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Abstract

The Mediterranean Sea is increasingly impacted by shipborne pollution, making the development of reliable operational oil spill forecasting systems a priority for environmental protection and maritime safety. The aim of this thesis is to study the behaviour of oil spills and to create a user-friendly WebGIS platform that can simulate the dispersion of pollutants in the Mediterranean Sea. The study presents a detailed Lagrangian modelling framework to investigate oil spill dynamics using multiple oceanographic forcing datasets. First, oil spill simulations are performed using only sea surface currents derived from three operational ocean models: Copernicus Marine Environment Monitoring Service (CMEMS), the Naval Hydrographic and Oceanographic Service (SHOM), and the French Research Institute for the Exploitation of the Sea (IFREMER). Comparing the models reveals that differences in ocean circulation fields are the main source of variability in the predicted trajectories. Subsequently, the simulations are extended to include additional physical processes affecting surface transport, such as Stokes drift and wind drag. These forcings are obtained from Copernicus ERA5 reanalysis and the MeteOcean-UniGe atmospheric and wave modelling system. The contribution of each forcing component is then assessed quantitatively. Additionally, the influence of both absolute and relative wind formulations on dispersion patterns is evaluated. For each simulation, the centroid of the oil slick is computed to track its trajectory and to quantify its spatial evolution and deformation over time. A Bayesian optimisation approach is applied to identify the optimal coefficients for weighting the contributions of Stokes drift and wind drag, providing a calibration of the transport parameters based on the data. The modelling approach is further strengthened by incorporating oil weathering processes and transitioning from inertial passive particles to particles that are characterised by mass and chemical behaviour. This allows for a more realistic representation of the fate and transformation of oil in the sea. All simulations are conducted using the Parcels Lagrangian framework, which enables flexible implementation of custom kernels to account for various physical and chemical processes. The methodology is validated through a real-life case study, which involves comparing simulated trajectories with Sentinel-1 SAR satellite imagery acquired in the days following the accident, as well as documented reports. The results demonstrate that including Stokes drift and wind forcing significantly improves trajectory prediction compared to simulations driven only by surface currents. Additionally, substantial variability between ocean models is observed, emphasising the importance of model selection in operational forecasting and supporting the adoption of a multi-model probabilistic approach. Bayesian calibration reduces trajectory errors further and improves agreement with observations. The incorporation of oil weathering processes serves to enhance the simulations' physical realism, thereby enabling the slick to evolve dynamically in accordance with the type of oil,

resulting in modifications to the mass, viscosity, spreading behaviour, and the influence of droplet entrainment under wind and wave action. Finally, the validated Lagrangian modelling framework is implemented within a dedicated backend and frontend architecture, leading to the development of a user-friendly WebGIS forecasting tool capable of simulating the dispersion of particles involving combined surface currents, Stokes drift and wind forcing.

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Chapter 1

Introduction

1.1 Background and motivation

The Mediterranean Sea serves as a vital hub for maritime transits and recorded a significant increase in maritime transport in recent years: according to the most recent data, vessel traffic has increased by an average of 3.0-3.5% per year, peaking at around 4.0% in 2019 (Deandreis et al. 2022). Although transit experienced a significant decline in 2020 due to the pandemic, it fully recovered by 2021: the Mediterranean Sea accounts for approximately 10% of global cruises, which carried around 2.5 million passengers in 2019 and 19% of the world's freight traffic, mainly along the North African coast (Wecel et al. 2024). Mediterranean ports handle over 1.3 billion tonnes of goods annually, including 697 million tonnes of liquid bulk, which accounts for 40% of short sea shipping in 2022 (EUROSTAT 2024). Major ports, such as the Port of Valencia, handled over 12.2 million tonnes of goods in the first two months of 2024 alone, highlighting the increasing cargo volumes across the region (Valenciaport 2024). Tanker traffic plays a crucial role in this, with approximately 7.5 million barrels of oil per day (10% of global seaborne oil) transiting the Suez Canal in 2023 (IEA 2023). Italy and Spain each handle more than 137 million tonnes of liquid bulk annually, further underscoring the significance of tanker traffic in Mediterranean trade routes (EUROSTAT 2024). The intensity and spatial distribution of maritime traffic are clearly illustrated by the map of vessel route density shown in Figure 1.1. The map, produced by the European Maritime Safety Agency (EMSA) in 2019 with a spatial resolution of 1 km and made available through EMODnet Human Activities, an European Commission initiative, which represents the annual number of ship routes per square kilometre derived from the Automatic Identification System (AIS) data. The red areas highlight the main shipping routes, particularly along the Italian and North African coasts and in the eastern Mediterranean. This confirms the high concentration of traffic along specific routes between major ports and through strategic points.

The high volume of maritime traffic in the Mediterranean Sea exerts considerable pres-

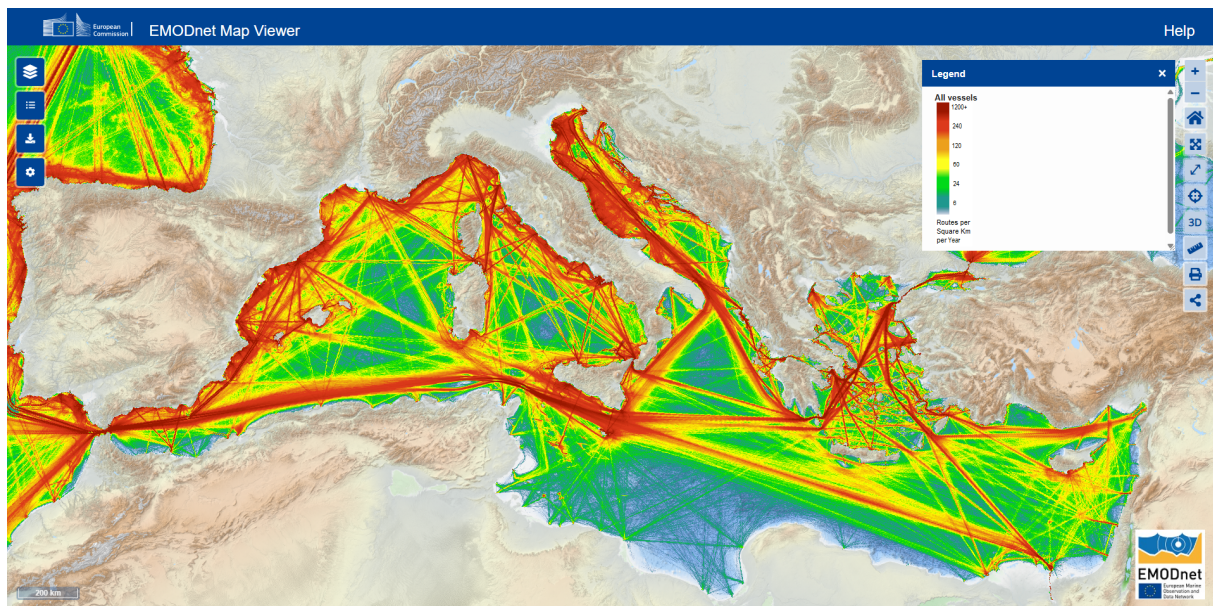


Figure 1.1: Vessel route density map (routes per km² per year) at 1 km resolution in the Mediterranean Sea. Produced by EMSA (2019) and distributed through EU EMODnet Human Activities. Last revision: 9 February 2026.

sure on an already fragile ecosystem. As shipping activity increases, so do environmental concerns, including acoustic and chemical pollution, an increased risk of collisions with marine life, and oil spills that can severely impact marine biodiversity.

A report from the European Maritime Safety Agency (EMSA) recorded approximately 2'066 oil spills of varying magnitudes in the Mediterranean between 2015 and 2017 (Polinov et al. 2021). Recent satellite monitoring highlights that the extent of oil pollution may be even greater than what is officially reported and validated as spill incidents. According to data reported by the European Environment Agency, based on EMSA's CleanSeaNet service, 7'513 possible oil spills were detected in European seas, including the Mediterranean, in 2023. These observations are derived from satellite images and represent potential pollution events rather than confirmed spills. CleanSeaNet identifies anomalies on the sea surface that could correspond to oil slicks, but could also include natural surfactants or false positives. Similarly, a satellite assessment conducted by SkyTruth using the Cerulean platform identified 757 oil slicks in the Mediterranean Sea between July 2020 and January 2024, covering approximately 1.9 million hectares of sea surface, as shown in Figure 1.2. Most of these patches are associated with identifiable vessels, suggesting persistent pollution along major shipping routes. However, as with CleanSeaNet detections, these observations are based on automated SAR analysis and machine learning classifications and do not necessarily correspond to legally confirmed spill events. These data indicate that, while officially reported incidents provide essential information on major spills, satellite observations reveal a broader picture of recurrent and widespread oil pollution in the Mediterranean Sea.

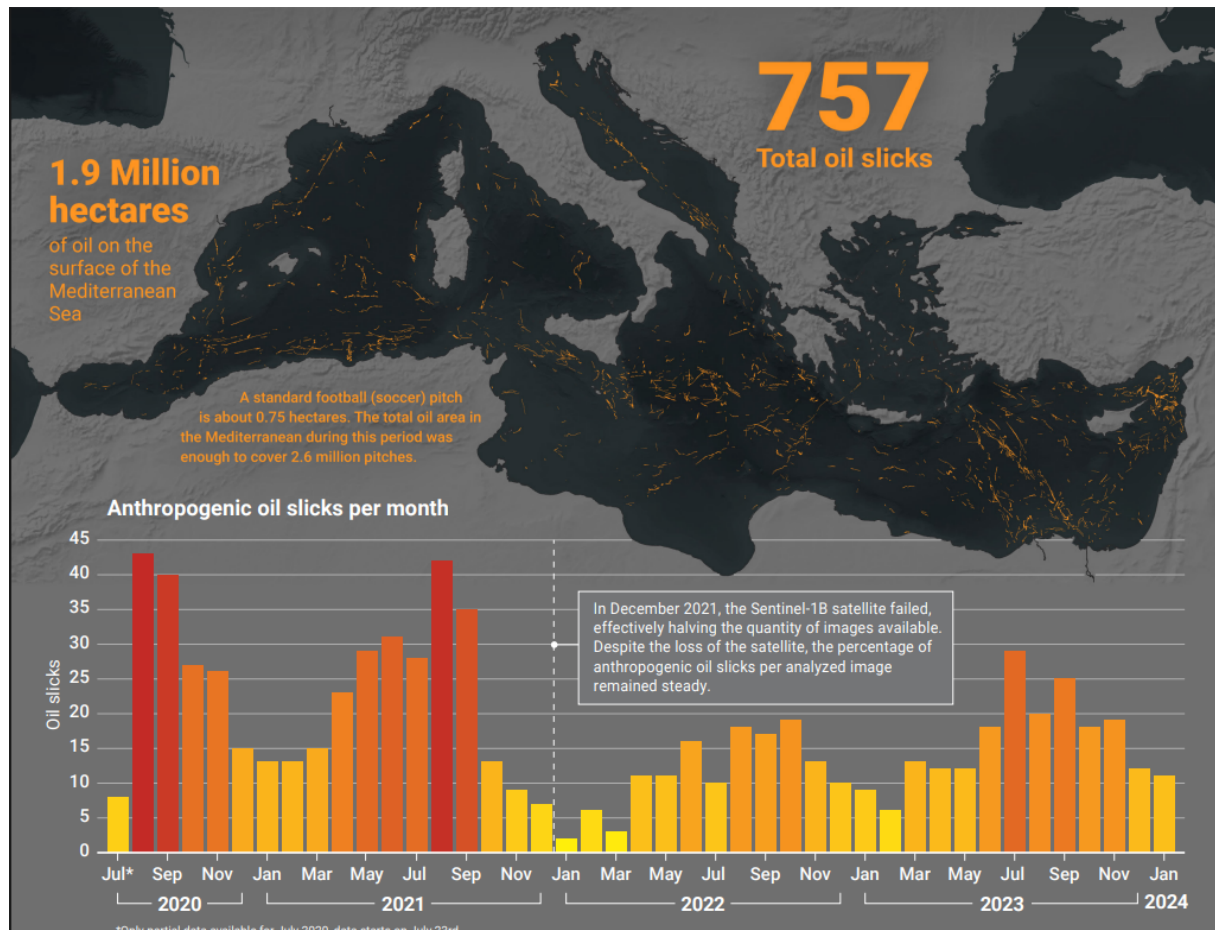


Figure 1.2: Spatial distribution and temporal frequency of anthropogenic oil slicks detected in the Mediterranean Sea between July 2020 and January 2024. The lower panel shows the monthly variability of detected slicks. Source: SkyTruth, *Mediterranean Sea - Chronic Oil Pollution Analysis* (2024).

In this scenario, continuous research into oil spillage is extremely important, since even a single event can cause severe environmental impact. The extent of damage caused by an oil spill depends on several factors: the quantity of oil spilled, its behaviour in the marine environment, the chemicals involved, the sensitivity of the affected marine area, and the wind and weather conditions at the time of the incident. Improving precision and quality of oil dispersion fate prediction is crucial for limiting the environmental impact of accidental spills. Central to this research is the dispersal of oil spills in marine areas and the modulating role of sea surface currents, wind, and wave action. It is important to note that wave action involves both the horizontal transport of buoyant oil and the vertical intrusion into the water column (Cao et al. 2021).

1.2 Thesis objectives and document structure

This research aims to provide a comprehensive investigation of the physical and chemical processes that govern oil spill dynamics. Specifically, the thesis intends to develop a user-friendly WebGIS platform that can simulate potential oil spill scenarios in forecast mode. This operational tool is designed to support decision-making during emergency response and mitigation activities. The study focuses on the Mediterranean Sea basin, a region characterised by complex circulation patterns and high environmental vulnerability. The first part of this study compares various oceanographic forcing datasets by applying a consistent methodology to evaluate their efficiency and accuracy in predicting the temporal evolution of oil spills, which is an essential component of effective marine pollution prevention and preparedness. This study employs a Lagrangian Particle Tracking (LPT) model (Van Sebille et al. 2023), recognized for its effectiveness in replicating realistic scenarios, to extrapolate the probabilistic distribution of oil spill trajectories. From the simulations, key metrics such as the centroid of spill clusters and their spatial distribution, are analysed. An analysis of the coefficients of the wind and wave components in particle transport is conducted, using Bayesian optimisation to align the values with the reference positions. Furthermore, a comparison is made between absolute and relative wind in order to determine the optimal choice. Finally, the weathering of the oil is incorporated into the simulations to make them more realistic, taking into account the physical and chemical components of the release. The results obtained are based on a real accident occurred on the 2018 Capo Corso collision (Figure 1.3), which caused significant environmental damage by releasing approximately 600 cubic meters of heavy fuel oil into the Mediterranean Sea, impacting marine ecosystems and coastal areas (REMPEC 2019).

This thesis is structured into six main chapters, with the addition of an appendix at the end of the document. The initial chapter 1 establishes the foundation for the research study by delineating the primary motivations behind it, the objectives that have been delineated,



Figure 1.3: Capo Corso cargo vessel collision in the Ligurian Sea (7 October 2018), resulting in a significant oil spill threat along the French coastlines. Source: Daily Mail (2018).

and a concise synopsis of the analytical procedures that will be employed. The second chapter 2 describes the relevant scientific literature and outlines the main approaches adopted in previous studies, providing the context for this work. The third chapter 3 provides a detailed description of the oceanographic and atmospheric datasets used as input for the Lagrangian Particle Tracking (LPT) model and outlines the methodology adopted to analyse the spill evolution and its main characteristics. Chapter 4 presents the results obtained from the different simulations. Chapter 5 presents the WebGIS interface developed for oil spill forecasting, describing both the backend and frontend components. Finally, chapter 6 discusses the main findings, highlights the limitations of the study, and outlines possible future developments.

Chapter 2

Literature Review

2.1 Theoretical framework of oil spill transport

Oil spills in marine environments are governed by a number of physical and chemical processes which interact with each other at multiple spatial and temporal scales. In the surface layer, oil slicks are mainly transported horizontally by the induced processes of sea currents, wave-induced Stokes drift and wind acting on the sea surface. In addition, the spreading and deformation of the slick is contributed to by turbulent diffusion and sub-grid scale mixing. The contribution of each process depends on the spatial scale considered, the event duration, and the environmental conditions at the time of the spill. As mentioned, surface advection is usually expressed as a linear combination of Eulerian sea surface currents and additional contributions from wind and waves. Previous studies have demonstrated that wind forcing plays a role in the transport of oil through an empirical wind-induced drift term (Abascal et al. 2009; De Dominicis et al. 2013). Although the effective value of the wind drag coefficient depends on oil properties, sea state, and turbulence near the surface, it is typically assumed to range between 2% and 3% of the wind speed (Spaulding 2017). This range is widely adopted in operational modelling, but it should be considered as an effective parameter rather than a universal constant. This is due to the fact that most circulation models only partially resolve processes near the surface. Specifically, processes such as the direct wind drag on floating oil, the Stokes drift induced by the waves, turbulent mixing in the near-surface layer, and vertical shear in the uppermost ocean layer are typically only partially represented or not included in standard operational models.

Wave action affects oil transport in two main ways. The first is horizontal, through a process known as Stokes drift, while the second is vertical and involves droplet entrainment and turbulent mixing. Research has shown that disregarding Stokes drift can result in systematic trajectory errors, especially in moderate to strong wave conditions (Tamtare et al. 2021; Yang et al. 2026). The Stokes drift component is particularly important for

buoyant surface pollutants, as it can significantly modify the predicted locations of their impact on the shoreline. Its vertical decay with depth makes it difficult to represent, since the transport experienced by oil droplets depends on their vertical distribution within the water column. In the case of the oil slick, its evolution is influenced not only by advection, but also by turbulent diffusion. The growth of particle clouds is described by Lagrangian dispersion theory through relative dispersion metrics, which show distinct regimes depending on the time scale and flow structure (LaCasce 2008). These behaviours are particularly relevant in coastal and semi-enclosed basins such as the Mediterranean Sea, where mesoscale variability strongly influence transport pathways (d’Ovidio et al. 2004).

In addition to physical transport, oil undergoes various weathering processes such as evaporation, emulsification, spreading, photo-oxidation, biodegradation, and droplet entrainment. These processes alter the density, viscosity and buoyancy of oil progressively, which influences its transport pathways and ability to remain in the marine environment (Spaulding 2017). Weathering has been studied using both laboratory experiments and numerical modelling. Different modelling methods have been employed, including simulations of mass transfer, emulsification kinetics and density evolution. This allows for dynamic interaction between oil properties and hydrodynamic forces (Horn et al. 2024). Particular attention has been focused on the processes of wave-induced droplet breakup and turbulent entrainment, since the distribution of droplet sizes has a significant impact on resurfacing timescales and vertical dispersion. Entrainment models based on processes show that breaking wave energy dissipation is linked to the formation and resurfacing rates of droplets (Johansen et al. 2015). This highlights the importance of accurately representing the upper part of the ocean turbulence in oil spill simulations.

2.2 Sensitivity to environmental forcing and model uncertainty

The accuracy of oil spill trajectory predictions depends not only on the modelling framework itself, but also on the quality and resolution of the environmental forcing fields used. Since ocean circulation models differ in terms of their spatial resolution, data assimilation strategies, vertical discretisation and boundary conditions, there is the potential for significant variability in the predicted surface currents. Previous studies have demonstrated that errors and variability in the underlying velocity fields can have a significant impact on the accuracy and separation of simulated trajectories. Also, small uncertainties in near-surface velocity fields can become more significant over time due to the non-linear and chaotic nature of Lagrangian transport (d’Ovidio et al. 2004; Liu and Weisberg 2011). Furthermore, Johannes Röhrs et al. (2012) showed that inaccuracies in representing

near-surface current shear and Stokes drift can result in systematic drift errors. There are several sources of uncertainty when it comes to oil spill modelling. These include structural model uncertainty, errors in forcing datasets, limited resolution of submesoscale processes and empirical parameter selection (Liu and Weisberg 2011; Spaulding 2017). Additional challenges are presented by semi-enclosed basins such as the Mediterranean Sea due to complex coastline geometry, mesoscale eddies, and strong regional variability. In such contexts, the choice of forcing dataset can have a significant impact on both the length of the trajectory and the timing and location of shoreline impact. Although several studies have examined the impact of wind and the inclusion of Stokes drift on trajectory accuracy, as described in section 2.1, comparisons between multiple ocean products within a consistent Lagrangian framework remain limited. Therefore, a comparison of high-resolution datasets is necessary to strengthen the robustness and reliability of oil spill forecasting systems.

2.3 Lagrangian oil spill modelling frameworks

A fully integrated operational oil spill forecasting system generally encompasses several interconnected components such as spill detection algorithms based on remote sensing data, real-time forcing from atmospheric and ocean forecast systems, data assimilation procedures to constrain model trajectories, systematic model evaluation against observational data, and the derivation of hazard or risk indicators to support emergency response decision-making. The models reviewed in this section represent the Lagrangian modelling component of such systems, a core element that can be integrated into broader operational pipelines. Over the past few decades, many operational oil spill models have been developed to simulate the transport and fate of oil under realistic environmental conditions. Most of these models use on Lagrangian particle tracking approaches within hydrodynamic and atmospheric forcing frameworks. The Lagrangian formulation is particularly appropriate for oil spill applications because it accurately represents the movement and dispersion of individual oil parcels in response to time-dependent forces. A review of oil spill tracking methods highlights the significance of Lagrangian particle models, which are widely used to simulate the transport and dispersion of oil in marine environments. These models track the fate of oil spills under the influence of ocean currents, wind, and turbulence, providing detailed insights into oil spill dynamics. GNOME (General NOAA Operational Modelling Environment), a widely used model, simulates the fate and transport of spilled oil by integrating both environmental and chemical processes (Beegle-Krause 2001). Thanks to its operational efficiency and relatively simple configuration, GNOME has been extensively applied in emergency response scenarios. MEDSLIK-II, another well-known Lagrangian model used in the Mediterranean Sea, predicts oil spill trajectories and assesses risks by incorporating hydrodynamic and atmospheric data (De Dominicis et al. 2013). Its

application in semi-enclosed basins has demonstrated the importance of high-resolution forcing fields in reproducing realistic transport pathways and shoreline impact locations. The OILTRANS model focuses on simulating the transport and degradation of oil spills in three-dimensional hydrodynamic environments (Berry et al. 2012). By explicitly resolving vertical processes, it allows a more comprehensive description of oil fate beyond purely surface transport. OpenDrift, a more recent framework, enables the simulation of oil and other substances' trajectories in complex oceanic environments using advanced Lagrangian tracking techniques (Dagestad et al. 2018). Its modular structure allows flexible integration of different forcing datasets and particle parametrisations, making it particularly suitable for research-oriented applications where sensitivity testing and methodological development are required. The MOHID Oil Spill model is integrated within the MOHID water modelling system. It combines Lagrangian particle tracking with three-dimensional hydrodynamic fields and detailed weathering modules, including processes such as evaporation, emulsification and dispersion (de Pablo et al. 2020). This flexibility enables its use in both coastal and open-sea environments, including case studies in the Mediterranean. Regional forecasting systems have also been implemented for specific regions, such as the Mediterranean basin. The POSEIDON oil spill forecasting system, for example, operates in the Eastern Mediterranean and uses a Lagrangian framework to integrate atmospheric and oceanographic forecasts, providing operational predictions for emergency response purposes (Annika et al. 2001). This model emphasise the importance of high-resolution regional circulation models and data assimilation in improving spill trajectory predictions in complex coastal areas. In addition to academic and publicly available models, commercial platforms are widely used in industrial and consultancy contexts. OSCAR (Oil Spill Contingency and Response) model developed by SINTEF is another advanced oil spill modelling system widely used in operational and risk assessment contexts (Aamo et al. 1997). OSCAR couples hydrodynamic forcing with comprehensive oil weathering parametrisations, enabling the simulation of surface, subsurface and shoreline processes. This makes it particularly suitable for conducting scenario-based environmental impact assessments, which are an essential part of environmental management. Furthermore, commercial and semi-operational platforms, such as the MIKE 3 Oil Spill module powered by DHI, adopt a Lagrangian approach embedded within three-dimensional hydrodynamic models. This allows the simulation of the fate of oil under varying stratification and coastal forcing conditions (DHI 2023). These models are frequently used in environmental impact assessments and contingency planning studies in Mediterranean coastal zones. Few studies have systematically compared the impact of different input datasets, such as atmospheric forcing, ocean currents, and wind fields on the performance of these models. One study, using MEDSLIK-II, investigated the impact of different ocean and atmospheric forcings on oil spill simulations, showing significant variability in the results depending on the quality and resolution of the input data (Lyubartseva et al. 2015). This variability highlights

the intrinsic sensitivity of the predictions of the Lagrangian trajectories of the particles to the underlying circulation model and atmospheric forcing. Some studies have shown improved accuracy in oil spill simulations when wind, Stokes drift and sea surface currents are combined. Abascal et al. (2009) demonstrated that the inclusion of these forcings significantly improved model predictions when calibrated against drift data during the Prestige oil spill. Similarly, Yang et al. (2021) highlighted the critical role of Stokes drift in improving trajectory predictions during the Sanchi oil spill. These findings reinforce the importance of integrating multiple environmental forcings to enhance oil spill trajectory modelling and reduce systematic drift errors. Increasing the accuracy of ocean prediction models is therefore fundamental to improving oil spill response strategies and mitigating environmental impacts. In a broader perspective, these modelling tools are pillars of the Blue Economy, offering potential for economic growth, environmental sustainability, job creation, and active support in decision-making (Antonio Novellino et al. 2024).

2.4 Identified research gaps

The review of the existing literature highlights several open challenges. The use of a consistent Lagrange framework for the systematic comparison of multiple high-resolution ocean circulation datasets is an area that has not been extensively explored. In operational contexts, the probabilistic calibration of wind and Stokes drift coefficients using formal optimisation techniques is rarely implemented. Moreover, the propagation of forcing uncertainty into shoreline impact predictions is not always clearly quantified. The limited integration of advanced weathering processes within flexible, Lagrangian frameworks, coupled with the gap between modelling tools designed for research purposes and user-friendly, operational forecasting interfaces, highlights the need for methodological development. Specifically, processes such as evaporation, emulsification, photo-oxidation, biodegradation, droplet entrainment, buoyancy-driven resurfacing, and turbulence-induced vertical mixing are often simplified, parameterised independently, or only partially coupled with the hydrodynamic transport processes in most existing Lagrangian frameworks. In addition, representing the temporal evolution of oil properties, such as density, viscosity, and droplet size distribution, together with their feedback on transport and vertical dispersion, remains computationally and physically challenging in operational and research-oriented Lagrangian frameworks. These limitations are addressed in the present Thesis through the explicit implementation of a coupled weathering module, as described in Section 3.6, where oil fate processes are resolved at the particle level and coupled with the Lagrangian transport framework to provide a more physically complete representation of oil spill evolution. This is particularly pertinent in the context of the Mediterranean Sea, where dense maritime traffic, complex circulation patterns and high environmental vulnerability necessitate further research and the development of reliable forecasting systems. This research builds on existing

literature by comparing three operational ocean circulation datasets within a unified, Lagrangian modelling framework. It implements Bayesian optimisation to calibrate wind and Stokes drift contributions based on observational constraints. Weathering processes are incorporated to enhance physical accuracy, and the framework is integrated into a web-based geographic information system for operational forecasting.

Chapter 3

Data and Methods

3.1 Forcing datasets

The complexity of modelling the ocean dynamics leads to considerable variability in the results depending on the models employed to describe the different physical processes. Different current fields obtained through different oceanographic models are then adopted. The main sources of inaccuracy include i) the non-linearity of the Navier-Stokes equations and the chaotic nature of the ocean circulation, that can lead to large temporal and spatial differences due to small variations in initial conditions (Visconti and Ruggieri 2020), ii) the lack of small-time and space resolution that leads to a parametrization of turbulent dynamics and no information at the sub-grid scale (Furuichi and Hibiya 2015), iii) the uncertainties in forcing fields, initial conditions, and boundary conditions can introduce errors in the representation of ocean state variables, particularly in regional models that depend on larger-scale simulations for their boundary conditions (Moore et al. 2011). To overcome these drawbacks, ocean models adopt various strategies, including stochastic approaches where undefined parameters are determined by a probability distribution, and data assimilation techniques that minimize errors by comparing with real ocean data using methods such as HF radar or drifter (Berta et al. 2014; Sayol et al. 2014).

3.1.1 Ocean currents

This study utilizes three distinct datasets from different ocean circulation models to compare their effectiveness in reproducing oil spill trajectories. These datasets are selected based on their spatial resolution, temporal coverage, and availability of essential variables. The analysis evaluates how well each model represents ocean currents that influence spill dispersion. All model data used in this study are freely available, ensuring accessibility and facilitating broader application. Specifically, sea surface current data from the following models are used:

- Copernicus Marine Environment Monitoring Service (CMEMS)

- Naval Hydrographic and Oceanographic Service (SHOM)
- French Research Institute for the Exploitation of the of the Sea (IFREMER)

The sea surface current dataset used from the Copernicus Marine Service (CMEMS) is the Mediterranean Sea Physics Reanalysis (Med MFC). The horizontal grid resolution of the model is $1/24^\circ$ (about 4-5 km) and the unevenly spaced vertical levels are 141 (Escudier et al. 2020). The surface level is used for the first part of the study, since the dataset with a temporal resolution of one hour only provides sea surface data. This model is forced with the ECMWF ERA5 climate model and data assimilation includes observations from satellite altimetry, in situ temperature, and salinity profiles. For the weathering analysis, the same CMEMS reanalysis product is employed, but using the dataset with daily temporal resolution, as it provides the full three-dimensional current field across all vertical levels. This allows for a consistent representation of subsurface dynamics relevant to weathering processes. For the purposes of this study, only the upper ~ 50 m of the water column are considered, corresponding to the first 16 vertical levels. This depth range is selected based on the physical processes governing oil weathering, which predominantly occur within the near-surface layer where turbulence, wave-induced mixing, and vertical shear are most active. The same CMEMS reanalysis product is used in the weathering analysis, but the dataset with daily temporal resolution is chosen, as this provides the full three-dimensional current field across all vertical levels. This allows for a reliable representation of the subsurface dynamics that are relevant to weathering processes. For the purposes of this study, the upper ~ 50 m of the water column are considered, corresponding to the first 16 vertical levels. This depth range has been selected based on the physical processes that govern oil weathering, which predominantly occur within these layers.

The second dataset, provided by SHOM (Shom 2017), is based on the HYCOM 3D (Hybrid Coordinate Ocean Model). This model, referred to as HYDRODYN-SURF_HYCOM 3D-SURF_R2000_MEDOC-NOR, is a specific configuration of HYCOM designed to simulate sea surface velocity with an hourly temporal resolution. It provides daily forecasts and operates at a spatial resolution of approximately 1.8 km. While the model does not generate reanalysis data, its archived outputs, available from the first of January 2016, represent the best analyses obtained from weekly simulations, with data assimilation applied only after June 2022. The model is forced by atmospheric data from the ARPEGE EURAT01 model developed by Météo-France, providing wind fields, surface pressure, and other meteorological variables. Additionally, data assimilation is incorporated from satellite observations, including sea surface height (SSH) derived from altimetry, sea surface temperature (SST), and in situ temperature and salinity profiles.

The third dataset, provided by IFREMER (Garnier et al. 2014), was developed as part of the MARC project, Modelling and Analysis for Coastal Research. This dataset is

based on the Ifremer MARS3D model, which simulates ocean circulation, biogeochemistry, and sediment dynamics, along with the WAVEWATCH III wave model. The latter was developed by an international consortium coordinated by NOAA, with contributions from the LOPS (Laboratory for Ocean Physics and Satellite Remote Sensing) research unit. The ocean circulation model has a spatial resolution of approximately 1.2 km and a temporal resolution of three hours. The MARS3D model is forced by atmospheric data from the ECMWF ERA5 reanalysis, which provides wind fields, surface pressure, and other meteorological parameters essential for surface forcing. Additionally, it is coupled with the WAVEWATCH III model to account for wave effects, particularly in coastal regions. The model also integrates data assimilation from various sources, including satellite-derived sea surface temperature, sea surface height from altimetry, and in situ temperature and salinity profiles from the European Marine Observation and Data network - Physics (Míguez et al. 2019).

	CMEMS Med MFC	SHOM HYCOM3D	IFREMER MARC
Model	NEMO	HYCOM 3D	MARS3D + WAVEWATCH III
Configuration	Mediterranean Sea Physics Reanalysis (Med MFC)	HYDRODYN-SURF_HYCOM3D-SURF_R2000_MEDOCNORD	MARC Project (Modelling and Analysis for Coastal Research)
Type	Reanalysis	Best Analysis of forecast	Hindcast
Horizontal resolution	1/24° (~4–5 km)	1/60° (~1.8 km)	~1.2 km
Vertical levels	141	50	60
Temporal resolution	1 h (surface), daily (3D)	1 h (surface), daily (3D)	3 h
Atmospheric forcing	ECMWF ERA5	ARPEGE EURAT01 (Météo-France)	ECMWF ERA5
Data assimilation	Satellite altimetry, in situ T&S profiles	Spectral nudging from MERCATOR PSY4 (from June 2022)	Satellite SST, SSH altimetry, in situ T&S (EMODnet)
Archive availability	From 01/01/1987	From 01/01/2016	From 05/01/2001
Variables	Sea surface currents; 3D currents for weathering	Sea surface currents	Sea surface currents

Table 3.1: Summary of the oceanographic datasets used in this study.

3.1.2 Wind and waves forcing

For the wave-induced Stokes drift and the 10m-wind, two models with very different spatial resolution have been used: the first ERA5 is the fifth generation ECMWF reanalysis for the global climate and weather for the past eight decades, produced by the European Centre for Medium-Range Weather Forecasts (ECMWF) and distributed in the Copernicus Climate Change Service (C3S) (Hersbach et al. 2020). An estimate of uncertainty is provided by a 10-member ensemble, where each member runs the model with slight variations in observational data and parameters, producing a set of simulations every three hours to account for uncertainty related to observational and model errors. The spatial resolution of the atmospheric data is 31 km (0.28125°) for the high-resolution forecast (HRES), while the ensemble of data assimilation (EDA) has a resolution of 63 km (0.5625°). For wave data, ERA5 uses a different grid, with a resolution of 0.36 degrees for HRES and 1.0 degree for EDA. The two variables used are the 10-m wind velocity ($\vec{u}_w$) and the Stokes drift ($\vec{u}_s$).

The second model is the atmospheric and wave hindcast developed by the MeteOcean research group of the University of Genoa (Italy). The atmospheric modelling and downscaling is done with the non-hydrostatic mesoscale Weather Research and Forecast (WRF) model version 3.4 (Skamarock et al. 2008) with an approximately 10-km resolution Lambert Conic Conformal grid over the entire Mediterranean Sea. Initial and boundary conditions are obtained from the National Center for Environmental Prediction (NCEP) Climate Forecast System Reanalysis for the period 01/01/1979 – 31/03/2011 (Saha et al. 2010, CFSR) and Climate Forecast System Version 2 01/04/2011–today (Saha et al. 2014, CFSv2) with a 3-hour and $0.5 \times 0.5^\circ$ temporal and spatial resolution, respectively. For additional details of the WRF model configuration and its performance in the Mediterranean Sea the reader is referred to Cassola et al. (2016) and Ferrari et al. (2020). The wind fields from the WRF model are used as forcing for the third-generation wave model Wavewatch III (version 5.16; Tolman et al. 2014, hereinafter WW3) with the source terms of growth/dissipation ST4 (Ardhuin et al. 2010; Raschle and Ardhuin 2013) providing hourly wave climate integrated parameters, i.e. significant wave height H_s , from 1979 to 2025 in the Mediterranean Sea using a regular grid of longitude 0.127° and latitude 0.09° , corresponding to ≈ 10 km (Besio et al. 2016; Lira-Loarca et al. 2022; Mentaschi et al. 2013, 2015).

3.1.3 Satellite SAR Imagery

The satellite data used in this study consist of Synthetic Aperture Radar (SAR) images acquired by the Copernicus Sentinel-1 mission, which are employed to validate the Lagrangian oil spill simulations by comparing the simulated particle distributions with the observed oil slick extent. Sentinel-1 is a two-satellite constellation (Sentinel-1A and Sentinel-1B) operating in C-band SAR at 5.405 GHz. According to the Copernicus SentiWiki platform, the two satellites orbit at approximately 180° offset from each other, allowing images of the same region to be acquired every 12 hours. Each satellite revisits the same area every 6 days, but their combined operation allows, under favourable orbital conditions, repeat coverage of the same area at intervals of less than 24 hours. The images are acquired in Interferometric Wide (IW) Swath mode, Ground Range Detected (GRD) format, with a spatial resolution of approximately 10 m and a swath width of 250 km (Torres et al. 2012). VV polarisation is adopted, as it is particularly sensitive to sea surface roughness and therefore provides better contrast between open water and oil-covered areas compared to VH polarisation. In SAR imagery, oil spills appear as dark patches of anomalously low radar backscatter, since the oil film dampens the capillary waves that are normally responsible for the radar return signal. However, the interpretation of SAR imagery for oil spill detection is subject to several limitations. Dark patches of reduced backscatter can also originate from natural or anthropogenic phenomena unrelated to oil pollution,

commonly referred to as look-alike features. These include areas of reduced wind speed, biogenic surfactant films, rain cells, and ship wakes, all of which can produce a similar dampening of capillary waves (Alpers et al. 2017). In the present study, the SAR images are used in conjunction with the known spill location and timing of the accidental release, which provides strong contextual evidence supporting the identification of the observed dark patches as oil-related features rather than look-alike phenomena. All images are retrieved from the Sentinel Hub platform, which provides operational access to Sentinel-1 data with orthorectification and geometric correction already applied.

3.2 Lagrangian particle tracking model

The particle dispersion simulation is analysed using the Lagrangian Particle Tracking Model Ocean Parcels, which effectively simulates the displacement of virtual particles influenced by ocean currents. This model utilizes Eulerian fluid information, such as velocity fields, to integrate particles' trajectories (Seville et al. 2018). Various interpolation techniques, including bilinear, trilinear, and spline interpolation, are employed to create continuous velocity fields within grid cells. To accurately estimate the evolution in time of an oil slick, it is essential to consider not only the surface current component but also the drag exerted by the wind on the ocean surface and the Stokes drift. This is because these processes significantly influence the movement of the oil slick. To account for them, the east and north components of the velocity field are calculated as follows,

$$\vec{u} = \vec{u}_c + \alpha \cdot \vec{u}_s + \beta \cdot \vec{u}_w \quad (3.1)$$

where $\vec{u}_c$ is the sea surface current velocity provided by ocean circulation models described in the paragraph 3.1.1, which already include the effect of atmospheric forcing such as wind stress, $\vec{u}_s$ is the Stokes velocity, $\vec{u}_w$ is the wind velocity, while α and β are respectively the Stokes drift and wind coefficients. The additional wind term accounts for the direct wind drag acting on the oil slick, which is not explicitly represented in the Eulerian current fields.

The MeteOcean-UniGe hindcast does not contain the Stokes drift data, so the latter is calculated through the variables in the dataset. Since the case study is mainly in a deep water region, the equation (3.2) for the Stokes drift approximation is applied (N. Kumar et al. 2017)

$$[U_s, V_s] = \sigma \cdot ka^2 \cdot \exp(2kz) \cdot [\cos(\theta), \sin(\theta)] \quad (3.2)$$

where σ is the dispersion number, in deep water evaluated as $\sigma^2 = g \cdot k$, k is the wavenumber, g is the gravitational acceleration, $a = H_s/2$ is the wave amplitude, z is the water depth and θ is the peak wave direction.

Equation (3.1) allows for the quantification of the relative contributions of each factor

to the overall movement of the oil slick, providing a more comprehensive understanding of the complex interactions at play. By incorporating these additional contributions, the accuracy of our predictions can be improved, ultimately informing more effective decision-making in oil spill response and environmental damage assessment.

The movement of particles is influenced by advection and diffusion. Advection refers to the horizontal transport of particles driven by ocean and wind currents, which primarily determines the trajectory of the particles. Diffusion describes the spread of particles due to their individual irregular movements. Dispersion, representing the overall trend of particle clusters, increases rapidly over short to intermediate time scales and linearly over larger scales, eventually reaching a constant value (Abernathy et al. 2022; Lacasce and Mahadevan 2006). In this study, the diffusion coefficient are selected based on the model’s resolution and considered as small-scale noise affecting particle movements.

