DIOGO MENDES MOREIRA

A GENERIC OPERATIONAL TOOL FOR EARLY WARNING OIL SPILLS - APPLICATIONS TO CARTAGENA BAY (COLOMBIA) AND THE COAST OF ALGARVE

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Master's in Marine and Coastal Systems

Work done under the supervision of: Prof. Dr. Flávio Martins & Dr. João Janeiro

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Declaration of authorship of the work

I declare that I am the author of this work, which is original and unpublished. Authors and works consulted are duly cited in the text and are included in the list of references included.

ABSTRACT

Over the past 10 years, the record of oil spills per year has decreased, with the majority being of a medium size (between 7 and 700 tonnes) followed by larger scale events, with volumes greater than 700 tonnes. Even though the frequency of spill events has been decreasing, the size and quantity of oil tanker ships have been growing, which will increase the hazard level of a spill. These issues, highly motivate the creation of projects focused on dealing with ocean pollution. This thesis was developed in accordance with two of these projects: "BASIC-Building Resilience in Cartagena Bay" and "ASTRiiS-Atlantic Sustainability Through Remote and In-situ Integrated Solutions". The BASIC project focuses on monitoring water quality and creating a mathematical model to predict hydrodynamic conditions and identify pollution in Cartagena Bay. The resulting product will be used by CARDIQUE Corporation and local authorities. The ASTRiiS Project, involving organizations like the Technical Institute of Lisbon and CIMA at the University of the Algarve, seeks to develop customizable information services and products to be implemented in key sectors of the blue economy with growth potential. Thus, spill predictions are a crucial component of monitoring because they enable a more effective response to the accident by assessing the impact beforehand and better developing a strategy to mitigate the environmental impact. The most important oil weathering processes in seawater are most commonly computed by Lagrangian models, which provide these predictions. These processes, which represent the interaction of hydrocarbons with seawater, are: Spreading, Evaporation, Dispersion, Dissolution and Emulsification. The models are able to forecast the geographical and temporal propagation of the oil spill slick with the support of the hydrodynamic and atmospheric forcing from external numerical models, which are required to compute these processes. The three most crucial factors out of these are wind, currents, and water temperature, which are all applied to calculate how spills behave in different parts of the world. The objective of the thesis is to create a generic Python-based program that will serve as the link between the user and the oil spill model, serving as an Early Warning System Tool (EWS-Tool) in response to oil spills, adaptable to any region of the globe. The MOHID Lagrangian module will be adapted to the region of Cartagena Bay, Colombia, and, the Coastal Region of Algarve to assess the oil spill events. Furthermore, the operational models BASIC, SOMA, CMEMS, AMSEAS, SKIRON and GFS will supply the hydrodynamic and atmospheric variables, which will serve as the foundation for the simulation forcing. Essentially, the EWS-Tool must read the user simulation information from a web form and send the results for the user email with a report of the simulation results. Furthermore, the EWS Tool entered a testing phase where different users tested it in order to find improvements. The results showed that, by adapting the tool to two different regions, the tool can be easily used in different scenarios and adapted to other pollutants in any other region of the globe. Additionally, the base created in this work will allow the development in the future of new models capable of further reducing hydrocarbon pollution in the environment, track other types of pollution, including microplastics, and even assist in search and rescue operations.

Keywords: Ocean Modelling, Oil Modelling, Operational Models, BASIC, SOMA, Cartagena Bay, Algarve.

RESUMO

A presente tese foi desenvolvida no âmbito de dois projetos de investigação, o “BASIC- Building Resilience in Cartagena Bay” e o ASTRiiS- “Atlantic Sustainability Through Remote and In-situ Integrated Solutions”. O Projeto BASIC visa desenvolver um programa de monitorização da qualidade da água e um sistema de modelação matemática capaz de prever as condições hidrodinâmicas e rastrear possíveis tipos de poluição na baía. Além disso, pretende apoiar a comunidade de Cartagena, unindo esforços com investigadores e instituições governamentais para melhorar o fornecimento e a qualidade da água potável. O produto final resultante deste trabalho será explorado pela Corporação CARDIQUE e pelas autoridades da baía. O Projeto ASTRiiS está a ser desenvolvido por um conjunto de organizações, incluindo o Instituto Técnico de Lisboa e o Centro de Investigação Marinha e Ambiental (CIMA) da Universidade do Algarve. O objetivo principal é desenvolver conhecimento técnico e científico para conceptualizar e implementar um conjunto de serviços e produtos de informação integrados e personalizáveis que serão aplicados e explorados em sectores-chave da economia azul com elevada margem de desenvolvimento.

Ambos os projetos visam a diminuir o impacto da poluição ambiental, tanto por derrames de petróleo como por qualquer outra fonte. Atualmente, o registo de derrames de petróleo por ano diminuiu, sendo a maioria de dimensão média (entre 7 e 700 toneladas), seguida de eventos de maior escala, com volumes superiores a 700 toneladas. Apesar de a frequência dos derrames ter vindo a diminuir, a dimensão e a quantidade de navios petroleiros têm vindo a aumentar devido à necessidade acrescida deste tipo de recurso, o que por sua vez aumenta o risco de derrames de hidrocarbonetos.

Assim, as previsões de derrames são uma componente crucial da monitorização, pois permitem uma resposta mais eficaz ao acidente, avaliando antecipadamente o impacto, ajudando a desenvolver uma melhor estratégia para atenuar o impacto ambiental. Os processos mais importantes de degradação do petróleo na água do mar são normalmente calculados por modelos Lagrangianos, que fornecem estas previsões. O modelo é capaz de prever a propagação espacial e temporal da mancha de hidrocarbonetos baseando-se nos dados fornecidos por modelos hidrodinâmicos e atmosféricos, que são necessários para calcular estes processos, e prever o comportamento do hidrocarboneto na água do mar. Estes processos, que representam a interação dos hidrocarbonetos com a água do mar, são: o Espalhamento, a Evaporação, a Dispersão, a Dissolução e a Emulsificação. Os três fatores mais importantes são o vento, as correntes e a temperatura da água, que são todos aplicados para calcular o comportamento dos derrames em diferentes partes do mundo.

O objetivo da tese é criar um programa genérico baseado em Python que servirá de ligação entre o utilizador e o modelo de derrame de petróleo, servindo como uma Ferramenta de Sistema de Alerta Rápido (EWS-Tool) em resposta a derrames de petróleo, adaptável a qualquer região do globo. O modelo Lagrangiano MOHID, será adaptado à região da Baía de Cartagena, Colômbia, e à Região Costeira do Algarve para avaliar os eventos de derrames de petróleo. Além disso, os modelos operacionais BASIC/AMSEAS e GFS irão fornecer as variáveis hidrodinâmicas e atmosféricas, respetivamente, que servirão de base para o forçamento da simulação. O programa lê as linhas de um formulário web preenchido pelo utilizador e utiliza-as para executar a simulação. No final será enviado um e-mail ao utilizador com um relatório da simulação e três imagens que mostram o transporte da mancha de petróleo ao longo de um período de três dias. A EWS Tool entrou numa fase de testes onde diferentes utilizadores a testaram para providenciar sugestões para melhorias ao programa. Os resultados mostraram que, ao adaptar a ferramenta a duas regiões diferentes, pode ser facilmente utilizada em cenários diferentes e adaptada a outros poluentes em qualquer outra região do globo. Além disso, a base criada neste trabalho permitirá o desenvolvimento, no futuro, de novos modelos capazes de reduzir ainda mais a poluição por hidrocarbonetos no meio ambiente, rastrear outros tipos de poluição, incluindo microplásticos, e até ajudar em operações de busca e salvamento.

Palavras-chave: Modelação Oceânica, Modelação de Hidrocarbonetos, Modelos Operacionais, BASIC, SOMA, Baía de Cartagena, Algarve.

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CONTENTS

INDEX OF FIGURES

INDEX OF TABLES

1 INTRODUCTION

Accidents regarding hydrocarbons in the ocean are becoming less frequent in recent days. In the last century, the average large scale oil spill per year was approximately 79, being reduced to 5 in the past years (ITOPF, 2023). The most frequent accidents are of a medium size (between 7-700 tonnes), followed by a low percentage of large-scale events (>700 tonnes). Given the increase in petroleum demand, mainly as a cheap energy source, the number of vessels that export them have been highly increasing, as well as its volume (ITOPF, 2023). This increases the hazard level per transportation, although fewer oil spill accidents are being registered. Hence the importance of the increasing efforts made to prevent such accidents. The advances in technology have enabled the tracking of an oil spill in an effective way, with more advanced spill models capable of predicting the spatial and temporal variation of a spill, and even artificial intelligence capable of detecting an oil spill via satellite imagery (De Kerf et al. 2020; Singh et al. 2022).

The prediction of an oil spill slick in the ocean depends on his interaction with the water, which also depends on the processes occurring in the ocean. These processes originate the ocean drift, which is the main influence on the transport of the oil, and is further influenced by the surface currents, by the stokes drift (a specific type of drift influenced by waves), and the wind drag effect acting on the ocean surface, (Malan et al, 2019). The effect of the ocean drift is important not only for keeping track of oil spill accidents, but also spatial detection of plastics, and supporting search and rescue operations. The oil spill accidents, as explained above, are prone to happen, and a better understanding of the processes involved is a step forward to minimize their impact.

This falls under a specific branch of science called Operational oceanography, which is responsible for monitor and forecast, in near real time, the continuous processes of the ocean and atmosphere, resulting in their quick interpretation and dissemination, which also contributes to a more precise prediction of the state of the ocean. Monitoring and forecasting services are powerful tools to respond to this demand of ocean state prediction and understanding (Sotillo, 2022). For these, the tools used are the Lagrangian models, which can compute and predict the ocean drift and the weathering of oil, based on the transport equations in their Lagrangian form. However, these models need to compute a variety of complex ocean processes (chemical, biological and physical), thus becoming very challenging to realistically simulate their behavior. Realistically simulating all these processes requires a high level of complexity, compelling the operational modeling systems to be coupled with forcing models and subsequently validated by comparison with in situ data. The forcing models, are frequently employed in a variety of sectors, such as energy generation, water management, transportation, and weather forecasting. The set of mathematical equations that describe the behaviour of the system being modelled make part of the operational modelling system, along with the set of input data and a computer software used to solve the equations and produce predictions. One of the key benefits of operational modelling systems is their ability to provide real-time forecasts and projections of a system's behaviour (Giannaros et al. 2014). Systems for operational modelling also have certain limitations. Models always represent a simplified version of the reality and might not accurately reflect the complexity and diversity of the system being studied. Furthermore, running operational models frequently requires a large quantity of data and computational resources, which can be both expensive and time-consuming (Semmendinger et al. 2022). Two examples of local operational systems are the BASIC system and the SOMA system (Janeiro et al. 2017; Mendonça, 2020), both maintained by CIMA at University of Algarve, and managed by a tool called SMS-Coastal, a python system capable of managing simulations of coastal operational models, developed by Mendonça, (2020). The BASIC operational system also has meaningful limitations, such as the absence of a built-in GUI, which makes it challenging for some users to navigate. However, it has a built-in interface for data visualization that can be accessed by: http://bahiacartagena.omega.eafit.edu.co/. As for the SOMA Operational System, the data is being stored in a virtual machine hosted in the University of Algarve (UAlg) and in a Thredds Data Server (TDS) that is also hosted in UAlg servers, to make the data available to other institutions.

As preciously said, the most important processes that dictate the behaviour of a hydrocarbon in the water are called, weathering processes. They depend on the hydrodynamic and atmospheric conditions, as well as on the oil-specific characteristics. These processes include: Spreading, evaporation, dissolution, emulsification, dispersion, microbial degradation, and the interaction between oil and sediments, being the most important processes in order to predict the persistence and behaviour of petroleum in seawater (Wang et al. 1999). Each of these processes is represented by a mathematical equation that is implemented into the Lagrangian model, to compute the persistence of this pollutant in the ocean, as well as the impact that may have in the long term. This allows to make a better management of the cleaning resources, in order to reduce their impact on the environment.

The most important step towards the decreasing impact of hydrocarbons in the environment is the connection between the stakeholders that export and import this type of energy source to attend the population needs, and an operational system that can predict the oil spill. If this connection is well established, it can provide to the stakeholders an effective way to decide what types resources must be applied in order to suit their necessities, and at the same time avoid unnecessary accidents and further impact on the environment (She et al, 2020; Sotillo, 2022).

The focus areas of this work are Cartagena Bay, Colombia and the Coast of Algarve, in Portugal. In the next sections, a brief introduction of the geographic systems is given.

1.1 Study Area

Cartagena bay is located on the north coast of Colombia, in the Caribbean Sea. As seen in the map in Figure 1, the flux of freshwater to the bay is determined by its major contributor, the Magdalena River basin, part of which flows through the Dique Canal, a large man-made channel connecting the bay to the Magdalena River. Wind-driven circulation, freshwater discharge and tidal forcing dictates the water transport in the bay. The bay has estuarine conditions being connected to the Caribbean Sea through two bars. It possesses a highly stratified upper water column with low salinity and high turbidity at the surface, mainly driven by the Dique Canal, and a less dynamic lower layer of saline water, with maximum depths of about 30m (Tosic et al. 2019a, 2019b). Cartagena Bay has semi-diurnal tides, with two high tides and two low tides every day. The tidal range, or the variation in water level between high and low tide, normally ranges from 0.5 to 1.5 meters, depending on factors such as moon phase and time of year. The wind patterns in Cartagena Bay are influenced by the prevailing easterly trade winds that blow from east to west over the Caribbean Sea, causing surface currents in the bay to flow from east to west, pushing water towards the bay's western end. In addition to tidal currents, Cartagena Bay suffers residual currents, which are longer-term currents driven by various factors such as wind, temperature, and salinity gradients. These currents can cause a net circulation of water within the bay, influencing its hydrodynamic behavior. For example, the prevailing easterly trade winds can cause surface currents in the bay to flow from east to west, while temperature and salinity gradients can drive density-driven currents, in which denser water sinks and flows along the bottom while lighter water rises and flows along the surface, resulting in a vertical circulation pattern. The combination of tidal currents and residual currents within Cartagena Bay can result in complex and dynamic flow patterns, with water traveling in different directions and velocities at different times of day and under different weather conditions. These currents can have an impact on many elements of coastal management, such as sediment movement, water quality, and navigation. Understanding the features and dynamics of these currents is therefore critical for understanding the hydrodynamic behavior of Cartagena Bay and its coastal environment.

There are two main marine ports inside the bay, Puerto Bahia and Puerto de Cartagena. Puerto Bahía is Colombia's most modern maritime multipurpose terminal, located at the southeast region of Cartagena Bay. However, its primarily function is as a marina and residential development, not a commercial port for oil export, being just a connection point to the principal port. Puerto de Cartagena, is a major commercial port on Colombia's Caribbean coast. It is regarded as one of the most important ports in the Caribbean region, as well as Colombia's largest port in terms of total cargo volume. The port's strategic location on the Caribbean Sea allows for easy access to shipping lanes connecting North America, South America, Europe, and Asia. It is a major trade hub for Colombia and other countries in the region, as well as a key entry point for goods such as oil, coal, and other agricultural products (Sánchez-Catalán et al. 2020). The port has five terminals in total, four of which are for general cargo and one for containers. It also has a specialised bulk oil and liquid terminal. The port has modern infrastructure, equipment, and technology to handle various types of cargo, as well as a large capacity for containers and general cargo storage (Sánchez-Catalán et al. 2020). This makes it a strategically located and well-equipped commercial port that plays a vital role in the economy of Colombia and the Caribbean region.

Due to this pressure for industrialization, various records of pollution in the sediments, biota, and waters have been observed (Parga-Lozano et al, 2002; Tosic et al. 2019a, 2019b; Caballero-Gallardo et al, 2020). This pollution is related to the several industrial facilities present in the area, such as chemical and oil refineries, which are known to release pollutants into the water. High amounts of contamination have resulted from this, which may be damaging to aquatic life and the humans who rely on the bay for food and water. The oil spill accidents that take place in the bay are also connected to the water contamination.

