low-dimension
Strength	Escaping local optima	Diversity of solutions	Simplicity and speed
Weakness	Computationally expensive	Premature convergence	May miss global optima

In the Lagrangian field, the evolution of the particle in space and time are functions of the position of the particle and the velocity from the Hydrodynamic (CIMATORIBUS; LEMMIN; BARRY, 2019), using Lagrangian passive tracer (SOROKIN; SHELOPUT, 2019; WICHMANN et al., 2019). The mathematical description is observed in Eq. (1):

$$\frac{dx}{dt} = v(t), \quad \frac{dv}{dt} = F(x,t) \qquad \text{Eq. (1)}$$

where x(t) is the position of the particle vector at time *t*, *v(t)* is the velocity vector, and *F(x,t)* represents the net forces.

While the forward problem provides the initial condition (*x0*, *v0*) at $t = 0$ and the force field $F = (x,t)$, the computation of the trajectory *x(t)* and *v(t)* becomes straightforward by solving the system of differential equations.

On the other hand, the inverse problem aims to look in reverse (LUGON JUNIOR; SILVA NETO, 2011). Given the observed position of a particle (or group of particles), it aims to find a single or more parameter from the initial conditions, such as x_0 and v_0.

One significant challenge in inverse problems in water resources is the ill-posedness and noise in the observations, as measurement errors in $x_{obs(t)}$ may propagate over time into the computational force field (ARGOUL, 2012; BEVEN, 2009). This challenge becomes even more significant in grids of higher resolution, where small changes may lead to large deviations. In addition, the non-uniqueness nature of the system may result in similar results though the initial conditions differ. In other words, a group of particles emitted from varied pairs of coordinates in the domain may coincide in the same result (MOURA NETO; DA SILVA NETO, 2013).

In order to reduce this challenge, regularisation methods are employed (ROUCHIER, 2018). For example, the force field could be reconstructed by minimising the cost function τ as in Eq. (2).

$$\tau = \int_0^T \|x_{obs}(t) - x_{model}(t)\|^2 dt + \lambda R|F|, \quad \text{Eq. (2)}$$

Where $x_{model(t)}$ is the point in the trajectory of the particle, R|F| is the regularisation term, τ is the total time of integration, and $\lambda > 0$ controls the balance between data fitting and regularisation. Thus, given the $x_{obs(t)}$ and F, the initial conditions may be described by Eq. (3)

$$(x_0^*, v_0^*) = \arg\min_{x_0, v_0} \tau, \quad \text{Eq. (3)}$$

5. Uncertainty In The Forward Problem

Lagrangian models often combine deterministic and stochastic elements (e.g random walk based on diffusion coefficients) to compute velocity field, reflecting system uncertainty - as seen in Eq. (4) (BREIVIK et al., 2012; DAGESTAD et al., 2018; DE DOMINICIS et al., 2013; LUGON JR et al., 2019).

$$\frac{\partial \mathrm{r}}{\partial \mathrm{t}} = \mathrm{u}(\mathrm{r}, \mathrm{t}) + \xi(\mathrm{t}), \quad \text{Eq. (4)}$$

where r is the position vector in the three dimensions $[x, y, z]^T$, u(r, t) is the velocity field $\left[u_x(x, y, z, t), u_y(x, y, z, t), u_z(x, y, z, t)\right]^T$, and uncertainties $\left[\xi_x(t), \xi_y(t), \xi_z(t)\right]^T$.

The deterministic process is straightforward. However, the uncertainty solution is designed by Lagrangian model creators as a pseudorandom function.

For instance, (PILECHI; MOHAMMADIAN; MURPHY, 2022) suggest as a naïve random walk solution the use of a constant diffusive coefficient parameter in the domain during the simulation time, as seen in Eq. (5). The pseudorandom value is a computational expression to indicate that values are not truly random, as computers are deterministic machines, there are protocols to obtain the pseudorandom values (MEACHAM; BERLOFF, 2023; PASQUALINI; PARTON, 2020). These pseudorandom values appear random due to the sequence exhibiting statistical properties of randomness, though the sequence can be predicted given the initial conditions (ÁLVAREZ; MARTÍNEZ; ZAMORA, 2022).

$$\Delta Pos_{x,y,z} = R\sqrt{2K\Delta t} \quad \text{Eq. (5)}$$

where the difference in position $Pos_{x,y,z}$ is yielded from a pseudorandom value (R) and the diffusive coefficient (K).