The PTM is implemented through *Parcels*, a tool designed to simulate the trajectories of passive particles. The key components of the model used in this study include the representation of particle motion within an existing flow field based on hydrodynamic data. Specifically, eastward (u) and northward (v) surface velocities are used to simulate horizontal particle motion. Horizontal diffusivity is parametrised by the Kh_zonal and $Kh_meridional$ fields, representing zonal and meridional diffusivity, respectively. The *AdvectionDiffusionEM* kernel, based on the Euler-Maruyama scheme, is used in this study to integrate the particle motion, including both advection and diffusion processes. The equation governing the diffusion component of particle movement is the following:

$$\Delta x_{diff} = \sqrt{2, K_h \cdot \Delta t} \cdot \mathcal{N}(0, 1) \quad (3.3)$$

where Δx_{diff} is the stochastic displacement due to sub-grid scale diffusion, K_h is the local horizontal diffusivity, a combination of Kh_zonal and $Kh_meridional$ from the input data, Δt is the time step and $\mathcal{N}(0, 1)$ is a random value drawn from a standard normal distribution, introducing the stochastic noise. This approach adds a random walk component to the particles, simulating the sub-grid scale diffusion due to small-scale turbulence that cannot be resolved directly by the model’s grid. In addition, the process of subdiffusion, characterised by the sublinear growth of the mean square displacement (Hulianytskyi 2022), is included in the diffusivity term and accounted for within the *Parcels* kernel (Van Sebille et al. 2023). To simplify the analysis, virtual particles without mass are considered. The first step in the analysis is to design a system capable of representing the probability distribution of particles in selected areas. The probability distribution is achieved by constructing a regular grid within the analysis region. Finally, the simulation runs over a defined period of time with a specific time step to simulate real conditions observed in the field.

3.3 Mixing processes

In this section the aim is to provide detailed information on the characteristics and movement of an oil slick.

Once the particles trajectories are obtained through Parcels, the probability density map is constructed. For each time step, the number of particles passing through each grid cell (areal bin) is counted and normalised by dividing by the total number of particles present in the entire domain area. This method evaluates the probability density, calculated by the equation (3.4), resulting in an experimental distribution that reflects the dispersion patterns of the particles:

$$P(x, y, t) = \frac{n(x, y, t)}{N} \quad (3.4)$$

where n is the number of particles present in a single cell, corresponding to a single simulation, and is both space and time dependent. N is the total number of particles released at the beginning of the simulation. This is employed to construct a map of the distinct probability of each model simulation and to determine which area exhibits a higher concentration of particles.

The centroid of each individual cloud of dispersed particles is then calculated as the average of the x and y positions of the particles present in the cloud, at each time step. Specifically, the components of the centroid, $\bar{x}(t)$, $\bar{y}(t)$, are evaluated using Equations (3.5) as follows

$$\bar{x}(t) = \langle x_i(t) \rangle, \quad \bar{y}(t) = \langle y_i(t) \rangle \quad (3.5)$$

where $x_i(t)$ and $y_i(t)$ are the coordinates of the i -nth particle at the time t . From the centroids information the absolute and relative distances can be computed, in order to evaluate the trajectory covered by the simulations. The absolute distance (D_{b0}) represents the displacement of each centroid from its initial position over time (Fig. 3.1a). The relative distance, D_b , is defined as the sum of the individual segments connecting each centroid to the next one.

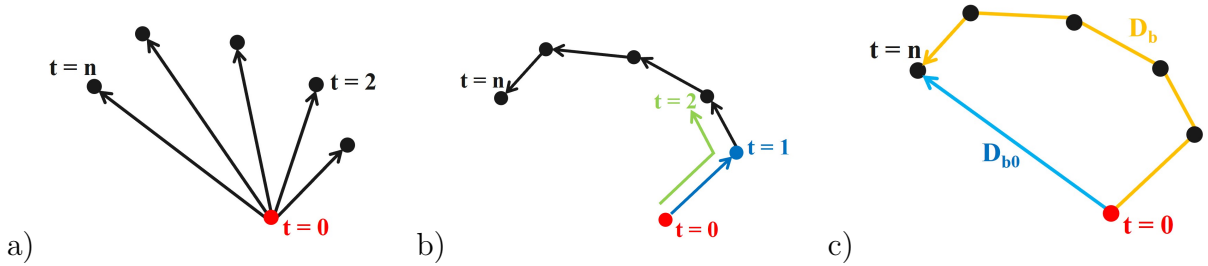


Figure 3.1: a) Absolute distance D_{b0} ; b) Relative distance D_b ; c) Comparison between absolute and relative distance at the final time step.

Consequently, the absolute distance, D_{b0} , is defined following Equation (3.6)

$$D_{b0}(t) = \sqrt{(\bar{x}(t) - \bar{x}(0))^2 + (\bar{y}(t) - \bar{y}(0))^2} \quad (3.6)$$

where $(\bar{x}(t), \bar{y}(t))$ is the position of centroid over time and $(\bar{x}(0), \bar{y}(0))$ is the position of centroid at time zero. The relative distance instead provides the measure of the total path travelled by the centroid up to time t and is represented by Equation (3.7)

$$D_b(t) = \sum_{j=1}^t \sqrt{(\bar{x}(j) - \bar{x}(j-1))^2 + (\bar{y}(j) - \bar{y}(j-1))^2} \quad (3.7)$$

where $\bar{x}(j)$ and $\bar{y}(j)$ are the coordinates of the centroid at time j .

Another mixing property of interest in this study is the overall displacement of the particles, i.e. the degree of dispersion. Specifically, the relative dispersion of the particles with respect to the position of the centroid over time is calculated (Eq. 3.8).

$$R^2(t) = R_x^2(t) + R_y^2(t) \quad (3.8)$$

The two components of Eq. (3.8) are the dispersion in time in the direction of x and in the direction of y , respectively, and are reported in Eq. (3.9)

$$R_x^2(t) = \langle [x_i(t) - \bar{x}(t)]^2 \rangle, \quad R_y^2(t) = \langle [y_i(t) - \bar{y}(t)]^2 \rangle \quad (3.9)$$

where $x_i(t)$ and $y_i(t)$ represent the position of the i -nth particle at time t . $\bar{x}(t)$ and $\bar{y}(t)$ correspond to the position of the centroid of the cluster at each single time t . The relative dispersion will allow to measure quantitatively the spread of the particle cloud, capturing both the magnitude of the dispersion and the directions in which the particles are spreading. It helps to assess the anisotropy of the deformation of the cluster along its trajectory, indicating whether the dispersion is more along certain directions or uniform.

As satellite images are available, an accuracy analysis of the simulations is also conducted by comparing the output obtained with the data recorded by the SAR sensors. To achieve this, the distance in kilometers is evaluated between the centroids of particle dispersion simulations and the centroid of the observed SAR image for the temporal instants available (Eq. 3.10).

$$D_{\text{centroid}} = \sqrt{(\bar{x}(t) - x_{\text{SAR}})^2 + (\bar{y}(t) - y_{\text{SAR}})^2} \quad (3.10)$$

where $(\bar{x}(t), \bar{y}(t))$ are the coordinates of the simulation centroid at the given instant and

$(x_{\text{SAR}}, y_{\text{SAR}})$ are the coordinates of the SAR image centroid. This provide a quantitative measure of spatial agreement between simulated and observed oil spill locations. The

number of simulated particles intersecting the slick detected by Sentinel-1 is also calculated for each of the three time instants.

The ratio N_{in} / N_{tot} , representing the proportion of particles within the SAR slick, is also determined.

$$P_{in} = \frac{N_{in}}{N_{tot}} \times 100 \quad (3.11)$$

where P_{in} represents the percentage of particles, N_{in} is the number of particles inside the SAR image, and N_{tot} is the total number of particles for the specific simulation. This value is expressed as a percentage (Eq. 3.11), and indicates the ability of the simulations to reproduce the observed spill.

It is worth noting that additional quantitative metrics for the satellite-based evaluation of oil spill model outputs have been proposed in the literature. (Keramea et al. 2023) present a comprehensive framework for comparing simulated trajectories with SAR-derived oil spill patterns, including a range of spatial and geometrical indicators. While the present work adopts the centroid distance and the percentage of particles intersecting the observed SAR slick as evaluation metrics, more comprehensive frameworks remain a valuable reference for future model evaluation efforts.

3.4 Bayesian optimization for coefficient calibration

The physical processes responsible for the transport of surface oil and their Lagrangian representation are described in Section 3.2. As outlined, particle advection is driven by a near-surface velocity field, which is the result of the combined effects of ocean currents, Stokes drift caused by waves and wind drag. Following Eq. (3.1), the advective velocity is expressed as a linear combination of these contributions. The dimensionless coefficients, α and β , control the relative impact of Stokes drift and wind forcing.

The wind coefficient β has previously been studied in the literature and is generally assumed to fall within the narrow range of 0.02 and 0.03, based on empirical observations and field experiments (ASCE 1996; Spaulding 2017). Nevertheless, the actual impact of wind force on oil transport is influenced by several factors, including sea state, oil properties, and unresolved turbulence in proximity to the surface. The coefficient α , which governs the contribution of Stokes drift, is less defined, as it depends on the wave spectrum, the vertical distribution of velocities induced by waves, and the depth at which the particles are assumed to move (Bremer and Breivik 2018). Consequently, the contribution of Stokes drift is usually included in its entirety or scaled through a coefficient in practical applications. This reflects the uncertainties in the coupling between waves and particles, as well as the differences in model formulations (Abascal et al. 2009). Therefore, both coefficients are treated as effective parameters rather than as intrinsic physical constants. The previous analyses in this research relied on a sensitivity analysis approach to calibrate

these transport parameters, involving multiple simulations using different values of α and β until satisfactory agreement with observations is achieved. Although this strategy is intuitive, it becomes progressively more challenging with non-linear, computationally demanding Lagrangian particle simulations, particularly when exploring a wide range of parameters is necessary.

In the present case, these methodological limitations are aggravated by the limited and diverse nature of the available observational data. The only information available about the event consists of three satellite images acquired during the initial phase of the spill (Table 4.2), and reports indicating that oil reached the coast of Pampelonne beach in southern France on the morning of 16 October 2018 (CEDRE 2019). Although coast contamination has been confirmed, neither the precise arrival time nor the location of the impact has been documented, given that the affected beach segment extends over several kilometres. Under these conditions, direct calibration of the transport parameters is not easily achieved under these conditions. Therefore, a set of explicit assumptions is introduced to allow the coefficients to be calibrated systematically and reproducibly.

Within this framework, the estimation of α and β is formulated as a Bayesian optimisation problem. Bayesian optimisation is a global optimisation technique that is specifically designed for expensive black-box objective functions, for which gradient information is either unavailable or unreliable. This method uses a probabilistic surrogate model, typically a Gaussian process, to estimate the objective function and quantify uncertainty in unexplored regions of the parameter space. The process of selecting new parameter combinations sequentially is guided by an acquisition function, which balances exploration and exploitation (Shahriari et al. 2016).

The calibration problem (Eq. 3.12) is formulated as

$$(\alpha^*, \beta^*) = \arg \min_{\alpha, \beta} J(\alpha, \beta), \quad (3.12)$$

where $J(\alpha, \beta)$ is an objective function that measures the discrepancy between the simulated oil trajectories and the corresponding observations. As the observational dataset is both limited and varied, it is not possible to rely on a single, simple objective function for calibration. To incorporate the available information into the calibration procedure, a representative impact point is introduced as a substitute for the location where the oil first reached the coast. This point is located at the centre of the affected area of Pampelonne beach. For the long-term calibration, optimisation is performed with respect to a constraint defined by the point of impact on the coast (43°14'94" N, 9°28'47" E) and an associated reference arrival time (16 October 2018 at 09:00). Once the calibration problem is defined, the analysis is organised to examine the behaviour and consistency of the transport coefficients across different spatial and temporal scales. Initially, long-term calibration is achieved by utilising the available information on the final stage of the event: the arrival

of oil on Pampelonne beach’s shoreline. The purpose of the long-term calibration is to estimate the cumulative effect of advection processes that occur over several days. This provides an effective method of determining the transport coefficients that influence the long-term evolution of the spill. Three objective formulations are considered for calibration based on the coast in order to assess the sensitivity of the inferred coefficients to the definition of the shoreline impact. In all formulations, the objective function is constructed as a combination of spatial and temporal discrepancies. In the first formulation, the spatial component is defined as the distance between the centroid of the simulated oil distribution and a reference impact point at the centre of the affected beach. The time component takes into account the time difference between the moment when the arrival of the oil is simulated and is expressed as follows:

$$J_{\text{LT,cent}} = \left(\frac{d_{\text{cent}}}{L_0} \right)^2 + \left(\frac{\Delta t}{T_0} \right)^2 \quad (3.13)$$

where d_{cent} is the distance between the simulated centroid and the coast impact point, and Δt is the temporal mismatch. L_0 and T_0 are characteristic spatial and temporal scales used to normalise the distance and time errors, respectively.

In the second long-time formulation, shoreline impact is defined as the particle–time sample in the simulation that minimises the combined spatial and temporal discrepancy in relation to a reference point and time for impact on the coastline. For each simulation, the difference is calculated for all particle positions and output times. The particle–time sample that minimises this discrepancy is then selected. In this context, a particle–time sample refers to a specific particle position evaluated at a given simulation output time. In this formulation, spatial mismatch is computed as the distance between the simulated particle position and the reference impact point on the shoreline. Meanwhile, temporal displacement is defined as the absolute difference between the simulation time and the reference arrival time. The corresponding objective function is expressed as follows:

$$J_{\text{LT,part}} = \left(\frac{d_{\text{part}}}{L_0} \right)^2 + \left(\frac{\Delta t}{T_0} \right)^2 \quad (3.14)$$

where d_{part} represents the distance between the shoreline impact point and the simulated particle position, and Δt is the absolute temporal discrepancy with respect to the reference time.

In addition to the particle–time formulation described above, a more precise long-time calibration strategy based on the initial arrival of individual particles at the coast impact point is also considered. This alternative formulation explicitly accounts for the early arrival of isolated particles, which may precede the bulk of the oil slick. Here, the shoreline impact is defined as the first simulation time at which at least one Lagrangian particle enters the specified area around the reference impact point. Due to the uncertainty

surrounding the reported impact location and arrival time, the affected area is defined as a circular region with a radius of 2 km centred on the shoreline reference point. While the arrival time is considered acceptable only if it falls within a period of ± 2 h around the reference time (16 October 2018 at 09:00). Both constraints are applied as acceptance criteria rather than as explicit components of the objective function. For admissible first-arrival events, the spatial mismatch is computed as the distance between the impact point and the first-arriving particle. Meanwhile, the temporal discrepancy is defined as the absolute difference between the time of first arrival and the reference time. The objective function has the same non-dimensional form as in Eq. (3.14). Simulations in which no particles reach the prescribed vicinity or in which the first arrival occurs outside the temporal window are excluded from the optimisation process by assigning a large numerical penalty value to the objective function.

The analysis compares the coefficients obtained using these long-time objective functions to evaluate how sensitive the estimated transport parameters are to the chosen coastal impact representation, and whether the resulting estimates remain consistent under different yet plausible definitions. Additionally, the robustness of the Bayesian optimisation procedure for the calibration of the coastline based on the particles-to-point metric is examined by comparing different acquisition functions, such as:

- Expected Improvement (EI),
- Probability of Improvement (PI),
- Lower Confidence Bound (LCB),
- Adaptive strategy (`gp_hedge`).

These acquisition functions represent different exploration-exploitation strategies. EI and PI prioritise regions of the parameter space that are expected to improve upon the current best solution. LCB explicitly balances predicted performance and model uncertainty, while `gp_hedge` dynamically combines multiple strategies during the optimisation process. This comparison enables to assess how sensitive the predicted coefficients are to the choice of acquisition strategy.

The calibration is then repeated on a smaller spatial and temporal scale, incorporating information from three satellite-derived slick observations acquired during the incident's initial phase. In this case, the objective function includes further details on the extent of the observed slicks. For each satellite acquisition, the objective function combines three components: a spatial term based on the distance between the simulated and observed slick centroids, a term accounting for the difference in time between the simulation and observation within a given period and a third term quantifying the number of simulated particles within the observed slick area. For the given satellite observations, the short-term objective function is written as Eq. (3.15):

$$J_{\text{ST}} = \left(\frac{d_{\text{cent}}}{L_0} \right)^2 + \left(\frac{\Delta t}{T_0} \right)^2 + (1 - p_{\text{in}})^2 \quad (3.15)$$

where p_{in} is the fraction of simulated particles detected inside the observed slick area. The total short-term objective function is obtained by adding the contributions of the three satellite acquisitions, selecting for each acquisition the minimum deviation within a predefined time window around the time of observation.

All experiments are performed using the `scikit-optimize` Python library, which employs the `gp_minimize` algorithm. Two stopping criteria are defined in advance for each Bayesian optimisation run: a maximum number of iterations, which limits the computational resources available, and a target value for the objective function corresponding to an acceptable minimum error. Optimisation is stopped as soon as either condition is met. The target value of the objective function is estimated based on predefined physical tolerances, requiring the spatial discrepancy to be below a specified distance threshold and the temporal difference to be within a specific time threshold. These tolerances are converted into a non-dimensional target error using the normalization scales applied to the objective function. This ensures consistency between the stopping criterion and the physical interpretation of the calibration. The sets of coefficients obtained from the long-time and small-time calibrations are then compared to assess their consistency and their agreement with values commonly adopted in the literature.

To better assess the consistency of the transport coefficients inferred through the Bayesian optimization across different temporal scales, an additional set of Lagrangian diagnostics is considered. In particular, the evolution of the absolute Lagrangian dispersion is examined through the mean squared displacement (MSD), defined as

$$a^2(t) = \langle |\mathbf{r}_i(t) - \mathbf{r}_i(t_0)|^2 \rangle \quad (3.16)$$

where $\mathbf{r}_i(t)$ is the position of the i -th particle at time t , and $\langle \cdot \rangle$ represents an ensemble average. The MSD is a classical Lagrangian metric used to quantify the temporal growth of particle-cloud spread and to identify finite-time dispersion regimes. Finite-time scaling behaviours are analysed by fitting local power-law relationships of the form

$$a^2(t) \sim C t^p \quad (3.17)$$

where the exponent p acts as an effective indicator of the rate of dispersion growth over a selected time interval. These exponents are not interpreted as asymptotic turbulence scalings, but rather as empirical descriptors that reflect how the simulated transport responds to the calibrated coefficients within distinct temporal windows. A second diagnostic quantity is the Lagrangian integral time scale T_L , defined as the integral of the velocity autocorrelation function up to its first zero crossing. This time scale represents

the characteristic duration over which particle velocities remain correlated, and therefore provides a reference for distinguishing between short-time (memory-dominated) and long-time (decorrelated) transport behaviour. In addition, a diagnostic transition time T_s is evaluated from the temporal evolution of the local logarithmic slope of $a^2(t)$. This time marks the onset of a reduction in the effective dispersion exponent and signals a change in the finite-time scaling regime. Unlike T_L , the time T_s is not a dynamical invariant of the flow, but an empirical indicator extracted from the simulation. These diagnostic quantities are used in the results section to analyse the scale dependence of the calibration and to investigate the consistency between the transport coefficients inferred from short-time satellite constraints and those derived from long-time shoreline impact information.

3.5 Absolute and relative wind comparison

Wind forcing is one of the main drivers of surface transport in oil spill and floating particle simulations. Its influence manifests both indirectly, through wind-driven ocean circulation and wave generation, and directly, through aerodynamic drag acting on the exposed portion of floating oil or objects (Spaulding 2017). However, operational and research models may include terms induced by the wind using different formulations, and the distinction between atmospheric forcing and motion relative to an object is not always made explicit. In such cases, particular care is required to ensure physical consistency and to avoid potential overestimation of wind-related effects when multiple wind-driven processes are combined (Dagestad and Johannes Röhrs 2019a). This section clarifies the physical meaning of absolute and relative wind and discusses their respective roles in surface oil spill modelling. In many oil spill studies, the transport induced by the wind is parametrized in terms of a wind drag or windage contribution, which implicitly represents the motion of floating oil relative to the surrounding air-sea system. While this approach is physically motivated, different implementations may lead to different representations of wind effects. On this basis, a systematic comparison between simulations using absolute and relative wind formulations is performed, with a specific focus on the resulting differences in model outputs obtained using CMEMS surface currents and MeteOcean-UniGe wind and wave forcing. The use of absolute wind in previous simulations is consistent with common practice in operational oil spill modelling and provides physically meaningful results when combined with wind-driven currents and wave fields. The analysis is structured in three main steps to provide a comprehensive assessment of the impact of the wind formulation. First, a direct comparison is performed between simulations forced by absolute and relative wind. Secondly, the differences are quantified by examining the temporal evolution of the distance between particle cloud centroids in absolute terms and using a non-dimensional metric. These are then evaluated with and without the diffusion term. Finally, a Lagrangian velocity autocorrelation analysis is performed to investigate the

effect of the wind formulation on the temporal structure of particle motion, considering the absolute and relative wind simulations with diffusion.

The absolute wind is defined as the velocity of air relative to a fixed Earth reference frame, Eq. (3.18). It corresponds to the wind provided by atmospheric reanalyses and numerical weather prediction models, both of which estimate the atmospheric flow in an Earth-fixed reference frame, and is typically referenced at 10 m above sea level:

$$\vec{u}_w^{\text{abs}} = \vec{u}_{\text{air/Earth}} \quad (3.18)$$

Absolute wind represents the primary atmospheric forcing acting on the ocean surface and is therefore the appropriate quantity for driving air–sea interaction processes. It is used to compute surface wind stress and to force ocean circulation and wave models, leading to Ekman transport, wind-driven Eulerian currents, and wave generation, as well as the associated Stokes drift (Spaulding 2017). The relative wind, instead, is defined as the velocity of air relative to the moving ocean surface, or, equivalently, relative to the motion of a floating object assumed to be largely advected by the surface current (3.19), (Dagestad and Johannes Röhrs 2019b):

$$\vec{u}_w^{\text{rel}} = \vec{u}_w^{\text{abs}} - \vec{u}_c \quad (3.19)$$

From a physical perspective, the aerodynamic force exerted on floating objects, including oil slicks, surface drifters and marine debris, depends on the velocity difference between the air and the object. This quantity corresponds to the relative wind, defined as the wind velocity with respect to the moving ocean surface. Because the aerodynamic drag acting on floating material is controlled by the relative motion between air and water, the use of relative wind provides a physically consistent representation of the direct wind forcing on surface particles (Lehr et al. 2002).

At the same time, the indirect influence of wind on surface transport arises from the oceanic response to atmospheric forcing. Wind generates wind-driven circulation, wave fields, and the associated Stokes drift, which are typically included in oil spill models through prescribed ocean current and wave-induced drift fields (Ardhuin et al. 2009). These components represent the integrated response of the ocean to the atmospheric forcing and therefore already account for an important fraction of the transport driven by the wind affecting floating material. In addition to these indirect effects, floating oil and surface particles also experience a direct aerodynamic drag due to the portion of the slick exposed to the atmosphere. This contribution is commonly parametrized as a fraction of the wind velocity acting on the particles, Eq. (3.1). In practical applications, the wind term can be expressed either using the absolute wind velocity or the relative wind velocity, depending on the modelling framework and on how the wind-driven ocean response is represented. The use of absolute wind in this formulation is widely adopted in operational

oil spill models and offers a simple method of accounting for direct wind forces acting on floating material. However, since ocean currents and Stokes drift are largely generated by atmospheric forcing, including these components alongside a direct wind term based on absolute wind may result in a partial overlap of effects driven by the wind.

For this reason, some studies have highlighted that the use of relative wind may provide a more physically consistent formulation of the drag term, as it explicitly accounts for the motion of the underlying ocean surface (Dagestad and Johannes Röhrs 2019a). When absolute wind is used together with wind-driven currents and Stokes drift, part of the wind influence may be implicitly counted more than once, potentially leading to an overestimation of particle velocities. This issue may be particularly relevant in semi-enclosed basins such as the Mediterranean Sea, where strong atmospheric forcing and energetic wave conditions can enhance the coupling between wind-driven currents and wave-induced transport (Liubartseva et al. 2018). In light of the conceptual differences and potential inconsistencies outlined, this thesis examines the impact of using absolute versus relative wind in the direct wind drag term of surface particle simulations. The analysis focuses on floating particles constrained to the sea surface, aiming to quantify the effect of the wind reference frame choice on particle trajectories, dispersion patterns and the temporal evolution of spatial metrics such as particle cloud centroids. The effect of the wind drag formulation is isolated by making a controlled comparison in which all model components, including ocean currents and Stokes drift, remain identical and only the reference frame used to compute the direct wind drag term varies. This approach enables the specific impact of absolute versus relative wind formulations to be evaluated, while maintaining the complete coupled representation of wind-driven ocean processes. Surface currents used in this study are Eulerian velocities described in detail in section 3.1.1. These currents represent the resolved surface ocean circulation and include both geostrophic and ageostrophic components. They are therefore used as a substitute for surface water velocity when calculating the effects of relative wind on floating particles.

In addition to the absolute centroid distance expressed in kilometres, a non dimensional measure of the separation is introduced in order to interpret the divergence between the two simulations relative to the spatial scale of the particle cloud itself. While the distance in km provides an operationally meaningful estimate of the offset between the two solutions, it does not account for the concurrent growth of the particle cloud due to dispersion processes. To address this, a normalized separation is defined as

$$d^*(t) = \frac{d(t)}{L_n(t)} \quad (3.20)$$

where $d(t)$ is the distance between the centroids of the absolute and relative wind simulations, and $L_n(t)$ is a characteristic length scale of the particle cloud at time t . The quantity $L_n(t)$ is computed as the mean square root distance of particles from their centroid

and represents the ensemble’s instantaneous spatial extent. This approach allows the robustness of the observed differences between the two wind formulations to be evaluated with respect to the inclusion or exclusion of unresolved-scale diffusion.

In order to isolate the effect of the wind formulation, it is also necessary to consider the role of stochastic diffusion, which is included in all simulations presented so far in addition to the advective terms. This diffusive term is introduced to account for unresolved subgrid-scale processes, such as small-scale turbulence and flow variability, which are not explicitly represented by the resolved velocity fields. The inclusion of stochastic diffusion is a common and widely accepted practice in Lagrangian particle modelling, particularly in oceanographic applications, as it allows for a more realistic spreading of particle clouds (LaCasce 2008). Nevertheless, the use of additional diffusive terms remains a subject of debate in the literature. Several studies have highlighted that, if not carefully calibrated, stochastic diffusion may lead to excessive dispersion, potentially masking physically meaningful differences between model configurations or forcings (Berloff et al. 2002). To assess the influence of the diffusive parametrisation on the results presented in this study, a dedicated comparison is performed between simulations including stochastic diffusion and simulations without diffusion. For consistency, the same analysis framework is adopted in both cases, focusing on the comparison between absolute and relative wind formulations and on the temporal evolution of the distance between the centroids of the simulated particle clouds.

Following the assessment of the impact of absolute and relative wind formulations on particle dispersion, it is evident that the distance between the ensemble centroids remains minimal, with maximum differences amounting to a few kilometres at most. This suggests that the mean advective transport of the oil spill is only weakly affected by the chosen wind formulation. However, diagnoses are primarily sensitive to large-scale, temporally averaged transport, meaning that they can mask differences in the underlying dynamic processes governing particle movement. To further investigate whether the choice of wind forcing formulation affects not only the mean advective transport but also the underlying particle motion dynamics, a Lagrangian velocity autocorrelation analysis is performed on the particle trajectories obtained from the absolute and relative wind simulations, considering the diffusion. This approach enables the characterisation of the temporal persistence of velocity fluctuations along particle trajectories, providing insight into the transition from locally coherent motion to effectively decorrelated transport (LaCasce 2008). The Lagrangian velocities are calculated for each particle trajectory from the successive positions of the particles, and are decomposed into fluctuating components by removing the ensemble’s average velocity at each time interval. This decomposition isolates the stochastic component of the motion associated with turbulent and fluctuations induced by the wind, thereby eliminating the contribution of large-scale mean advection (Sawford and Guest 1991). The autocorrelation of the Lagrangian velocity is then estimated

by considering the diagonal components of the Lagrangian velocity correlation tensor. Assuming statistical stationarity of velocity fluctuations, the normalised autocorrelation function is presented in the following equation 3.21

$$R_{ii}^L(\tau) = \frac{\langle u'_i(t) u'_i(t + \tau) \rangle}{\langle u'^2 \rangle}, \quad i = x, y \quad (3.21)$$

where u'_i is the fluctuating velocity component in the zonal (x) or meridional (y) direction, τ is the time lag, and brackets indicate an ensemble average over particles. Only the diagonal terms of the correlation tensor are considered, as the focus of this analysis is on the temporal persistence of velocity fluctuations along each coordinate direction. The autocorrelation functions are computed separately for the zonal and meridional components and subsequently averaged over all particle trajectories to obtain ensemble-mean estimates of $R_{xx}^L(\tau)$ and $R_{yy}^L(\tau)$.

The Lagrangian decorrelation time scale T_L is computed as the time integral of the autocorrelation function (Eq. 3.22),

$$T_L = \int_0^\infty R_{ii}^L(\tau) d\tau, \quad (3.22)$$

which is evaluated up to the first zero crossing of $R_{ii}^L(\tau)$ in order to minimize the influence of noise at large time lags (LaCasce 2008).

3.6 Oil weathering processes

Until now, the dispersion of oil spills is been modelled by treating oil particles as passive Lagrangian tracers, advected by ocean currents, wind-induced drift, and wave-driven Stokes transport. This simplified approach allows the hydrodynamic contribution to the spill evolution to be isolated and quantified, providing a reference scenario against which additional processes can be evaluated. However, such an approach neglects the intrinsic time-dependent evolution of oil properties once released into the marine environment. In reality, the physical properties and transport behaviour of oil particles are modified by their rapid compositional and rheological changes (Spaulding 2017).

Following a spill, oil undergoes a series of physical and chemical transformations collectively known as weathering (Fig. 3.2).

These processes include evaporation, emulsification, spreading, photo-oxidation, and biodegradation (Keramea et al. 2021). During the first hours to days after release, evaporation and emulsification typically dominate the evolution of oil properties. Evaporation preferentially removes lighter and more volatile fractions, leading to a reduction in mass and an increase in viscosity (Mishra and G. S. Kumar 2015). Emulsification promotes the incorporation of water droplets into the oil phase, altering its rheological behaviour

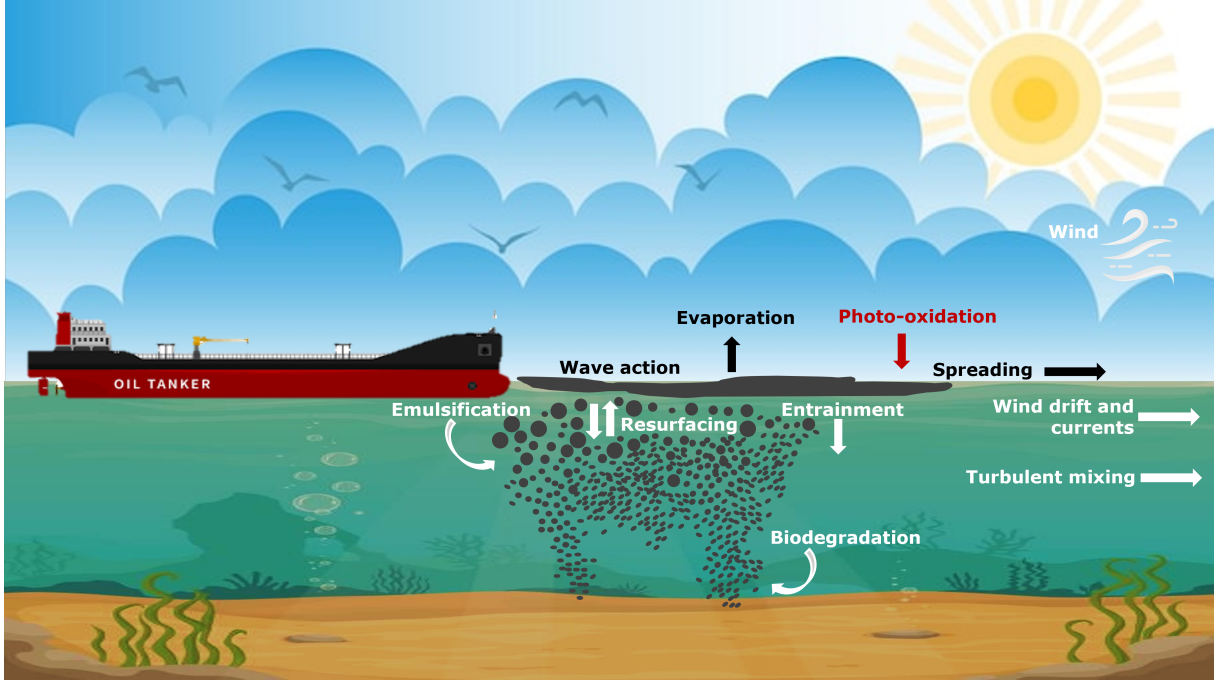


Figure 3.2: Schematic representation of the weathering processes that oil undergoes after spillage.

and increasing its effective viscosity and density (Spaulding 2017). Nonetheless, for simulations lasting to ten days or more, longer-term processes such as photo-oxidation and biodegradation can also contribute to the progressive transformation of the oil composition and persistence in the marine environment (Brakstad et al. 2015; Ward et al. 2018). Although these processes generally act on slower timescales compared to evaporation, they may affect oil weathering pathways and residual mass in multi-day simulations. These weathering processes have a cumulative effect on key oil properties such as mass, viscosity, density, interfacial tension and droplet size distribution, modifying them over time. These changes directly impact vertical transport mechanisms, such as entrainment by breaking waves, buoyancy-driven resurfacing and turbulent mixing (J. Röhrs et al. 2018). Therefore, weathering not only alters the internal state of the oil, but also indirectly influences horizontal dispersion by modifying the vertical distribution of droplets and their exposure to depth-dependent current velocities and wind forcing.

In this study, weathering is explicitly incorporated within the Lagrangian modelling framework using the Parcels toolbox, where oil weathering is resolved at the particle level through a modular set of Lagrangian kernels. Each particle carries its own evolving physicochemical properties, including mass, density, viscosity, water fraction, interfacial area, diameter, and compositional cuts, which are dynamically updated at every time step. Compared to simplified bulk formulations frequently adopted in operational models (Lehr et al. 2002), the present implementation resolves weathering processes at a finer level of detail. In particular, evaporation is represented through a multi-cut pseudo-component scheme

in which individual distillation fractions experience vapour-pressure-dependent mass loss, allowing the compositional evolution of the oil to be explicitly tracked. Wave-induced entrainment is modulated by the evolving viscosity of the oil, thereby introducing a feedback between rheological changes and vertical mixing efficiency. The onset of emulsification is not prescribed a priori but is dynamically linked to both the degree of evaporation and viscosity thresholds, ensuring a physically consistent transition toward water-in-oil emulsion formation. Furthermore, droplet diameters are stochastically resampled during wave-breaking events to reproduce a dynamically evolving droplet size distribution, while cumulative photo-oxidative exposure is tracked to account for progressive surface weathering effects over multi-day simulations. The governing mathematical formulations and parametrisations associated with each of these processes are presented in detail in the following sections.

The implementation follows a modular approach. First, a dedicated particle class is defined to include the relevant physicochemical properties of the oil, with separate parameter sets for a light crude oil and a heavy fuel oil. These properties include initial density, viscosity, mass, and additional parameters required by the weathering formulations. The oil-specific properties are obtained from the NOAA ADIOS (Automated Data Inquiry for Oil Spills) database, which provides standardised physicochemical and compositional information for a wide range of petroleum products. In particular, the light crude oil corresponds to the Saharan Blend (AD02316), while the heavy oil is represented by Albion Heavy Synthetic (EC01172). A summary of the key physicochemical properties adopted for each oil type is provided in Table 3.2. The selected light oil has a lower density and significantly lower viscosity than the heavy oil, meaning it will behave very differently during weathering processes. In addition, different droplet size ranges are considered for the two oil types, reflecting their distinct properties. The light oil is more susceptible to fragmentation under wave breaking due to its smaller diameter ranges, whereas the heavy oil’s larger diameter ranges are due to its higher viscosity and resistance to breakup (Johansen et al. 2013). Consequently, the particles are not all the same size. Each Lagrangian element is assigned an individual droplet diameter, which is sampled from a lognormal distribution. This approach ensures that diameters remain within physically consistent limits while preserving statistical variability. Furthermore, during stochastic entrainment events induced by wave breaking, the diameters of the droplets are resampled according to the same oil-dependent distribution. This allows for a heterogeneous and dynamically evolving representation of the submerged oil.

Oil type	Density [kg/m ³]	Viscosity [Pa · s]	Diameter [µm]
Saharan Blend	807.8	0.004	10.0-500.0
Albian Heavy Synthetic	937.0	0.160	100.0-1000.0

Table 3.2: Characteristic properties of light and heavy oil.

Subsequently, a series of dedicated kernels are introduced to represent individual weathering processes, such as evaporation, emulsification, photo-oxidation, and biodegradation, which dynamically update particle properties at each time step. The mathematical formulations and parametrisations adopted for each process are presented in detail in the following sections.

The objective is therefore to quantify the impact of explicitly resolved weathering processes on simulated oil spill dispersion. This is achieved through a systematic comparison between simulations performed with and without weathering parametrizations, and by analysing the contrasting behaviour of light and heavy oils. Particular attention is given to the relationship between changes in oil properties and vertical transport processes, and to the effect of these mechanisms on the spatial spread and accuracy of forecasts in the days following a spill.

The interaction between evaporation, emulsification, viscosity growth, density increase, entrainment suppression and buoyancy-driven resurfacing creates a highly non-linear feedback system. Changes in oil composition modify rheological properties, which regulate droplet breakup, entrainment probability, and vertical redistribution. Consequently, weathering not only alters the mass of the oil, but also dynamically controls the vertical structure of the spill and its interaction with depth-dependent hydrodynamic forces. Light oils typically undergo rapid evaporation in the early stages while maintaining relatively low viscosities, favouring droplet fragmentation and enhanced vertical exchange shortly after release. In contrast, heavier oils exhibit limited evaporation, but stronger viscosity growth and higher emulsification potential. The resulting increase in density and viscosity suppresses entrainment efficiency, promoting thicker slick formation and prolonged surface persistence. The explicit, particle-resolved representation adopted in this study allows us to quantify directly how evolving physicochemical properties modulate vertical distribution and consequently influence horizontal dispersion forecasts.

Despite its physical basis, the weathering model relies on empirical parametrisations and simplified representations of oil chemistry. In particular, the pseudo-component approach neglects interactions between components and assumes homogeneous oil properties within each particle. Furthermore, direct validation is not possible in this case because information on the weathering processes during the event is unavailable.

3.6.1 Horizontal Transport Framework

The horizontal transport of oil particles in the current weathering configuration is based on the previously described hydrodynamic framework. Advection is driven by ocean currents, wind-induced drift and wave-induced Stokes transport. These factors determine the large-scale displacement of surface and subsurface particles. This current, wind and wave formulation provides the transport model's baseline dynamical structure and governs the

horizontal displacement of particles at every time step. The weathering processes introduced in this chapter do not modify the hydrodynamic forcing directly, but rather influence horizontal dispersion indirectly by altering the vertical distribution, buoyancy, entrainment frequency and droplet size. Consequently, changes in the physicochemical properties of the oil feed back into horizontal transport through depth-dependent current shear and wave-induced velocity profiles. The following sections therefore describe additional processes that interact with the horizontal advection framework previously defined.

3.6.2 Evaporation

Evaporation is typically the primary weathering process in the initial hours following an oil spill, especially for light and medium crude oils (Fingas 2011). The process involves the preferential volatilisation of low-molecular-weight, high-vapour-pressure hydrocarbons from the oil slick into the atmosphere. This process is governed by thermodynamic equilibrium at the oil–air interface, as well as by mass transfer across the atmospheric boundary layer. Transfer rates are strongly influenced by factors such as wind speed, temperature, oil composition and slick thickness (Keramea et al. 2021). As the more volatile fractions are removed, the residual oil becomes increasingly enriched with heavier compounds. This leads to an increase in viscosity and density over time (Mishra and G. S. Kumar 2015).