This level of contamination of the water in the bay motivated the creation of a project to deal with this pollution situation, which is precisely where the work developed in this thesis is inserted. The project is called “BASIC - Building Resilience in Cartagena Bay”, financed by Cardique, an environmental agency in Colombia. This project is partnered with the Centre for Marine and Environmental Research (CIMA-UAlg) and Escuela de Administración, Finanzas e Instituto Tecnológico (EAFIT) to help accomplish its goals. The project aims to develop a monitoring program for water quality and a mathematical modelling system capable of forecasting hydrodynamic conditions and tracking possible types of pollution in the bay. Additionally, it aims to support the community of Cartagena by joining forces with researchers and governmental institutions to improve the supply and quality of drinkable water. The final product resulting from this work will be explored by the CARDIQUE Corporation and the authorities of the bay.

As was mentioned earlier, the region is significantly impacted by the export of petroleum as well as other chemical pollutants. As a result, over time, there have been numerous oil spills there. Cartagena Bay has been fortunate to avoid significant oil spills, however the heavy exportation of oil poses potential disastrous consequences. Even if an accident occurs outside the region, the scale of the spill can indirectly affect the area. An illustration of this is the SS Atlantic Empress oil spill, which occurred on July 19, 1979, when the oil tanker collided with the Greek bulk carrier Aegean Captain in the Caribbean Sea, approximately 11 miles off the coast of Tobago (ITOFT, 2003). Unfortunately, efforts to contain and minimize the environmental impact of the spill were hindered by the disaster's magnitude, adverse weather conditions, and the remote location of the incident. Consequently, substantial quantities of crude oil were released into the surrounding waters, leading to significant damage to marine life, coastal ecosystems, and local economies. Although it remains challenging to determine the exact extent of the environmental impact and the total amount of oil spilled, estimates suggest that between 20 and 50 million gallons of crude oil contaminated coastlines in Trinidad and Tobago, Venezuela, and neighbouring countries. The Atlantic Empress collision prompted international efforts to mitigate the environmental damage caused by such incidents and emphasized the necessity for improved safety regulations and practices in the shipping industry, particularly concerning oil tankers and the transportation of hazardous materials.

While the Atlantic Empress collision did not directly impact Cartagena Bay, it serves as a vivid reminder of the constant vigilance and proactive measures required to protect the bay's sensitive marine ecosystem and coastal area from potential oil spills and other adverse environmental consequences.

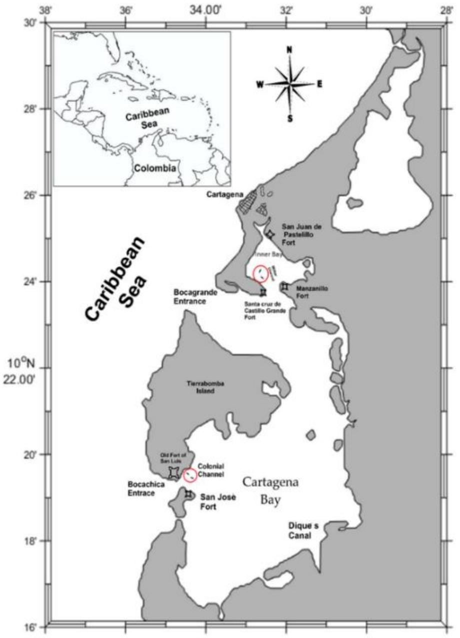


Figure 1 *- Map of Cartagena Bay (source: Quintana-Saavedra et al, 2023)*

The Coast of Algarve is a region in southern Portugal known for its stunning beaches, sunny weather, and beautiful coastline. It is a popular touristic destination, attracting millions of visitors each year. The region's coastline is characterized by a diversity of coastal features, such as long sandy beaches, rocky cliffs, and estuaries, which create complex hydrodynamic conditions. Waves and tides play an important role in shaping the Algarve's coastline, influencing sediment transport, erosion rates, and the distribution of marine organisms. In addition to waves and tides, the Algarve's hydrodynamics is influenced by a range of oceanic circulation patterns, including the Gulf Stream, a warm ocean current that originates in the Gulf of Mexico and flows north-eastward towards Europe. As it passes by the Algarve, the Gulf Stream brings warm water and marine organisms to the region, contributing to the region's rich marine biodiversity. The Algarve's hydrodynamics is also influenced by the region's climate, which is characterized by a Mediterranean climate with mild, wet winters and hot, dry summers. This region's ocean circulation follows a definite seasonal pattern, being influenced by southerly winds throughout the winter, which causes a poleward surface circulation along the west coast. Prevalent northerly winds in late spring and summer cause upwelling conditions, which are typified by a cold southward flow along the western coast. At the same time, westerly winds push the upwelled water along the southern coast in an easterly direction. A coastal counter-current develops along the coast during times of reduced northerly winds, transporting warm waters westward before turning northward at Cape St. Vincent (Rosas et al. 2021). Understanding these conditions is important for coastal management and infrastructure development in the region, including decisions about beach nourishment projects and erosion management strategies. The Algarve region, known for its tourism and fisheries industries, could be severely impacted by oil spill events, which fortunately do not occur frequently in the area. Tourism is a major source of revenue for the region, and an oil spill could have devastating effects such as cancellations of hotel reservations, restaurant closures, and loss of income for tourism-related companies. The negative visual impact of oil-contaminated beaches could also harm the region's image as a travel destination, resulting in fewer visitors and further financial losses for local businesses (Graça, 2016). In addition to tourism, the fisheries industry in the Algarve region, which includes commercial, leisure, and shellfish harvesting, could also be significantly affected by an oil spill. The spill could result in direct mortality of fish and other marine life, as well as contamination of fish populations and their food supplies, leading to declining fish populations and reduced capture. This would have financial implications for the fishing sector and impact the livelihoods of local fishing communities who rely on the sea for their way of life. Furthermore, the Algarve region is home to important natural parks, such as the Ria Formosa Natural Park and the Costa Vicentina Natural Park, which are rich in aquatic life. The risk of an oil spill along the coast can have significant impacts on maritime traffic, coastal ecosystems, and the overall environment (Santos & Andrade, 2009; Frazão Santos, Carvalho & Andrade, 2013). Maritime traffic can be directly impacted by an oil spill as it can lead to the closure of shipping lanes, ports, and harbours. Spilled oil can create hazardous conditions for vessels, hindering navigation and posing risks to ships and crew. The clean-up operations following a spill can also disrupt maritime activities, resulting in delays, detours, and increased costs for shipping companies and traders., which raises concerns from environmental groups regarding potential risks to the coastal ecosystems (ITOPF, 2023). Efforts to prevent and mitigate the impact of oil spills in the Algarve region are crucial to protect its tourism and fisheries industries, as well as the environment and the livelihoods of local communities (Santos & Andrade, 2009; Santos, Carvalho & Andrade, 2013).

This includes implementing strict regulations, preparedness and response plans, and investing in technologies for early detection and containment of oil spills. Additionally, raising awareness about the importance of protecting the marine environment and promoting sustainable practices in the tourism and fisheries sectors can contribute to safeguarding the Algarve region's economy and natural resources for future generations (Janeiro et al. 2014 & 2017). The focus on the coast of Algarve, also falls on a project named ASTRiiS- “Atlantic Sustainability Through Remote and In-situ Integrated Solutions”. The project is being developed by a number of organizations, including the Instituto Técnico de Lisboa and CIMA at the University of Algarve. The primary goal is to develop technical and scientific knowledge in order to conceptualize and implement a set of seamlessly integrated and customizable information services and products that will be applied and exploited in key sectors of the blue economy with high development and value creation.

1.2 Thesis Goal

The work developed in this thesis, aims to provide a generic tool to support the tracking of hydrocarbons in the ocean, with the capability of being adapted to track other types of pollution or object (such as, microplastics, other hazardous noxious substances, waste waters, person lost in sea), in any region of the globe. For demonstration purposes, the MOHID Modelling system will be adapted to oil spills in Cartagena Bay and in the coast of Algarve, to further test the tool’s adaptability. A python-based program will be developed, capable of automating the oil spill simulations as they are requested by the user in a web form questionnaire. This thesis is divided into 6 chapters, the first of which is the Introduction. In Chapter 2, a literature review of oil spill models will be provided, by explaining the different functions of the models and a brief explanation of the equations used to compute these simulations. In Chapter 3, will be explained the tool developed in more detail, by explaining the specific modules and functions of python used in the script. In Chapter 4, the results are present, and the respective discussion in Chapter 5. Finally, in Chapter 6 the final conclusions of the thesis are presented.

2 STATE-OF-THE-ART

As oil spills pose a significant risk to both marine ecosystems and human health, predicting their behavior and potential impact is of critical importance. Therefore, understanding the advanced methodologies used in oil spill modelling is fundamental for effective prevention, response, and mitigation strategies. This chapter provides a comprehensive overview of the current state of oil spill modelling, highlighting the progress that has been achieved in the field, the existing gaps in knowledge, and the opportunities for further advancements.

2.1 Oil Spill Models

These models can predict the movement of oil spills based on ocean currents, wind, and waves, which are then used to forecast where and how the oil will spread over time. Based on these factors, they can also predict how the oil will disperse in the water column, allowing them to determine the concentration of oil in different parts of the ocean (Fingas, 2011). Furthermore, it can predict how long will the oil take to degrade based on the oil weathering processes, allowing to assess the potential effects on marine organisms as well as the effectiveness of various response strategies.

Oil spill models are classified into three generations based on their evolutionary stages. The first generation of transport models are primarily based on physical oceanographic data and simple mathematical algorithms, such as the drift model. Second-generation models use numerical algorithms to simulate oil movement and incorporate more advanced oceanographic data, such as wind and current information. The third-generation models combine real-time data from satellites, remote sensing, and In-situ measurements to provide high-resolution predictions of oil spill transport and behaviour (Berry et al. 2012, Keramea et al. 2021). They also consider wave dynamics, atmospheric conditions, and oil weathering.

The more recent generations of oil spill models follow a similar structure to their predecessors, utilizing Langrangian-based methods for transport processes and employing separate algorithms for fate processes. Among the Lagrangian methods used for transport prediction, the random walk method is the most commonly employed and forms the lowest level in the hierarchy. Hydrodynamic and atmospheric conditions, such as wind, currents, and waves, are obtained from models or observation systems like buoys or satellites. Oil spill models simulate transport by tracking Lagrangian oil particles, which can be categorized into different size classes (Spaulding, 2017). Fate processes are modelled differently on various regions of the ocean, including the water column, seabed, shoreline, and sea surface, accounting for changes in oil composition and physical characteristics over time, such as viscosity, density, and interfacial tension. Modern oil spill models not only provide predictions but also assess the level of uncertainty, which is crucial for timely, effective, and cost-efficient response actions. Uncertainties arise from input fields, internal model dynamics, and limited observational data. Ensemble forecasts play a critical role in improving prediction accuracy, considering the multitude of uncertain factors involved (Keramea et al., 2021). Furthermore, the new generation models incorporate spill and drifter monitoring to enhance slick forecasting. They utilize satellite Synthetic Aperture Radar (SAR) imagery and data to identify potential oil slicks. Detailed information on current oil spill remote sensing methods can be found in review papers by Fingas and Brown, 2017. The scientific community has focused its efforts on improving 4D predictions by retrospectively modeling oil spills to trace back to their source and identify the origin of the slick. Combining this back-propagation technique with the functionality of the Automatic Identification System (AIS) allows for pinpointing the causes of oil spills (Keramea et al., 2021). The model system ADIOS (Automated Data Inquiry for Oil Spills) is frequently used to forecast the movement and outcome of oil spills in the marine environment, and consists on a group of oil weathering models that are frequently used in the oil spill models like MOHID (Keramea et al. 2021). The National Oceanic and Atmospheric Administration (NOAA) employs GNOME, an open-source Lagrangian model, within their Hazardous Materials Response Division, using the ADIOS as a supportive model. GNOME is specifically designed to forecast the movement and behavior of pollutants and oil spills, accounting for factors such as wind, currents, tides, and spreading. Its comprehensive features include 3D particle transport, compatibility with various hydrodynamic models and field data, wind surface transport through the concept of 'leeway,' open-source code availability, backward simulation capabilities, incorporation of oil weathering algorithms from the integrated ADIOS oil database, interaction with sea ice based on concentration and velocity, shoreline interaction (beaching), and an integrated response options calculator (ROC) for evaluating spill response systems' performance (Keramea et al., 2021). Additionally, a Python framework called PyGNOME has been developed to facilitate the utilization of GNOME, enabling web-based batch processing, testing, and visualization of model output through a Geographic Information System (GIS). The model is designed to be user-friendly, featuring an intuitive interface that allows users to run simulations quickly. It relies on various input data, including ocean currents, wind patterns, and detailed information about the spilled oil, such as density, viscosity, and composition. Nevertheless, it is important to note that oil spill models still face challenges in accurately replicating certain complexities and variations found in real-life scenarios, such as the influence of subsurface currents and internal waves (Lehr et al., 2012; Keramea et al., 2021).

For this work, the model MOHID was chosen due to its wide range of applications, which include coastal and estuarine modelling, river modelling, and lake modelling. MOHID is an abbreviation for Modelo Hidrodinâmico, which means Hydrodynamic Model, and was the model's original purpose when it was created in 1985. The MOHID Water Modelling System is written in ANSI FORTRAN 95, integrating various numerical models. It is an integrated modeling tool capable of simulating physical and biogeochemical processes in both the water column and sediments, as well as coupling with the atmosphere (MOHIDWiki, 2008). Mohid Water Modelling System is organised in a hierarchical modular structure and currently consists of over 60 modules. Each module is in charge of managing a specific type of information while performing a specific function or process, inserted into three main categories of environmental systems, air, water, and land. MOHID is an open-source model with a user-friendly interface that makes it simple for users to set up and run simulations. It has the capability to combine with other models, such as wave and sediment transport models, to provide a more complete representation of the system under consideration. One significant advantage of MOHID over other oil drift models like GNOME is its Lagrangian module, which allows online Lagrangian simulations coupled with the respective hydrodynamic simulation. This feature greatly enhances the precision of particle trajectories and oil weathering processes. However, it is important to note that these simulations can be computationally demanding, and therefore, the use of high-performance computing resources is crucial for efficient execution. By utilizing such resources, the oil spill model integrated within MOHID can effectively compute the properties of the weathering of hydrocarbons, providing valuable insights into the fate and behavior of oil spills.

The weathering processes, mentioned above, are computed by the oil spill models due to a collection of different algorithms, each of which describes an individual fate process. In order to track the spatial and temporal variation of the spill, the spill models must consider the oil weathering processes, being a key impact on the size of the oil slick and the concentrations of the oil components, both dissolved and in particulate form. The oil weathering processes consist of spreading, evaporation, dispersion, dissolution, and emulsification, as illustrated in Figure 2.