Accordingly, it was provided with a modified diffusive term to enhance naïve random walk in Eq. (6) (PILECHI; MOHAMMADIAN; MURPHY, 2022).

$$Diff = \left(\frac{\partial K}{\partial X}\right) + \left\{R\sqrt{\left[2K\left(P_{(t)} + \left(\frac{1}{2}\right)\left(\frac{\partial K}{\partial P}\right)\Delta t\right)\right]\Delta t}\right\} \quad \text{Eq. (6)}$$

where P(t) is the position of the particle in the coordinates x,y, and z during the simulated time.

Another group of researchers (SUMMERS et al., 2023) obtained a random walk based on Eq(7).

$$r_{n+1} = r_n + (v + \nabla K)\Delta t + R \odot \sqrt{6K\Delta t}, \quad \text{Eq. (7)}$$

where r is the position at step *n* in the coordinates $[X_n, Y_n, Z_n]^T$, v is the velocity vector in the three components $[U, V, W]^T$, ∇K is the gradient of the diffusive coefficients $\left[\frac{\partial x}{\partial K_x}, \frac{\partial y}{\partial K_y}, \frac{\partial z}{\partial K_z}\right]^T$, K the diffusive coefficient vector $\left[K_x, K_y, K_z\right]^T$ and R the random walk variable $[R_x, R_y, R_z \sim N(-1,1)]$. $\odot$ denotes element-wise multiplication.

(PERIÁÑEZ, 2020) uses an alternative naïve random walk for horizontal dispersion as seen in Eq. (8)

$$D_h = \sqrt{12K_h\Delta t} \quad \text{Eq. (8)}$$

where K_h is the horizontal diffusivity term and D_h the random walk in horizontal axis.

The MOHID platform, designed by the research group MARETEC in Instituto Superior Tecnico in Lisbon uses a method adopted from Sullivan and Allen (ALLEN, 1982; SILVA et al., 2013; SOUZA et al., 2021; SULLIVAN, 1971). Considering the mixing lengths and standard deviation of the turbulent velocity (RODRIGUES, 2012). The turbulent dispersion of particles can be characterized by the relationship between the mixing length (L) and the turbulent velocity (u′), where the turbulent time scale is given by $dT = L\sqrt{u' \cdot u'}$. This describes the duration a particle maintains its turbulent velocity before undergoing a new random step. The spatial dispersion is governed by $\frac{d}{dt}(x^2)$, which shows that the rate of change of the squared position is proportional to both the particle's position (x) and its turbulent velocity (u′).

The Opendrift platform uses the (VISSER, 1997) method for vertical motion. This method consists of a combination of deterministic movement due to buoyancy ($w\Delta t$) and a random component due to turbulent mixing $\sqrt{(2K\Delta t)} * N(0,1)$. The platform iterates this process for the total simulation time to yield the vertical mixing over the larger time step. The horizontal random walk is based on diffusivity $\Delta x, \Delta y \sim \sqrt{(2D_t)} * N(0,1)$.

6. Beaching and outside of the domain

Particles in longer simulations can move beyond model boundaries, including beaching—particles retained at shorelines due to sediment interaction, for example. While no standard beaching parameterisation was identified in publications, common approaches consider (i) distance thresholds, (ii) beaching probabilities, and (iii) trapping boundaries (BRABO et al., 2022; DE CARVALHO; BAPTISTA NETO, 2016; JIMÉNEZ MADRID; GARCÍA-LADONA; BLANCO-MERUELO, 2016). Beaching probability (P_{beach}) considers hydrodynamic (H) and atmospheric (A) conditions, and boundary characteristics (B) (Eq.9).

$$P_{beach} = f(H, A, B) \quad \text{Eq. (9)}$$

Naturally, it is expected that higher resolution will allow better representation, however, for beaching processes, it is unclear whether very high resolution will offer significant insights over lower resolutions.

Beaching rates are often calculated using Eq. (10).

$$R_{beaching} = \frac{N_{beached}}{N_{total}} \quad \text{Eq. (10)}$$

where the beaching rate ($R_{beaching}$) will be a rate between the percentage of particles ($N_{beached}$) that is assumed to beach in the total number of particles in the system (N_{total}).