Since crude oil is a complex, multi-component mixture, evaporation cannot be accurately represented as a single process of overall mass loss. Instead, a compositional approach is necessary to account for the differential volatility of its constituents. In the present model, evaporation is modelled using a pseudo-component formulation based on distillation cuts, which is consistent with thermodynamic models of atmospheric alteration such as ADIOS (Lehr et al. 2002). The oil is divided into N pseudo-components, each corresponding to a range of boiling points. Each component is characterised by an initial mass m_i , a molecular weight MW_i , and a vapour pressure $P_{vap,i}$. This simplified model maintains the volatility spectrum of oil while remaining computationally efficient, allowing the compositional evolution of the slick over time to be solved explicitly.

The evaporation rate of each pseudo-component is derived from a mass transfer formulation based on boundary layer theory (Stiver and Mackay 1984). Assuming local thermodynamic equilibrium at the oil–air interface and wind-controlled transport through the atmospheric boundary layer, the mass loss of component i is expressed in Eq. 3.23.

$$\frac{dm_i}{dt} = - \frac{AKP_{vap,i}}{RT_w} \frac{m_i/MW_i}{\sum_j m_j/MW_j} \quad (3.23)$$

where A is the area of the smooth surface, K is the mass transfer coefficient, $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$ is the universal gas constant, and T_w is the sea surface temperature. The molar fraction term ensures that the contribution of each pseudo-component to the total evaporative flux is modulated by its relative abundance, thus preserving compositional

consistency.

The mass transfer coefficient K is parametrised as a function of the 10 m wind speed U_{10} following a gradual transition between weak and strong wind regimes:

$$K_{\text{low}} = 0.0025 U_{10}^{0.78}, \quad K_{\text{high}} = 0.06 U_{10}^2 \quad (3.24)$$

and

$$K(U_{10}) = \begin{cases} K_{\text{low}}, & U_{10} \leq U_1 \\ (1-s) K_{\text{low}} + s K_{\text{high}}, & U_1 < U_{10} < U_2 \\ K_{\text{high}}, & U_{10} \geq U_2 \end{cases} \quad (3.25)$$

where

$$s = \xi^2(3 - 2\xi), \quad \xi = \frac{U_{10} - U_1}{U_2 - U_1} \quad (3.26)$$

with $U_1 = 6\text{ms}^{-1}$ and $U_2 = 14\text{ms}^{-1}$, while ξ is a normalised wind-speed variable in the interval $[0, 1]$ and s is a cubic smooth step interpolation function ensuring a continuous transition between the two wind regimes. This scaling reflects the increased turbulent transfer that occurs at higher wind speeds, and it captures the transition towards wave-enhanced evaporation in energetic conditions (Stiver and Mackay 1984). The cumulative evaporated fraction is then computed as

$$E(t) = 1 - \frac{\sum_i m_i(t)}{\sum_i m_i(0)} \quad (3.27)$$

Unlike in bulk evaporation formulations, the current implementation updates the mass of each component individually at each time step. This prevents volatile fractions from being instantly and artificially removed, while providing consistent feedback on the evolution of density and viscosity, which depend explicitly on the composition of the oil mixture as it changes. Finally, evaporation is constrained by an oil-dependent maximum evaporative fraction E_{max} , reflecting compositional limits observed experimentally for different crude types (Fingas 2011). Specifically, E_{max} is set to 0.45 for the light oil (Saharan Blend) and 0.12 for the heavy oil (Albian Heavy). This constraint stops the mass from decreasing too much once the volatile fraction has been consumed.

3.6.3 Emulsification

Emulsification is the process by which seawater is incorporated into the oil phase to form a water-in-oil emulsion. Under the action of waves and turbulence, water droplets become trapped in the oil matrix and are stabilised by natural surfactants such as resins and asphaltenes. This process can substantially alter the physical properties of the slick, resulting in an increase in volume, density and, above all, viscosity. It often leads to the formation of persistent mousse-like structures. Emulsification is therefore one of the

dominant alteration mechanisms controlling the persistence of oil at sea (Lehr et al. 2002).

In this model, water absorption is represented using a first-order kinetic formulation that describes the relaxation of the volumetric water fraction W towards a maximum value dependent on oil $W_{\max}$:

$$\frac{dW}{dt} = k_{\text{emul}}(W_{\max} - W) \quad (3.28)$$

where $W_{\max}$ represents the maximum stable water content possible for a given type of oil, set to 0.70 for the light oil and 0.89 for the heavy oil. This formulation is consistent with operational ageing models, in which emulsification is considered a relaxation process limited by the intensity of the mixing process and the properties of the oil. (Fingas 2011; Lehr et al. 2002).

The kinetic coefficient k_{emul} depends on the mixing caused by the wind and the viscosity of the oil and is expressed as

$$k_{\text{emul}} = \frac{F_{\text{bw}}(U_{10})}{\tau_{\text{emul}}} \left(\frac{\nu_{\text{ref}}}{\nu} \right)^\alpha \quad (3.29)$$

where $F_{\text{bw}}(U_{10})$ is a proxy for wind-dependent breaking waves, τ_{emul} is an oil-specific emulsification time scale set to 2.0 days for both oil types, ν is the evolving kinematic viscosity of the oil, $\nu_{\text{ref}} = 5.0 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ is a reference viscosity, and α is an empirical exponent set to 1.6 for the light oil and 2.2 for the heavy oil. This structure reflects the increase in water incorporation in the presence of stronger wind and the slowdown associated with increased viscosity. The breaking wave proxy F_{bw} is defined as:

$$F_{\text{bw}}(U_{10}) = \max(0, \min(0.03(U_{10} - 5), 0.3)) \quad (3.30)$$

and is set to zero for $U_{10} \leq 5 \text{ m s}^{-1}$. The coefficient 0.03 and the upper bound of 0.3 are empirical values adopted to ensure physically plausible emulsification rates across the range of wind conditions encountered in the simulation. The density of oil evolves according to a volumetric mixing rule:

$$\rho_{\text{oil}} = (1 - W)\rho_{\text{oil},0} + W\rho_w \quad (3.31)$$

where $\rho_{\text{oil},0}$ is the initial density of the oil and ρ_w is the density of seawater. The maximum achievable water fraction $W_{\max}$ depends on the composition of the oil and reflects compositional controls such as resin and asphaltene content, which determine the stability of the emulsion. Light crude oils typically achieve lower equilibrium water contents than heavier crude oils (Fingas 2011). In addition to changing the density, emulsification significantly increases viscosity, reducing wave-induced entrainment efficiency and introducing feedback between atmospheric disturbance and hydrodynamic response (see Section 3.6.7).

3.6.4 Spreading

Surface spreading is the term used to describe the lateral expansion of an oil slick immediately after its release, due to the action of gravitational forces on a layer of buoyant fluid over denser seawater. This process is driven by the difference in density between the oil and the water, but is resisted by viscous stresses and interfacial tension. Classical spreading theory identifies two distinct regimes: gravity–inertia and gravity–viscous (Fay 1971). The spreading process is applied to particles located at the surface, following an analytical formulation derived from the axisymmetric scaling laws proposed by Fay (1971). The evolution depends on the relative buoyancy

$$B = \frac{\rho_w - \rho_{oil}}{\rho_w} \quad (3.32)$$

where $\rho_w = 1025 \text{ kg m}^{-3}$ is the density of seawater and ρ_{oil} is the evolving oil density, set to 807.8 kg m^{-3} for the light oil (Saharan Blend) and 937.0 kg m^{-3} for the heavy oil (Albian Heavy) at the time of release. This represents the reduced gravity effect $g' = gB$, and on the initial released volume V_0 . A transition time scale t_0 separates the early gravity–inertia regime from the later gravity–viscous regime:

$$t_0 = \left(\frac{C_t V_0}{\nu_w g B} \right)^{1/3}, \quad C_t = \left(\frac{1.21}{1.53} \right)^4 \quad (3.33)$$

where $\nu_w = 1.0 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ is the kinematic viscosity of water, g is gravitational acceleration and V_0 is the initial volume per particle, computed as the ratio of the initial particle mass to the oil density, yielding $V_0 = 1.24 \text{ m}^3$ for the light oil and $V_0 = 1.07 \text{ m}^3$ for the heavy oil. The dimensionless constant C_t is obtained from the axisymmetric spreading coefficients reported by Fay (1971), through algebraic matching of the gravity–inertia and gravity–viscous regimes. For $t < t_0$, the slick area follows the gravity–inertia scaling:

$$A = C_{GI} \left(\frac{V_0^5 g B}{\nu_w} \right)^{1/6}, \quad C_{GI} = \frac{\pi 1.21^4}{1.53^2} \quad (3.34)$$

where the prefactor C_{GI} is constructed from the axisymmetric inertial spreading coefficient reported by Fay (1971), combined with the geometric relation $A = \pi R^2$. For $t > t_0$, the gravity–viscous regime dominates and the area evolves as

$$A = C_{GV} \left(\frac{V_0^2 g B}{\sqrt{\nu_w}} \right)^{1/3} t^{-1/2}, \quad C_{GV} = \pi 1.45^2 \quad (3.35)$$

where C_{GV} is analogously derived from the axisymmetric gravity–viscous spreading coefficient given by Fay (1971). A maximum spreading area, $A_{\max}$, is imposed as a model constraint to prevent expansion becoming unrealistic over prolonged simulation times. Specifically, $A_{\max}$ is set to $1.0 \times 10^5 \text{ m}^2$ for the light oil and $7.0 \times 10^4 \text{ m}^2$ for the heavy

oil, reflecting the distinct initial contrasts of the two oil types. Since oil density evolves dynamically through evaporation and emulsification, the relative buoyancy varies over time, creating a feedback loop between weathering and lateral spreading. Consequently, oils experiencing stronger density changes may exhibit modified spreading behaviour over time.

3.6.5 Photo-Oxidation

Photo-oxidation is the process by which petroleum hydrocarbons are transformed by solar radiation, particularly within the ultraviolet and visible light spectrum. Significant photochemical changes to floating oil have been seen in the lab and in the field. These changes can happen in a matter of hours or days when the oil is exposed to sunlight (Ward et al. 2018). These transformations lead to the incorporation of oxygen into hydrocarbon molecules, thereby increasing their polarity, density and viscosity. Photo-oxidation is modelled as a process whose rate is proportional to the quantity of oil present:

$$\frac{dm}{dt} = -k_{\text{photo}} m \quad (3.36)$$

where k_{photo} is an effective photo-oxidation rate constant, parameterised through a characteristic time scale τ_{ox} as $k_{\text{photo}} = I(z, t)/\tau_{ox}$, with $\tau_{ox} = 12$ days for the light oil and $\tau_{ox} = 20$ days for the heavy oil. As photochemical reaction rates depend on the amount of available light, the rate constant is assumed to be proportional to local light intensity:

$$k_{\text{photo}}(z, t) = \alpha I(z, t) \quad (3.37)$$

where α is an empirical photoreactivity coefficient and $I(z, t)$ is the irradiance at depth z and time t . The attenuation of light in seawater is described by Beer-Lambert's law:

$$I(z, t) = I_0(t) e^{-k_d z} \quad (3.38)$$

where $I_0(t)$ is the surface irradiance considered active between 06:00 and 18:00 local time and $k_d = 2.0 \text{ m}^{-1}$ is the diffuse attenuation coefficient, corresponding to a light penetration depth of 0.5 m representative of coastal Mediterranean conditions. Integration of Eq. 3.36 yields

$$m(t) = m_0 \exp \left(- \int_0^t k_{\text{photo}}(z, \tau) d\tau \right) \quad (3.39)$$

which shows that oil transformation depends on the cumulative light exposure, in line with laboratory observations of dose-dependent photo-oxidation (Ward et al. 2018). Photo-oxidation is activated after an initial delay of 48 hours with a gradual 24-hour activation ramp, and is applied only to particles located within 1 m of the surface.

3.6.6 Biodegradation

Biodegradation is the process by which naturally occurring marine microorganisms transform hydrocarbons. Oil components can be metabolised by specific bacterial communities as sources of carbon and energy, with the resultant biomass, carbon dioxide and intermediate oxidation products being produced. The rate at which this process occurs depends on various environmental factors, such as temperature, nutrient availability, oxygen concentration and oil composition. Lighter and more bioavailable hydrocarbons are generally degraded more rapidly than heavier, more complex fractions, such as resins and asphaltenes, which are more resistant to microbial attack (Prince and Clark 2004). Biodegradation is represented by a simplified first-order decay formulation that is applied to the remaining oil mass:

$$\frac{dm}{dt} = -k_{bio} m, \quad (3.40)$$

where k_{bio} is the effective biodegradation rate constant. In the present implementation, k_{bio} is specified by a constant half-life $t_{1/2}$, such that

$$k_{bio} = \frac{\ln 2}{t_{1/2}}, \quad (3.41)$$

with $t_{1/2} = 30$ days. This choice provides a simple representation of biodegradation that is consistent with the time scales reported in laboratory and field studies under typical marine conditions (Brakstad et al. 2018). Biodegradation generally occurs more slowly than evaporation and emulsification. This is in the days immediately following an oil spill. However, it becomes increasingly relevant over multi-week to monthly timescales. Therefore, while its contribution is limited in short-term simulations (7–14 days), it facilitates the long-term removal of oil from the system in a consistent manner.

3.6.7 Droplet entrainment

Entrainment is the process by which surface oil droplets are injected into the water column due to wave breaking and turbulent shear. When breaking waves collapse, they generate strong local turbulence and shear stresses that can overcome the forces of interfacial tension and buoyancy, fragmenting the surface slick into droplets that are then transported below the surface. The efficiency of this process depends on the balance between inertial, viscous, and interfacial forces, and is therefore commonly described using dimensionless numbers such as the Weber and Ohnesorge numbers (Li et al. 2017). The Ohnesorge number expresses the ratio between viscous and interfacial forces:

$$Oh = \frac{\mu_{oil}}{\sqrt{\rho_{oil}\sigma d}} \quad (3.42)$$

where μ_{oil} is the dynamic viscosity, ρ_{oil} is oil density, σ interfacial tension, set to 0.0205 N m^{-1} for the light oil and 0.030 N m^{-1} for the heavy oil, and d droplet diameter. While the Weber number represents the ratio between inertial forces associated with wave motion and interfacial tension:

$$We = \frac{\rho_w g H_s d}{\sigma} \quad (3.43)$$

where ρ_w water density, g gravitational acceleration, H_s significant wave height, d droplet diameter and σ interfacial tension. Following semi-empirical formulations derived from laboratory and field experiments, the entrainment rate is expressed as (Reed et al. 2009):

$$Q = 4.604 \times 10^{-10} We^{1.805} Oh^{-1.023} F_{bw} \quad (3.44)$$

where F_{bw} is the fraction of breaking waves, defined as in Eq. 3.30. The probability of entrainment over a time step Δt is then:

$$P = 1 - e^{-Q\Delta t} \quad (3.45)$$

To account for the strong suppression of droplet formation at high viscosities, the entrainment rate may be further reduced by a viscosity-dependent correction factor:

$$Q^* = Q \left(\frac{\nu_{ref}}{\nu_{oil}} \right)^\alpha \quad (3.46)$$

where $\nu_{ref} = 5.0 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ is a reference viscosity, ν_{oil} is the dynamic viscosity, and $\alpha = 0.40$ is an empirical exponent reflecting experimentally observed viscosity thresholds for droplet breakup. Upon entrainment, droplet diameters are resampled at random from a distribution specific to the type of oil, allowing representation of dynamically evolving droplet size spectra. Additionally, a cool-down counter prevents unrealistic repeated entrainment events within successive time steps, ensuring physically consistent stochastic behaviour.

3.6.8 Buoyancy-driven resurfacing

Buoyancy-driven resurfacing describes the vertical motion of submerged oil droplets caused by the density contrast between oil and seawater. Once entrained below the surface, droplets experience an upward (or, in the limiting case of negatively buoyant droplets, downward) buoyant forcing that competes with turbulent mixing and downward advection (Boufadel et al. 2023). In the present model, the terminal vertical velocity is computed from Stokes' law in the low Reynolds number regime for small, approximately spherical droplets (Zhao et al. 2015):

$$w_{rise} = \frac{2g}{9\nu_w} \left(1 - \frac{\rho_{oil}}{\rho_w}\right) r^2 \quad (3.47)$$

where g is gravitational acceleration, $\nu_w = 1.0 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ is the kinematic viscosity of seawater, ρ_{oil} and ρ_w are oil and seawater densities, respectively, and r is the droplet radius. When $\rho_{oil} < \rho_w$, the buoyancy term is positive and droplets tend to resurface unless retained by turbulent mixing and when $\rho_{oil} \geq \rho_w$, the same formulation predicts neutral buoyancy or sinking. To account for departures from creeping-flow conditions, the model evaluates the Reynolds number based on the Stokes velocity and, for sufficiently large buoyant droplets (here $Re > 50$), switches to a higher-Reynolds drag scaling.

Since ρ_{oil} and droplet diameter evolve dynamically through weathering processes such as evaporation and emulsification, the buoyancy contrast and size distribution vary over time. Consequently, resurfacing becomes fully time-dependent and directly linked to the physicochemical evolution of the oil.

3.6.9 Turbulent Mixing

Turbulent mixing describes the vertical redistribution of submerged oil droplets caused by turbulence generated by wind forcing, wave breaking, and shear-driven instabilities in the upper ocean. In the near-surface layer, turbulent kinetic energy enhances vertical dispersion, counteracting buoyancy-driven resurfacing and promoting intermittent subsurface transport (Tkalic and Chan 2002). In the present model, vertical turbulent mixing is represented through a K-profile parametrization, in which the eddy diffusivity varies with depth inside the mixed layer. Within the mixed layer, the local vertical diffusivity is expressed as

$$K_z(z) = K_z^0 z^* (1 - z^*)^2 \quad (3.48)$$

where K_z^0 is a reference vertical diffusivity coefficient provided by the hydrodynamic forcing and z^* is a non-dimensional vertical coordinate normalised by the mixed-layer depth.

$$z^* = \frac{z + z_0}{MLD + z_0} \quad (3.49)$$

MLD is the mixed-layer depth, and z_0 is a surface roughness length scale derived from wind speed and wave age, with a default wave age of $\chi = 35$ adopted in the absence of explicit information, representative of fully developed sea conditions. This formulation ensures that diffusivity decreases smoothly at both the surface and the base of the mixed layer. The vertical displacement over a time step Δt follows a stochastic differential formulation consistent with depth-dependent Fickian diffusion and the correction proposed by Visser (1997):

$$\Delta z = \frac{\partial K_z}{\partial z} \Delta t + \mathcal{R} \sqrt{2K_z \Delta t} \quad (3.50)$$

where $\mathcal{R}$ is a random variable drawn from a bounded uniform distribution in the interval $[-1, 1]$ and $\partial K_z / \partial z$ is the gradient of the diffusivity profile. The deterministic correction term prevents spurious drift when the diffusivity varies with depth. Turbulent mixing continuously acts on submerged droplets, competing with buoyancy-driven resurfacing. As the size and density of the droplets evolve dynamically through weathering, the balance between turbulent retention and buoyant rise becomes dependent on time and oil type.

3.7 Case study: The 2018 Capo Corso Oil Spill

A real-case scenario is analysed to validate the proposed methodology. The selected case study is the collision that occurred on October 7, 2018, at 07:00 UTC between two vessels off the coast of Corsica in the Northern Tyrrhenian Sea (Mediterranean Sea), as shown in Figure 3.3.



Figure 3.3: Left panel: Geographic location of the collision site ($43^{\circ}14'94''$ N, $9^{\circ}28'47''$ E). Top right panel: Depiction of the ship collision at the moment of impact (REMPEC 2019). Bottom right panel: Evidence of hydrocarbon contamination observed on the shore of Pampelonne Beach, France, following the collision (CEDRE 2019).

At the time of the collision, the weather conditions were optimal with perfect visibility (10-m wind speed under 2 m/s). The collision occurred in French waters, 30 km north-east

of Cap Corse. The two vessels involved were the ro-ro ferry *Ulysses*, owned by a Tunisian company, and the container vessel *CLS Virginia*, owned by Cyprus Sea Lines, which was at anchor. The impact caused a spill of six hundred tonnes of fuel from the hull over a distance of about 20 kilometres. Despite the monitoring and clean-up operations carried out by the Coast Guard, the oil slick was carried by the currents for many kilometres in the Ligurian Sea, westwards towards the French coast. A few days later, on the morning of the 16th of October, hydrocarbons from the accident were detected on the beach at Pampelonne, near Saint-Tropez (CEDRE 2019). The area affected by the incident is part of an area with an extremely fragile ecosystem of great environmental interest, specifically the Pelagos Sanctuary, which is recognized for its significant biodiversity and the presence of various marine mammals (Fossi et al. 2013). For validation and calibration, the following reliable sources are used: satellite imagery from Sentinel-1 SAR sensors captured during the first three days after the incident, and multiple reports of hydrocarbon beaching along the French coastline. The first confirmed observation was recorded on October 16 at Pamplonne Beach near Saint-Tropez, with subsequent detections reported in surrounding areas in the following days.

Chapter 4

Results

Note

Part of this chapter presents some of the results that have been published on:
Scotto, B. M., Lira Loarca, A., Novellino, A., and Besio, G. (2025). "Dispersion monitoring services in the Mediterranean Sea: A multi-model statistical approach". *Marine Pollution Bulletin*, Volume 222, Part 2, 2026, 118574. ISSN: 0025-326X. DOI: <https://doi.org/10.1016/j.marpolbul.2025.118574>

The first stage of the work is focused on analysing the role of the horizontal motion of the ocean in particles dispersion by carrying out simulations of a scenario driven solely by sea surface currents ($\vec{u}_c$) for all three ocean circulation models described in §3.1.1 and performed an in-depth comparison of the different behaviour for the different models. These results are presented in §4.1. The second step and scenario takes a more comprehensive approach, incorporating all relevant forcings: sea surface currents ($\vec{u}_c$), wind fields at 10-meter height ($\vec{u}_w$), and Stokes drift ($\vec{u}_s$). Wind and wave data are obtained from the MeteOcean-UniGe and ERA5 datasets, as detailed in §3.1.2. This resulted in six different simulations, combining the three current models (CMEMS, SHOM, and IFREMER) with the two wind-wave models (ERA5 and MeteOcean-UniGe) whose results are presented in §4.2. Section §4.3 presents the analysis of Lagrangian mixing properties, including the relative and absolute dispersion metrics, the centroid evolution, and the spreading of the particle cloud under different forcing configurations.

For all the simulations described above, the setup is simplified by assuming an instantaneous dispersion, rather than a gradual and continuous release as would occur in a real event. This assumption is made because no information is available regarding the temporal evolution of the release itself. Nevertheless, §4.4 investigates a scenario with a gradual release of pollutants based on empirical assumptions.

Given the different possible formulations of wind forcing in Lagrangian transport models, a comparative analysis is carried out for simulations forced by absolute and

relative wind with the results presented in §4.6. Finally, Section 4.7 presents the impact of oil weathering processes on particle dynamics, including changes in mass, viscosity and vertical distribution, and how these changes influence transport and dispersion patterns.

All simulations are carried out using the same consistent framework and configuration. Each model run began at 7th October 2018 at 07:00 UTC, from the same release location at 43°14'94"N, 9°28'47"E, with 800 particles released instantly and a simulation duration of 13 days.

4.1 Oil spill dispersion forced by surface currents alone

Figure 4.1 shows the temporal evolution of the oil spill and the probability density map (Eq. 3.4) for the simulations forced with the three ocean circulation models: CMEMS (blue), SHOM (green) and IFREMER (orange). At the initial stages, the concentration is at its highest due to the instantaneous release from the source. However, the values remain relatively low because the particles are initially distributed over a large area, spanning more than one grid cell, as estimated using the first available satellite images. Over time, this concentration decreases significantly as the particles disperse over a larger area. The significance of this study lies in identifying the areas with the highest pollutant concentration. As shown in Figure 4.1, these correspond to the darkest-coloured regions, where the experimental probability, defined in Equation 3.4, reaches its maximum value of ~ 0.008 across the three models. This information can help to guide the implementation of containment measures in response to such emergencies. A significant difference in the temporal evolution of the oil slick can be observed between simulations corresponding to the three current forcings (IFREMER, SHOM, and CMEMS), as shown in Figure 4.1. This variation is primarily due to the inherent challenges in modelling highly variable ocean currents and the subgrid-scale estimates. Even small variations in the initial conditions can lead to substantially different outcomes. Despite these differences, all models generally show a westward movement toward the French coast. This behaviour is primarily driven by the dominant mesoscale circulation patterns in the Mediterranean Sea during the simulation period. These mesoscale structures, such as persistent eddies and large-scale current systems, operate at spatial and temporal scales that govern the overall transport of surface waters (Millot and Taupier-Letage 2005). While the detailed trajectories differ due to model-specific dynamics and resolution, the main advection pathway remains similar, leading the simulated oil spills towards the same general impact area. Notably, the IFREMER simulation reached greater distances more quickly than both the CMEMS and SHOM simulations. The duration of the event is based on actual observations, as crude oil was found on the beach at Pampelonne (marked by the red dot on the map) on

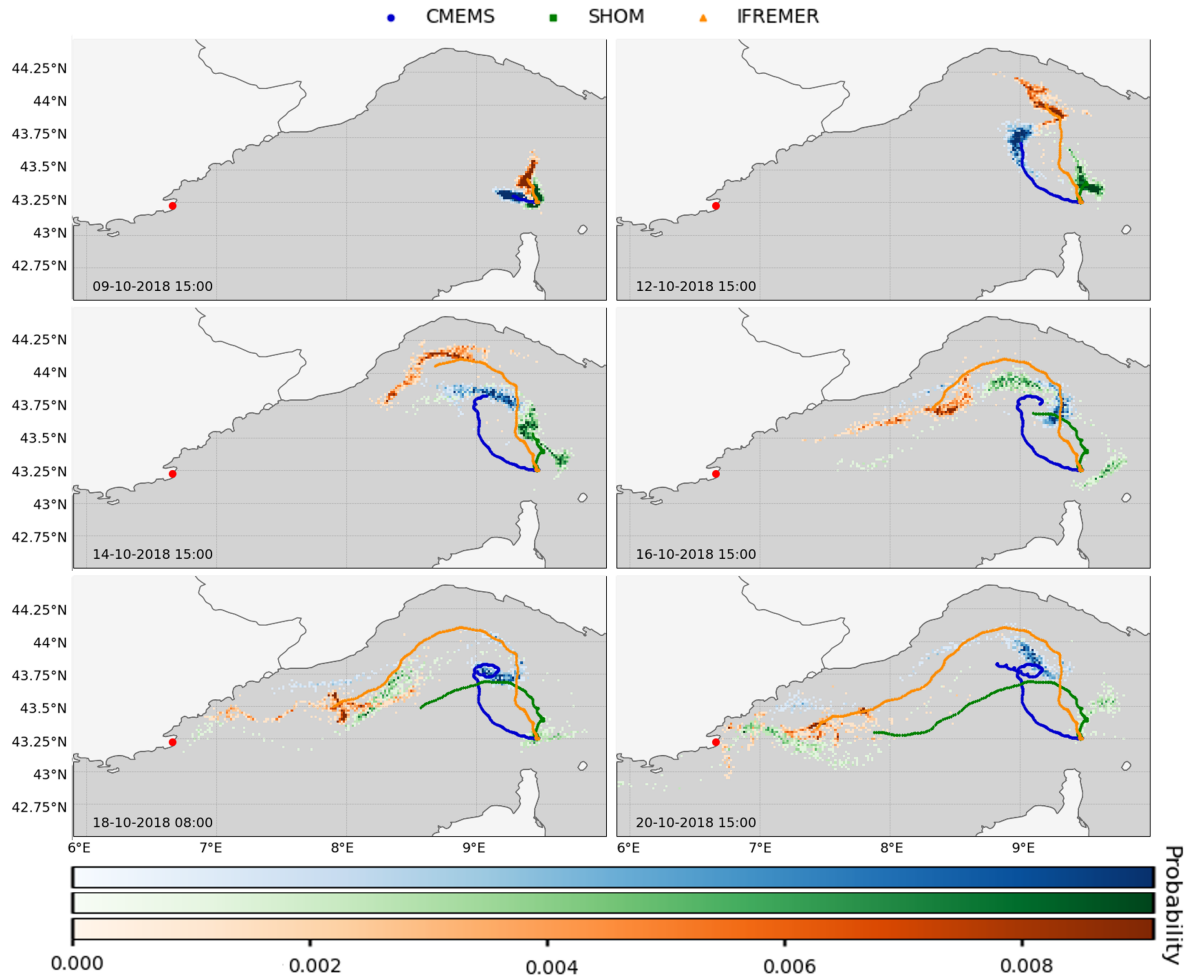


Figure 4.1: Evolution of oil spills with relative probability for the three models and trajectory followed by the centroid, considering only sea surface currents forcing. From top-left to bottom-right: 09/10/2018 15:00, 12/10/2018 15:00, 14/10/2018 15:00, 18/10/2018 15:00, 20/10/2018 08:00, 23/10/2018 08:00. The red dot represents the area of impact on the beach of Pampelonne in France, when traces were found on the 16/10/2018 presumably in the early morning.

October 16, more than a week after the incident. However, none of the three simulations predicted the oil slick reaching the coastline by that date, suggesting that additional forcing factors, not accounted for in this currents-only scenario, may have influenced the spill's trajectory. After a two-day delay, on the 18 October, both the IFREMER at 23:00, and SHOM at 01:00 simulations depicted particles near the French coast, likely impacting the Saint-Tropez promontory. The CMEMS model showed a larger delay compared to the other two, as the oil spill is directed into a vortex between Corsica and Liguria, arriving on the near the coast on the 22 October at 23:00. Although the SHOM model uses archived forecast data instead of reanalysis products, its results are not significantly different from those of the CMEMS and IFREMER models. In fact, the SHOM simulations predict the impact area around the same time as IFREMER, suggesting that SHOM performs reliably as a forecasting tool, even when compared to reanalysis-based models. It is important to note that even though the CMEMS and IFREMER models are based on reanalysis data, they exhibit noticeable differences in trajectories and dispersion patterns. This highlights the inherent variability between models and underscores the influence of their respective configurations and forcings. After impacting the coast, the oil slick was pushed further south-west by currents (Fontana 2018). As shown in Figure 4.1, bottom-left, the simulations accurately exhibit the presence of particles along the French coast after the 20th of October, with event the CMEMS simulation showing particles arriving at the impact zone near Saint Tropez, albeit with a delay of many days than expected.

4.2 Oil spill dispersion with combined surface currents, wind and Stokes drift forcing from multiple models

The second scenario presents the integration of the 10-meter wind field and Stokes drift forcing to improve the understanding of dispersion driving processes. Data from the ERA5 and MeteOcean-UniGe models will be used in combination with the currents from CMEMS, SHOM and IFREMER leading to 6 different simulations. This approach is motivated by the significant differences in resolution between the two climate models, allowing a comparison of their results and providing a comprehensive view of the dispersion dynamics of the oil spill. We have divided this scenario into different sub-cases in order to evaluate the role of each forcing (currents, wind, waves) and their combination:

- Combined forcing of surface currents, 10-m wind field and Stokes drift
- Combined forcing of surface currents and 10-m wind field
- Combined forcing of surface currents and Stokes drift

4.2.1 Sea surface currents combined with wind field and Stokes drift forcing

The first sub-case represents the simulations with currents from the three ocean circulation models in combination with both 10-m wind field and Stokes drift forcing from ERA5 and MeteOcean-UniGe. For the MeteOcean-UniGe simulations, the northward and eastward velocities of Stokes drift are calculated using Equation (3.2). The LPT model is forced by the combination of all three forcing following Eq. (3.1) where the β and α need to be evaluated. For this a sensitivity analysis has been carried out to find the optimal β and α based on the knowledge of the area and time-of-impact of the oil spill at the French coast. Initially, the same coefficients for α and β are used, specifically $\alpha = 0.3$ and $\beta = 0.02$ for the ERA5 and the MeteOcean-UniGe simulations for all three ocean model combinations. However, for the IFREMER model, it was necessary to adjust these coefficients in both scenarios to obtain a more reliable simulation, according to the only two evidences relating to the specific case study (i.e. the area of impact and satellite images). Consequently, for CMEMS and SHOM the original values, $\alpha = 0.3$ and $\beta = 0.02$ for ERA5 and MeteOcean-UniGe are maintained, while for IFREMER coefficients are changed to $\alpha = 0.3$ and $\beta = 0.03$ for the simulations in combination with ERA5 and MeteOcean-UniGe. The final α and β values are reported in Table 4.1. The coefficients are strongly influenced by the specific weather and sea conditions, seasonality and oil spill characteristics. These coefficients should be interpreted as preliminary estimates derived from a sensitivity analysis aimed at providing an initial assessment of the influence of wind and wave forcing on particle transport. Section 4.5 will carry out a more systematic and quantitative optimisation of α and β using a Bayesian approach. Figures 4.2 and 4.3 show the progressive trajectories of the oil slicks for the simulations of surface currents in combination with ERA5 and MeteOcean-UniGe, respectively. As observed, for both ERA5 and MeteOcean-UniGe there is a clear improvement, in terms of expected oil-spill trajectory, from the previous simulations that are forced with only sea surface currents.

	CMEMS	SHOM	IFREMER
α	0.3	0.3	0.3
β	0.02	0.02	0.03

Table 4.1: α and β coefficients for the simulations

The MeteOcean-UniGe model, which has a higher grid resolution than the ERA5 model, presents an improvement in the accuracy of the simulations with reduced particle diffusion and a slight better precision in predicting the impact area on the French coast as shown in Figure 4.3. The three simulations maintain a certain difference between their trajectories, but the general trends are very similar to those shown in Figure 4.2. With the introduction of the coefficients chosen according to each model, all the simulations arrive

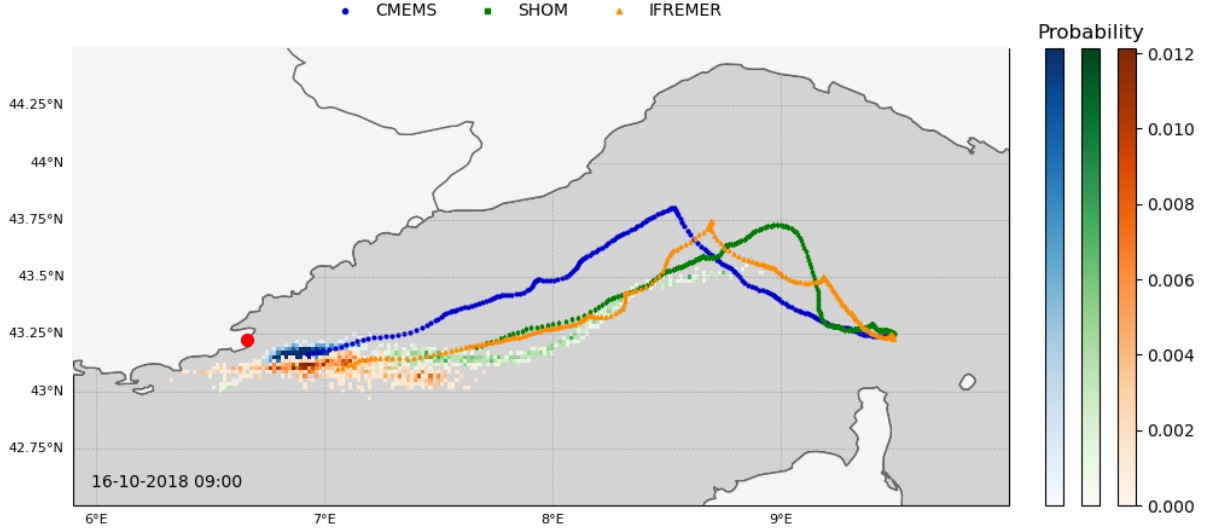


Figure 4.2: Evolution of oil spills with relative probability for the three surface currents models (CMEMS, IFREMER and SHOM) in combination with ERA5 wind field and Stokes Drift forcing on the 16th October 2018 09:00.

at the area of impact on the French coast on the same day and no longer on different dates as in the case of the simulations with currents alone. It is also worth noting that the CMEMS model, which in Figure 4.1 shows a vortex at the height of the Ligurian coast, is no longer present in the two results in Figures 4.2 and 4.3, which show a trajectory more similar to that of IFREMER and SHOM. Finally, it can be noted how the diffusion of the particles present in the case of the currents is no longer so marked in the results obtained by implementing the wind and Stokes drift, improving the achievement of the impact area where hydrocarbons were actually found on the French coast and not in other areas where this did not occur.

To further evaluate the accuracy of the results, the simulated oil slick distributions are compared with Sentinel-1 SAR imagery of the oil slick (Magrì et al. 2021) acquired in the days following the accident (see Section 3.1.3). The specific images used, identified by their product IDs, are listed in Table 4.2.

The acquisition of usable imagery is made possible by favourable wind conditions, with speeds ranging from 2 to 10 m/s on 8 and 9 October (Espedal and Wahl 1999).

Figure 4.4 illustrates in the left panel three time instants at which the slick is detected by the satellite, represented by the red outline, in comparison with the simulations carried out with the three ocean circulation models surface currents in combination with MeteOcean-UniGe wind field and Stokes drift. The right panel shows the corresponding satellite images. It can be observed that although the speed of movement differs, the simulation derived from the CMEMS model is the one that most closely aligns with the actual slick points for MeteOcean-UniGe. As mentioned, the MeteOcean-UniGe simulations present a lower dispersion of the oil slick, in agreement with the satellite images.

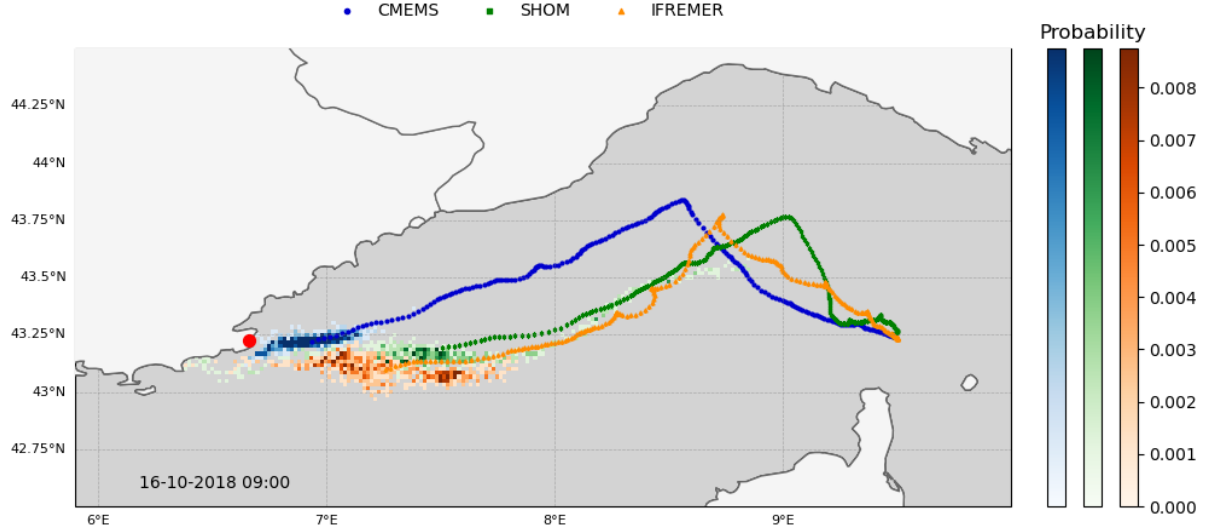


Figure 4.3: Evolution of oil spills with relative probability for the three surface currents models (CMEMS, IFREMER and SHOM) in combination with MeteOcean-UniGe wind field and Stokes Drift forcing on the 16th October 2018 09:00.