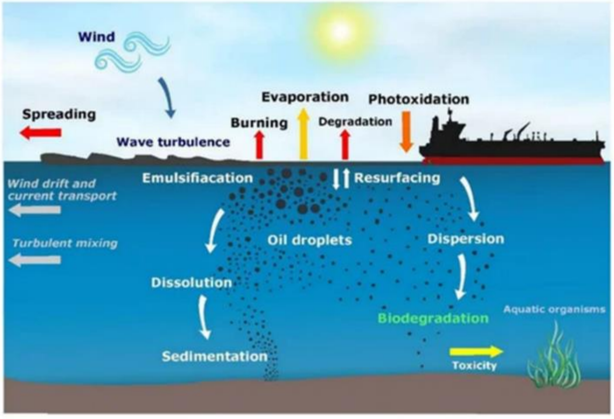


Figure 2 *- Oil Weathering processes in the water (Keramea et al. 2021)*

The horizontal expansion of a slick, caused by forces including gravity, inertia, viscosity, and interfacial tension is known as spreading. It is a crucial phase in the early stages of the transformation of the slick since weathering processes tend to alter the mass and characteristics of the slick. Slick area and thickness are important parameters in oil models, because, under free-surface conditions, they have a significant impact on weathering processes including evaporation and dissolution. The initial slick area of a spill is determined by an equation derived from Fay's solutions (Fay,1969). This equation was proposed by Fay by adjusting experimental results to a curve during the first phase of the spreading after a point discharge. This first phase is frequently very short in time (order of a few hours) and only inertia and gravity forces are present. It is thus not simulated explicitly in the models, and is used to set the initial area of the spill (Keramea et al. 2021). The initial area is calculated as follows:

$$A_0 = \pi \frac{k_2^4}{k_1^4}\left(\frac{\Delta V_0^5}{v_w}\right)^{\frac{1}{6}}$$

where A_0 is the initial area of the spill, $\Delta = \frac{\rho_w - \rho_0}{\rho_w}$ is the density of water, ρ_0 is the oil density, V_0 is the volume of the oil spilled, v_w is the water kinematic viscosity and, $k_1 =$

0.57 and k_2 = 0.725, which are a sensitivity parameter introduced by the user and dependent on the mesh geometry (Fay, 1969).

Evaporation is represented in models as an evaporative exposure algorithm, where the flux of volatiles to the atmosphere is determined by the molar volume of the compounds, vapor pressure, and molecular weight (Karamea et al. 2021; Berry et al. 2012). All these characteristics are related to the boiling point of the components of the oil, which need to be specified before running the model. The oil evaporation process is estimated using the analytical method of Stiver and Mackay (1984), also known as the evaporative exposure method, given by the equation:

$$\frac{dF_e}{dt} = \frac{K_e A_S}{V_0} exp\left(A - \frac{B}{T}(T_0 + T_G F_e)\right)$$

where, F_e is the volume fraction of evaporated oil, T is the oil temperature, T_0 represent the initial boiling point, T_G is the gradient of the distillation, A_s is the oil slick area, V_0 is the initial oil volume, A and B are empirical constants with values of A = 6.3 and B = 10.3, and K_e is the mass transfer coefficient, determined by a formulation proposed by Buchanan & Hurford (1988).

Surface oil dispersion is defined as the breakdown of a coherent oil slick into small droplets and their entrainment into the water column. The action of waves, particularly breaking waves and upper layer turbulence, is primarily responsible for slick breakup. Furthermore, wave action can break up an oil slick and push the resulting oil droplets down into the water column to a depth determined by the breaking wave energy. To compute dispersion in MOHID, two methods are available. The first was proposed by Delvigne and Sweeney (1988), which uses wave energy, using the following equation:

$$\frac{dm_d}{dt} = c_{oil} D_{ba}^{0.57} f_s F_{wc} d_0^{0.7} \Delta d$$

where f_s is the surface fraction covered by oil, d_0 is the droplet diameter; Δd is the oil droplets diameters range around d_0, and c_{oil} is a parameter experimentally determined which depends on oil type. The second method, and the one used in this study, was proposed by Daling et al. (1980), that gives the vertical dispersion as a function of wind velocity squared, given by the equation:

$$\frac{dm_d}{dt} = 0.11 m_{oil} \frac{(1+W)^2}{1 + 50\mu^{1/2} h\sigma}$$

where m_{oil} is the oil mass that remains in surface, μ is the oil dynamic viscosity, h is the slick thickness (cm), W is the wind velocity (m/s) and σ is oil-water interfacial tension.

Dissolution is the process in which the oil droplets mix with the water, and is a process that is rarely considered in numerical models because its impact on the oil mass balance is negligible, as less than 1% of the oil spilled dissolves. However, it is significant from a toxicological standpoint because the components of the oil that tend to dissolve are the most toxic and volatile ones (Keramea et al.2021). Cohen et al., 1980 estimated the dissolution rate as the rate at which the soluble fraction of the oil breaks down into small particles that mix with water to form a homogeneous mixture, given by the formula:

$$\frac{dDiss}{dt} = Kf_sA_sS$$

Where $\frac{dDiss}{dt}$ is the variation of the dissolution of oil over time, f_s is the surface fraction covered by oil, A_s is the oil slick area and S is the oil solubility in water, given by Huang (1983).

Emulsification is the process by which water-in-oil emulsions, also known as "chocolate mousse," are formed. Evaporation decreases the volume of the surface slick, whereas emulsification increases it. The turbulent energy present in the water can cause small droplets of water to mix with the oil, resulting in the formation of an emulsion. The amount of water droplet size distribution affects the emulsion's viscosity and temporal stability. The equation proposed by Daling et al. (1980) is used to estimate the variation of the water volume fraction incorporated in the emulsion, as follows:

$$\frac{dF_{wv}}{dt} = K_w(1+W)^2\left(1-\frac{F_{wv}}{F_{wv}^{final}}\right)$$

where F_{wv} is the water volume fraction incorporated in emulsion, F_{wv}^{final} is the final volume fraction of water incorporated in emulsion, and K_w is an empirical constant, introduced by the model user. The default value in MOHID is 1.6×10^{-6} (MOHIDWiki, 2008).

Thus, hydrocarbon fate models must be well configured, using these equations and the correct set of parameters, to support the response to an oil spill accident, aiming to access and prevent its impact on the environment (Sebastião et al. 1995).

To compute the transport of the particle of oils, or their fate, the oil spill models use the concept of tracers. A tracer can be a water mass for a physicist, a sediment particle for a geologist, and a molecule for a chemist. The tracers' movement can be influenced by the hydrodynamic module's velocity field, the wind from the surface module and the spreading velocity from the oil dispersion module (MOHID Modelling System Description, 2006). Tracers are "born" at origins, and tracers from the same origin have the same set of properties. Tracer emission patterns differ depending on the origin, which can be classified as "Point Origin" (emits at a specific point), "Box Origin" (emits over an area), or "Accident Origin" (emits in a circular pattern around a point).

The third option was chosen for this study to better represent the unpredictability of an oil spill accident (Keramea et al. 2021). The Lagrangian module interacts with the oil dispersion module to simulate oil dispersion, and the Lagrangian module uses the water quality module's feature to simulate water quality evolution. The major factor responsible for particle movement (or tracer movement) is generally the mean velocity. The spatial coordinates of a particle are given by the definition of velocity:

$$\frac{dx_i}{dt} = U_{i(x_i,t)}$$

Where:

$$U_i = u_{1i} + u_{2i} + u_{3i} + u_{4i} + u_{5i} + u_{6i}$$

Where U_i stands for the total velocity of the particle, consisting on the sum of u_{1i}, the velocity currents, u_{2i}, the velocity induced by the direct action of the wind drag, u_{3i}, the velocity due to the effect of ocean wave (Stokes drift), u_{4i}, the velocity due to horizontal surface spreading of the oil, u_{5i}, the random velocity due to isotropic turbulent mixing and u_{6i}, the velocity with which oil particles disperse in the water column (Suh, 2006). The hydrodynamic modulus is used to determine u_{1i}, the Lagrangian modulus is used to calculate u_{2i} and u_{3i}, and the MOHID oil module is used to calculate u_{4i} and u_{6i}. The mixing length and the standard deviation of the turbulent velocity component, as indicated in the hydrodynamic model's turbulence closure scheme, are used to calculate the random particle displacement due to turbulence u_{5i} in the MOHID oil module in accordance with Allen's (1982) instructions. The model's operation and setup will be thoroughly explained in Chapter 3.

3 METHODOLOGY

The thesis aims to develop a generic tool that supports the tracking of various types of pollution, such as microplastics, hydrocarbons, hazardous noxious substances, and wastewater. The methodology developed for this tool can be applied in any region of the world, serving as an Early Warning System Tool (EWS-Tool). The tool utilizes the MOHID Modeling system, which provides Lagrangian simulation of oil spills. As a demonstration, the tool is adapted for two specific regions: Cartagena Bay and the coast of Algarve. These regions serve as test cases to test the tool's adaptability. At the core of the tool is a Python-based program designed to automate oil spill simulations based on user requests submitted through a web form questionnaire. The program reads the user inputs from the web form using a CSV file and generates the necessary simulation instructions to run the desired scenario. To run the simulations the hydrodynamic and atmospheric forcing are necessary, which will be extracted from the BASIC (Cartagena Bay) and SOMA (Algarve) operational systems maintained by University of Algarve. Additionally, using the forcing and the lagrangian simulation files, the program generates maps of the oil spill simulations, which are included in the report sent to the user. All these steps are explained in detail in the next sections.

3.1 BASIC Operational System

The basis of the Cartagena Bay oil spill model is centred around the operational system BASIC. This system is capable of forecasting and hindcasting a variety of physical parameters such as water level variation, salinity, water surface temperature, and current velocity, with a resolution grid of 75 m. The data is produced hourly for each day, being composed by both 3D and surface datasets, in HDF5 format. However, the lagrangian model in MOHID cannot read more than one HDF5 file at the same time, so an external tool “Merger” is used to compile the hourly files into a single file that corresponds to 3 days of forecast for each variable mentioned above. In Figure 3, two examples of the BASIC forecast data from the surface layer are shown. Pictures were created with the OpenFlows FLOOD program interface.

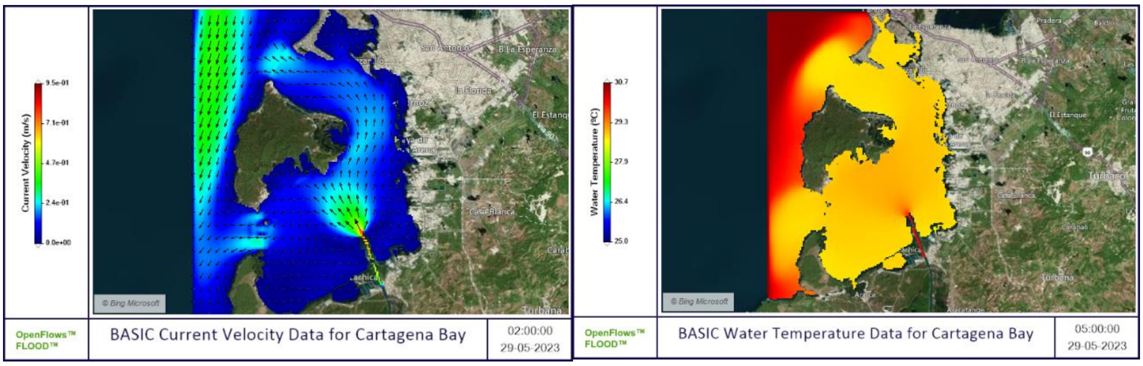


Figure 3 *- BASIC Forecast Data for Cartagena Bay (created with OpenFlows FLOOD).*

3.2 SOMA Operational Model

The Algarve Operational Modelling and Monitoring System (SOMA) was developed to address the specific requirements of predicting the sea state and trajectory of oil spills along the Algarve coast (Janeiro et al., 2017). SOMA is built within the framework of the MOHID modeling system, which is considered a suitable and robust tool for downscaling approaches. This choice of architecture ensures the reliability and efficiency of the model (Janeiro et al., 2017; Mendonça, 2020). The operational model consists of two grid levels: Level 1, with a 2 km resolution grid and Level 2, with an increased resolution of 1 km. Both grids use a vertical discretization with 50 cartesian layers. The output data files are generated hourly for the Level 1 grid and every half hour for the Level 2 grid. The SOMA model was specifically selected to support oil spill simulations along the Algarve coast due to its capabilities and suitability for the task. Figure 4, illustrates two maps showcasing the data from the surface layer of the SOMA operational model, representing current velocity and water temperature for the coastal area of Algarve.

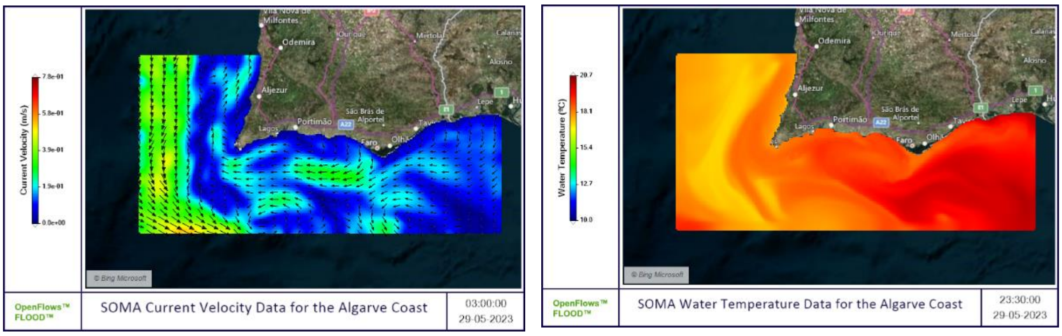


Figure 4 *- SOMA Hydrodynamical Forecast Data for the Coast of Algarve (created with OpenFlows FLOOD).*

3.3 Oil spill model Setup

To accomplish the goals of this study, a multi-grid Lagrangian oil model was adapted and used to predict the fate of potential oil spills in the study areas. In a multi-grid model, the domain is divided into a hierarchy of grids, often referred to as levels. Each grid level represents a different level of resolution, with the finest grid providing the highest level of detail. The idea behind the lagrangian multi-grid approach is to provide to the particles the best forcing available at a certain position. In this method, for each time step and for each particle, the hydrodynamic forcing is interpolated using the best solution existent in the grid hierarchy.

In this work the Lagrangian model was chosen to be run in off-line mode. In this mode the Lagrangian model uses forcing data from external hydrodynamical and atmospheric operational models, which provide spatial and temporal variation of wind, currents, water temperature, and waves. Alternative sources of data were also considered acting as redundancy. The model tries to integrate all possible processes to make the simulation as close to reality as possible. It applies the particle transport and oil weathering equations, described in the previous chapters, including the oil weathering processes, such as Emulsification, Dispersion, Evaporation, Dissolution, and Spreading.

For the region of the Cartagena Bay, the hydrodynamical and atmospheric forcing, are provided by the operational system BASIC and by the operational model SKIRON, respectively. A large set of other parameters is needed to run the simulation. Those parameters are written in two separate DAT files. For MOHID to understand the parameters they must be written with specific keywords that work as commands for MOHID to execute and compute. Two files must be configured for every simulation: the Lagrangian.dat and the Model.dat. The Lagrangian.dat file includes all the physical parameters from the operational models that are needed to compute the ocean drift (wind, currents, temperature, and salinity), as well as the characteristics of the oil, seen more thoroughly in the next subchapter. The second file is used to set the time of the start and end of the simulation, as well as the time step. In this work a maximum of three days was considered for the simulation which is the average time taken by an oil slick to reach land in the bay.

In the Algarve region the main differences are in the hydrodynamical forcing, which in this case come from the University of Algarve's Operational Model SOMA. The only difference between the two separate DAT files is a change in the spill accident coordinates. The tool's code will also need to be modified slightly, which involves the extraction of the forcing and a change in the directories for the necessary files.

3.4 Early Warning System Tool

The oil spill Early Warning System Tool (EWS-Tool) consists in a program, written in python, developed to automatize the Lagrangian simulation for the oil spills. An illustrative diagram of the functionalities of the program is shown in Figure 5. The letters refer to the different actions executed by the program. As it starts running, it will keep checking a specific email address (A), designed to receive a notification every time the Google form is filled (B) and submitted. This works as the trigger for the rest of the program. Once it detects that a new notification was received, it reads the CSV file (C) with the most recent written line and extracts all the user inputs to separate variables. The information needed is: the user's name, the user email (to send the results), the institution\company to which the user belongs, the time of the submission, the simulation start date and time, the coordinates of the spill origin, the volume of the spill and the type of oil. 3 oil types are currently implemented. MOHID is very strict with the format of certain parameters, so the program will follow the conversion of the volume from US Gallons to Cubic Meters and separate the data with blank spaces, to allow MOHID to understand them. Following this, it will extract the hydrodynamic forcing from the operational system (BASIC or SOMA depending on the case) (D), and the atmospheric forcing from the respective data provider (GFS, AMSEAS or SKIRON) (E). Next it compiles the daily files (F) into a 3-day HDF5 single file. After all this is done, it creates the MOHID files Lagrangian.dat and Model.dat with the instructions to run the simulation (G). Finally, the program executes the MOHIDWater.exe (H) which is executed in a specific virtual machine hosted in the UAlg servers. After the simulation is done, the program checks the model logs for possible errors (I). If an error is detected, the user receives an error message (J). In case the simulation ran without errors, the program will create a report of the results (K), with maps of the oil spill behaviour along the three days and send it to the user email (L).