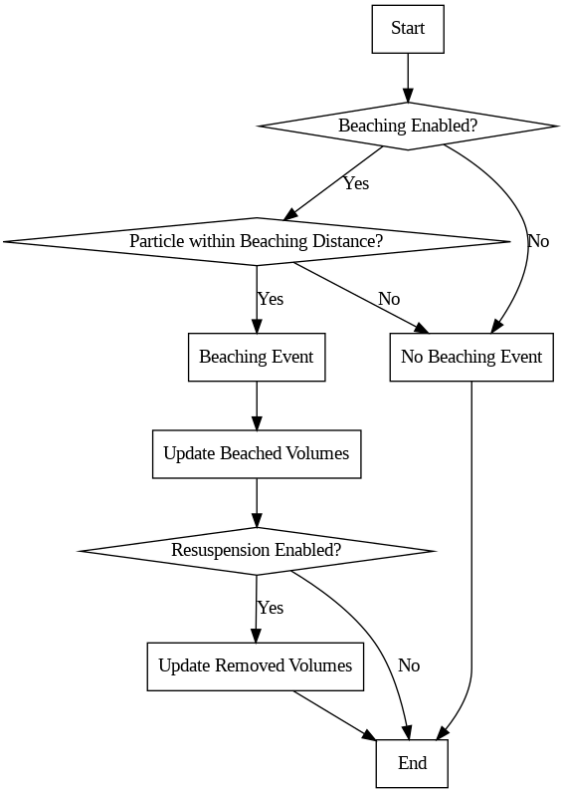
Periáñez (2020) defined the beaching process as the moment a particle reaches the shoreline during a simulation. Once a particle is considered beached, it will remain stationary. Matsushita et al. (2022) on the other hand, defined beaching based on a predefined minimum depth. In this example, when a particle reaches a grid cell with a depth of 20 meters (the minimum depth set in their model), it is classified as beached and the tracking of the particle ceases. Onink et al. (2021) used a stochastic beaching model that considers a beaching zone extending 10 kilometres from the coastline. Within this zone, particles have a probability of beaching determined by a characteristic timescale.

These beaching methods are effective and simple for implementation. However, relevant surf-zone processes, wave run-up, tip currents, and shoreland topography may affect the beaching processes. Parameters to represent these effects were not identified in the publications.

It was identified models with and without the beaching process in publications. It is not possible to anticipate whether a simulation without beaching would be a limited simulation, as interactions with the continent shoreline must be carefully understood. It is reasonable to consider that in shoreland regions where sediment trapping is less likely, the beaching process may become irrelevant to the overall result.

The computational platform MOHID uses the method described in Fig. 6. The beaching process in MOHID is a combination of a deterministic distance check from the coastline and a probabilistic decision based on a beaching probability. The actual beaching event is a discrete decision made for each particle at each time step (RODRIGUES, 2012). The aftermath (accumulation and removal of beached material) is then handled separately. As particles approximate the defined beaching distance from the boundary cells, the *beaching probability* will systematically reduce the *volume of particles*. As real particles may have a temporary accumulation on shoreland, virtual particles may be dragged back partially or completely into the domain in case of *resuspension*, enhancing the realism of the method.

Figure 6: Flowchart of the MOHID Lagrangian beaching algorithm highlighting the calculation of the proximity to the coast and a probability assessment parametrised by the user.



In the Opendrift platform (DAGESTAD et al., 2018), the beaching occurs whenever particles reach the shoreland defined in the domain. No probability concept was identified in the open-source code for beaching processes. On the other hand, the MEDSLIK II platform (DE DOMINICIS et al., 2013) considers a more complex solution for the beaching of oil as demonstrated in Fig. 7. MEDSLIK initially beaches oil deterministically based on shoreline intersection. However, the amount of oil retained on the beach (due to adsorption) and the potential for resuspension are influenced by probabilistic calculations based on coastal type and random number generation, adding some stochasticity to the long-term beaching behaviour. The mathematical framework of MEDSLIK describes stranding occurring when the position of the particle, χ(x, y, t), intersects a coastline segment as seen in Eq. (11).

$$\chi(x, y, t) \in L_i \qquad \text{Eq. (11)}$$

Upon beaching, the particle's status changes ($\sigma = -L_i$), indicating the segment where beaching occurred), and the non-evaporative oil volume ($V_{NE(t)}$) begins to decrease due to adsorption, following a decay process ($V_{NE(t0)}$) describe in Eq(12)

$$V_{NE(t)} = V_{NE(t_0)} * 0.5^{\frac{t-t_0}{\tau_s}} \quad \text{Eq. (12)}$$

where t_0 is the time of beaching.