Image	Product ID
08/10/2018 07:28	S1A_IW_GRDH_1SDV_20181008T052757_20181008T052822_024040_02A081_CA4D
08/10/2018 19:21	S1B_IW_GRDH_1SDV_20181008T172145_20181008T172210_013064_01822C_B07F
09/10/2018 19:14	S1A_IW_GRDH_1SDV_20181009T171427_20181009T171452_024062_02A131_E887

Table 4.2: Sentinel-1 product IDs

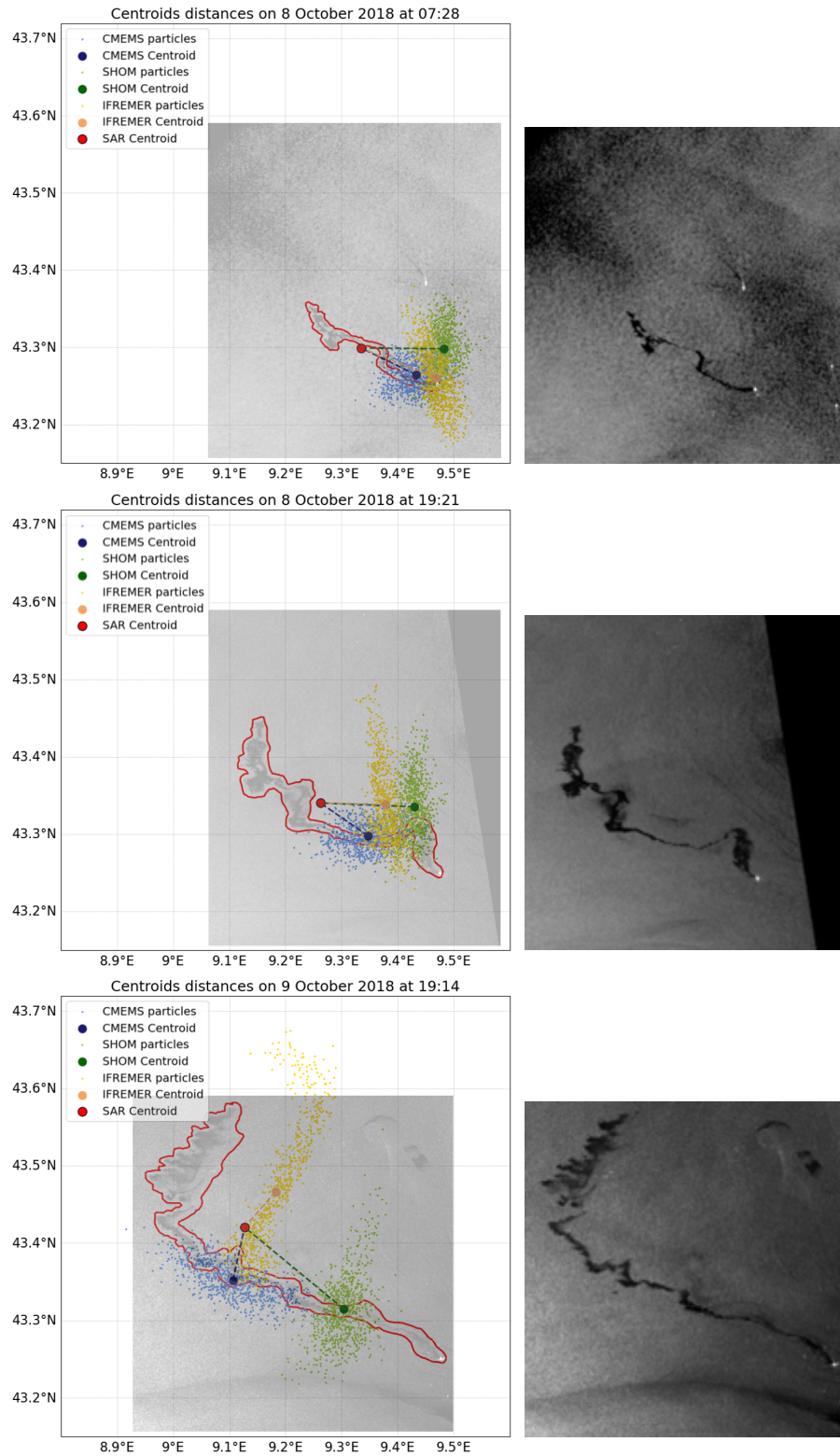


Figure 4.4: Left panel - Oil slicks trajectories simulated with three sea water velocity models in combination with Stokes drift and wind field forcing from MeteOcean-UniGe compared with SAR images from Copernicus Sentinel-1 at three different times (red outlines). Right panel - Corresponding satellite images, from top to bottom, 08/10/2018 at 7:28, 08/10/2018 at 19:21, 09/10/2018 at 19:14.

The results, giving the distances between the centroids of the simulations and that of the satellite images (Eq. 3.10) and the percentage of particles simulated for each model intersecting slicks detected by SAR (Eq. 3.11), for the three temporal instants are reported in Table 4.3 and reveal variations in percentages across the models, reflecting their relative performance in simulating the spill dynamics. These variations are related to the input characteristics of each simulation as well as the introduced α and β coefficients, although these vary only for the β coefficient of 0.01 between models.

Date and Time		CMEMS	SHOM	IFREMER
08/10/2018 07:28	P_{in} [%]	12.50	3.38	5.00
	D_{centroid} [km]	8.87	11.98	11.70
08/10/2018 19:21	P_{in} [%]	24.25	21.75	12.12
	D_{centroid} [km]	8.38	13.56	9.39
09/10/2018 19:14	P_{in} [%]	38.12	15.75	7.38
	D_{centroid} [km]	7.87	18.49	6.81

Table 4.3: MeteOcean-UniGe model. P_{in} - Percentage of particles detected inside the oil slick area for each instant of the SAR images. D_{centroid} - Distance between the centroids of particle dispersion simulations and the centroid of the observed SAR image.

The results demonstrate that the CMEMS model is the most accurate in this analysis, exhibiting the minimal distances between centroids and the highest percentage of simulated particles within the temporal image area, in comparison to the outcomes from the SHOM and IFREMER models.

The same procedure is then applied to simulations obtained with Stokes drift and wind data from ERA5, compared with satellite images at the three times. Figure 4.5 shows the results obtained, and what can be observed is a certain similarity in the trends of the models with the results obtained in Figure 4.4.

Table 4.4 shows the data obtained for the distance between the centroid of the satellite image and the centroids of the three simulations, and the percentage of particles falling within the area of the SAR image. It can be noted that, compared to the results obtained for the case of MeteOcean-UniGe, the simulations generally perform slightly worse, with larger values of distance between the centroids and lower percentages of particles within the area of the satellite image. Even in this case, at the first three instances, it is the CMEMS model that gives overall the best results.

4.2.2 Surface currents combined with wind field forcing

Figure 4.6 presents the results of the simulations forced with surface currents from the three ocean circulation models and wind field from ERA5. The coefficients used for the wind component, $\beta = 0.03$ for CMEMS and SHOM, while $\beta = 0.02$ for IFREMER, are the same as the one used in previous simulations. The results show that the slicks travel a

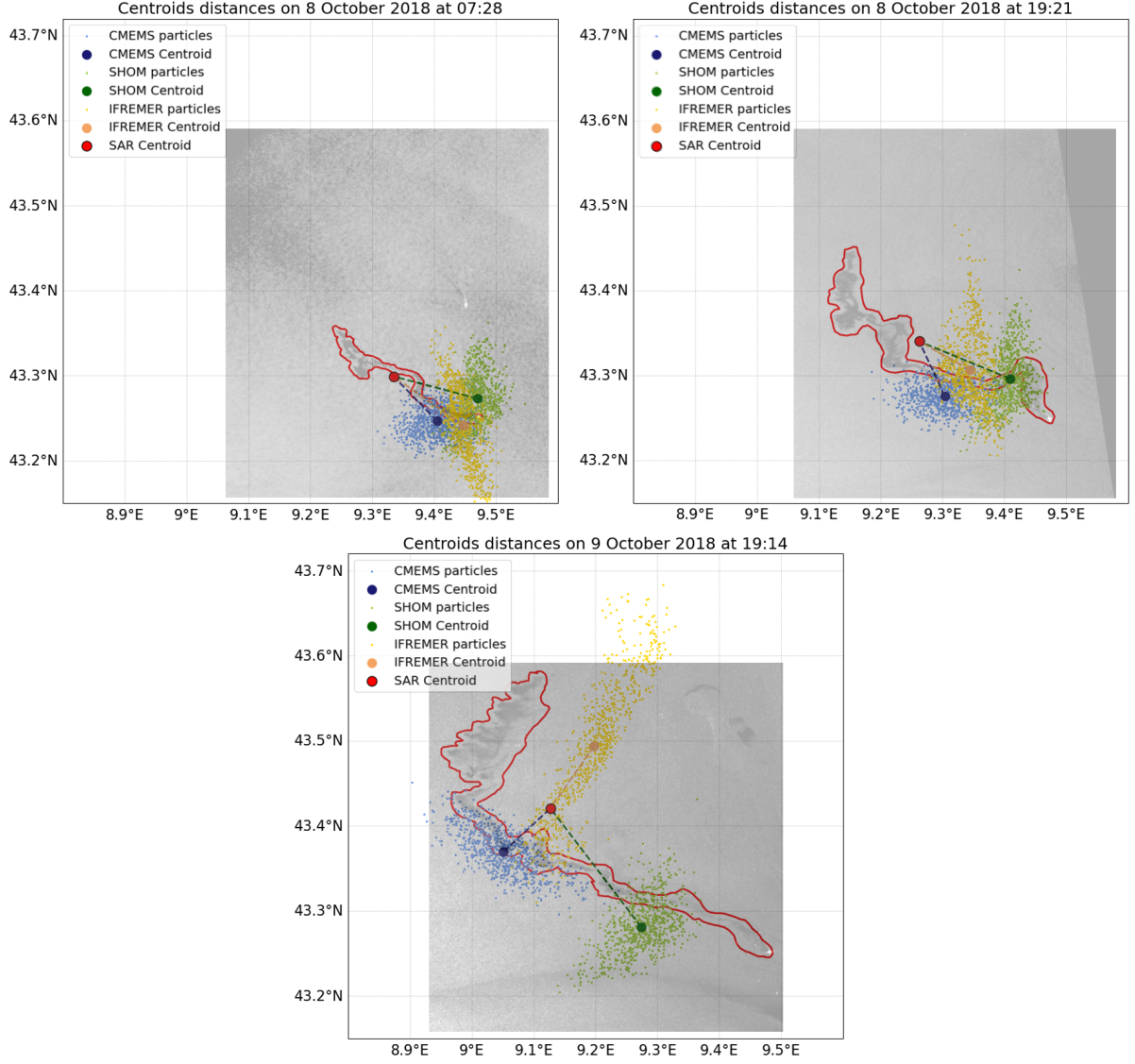


Figure 4.5: Oil slicks trajectories simulated with three sea water velocity models in combination with Stokes drift and wind field forcing from ERA5 model, compared with SAR images from Copernicus Sentinel-1 at three different times (red outlines). On the upper left, the 08/10/2018 at 7:28, in the upper right the 08/10/2018 at 19:21. and on the bottom, the position of 09/10/2018 at 19:14.

Date and Time		CMEMS	SHOM	IFREMER
08/10/2018 07:28	$P_{in} [\%]$	13.75	5.75	9.00
	$D_{centroid} [km]$	8.17	11.36	11.15
08/10/2018 19:21	$P_{in} [\%]$	13.25	25.87	12.38
	$D_{centroid} [km]$	7.87	12.85	7.62
09/10/2018 19:14	$P_{in} [\%]$	38.00	8.88	7.12
	$D_{centroid} [km]$	8.37	19.53	9.92

Table 4.4: ERA5 model. P_{in} - Percentage of particles detected inside the oil slick area for each instant of the SAR images. $D_{centroid}$ - Distance between the centroids of particle dispersion simulations and the centroid of the observed SAR image.

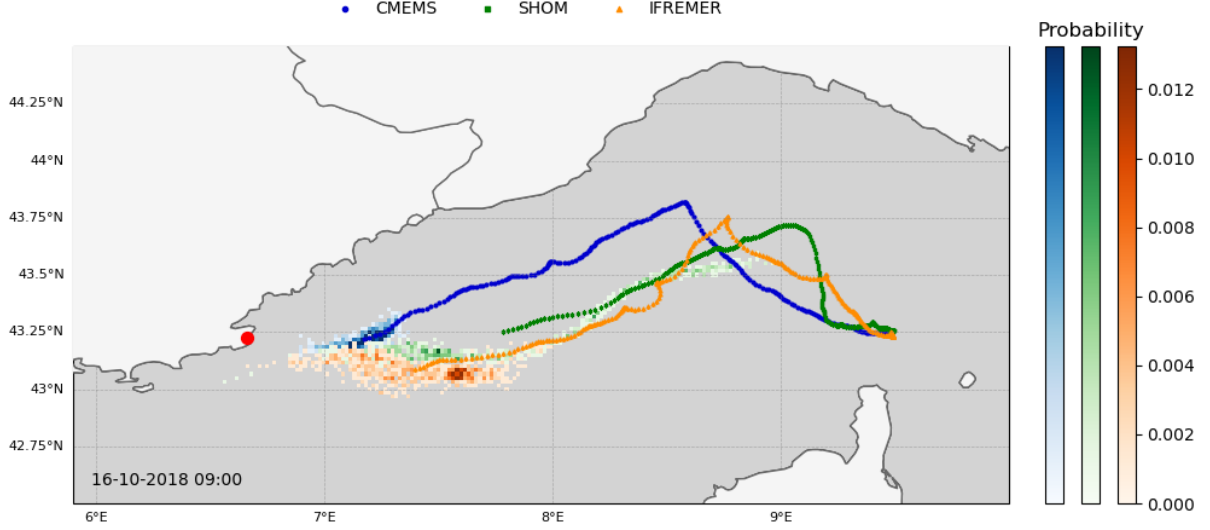


Figure 4.6: Evolution of oil spills with relative probability for the three surface currents models (CMEMS, IFREMER and SHOM) in combination with ERA5 wind field forcing on the 16th October 2018 09:00.

significant distance when the wind forcing is introduced. The wind, in particular, appears to contribute significantly to advection, accelerating the movement of particles on the water surface and increasing the area affected compared to what is observed with surface currents alone. This highlights the importance of wind in determining the overall behaviour and dispersion of particles on the water surface, as has already been demonstrated in others studies such as Prigent et al. (2017).

In this scenario, despite the low coefficient of wind, 2%-3%, its high magnitude nevertheless exerts a significant impact on the simulation. This is evidenced by Figure 4.7, which compares the wind and Stokes drift magnitudes at a point in the simulation domain (43°12'18"N, 7°30'32"E). A difference in order of magnitude reaching $\sim O(10^2)$ between wind and Stokes drift is observed which reflects the contribution of wind in the oil spill evolution.

Figure 4.8 presents the results of the simulations using surface currents from the three ocean models combined with wind field from the MeteOcean-UniGe model. The wind effect is applied with coefficients $\beta = 0.02$ for CMEMS and SHOM and $\beta = 0.03$ for IFREMER. The results indicate that the patches move a considerable distance when surface currents and wind are taken into account. However, with the chosen β , the calculated speed of movement is higher than that observed in the case study, i.e. the particles arrive sooner at the French coast than the expected impact date of 16/10/2018. Despite the lower coefficient, the impact of wind is substantial due to its magnitude (Fig. 4.7), contributing to the greater dispersion and rapid movement of particles on the water surface. It can be observed that the introduction of the wind component results in trajectories with a comparable overall trend across the three simulations, despite exhibiting differences in

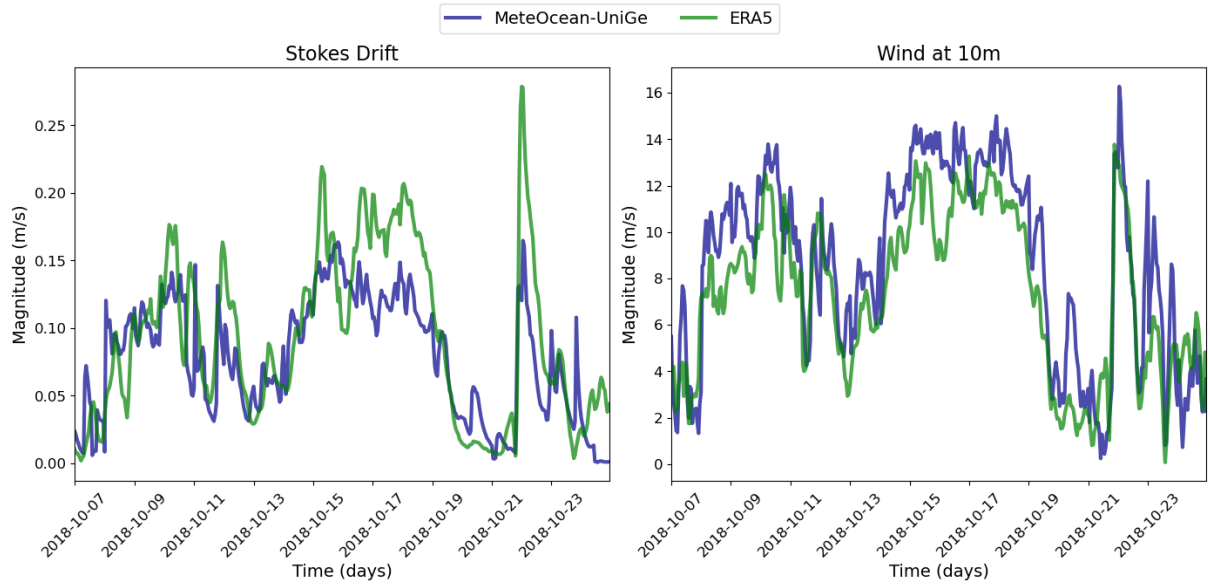


Figure 4.7: Comparison of the magnitude of Wind and Stokes drift for both ERA5 and MeteOcean-UniGe at the location of coordinates 43°12'18"N, 7°30'32"E.

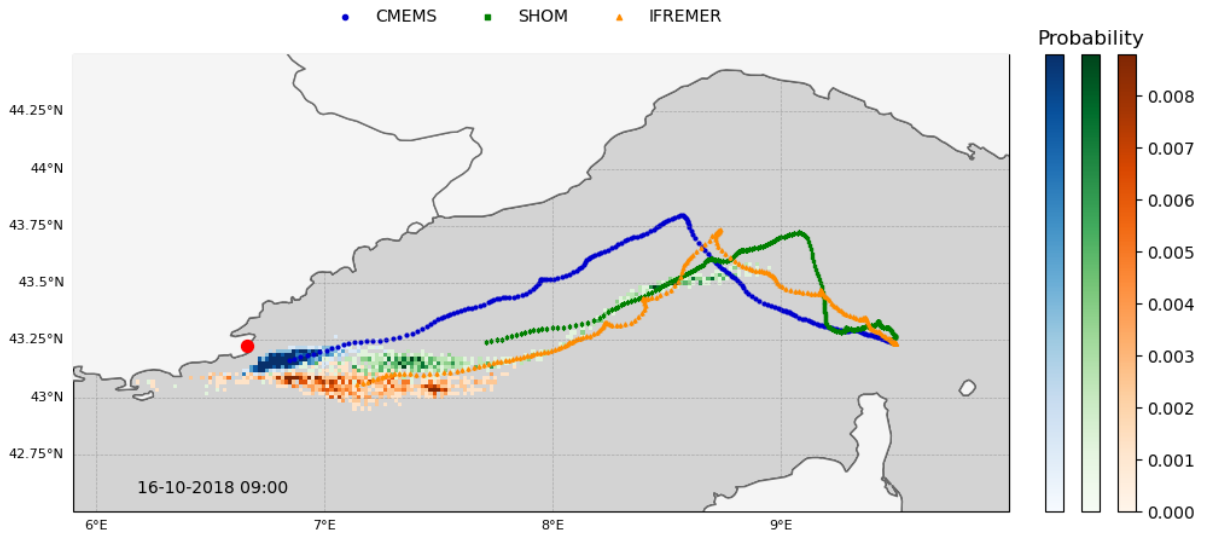


Figure 4.8: Evolution of oil spills with relative probability for the three surface currents models (CMEMS, IFREMER and SHOM) in combination with MeteOcean-UniGe wind field forcing on the 16th October 2018 09:00.

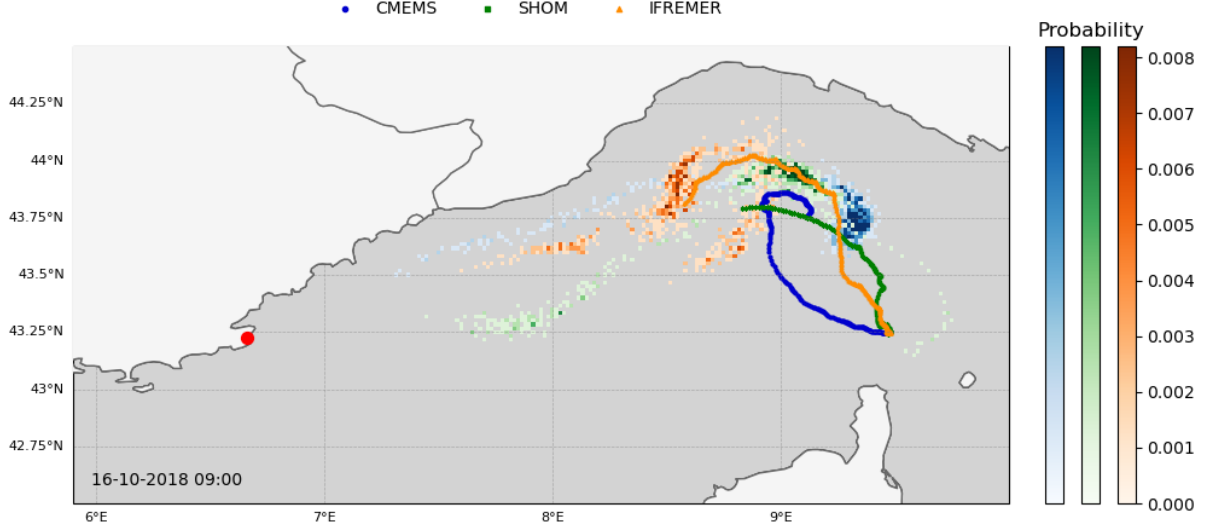


Figure 4.9: Evolution of oil spills with relative probability for the three surface currents models (CMEMS, IFREMER and SHOM) in combination with ERA5 Stokes Drift forcing on the 16th October 2018 09:00.

the reversal point from north-west to south-west. It is also of interest to note that the trajectory trends for the MeteOcean-UniGe model (Figure 4.8) and ERA5 (Figure 4.6) are rather similar, differing only in the speed at which the particles move towards the area of impact, with the MeteOcean-UniGe model exhibiting a faster rate of movement than ERA5.

4.2.3 Surface currents combined with Stokes drift forcing

Figures 4.9 and 4.10 illustrate the results of the simulations forced with the sea surface currents (CMEMS, SHOM and IFREMER) in combination with the Stokes drift induced by waves from ERA5 and MeteOcean-UniGe with $\alpha = 0.3$ for both the ERA5 and the MeteOcean-UniGe simulations.

From Figures 4.9 and 4.10, it is evident that the simulated trajectory differs significantly from what was observed in the previous results, where the wind component was considered. In this scenario, the Stokes drift component has a minimal impact on the advection process, whereas it contributes more in the general spatial distribution of the simulated spill. It is evident that the outputs of the current analysis exhibit a similarity to those obtained in previous simulations utilising only the sea surface currents in paragraph §4.1. This is a consequence of the low value of the α coefficient employed in the present analysis. The output of the MeteOcean-UniGe and ERA5 simulations demonstrates a high correlation in the trajectories of the simulations, with the primary distinction being in the diffusion of the particles. As illustrated in the ERA5 Figure 4.9, the CMEMS model simulation exhibits a notable divergence in particle diffusion compared to the results obtained with the MeteOcean-UniGe model simulations (Fig. 4.10).

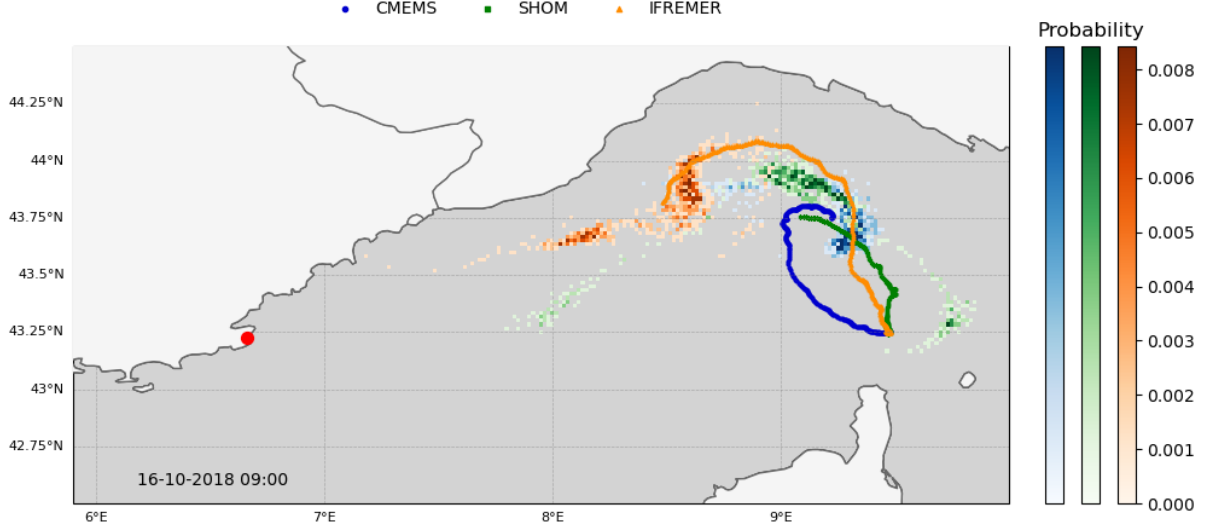


Figure 4.10: Evolution of oil spills with relative probability for the three surface currents models (CMEMS, IFREMER and SHOM) in combination with MeteOcean-UniGe Stokes Drift forcing on the 16th October 2018 09:00.

4.3 Mixing properties

A comparative analysis of the different mixing properties described in §3.3 is presented for the simulations carried out with the forcing combination of surface currents, wind and Stokes drift. Figures 4.11 and 4.12 present the relative dispersion R^2 , the absolute distance D_{b0} and the relative distance D_b , for the simulations carried out with the different forcing combinations of currents and ERA5 wind and Stokes drift. The graphs in Figure 4.11 indicate the total R^2 dispersion, and the two, x and y , components. A general trend of increasing dispersion over time is observed across all simulations in the three graphs. Notably, in the simulations that incorporate the wind and Stokes Drift factor in the bottom graph, there is a reduction in dispersion by almost an order of magnitude. This indicates that the two factors have a greater impact on particle advection than on particle dispersion.

In accordance with the data presented in Figures 4.12, it is evident that the absolute distance is consistently less than the relative distance. This is due to the fact that the absolute distance only accounts for the linear distance between the initial and final centroids, whereas the relative distance considers the entire path traced by the virtual particles. As previously evidenced in the results obtained in paragraph §4.2, the output for the case where sea surface velocity and Stokes drift are considered exhibits a trajectory for the three simulations that is half in value that of the simulation with wind contribution. This is also evident in Figure 4.12, which illustrates the results for the sea surface velocity with the Stokes drift contribution in the top panel. These results reach a maximum distance of 170 km for the IFREMER model. The results obtained for the graph on the top and on the bottom present a reaching distance of the trajectory of approximately 300

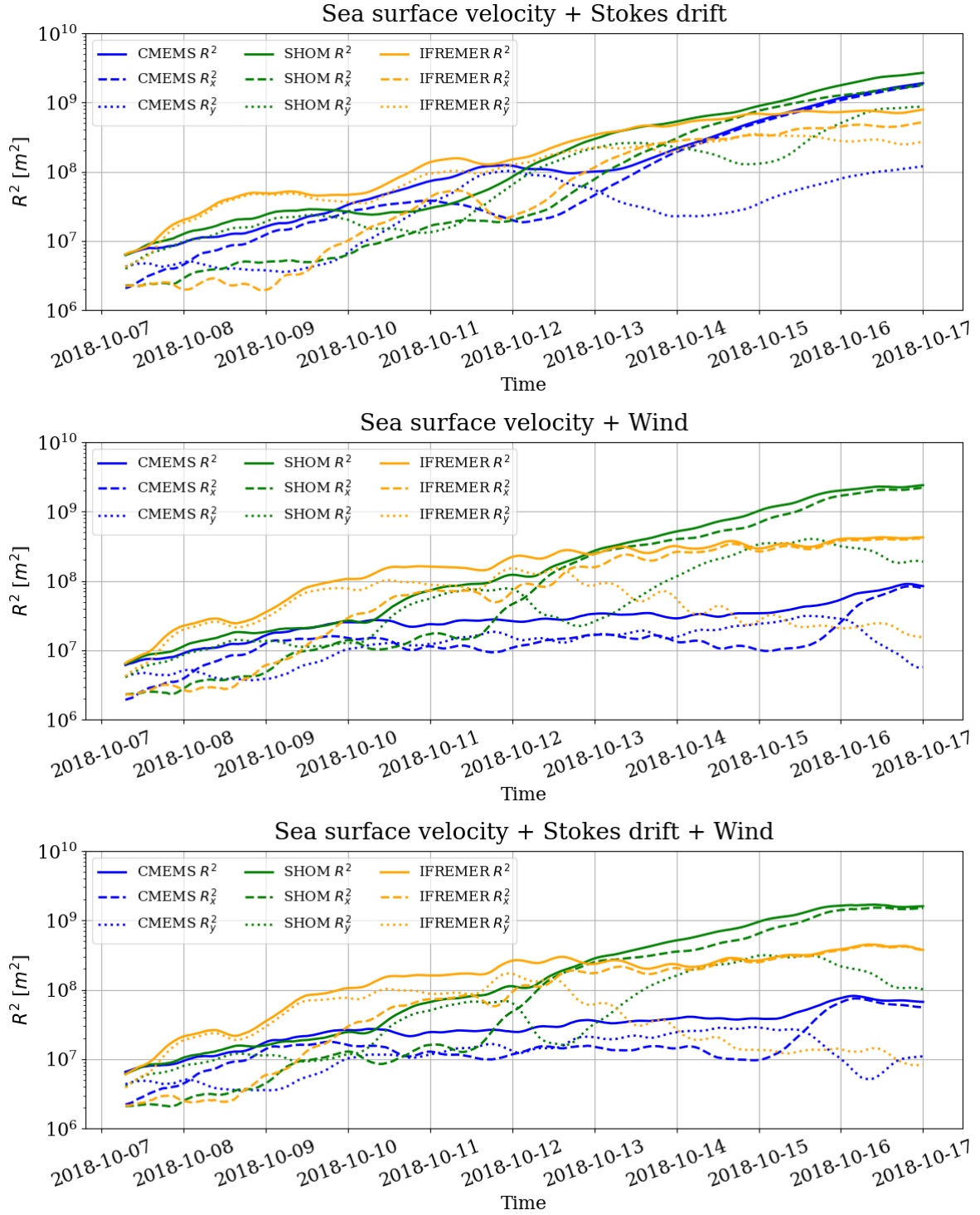


Figure 4.11: ERA5 Model - The graphs represent respectively the relative dispersion (continuous line) of the three models with bilogarhythmic trend and dispersion in x-direction (dashed line) and y-direction (dotted line).

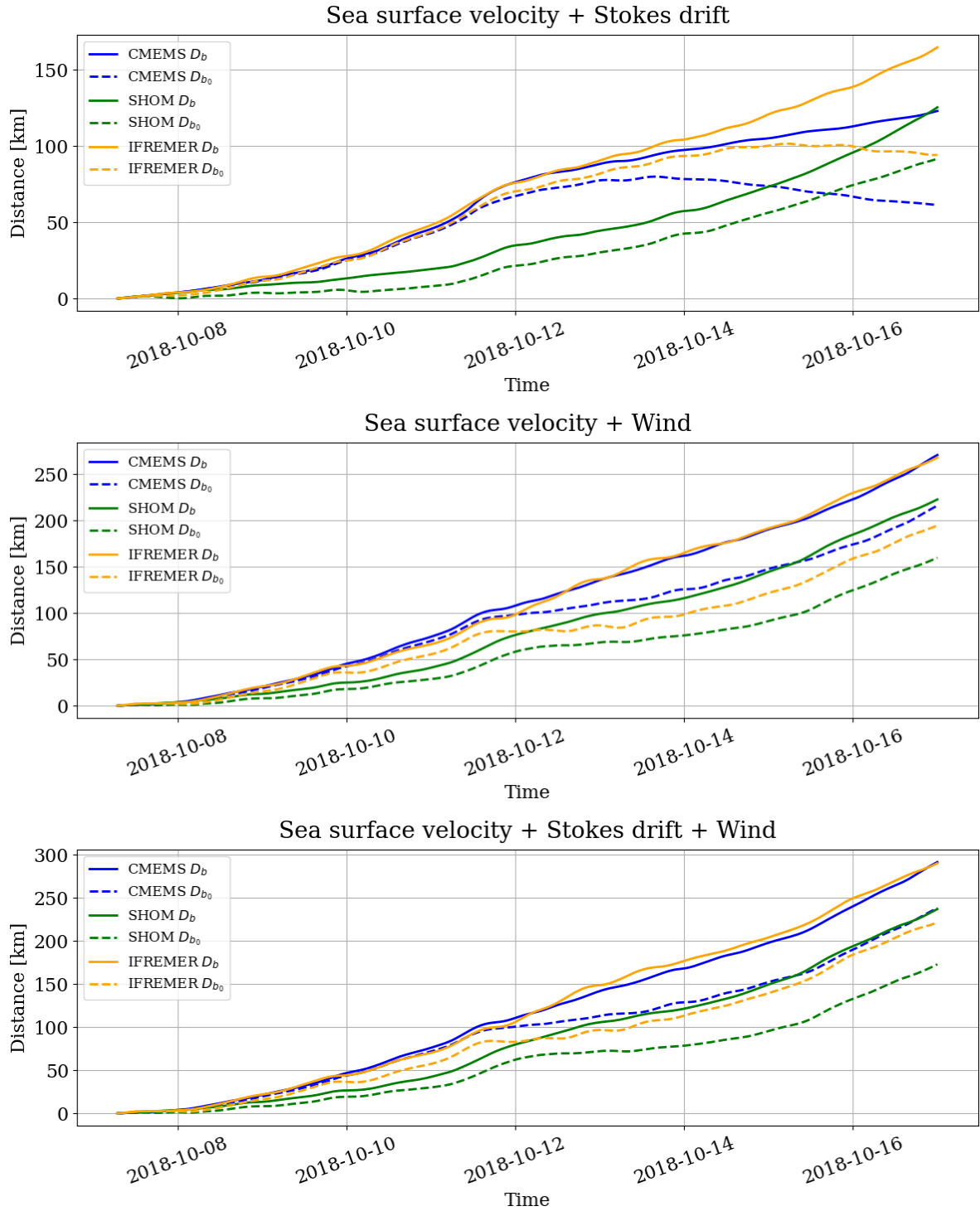


Figure 4.12: ERA5 Model - The graphs show the relative distance D_b (continuous line) and the absolute distance D_{b0} (dashed line) related to the three models. Top panel: results for sea surface velocity and Stokes drift contribution; Middle panel: results for sea surface velocity and wind component; Bottom panel: results for sea surface velocity, wind and stokes drift contributions.

km, which is almost twice the result obtained in the graph with sea surface velocity and Stokes drift contribution.

Similar trends are observed in the results obtained by MeteOcean-UniGe where Figure 4.13 represents the relative dispersion and the two components in x and y in the three cases of sea surface velocity, wind and Stokes drift. It can be observed that in all graphs, dispersion occurs gradually, increasing with time. It is interesting to note that the middle and bottom graphs show clear variations between the different simulations, with differences of more than an order of magnitude between the CMEMS and SHOM models.

Figure 4.14 presents graphical representations of the absolute and relative distances for the various combinations of simulations. Furthermore, the results obtained with the MeteOcean-UniGe model demonstrate that the graphs illustrating sea surface velocity and wind (middle panel) and sea surface velocity, wind and Stokes drift (bottom panel) exhibit a similar trend to the graphs in Figure 4.12. In particular, the graph representing sea surface velocity and Stokes drift reaches a distance of 175 km with the IFREMER model, while the other two graphs reach a distance of almost 300 km.

The graphs in Figures 4.15 and 4.16 depict the Probability Density Function (PDF) of the dispersion R^2 estimated at four time intervals, for every model, resulting in nine different lines in each graph. The PDF is then estimated numerically by counting how many particles fall within predefined intervals (bins) of R^2 and normalising the counts so that the area under the curve equals one.

The Figures 4.15 and 4.16, respectively, are derived from the ERA5 and MeteOcean-UniGe results and represent the probability density function of the relative dispersion in the three cases for each model simulation. The graphs illustrate the temporal evolution of the simulation at three distinct points in time. It is evident that in the period surrounding the release date, the probability density function (PDF) is higher than it is many days later, where the PDF becomes lower and more elongated. This phenomenon is reflected in the PDF graphs, which demonstrate that the particle cloud initially remains compact and then gradually expands over time.

4.4 Progressive release experiments

The results obtained in the previously analysed scenarios are based on the assumption of an instantaneous release, meaning that all particles are released simultaneously in a single location. This type of configuration is useful for isolating and analysing transport and weathering mechanisms, but not always represents the optimal or real-life scenario. Therefore, an additional experiment is conducted using the same modelling framework and parameter settings, but with the oil discharge distributed progressively over time. This study is based on sea surface currents from the Copernicus Marine Service, combined with wind and Stokes drift fields provided by the MeteOcean-UniGe model. In this set up, 30

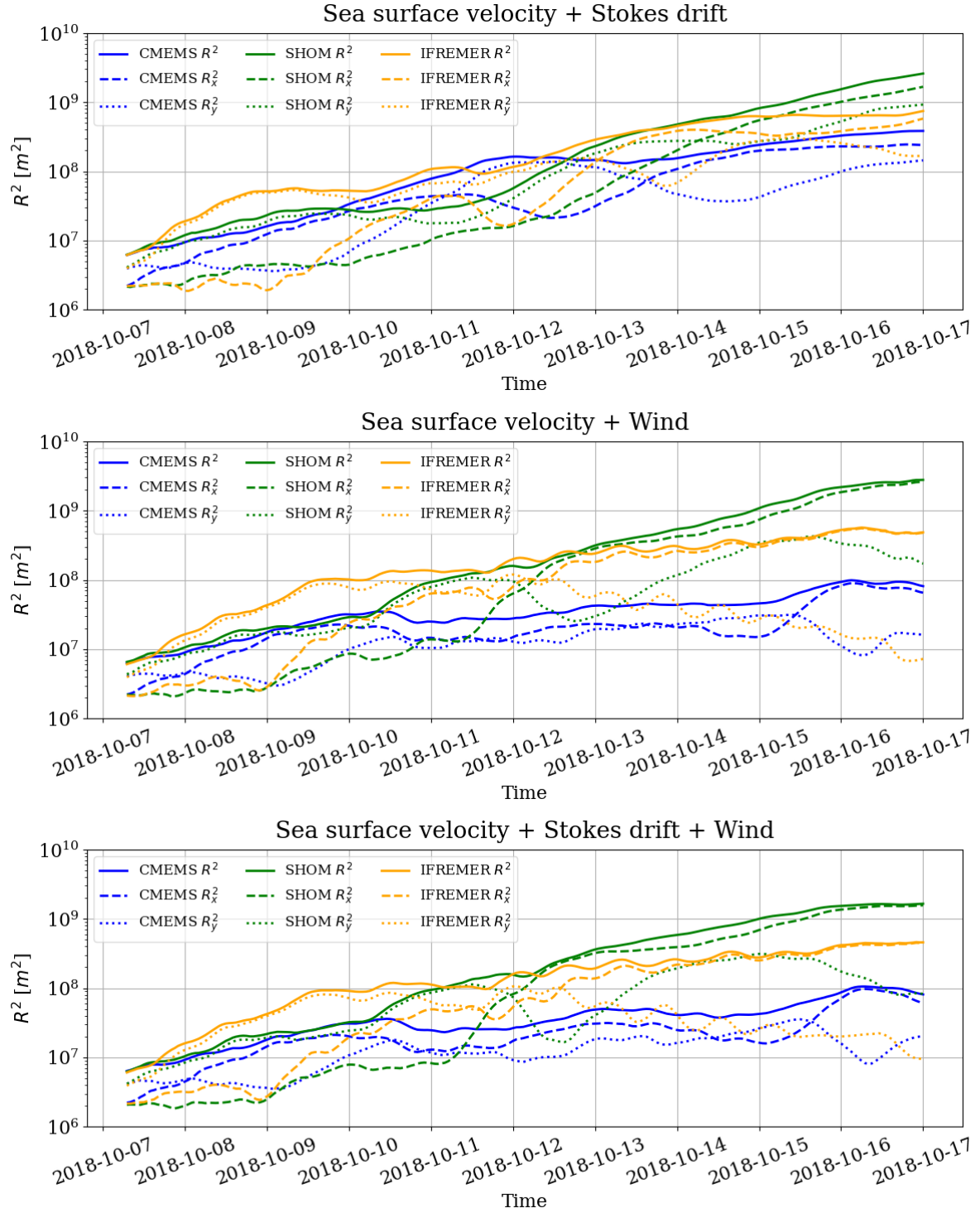


Figure 4.13: MeteOcean-UniGe Model - The graphs represent respectively the relative dispersion (continuous line) of the three models with bilogarhythmic trend and dispersion in x-direction (dashed line) and y-direction (dotted line).