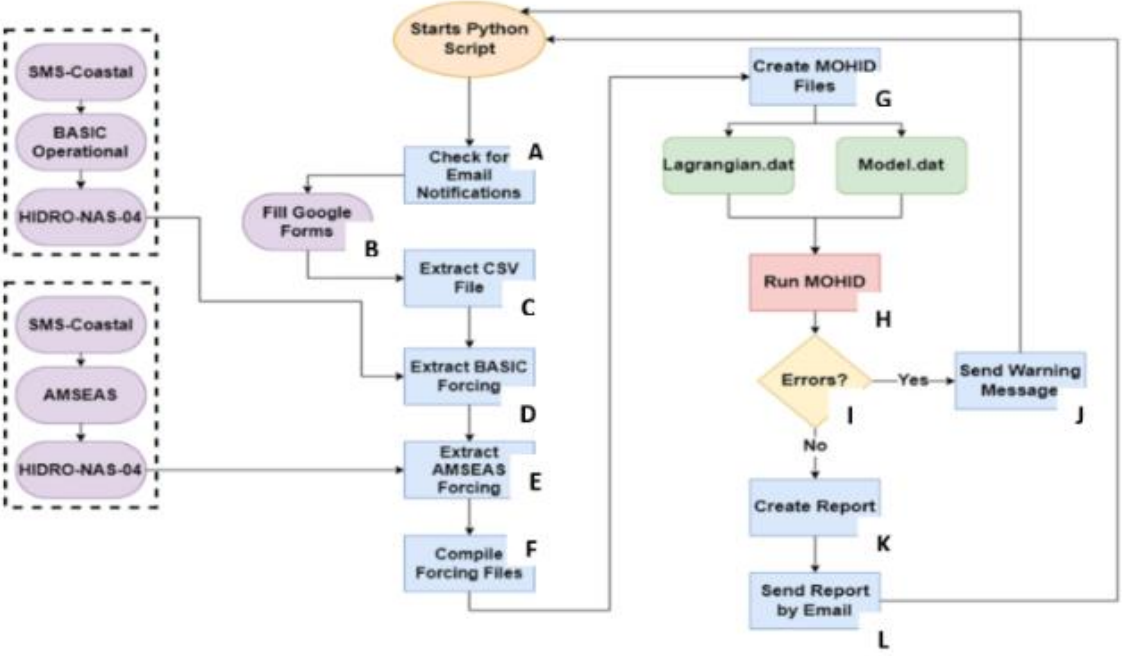
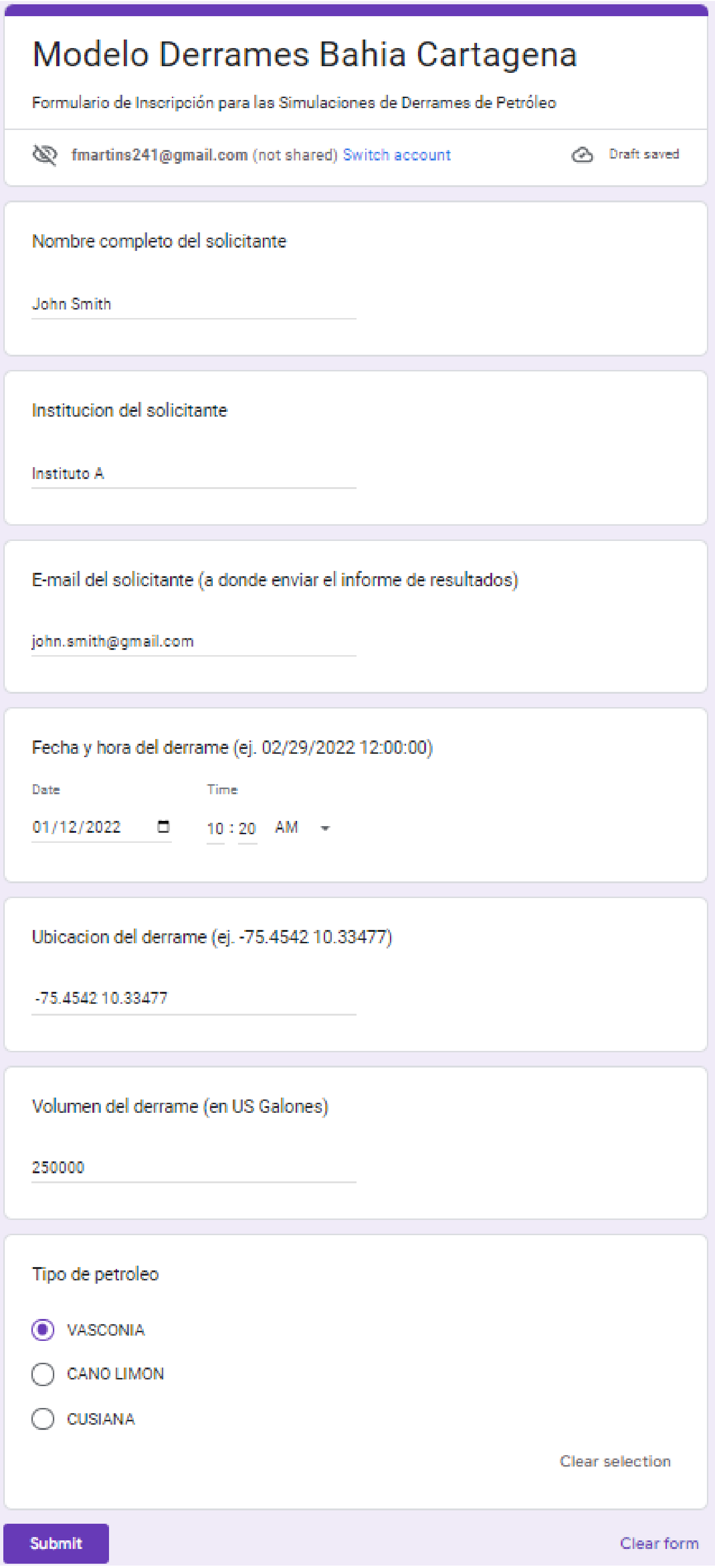


Figure 5 *- Diagram of the Early Warning System Tool.*

Figure 6 shows an example of a form with all the information given by the user for the BASIC case.



Modelo Derrames Bahia Cartagena

Formulario de Inscripción para las Simulaciones de Derrames de Petróleo

fmartins241@gmail.com (not shared)

Nombre completo del solicitante

John Smith

Institucion del solicitante

Instituto A

E-mail del solicitante (a donde enviar el informe de resultados)

john.smith@gmail.com

Fecha y hora del derrame (ej. 02/29/2022 12:00:00)

Date	Time
01/12/2022	10 : 20 AM

Ubicacion del derrame (ej. -75.4542 10.33477)

-75.4542 10.33477

Volumen del derrame (en US Galones)

250000

Tipo de petroleo

● VASCONIA
○ CANO LIMON
○ CUSIANA

Figure 6 *- Example of a filled online form.*

In the next sections the different actions performed by the EWS are explained in detail.

3.5 Python Script

The final version of the Oil Spill tool consists of a script that performs a variety of tasks in order to provide the final report of the oil spill simulation. These are grouped in 3 different Python functions: a function to get the information for the simulation and run it, another to extract and compile the forcing files and a third one to create the images of the simulation and write the report.

3.5.1 Email Trigger Loop

The first part of the script consists of a loop that continuously checks a specific email account, created exclusively to receive notifications from the Google Forms, whenever an entry form is filled and submitted. By using the *"imaplib"* module of python and the class IMAP, enables a creation of a SSL connection to the outlook servers and check if there is new emails in the inbox by selecting it with the *"email"* module. Then, an infinite *while* loop was created, always checking if there is a new email notification. Once it detects a new email, executes the main script for the simulation.

The loop continues, logging in and out of the email account. As the loop continues, connection errors or time outs may occur, which can be resolved by restarting the script and by setting a sleep timer, that makes the program wait one minute before logging again into the email searching for another simulation request. However, because this program requires almost no intervention, this error was captured inside a try/except that every time this error appears, the script is restarted automatically.

3.5.2 User inputs

Once the main script starts, the first thing it does is connecting to the Google Forms associated file to read the latest response. It will extract all the necessary information to run the simulation and create the report with the results. The Google Forms associated file is a comma separated value file, or CSV. To read the information with python, the "csv" and the "pandas" modules were used. The first module reads the file directly using the *"CSV.reader"* subclass and the second transforms it to a data frame enabling the selection of data in a column/rows type of structure. This enables to create variables that will correspond to the user's inputs for the simulation: user´s name, user's institution, user's email, time of submission, start date of the simulation, coordinates of the spill, volume of the spill and type of oil.

Some formatting and conversions must be made so that MOHID can read them correctly. This applies to the end date of the simulation which is computed using a datetime type variable. The end time is created automatically by adding three exact days to the start date of the simulation inputted by the user. The volume is also converted form US Gallons to Cubic Meters, in which 1 US Gallon = 0.0037854118 Cubic Meters. The characteristics of the oil are read from a separate csv file, extracted from the ADIOS database. At this moment it includes three different types of oil: Cano Limon, Vasconia and Cusiana.

3.5.3 Extraction of Forcing Data

The function responsible for extracting the forcing data is then called by the main script. It copies the respective HDF5 files from a network attached storage (NAS) and utilizes the MOHID Water Modeling System's Merger tool to compile all the files that correspond to three days' worth of hydrodynamic conditions. The Merger tool requires a user input file containing information about the files that will be merged and the name of the output file. To select the necessary files, the script creates the path to the data files by using the initial date variable from the user and constructs the file that has the year, the month and the day in the path. These files are the output results of the SOMA or the BASIC operational models.

Every time the script is activated by the email notification, a text file that contains this user input will be written in Python. The "glob" module of Python is used to build the list of HDF5 files required for the simulation, which are stored in the folders described above. Two log files will be generated when the Merger tool is used, one of which will show the program operating and the time it took to finish the operation (average 3 min) and the other will contain any errors that may have happened. If there is any error in the second log, the file merging failed, and the program must notify the user that the simulation failed. The second log must always be empty. The absence of data and the inability to locate the text file containing the instructions for merging the files are two possible reasons to produce an error. Assuming all went well with the forcing extraction, the script will continue to its following task.

3.5.4 Running MOHID

After the extraction of the forcing the script will perform the steps needed to execute MOHID. The simulation is based on a fixed set of MOHID input data files where only the files Lagrangagian.dat and Model.dat are modified. These files are created using the user's inputs and making use of if/else statements. The oil properties are obtained from an oil properties file constructed from the ADIOS database, as a function of the type of oil chosen by the user.

After the creation of the files, the script launches the MOHID executable which produces two log files. In this case, the approach used to determine whether there were any errors is to check for a line in the log file “run.txt” indicating that the simulation terminated successfully. Assuming the simulation was successful, the script continues to the creation of the pictures and production of the report. If any error has occurred, the script will deliver a report without any images indicating that issues were detected in the simulation. The simulation is the operation that takes the longest time, around 10 min, for both systems, Cartagena Bay and the coast of Algarve.

3.5.5 Creation of Simulation Maps

This function of the script begins as soon as the simulation terminates and has the objective of creating the maps for the report. Two HDF5 files, the Hydrodynamic file and the Lagrangian file, are required for this. The "h5py" and the "NumPy" modules are used to generate variables with the latitude, longitude, current velocity, and the thickness of the oil—a parameter used to describe the evolution of the oil spill slick.

Three maps are created from the simulation—one for each day—representing the evolution of the oil slick. A colour bar is used to indicate the thickness associated to each particle. The classes "pyplot", "cartopy" and "matplotlib" are used to produce the maps. The current velocity vectors are added to the map using the "cartopy" module, which offers a high-level interface for making maps and interfacing with raster and vector data. The simulation's visualization of the oil particles is made using a scatter plot and the class "pyplot". Lastly, the images are saved separately before they are inserted into the report and sent to the user’s email.

3.5.6 Create Report of the Results

The report is the tool's final result. The contents of this report provide assurance about the tool's efficiency. The report gives basic information about the simulation that was requested, including the simulation specifications and maps depicting the transport of the oil spill slick over the three days. The report is created automatically in python using the "FPDF" library. It allows to define how many pages the document will have, the size of the page, the letter font, and the orientation of the page. To reduce the number of lines of code required to create this, an image was created that includes all report static elements and was then inserted into the page created for the new document. Once the report's static elements have been inserted, the user inputs that were previously stored in separate variables are inserted and their position adjusted. Finally, the images with the simulation maps are added and adjusted to the report’s canvas. The report is then saved as a pdf document, ready to be sent to the user.

3.5.7 Sending the Report via Email

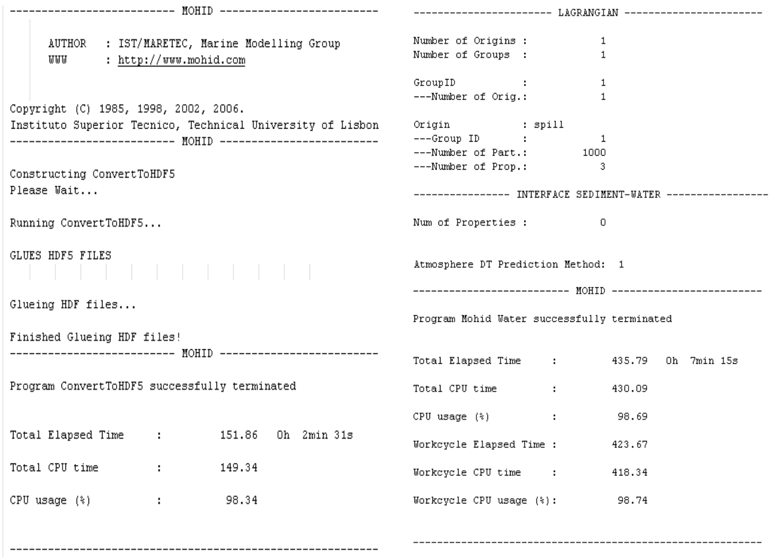
Finally, the script completes the task by sending the report with the results to the user. The sending action, as well as the writing and addition of annexes to the email message, is fully automatic. To accomplish this, the Python class "email. message" is extremely useful, as it is capable of creating a new email, writing the sender and receiver information, as well as the email text and adding the pdf. To send the email, the script uses the “email.sendmessage” class by first login to the email address created for this tool. Once the user receives it, the program successfully finishes the handling of the simulation and returns to the loop of checking new email notifications, until the user requests a new simulation using the entry form.

4 RESULTS

In this work, the main objective is to develop an Early Warning System (EWS) Tool rather than conducting tests on the hydrocarbon model. Previous studies, such as those by Janeiro et al. (2017) and Tosic et al. (2018, 2019a, 2019b), have already tested the hydrocarbon model, providing the necessary background for this thesis. The focus of the next two sections is not to analyze the results of the runs, but rather to observe the behavior of the EWS Tool in an operational scenario. The results presented here pertain to two specific systems: the Cartagena Bay in Colombia, which is part of the BASIC operational system, and the Coast of Algarve, which is part of the SOMA operational system. In the upcoming sections, the outcomes of these two experiments will be discussed, shedding light on the performance and effectiveness of the EWS Tool in practical situations.