τ_s is the half-life for seepage or adhesion, dependent on the coastal type (L_i)

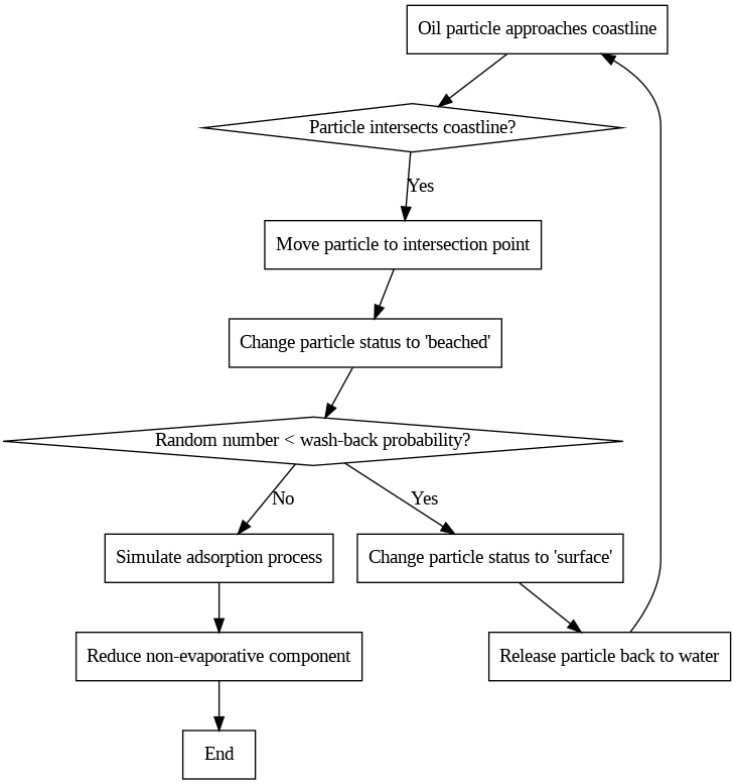
The particle's potential for resuspension is evaluated at each subsequent time step. A wash-back probability, P_w, is calculated based on a similar decay relationship (Eq. 13)

$$P_{w(t)} = 1 - 0.5^{\frac{t-t_0}{\tau_w}} \quad \text{Eq. (13)}$$

where τ_w is the half-life for wash-back (also coastal type dependent)

A random number ($0 \leq r \leq 1$) is generated. If r is less than P_w, the particle is resuspended, its status is updated ($\sigma = 0$), and it returns to the water column.

Figure 7: Flowchart of the MEDSLIK Lagrangian beaching algorithm.



7. General Discussion:

A significant challenge in Lagrangian modelling is the lack of a universal random walk solution due to the case-specific nature of particle dispersion. It can be inferred that the particle dispersion is governed by underlying physical processes, however, there are specific processes that cannot be anticipated to date. Hence, the random walk is addressed to mimic the maximum entropy state consistent with the constraints of the system.

The beaching process is inherent in natural systems and has to be carefully carried out. It was observed that platforms vary between probabilistic and more deterministic methods. Factors to further complicate a deterministic method involve heterogeneous coastlines, uncertainties inherent to hydrodynamic models, physical and chemical properties and the

interactions of the particles to be beached, resolution of the model, environmental uncertainties, and data limitation (BEVEN, 2009). However, the probabilistic approach balances the simplicity with some level of representativeness, especially for large-scale or data-sparse applications. Thus, the probabilistic method seems feasible and, to date, more appropriate than deterministic models for beaching particles. A criteria-based solution to determine the rate of beaching accumulation with further validation protocols would potentially enhance the beaching model. Confirmation will occur with validation protocols.

Rigorous validation of Lagrangian models against real-world observations is used to ensure their reliability in predicting contaminant transport (CLOUX et al., 2022; LAURENT et al., 2020). In a study of the transport of floating plastic, researchers validated their model results by comparing them to the distribution patterns observed in satellite-tracked Lagrangian drifters deployed in the same region (LIUBARTSEVA et al., 2016). This is a significant solution for floating particles on water, though it can be limited due to the capacity of observation. For example, if microplastic particles are not abundant, there might be challenges to observe small accumulations. A second study used the Global Drifter Program database for comparison (MATSUSHITA et al., 2022). Opposing different models or platforms is a potential solution for validation. This method may provide a better representation of an unbiased solution. However, it must be carefully observed that models are only significant if they are comparable to the real system.