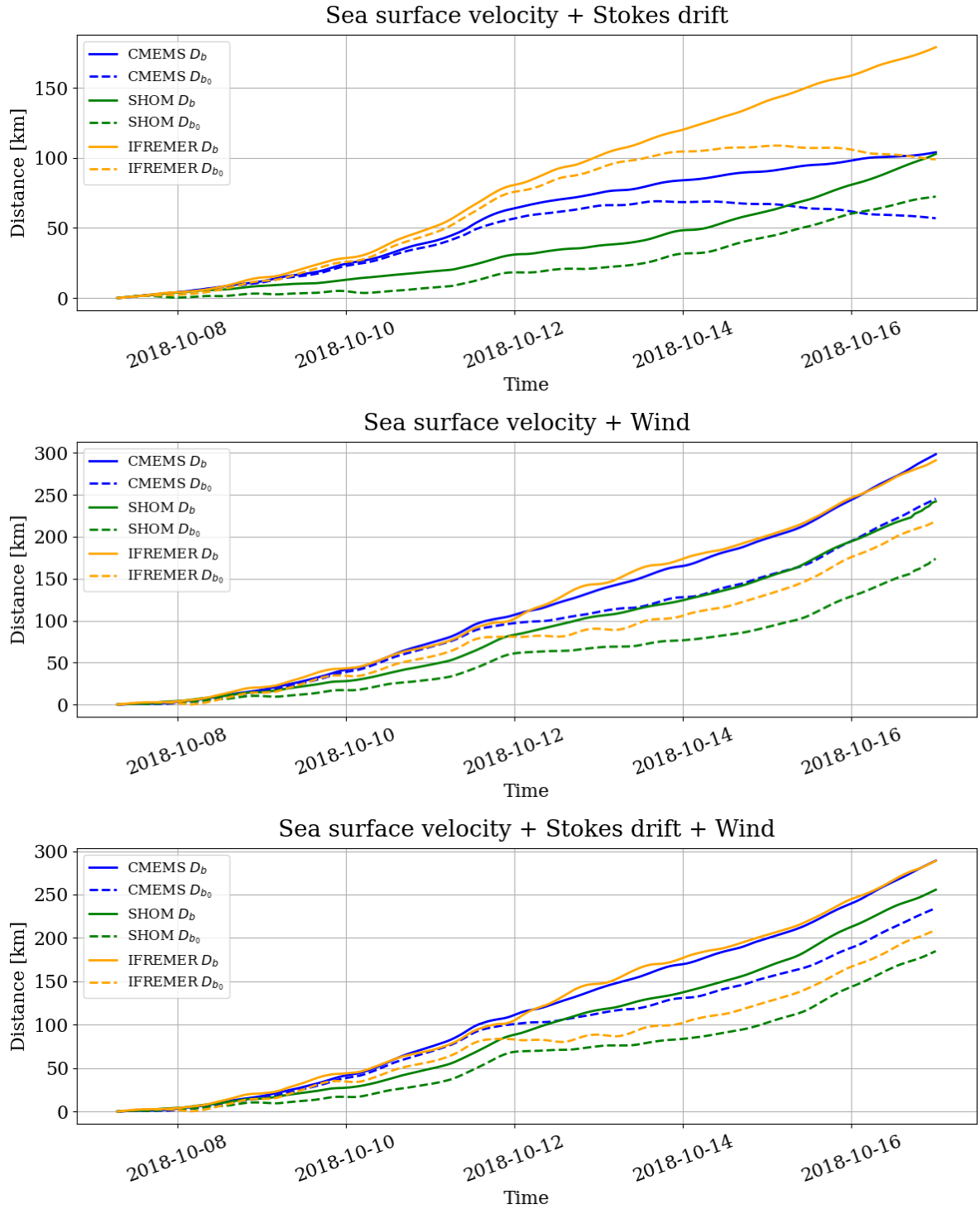


Figure 4.14: MeteOcean-UniGe Model - The graphs show the relative distance D_b (continuous line) and the absolute distance D_{b0} (dashed line) related to the three models. Top panel: results for sea surface velocity and Stokes drift contribution; Middle panel: results for sea surface velocity and wind component; Bottom panel: results for sea surface velocity, wind and stokes drift contributions.

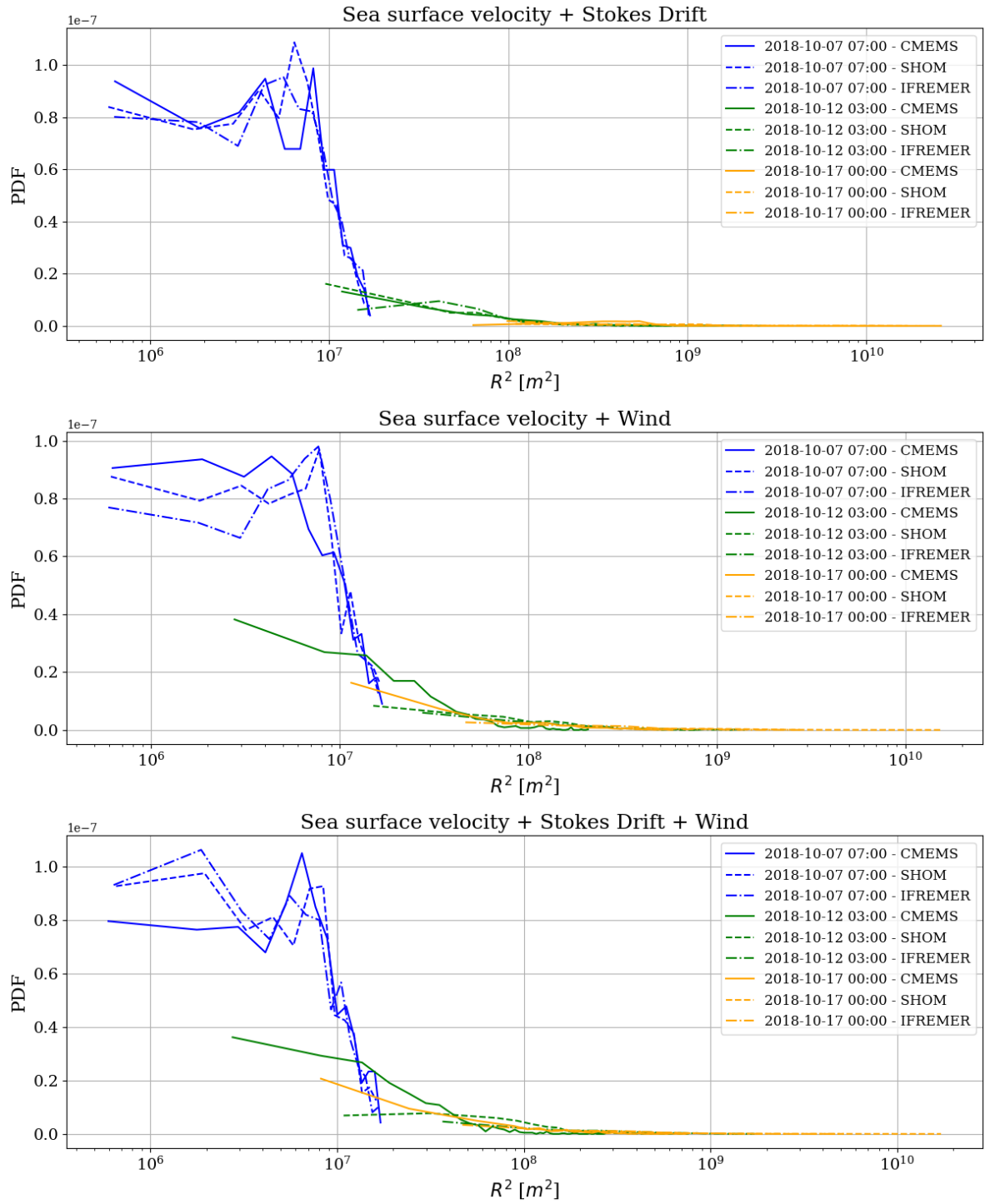


Figure 4.15: ERA5 Model - representation of probability density function (PDF) of R^2 in three different instants of time.

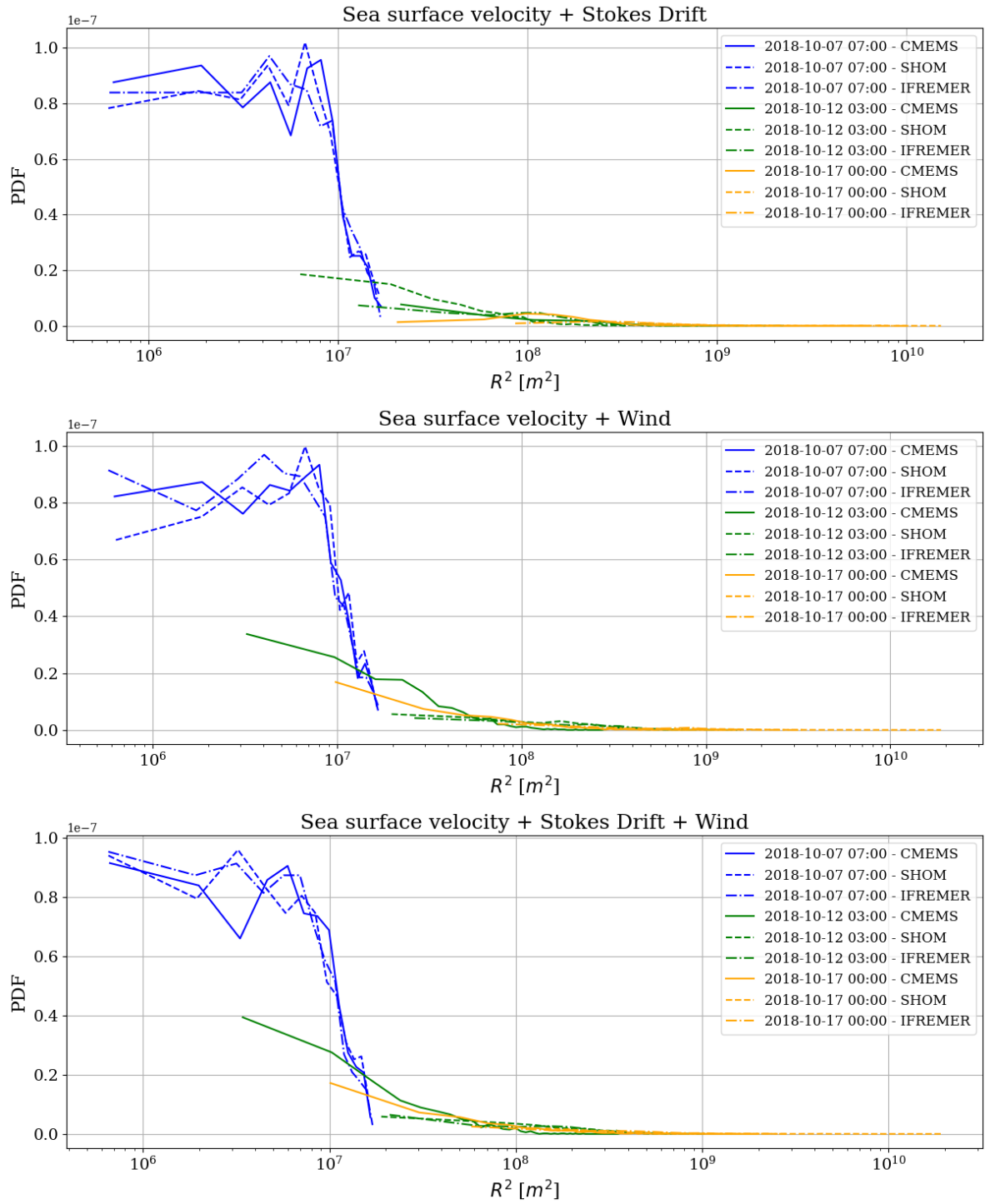


Figure 4.16: MeteOcean-UniGe Model - representation of probability density function (PDF) of R^2 in three different instants of time.

particles are released every 30 minutes for the first three days after the accident. This configuration is considered in this section as a plausible, although idealised, scenario in order to attempt to reconstruct the real event, despite the fact that detailed information on the true discharge rate and timing is unavailable. The main purpose of this analysis is therefore to assess whether this setup could provide useful insight and be adopted more confidently in future case studies where more complete observational data are available.

This approach, as can be seen in Figure 4.17, produces an evolution that broadly resembles the behaviour observed in the instantaneous release case, but with a persistent tailing structure resulting from the continuous addition of new particles. Progressive release therefore produces a temporally extended slick characterised by a more elongated spatial profile. A comparison is performed between instantaneous release (shown in orange), progressive release (shown in green) and three available satellite images. The results obtained, in particular the bottom figure, suggest that the simulation of progressive release more accurately reproduces the observed spatial evolution of the oil slick, especially in terms of extent and persistence over time. However, it should be noted that no detailed information is available regarding the exact rate of the actual discharge during the accident. Consequently, the adopted progressive release configuration is a plausible assumption rather than a reconstruction based on verified operational data. The release parameters can then be adjusted to represent alternative discharge scenarios, allowing the framework to be adapted for use in different types of analysis, such as sensitivity analysis.

From a quantitative perspective, the progressive release configuration introduces differences in the statistical properties of the particle cloud compared to the instantaneous release case. Since particles are continuously injected over time, the resulting distribution is characterised by a broader spatial extent and a more heterogeneous temporal structure. Given the increased spatial spreading associated with progressive release, lower probability values are expected due to the reduced particle concentration in each grid cell. Although the centroid trajectory is primarily controlled by the environmental forcing fields, in the case of progressive release it may exhibit slight deviations compared to the instantaneous release. This is due to the temporal distribution of particle injection, which introduces a superposition of trajectories at different stages of evolution, potentially leading to a delayed or smoothed centroid displacement. Despite these differences, the area and timing of shoreline impact remain similar to the instantaneous release case. This behaviour can be interpreted within the Lagrangian dispersion framework described in Section 3.3, where the evolution of the particle cloud depends on both advection and time-dependent spreading. In this context, the progressive release leads to a superposition of particles at different stages of their trajectories, resulting in a less concentrated and more elongated distribution. These results suggest that, while the temporal distribution of the source influences the spatial extent and concentration of the oil slick, the dominant transport pathways and shoreline impact are primarily determined by environmental forcing fields.

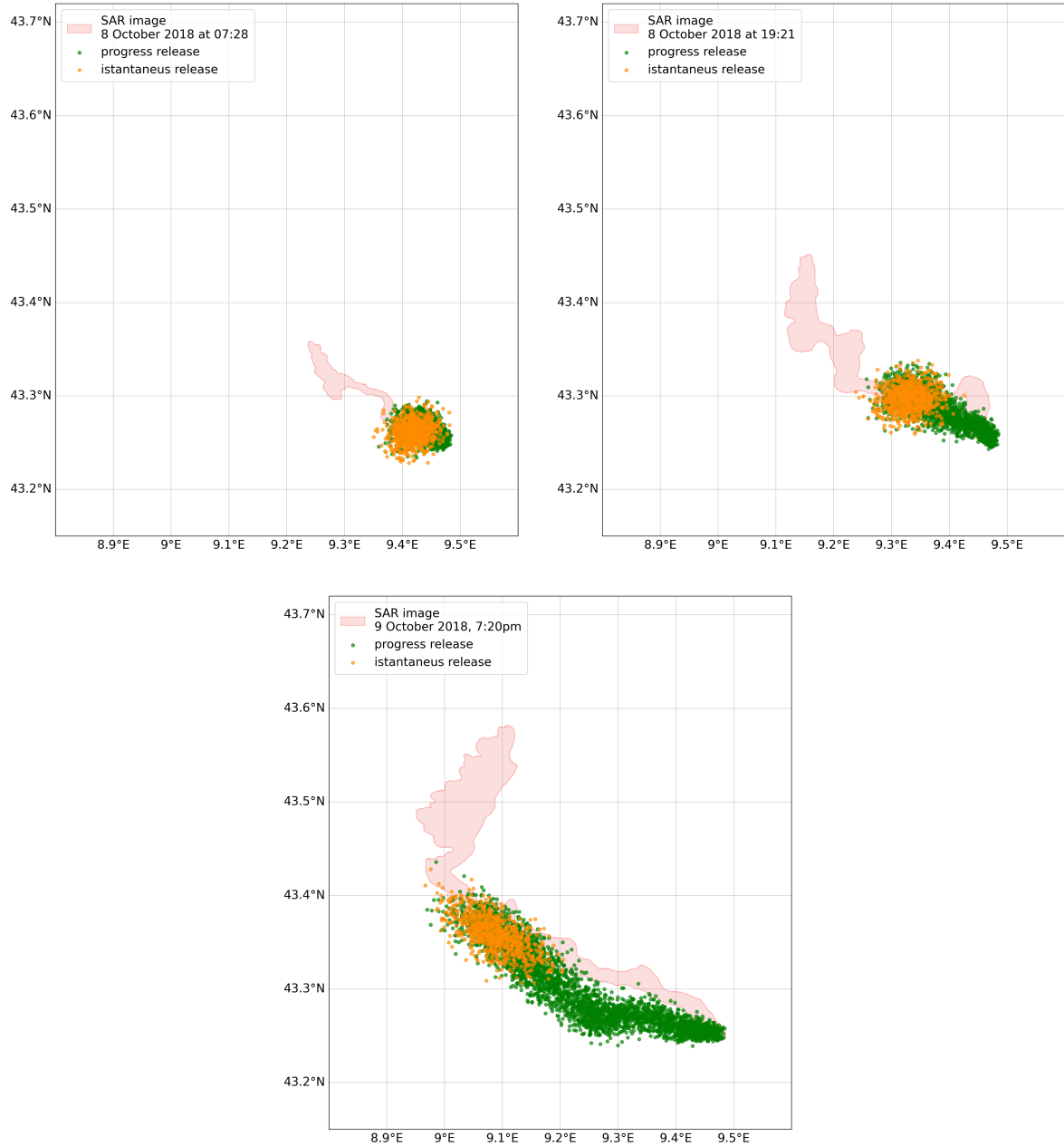


Figure 4.17: Oil slicks trajectories simulated with instantaneous release in orange and progressive release in green, compared with SAR images from Copernicus Sentinel-1 at three different times (red shape). On the upper left, the 08/10/2018 at 7:28, in the upper right the 08/10/2018 at 19:21. and on the bottom, the position of 09/10/2018 at 19:14.

4.5 Bayesian optimization results

In previous sections, the transport coefficients α and β are estimated using a sensitivity analysis to provide a preliminary qualitative evaluation of the influence of wind and wave forcing on particle transport. This section presents a systematic and quantitative calibration using a Bayesian optimisation approach introduced in §3.4. This refinement uses the limited observational information available for the case study: the position of the oil slick, derived from satellite imagery, and the reported area of impact along the French coastline. Specifically, the impact is said to have occurred on the Pampelonne beach in the early morning of 16 October 2018. As the available information refers to a relatively large coastal area and does not specify an exact arrival time, further assumptions are necessary. In this study, the shoreline impact location has been approximated by a representative point along the beach and the arrival time has been fixed at 09:00 on 16 October 2018. While these assumptions introduce a degree of uncertainty into the calibration process, they are necessary in order to define a well-posed optimisation problem. For this reason, Bayesian optimisation is applied as a refinement step following the initial sensitivity analysis. Where more precise observations are available, this approach would provide a more robust and objective estimation of the transport coefficients. To account for the different types of observational constraints available, two complementary calibration configurations are considered. The long-time configuration is defined by constraining the optimisation to the shoreline impact at Pampelonne Beach (16 October 2018), which corresponds to the final stage of the spill’s evolution. The small-time configuration, in turn, is based on three satellite observations acquired during the first two days after the accident and focuses on the early evolution of the oil slick. This distinction enables the transport coefficients to be evaluated across different temporal scales.

Within the long-time configuration, three alternative optimisation formulations are considered. The *centroid-point* approach evaluates the mismatch between the centroid of the simulated particle cloud and a fixed shoreline impact point, thus representing the bulk behaviour of the oil slick. The *particles-point* formulation instead identifies, at each simulation, the particle–time sample that minimises the combined space–time discrepancy with respect to the reference impact point and time, allowing for a more flexible representation of the arrival. Finally, the *first particles-point* approach defines the shoreline impact as the earliest arrival of any particle within a predefined spatial and temporal tolerance around the target, explicitly accounting for the leading edge of the spill. In the small-time configuration, a fourth formulation, referred to as *SAR-derived*, is adopted. In this case, the optimisation is constrained by satellite observations of the oil slick extent, combining information on centroid position, temporal alignment, and the fraction of particles overlapping the observed slick area.

The first outputs obtained by applying Bayesian optimization concerns the calibration

of the transport coefficients with respect to the shoreline impact point fixed along the coast of Pampelonne, assuming an arrival time of 16 October 2018 at 09:00. In this long-time configuration, the objective function is formulated using individual Lagrangian particles, and the calibration is based on identifying the simulated particle–time samples that minimise a combined space–time mismatch with respect to the prescribed shoreline impact point and reference arrival time. For this set-up, the maximum number of optimization iterations is fixed to 100, while the target value of the objective function is set to $J = 0.001$. This non-dimensional threshold is derived from physical tolerances, corresponding to minimum acceptable spatial distances from the impact point and temporal mismatches relative to the reference arrival time. The optimization is therefore terminated as soon as a combination of parameters (α, β) produces an objective value below this threshold, or when the maximum number of iterations is reached. For the optimization function, and based on values commonly reported in literature, α and β are restricted to the ranges $[0, 1]$ and $[0.01, 0.04]$, respectively. Within this framework, a series of optimization runs are performed using the different acquisition functions described in Section 3.4. The resulting optimal parameters and convergence properties are summarised in Table 4.5. As shown in the table, none of the optimization runs reaches the maximum number of 100 iterations, indicating that all acquisition strategies identify satisfactory solutions ($J \leq 0.001$) at an earlier stage of the optimization process. The smallest number of iterations is observed for the Probability of Improvement (PI) strategy, which converges after 26 iterations, whereas the largest number of iterations is required by the Lower Confidence Bound (LCB) strategy, which converges after 62 iterations. In all cases, the optimization identifies parameter combinations yielding values of the objective function well below the prescribed threshold, often by more than one order of magnitude. The estimated values of the wind drag coefficient β are consistent across the different acquisition functions and are in good agreement with the values obtained through the sensitivity analysis. In contrast, the values of the Stokes drift coefficient α exhibit a larger variability, both among the different acquisition strategies and with respect to the value inferred from the sensitivity-based approach. This behaviour can be partly attributed to the wider search interval adopted for α , defined over the range $[0, 1]$, compared to the narrower range imposed for β $[0.01, 0.04]$.

Focusing on the results obtained using the **gp_hedge** acquisition function, which is here treated as a flexible and adaptive strategy, further analysis is conducted to investigate the behaviour of the Bayesian optimization process in the parameter space. Figure 4.18 displays the full sequence of (α, β) pairs explored during the optimization process (48 iterations), with each iteration labelled sequentially and coloured according to the corresponding value of the objective function J . The colour scale highlights the progressive improvement of the optimization: darker colours indicate lower values of J , corresponding to parameter combinations closer to the prescribed target, whereas lighter colours tending towards green and yellow denote higher values of J and thus poorer agreement with the imposed

	Iterations	Best α	Best β	Minimum J
Sensitivity analysis	–	0.3	0.02 (CMEMS, SHOM) 0.03 (IFREMER)	–
PI	26	0.753	0.024	0.0001
EI	58	0.517	0.022	0.0001
LCB	62	0.719	0.022	0.0001
gp_hedge	48	0.659	0.023	0.0008

Table 4.5: Results of the long-time calibration of the transport coefficients. The table reports the optimal values of the Stokes drift coefficient α and wind drag coefficient β obtained from both the sensitivity analysis and the Bayesian optimisation. For each acquisition function, the number of iterations required to meet the stopping criterion and the minimum value of the objective function J , whose threshold was set at $J = 0.001$, are also reported.

space-time constraint. This visualisation allows tracking the evolution of the optimization trajectory in the parameter space and provides insight into the balance between exploration and exploitation achieved by the algorithm. For reference, the red diamond marks the pair (α, β) obtained from the sensitivity analysis performed in previous sections, while the yellow star identifies the optimal parameter combination found by the Bayesian optimization procedure. The comparison between these markers and the sampled points highlights both the departure from the sensitivity-based estimate and the region of the parameter space favoured by the optimization under the imposed objective formulation. Overall, the figure illustrates how the Bayesian optimization initially explores a broad region of the parameter space, sampling diverse combinations of α and β , before progressively concentrating the evaluations around a region associated with lower objective values. This behaviour reflects the adaptive nature of the **gp_hedge** strategy and demonstrates the convergence of the optimization towards an effective set of transport coefficients consistent with the shoreline impact constraint.

As expected from its formulation, the Bayesian optimization procedure aims at progressively reducing the combined space–time discrepancy encoded in the objective function, namely the spatial mismatch between the simulated particles and the shoreline impact point and the temporal mismatch with respect to the reference arrival time. To better illustrate this behaviour, Figure 4.19 shows the evolution of the two physical error components, the spatial error dx (expressed in kilometres) and the temporal error dt (expressed in hours), as a function of the optimization iteration number. The errors are displayed in two different graphs to highlight their differences. At the beginning of the optimization, large errors are observed, particularly for the spatial component dx , which exhibits pronounced peaks reaching values on the order of tens of kilometres. This behaviour reflects the exploratory phase of the Bayesian optimization, during which the algorithm samples a broad region of the parameter space to characterise the objective function and its variability, and therefore a monotonic decrease of the error is not expected. After approximately the first quarter of

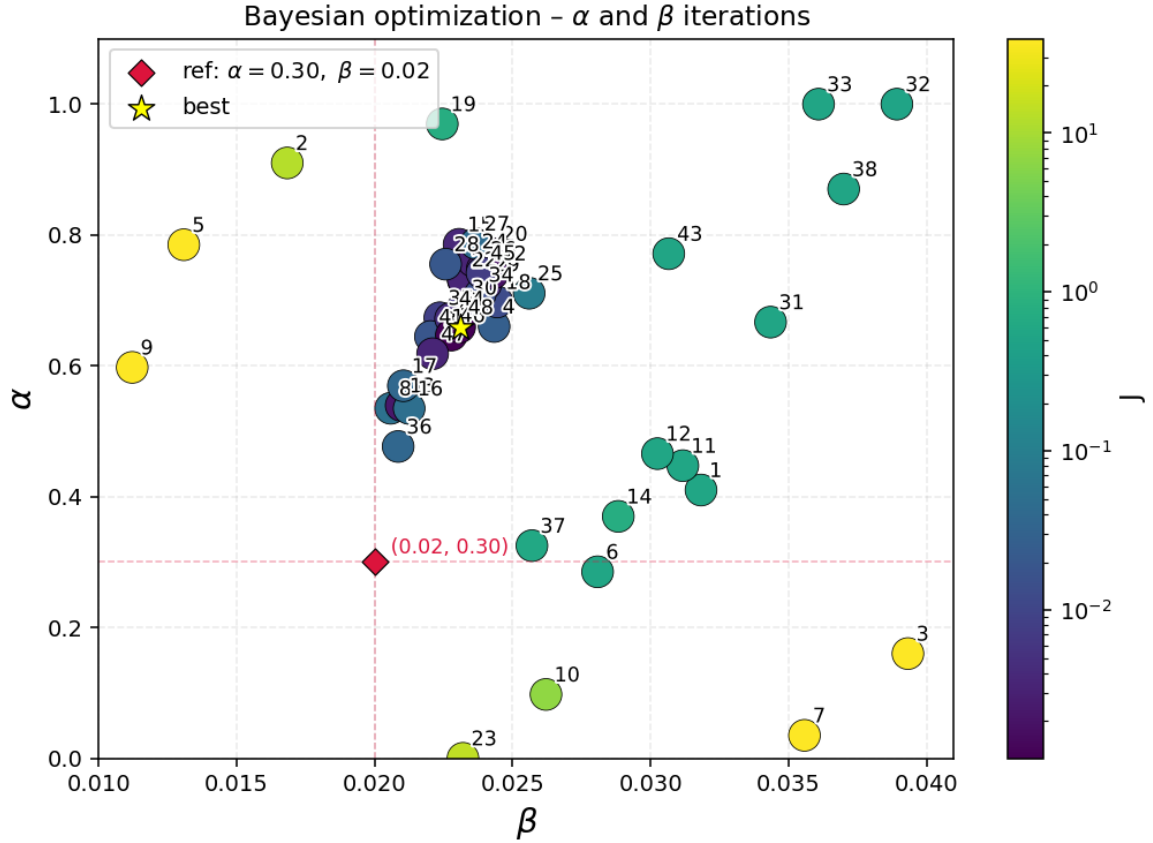


Figure 4.18: Evolution of the Bayesian optimization process in the (α, β) parameter space for the particles-to-point shoreline impact formulation using the `gp_hedge` acquisition strategy. Each point represents one optimization iteration and is coloured according to the corresponding value of the objective function J . The red diamond denotes the parameter pair obtained from the sensitivity analysis, and the yellow star marks the optimal combination identified by the Bayesian optimization.

the iterations, the spatial error progressively stabilises at significantly lower values with the final iterations presenting dx on the order of a few hundred metres, indicating that the optimization has identified a region of the parameter space associated with improved agreement with the shoreline constraint. Occasional spikes in dx observed at later stages correspond to exploratory evaluations introduced by the acquisition strategy to reduce the risk of premature convergence to local minima. In contrast, the temporal error component (dt) exhibits few initial exploratory peaks related to the initial sampling phase, followed by a rapid convergence to zero, where it remains stable for the rest of the optimisation. In the adopted particles-point formulation, dt is evaluated for the particle-time sample that minimises the objective function over all simulated particles and output times, rather than representing the arrival time of the bulk oil slick. Consequently, values of dt close to zero indicate that the best-matching particle is found at the reference output time. This behaviour is consistent with the temporal resolution of the forcing fields, and therefore the temporal error should be interpreted as being effectively constrained by both the objective function formulation and the temporal sampling of the model output, rather than as a continuous quantity that can be reduced below the intrinsic resolution of the forcing.

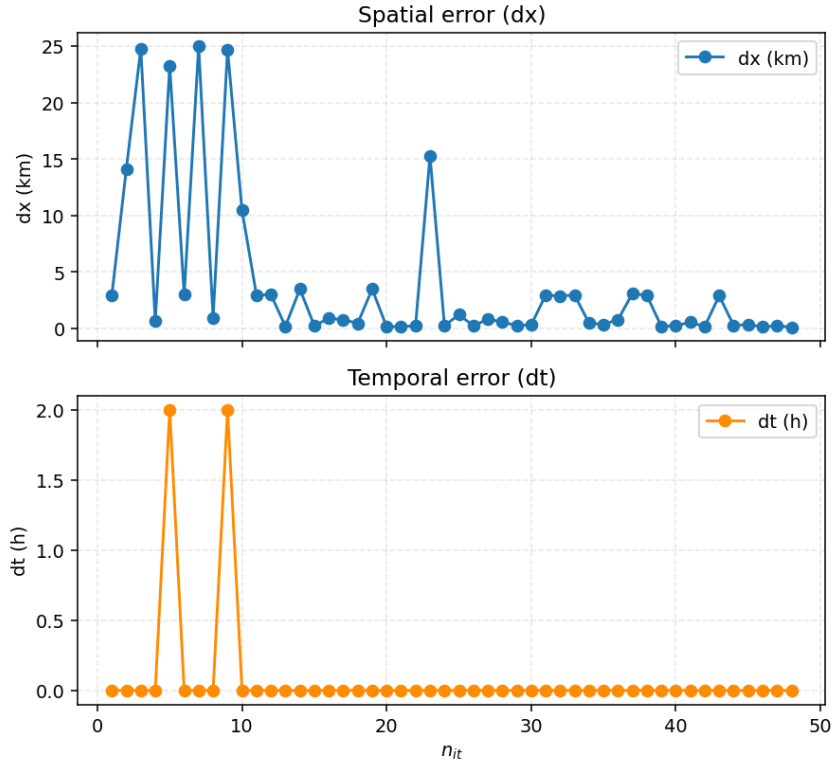


Figure 4.19: Evolution of the physical error components during the Bayesian `gp_hedge` optimization process for the particles-to-point shoreline impact formulation. The upper panel shows the spatial error d_x (in km), while the lower panel shows the temporal error d_t (in hours), both as a function of the iteration number.

Figure 4.20 illustrates the convergence behaviour of the Bayesian optimization by showing the evolution of the best-so-far value of the objective function as a function of the

iteration number. Each point represents the minimum value of the objective function J attained up to a given iteration, while the final optimal value identified by the optimization is highlighted by the red marker. The stepwise structure of the curve reflects the sequential nature of the optimization process. Extended plateaus are observed, during which the best-so-far error remains unchanged over several iterations. These plateaus indicate that the parameter combinations sampled in those iterations yield objective values higher than the current best solution and therefore do not improve the minimum achieved so far. Such behaviour is typical of Bayesian optimization and reflects the balance between exploratory and exploitative sampling guided by the acquisition function. Rapid decreases in the best-so-far error correspond to iterations in which the algorithm identifies a new region of the parameter space associated with a significantly lower mismatch. In the present case, the convergence occurs progressively, with successive reductions of the objective function by more than one order of magnitude, before stabilising close to the prescribed target value. The final iterations show only marginal improvements, indicating that the optimization has effectively converged towards a stable solution and that further evaluations are unlikely to produce substantial gains under the adopted objective formulation and stopping criteria.

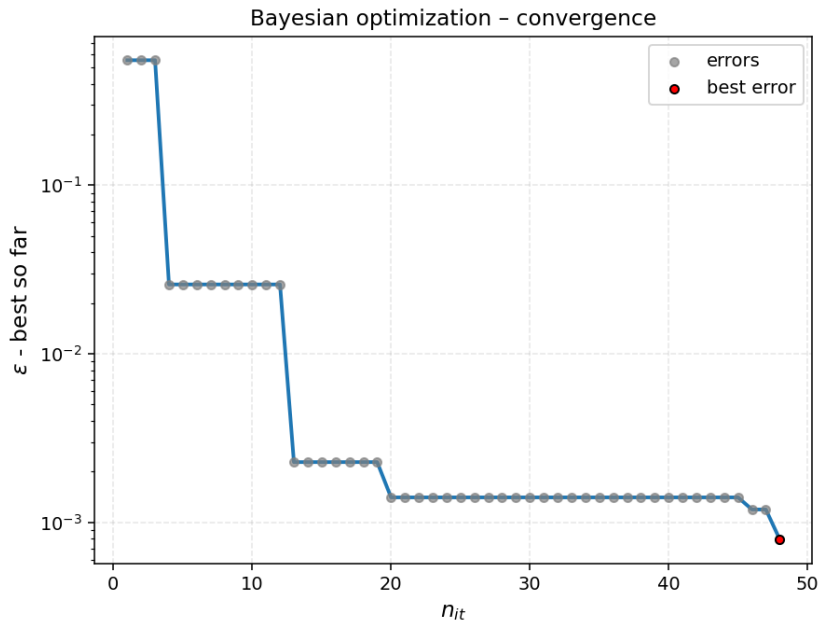


Figure 4.20: Evolution of the best-so-far value of the objective function J as a function of the iteration number. The red marker highlights the final optimal value reached by the optimization.

For the centroid-to-point shoreline scenario, for the calibration based on the comparison between simulated trajectories and SAR-derived slick observations, and for the first-arrival particle formulation introduced above, only the results obtained using the `gp_hedge` acquisition strategy are reported. This choice is motivated by both methodological and computational considerations. From a methodological perspective, `gp_hedge` provides an

adaptive optimisation strategy by dynamically combining standard acquisition functions (Expected Improvement, Probability of Improvement, and Lower Confidence Bound) according to their past performance, thereby reducing the sensitivity of the results to a single, fixed exploration-exploitation trade-off. From a computational perspective, the explicit identification of first-arrival events within prescribed spatial and temporal constraints substantially increases the cost of each objective function evaluation, making a systematic comparison across multiple acquisition functions impractical.

In all four configurations, the maximum number of optimisation iterations is fixed to 100 in order to ensure a consistent computational budget across the different calibration experiments. The stopping criterion based on the target value of the objective function is instead adapted to the considered specific formulation. For the centroid-to-point shoreline formulation and for the SAR-based calibration, the target value is set to $J = 1$, reflecting the increased dimensionality and complexity of the corresponding objective functions, which combine multiple spatial, temporal, and geometric components. In contrast, for the first-arrival particle formulation, a more stringent target value of $J = 0.1$ is adopted, consistent with the discrete and more restrictive definition of the shoreline impact event in this case. These choices ensure that the optimisation process is neither prematurely terminated nor excessively prolonged, while maintaining a physically meaningful interpretation of the stopping criteria across the different formulations.

Table 4.6 summarises the results obtained for the different calibration configurations considered in this study, namely the particles-to-point formulation, the first-arrival particle formulation, the centroid-to-point formulation, and the SAR-derived calibration. All optimisation experiments are performed using the instantaneous release of particles and the `gp_hedge` acquisition strategy, with a maximum number of 100 iterations. With the exception of the particles-to-point formulation, all configurations reach the maximum number of iterations before satisfying the prescribed stopping criterion, indicating an increased complexity of the corresponding calibration problems. In the case of the first-arrival particle formulation, the optimisation approaches the target objective value closely but does not fully satisfy it within the allocated computational budget, reflecting the restrictive nature of the spatial and temporal constraints imposed on the definition of the shoreline impact event. A particularly noteworthy result concerns the values of the transport coefficients inferred from the first-arrival particle calibration, for which both α and β are in very good agreement with the values previously estimated through the sensitivity analysis, confirming the ability of this formulation to accurately capture the dynamics governing the earliest particle arrivals on the shoreline. Across all configurations, the estimated values of the wind drag coefficient β remain remarkably consistent and close to 0.02, reflecting the relatively narrow and well-constrained search interval adopted for this parameter. In contrast, the optimal values of the Stokes drift coefficient α exhibit a pronounced dependence on the calibration strategy. In the SAR-derived calibration,

α reaches its upper bound, which corresponds to a full inclusion of the Stokes drift contribution in the advective velocity. While this choice improves the agreement with short-term satellite observations, it proves inconsistent when extended to long-term shoreline impact simulations, as the resulting trajectories lead to a simulated coastal arrival located significantly north of the observed contamination at Pampelonne beach, as illustrated in Figure 4.22. This result highlights the scale-dependent nature of the calibration problem and confirms that parameter values optimised for short-term, satellite-based observations cannot be directly transferred to long-term shoreline impact simulations without loss of accuracy.

Figure 4.21 shows a small-time comparison between the SAR-derived simulation (green) and the first particle-point simulation (orange), against the SAR-observed oil slick (red shapefile). At small-time scales (09 October 2018, 19:00), the SAR-derived simulation (in green) appears slightly better aligned with the actual slick shape, meaning that a larger fraction of particles may fall within the observed extent. However, the difference between the two simulations remains relatively modest.

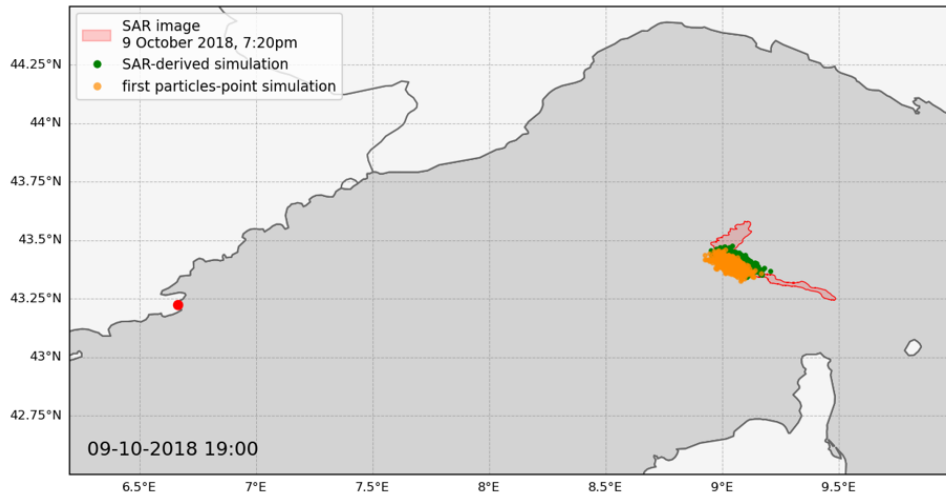


Figure 4.21: Short-time comparison (09 October 2018, 19:00) between the SAR-observed slick (red), the SAR-derived simulation (green), and the first particle-point simulation (orange). The SAR-derived configuration better reproduces the observed slick geometry at early times.