4.1 Cartagena Bay Reporting

The EWS-Tool will originate two log files: one of the Merger tools of MOHID, responsible for compiling the forcing files, and another for the Lagrangian Simulation, both seen in Figure 7.

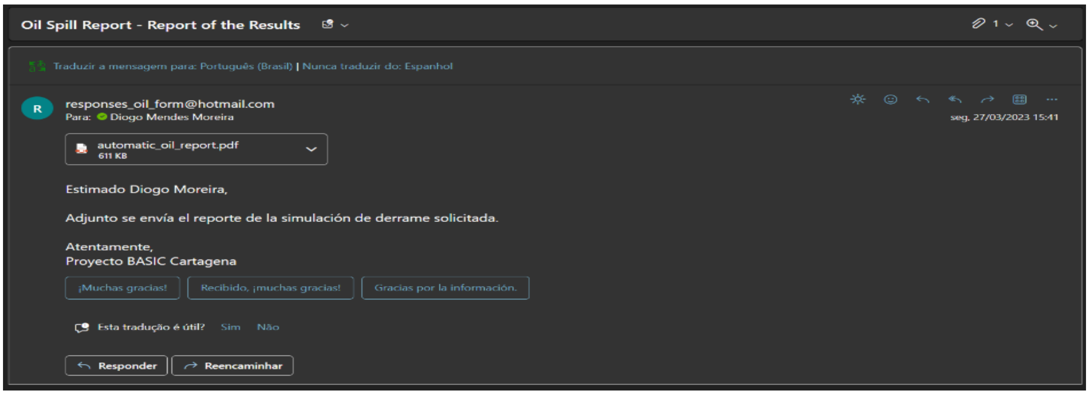


```
------------------------- MOHID -------------------------

     AUTHOR   : IST/MARETEC, Marine Modelling Group
     WWW      : http://www.mohid.com


Copyright (C) 1985, 1998, 2002, 2006.
Instituto Superior Tecnico, Technical University of Lisbon
------------------------- MOHID -------------------------

Constructing ConvertToHDF5
Please Wait...

Running ConvertToHDF5...

GLUES HDF5 FILES


Glueing HDF files...

Finished Glueing HDF files!
------------------------- MOHID -------------------------

Program ConvertToHDF5 successfully terminated


Total Elapsed Time     :         151.86   0h  2min 31s

Total CPU time         :         149.34

CPU usage (%)          :          98.34


---------------------------------------------------------
```

```
---------------------- LAGRANGIAN ----------------------

Number of Origins :            1
Number of Groups  :            1

GroupID           :            1
---Number of Orig.:            1

Origin            : spill
---Group ID       :            1
---Number of Part.:         1000
---Number of Prop.:            3

---------------- INTERFACE SEDIMENT-WATER ----------------

Num of Properties :            0


Atmosphere DT Prediction Method:  1

------------------------- MOHID -------------------------

Program Mohid Water successfully terminated


Total Elapsed Time     :         435.79   0h  7min 15s

Total CPU time         :         430.09

CPU usage (%)          :          98.69

Workcycle Elapsed Time :         423.67

Workcycle CPU time     :         418.34

Workcycle CPU usage (%):          98.74


---------------------------------------------------------
```

***Figure 7** - Merger and MOHID Log Files for Algarve Simulations*

After these processes are finished, the tool creates and sends a report to the user by email, as seen in the example in Figure 8. The report sent is similar to the one shown in Figure 9, in case one error was found during the simulation, or the one in Figure 10, if the simulation ran without errors. The average time of the whole process is about 15 min from filling the form until receiving the report in the email.



responses_oil_form@hotmail.com
Para: Diogo Mendes Moreira

seg, 27/03/2023 15:41

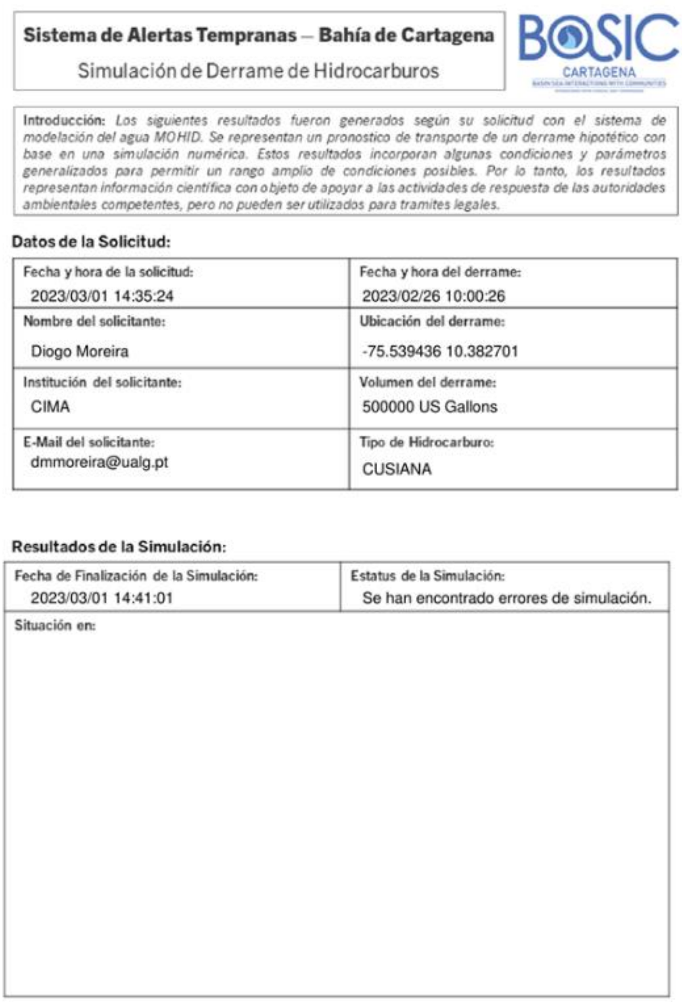
automatic_oil_report.pdf
611 KB

Estimado Diogo Moreira,

Adjunto se envía el reporte de la simulación de derrame solicitada.

Atentamente,
Proyecto BASIC Cartagena

Figure 8 - Automate Email with Report



Sistema de Alertas Tempranas – Bahía de Cartagena

Simulación de Derrame de Hidrocarburos

Introducción: *Los siguientes resultados fueron generados según su solicitud con el sistema de modelación del agua MOHID. Se representan un pronostico de transporte de un derrame hipotético con base en una simulación numérica. Estos resultados incorporan algunas condiciones y parámetros generalizados para permitir un rango amplio de condiciones posibles. Por lo tanto, los resultados representan información científica con objeto de apoyar a las actividades de respuesta de las autoridades ambientales competentes, pero no pueden ser utilizados para tramites legales.*

Datos de la Solicitud:

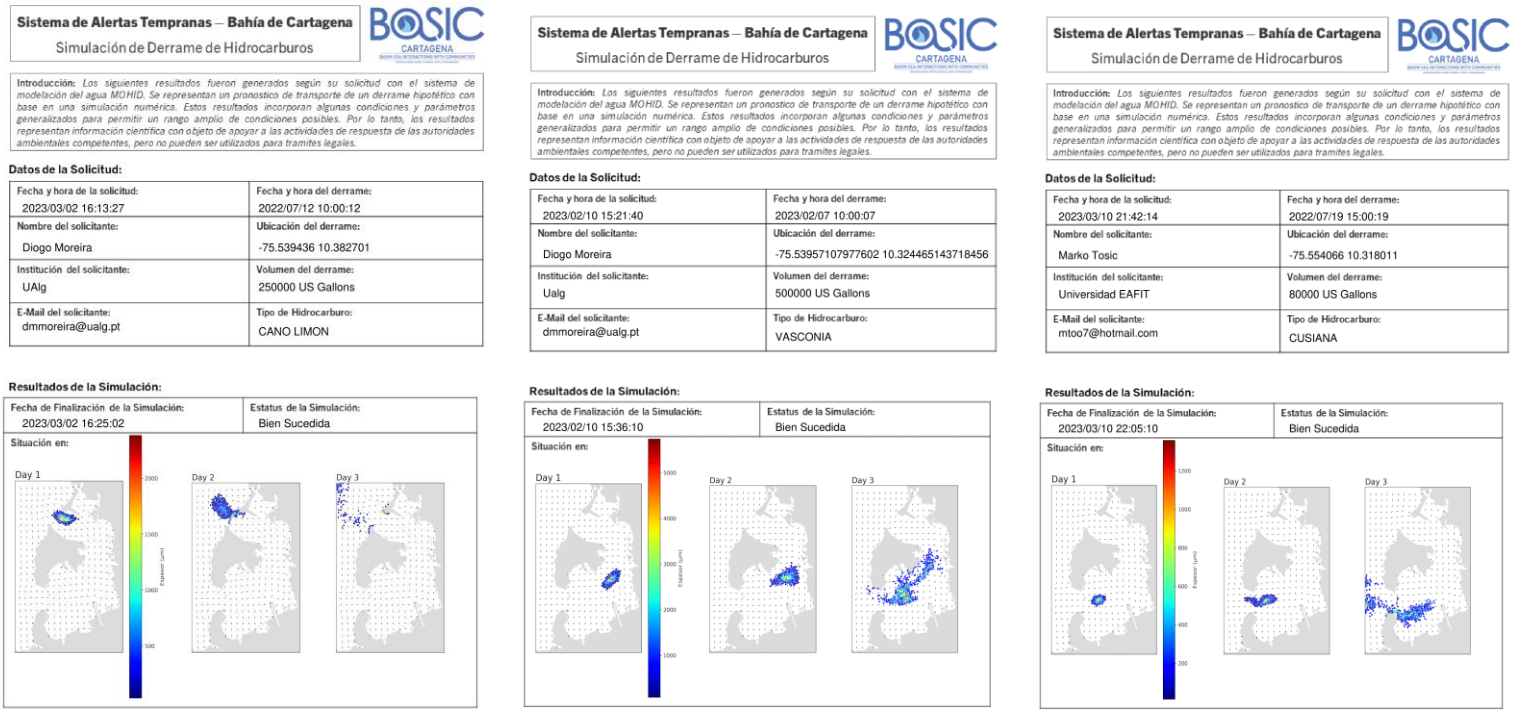
Fecha y hora de la solicitud: 2023/03/01 14:35:24	**Fecha y hora del derrame:** 2023/02/26 10:00:26
Nombre del solicitante: Diogo Moreira	**Ubicación del derrame:** -75.539436 10.382701
Institución del solicitante: CIMA	**Volumen del derrame:** 500000 US Gallons
E-Mail del solicitante: dmmoreira@ualg.pt	**Tipo de Hidrocarburo:** CUSIANA

Resultados de la Simulación:

Fecha de Finalización de la Simulación: 2023/03/01 14:41:01	**Estatus de la Simulación:** Se han encontrado errores de simulación.
Situación en:	

Figure 9 *- Cartagena Oil Simulation Error Message.*

For successful simulations, the EWS tool will create a report showing three successive states of the system. Figure 10 shows an example of reports for 3 different simulation requests, with different volumes, oil types, start days and discharge coordinates inside the bay. The reports are presented in Spanish, because they are destined for the Colombian Authorities and regional oil companies. The simulations are being performed at present in a virtual machine (VM) hosted at the IT infrastructure of University of Algarve. The VM has four Intel Xeon cores, 16GB RAM and 200GB high performance SSD disk.



Sistema de Alertas Tempranas – Bahía de Cartagena

Simulación de Derrame de Hidrocarburos

Introducción: *Los siguientes resultados fueron generados según su solicitud con el sistema de modelación del agua MOHID. Se representan un pronostico de transporte de un derrame hipotético con base en una simulación numérica. Estos resultados incorporan algunas condiciones y parámetros generalizados para permitir un rango amplio de condiciones posibles. Por lo tanto, los resultados representan información científica con objeto de apoyar a las actividades de respuesta de las autoridades ambientales competentes, pero no pueden ser utilizados para tramites legales.*

Datos de la Solicitud:

Fecha y hora de la solicitud: 2023/03/02 16:13:27	**Fecha y hora del derrame:** 2022/07/12 10:00:12
Nombre del solicitante: Diogo Moreira	**Ubicación del derrame:** -75.539436 10.382701
Institución del solicitante: UAlg	**Volumen del derrame:** 250000 US Gallons
E-Mail del solicitante: dmmoreira@ualg.pt	**Tipo de Hidrocarburo:** CANO LIMON

Resultados de la Simulación:

Fecha de Finalización de la Simulación: 2023/03/02 16:25:02	**Estatus de la Simulación:** Bien Sucedida

Situación en:

Sistema de Alertas Tempranas – Bahía de Cartagena

Simulación de Derrame de Hidrocarburos

Introducción: *Los siguientes resultados fueron generados según su solicitud con el sistema de modelación del agua MOHID. Se representan un pronostico de transporte de un derrame hipotético con base en una simulación numérica. Estos resultados incorporan algunas condiciones y parámetros generalizados para permitir un rango amplio de condiciones posibles. Por lo tanto, los resultados representan información científica con objeto de apoyar a las actividades de respuesta de las autoridades ambientales competentes, pero no pueden ser utilizados para tramites legales.*

Datos de la Solicitud:

Fecha y hora de la solicitud: 2023/02/10 15:21:40	**Fecha y hora del derrame:** 2023/02/07 10:00:07
Nombre del solicitante: Diogo Moreira	**Ubicación del derrame:** -75.53957107977602 10.324465143718456
Institución del solicitante: Ualg	**Volumen del derrame:** 500000 US Gallons
E-Mail del solicitante: dmmoreira@ualg.pt	**Tipo de Hidrocarburo:** VASCONIA

Resultados de la Simulación:

Fecha de Finalización de la Simulación: 2023/02/10 15:36:10	**Estatus de la Simulación:** Bien Sucedida

Situación en:

Sistema de Alertas Tempranas – Bahía de Cartagena

Simulación de Derrame de Hidrocarburos

Introducción: *Los siguientes resultados fueron generados según su solicitud con el sistema de modelación del agua MOHID. Se representan un pronostico de transporte de un derrame hipotético con base en una simulación numérica. Estos resultados incorporan algunas condiciones y parámetros generalizados para permitir un rango amplio de condiciones posibles. Por lo tanto, los resultados representan información científica con objeto de apoyar a las actividades de respuesta de las autoridades ambientales competentes, pero no pueden ser utilizados para tramites legales.*

Datos de la Solicitud:

Fecha y hora de la solicitud: 2023/03/10 21:42:14	**Fecha y hora del derrame:** 2022/07/19 15:00:19
Nombre del solicitante: Marko Tosic	**Ubicación del derrame:** -75.554066 10.318011
Institución del solicitante: Universidad EAFIT	**Volumen del derrame:** 80000 US Gallons
E-Mail del solicitante: mtoo7@hotmail.com	**Tipo de Hidrocarburo:** CUSIANA

Resultados de la Simulación:

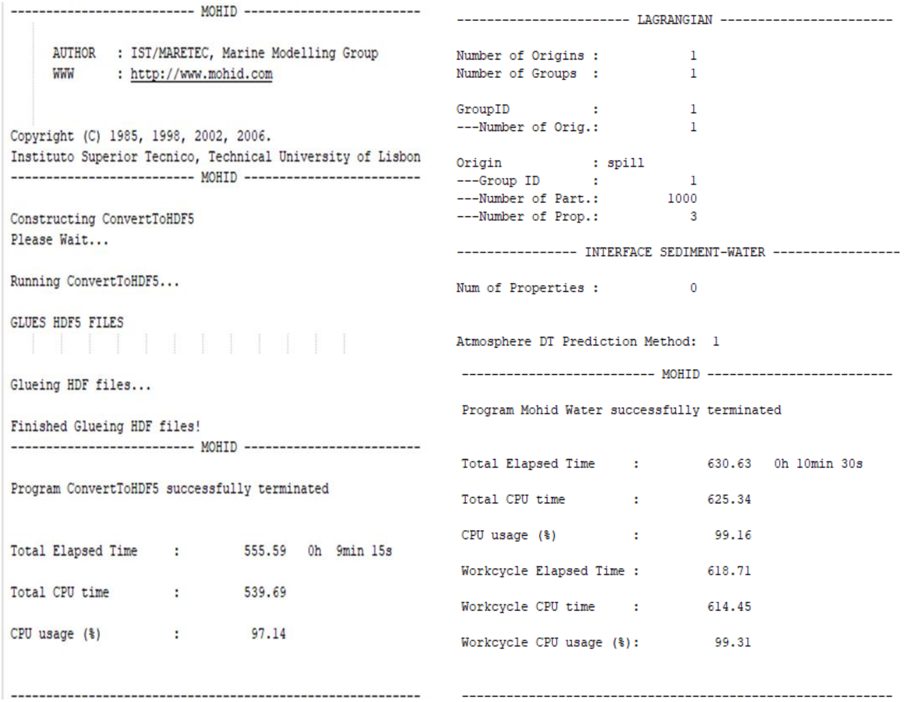
Fecha de Finalización de la Simulación: 2023/03/10 22:05:10	**Estatus de la Simulación:** Bien Sucedida

Situación en:

Figure 10 *- Reports of three different simulation requests for Cartagena Bay.*

4.2 Algarve Reporting

The tool developed in this work is generic, hence, the code can be applied to any other region of the world with minimum modifications. To further test the tool's adaptability, it was tested for the Algarve region, using the SOMA Operational System for the hydrodynamic forcing fields and the SKIRON system for the atmospheric forcing. Figure 11 shows the log files created when the Merger tool and the MOHID Lagrangian runs. These log files only differ in the process time, as will be explained in Chapter 5.