Another study investigating the transport of microplastics compared their model simulations to field data collected during surveys, noting areas of agreement and discrepancies in microplastic concentrations (POLITIKOS et al., 2020). Buoys and in-situ data collection are important means to ensure the initial conditions of the models. During this review, it was observed no protocol for measuring microplastic properties in the water resources, which could lead models to discrepancy from reality (PÄRT et al., 2023; YU et al., 2017). In addition, the distance of buoys may further complicate the data reliability between measuring points. Nevertheless, this buoys measurement method is observed the most reliable, to date, to incorporate the initial conditions in the system.

A group of researchers compared the model predictions of oil plumes with data from an older recorded experiment (CHEN et al., 2015; JIANG et al., 2021). This solution may be effective if boundary conditions and initial conditions are fairly similar. If the hydrodynamic is unchanged, the only factor that will vary the trajectory of oil particles unpredictably will be the Lagrangian random walk element. However, the random walk schemes in publications do not represent the main factor, but a minoritarian factor that will make small changes in the velocity field. The small change may allow particles to access other grid cells with different sensitivity. This is important to take into consideration, mainly for low-resolution simulations.

Most authors highlight the limited availability of real-world data, especially at the necessary temporal and spatial resolutions (BEVEN, 2009; CIMATORIBUS; LEMMIN; BARRY, 2019; DOBLER et al., 2019; FENG et al., 2019; KIM; KIM, 2024; RHOMAD et al., 2022), leading to challenges in comparing model output with observations (CHEN et al., 2015; CIMATORIBUS; LEMMIN; BARRY, 2019; GONZÁLEZ et al., 2019; MITCHELL et al., 2023). In addition, inaccuracies and uncertainties in input data, which can be widened through the model, significant computational demands for high-resolution simulations, and inherent model structural error due to necessary simplifications and approximations (CIMATORIBUS; LEMMIN; BARRY, 2019; JALÓN-ROJAS; WANG; FREDJ, 2019). The platforms converge in interpolation methods to provide a complete initial condition under the total of grid cells, satisfying the need for data in regions where it is scarce.

The groups that study the Lagrangian models mostly highlight the importance of enhancing model reliability. These include advancements in observation technology (GU et al., 2024) for more accurate and higher-resolution input data and/or comparison. In addition, it was observed that integrating Lagrangian and Eulerian methods for a more comprehensive understanding (BILGILI; PROEHL; SWIFT, 2016; DALLA et al., 2024; DU et al., 2020; GU et al., 2024) can improve parameterisation of crucial processes through focused laboratory and field studies (GONZÁLEZ et al., 2019; GU et al., 2024; HUNTER et al., 2022; LI et al., 2023; RHOMAD et al., 2022).

Another point of discussion is the reactive transport models. Though most Lagrangian models make use of the passive tracer concept without any reactive interaction, the biogeochemical processes can eventually interact with the

contaminant particles (e.g. microplastic) changing their passive behaviour (ALOSAIRI; AL-SALEM; AL RAGUM, 2020; GOLUBEVA; GRADOVA, 2024; GU et al., 2024; MITCHELL et al., 2023). Some authors found the solution in coupling between hydrodynamic Eulerian water properties and particle-tracking Lagrangian models implementing reactive transport models (ALOSAIRI; AL-SALEM; AL RAGUM, 2020; GOLUBEVA; GRADOVA, 2024; LAURENT et al., 2020; LI et al., 2023). This approach involves directly incorporating biogeochemical reactions, such as biofouling and degradation, into the properties of the Lagrangian models (GU et al., 2024). However, the input of some details of the particle behaviour should be carefully addressed and evaluated whether it is significant. For example, the weathering process for a large steel container might be irrelevant for a short-time simulation. On the other hand, particle processes in oil matter and microplastic particles could affect the tracer motion in a short-time simulation, and thus, are relevant for implementation (BALSEIRO et al., 2003; FINGAS, 2011; KOOI et al., 2017). Another observation is that reactive models may be challenging to describe in a more deterministic approach. Thus, a random walk solution seems feasible to incorporate the reactive models, except if these reactive models impact in significant difference.

As constant optimisation and innovative technology are implemented in modern computers, limiting factors in model processing can be reduced. For example, the overall observation is that the authors of publications highlight the balance between computational cost and model representativeness. The object-oriented solution in computational programming methods provided an important step to reduce computational challenges (BRAUNSCHWEIG et al., 2004). However, the more complex the model, the more computational consumption will be. Algorithm construction design can optimise data processing and reduce computational cost at a certain level. It is possible to identify in publications discussions about simulation benchmarks due to the algorithm design. However it must be acknowledged that the more computational capacity is provided, the more is demanded to obtain more realism in models.