However, as shown in Figure 4.22, the behaviour at larger time scales (16 October 2018, 09:00) reveals the limitations of the SAR-derived calibration. Although tuned to match short-term satellite observations, the associated coefficients lead to trajectories that do not reproduce the correct coastal arrival location and timing. In particular, the SAR-derived simulation (green) fails to reach the observed contamination point along the coastline, whereas the first particle-point simulation (orange) approaches the coastal area more consistently with the observed impact.

The comparison between long-term shoreline-based calibrations and short-term SAR-

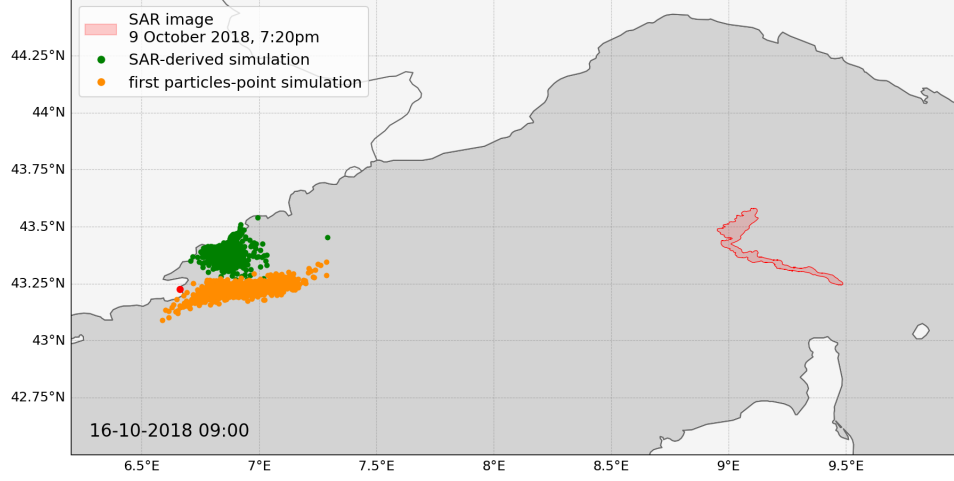


Figure 4.22: Large-time comparison (16 October 2018, 09:00) between the SAR-observed slick (red), the SAR-derived simulation (green), and the first particle-point simulation (orange). The SAR-derived calibration fails to reproduce the correct shoreline impact in space and time.

	Iterations	Best α	Best β	Minimum J
particles-point	48	0.659	0.023	0.0008
first particles-point	100	0.327	0.020	0.248
centroid-point	100	0.175	0.020	6.453
SAR-derived	100	1.000	0.020	5.016

Table 4.6: Results of the Bayesian optimisation using the `gp_hedge` acquisition strategy for the different calibration configurations considered in this study. The table reports, for each configuration, the number of iterations performed, the optimal values of the Stokes drift coefficient α and wind drag coefficient β , and the minimum value of the objective function J reached during the optimisation.

based calibrations reveals a clear scale dependence in the inferred transport parameters. While the wind drag coefficient β exhibits a remarkable consistency across all calibration strategies and temporal scales, with optimal values systematically close to 0.02, the Stokes drift coefficient α shows a markedly different behaviour. In particular, α tends to be significantly overestimated in the short-term calibration based on satellite observations, where the optimisation favours a full inclusion of the Stokes drift contribution in order to reproduce the early evolution of the surface slick. This choice, however, proves inconsistent when extended to long-term simulations, leading to erroneous shoreline impact locations and an overestimation of the cumulative wave-driven transport. The results therefore indicate that parameter values optimised against short-term observations cannot be directly transferred to long-term shoreline impact simulations, and that the calibration of α must explicitly account for the temporal scale and the physical processes dominating the transport at different stages of the spill evolution.

Following the comparison of small-time and long-time calibrations, an additional diagnostic analysis is performed to evaluate the scale dependence of the transport coefficients obtained. In particular, the evolution of the absolute Lagrangian dispersion is examined to determine whether the small-time calibration remains consistent as the simulation progresses beyond the Lagrangian velocity memory scale. Figure 4.23 shows the temporal evolution of dispersion for the SAR-derived (small-time calibrated) configuration, represented by the blue curve. Two power-law fits from Eq. 3.17 are performed in logarithmic space over selected early-time (orange) and late-time (green) windows. The estimated exponents are $p \approx 3.11$ for the early interval and $p \approx 2.44$ for the later one. These values describe the effective growth rate of dispersion within the chosen windows and are used here exclusively as empirical finite-time descriptors. Two characteristic time markers are included in Figure 4.23. The blue dotted line denotes the Lagrangian integral time T_L , obtained from the velocity autocorrelation function as the time up to its first zero crossing. This timescale indicates the decorrelation time of particle velocities. The purple dotted line marks the diagnostic transition time T_s , defined as the moment when the local slope of $a^2(t)$ falls below a prescribed threshold, indicating a change in the apparent growth regime. Unlike T_L , T_s does not correspond to a fundamental flow timescale. For reference, the red dashed line shows the SAR acquisition time, and the nearest model state is marked in red. The dark red vertical line corresponds to the coastline reference time (16 October 2018 at 09:00). In this configuration, the SAR observation occurs significantly earlier than the shoreline constraint, and the temporal separation between the two exceeds T_L . This implies that the small-time calibration informed by SAR imagery is applied to a dynamical regime that evolves beyond the velocity-memory timescale. The interpretation of the fitted scaling exponents and diagnostic times is still dependent on the chosen fitting windows and model configuration.

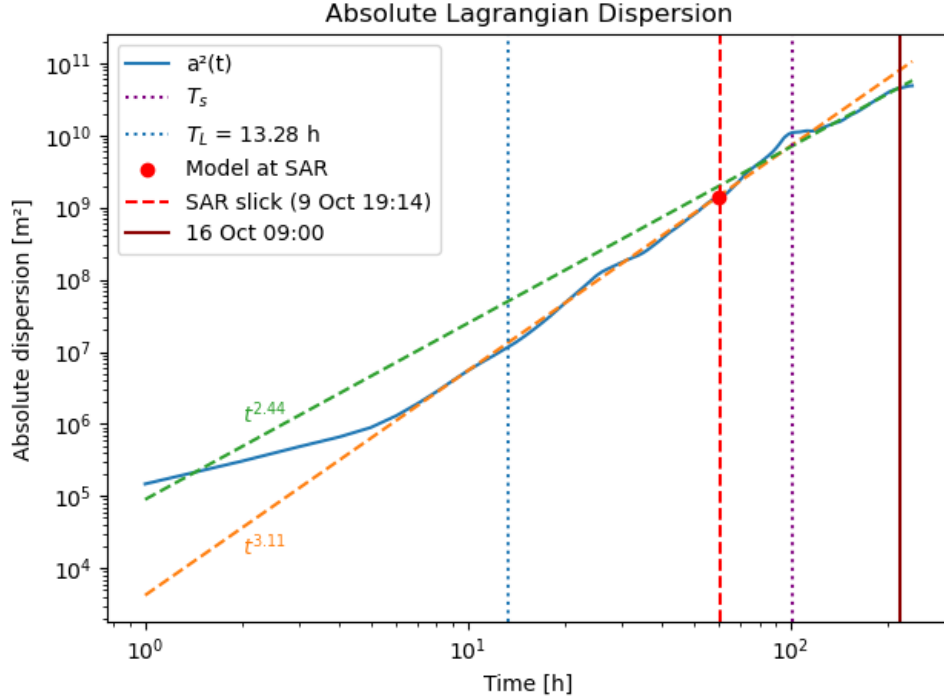


Figure 4.23: Representation of the absolute Lagrangian dispersion for the SAR-derived (small-time calibrated) configuration.

4.6 Absolute and relative wind

This section presents results that are based on a direct comparison between simulations performed using absolute and relative wind formulations. Unlike previous analyses, probability maps and centroid trajectories are not shown here. This is to improve the visual clarity of the particle dispersion patterns. The display of probability information is associated with the appearance of particles in low-density regions with very light colours, creating difficulty in the clear distinction between absolute and relative wind cases. Similarly, at certain stages of the simulation, the centroid positions evolving in time can be visually confused with individual particles, potentially misleading the interpretation of the dispersion dynamics. Representing all particles with uniform colours makes it easier to compare the two simulations. It is clear from these results that particles advected using absolute wind forcing (orange) travel slightly faster than those driven by relative wind forcing (green). Although this difference is slight, it is consistent throughout the simulation (4.24).

In order to quantitatively assess this behaviour, the distance between the centroids of the two simulated particle clouds is computed as a function of time. The resulting time series shows an increase in centroid separation from the beginning of the simulation, indicating gradual divergence between the absolute and relative wind solutions. The distance reaches a maximum shortly before the particles begin to interact with the coastline, after this point, a decrease is observed as expected (4.25). This reduction is due to the loss of particles

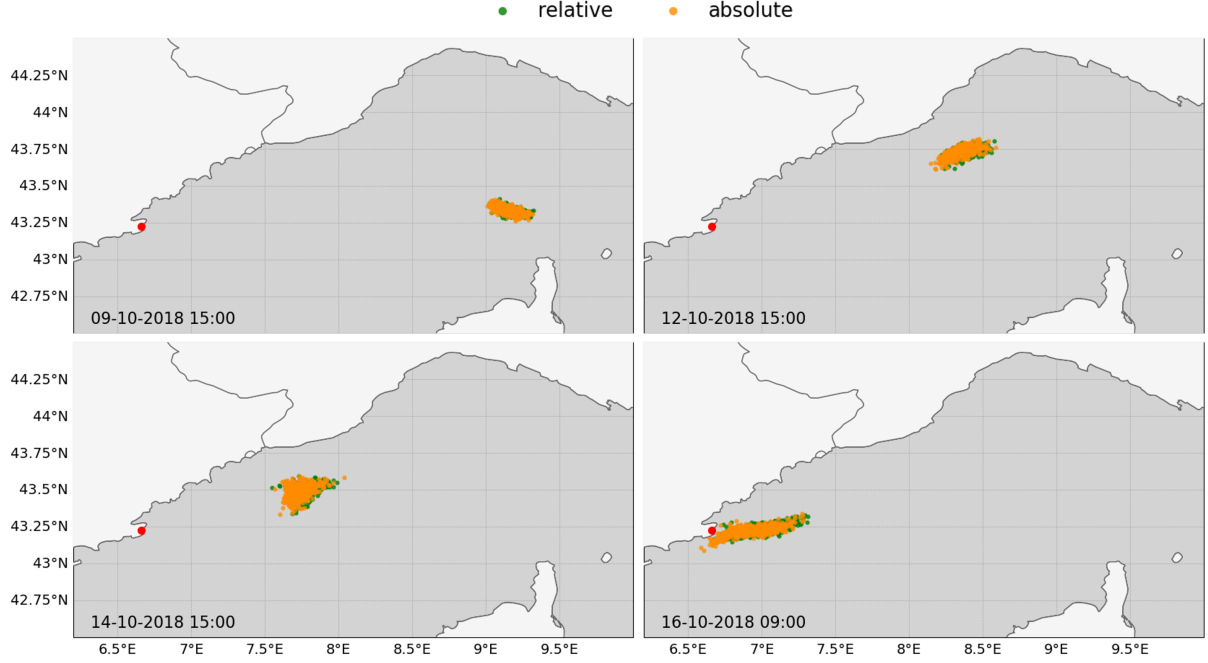


Figure 4.24: Evolution of oil spills with relative (green) and absolute wind (orange). From top-left to bottom-right: 09/10/2018 15:00, 12/10/2018 15:00, 14/10/2018 15:00, 16/10/2018 09:00. The red dot represents the area of impact on the beach of Pampelonne in France, when traces were found on the 16/10/2018 presumably in the early morning.

upon arrival at the coast and their subsequent beaching. This reduces the number of particles that contribute to the centroid calculation towards the end of the simulation. In addition to the centroid distance, the graph also shows the evolution of the characteristic cloud size $L_n(t)$ for each simulation, defined as the root mean square dispersion of particles around their centroid and plotted on the right axis. The dashed green line corresponds to the absolute wind case, while the dotted orange line corresponds to the relative wind case.

Even though the maximum distance between the two centroids is relatively small at around 5 km before coastal interaction, this result is significant nonetheless. It shows that even slight differences in how the wind drag term is formulated can cause measurable and consistent changes in particle trajectories over time. Previous studies have reported similar sensitivity of surface transport to parametrizations related to wind, particularly in regimes dominated by wind and waves (Dagestad and Johannes Röhrs 2019b). It is worth noting that the observed growth in centroid separation is likely to be limited by the finite duration of the simulation and by particle interaction with the coastline. Without such boundary constraints and over a longer simulation period, the cumulative effect of the different wind formulations could potentially lead to an increase in the separation between the two particle clouds.

The non dimensional results of the distances between the centroids are now presented. This method allows the centroid separation to be interpreted in relation to the cloud size, providing a scale-aware measure of the divergence between the two wind formulations, the

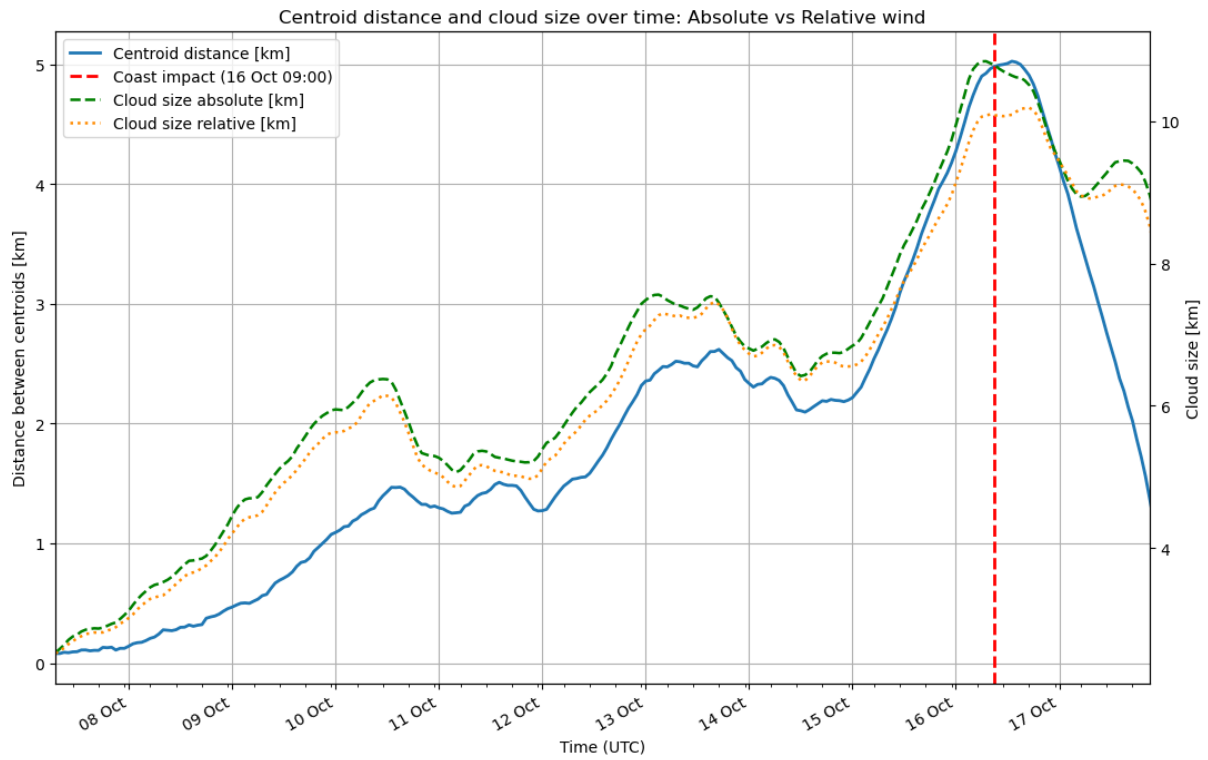


Figure 4.25: Evolution in time of centroids distance [km] between absolute and relative simulations. The dashed green line represents the cloud size for the absolute wind simulation, while the dotted orange line represents the cloud size for the relative wind simulation.

results are visible in Figure 4.26.

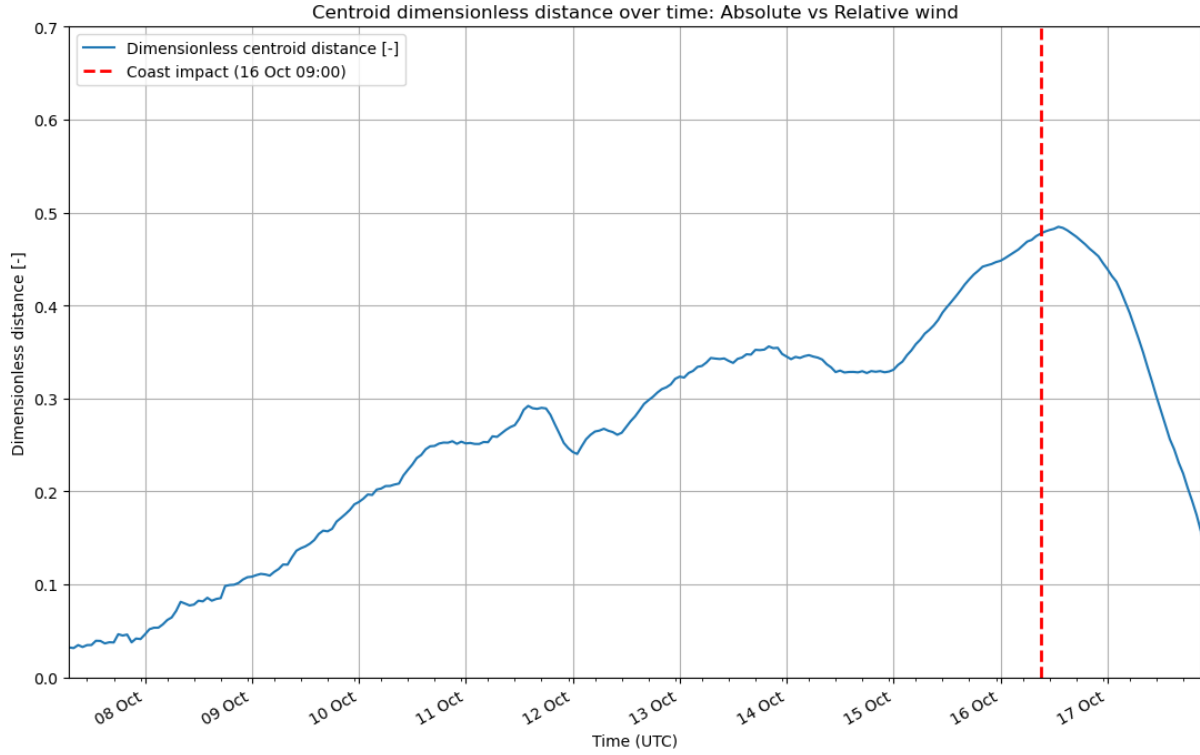


Figure 4.26: Evolution in time of centroids non dimensional distance between absolute and relative simulations.

Toward the final stages of the simulation particles begin to interact with the coastline, leading to progressive particle loss. Since both the centroid position and the cloud size $L_n(t)$ are ensemble-based quantities, their values may be influenced by this removal process. For this reason, the onset of coastal interaction is indicated in the figure by a vertical red line. Values of $d^*(t)$ after this time are interpreted with caution, as they may reflect not only dynamical differences between the wind formulations but also statistical changes in the particle ensemble.

On the basis of these findings, and considering the physical consistency of the relative wind formulation for representing direct aerodynamic drag, subsequent simulations and analyses presented in this thesis adopt the relative wind approach. The results obtained from the comparison between absolute and relative wind formulations in the absence of the diffusive term show an overall behaviour that is very similar to that observed in Figures 4.24 and 4.25. As in the simulations including diffusion, the particle cloud advected using absolute wind forcing (orange) exhibits a slightly faster propagation than the one obtained using relative wind forcing (green), although the difference between the two cases remains small.

This behaviour is also reflected in the temporal evolution of the distance between the centroids of the two particle clouds (Fig. 4.28). The centroid separation displays the same qualitative trend as in the diffusive case, with a gradual increase over time, reaching a

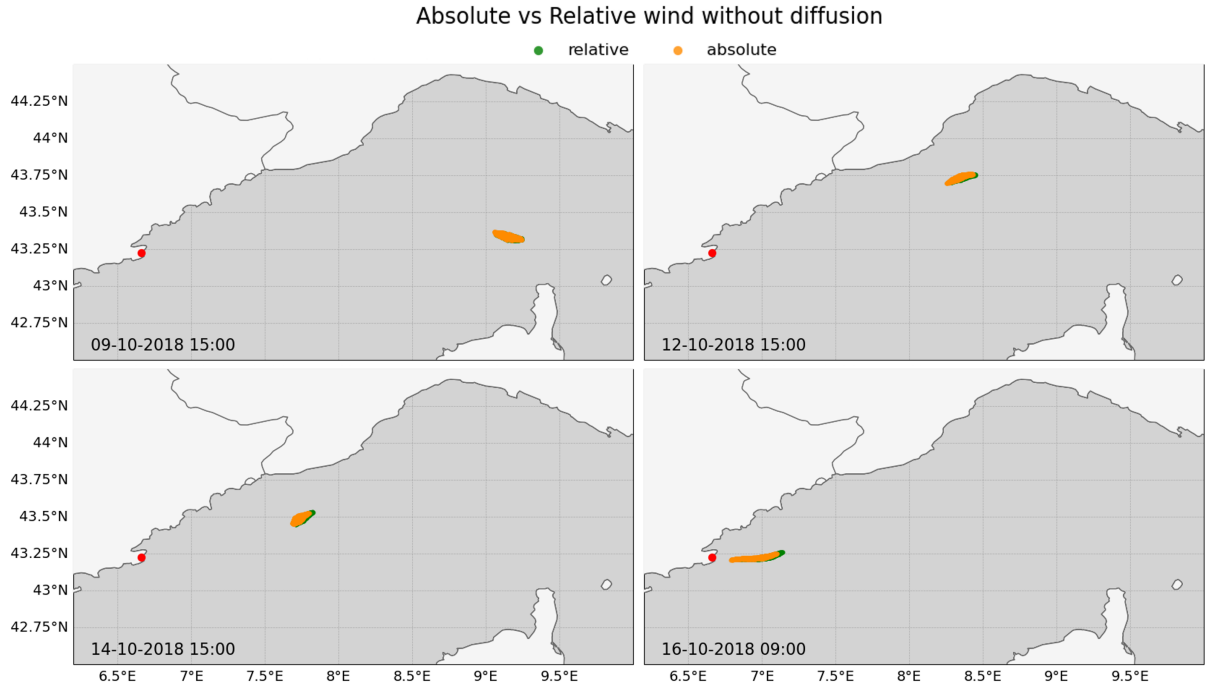


Figure 4.27: Evolution of oil spills with relative (green) and absolute wind (orange), without the diffusion component. From top-left to bottom-right: 09/10/2018 15:00, 12/10/2018 15:00, 14/10/2018 15:00, 16/10/2018 09:00. The red dot represents the area of impact on the beach of Pampelonne in France, when traces were found on the 16/10/2018 presumably in the early morning.

maximum distance of approximately 4 km, followed by a decrease once particles begin to interact with the coastline. This reduction is again associated with particle loss due to coastal arrival, which affects the centroid computation toward the final stages of the simulation. The figure also shows the corresponding evolution of the cloud size for the two simulations, with green indicating the absolute wind case and orange the relative wind case.

The non dimensional centroid separation $d^*(t)$ is also evaluated for the simulations without diffusion, and the corresponding results are shown in Figure 4.29.

An interesting aspect emerging from the simulations without diffusion is that, despite the removal of the stochastic spreading mechanism, the overall dynamical behaviour of the system remains almost unchanged. For this specific case, this suggests that the transport is primarily controlled by the advective component associated with the regional circulation, with diffusion playing a secondary role. However, this behaviour depends strongly on the specific environmental conditions of the event and generalisation is not possible.

The main difference with respect to the diffusive case is that the particle cloud occupies a smaller spatial area, which results in a delayed interaction with the French coastline. This effect is visible in Figure 4.27, where, in the bottom-right panel corresponding to 16 October at 09:00, the oil slick has not yet reached the reference coastal location, in contrast to the diffusive simulation. It should be noted that this delay is not indicative of an

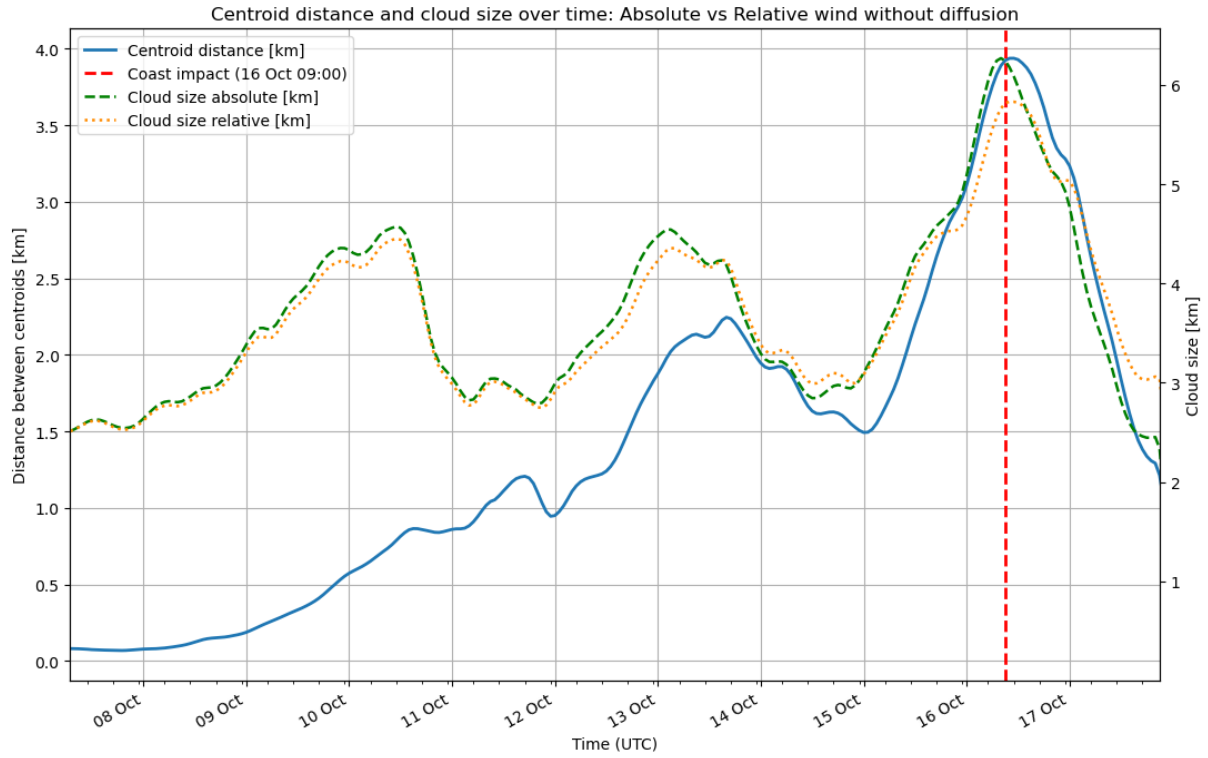


Figure 4.28: Evolution in time of centroids distance [km] between absolute and relative simulations without the diffusion component. The dashed green line represents the cloud size for the absolute wind simulation, while the dotted orange line represents the cloud size for the relative wind simulation, both without the diffusion component.

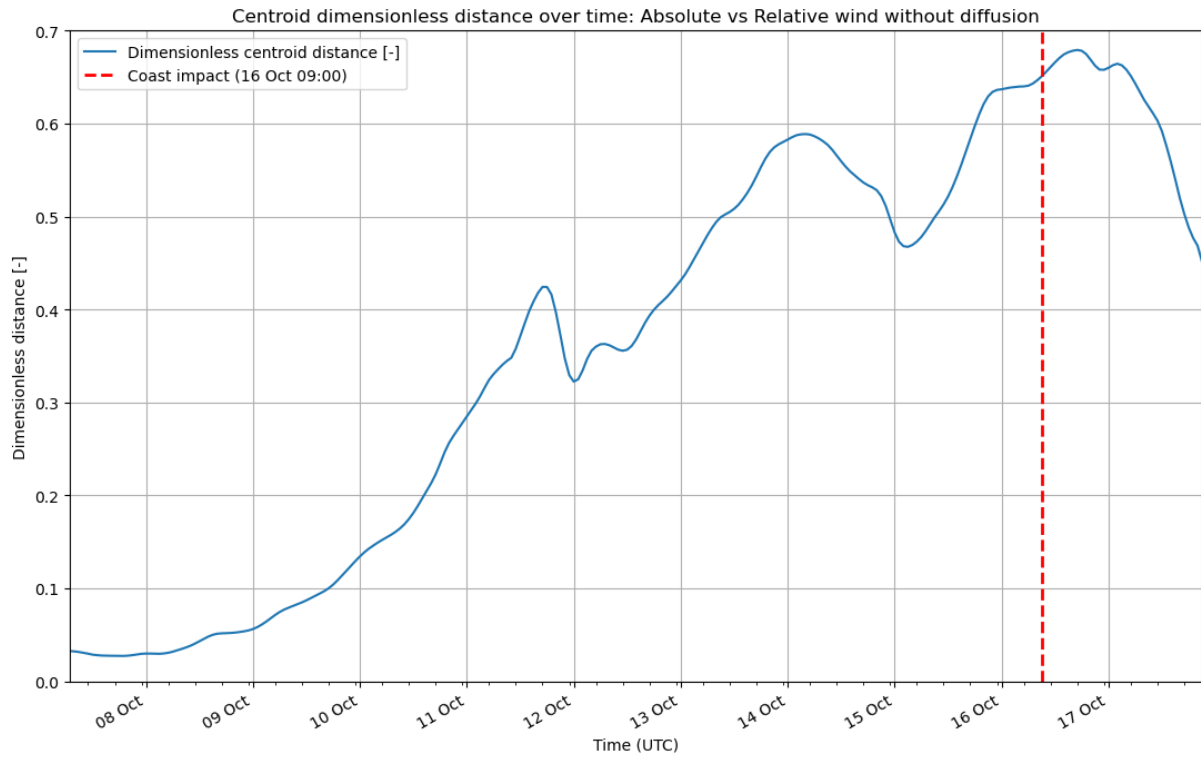


Figure 4.29: Evolution in time of centroids non dimensional distance between absolute and relative simulations without the diffusion component.

improved physical representation, but rather a direct consequence of using the same wind and wave coupling coefficients (α and β) adopted in the simulations including diffusion. Since stochastic diffusion contributes to the effective spreading and transport of particles, the removal of this term would require a re-tuning of the model coefficients to optimally reproduce the observed transport.

From Figure 4.30, the ensemble-mean Lagrangian velocity autocorrelation functions exhibit a rapid decay over the first few hours, indicating a short Lagrangian memory of velocity fluctuations. At longer time lags, weak oscillations around zero are observed, consistent with the progressive loss of correlation along particle trajectories.

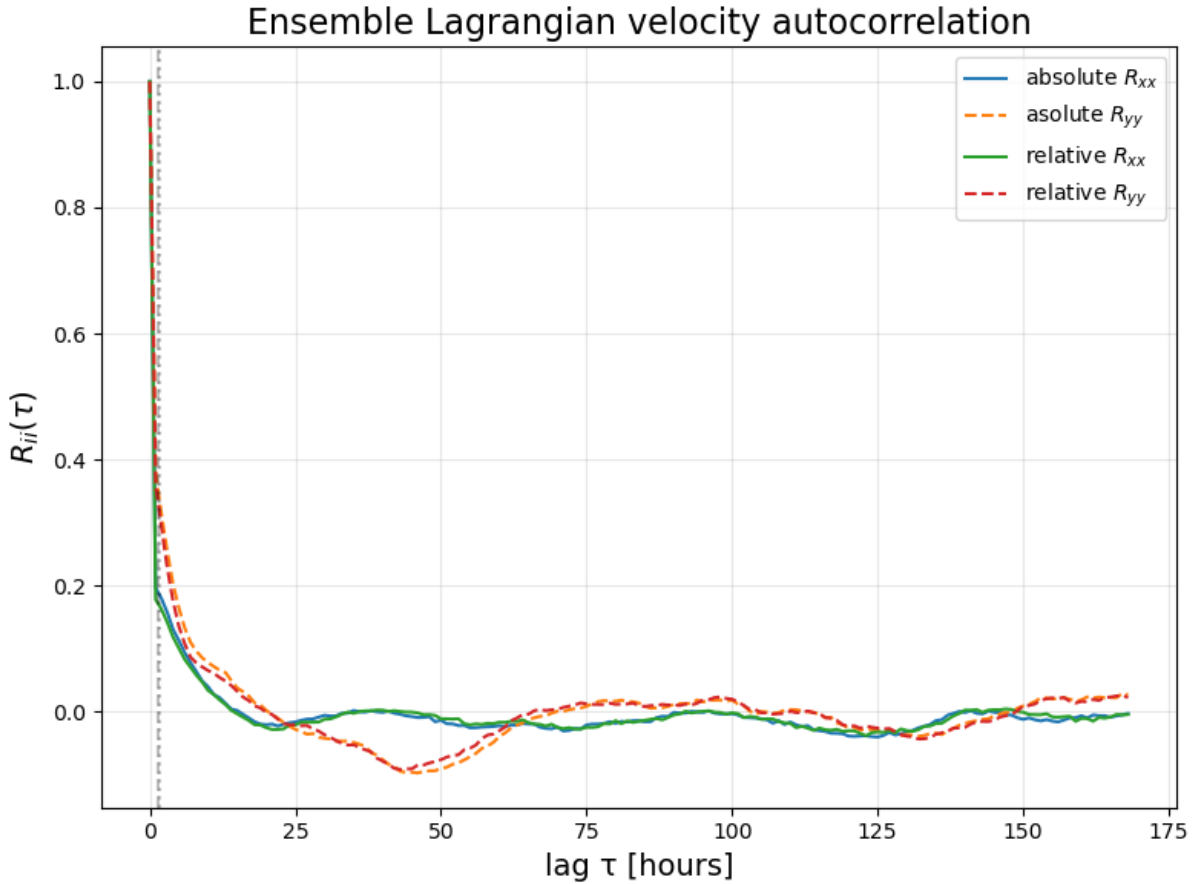


Figure 4.30: Ensemble-mean Lagrangian velocity autocorrelation functions $R_{xx}^L(\tau)$ and $R_{yy}^L(\tau)$ computed for particle dispersion simulations forced with absolute and relative wind formulations. Solid lines denote the zonal component (R_{xx}), while dashed lines denote the meridional component (R_{yy}).

Differences between simulations forced with absolute and relative wind formulations are primarily observed at short time scales comparable to the Lagrangian decorrelation time, while at longer time lags the autocorrelation functions converge toward near-zero values. A slightly slower decay is observed for the meridional component compared to the zonal one, suggesting a degree of anisotropy in the near-surface velocity fluctuations. The estimated decorrelation timescales are of the order of about 1-3 hours for both the zonal

and the meridional components, with slightly smaller values obtained when relative wind forcing is applied (Table 4.7). These values are consistent with previous observational and modelling studies of near-surface Lagrangian motion, suggesting that in the present configuration, the influence of relative wind is mainly expressed through short-time velocity fluctuations rather than through modifications of the mean advective transport. While the use of relative wind forcing results in measurable differences in the short-time behaviour of the Lagrangian velocity autocorrelation, the resulting decorrelation time scales T_L differ only marginally from those obtained using absolute wind forcing. This limited sensitivity reflects the fact that T_L primarily characterises the persistence of velocity fluctuations at short timescales, whereas the mean advective transport is dominated by larger-scale and longer-lived flow structures. As a consequence, modifications to the wind formulation mainly affect the high-frequency component of the Lagrangian velocity signal, while the integral time scale remains of the same order of magnitude.

	x	y
T_L absolute wind [h]	1.67	2.68
T_L relative wind [h]	1.55	2.38

Table 4.7: Lagrangian decorrelation time scales T_L , in hours, estimated from the ensemble-mean velocity autocorrelation for simulations forced with absolute and relative wind formulations.

This analysis shows that metrics based on centroids reveal only minor differences in large-scale transport between the absolute and relative wind formulations. However, Lagrangian velocity autocorrelation highlights small but consistent differences over short time scales. This indicates that the wind formulation mainly affects velocity fluctuations at high frequencies rather than mean advective transport. While these differences are physically meaningful, their overall impact on particle dispersion is limited in this case and may depend on specific environmental conditions.

4.7 Oil Weathering outcomes

The weathering results for the light oil case are illustrated in Figure 4.31. The droplet size distribution spans from 10 μm to 500 μm , consistently with the diameter interval prescribed in the numerical setup. The histograms on the left panel show the number of Lagrangian particles falling within each diameter or velocity bin. In other words, they show the numerical frequency distribution resulting from the imposed size spectrum. This distribution reflects the prescribed, truncated log-normal droplet size spectrum that is used to represent lower-viscosity oils. Under turbulent forcing, these oils are expected to exhibit increased breakup and the presence of smaller droplets. The rise velocity distribution, in the central panel, exhibits a strong concentration at low velocities, with a

maximum value of 0.0243 m s^{-1} . This behaviour is physically consistent with buoyancy-driven rise under low-to-moderate Reynolds number conditions. For smaller droplets, Stokes scaling provides a useful first-order approximation, implying that terminal rise velocity increases approximately with droplet diameter (the classical Stokes limit yields $w \propto d^2$). Consequently, the predominance of small droplets results in reduced rise velocities and longer periods of time spent within the water column. The velocity–depth scatter plot, shown in the right panel, further illustrates this relationship, demonstrating that droplets with lower rise velocities are distributed over a broader depth range and reach a maximum depth of 15.85 m. This suggests that smaller droplets are more susceptible to vertical turbulent mixing before they resurface. The colourbar represents the depths, with darker colours corresponding to particles located at greater depths and lighter colours, progressively shifting toward yellow, indicating droplets closer to the surface.

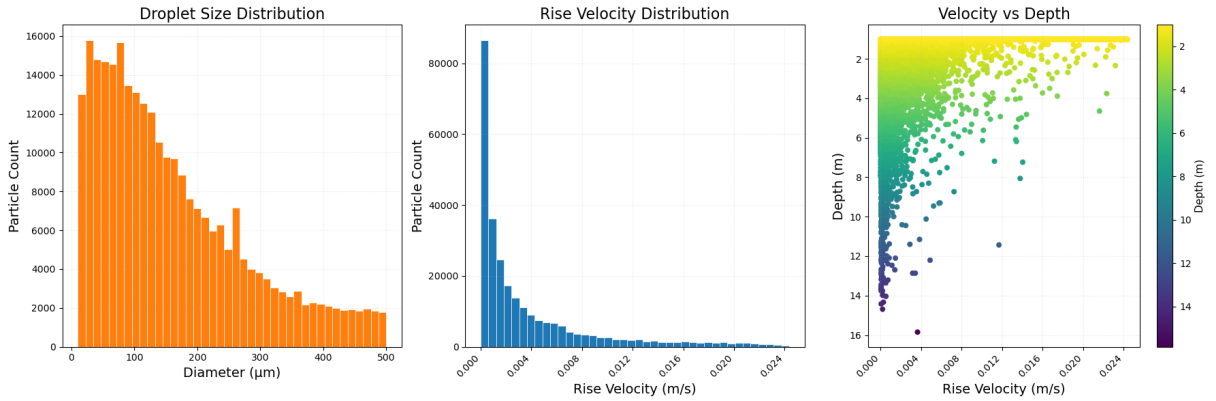


Figure 4.31: Weathering results for the light oil case. Left panel: droplet diameter distribution. Central panel: distribution of rise velocities. Right panel: velocity–depth scatter plot showing the relationship between rise velocity and vertical position.