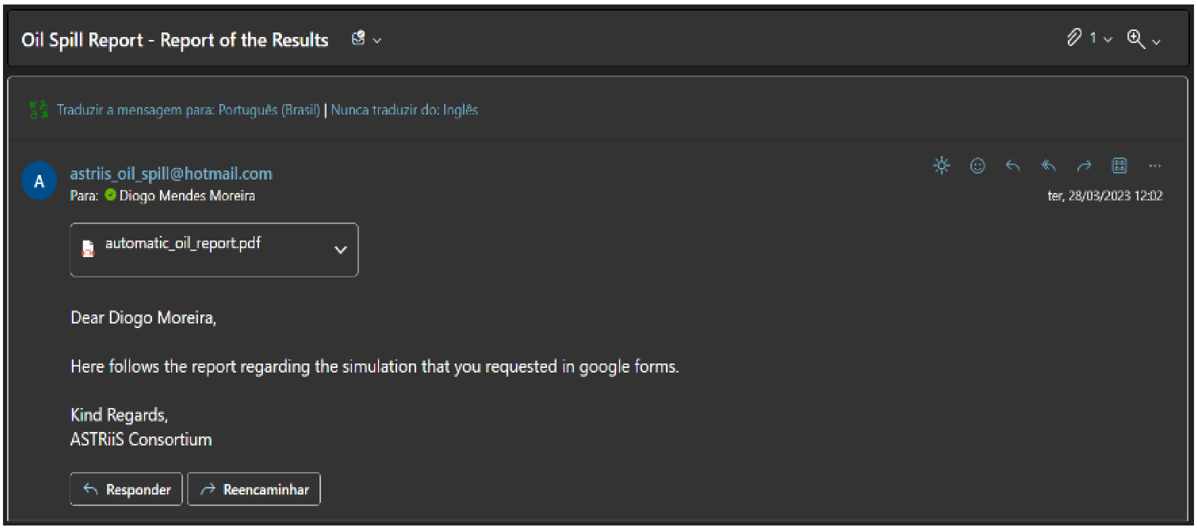


```
------------------------- MOHID ------------------------

     AUTHOR   : IST/MARETEC, Marine Modelling Group
     WWW      : http://www.mohid.com


Copyright (C) 1985, 1998, 2002, 2006.
Instituto Superior Tecnico, Technical University of Lisbon
------------------------- MOHID ------------------------

Constructing ConvertToHDF5
Please Wait...

Running ConvertToHDF5...

GLUES HDF5 FILES


Glueing HDF files...

Finished Glueing HDF files!
------------------------- MOHID ------------------------

Program ConvertToHDF5 successfully terminated


Total Elapsed Time     :         555.59   0h  9min 15s

Total CPU time         :         539.69

CPU usage (%)          :          97.14


--------------------------------------------------------
```

```
----------------------- LAGRANGIAN -----------------------

Number of Origins :            1
Number of Groups  :            1

GroupID           :            1
---Number of Orig.:            1

Origin            : spill
---Group ID       :            1
---Number of Part.:         1000
---Number of Prop.:            3

---------------- INTERFACE SEDIMENT-WATER -----------------

Num of Properties :            0


Atmosphere DT Prediction Method:  1

 ------------------------- MOHID -------------------------

 Program Mohid Water successfully terminated


 Total Elapsed Time     :         630.63   0h 10min 30s

 Total CPU time         :         625.34

 CPU usage (%)          :          99.16

 Workcycle Elapsed Time :         618.71

 Workcycle CPU time     :         614.45

 Workcycle CPU usage (%):          99.31


 ---------------------------------------------------------
```

Figure 11 *– Merger (left) and MOHID Lagrangian (right)) Log Files for Algarve Simulations*

As for the previous simulations, after these processes are finished, the tool creates and sends a report to the user by email. An example of this email can be seen in figure 12. Figure 13 shows an example of a report when errors were found during the simulation.



Oil Spill Report - Report of the Results

astriis_oil_spill@hotmail.com
Para: Diogo Mendes Moreira
ter, 28/03/2023 12:02

automatic_oil_report.pdf

Dear Diogo Moreira,

Here follows the report regarding the simulation that you requested in google forms.

Kind Regards,
ASTRiiS Consortium

Figure 12 *- Email for the Algarve Simulations.*

Early Warning System — Algarve

Oil Spill Simulation

Introduction: The following results were generated as per your request with the MOHID water modelling system. They represent a transport forecast of a hypothetical spill based on a numerical simulation. These results incorporate some generalized conditions and parameters to allow a wide range of possible conditions. Therefore, the results represent scientific information in order to support the response activities of the respective environmental authorities, but cannot be used for legal proceedings.

Request Information :

Date and time of the request: 2023/06/01 17:49	Start and End of the spill: 2020/04/21 10:00 - 2020/04/23 10:00
Name of the requester: Diogo Moreira	Spill coordinates: -8.20.56 36.9045
Institution of the requester: CIMA-UAlg	Spill Volume (cubic meters): 50000 m3
Requester's E-Mail: dmmoreira@ualg.pt	Type of oil: VASCONIA

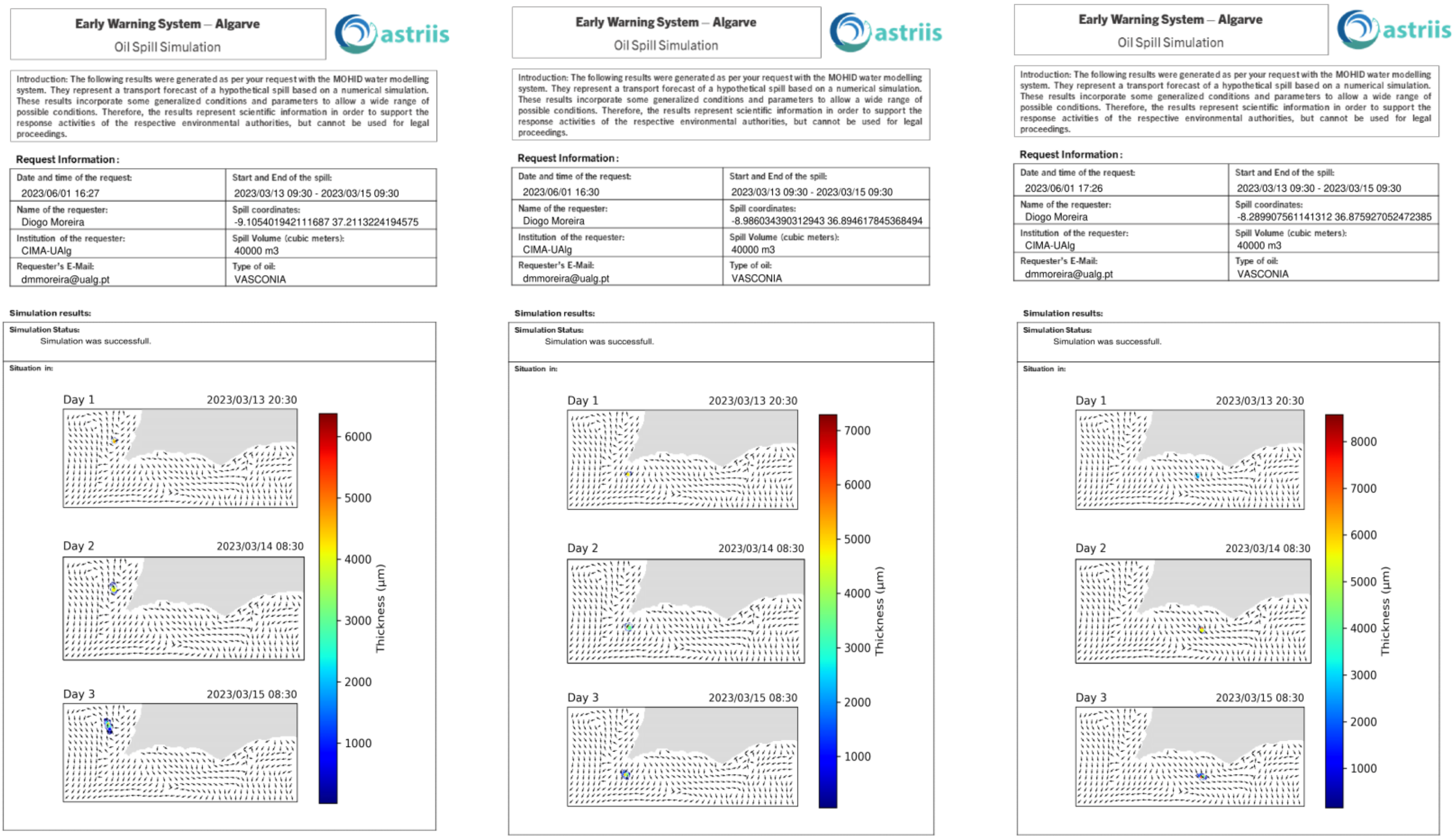
Simulation results:

Simulation Status:
Simulation Found errors

Situation in:

Figure 13 *– Algarve Oil Simulation Error Message.*

Figure 14 show the example of three reports of successful simulations, with different spill conditions. The reports in this case are presented in English, because they are developed as part of the international project ASTRiiS. Like the BASIC simulations, the process is executed in a similar VM, with the same characteristics. The average time of the whole process is about 20 minutes, which differs from the previous results. The explanation for this is related with the SOMA data files as will be further explained in Chapter 5.



Early Warning System – Algarve
Oil Spill Simulation

Introduction: The following results were generated as per your request with the MOHID water modelling system. They represent a transport forecast of a hypothetical spill based on a numerical simulation. These results incorporate some generalized conditions and parameters to allow a wide range of possible conditions. Therefore, the results represent scientific information in order to support the response activities of the respective environmental authorities, but cannot be used for legal proceedings.

Request Information:

Date and time of the request: 2023/06/01 16:27	Start and End of the spill: 2023/03/13 09:30 - 2023/03/15 09:30
Name of the requester: Diogo Moreira	Spill coordinates: -9.105401942111687 37.2113224194575
Institution of the requester: CIMA-UAlg	Spill Volume (cubic meters): 40000 m3
Requester's E-Mail: dmmoreira@ualg.pt	Type of oil: VASCONIA

Simulation results:

Simulation Status:
Simulation was successfull.

Situation in:

Early Warning System – Algarve
Oil Spill Simulation

Introduction: The following results were generated as per your request with the MOHID water modelling system. They represent a transport forecast of a hypothetical spill based on a numerical simulation. These results incorporate some generalized conditions and parameters to allow a wide range of possible conditions. Therefore, the results represent scientific information in order to support the response activities of the respective environmental authorities, but cannot be used for legal proceedings.

Request Information:

Date and time of the request: 2023/06/01 16:30	Start and End of the spill: 2023/03/13 09:30 - 2023/03/15 09:30
Name of the requester: Diogo Moreira	Spill coordinates: -8.986034390312943 36.894617845368494
Institution of the requester: CIMA-UAlg	Spill Volume (cubic meters): 40000 m3
Requester's E-Mail: dmmoreira@ualg.pt	Type of oil: VASCONIA

Simulation results:

Simulation Status:
Simulation was successfull.

Situation in:

Early Warning System – Algarve
Oil Spill Simulation

Introduction: The following results were generated as per your request with the MOHID water modelling system. They represent a transport forecast of a hypothetical spill based on a numerical simulation. These results incorporate some generalized conditions and parameters to allow a wide range of possible conditions. Therefore, the results represent scientific information in order to support the response activities of the respective environmental authorities, but cannot be used for legal proceedings.

Request Information:

Date and time of the request: 2023/06/01 17:26	Start and End of the spill: 2023/03/13 09:30 - 2023/03/15 09:30
Name of the requester: Diogo Moreira	Spill coordinates: -8.289907561141312 36.875927052472385
Institution of the requester: CIMA-UAlg	Spill Volume (cubic meters): 40000 m3
Requester's E-Mail: dmmoreira@ualg.pt	Type of oil: VASCONIA

Simulation results:

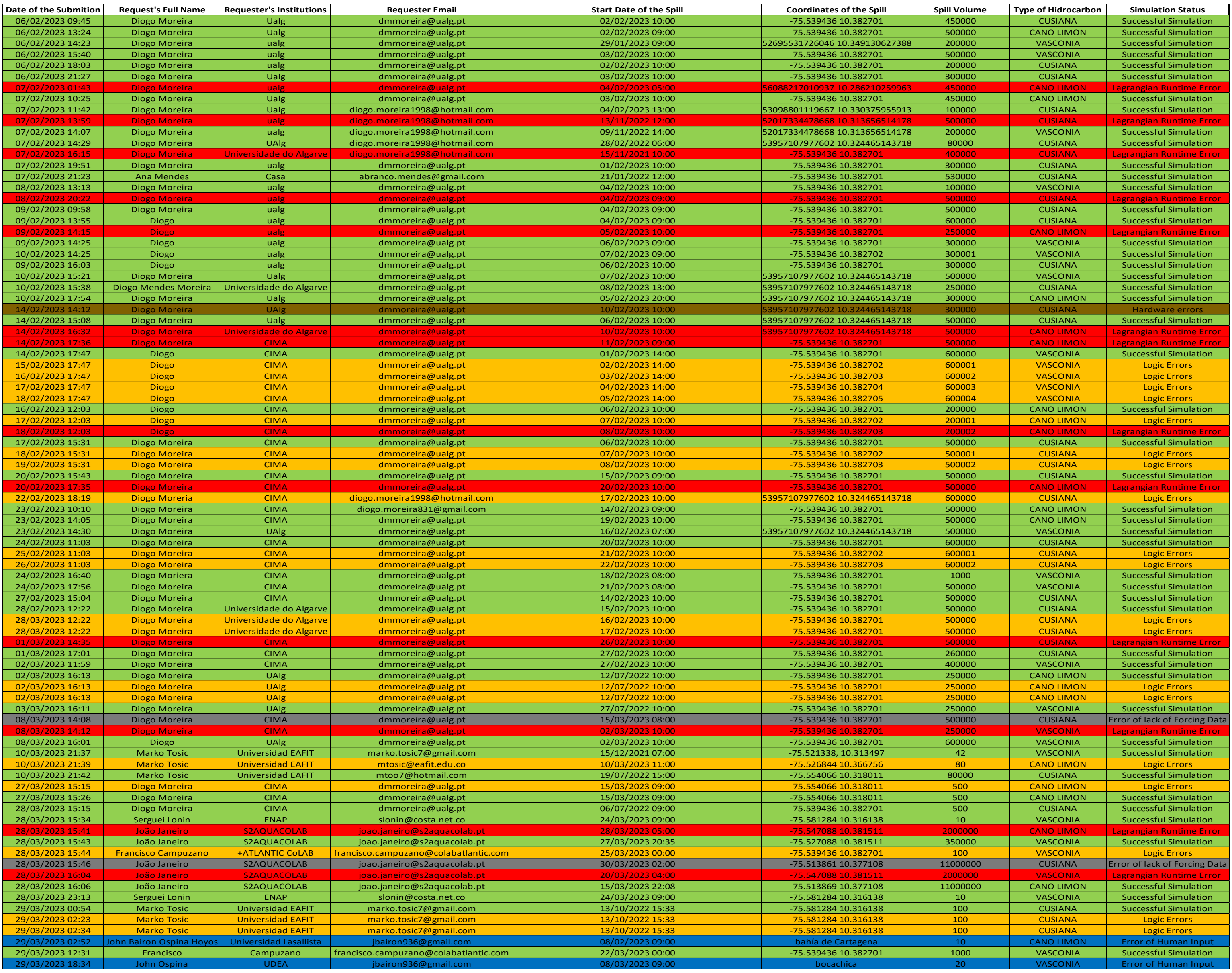
Simulation Status:
Simulation was successfull.