Solutions can be yielded from oversimplified models, which will be validated through rigorous criteria. If validation occurs, the model can be considered representative. There is no best model, but the model that mimics better the actual natural system. In addition, complexity must be carefully addressed in algorithms and models, as eventually specific parameters of complex systems will have lesser influence in the overall simulation. If computed with these less-influent parameters and models, it is likely to demand more computational cost for simulations that will not vary in representation significantly.

The initial conditions and final timestep output in Lagrangian models will provide the accumulation probability. In opposition, the trajectory between the initial and final steps may challenge to yield high representativeness. Few authors described a better representation of the trajectory based on satellite imagery and measurements (AL-SALEM; ALOSAIRI; AL-RASHED, 2017; TIAN; HUANG; LI, 2017), the reasonable limitation will be the particle accumulation visibility. A large oil slick similar to the DeepWater Horizon accident (CHEN et al., 2015; SAMMARCO et al., 2013) might be easier to observe in imagery than microplastic accumulation zones. Though long-term oil persistence by It is important to highlight that important improvements are constantly occurring in computational and observational capacities and most likely this limitation will reduce to smaller particles visualisation. A group of researchers from the University of Michigan reported a promising solution to observe small-scale particles using satellite-based radar measurements of ocean surface roughness (EVANS; RUF, 2022). The key principle behind this method is the hypothesis that microplastics, or tracers associated with them (like surfactants), suppress the roughening of the ocean surface caused by wind. The study found a strong correlation between mean square slope anomalies and microplastic concentrations predicted by various models, suggesting the potential of this method for monitoring ocean microplastics from space.

For the case that initial condition is unknown the inverse problem method poses a potential solution (LUGON JUNIOR; SILVA NETO, 2011). However, cost function decision must be carefully addressed. The few authors identified in the publications used a minimisation of least squared method. This method aligns with the assumption of Gaussian noise in measurements. If the observation errors are normally distributed, the least-squares approach is equivalent to maximising the likelihood of the observed data (BEVEN, 2009; MOURA NETO; DA SILVA NETO, 2013). This makes it statistically optimal under these assumptions. However, studies over absolute error minimisation, robust loss function, and others, are not observed in the publications in the used database.

Finally, reducing stochasticity is a reasonable solution to provide more representative models. The physical forces and uncertainties are a challenge in many sciences, though highly useful to implement the fuzzy realism of the system. Nevertheless, a robust review of random walk methods is necessary to understand better the influence and constraints of this realism factor.

The random values generator algorithms may be limited into a biased solution (ÁLVAREZ; MARTÍNEZ; ZAMORA, 2022). Some solutions describe a method using inverse problem methodology with elliptic curve functions to force an unpredictable noise in the results (HAIDER; BLANCO; HAYAT, 2024). Another group of research combine an evolutionary algorithm to generate an initial high-quality seed with a deterministic method that iteratively modifies and hashes this seed to produce a stream of cryptographically secure random values (RYAN et al., 2022). The use of hashing forces that the output values are potentially unpredictable and exhibit the desired characteristics of randomness. Though the philosophy of what is a random value, and a pseudorandom value may be inconclusive, complex solutions with many noisy functions may provide sufficient randomness for modelling. However, the validation will confirm whether or not the randomness method was effective.

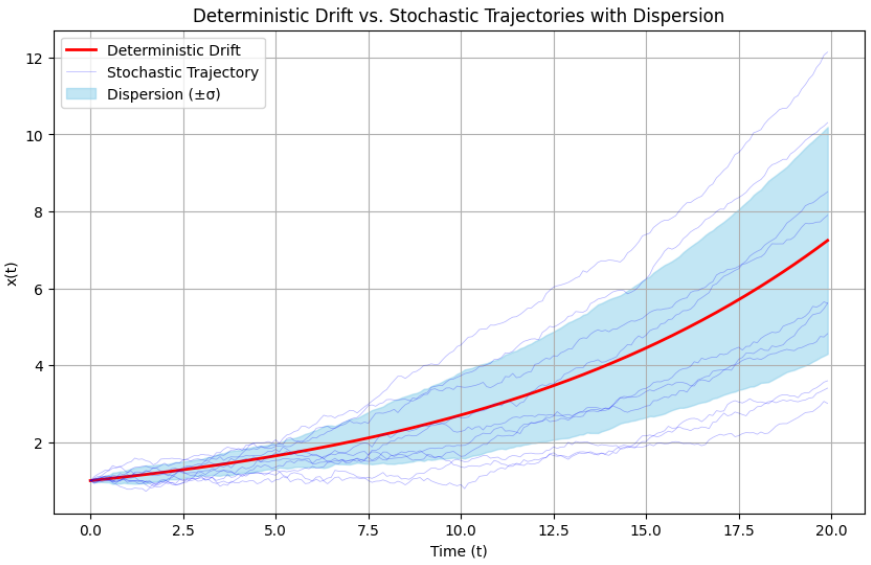
It is clear that the Lagrangian models provide important tools to understand, monitor, and anticipate environmental impacts in environmental engineering. Efforts in trajectory prediction robustness is an improvement that coincides with interests in mitigation and cleanse programmes.