The results for heavy oil are shown in Figure 4.32. The particle diameters are larger than in the light oil case, as the the model parameters are defined to represent the physical properties of heavier oil types. This reflects the decrease in fragmentation resulting from the oil’s higher viscosity and the size distribution is shifted toward larger diameters compared to the light oil case. The different shapes of the droplet size histograms are not only due to the imposed diameter ranges, but are primarily due to the parameters of the truncated lognormal sampling method used in each case. In the light oil simulation, for example, the larger dispersion parameter leads to a higher concentration of droplets near the lower bound of the prescribed interval. The smaller dispersion parameter used for the heavy oil case, on the other hand, produces a narrower, less asymmetric distribution with droplet sizes distributed more evenly around the central portion of the range. The corresponding rise velocity distribution for heavy oil is therefore shifted toward higher values, reaching a maximum of 0.03 m s^{-1} . An increase in droplet size directly leads to a more rapid rise to the surface, reducing the time spent within the water column. The

velocity–depth relationship confirms this, showing faster vertical transport and a maximum depth of 12.84 m. The absence of very small droplets limits the persistence of the oil phase at greater depths.

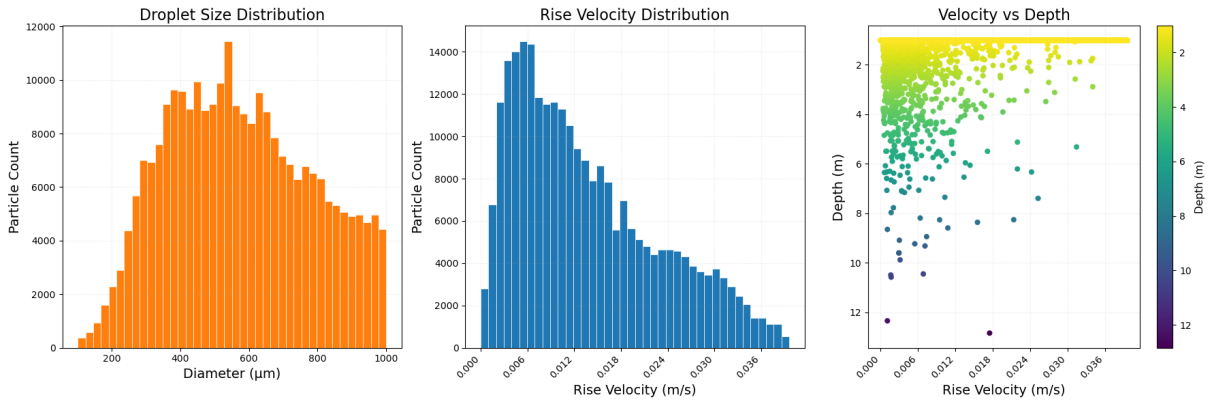


Figure 4.32: Weathering results for the heavy oil case. Left panel: droplet diameter distribution. Central panel: distribution of rise velocities. Right panel: velocity–depth scatter plot showing the relationship between rise velocity and vertical position.

Table 4.8 presents a summary of the diameter ranges and resulting dynamical metrics. The comparison reveals a consistent pattern of physical behaviour with the case involving light oil, characterised by smaller droplets, exhibits lower rise velocities and deeper vertical depth. In contrast, the case involving heavy oil, dominated by larger droplets, shows faster resurfacing and reduced maximum depth.

It is important to emphasise that these differences arise from the intrinsic physical scaling of buoyant rise and the intervals of defined droplet sizes adopted in the simulations.

	Light Oil	Heavy Oil
Minimum droplet diameter (μm)	10.0	100.7
Maximum droplet diameter (μm)	500.0	999.9
Maximum rise velocity (m s^{-1})	0.0243	0.0396
Maximum depth (m)	15.85	12.84

Table 4.8: Droplet diameter ranges and resulting dynamical metrics for the light and heavy oil simulations.

The slower rise of smaller droplets is a direct consequence of the balance between buoyancy and viscous drag. Under Stokes-type conditions, the buoyant force is proportional to the volume of the droplet, while the viscous resistance is proportional to the diameter of the droplet. At terminal velocity, this results in a quadratic dependence of rise velocity on droplet diameter ($w \propto d^2$). Therefore, the influence of viscous drag on smaller droplets is relatively stronger compared to the influence of buoyant forcing, resulting in reduced rise velocities.

The temporal evolution of the submerged particle fraction for both heavy and light oil is reported in Figure 4.33. Throughout the simulation, a clear difference between the

two oil types is observed with the light oil (blue line in the upper graph) consistently exhibits non-zero submerged fractions, which can become relatively high during energetic conditions. The heavy oil (orange line in the upper graph), however, shows very low submerged percentages over the entire period, with only moderate increases during stronger wave events. This behaviour is in line with the intrinsic properties of the two oils. The lighter oil, characterised by lower density and viscosity, is more easily entrained below the surface by wave-induced turbulence and breaking processes. In contrast, the heavier oil is less responsive to surface forcing and tends to remain closer to the surface as its physical properties limit vertical mixing. In all panels, a black dashed vertical line indicates the time at which the oil slick reaches the coastline. After this point, a decrease in the submerged light fraction can be seen in the top panel, even though the waves remain energetic. This reduction is not due to weakening of the sea state, but rather to the gradual accumulation of particles on the coastline, which reduces the number of particles in the water column and limits further entrainment. Two main entrainment events are clearly visible in the upper panel, occurring around 11 and 15–16 October. During these periods, the submerged fraction of the light oil increases noticeably, whereas the heavy oil shows only minor peaks. These events coincide with the wave conditions shown in the middle panel, where there is a substantial increase in the significant wave height. The simultaneous growth of H_s and T indicates the development of a more energetic sea state. The lower panel shows the deep-water wave steepness, computed as $S = H_s/(gT^2)$. Although steepness increases during these energetic events, the enhancement is primarily driven by the growth in H_s . In physical terms, greater wave heights imply higher wave energy and increased turbulence caused by breaking waves, which promotes the entrainment of droplets below the surface. However, the persistence of submerged particles is not only controlled by wave forcing, but also by droplet rise velocity. Smaller light-oil droplets remain within the water column for longer once entrained, resulting in sustained submerged fractions. In contrast, larger heavy-oil droplets resurface more rapidly. These results suggest that the intensity of entrainment is influenced by wave energy, while the duration of subsurface presence is governed by buoyant dynamics dependent on droplet size.

The spatial and temporal evolution of the oil slick under atmospheric conditions is illustrated in Figure 4.34 for light oil and in Figure 4.35 for heavy oil, showing different time intervals. In these maps, the colour of the particles represents their vertical position, with yellow tones indicating droplets located near the surface and progressively darker shades corresponding to greater depths. The background layer shows the significant wave height, allowing a qualitative assessment of the relationship between wave conditions and the vertical distribution of particles. In the case of light oil, the slick exhibits significant vertical variability over time, right from the early stages. During periods of increased wave activity, a greater number of particles appear darker in colour, indicating a greater presence in the subsoil. This behaviour is consistent with wave-induced entrainment,

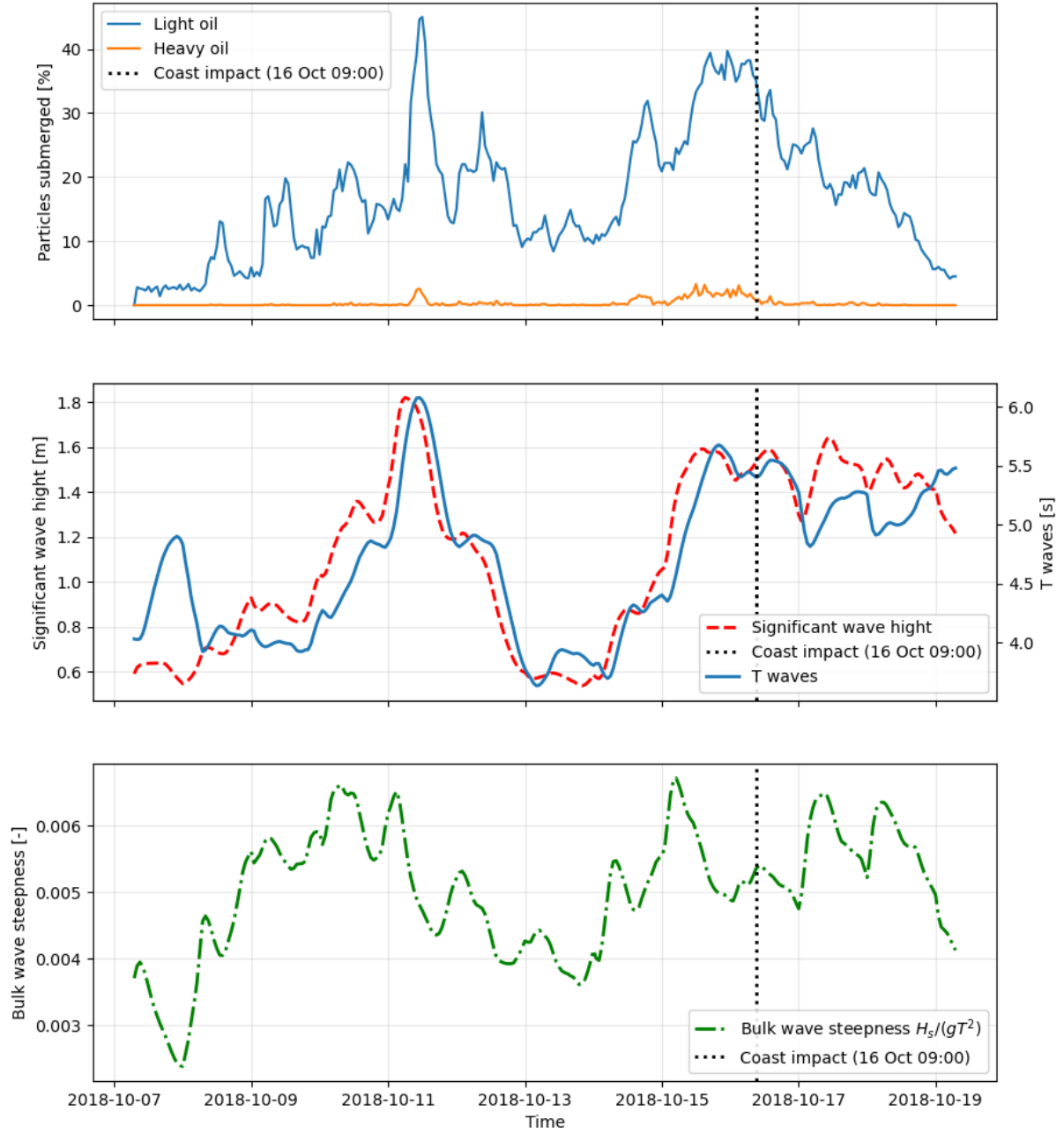


Figure 4.33: Upper panel - Temporal evolution of the submerged particle fraction for light and heavy oil. Middle panel - Combined significant wave height H_s and mean wave period T . Lower panel - Bulk deep-water wave steepness. The black dashed vertical line indicates the time at which the oil slick reaches the coastline.

associated with the relatively slow rise rate of smaller droplets. These droplets remain within the water column for long periods once they have been dragged downwards. As the waves become more intense, the slick spreads horizontally and develops a thicker vertical structure, with particles occupying intermediate depths before gradually resurfacing. In addition to greater vertical variability, the light oil slick spreads more horizontally over time. Its lower viscosity makes it more susceptible to deformation and lateral spreading, resulting in an increase in surface area. In contrast, heavy oil remains predominantly confined to the surface throughout the simulation. Although transient particles are observed below the surface during periods of intense wave activity, these are only present for a limited time and over a limited area. Larger droplet diameters result in a more rapid increase in buoyancy, reducing the persistence of concentrations below the surface even when entrainment occurs. Therefore, the vertical structure of the heavy oil slick is thinner than that of the light oil slick. In addition, the higher viscosity and increased emulsification of heavy oil make it more resistant to deformation, limiting its horizontal spread. As a result, the heavy oil slick remains more compact in a smaller area than the light oil slick. The figures illustrate the combined impact of wave force and buoyancy dynamics as a function of droplet size. While significant wave heights favour vertical particle displacement, the duration and spatial extent of underwater dispersion are strongly modulated by the rise velocity of the droplets.

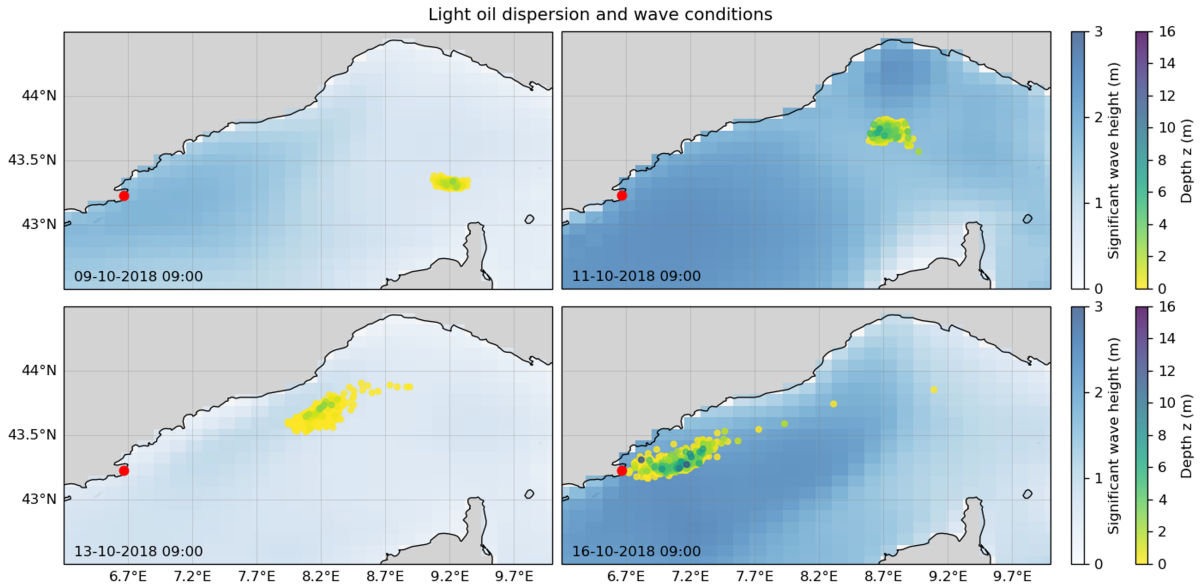


Figure 4.34: Spatio-temporal evolution of the light oil slick under weathering conditions. Each panel represents a selected time step from the simulation. Particle colour represent vertical position. The background layer shows the significant wave height (H_s).

Since recent results have shown that light and heavy oil evolve differently during dispersion simulation, a comparison is made between the two types of oil and passive particles. Figure 4.36 shows that, over time, the heavy oil slick (in orange) moves

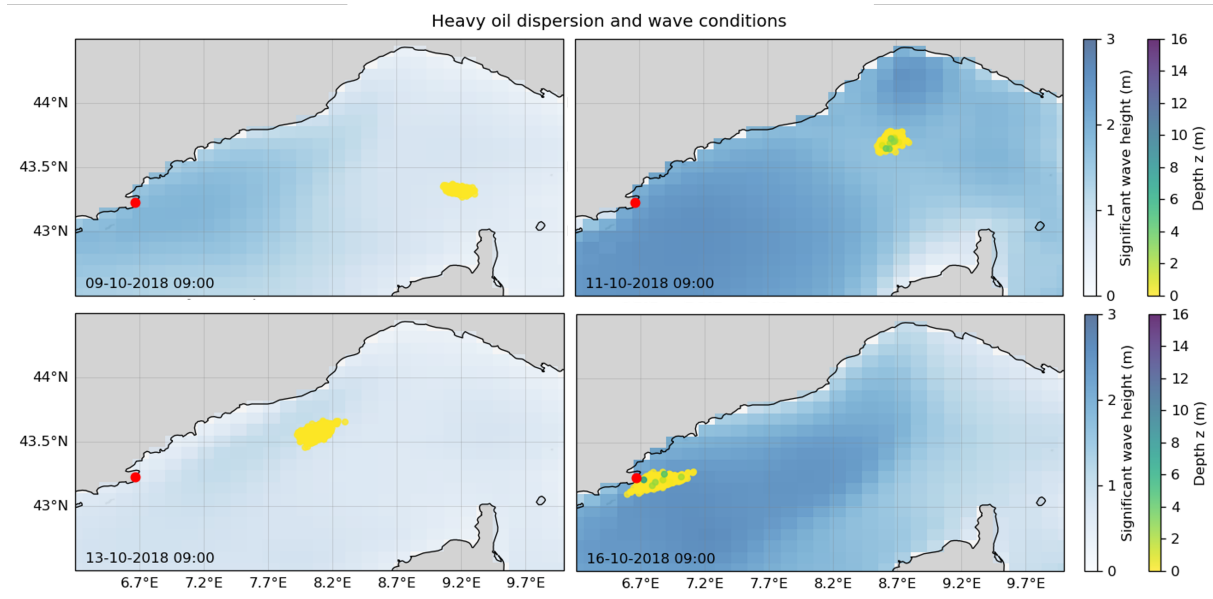


Figure 4.35: Spatio-temporal evolution of the heavy oil slick under weathering conditions. Each panel represents a selected time step from the simulation. Particle colour represent vertical position. The background layer shows the significant wave height (H_s).

horizontally faster than the light oil slick (in green). This apparent increase in propagation speed is due not only to intrinsic differences in density, but also to the vertical distribution of the droplets. Heavy oil droplets, characterised by larger diameters and higher rise velocities, tend to remain close to the surface. Since horizontal current velocities are generally stronger in the upper layer, particles confined to the surface undergo more intense advection. In contrast, light oil droplets are more frequently entrained below the surface and remain at intermediate depths for longer. Here, horizontal currents are typically weaker due to vertical shear. Consequently, the light oil slick has a lower average horizontal transport velocity than the heavy oil slick. The transport behaviour of massless particles, which follow the velocity field without buoyancy or drag dynamics, provides a reference that highlights the impact of vertical processes on the horizontal evolution of the slick. The passive particle slick (in blue) shows transport behaviour more similar to that observed in the case of heavy oil. Since passive particles are confined to the surface layer, they are continuously exposed to higher horizontal velocities and transport caused by wind. In contrast, a significant portion of light oil droplets are distributed below the surface, where horizontal velocities are reduced due to vertical flow. This difference in vertical distribution results in distinct effective horizontal transport velocities.

The temporal evolution of the main oil properties during the simulation provides further insight into the weathering processes and their mutual interactions. The Figure 4.37 shows the normalised total oil mass as a function of time. Both oil types show progressive mass reduction, though the decrease is significantly more pronounced for the light oil. It should be noted that the apparent drop in the mass of heavy oil to zero does not reflect its

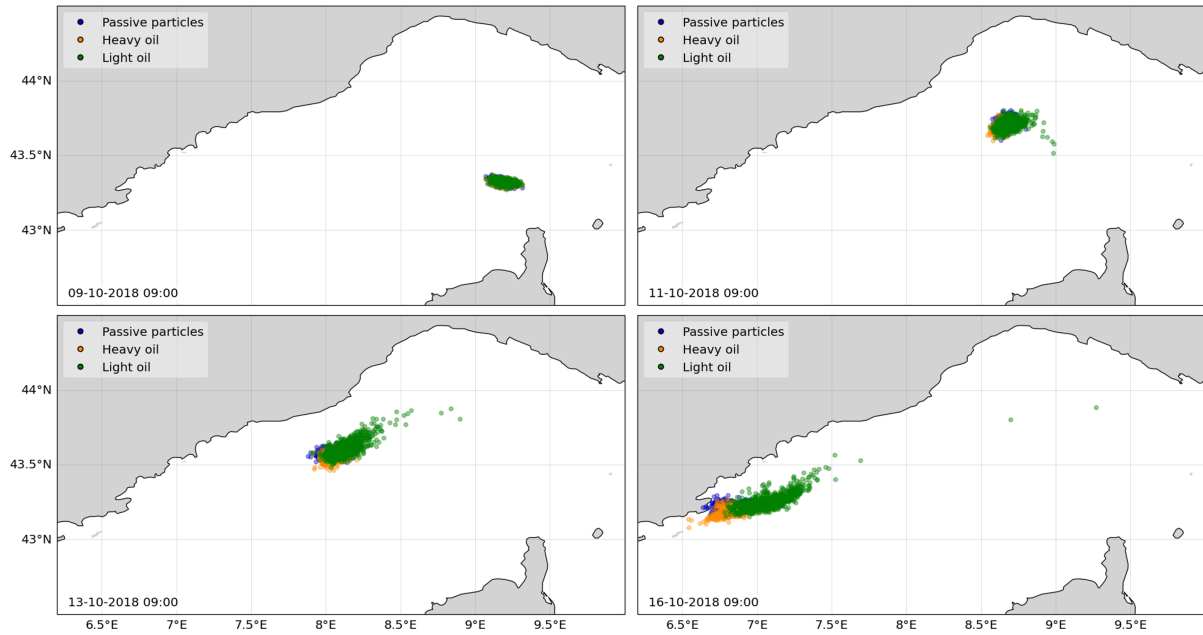


Figure 4.36: Comparison of simulations between light oil (in green), heavy oil (in orange), and passive particles (in blue) at different timesteps.

complete physical removal by weathering processes. This is because, at a certain stage in the simulation, the slick reaches the coastline (indicated in the figure by a red dashed line), and the particles that have been beached are no longer included in the water column mass calculation.

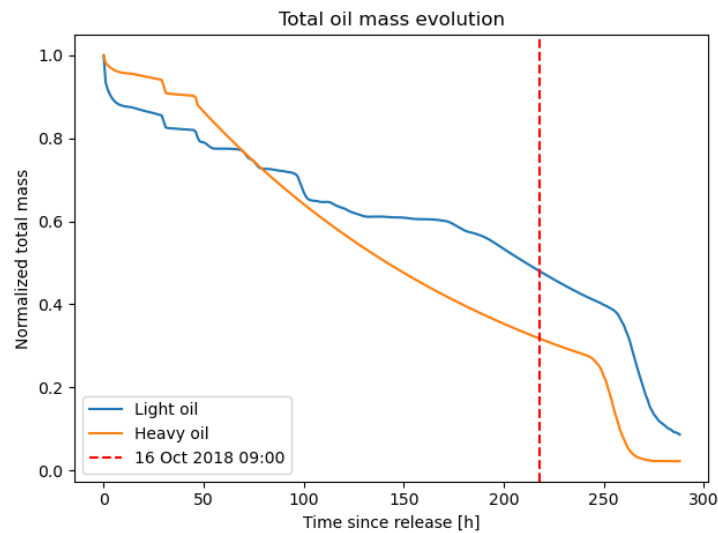


Figure 4.37: Normalised total oil mass as a function of time is shown in orange for heavy oil and in blue for light oil.

The behaviour of mass evolution is strictly associated with evaporative losses, as can be seen in Figure 4.38. These losses dominate the early stages of the simulation. Light oil, characterised by a higher proportion of volatile components, exhibits a rapid increase in its evaporated fraction, reaching around 45% of the initial mass. In contrast, heavy

oil shows a much lower evaporation rate, stabilising at around 12%, reflecting its lower content of light fractions and reduced volatility. It should be noted that this upper limit is a constraint imposed by the model configuration through the prescribed maximum evaporative fraction, rather than an emergent property of the simulation.

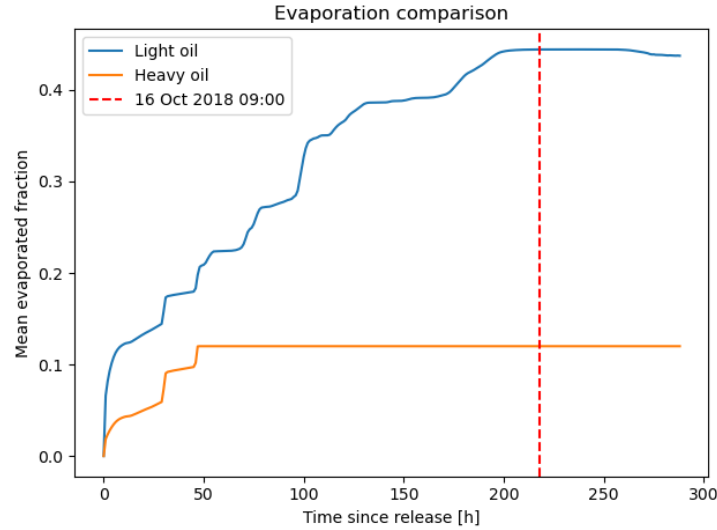


Figure 4.38: Mean evaporated fraction as a function of time is shown in orange for heavy oil and in blue for light oil.

The direct connection between evaporation and mass reduction is evident when comparing the two figures (4.37 and 4.38). The rapid decrease in total mass during the initial phase closely mirrors the rapid growth in the evaporated fraction, particularly in the case of light oil. As the process of evaporation progresses, the chemical composition of the remaining oil changes, with the lighter components being removed first. This compositional shift leads to a progressive increase in viscosity, as can be seen in Figure 4.39. Both oil types exhibit a consistent rise in kinematic viscosity over time, though the heavy oil consistently exhibits higher values throughout the simulation. This increase in viscosity is consistent with the removal of low-molecular-weight fractions and the ageing of the residual oil.

At the same time, emulsification contributes to the further modification of the oil properties. Figure 4.40 illustrates the evolution of the mean water fraction incorporated into the oil phase. The heavy oil undergoes a higher degree of emulsification than the light oil, reaching water fractions of around 14%, while the light oil stabilises at around 9%. This behaviour is consistent with the greater stability of water-in-oil emulsions in more viscous systems, where the higher internal resistance limits droplet coalescence and promotes water retention within the oil matrix. Therefore, the combined effects of evaporation and emulsification reinforce the observed increase in viscosity over time.

Simultaneous changes in mass loss, evaporative fraction, viscosity and water content demonstrate a clear progression in weathering. Initially, evaporation drives rapid mass

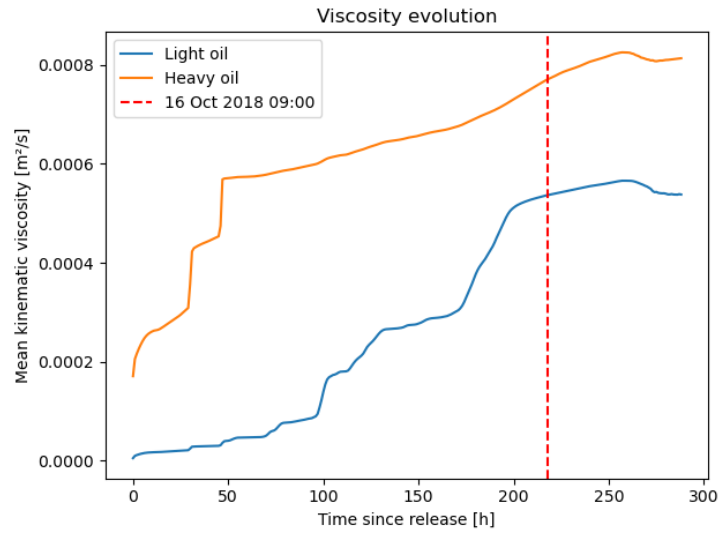


Figure 4.39: Mean viscosity as a function of time is shown in orange for heavy oil and in blue for light oil.

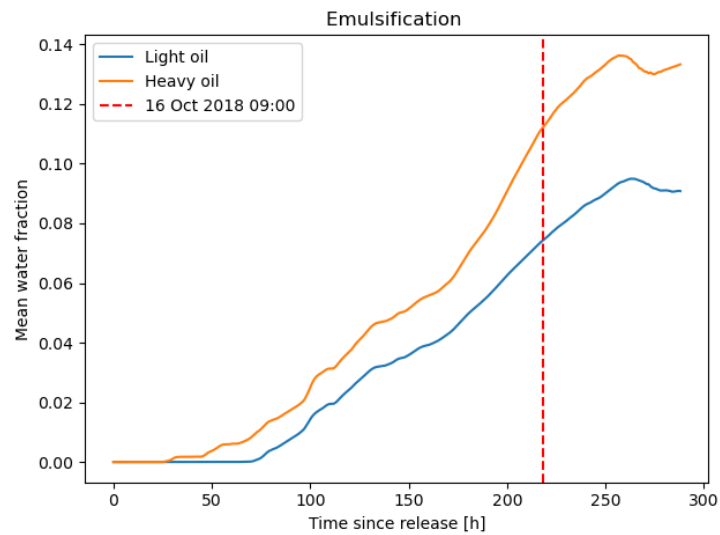


Figure 4.40: Mean water fraction emulsified as a function of time is shown in orange for heavy oil and in blue for light oil.

reduction and compositional change, while emulsification progressively alters the viscosity of the oil. The vertical redistribution driven by wave-induced droplet entrainment and buoyancy-driven resurfacing further modulates horizontal transport, with light oil experiencing reduced advection due to its prolonged subsurface residence and smaller droplet rise velocities, while heavy oil remains predominantly confined to the surface and undergoes stronger wind-driven horizontal transport. The differences observed in light and heavy oil scenarios reflect their distinct physical properties, confirming that the model reproduces the expected qualitative behaviour of crude oil weathering processes. It should be noted that sedimentation of denser oil compounds is not represented in the current implementation. As density increases through emulsification, particularly in the heavy oil case, gravitational settling toward the seabed is not accounted for. This is acknowledged as a limitation of the present framework and is identified as a relevant direction for future development.

Chapter 5

WebGIS interface for oil spill forecasting

One of the main objectives of the research is not only to provide a comprehensive investigation of the physical and physicochemical processes governing oil spill evolution at sea, including transport, diffusion, and weathering mechanisms, but also to develop an operational WebGIS interface designed to support rapid response scenarios. The proposed dashboard is designed to be user-friendly while remaining scientifically accurate. It is intended to be a decision-support tool capable of running oil spill simulations in forecast mode. Starting from user-defined initial conditions (e.g. release location, start time, oil type and simulation duration) the system will perform Lagrangian dispersion simulations and automatically produce associated diagnostic outputs, such as the temporal evolution of the slick centroid and graphical summaries of key performance indicators. From a software architecture perspective, the platform follows a modular client–server structure composed of a backend and a frontend layer. The backend is responsible for numerical processing, execution of the dispersion model, environmental data handling, and automated generation of outputs. It includes both autonomous components, such as environmental data ingestion and preprocessing routines, and modules that dynamically receive parameters from the frontend. The frontend represents the visualization and interaction layer, providing an interactive WebGIS environment for parameter input, real-time monitoring of simulation progress, and exploration of model outputs through dynamic cartographic and graphical tools. This modular architecture ensures flexibility, scalability, and future extensibility, allowing the integration of additional features.

5.1 Backend infrastructure

The backend infrastructure is entirely developed in Python and is structured around a single entry point, *main.py*, which simultaneously manages two main components: a background

worker responsible for data preparation and an API layer that exposes computational services. This unified architecture ensures that data updates and simulations initiated by users can run concurrently while remaining logically synchronised. All operations described up to the dispersion request phase are completely internal to the backend. The system autonomously monitors, downloads, pre-processes, and harmonises environmental data without requiring any interaction from the frontend. The backend only waits for the user-defined input parameters to be sent via the API once this preparatory phase is complete. The worker component is designed to ensure that the system always uses the latest environmental data. Every hour, the system checks for the existence and last modification date of the file containing wind and wave data (*ww3_forecast_gridded.nc*). If a newer version is detected, the file is downloaded again and replaces the previous local copy. At the same time, the system checks whether updated surface current fields are available from Copernicus Marine Service products. If new oceanographic data is released, it is automatically retrieved and integrated into the modelling workflow. While wind and wave forecasts are provided by MeteOcean-UniGe, surface current fields come from Copernicus operational products. This automated monitoring mechanism ensures that the computational pipeline always uses the most recent forcing datasets, thus maintaining the reliability of the forecasts and ensuring operational readiness. Once the updated file has been successfully retrieved, a sequence of processing steps is initiated. These include the calculation of wave-related derived quantities, such as wavelength and Stokes drift, as well as the retrieval of oceanographic fields from Copernicus Marine services. All meteorological and oceanographic datasets are then interpolated onto a common uniform grid with a spatial resolution of 4 km. This re-gridding step ensures spatial consistency between heterogeneous data sources and prevents numerical inconsistencies during the dispersion modelling step. After harmonising the resolution and structure, the final velocity fields used in the dispersion model are calculated, integrating the relevant physical contributions. Since these datasets can be large and memory-intensive, the Python library Dask is used to optimise memory usage and enable parallel and lazy evaluation of array operations, thereby improving computational efficiency and scalability.

At the end of the pre-processing workflow, a global variable stored in *job_has_run.py* is updated. This variable acts as a synchronisation flag between the worker and the API. When its value is set to True, the system signals that the preparation of environmental data has been completed and that the backend is ready to accept user-driven simulation requests. Until that moment, the backend remains in an initialisation state.

The API layer exposes several endpoints that enable interaction with the system. A dedicated */status endpoint*, accessible via a GET request, provides a lightweight mechanism that allows the frontend to check the availability of the system. If the pre-processing pipeline has been successfully completed, the endpoint returns *System is ready*, otherwise it reports *System is initialising*. This mechanism allows the frontend to determine when it

is appropriate to send simulation requests.

Once the backend has reached the ready state, it waits for the frontend to provide the user-defined simulation parameters. The main computation service is provided by the */dispersions endpoint*, which accepts POST requests containing a JSON payload. The payload includes parameters such as wind and wave weighting coefficients (α , β), simulation start time, release location, and additional configuration parameters, including field size. After receiving these inputs from the frontend, the backend takes over processing and starts the dispersion simulation. Particle release is configured according to the parameters provided, the model is run, and the output is generated in GeoJSON format, structured by time interval. Since this calculation can be resource-intensive and time-consuming, the response is provided using a streaming mechanism: features are returned incrementally as they become available, rather than waiting for the entire simulation to complete. After producing the dispersion output, the backend can also process it further through the */centroids endpoint*, which calculates the spatial centroids of the particle cloud at each time interval. In this way, once user inputs are received, the backend reactivates its internal computational workflow to perform both dispersion and centroid calculations before returning the results to the client. The architecture clearly separates autonomous data preparation from user-initiated simulations. First, the backend operates independently to update and harmonise all forcing data. It then enters a waiting state until the frontend provides the necessary parameters. Once these inputs are received, the computational pipeline resumes within the backend. This ensures that dispersion and centroid analyses are performed in a controlled and consistent manner, while maintaining responsiveness through streaming-based communication.

5.2 Frontend - User interface

The frontend component of the platform is designed as an interactive WebGIS environment that allows users to configure, launch, and analyse Lagrangian simulations through a web browser. It is implemented using Angular, a TypeScript-based, open-source frontend framework developed by Google that is widely used for creating single-page applications (SPAs). Angular provides a component-based architecture in which the application is divided into modular, reusable elements, each of which is responsible for a specific function (e.g. the simulation setup panel, the map viewer or the diagnostics section). This architecture improves maintainability, scalability and separation of concerns, all of which are important in scientific applications where computational workflows, visualisation layers and user interaction must remain logically decoupled. Angular also supports reactive programming through RxJS, enabling the interface to be updated dynamically as soon as new simulation data becomes available from the backend.

The frontend communicates directly with backend services via RESTful APIs, lever-

aging the `HttpClient` module in Angular. This client–server architecture ensures a clear separation between the computational engine and the visualisation layer. User-defined simulation parameters are transmitted to the backend via structured JSON requests, and results are retrieved asynchronously once available. This decoupling approach aligns with established best practices in distributed web-based systems (Fielding 2000) and the FAIR data principles for scientific workflows (Wilkinson et al. 2016), which emphasise interoperability and accessibility. The asynchronous communication model enables the monitoring of simulation progress and the progressive rendering of outputs without blocking the user interface.

Geospatial visualisation is implemented through Leaflet, a lightweight, open-source JavaScript library widely used for creating interactive maps. Leaflet enables the dynamic rendering of the Mediterranean basin, including base maps and geospatial overlays. Simulation outputs, which are usually provided in GeoJSON format, can be displayed as evolving particle clouds, centroid trajectories and deformation patterns. The library supports time-dependent layer updates, enabling the progressive visualisation of dispersion processes. Leaflet’s efficiency and flexibility make it particularly well-suited to environmental and oceanographic web geographic information system (WebGIS) applications, where large spatial datasets must be rendered interactively (Haklay and Weber 2008).

In addition to spatial visualisation, quantitative diagnostics are displayed using Highcharts, an interactive JavaScript charting library. Highcharts is used to generate time-series plots and comparative diagnostics derived from simulation results. These include the relative distance between the simulated centroid and a reference position, the temporal evolution of slick deformation in the x and y directions, and the centroid position trace. The interactivity of the plots (zooming, tooltips and dynamic updates) enhances interpretability and facilitates exploratory data analysis. Although Highcharts is not a specialised scientific plotting framework, its robustness and responsiveness make it ideal for web-based analytical dashboards. A central objective of the frontend is to provide a simulation configuration interface that is both scientifically accurate and flexible.

The created dashboard is included as a result of the RAISE project and can be accessed via the following link: https://s4raise.it/dssmare/dispersion_v2/.

RAISE Liguria (Robotics and AI for Socio-economic Empowerment) is a regional innovation ecosystem based in Liguria, Italy, funded under the Italian National Recovery and Resilience Plan (PNRR). It aims to strengthen research and technology transfer in the fields of robotics and artificial intelligence, as well as industrial innovation. This is being achieved by fostering collaboration between universities, research centres, companies and public institutions, in order to support socio-economic development and digital transformation in the region.

When accessing the dashboard, the initial view in Figure 5.1 displays a map centred on and zoomed in over the Ligurian Sea area. Users can adjust the zoom level using the



Figure 5.1: Initial view of the WebGIS dashboard, displaying the default map centred on the Ligurian Sea.

"+" and "-" controls in the bottom right corner of the interface to enlarge or reduce the spatial scale of the visualisation.

Although the default view focuses on the Ligurian Sea, simulations can be performed over the entire Mediterranean basin, which represents the full spatial domain available within the system. In the upper-right corner of the dashboard, an information button is provided. By clicking on this icon, a pop-up window opens, shown in Figure 5.2, containing details about the dashboard functionalities and the datasets used to generate the dispersion simulations.

To initiate the simulation, the user must first specify the release location within the Mediterranean basin. In the top-right corner of the dashboard, a panel displays the latitude and longitude of the currently selected point. As the cursor moves across the map, these coordinates update dynamically, allowing precise selection of the desired release position. Once the point is selected, a panel will appear on the dashboard, in which the user specifies the number of Lagrangian particles and determine the release diameter. This represents the spatial extent of the initial spill (Fig. 5.3). These parameters directly influence the initial conditions of the transport simulation. While increasing the number of particles generally improves the statistical representation of dispersion processes, it also increases the computational cost. Therefore, the interface enables users to strike a balance between accuracy and performance.

The selector also allows the specification of transport weighting coefficients, denoted α and β , which represent the relative contributions of wave-induced transport (Stokes drift) and wind forcing, respectively. From a modelling perspective, these coefficients directly influence the effective advection velocity applied to particles and enable controlled

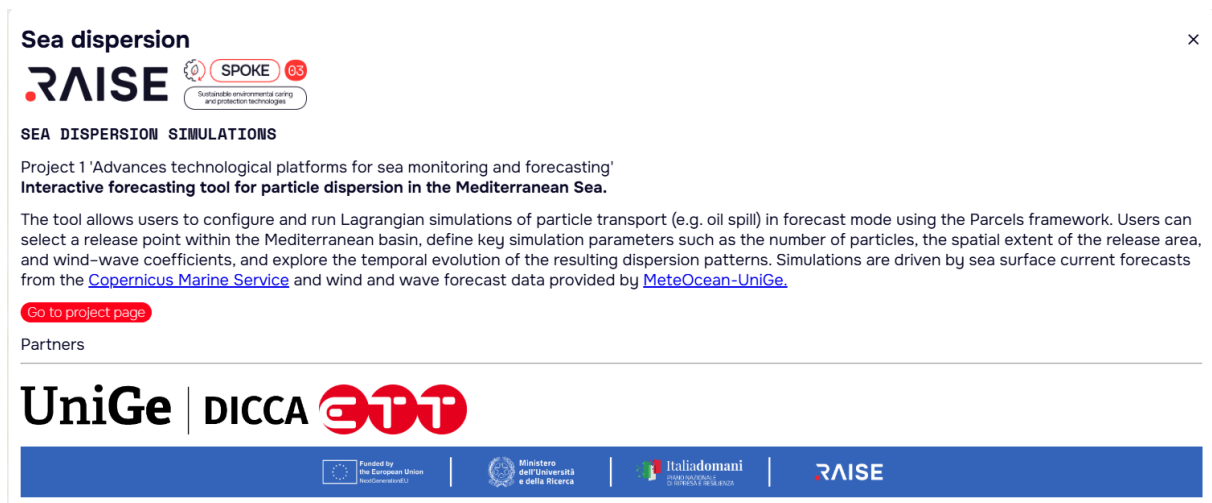


Figure 5.2: Information panel of the WebGIS interface. It summarises the system functionalities and the oceanographic and atmospheric datasets employed for the dispersion simulations across the Mediterranean basin.