Situation in:

Figure 14 *- Reports of three different simulation requests for the coast of Algarve.*

4.3 Testing phase

After completion, the EWS Tool underwent a testing phase, which was subsequently followed by a period of improvements. The links containing the tool's entry form were shared with partners and final users of the projects for testing purposes. Towards the end of the testing phase, a comprehensive registry of all requests and their outcomes was compiled, specifically for the Cartagena case study, as seen in Figure 15. The encountered errors were categorized into five types: i) Error due to Human Input, ii) Logic error in the tool, iii) Error due to no forcing data, iv) Lagrangian Runtime error, and v) Hardware Error. Each error category is associated with a distinct color, as specified in Table 1. Additionally, a calculation was performed to determine the percentage of errors and successful simulations relative to the entire set of tests, as outlined in Table 1. Further elaboration on each error type will be presented in Chapter 5.



Date of the Submition	Request's Full Name	Requester's Institutions	Requester Email	Start Date of the Spill	Coordinates of the Spill	Spill Volume	Type of Hidrocarbon	Simulation Status
06/02/2023 09:45	Diogo Moreira	Ualg	dmmoreira@ualg.pt	02/02/2023 10:00	-75.539436 10.382701	450000	CUSIANA	Successful Simulation
06/02/2023 13:24	Diogo Moreira	Ualg	dmmoreira@ualg.pt	02/02/2023 09:00	-75.539436 10.382701	500000	CANO LIMON	Successful Simulation
06/02/2023 14:23	Diogo Moreira	ualg	dmmoreira@ualg.pt	29/01/2023 09:00	52695531726046 10.349130627388	200000	VASCONIA	Successful Simulation
06/02/2023 15:40	Diogo Moreira	ualg	dmmoreira@ualg.pt	03/02/2023 10:00	-75.539436 10.382701	500000	VASCONIA	Successful Simulation
06/02/2023 18:03	Diogo Moreira	ualg	dmmoreira@ualg.pt	02/02/2023 10:00	-75.539436 10.382701	200000	CUSIANA	Successful Simulation
06/02/2023 21:27	Diogo Moreira	Ualg	dmmoreira@ualg.pt	03/02/2023 10:00	-75.539436 10.382701	300000	CUSIANA	Successful Simulation
07/02/2023 01:43	Diogo Moreira	ualg	dmmoreira@ualg.pt	04/02/2023 05:00	56088217010937 10.286210259963	450000	CANO LIMON	Lagrangian Runtime Error
07/02/2023 10:25	Diogo Moreira	Ualg	dmmoreira@ualg.pt	03/02/2023 10:00	-75.539436 10.382701	450000	CANO LIMON	Successful Simulation
07/02/2023 11:42	Diogo Moreira	Ualg	diogo.moreira1998@hotmail.com	04/02/2023 13:00	53098801119667 10.330375955913	100000	CUSIANA	Successful Simulation
07/02/2023 13:59	Diogo Moreira	ualg	diogo.moreira1998@hotmail.com	13/11/2022 12:00	52017334478668 10.313656514178	500000	CUSIANA	Lagrangian Runtime Error
07/02/2023 14:07	Diogo Moreira	ualg	diogo.moreira1998@hotmail.com	09/11/2022 14:00	52017334478668 10.313656514178	200000	VASCONIA	Successful Simulation
07/02/2023 14:29	Diogo Moreira	UAlg	diogo.moreira1998@hotmail.com	28/02/2022 06:00	53957107977602 10.324465143718	80000	CUSIANA	Successful Simulation
07/02/2023 16:15	Diogo Moreira	Universidade do Algarve	diogo.moreira1998@hotmail.com	15/11/2021 10:00	-75.539436 10.382701	400000	CUSIANA	Lagrangian Runtime Error
07/02/2023 19:51	Diogo Moreira	ualg	dmmoreira@ualg.pt	01/02/2023 10:00	-75.539436 10.382701	300000	CUSIANA	Successful Simulation
07/02/2023 21:23	Ana Mendes	Casa	abranco.mendes@gmail.com	21/01/2022 12:00	-75.539436 10.382701	530000	CUSIANA	Successful Simulation
08/02/2023 13:13	Diogo Moreira	ualg	dmmoreira@ualg.pt	04/02/2023 10:00	-75.539436 10.382701	100000	VASCONIA	Successful Simulation
08/02/2023 20:22	Diogo Moreira	ualg	dmmoreira@ualg.pt	04/02/2023 09:00	-75.539436 10.382701	500000	CUSIANA	Lagrangian Runtime Error
09/02/2023 09:58	Diogo Moreira	ualg	dmmoreira@ualg.pt	04/02/2023 09:00	-75.539436 10.382701	500000	CUSIANA	Successful Simulation
09/02/2023 13:55	Diogo	ualg	dmmoreira@ualg.pt	04/02/2023 09:00	-75.539436 10.382701	600000	CUSIANA	Successful Simulation
09/02/2023 14:15	Diogo	ualg	dmmoreira@ualg.pt	05/02/2023 10:00	-75.539436 10.382701	250000	CANO LIMON	Lagrangian Runtime Error
09/02/2023 14:25	Diogo	ualg	dmmoreira@ualg.pt	06/02/2023 09:00	-75.539436 10.382701	300000	VASCONIA	Successful Simulation
10/02/2023 14:25	Diogo	ualg	dmmoreira@ualg.pt	07/02/2023 09:00	-75.539436 10.382702	300001	VASCONIA	Successful Simulation
09/02/2023 16:03	Diogo	ualg	dmmoreira@ualg.pt	06/02/2023 10:00	-75.539436 10.382701	300000	CUSIANA	Successful Simulation
10/02/2023 15:21	Diogo Moreira	Ualg	dmmoreira@ualg.pt	07/02/2023 10:00	53957107977602 10.324465143718	500000	VASCONIA	Successful Simulation
10/02/2023 15:38	Diogo Mendes Moreira	Universidade do Algarve	dmmoreira@ualg.pt	08/02/2023 13:00	53957107977602 10.324465143718	250000	CUSIANA	Successful Simulation
10/02/2023 17:54	Diogo Moreira	Ualg	dmmoreira@ualg.pt	05/02/2023 20:00	53957107977602 10.324465143718	300000	CANO LIMON	Successful Simulation
14/02/2023 14:12	Diogo Moreira	UAlg	dmmoreira@ualg.pt	10/02/2023 10:00	53957107977602 10.324465143718	300000	CUSIANA	Hardware errors
14/02/2023 15:08	Diogo Moreira	Ualg	dmmoreira@ualg.pt	06/02/2023 10:00	53957107977602 10.324465143718	500000	CUSIANA	Successful Simulation
14/02/2023 16:32	Diogo Moreira	Universidade do Algarve	dmmoreira@ualg.pt	10/02/2023 10:00	53957107977602 10.324465143718	500000	CANO LIMON	Lagrangian Runtime Error
14/02/2023 17:36	Diogo Moreira	CIMA	dmmoreira@ualg.pt	11/02/2023 09:00	-75.539436 10.382701	500000	CANO LIMON	Lagrangian Runtime Error
14/02/2023 17:47	Diogo	CIMA	dmmoreira@ualg.pt	01/02/2023 14:00	-75.539436 10.382701	600000	VASCONIA	Successful Simulation
15/02/2023 17:47	Diogo	CIMA	dmmoreira@ualg.pt	02/02/2023 14:00	-75.539436 10.382702	600001	VASCONIA	Logic Errors
16/02/2023 17:47	Diogo	CIMA	dmmoreira@ualg.pt	03/02/2023 14:00	-75.539436 10.382703	600002	VASCONIA	Logic Errors
17/02/2023 17:47	Diogo	CIMA	dmmoreira@ualg.pt	04/02/2023 14:00	-75.539436 10.382704	600003	VASCONIA	Logic Errors
18/02/2023 17:47	Diogo	CIMA	dmmoreira@ualg.pt	05/02/2023 14:00	-75.539436 10.382705	600004	VASCONIA	Logic Errors
16/02/2023 12:03	Diogo	CIMA	dmmoreira@ualg.pt	06/02/2023 10:00	-75.539436 10.382701	200000	CANO LIMON	Successful Simulation
17/02/2023 12:03	Diogo	CIMA	dmmoreira@ualg.pt	07/02/2023 10:00	-75.539436 10.382702	200001	CANO LIMON	Logic Errors
18/02/2023 12:03	Diogo	CIMA	dmmoreira@ualg.pt	08/02/2023 10:00	-75.539436 10.382703	200002	CANO LIMON	Lagrangian Runtime Error
17/02/2023 15:31	Diogo Moreira	CIMA	dmmoreira@ualg.pt	06/02/2023 10:00	-75.539436 10.382701	500000	CUSIANA	Successful Simulation
18/02/2023 15:31	Diogo Moreira	CIMA	dmmoreira@ualg.pt	07/02/2023 10:00	-75.539436 10.382702	500001	CUSIANA	Logic Errors
19/02/2023 15:31	Diogo Moreira	CIMA	dmmoreira@ualg.pt	08/02/2023 10:00	-75.539436 10.382703	500002	CUSIANA	Logic Errors
20/02/2023 15:43	Diogo Moreira	CIMA	dmmoreira@ualg.pt	15/02/2023 09:00	-75.539436 10.382701	500000	CUSIANA	Successful Simulation
20/02/2023 17:35	Diogo Moreira	CIMA	dmmoreira@ualg.pt	20/02/2023 10:00	-75.539436 10.382701	500000	CANO LIMON	Lagrangian Runtime Error
22/02/2023 18:19	Diogo Moreira	CIMA	diogo.moreira1998@hotmail.com	17/02/2023 10:00	53957107977602 10.324465143718	600000	CUSIANA	Logic Errors
23/02/2023 10:10	Diogo Moreira	CIMA	diogo.moreira831@gmail.com	14/02/2023 09:00	-75.539436 10.382701	500000	CANO LIMON	Successful Simulation
23/02/2023 14:05	Diogo Moreira	CIMA	dmmoreira@ualg.pt	19/02/2023 10:00	-75.539436 10.382701	500000	CANO LIMON	Successful Simulation
23/02/2023 14:30	Diogo Moreira	UAlg	dmmoreira@ualg.pt	16/02/2023 07:00	53957107977602 10.324465143718	500000	VASCONIA	Successful Simulation
24/02/2023 11:03	Diogo Moreira	CIMA	dmmoreira@ualg.pt	20/02/2023 10:00	-75.539436 10.382701	600000	CUSIANA	Successful Simulation
25/02/2023 11:03	Diogo Moreira	CIMA	dmmoreira@ualg.pt	21/02/2023 10:00	-75.539436 10.382702	600001	CUSIANA	Logic Errors
26/02/2023 11:03	Diogo Moreira	CIMA	dmmoreira@ualg.pt	22/02/2023 10:00	-75.539436 10.382703	600002	CUSIANA	Logic Errors
24/02/2023 16:40	Diogo Moriera	CIMA	dmmoreira@ualg.pt	18/02/2023 08:00	-75.539436 10.382701	1000	VASCONIA	Successful Simulation
24/02/2023 17:56	Diogo Moreira	CIMA	dmmoreira@ualg.pt	21/02/2023 08:00	-75.539436 10.382701	500000	VASCONIA	Successful Simulation
27/02/2023 15:04	Diogo Moreira	CIMA	dmmoreira@ualg.pt	14/02/2023 10:00	-75.539436 10.382701	500000	CUSIANA	Successful Simulation
28/02/2023 12:22	Diogo Moreira	Universidade do Algarve	dmmoreira@ualg.pt	15/02/2023 10:00	-75.539436 10.382701	500000	CUSIANA	Successful Simulation
28/03/2023 12:22	Diogo Moreira	Universidade do Algarve	dmmoreira@ualg.pt	16/02/2023 10:00	-75.539436 10.382701	500000	CUSIANA	Logic Errors
28/03/2023 12:22	Diogo Moreira	Universidade do Algarve	dmmoreira@ualg.pt	17/02/2023 10:00	-75.539436 10.382701	500000	CUSIANA	Logic Errors
01/03/2023 14:35	Diogo Moreira	CIMA	dmmoreira@ualg.pt	26/02/2023 10:00	-75.539436 10.382701	500000	CUSIANA	Lagrangian Runtime Error
01/03/2023 17:01	Diogo Moreira	CIMA	dmmoreira@ualg.pt	27/02/2023 10:00	-75.539436 10.382701	260000	CUSIANA	Successful Simulation
02/03/2023 11:59	Diogo Moreira	CIMA	dmmoreira@ualg.pt	27/02/2023 10:00	-75.539436 10.382701	400000	VASCONIA	Successful Simulation
02/03/2023 16:13	Diogo Moreira	UAlg	dmmoreira@ualg.pt	12/07/2022 10:00	-75.539436 10.382701	250000	CANO LIMON	Successful Simulation
02/03/2023 16:13	Diogo Moreira	UAlg	dmmoreira@ualg.pt	12/07/2022 10:00	-75.539436 10.382701	250000	CANO LIMON	Logic Errors
02/03/2023 16:13	Diogo Moreira	UAlg	dmmoreira@ualg.pt	12/07/2022 10:00	-75.539436 10.382701	250000	CANO LIMON	Logic Errors
03/03/2023 16:11	Diogo Moreira	UAlg	dmmoreira@ualg.pt	27/07/2022 10:00	-75.539436 10.382701	250000	VASCONIA	Successful Simulation
08/03/2023 14:08	Diogo Moreira	CIMA	dmmoreira@ualg.pt	15/03/2023 08:00	-75.539436 10.382701	500000	CUSIANA	Error of lack of Forcing Data
08/03/2023 14:12	Diogo Moreira	CIMA	dmmoreira@ualg.pt	02/03/2023 10:00	-75.539436 10.382701	250000	VASCONIA	Lagrangian Runtime Error
08/03/2023 16:01	Diogo	UAlg	dmmoreira@ualg.pt	02/03/2023 10:00	-75.539436 10.382701	600000	VASCONIA	Successful Simulation
10/03/2023 21:37	Marko Tosic	Universidad EAFIT	marko.tosic7@gmail.com	15/12/2021 07:00	-75.521338, 10.313497	42	VASCONIA	Successful Simulation
10/03/2023 21:39	Marko Tosic	Universidad EAFIT	mtosic@eafit.edu.co	10/03/2023 11:00	-75.526844 10.366756	80	CANO LIMON	Logic Errors
10/03/2023 21:42	Marko Tosic	Universidad EAFIT	mtoo7@hotmail.com	19/07/2022 15:00	-75.554066 10.318011	80000	CUSIANA	Successful Simulation
27/03/2023 15:15	Diogo Moreira	CIMA	dmmoreira@ualg.pt	15/03/2023 09:00	-75.554066 10.318011	500	CANO LIMON	Logic Errors
27/03/2023 15:26	Diogo Moreira	CIMA	dmmoreira@ualg.pt	15/03/2023 09:00	-75.554066 10.318011	500	CANO LIMON	Successful Simulation
28/03/2023 15:15	Diogo Moreira	CIMA	dmmoreira@ualg.pt	06/07/2022 09:00	-75.539436 10.382701	500	CUSIANA	Successful Simulation
28/03/2023 15:34	Serguei Lonin	ENAP	slonin@costa.net.co	24/03/2023 09:00	-75.581284 10.316138	10	VASCONIA	Successful Simulation
28/03/2023 15:41	João Janeiro	S2AQUACOLAB	joao.janeiro@s2aquacolab.pt	28/03/2023 05:00	-75.547088 10.381511	2000000	CANO LIMON	Lagrangian Runtime Error
28/03/2023 15:43	João Janeiro	S2AQUACOLAB	joao.janeiro@s2aquacolab.pt	27/03/2023 20:35	-75.527088 10.381511	350000	VASCONIA	Successful Simulation
28/03/2023 15:44	Francisco Campuzano	+ATLANTIC CoLAB	francisco.campuzano@colabatlantic.com	25/03/2023 00:00	-75.539436 10.382701	100	VASCONIA	Logic Errors
28/03/2023 15:46	João Janeiro	S2AQUACOLAB	joao.janeiro@s2aquacolab.pt	30/03/2023 02:00	-75.513861 10.377108	11000000	CUSIANA	Error of lack of Forcing Data
28/03/2023 16:04	João Janeiro	S2AQUACOLAB	joao.janeiro@s2aquacolab.pt	20/03/2023 04:00	-75.547088 10.381511	2000000	VASCONIA	Lagrangian Runtime Error
28/03/2023 16:06	João Janeiro	S2AQUACOLAB	joao.janeiro@s2aquacolab.pt	15/03/2023 22:08	-75.513869 10.377108	11000000	CANO LIMON	Successful Simulation
28/03/2023 23:13	Serguei Lonin	ENAP	slonin@costa.net.co	24/03/2023 09:00	-75.581284 10.316138	10	VASCONIA	Successful Simulation
29/03/2023 00:54	Marko Tosic	Universidad EAFIT	marko.tosic7@gmail.com	13/10/2022 15:33	-75.581284 10.316138	100	CUSIANA	Successful Simulation
29/03/2023 02:23	Marko Tosic	Universidad EAFIT	marko.tosic7@gmail.com	13/10/2022 15:33	-75.581284 10.316138	100	CUSIANA	Logic Errors
29/03/2023 02:34	Marko Tosic	Universidad EAFIT	marko.tosic7@gmail.com	13/10/2022 15:33	-75.581284 10.316138	100	CUSIANA	Logic Errors
29/03/2023 02:52	John Bairon Ospina Hoyos	Universidad Lasallista	jbairon936@gmail.com	08/02/2023 09:00	bahía de Cartagena	10	CANO LIMON	Error of Human Input
29/03/2023 12:31	Francisco	Campuzano	francisco.campuzano@colabatlantic.com	22/03/2023 00:00	-75.539436 10.382701	1000	VASCONIA	Successful Simulation
29/03/2023 18:34	John Ospina	UDEA	jbairon936@gmail.com	08/03/2023 09:00	bocachica	20	VASCONIA	Error of Human Input