8. Accumulated Randomness

Though computational platforms and users constantly use random walk schemes, a reasonable question is implied whether the random walk should be implemented in Lagrangian models. The reason for this discussion is due to the inherent uncertainties adjustments in hydrodynamic and atmosphere models (FENG et al., 2019; STERL; DELANDMETER; VAN SEBILLE, 2020). To address this item, a representation of a python code was developed with a deterministic behaviour and a stochastic behaviour from Eq. (4). Multiple trajectories were observed by the adding of a random noise term at each time step to the deterministic step. The random noise was modelled using a Gaussian distribution, injecting randomness into the behaviour of the system. The programming lines are based on the following python-like pseudocode and representation is displayed in Fig. 8.

Figure 8: Simulation of a stochastic differential equation with linear drift without random walk. The thick blue line represents the deterministic solution; thinner lines show ten stochastic trajectories.

```
function stochastic_simulation(num_simulations, t_end, dt, u_x):
 x_stoch = zeros((num_simulations, int(t_end/dt)+1))  # Initialize; +1 for t=0
 x_stoch[:, 0] = 1 #Initial condition
 for sim in range(num_simulations):
  for t in range(int(t_end/dt)): #range excludes last value (t_end)
   noise = random.gauss(0, 0.5)
   x_stoch[sim, t+1] = x_stoch[sim, t] + u_x(x_stoch[sim, t], 0, 0, t*dt) * dt + noise * dt
 return x_stoch
```

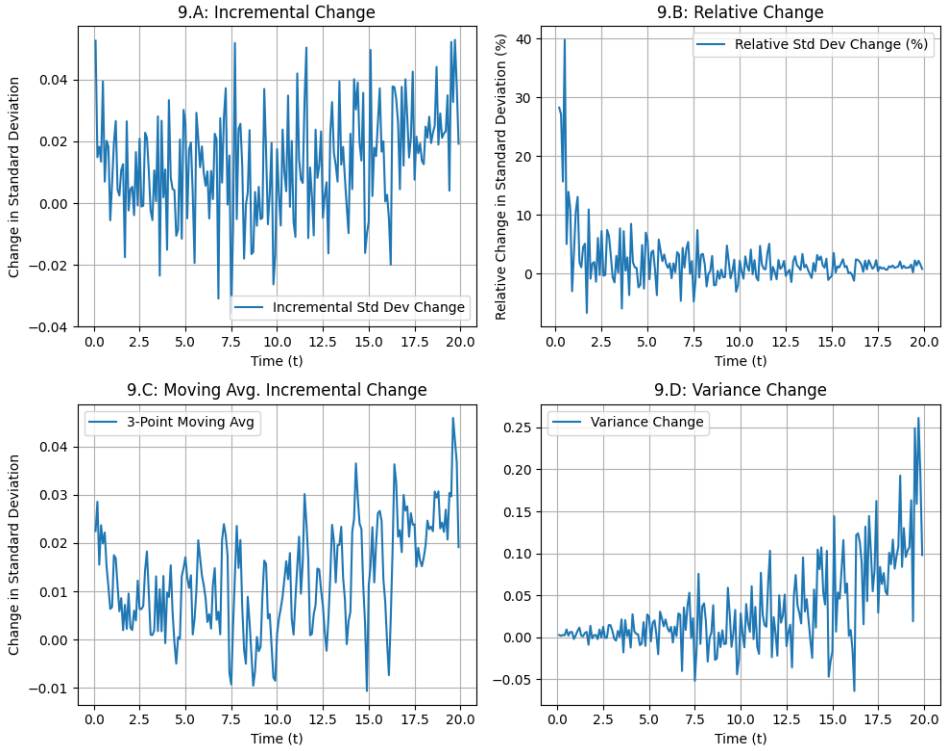


As expected, the use of a random noise within as an increment to the deterministic function provided dispersion. The total dispersion at this example (t=20) was 2.55 metres. This factor represents the impossibility of predicting where a single particle will be in the t=20 seconds. It could be inferred by this graph that a particle can be anywhere ± 2.55 metres of distance from the deterministic prediction, assuming a roughly normal distribution. More precisely, assuming a normal distribution, approximately 68% of the particles would be within one standard deviation (2.55 metres) of the mean position (represented by the deterministic trajectory), 95% within two standard deviations (5.1 metres), and so on.