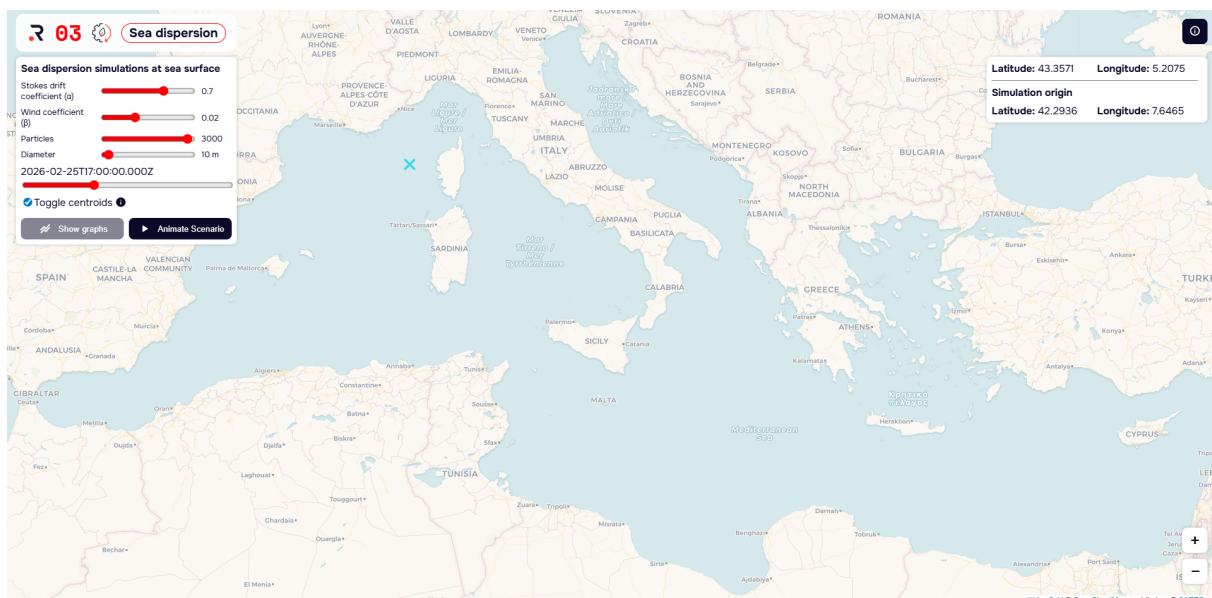


Figure 5.3: Release point selection and initial condition setup for the Lagrangian dispersion simulation.

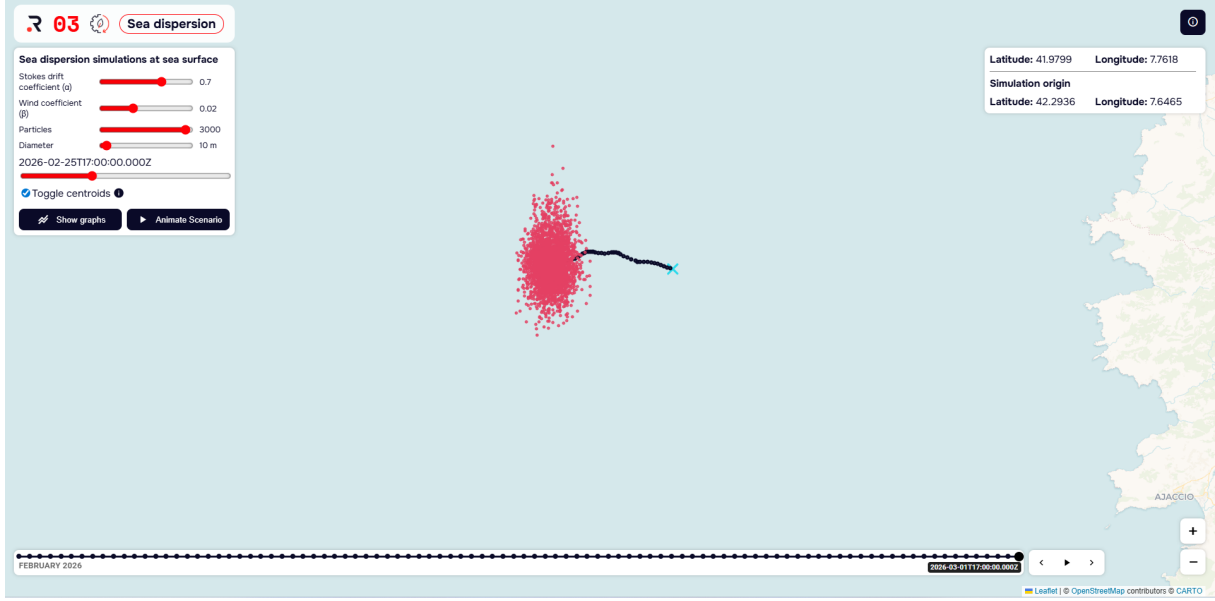


Figure 5.4: Animated Lagrangian dispersion simulation with centroid evolution displayed on the WebGIS map, represented by black dots.

exploration of different forcing scenarios. In the current configuration, α can be selected within the range $[0, 1]$ with increments of 0.1, allowing users to modulate the contribution of Stokes drift from null influence to full weighting. The coefficient β , derived from values commonly reported in the literature for wind drag in oil spill modelling, can be selected within the interval $[0.01, 0.04]$, with increments of 0.01. Although the interface facilitates scenario exploration through adjustable parametrisation, the physical consistency and scientific validity of the selected coefficients must be carefully evaluated, as inappropriate choices may significantly affect trajectory predictions.

Once a simulation is launched by clicking on *Animate Scenario*, the particle dispersion is progressively visualised on the map (Fig. 5.4). The animation displays the temporal evolution of the Lagrangian particles during the forecast period. After the simulation has completed, additional diagnostic features become available. By activating the *Toggle centroids* option in the control panel, the temporal evolution of the oil slick centroid can be displayed. The centroid positions appear as black markers on the map, representing the trajectory of the slick over time. At the bottom of the interface, a temporal slider allows users to select a specific time frame within the simulation period. When a given instant is selected, the map updates dynamically to show the particle distribution and the corresponding centroid position associated with that time.

In addition, the diagnostic plots can be generated in the plotting panel by clicking on *Show graphs*. In Figure 5.5, the relative distance metric represents the cumulative displacement of the oil slick centroid from the initial release point up to each time step, computed according to Eq. 3.7. In Figure 5.6, the relative dispersion with the x and y deformation metrics describe anisotropic spreading of the slick, computed according to

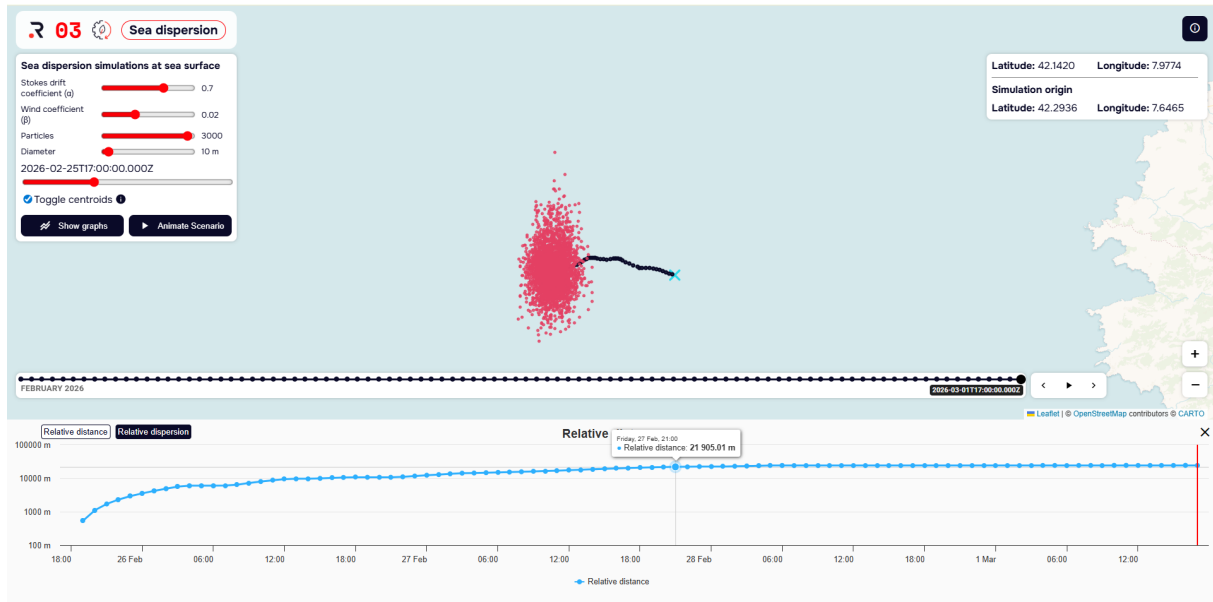


Figure 5.5: Time evolution of the relative distance between simulated and observed oil slick centroids. The red vertical bar indicates the time instant selected through the temporal slider.

Eq.3.8 and 3.9, offering insight into how the slick evolves in both time and space. Within the diagnostic plots, a red vertical bar indicates the time instant selected through the temporal slider, ensuring temporal consistency between the spatial visualisation on the map and the quantitative metrics shown in the graphs. The centroid trace summarises the bulk transport pathway of the spill and serves as a compact descriptor of large-scale advection.

Despite its operational capabilities, the current version of the dashboard presents some limitations that must be acknowledged. First, its use is primarily intended for experienced users, as the selection of the transport coefficients α (Stokes drift weighting) and β (wind drag coefficient) requires informed judgement. While β is generally constrained within a relatively narrow range, commonly around 0.02 in oil spill applications, the appropriate choice of α is more variable and may depend on seasonal circulation patterns and specific atmospheric or wave conditions. An incorrect parametrisation may therefore significantly influence the simulated trajectories. Secondly, the dashboard currently only implements passive inertial particles with no mass or explicit oil alteration processes. This design choice is motivated by computational constraints in an operational forecasting context. While including alteration processes only moderately increases the computation time of the simulation code, the main limitation stems from the three-dimensional input fields required for ocean currents. These datasets require significant memory and increase the necessary resources when combined with additional physicochemical processes.

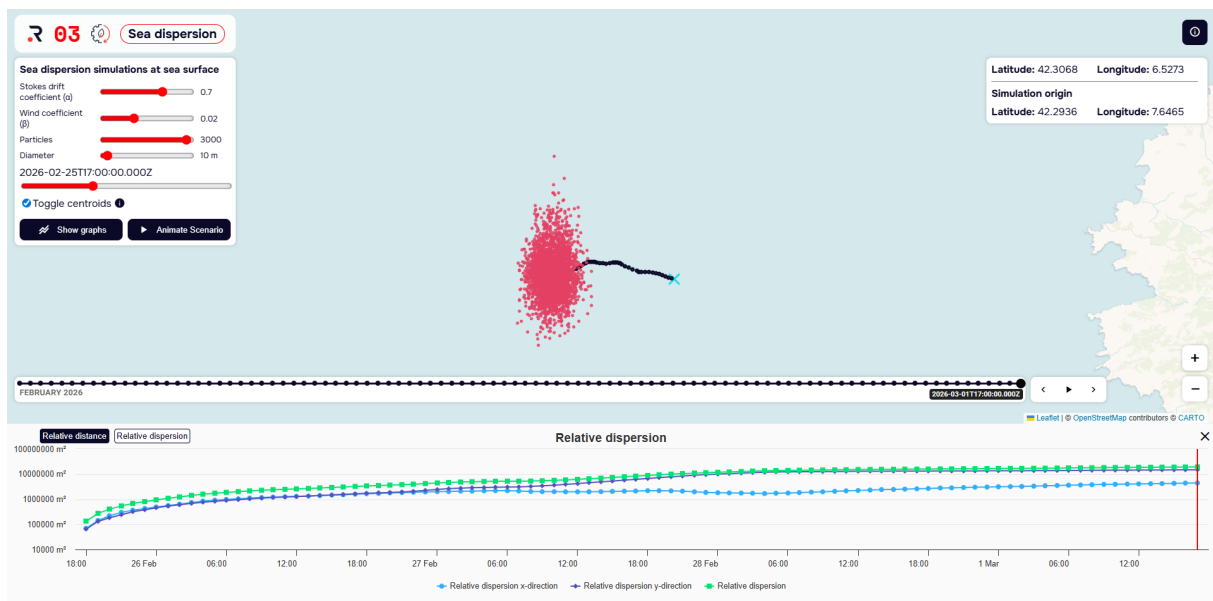


Figure 5.6: Relative dispersion and x , y deformation metrics of the oil slick centroid, representing anisotropic dispersion along the zonal and meridional directions in time. The red vertical bar indicates the time instant selected through the temporal slider.

Chapter 6

Conclusions and Future perspectives

This research highlights the significant differences between oceanographic and climate models used to simulate oil spill dispersion in the Mediterranean Sea. A systematic comparison of CMEMS, SHOM, and IFREMER circulation products combined with various wind and wave factors demonstrates that small variations in model structure, spatial resolution, boundary conditions, and data assimilation strategies can result in notable differences in dispersion patterns. Adopting an identical particle release configuration for all model combinations ensured methodological consistency and enabled robust cross-comparisons of trajectories, centre of gravity evolution, and coast impact times. Despite the models' structural differences, the simulations generally predict a westward shift of the oil slick toward the French coast in the Corsica case study. However, the timing, intensity, and deformation characteristics of the slick varied substantially. These discrepancies confirm that uncertainties in near-surface velocity fields propagate non-linearly over time, amplifying differences in multi-day simulations and directly affecting predictions of coastal impact. The results clearly demonstrate the crucial role of environmental forcings in addition to surface currents. Wind-induced transport significantly accelerates and increases the size of oil slicks, creating stronger and more coherent advection patterns than currents alone produce. Although Stokes drift contributes to the horizontal transport of floating pollutants, its impact in this scenario is secondary to wind forcing, primarily due to the greater magnitude of wind velocities during the analysed event. Even when relatively large scaling coefficients are assigned to the Stokes component, wind forcing dominates the resulting transport. This finding does not imply that Stokes drift is generally negligible, but rather that its relative importance depends heavily on the specific event and must be evaluated within the context of the particular hydrodynamic conditions.

An important result of this work is the comparison between absolute and relative wind formulations. Although the short-term differences between the two approaches appear moderate, their cumulative effects over several days become significant. The relative wind formulation accounts for the difference between wind and surface current velocities. This modification to the effective drag experienced by particles leads to different timing in

centroid trajectories and different decorrelation timescales. Analysing centroid separation and non dimensional distance metrics reveals progressive divergence between the two simulations. The computation of Lagrangian velocity autocorrelation functions also reveals differences in decorrelation timescales, indicating that the adopted wind representation directly influences the temporal memory of particle motion. These results imply that choosing between the absolute and relative wind formulations is not just a technical detail but a physically relevant modelling decision that can affect the timing of shoreline impacts and hazard assessments.

A key methodological development in this thesis is the use of Bayesian optimisation to calibrate the Stokes drift and wind drag coefficients. Unlike traditional sensitivity analysis, which relies on iterative manual tuning of parameters and can become inefficient and potentially biased in non-linear systems, the Bayesian framework enables a probabilistic exploration of the parameter space. In contrast, the Bayesian framework allows for a probabilistic exploration of the parameter space, striking a balance between exploiting promising regions and exploring uncertain combinations. The optimisation results show that the optimal values of α and β are dependent on the event in question and the temporal horizon of interest. It is notable that parameter combinations calibrated to minimise short time centroid errors do not necessarily minimise long time discrepancies in shoreline impact. This emphasises the multi-scale nature of oil spill dispersion and the importance of consistently aligning calibration objectives with operational priorities. When fixed reference points or well-defined observational targets are available, the proposed optimisation approach is particularly relevant. In such cases, the objective function can be expressed in terms of measurable quantities, such as the location of the shoreline impact, the timing of the impact, or the centroid distance from the observed slicks. This allows for a calibration that is both physically meaningful and quantitatively constrained. In this study, short-time SAR images gave us information about where the incident took place, but we had to estimate where the shoreline had been impacted based on reports. Under these conditions, while the optimisation process remains effective, it is inherently conditioned by the uncertainty associated with the assumed impact point. However, when accurate, precisely geolocated impact observations are available, the Bayesian framework becomes even more efficient and robust as it directly minimises discrepancies against clearly defined targets and reduces uncertainty in parameter selection. The adoption of Bayesian optimisation represents a methodological contribution that can be extended to other Lagrangian transport applications, particularly in contexts where observational constraints can be explicitly incorporated into the calibration strategy, beyond the specific numerical values obtained.

Incorporating oil weathering processes enhances the physical realism of the modelling framework. Transitioning from passive surface particles to particles characterised by evolving mass, density, viscosity, and droplet size distribution enables the simulations to

capture key transformation mechanisms that influence the fate of oil. Comparing light and heavy oil scenarios reveals substantial differences in evaporation rates, emulsification behaviour, viscosity increases and submerged particle fractions. The introduction of vertical redistribution through wave induced droplet entrainment and resurfacing processes driven by buoyancy is not possible within a purely two-dimensional framework. The evolution of droplet diameter distributions and their associated rise velocities shows that oil transport is dynamically linked to its chemical and physical state. Heavier oils, in particular, exhibit lower percentage of particles being entrained in the water column and slower resurfacing. While lighter oil shows really high presence of droplets in the layers below the surface, altering horizontal dispersion patterns and shoreline contamination risk. These findings confirm that neglecting weathering could result in overly simplified transport predictions and inaccurate environmental impact assessments.

The Corsican oil spill case study demonstrates the operational relevance of the developed framework. A quantitative comparison with Sentinel-1 SAR imagery using centroid distance metrics and particle-slick intersection percentages demonstrates the model's capacity to reproduce observed slick evolution, while also revealing residual mismatches. The framework therefore offers predictive capabilities and diagnostic insights into the mechanisms controlling dispersion. Finally, integrating the modelling framework within a WebGIS platform is a concrete step towards operational application. The developed backend and frontend architecture enables scenario-based simulations and the interactive visualisation of centroid evolution and dispersion metrics, improving accessibility for decision support. This study demonstrates the direct benefits of developing integrated ocean forecasting systems that combine physical modelling, parameter calibration, and visualisation tools to support environmental protection and emergency response efforts.

6.1 Limitations and future perspectives

Although the results of this research demonstrate the robustness and applicability of the proposed framework, several limitations must be acknowledged. First, the present analysis is based primarily on a single, well-documented case study. While the Corsican event provides a valuable opportunity to validate the results against satellite observations, it cannot be assumed a priori that the optimized coefficients and dispersion behaviour can be transferred to different meteorological, seasonal, or oceanographic regimes. Oil spill dynamics are strongly event-dependent, so a broader, multi-case evaluation is necessary to assess the calibration strategy's general applicability across contrasting environmental conditions. Treating the Stokes drift and wind resistance coefficients, α and β , as constants during each simulation is a simplifying assumption. In reality, these parameters are not intrinsic constants, but effective coefficients that depend on evolving air-sea interaction processes. Their magnitude is influenced by sea state, such significant wave height,

wave steepness, and breaking intensity, wind intensity and direction, and the turbulent structure of the upper ocean layer. Since these environmental conditions vary over time, even on a daily scale, and may exhibit seasonal modulations, the assumption of fixed coefficients may not fully capture the temporal variability of the coupling between wind and waves with surface transport. Representing α and β as static effective parameters improves numerical stability and tractability, particularly in an optimization framework. However, this assumption may limit the physical realism of longer simulations or forecasts over multiple days in which atmospheric forcing and sea state evolve significantly. A parametrization dependent on time and state of these coefficients would provide a more dynamically consistent representation of air-sea coupling processes. Finally, while the WebGIS platform shows that the developed framework is operationally feasible, its current implementation primarily focuses on advection-diffusion processes with simplified parameter control. The complete atmospheric alteration module, including dynamic mass evolution and vertical redistribution, has not yet been fully integrated into the operational user interface. Therefore, the current WebGIS configuration should be considered a prototype rather than a mature forecasting system.

Several research directions emerge from this work. A primary development concerns the introduction of dynamic, state-dependent parametrisations of α and β . Instead of constant coefficients, future models could link wind and Stokes contributions to different state of the meteocean framework. This would allow for a more physically consistent representation of time-varying air-sea-oil interactions, which is an important consideration in this field. Extending the optimization framework to calibration across multiple events and combining it with systematic cross-validation procedures would improve the robustness and general applicability of the estimated parameters. Additionally, adopting probabilistic ensemble forecasting approaches would allow for a more rigorous quantification of predictive uncertainty and enable the derivation of confidence intervals for shoreline impact timing and location. From an operational perspective, the full integration of weathering processes into the WebGIS platform is a future objective. Allowing users to select oil type, simulate mass evolution, and account for vertical redistribution would significantly improve the system's decision-support capabilities.

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Appendix A

In situ observations and data density mapping

The simulation of pollutant and oil spill dispersion relies on the accurate representation of ocean surface and near-surface dynamics. Lagrangian dispersion models are forced by Eulerian fields such as ocean currents, wind and waves, whose uncertainties directly propagate into particle trajectories, affecting transport pathways, spreading rates and accumulation patterns. For this reason, the reliability of dispersion modelling depends critically on the quality, spatial coverage and temporal consistency of the meteo-oceanographic fields used as input (Sebillé et al. 2018). These forcing fields are themselves the output of numerical ocean, wave and atmospheric models, whose realism depends on their ability to represent physical processes and to be constrained by observations. Independent in situ observations play a fundamental role in assessing the realism of these forcing fields. They provide the only direct measurements against which numerical models can be calibrated and validated, enabling the identification of systematic biases, scale-dependent errors and regime-dependent model limitations. In regions or periods where in situ observations are sparse or absent, dispersion model results must be interpreted with increased caution, as uncertainty cannot be adequately constrained. Understanding where and when in situ observations of currents, waves and wind are available is therefore a prerequisite for a transparent evaluation of dispersion modelling results. Density maps offer a synthetic way to visualise this availability, linking model reliability to observational support and highlighting areas where uncertainty is intrinsically higher due to lack of measurements.

High-quality in situ observations are a fundamental aspect of oceanography and climate science, underpinning process understanding, numerical model development, data assimilation and climate services (Centurioni et al. 2019; Speich et al. 2019). Measurements of ocean currents, waves, wind, temperature and salinity are essential to describe ocean variability and to constrain meteo-oceanographic models across spatial and temporal scales. In situ data are collected by sensors mounted on a wide range of observing platforms, including underwater gliders, moorings, Argo floats, drifting buoys, HF radars, research

and container vessels, and other fixed or mobile systems. Each platform is characterised by its own sampling frequency, spatial representativeness and parameter set, and no single observing system can capture the full complexity of the ocean (Liblik et al. 2016). Only the integration of heterogeneous platforms provides sufficient observational evidence to describe ocean dynamics and their variability. In addition to data availability, the effective use of in situ observations for modelling applications requires transparent documentation of measurement accuracy, uncertainty, quality control procedures, and processing workflows. Without this information, it is difficult to determine whether discrepancies between models and observations are due to model deficiencies or observational limitations.

Despite significant progress in data integration and open-access infrastructures, critical gaps still limit the full scientific and operational value of in situ observations. These gaps extend beyond data volume and include uneven spatial and environmental coverage, fragmented standards and quality control practices, incomplete and non-standard metadata, and weak traceability between datasets and the measurement and processing protocols that produced them (A. Novellino et al. 2024). Spatial coverage remains highly heterogeneous. Deep-ocean observations below approximately 2000 m are sparse compared to upper-ocean measurements, while dynamic interfaces such as the air–sea and land–sea boundaries are often under-sampled despite their importance for wind forcing, wave generation and surface transport. Polar and remote regions are particularly affected by logistical and infrastructural constraints, resulting in persistent observational gaps. From a data integration perspective, heterogeneity in variable naming, quality control philosophies and documentation of processing steps complicates automated cross-dataset analyses and increases the effort required for harmonisation. A key limitation for modelling applications is the frequent lack of sensor-level metadata, such as sensor type, calibration procedures and nominal accuracy. This limits the ability to quantify observational uncertainty and to objectively evaluate model–data differences. In addition, the explicit linkage between datasets and community-endorsed best practices is rarely machine-readable, reducing reproducibility and complicating the selection of datasets suitable for model validation. These limitations directly affect meteo-oceanographic and dispersion modelling, as uncertainty in forcing fields cannot be rigorously constrained where observational support is weak or poorly documented.

In this context, density maps are used to quantify the spatial and temporal availability of in situ observations. A density map represents, for each grid cell, the number of recording days associated with a given parameter, providing a synthetic overview of observational coverage. While density maps do not assess data quality directly, they highlight where observations exist, where they are sparse or absent, and where model validation is more or less constrained by empirical evidence. Density maps should therefore be interpreted as indicators of observational support rather than proxies for data quality. The methodology described here focuses on currents, waves and wind, which are the

primary forcing parameters used in this thesis for dispersion modelling. Density maps derived from in situ observations allow a first-order assessment of whether observational coverage is sufficient to support model evaluation in the regions and periods of interest.

A.1 Data sources

At the European level, EMODnet Physics provides harmonised access to in situ observations of ocean physics, including currents, waves and wind, through standardised services such as ERDDAP, WMS and WFS. EMODnet Physics federates data from major European and international data integrators, offering one of the most comprehensive catalogues of physical ocean observations currently available.

EMODnet Physics is one of the seven domain-specific components of the European Marine Observation and Data Network (EMODnet), which provides free and unrestricted access to physical oceanographic data and data products. Through several development phases, EMODnet Physics has established itself as an operational service providing standardised, high-quality marine data in support of EU policies such as the Marine Strategy Framework Directive, the Marine Spatial Planning Directive and the European Green Deal. Integrated into the EMODnet Central Portal, EMODnet Physics improves the accessibility and interoperability of marine data and serves as a resource for monitoring and sustainability efforts. Its objectives include the further development of operational services to provide seamless access to key physical parameters, together with the adoption of international data standards and open-data practices.

EMODnet Physics organizes marine data by categorizing it into three key levels: in-situ data, data collection, and products.

- In-situ data consists of time series or profiles sampled by various platforms (e.g., CTDs, tide gauges, HF radars) .
- Data collections are groupings of similar in-situ data harmonized using common standards (e.g., salinity or temperature datasets across multiple platforms), organized using the P33-controlled NVS vocabulary . This allows seamless integration of metadata, linking terms like “salinity” to specific parameters and features such as time series or profiles.
- Products result from processing data into value-added outputs, such as climatologies or reanalysis datasets .

The platform ensures harmonized metadata, interoperability, and free access to data and products through standard protocols (e.g., ERDDAP, WMS/WFS), all integrated into the EMODnet Central Portal. Data collections provide the list of the platforms and

the temporal and geographical boundary information, while the full data are available in single platform data files.

Although the start and end dates of the datasets are available, the current structure lacks detailed temporal distribution of the data, such as monthly time steps. This limitation prevents the extraction and slicing of temporal information from the available data. To overcome this limitation and to support the construction of density maps, it is necessary to develop a dedicated dataset starting from the individual platform data files listed in each data collection. Each P33 data collection consists of one or more P01 collections, where a P01 collection includes either time series data or profile data.

A.2 Data density maps methodology

To quantify the spatial and temporal availability of in situ observations, data are aggregated on a regular $1^\circ \times 1^\circ$ spatial grid. The aggregation is performed on a monthly basis, and the density of observations within each grid cell is defined as the total number of days in which at least one measurement is available during the selected month. Formally, the density can be expressed as following Eq. A.1:

$$D(x, y, t) = \sum_{d \in t} I_{x,y}(d), \quad (\text{A.1})$$

where $D(x, y, t)$ represents the data density at the grid cell centred at (x, y) for the month t , and $I_{x,y}(d)$ is an indicator function equal to 1 if at least one measurement is available within the grid cell on day d , and 0 otherwise. With this definition, the density D ranges from 0 to the total number of days in the selected month.

This approach provides a synthetic representation of the temporal availability of in situ observations, highlighting how frequently measurements have been collected for a given parameter at different locations. Density maps therefore allow the identification of well-sampled regions, as well as areas and periods characterised by sparse or absent observations. As discussed in the previous sections, these maps describe observational support and should not be interpreted as direct indicators of data quality.

The density datasets generated for this study are made available through ERDDAP services for the following parameters:

- Currents: https://erddap.s4oceandata.eu/erddap/griddap/DENSITY_EWCT_NSCT.html
- Waves: https://erddap.s4oceandata.eu/erddap/griddap/DENSITY_WAVES.html
- Wind: https://erddap.s4oceandata.eu/erddap/griddap/DENSITY_WINDS.html

The visualisation interface is implemented as a Python-based interactive dashboard developed within a Google Colab notebook environment. The dashboard is designed to allow users to explore the spatial and temporal availability of in situ observations across the processed parameters. Users can interactively filter the data by physical parameter, geographic region, temporal interval and depth range. The interface is designed to be extensible and can incorporate additional metadata-based filters, such as platform type or data source (e.g. specific buoys, vessels or fixed stations), to further refine data selection.

The Google Colab notebook implementing the density map dashboard is available at: *Google Colab Density Maps*.

Figure A.1 shows the developed dashboard interface. Once the user defines the desired filter configuration, the dashboard computes and displays the corresponding density map using a colour scale ranging from low to high data density. The colour bar indicates the number of days with available measurements within each grid cell. The resulting maps provide an intuitive visual representation of where and how frequently in situ observations are collected over the selected time period and spatial domain.

The image shows a web-based filtering interface for an interactive dashboard. It includes several controls for selecting data parameters and ranges:

- Parameter:** A dropdown menu currently set to "Currents".
- Min latitude:** A slider ranging from -90.00 to 90.00.
- Max latitude:** A slider ranging from -90.00 to 90.00.
- Min longitude:** A slider ranging from -180.00 to 180.00.
- Max longitude:** A slider ranging from -180.00 to 180.00.
- Start month:** A date input field set to "2018-01".
- End month:** A date input field set to "2019-01".
- Color bar:** A dropdown menu currently set to "Green to red".
- Min depth:** A slider ranging from 0 to 10000.
- Max depth:** A slider ranging from 0 to 10000.

Figure A.1: Filtering interface of the interactive dashboard for in situ data density maps, enabling parameter, spatial, temporal and depth selection.

A.3 Density maps results for the year 2018

As discussed in the previous sections, density maps provide a synthetic representation of the spatial and temporal availability of in situ observations for key physical parameters relevant to dispersion modelling. In this section, the results are presented for the year 2018, corresponding to the period of the incident analysed in this thesis, with a specific focus on ocean currents, wind and waves. The density maps are produced on a global scale, providing a comprehensive overview of the worldwide distribution of in situ observations. However, given the geographical relevance of the case study, particular attention is focused on the Mediterranean Sea, where the dispersion simulations are performed. The Mediterranean is therefore the region of interest for interpreting the results presented in this section.

The adopted platform-agnostic aggregation approach allows all available observations to contribute to the density estimates, regardless of platform type. While this ensures a comprehensive overview of data availability, it also implies that the resulting maps do not differentiate between observing systems with different sampling strategies, sensor accuracies or applied best practices. As a consequence, the density maps should be interpreted as indicators of observational support rather than as measures of data quality.

The following figures present the density maps for currents, wind and waves for the year 2018, aggregated on a monthly basis and integrated over the full available depth range. For each grid cell, the maps represent the number of days with at least one recorded measurement during the selected period. These results provide a first-order assessment of where and when in situ observations are available to support the validation and interpretation of the dispersion simulations presented in the following sections.

As shown in Figure A.2, the density map for ocean currents indicates a generally homogeneous observational coverage throughout the year. Large portions of the domain are characterised by green colours, corresponding to approximately one day with available measurements per week, while red areas indicate locations where current observations are available on a daily basis over the entire year. Overall, the spatial and temporal coverage of in situ current data in the Mediterranean Sea during 2018 can be considered very good.

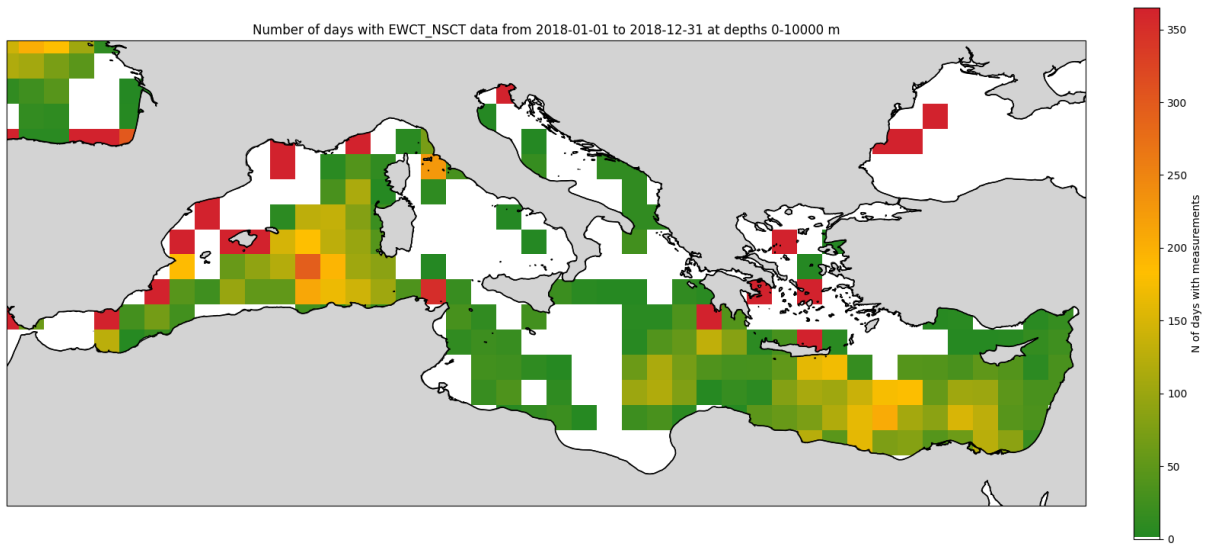


Figure A.2: Data density map showing the number of days with available in situ currents measurements aggregated over the 12 months of 2018 in the Mediterranean Sea.

Figures A.3 and A.4 show the density maps for wave and wind observations, respectively. In both cases, a very similar spatial pattern emerges, characterised by a generally sparse observational coverage, with measurements primarily concentrated in coastal areas. The highest data availability is observed in the north-eastern part of the basin and in the Greek region.

Despite the limited spatial extent of the observations, most of the available wave and

wind measurements exhibit continuous temporal coverage, corresponding to daily records over the entire year. These locations are indicated by red colours in the maps, denoting the presence of measurements on nearly every day of 2018.

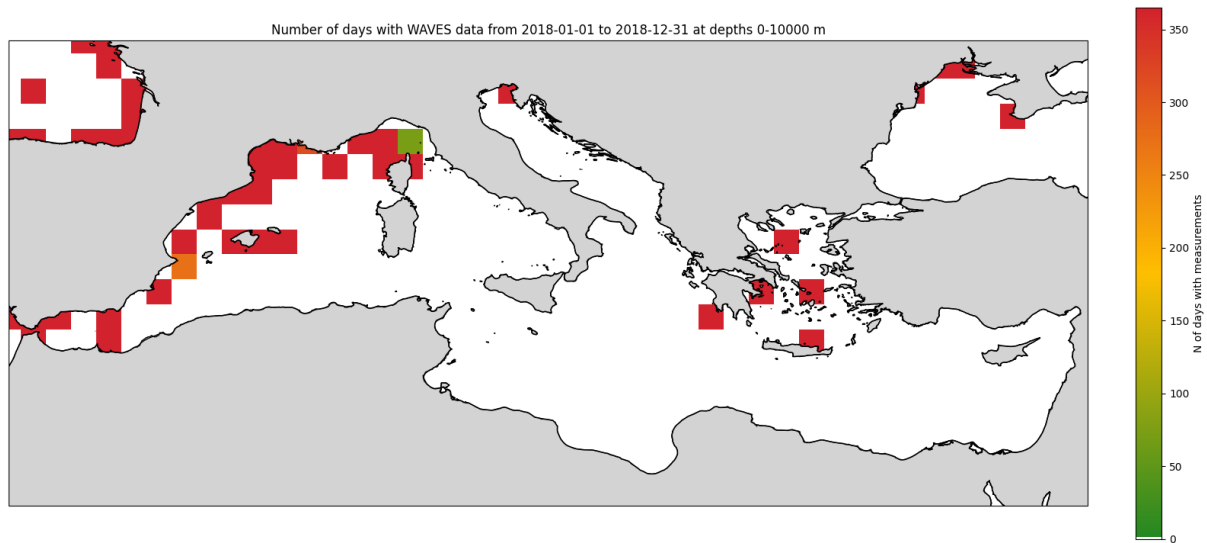


Figure A.3: Data density map showing the number of days with available in situ waves measurements aggregated over the 12 months of 2018 in the Mediterranean Sea.

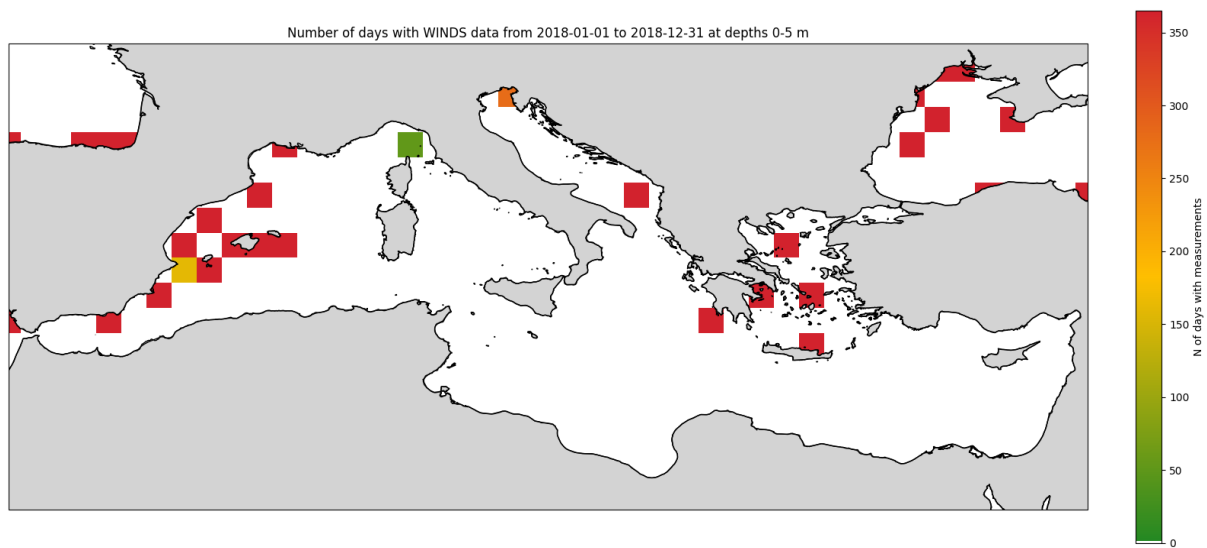


Figure A.4: Data density map showing the number of days with available in situ wind measurements aggregated over the 12 months of 2018 in the Mediterranean Sea.

The density maps highlight a heterogeneous distribution of in situ observational coverage across the domain and among the different parameters, reflecting the uneven spatial and temporal distribution of observing platforms. This variability influences the extent to which meteo-oceanographic fields can be evaluated using independent in situ data during the period of interest. Since ocean circulation, wind and wave models are constrained, directly or indirectly, by the available observations through initialisation,

assimilation and validation procedures, the spatial and temporal distribution of in situ data also affects the level of confidence that can be attributed to the model-derived fields used to force dispersion simulations. In this sense, the density maps provide a useful contextual framework for the interpretation of the dispersion results presented in the following chapters, supporting the identification of regions where model–data comparison is better constrained and areas where the limited availability or integration of observations calls for a more cautious interpretation of the results.