The validation is crucial for comparing the observed dispersion in real world to the simulated dispersion of 2.55. Assuming that the hydrodynamic is sufficiently validated, a significant mismatch might suggest that your noise parameters, drift function, or other model assumptions need to be adjusted.

An additional method to scrutinise the impact of random walk in Lagrangian model is depicted in Fig. 9. Four statistical interpretation to calculate the dispersion growth over the timestep: (i) incremental standard deviation, (ii) relative change in standard deviation, (iii) growth rate variance, (iv) moving average of incremental change (for smoothing). The relevance of method (i) is to calculate the simple standard deviation between consecutive timesteps, the method (ii) will yield the percentage change in standard deviation relative to the immediately previous timestep. The method (iii) will analyse the growth rate considering the variance. And the last method (iv) the moving average is expected to reveal trends from the noisy increment.

Figure 9: Characterising the temporal evolution of particle dispersion. (9. A) Raw incremental changes in standard deviation show short-term fluctuations. (9. B) Relative change highlights the percentage change in dispersion per timestep, decaying over time. (9. C) A 3-point moving average smooths the incremental change in standard deviation, revealing an increasing trend. (9. D) Variance change emphasises periods of significant dispersion shifts, especially towards the end of the simulation.



The statistical analysis of particle dispersion reveals a complex, non-constant growth pattern. The spread of particles does not increase uniformly over time, as evidenced by the fluctuating incremental and relative changes in standard deviation. This suggests that the underlying processes driving dispersion are not static but evolve over time. While the moving average and variance change indicate a potential acceleration of dispersion growth, particularly towards later times, further investigation with longer simulation times may provide more insights. This acceleration could be due to positive feedback mechanisms or changes in the dominant dispersion processes. The generally decaying, yet oscillating, relative change in standard deviation hints at a decreasing rate of spread relative to the current dispersion.

However, it's crucial to acknowledge the limitations of this analysis. The conclusions are drawn from a finite simulation time and are contingent on the specific model assumptions, including the chosen noise model and the number of stochastic simulations. The Gaussian noise model might not fully capture the complexity of real-world stochasticity, and a limited number of simulations could affect the statistical robustness of the findings. Different models and noise characteristics might lead to different dispersion patterns.

Looking ahead, these findings suggest that real-world particle dispersion is likely to exhibit similar complexities and non-constant growth, influenced by a multitude of environmental factors. This poses challenges for accurately predicting long-term spread and the need for the incorporation of stochasticity in real-world simulations. Accumulated random processes may also influence the model overall Lagrangian (e.g wind, hydrodynamic, waves). Model calibration and validation against observed dispersion patterns are essential for refining model parameters and improving predictive accuracy.

9. Conclusion

In conclusion, it is observed that the important role Lagrangian models have in simulating the trajectory of the particles in the water resources. The strategy will depend on parameters and input data that are approximated to the observed system. However, there might be a challenge to address the initial parameters and inverse problem methods are potentially useful to fill these gaps.

The observed publications showed a balance between deterministic with a stochastic increment to address beaching and motion. Though publications described various solutions for random walk, it still becomes valid as far as the validation process confirms. The model must represent the realism of the natural system, and the entropy cannot be fully covered by the framework. For this reason, even the stochasticity of Lagrangian models must be carefully addressed, as random processes for the background hydrodynamic and atmosphere solution may represent sufficient randomness.

It will be an important improvement to more research on random walk solutions, beaching, and inherent uncertainties to confirm the efficiency of probabilistic solutions in these models, especially in long-term simulations where numerical diffusion may significantly affect the models. Whilst for inverse problems, the use of other methodological frameworks will allow researchers to identify advantages and disadvantages of minimum least squared methods to reach the input parameter for Lagrangian models.

Though computational cost is still a common discussion in publications, improvements and optimisation in the algorithm logic may deliver a potential computational cost saving.

Ultimately, the focus on mitigating and cleaning environmental impacts can be effectively achieved by Lagrangian model users. Offering a solution for the impacted environment. Enhancing models may allow cost savings and rapider solutions.

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