Figure 15 *- Registry of the Simulations during the testing phase.*

Table 1 - Statistics of the events encountered during the test phase

Type of event	Number of occurrences	% of total simulation
Successful Simulation (green)	50	43%
Error due to human input (blue)	2	2%
Logic error in the tool (orange)	19	16%
Error due to no forcing data (grey)	1	1%
Lagrangian runtime error (red)	13	11%
Hardware error (brown)	1	1%
Total	**86**	**100%**

In the next chapter the results shown in this chapter will be thoroughly analyzed and explained.

5 DISCUSSION

5.1 Oil Spill Simulations

As seen in Chapter 4, the EWS Tool acting for Cartagena Bay generates a number of results, such as the log files shown in Figure 7. These files are not important from the standpoint of the user, but they are very useful for the programmer to check if the program is running in accordance with the request. The logs shown in Figure 7 are called Run Logs, and they show the display text of the Merger and MOHID runs. Two additional log files called, Log Error, will only be created if errors are detected during the process. When the program detects an error during any of these processes, it immediately jumps to the creation of the report shown in Figure 10, displaying an error message with no maps. The error report is generated only if an error occurs during the Merger or the MOHID Lagrangian processes. The errors that can occur with the Merger Tool are related to the BASIC or SOMA forcing data. One possible reason for an error to occur is to request a simulation prior to the start of operation of the operational model. BASIC data starts at 20th of October 2021, and SOMA data starts at 21st of April 2020. Since there is no forcing data prior to those dates, if the user selects any date before that, the simulation cannot be performed. Another possible source of errors is due to storing access. The data is stored in a NAS units, so any issues with this equipment (such as power failure or internet failure) will generate an error. The storage is in the process of being transferred to the IT infrastructure of the University. This will be a more controlled environment, reducing the possibility of errors. The MOHID Lagrangian errors are highly dependent on the user inputs, particularly the coordinates and the user email. If the coordinates are outside the domain, the MOHID cannot compute the simulation. A similar situation happens if the user chooses an origin in land. Furthermore, the user is asked to write an email address to receive the report; if this address is misspelled, the program will not send the report to the user and may break the entire program. The text in the email the user receives is always the same, as seen in Figure 8, even in case of an error, the only thing that changes is the report content. For the case study of the Coast of Algarve, the time it takes to complete the Merger Tool and the MOHID simulation, increases to 10 minutes for each, as seen in the logs of Figure 11. This increase is due to the extraction of the forcing data, which is now provided by SOMA, and, as stated in previous chapters, the number of files is doubled due to the half-hourly files. As a result, compiling and extracting these files extends the overall process time. Aside from that, the log files work exactly as for the Cartagena Bay simulation, with no changes to the EWS Tool original code.

If the simulation runs without errors, the report shown in Figure 10 will be created. The examples shown were performed in various locations throughout the bay to provide a better understanding of the oil behavior within Cartagena Bay. The first is in the northern region of the Bay, which is also home to Puerto de Cartagena, one of the Caribbean's most important ports. Despite the relatively high volume of oil spilled, minor concentrations of oil enter the port, with the majority circulating outside the bay. The second map was in the Bay's middle region, with a very high volume of oil spilled of 500000 US Gallons, approximately 670 tons. Since a high volume of oil still remains inside the bay after three days, it is possible to say that the impact on the environment is more severe in this scenario due to the oil's presence in the bay for more than three days. The third and last report, displays a scenario in the Bay's southernmost region, with approximately 110 tons of oil spilled. This scenario is very similar to the first one in that the majority of the oil spilled leaves the Bay by the third day. The oil flushing although is done by the south bar (Boca Chica).

The reports in Figure 14 differ from those in Cartagena Bay in their structure. The first point to mention is how the maps are organized, which was done in by stacking the images on top of each other to have a better visualization of the simulation. The simulations in the reports followed a similar methodology to the Cartagena Bay simulations, with three different simulation requests in different locations of the model domain, for the same day and with the same volume of oil spilled to better understand the behaviour of the oil slick. The Algarve region is heavily influenced by the Mediterranean water, with a dominant current flowing from East to West and some vortices formation, and strong upwelling currents, which are quite demanding for the model. The first discharge is located on the west coast of Algarve, where there is a strong northward current, preventing the oil slick from reaching the coast. The oil slick's origin point was near the coast, but by the third day, it was visibly moving north away from the coast. The second discharge was requested offshore of Sagres. The volume spilled was very high (40 000 m3) and some of the oil reaches the coast by the second day, even if the concentration is very low. The third day of the simulation shows the oil slick approaching the coast of Sagres, with the thickness of the oil increasing, which can cause severe problems for marine and human life. The third simulation is located in front of Portimão, where the oil slick is heavily influenced the upwelling currents. In the maps is seen the oil slick being transported away from the coast and towards the east, which can be an indicator of an upwelling event, which pushes the oil at the surface away from the coast. The interaction of the currents with the oil greatly diffuses it, causing the oil concentration to decrease over time.

5.2 Testing Phase

The testing phase lasted approximately 2 months, following the development of the EWS Tool, with a total of 86 tests. During this phase the link to the simulation's input form was shared with partners of the BASIC Project, namely Marko Tosic from Universidad Escuela de Administración, Finanzas e Instituto Tecnológico (EAFIT), João Janeiro from S2AQUAcoLAB, Francisco Campuzano from +ATLANTIC CoLAB, Sergei Lonin from Escola Nacional de Administración Pública (ENAP) and John Ospina from Universidad Lasallista. This demanded several types of tests in order to completely analyse the tool and pinpoint the improvements that need be made. Figure 15 depicts the registry of tests performed for the Cartagena Bay Simulations, where all of the inputs chosen by the user and the corresponding simulation status are shown using color coding, for each type of error and a correspondent percentage of error and successful simulations, indicated in Table 1, where the biggest percentage going to the successful simulations with 43%. The following section explain in detail each type of error encountered.

5.2.1 Human Input Errors

Human input errors can occur as a result of incorrect inputs provided by the user. These errors are typically attributed to lack of familiarity with the tool, which originates inputs in the wrong format or out of the bounds of the model. Typical errors of this category encountered during the test phase were:

a) Wrong format of the spill coordinates, where users may have provided coordinates using the wrong coordinate system or inputting latitude and longitude values in the wrong order;
b) Spill coordinates outside the simulation area, where users have inputted spill coordinates that fall outside the designated simulation area, leading to errors in the lagrangian model;

c) Simulation dates outside the range of available forcing data, where users may have selected simulation dates where there is no available data, within the range of available forcing data, as previously explained, preventing the lagrangian simulation from running;
d) Incorrect spelling of the email, where users may have made spelling mistakes or typos when providing their email address, which results in not receiving the email with the simulation results.

These errors, identified to have a weight of 2% during the testing phase, indicate that the majority of users were already familiar with the oil spill tool. This is a positive aspect, considering that a higher percentage of errors can be expected once the tool is distributed to the general public. To mitigate these errors and improve user understanding, it is recommended to enhance the clarity and conciseness of the explanations provided for each question. By simplifying the language used in the form's instructions and effectively communicating the purpose of each question, users can better comprehend the required inputs and reduce the likelihood of errors. This can be achieved, by transitioning to a more elaborate web form that will greatly decrease the occurrence of such errors, as it will allow for better explanations to guide users on what information needs to be inputted and how.

5.2.2 Logic Errors in the tool

The errors in this category are caused by logical flaws within the EWS Tool itself, and represent the highest percentage of error, with 16%. These errors are not influenced by user input but rather arise from errors in the underlying algorithms, calculations, or programming code. Logic errors can lead to incorrect results or unexpected behavior of the tool. Typical errors of this category encountered during the test phase were:

a) Discarding simulation requests when more than one new request is entered while the simulation is being performed;
b) Program redo the simulation without any request being submitted;
c) Breaking of the program due to the too many attempts at logging in and out of the email.

All the errors have been resolved through modifications made to the tool's code. The first error (a) was addressed by changing the method of detecting new requests. Initially, the tool inspected the mail inbox, considering only the last received email as a new request. In the new version, the tool directly checks the .CSV file generated by Google Forms to detect new lines. It then loops over the file to determine if the submission date is higher or lower than the previous one, running the corresponding simulation. Once the simulation is complete, the tool moves on to the next one, ensuring no simulations are ignored. This modification also resolves the second error (b), which occurred when SPAM emails triggered the EWS Tool without any simulation request, leading to the repetition of the last simulation in the file. With the improvement, SPAM emails do not create entries in the .CSV file, preventing the tool from triggering repeated simulations. Lastly, the errors of type (c) were easily avoided by adding a "time.sleep" of 30 seconds after each simulation and during the tool's waiting period for new simulations. This function allows the tool to wait for 30 seconds before checking the .CSV file again.

These modifications have significantly reduced the risk of such errors, although it is still possible to encounter new situations related with logic misfits of the tool in the future.

5.2.3 Errors due to lack of forcing data

These errors arise when one of the operational models supplying data to the Lagrangian model fails. At the moment, the Lagrangian model utilizes hydrodynamic forcing from the BASIC for Cartagena and SOMA for the coast of Algarve operational systems, as well as SKIRON and AMSEAS for meteorologic forcing. The tool extracts the necessary data from the storage location, including the local storage location. These errors are considered external to the tool, and no remediation action was taken during the test phase. However, one modification that can be considered in the future is the implementation of redundancy. This involves systematically extracting alternative forcing fields and utilizing them in case of failure of the primary data providers.

5.2.4 Lagrangian model errors during runtime

The Lagrangian model occasionally encountered a runtime error, the exact cause of which remained undetermined due to its intermittent nature. Even when utilizing the same initial conditions, it didn’t always reproduce the error. It should be noted that the random component in the velocity of Lagrangian particles yields different results for each run, even with identical initial conditions. In an effort to address this issue, several potential error sources were examined and modified. Firstly, the land definition was adjusted from a polygon to the bathymetry to prevent any potential errors related to the land polygon. Secondly, the beaching distance was increased to avoid any potential misallocation of particles onto land during beaching. Lastly, a loop was implemented in the tool to detect runtime errors and rerun the simulation if such an error occurred. While this solution proved effective, it is considered temporary until a thorough understanding of the root cause behind the exception can be achieved.

5.2.5 Hardware Errors

This category of errors is related to physical issues occurring in the IT infrastructure. Typical errors of this category can be:

a) Power failure;
b) Internet Failure;
c) Internet Attack;
d) Issues with the NAS storage units.

The Lagrangian model is running in a dedicated server located in the UAlg’s IT infrastructure. This infrastructure is (in principle) resilient to most of the aforementioned events: The power is protected by UPS systems and possess an emergency electric generator. It is enclosed in a fireproof, positive pressure room to prevent impact from external fires. An active cybersecurity policy is in place to prevent cyberattacks. The same infrastructure is used to operate the BASIC and SOMA systems, which also gives confidence in the hydrodynamic forcing used by the tool. The only section of the system that is less protected is the storage units used to extract the forcing. At the moment they are based in NAS units located outside the infrastructure. There are plans however, to include the storage also inside the perimeter of the IT infrastructure. The forms and the E-Mail account used are Google native, which also give good guarantees of stability.

During the entire test phase, only one failure of this type has occurred, related with type (d). Credentials are needed to have access to the NAS storage. When the units are restarted, it is necessary to input the credentials again. If the program tries to access it without the credentials, it breaks. To avoid this the type of error credentials are now memorized inside the virtual machine.

5.2.5 Report improvements

Following the testing phase, a few improvements were suggested by different users, regarding the reports. The suggestions were centred around the maps of the oil spill simulation. Users recommended modifications such as adjusting the position and size of the maps to enhance visibility and usability. Additionally, they suggested refining the colorbar units to provide clearer representation of the data. Furthermore, adding dates to the maps would help users identify which day each image represents, providing a time reference for the simulation results. Other suggestions for enhancements focused on the report's aesthetics and the hour being changed to Colombia time zone. All these modifications were implemented.

The testing phase, as well as the useful feedback provided by users, resulted in significant improvements to the program. As a result, all errors were successfully fixed resulting in a series of successful simulations. Nonetheless, continual monitoring of the tool is required to quickly correct any unforeseen problems that may occur.

6 CONCLUSION

The main objective of the study was successfully accomplished by developing a versatile tool using the Python programming language. This tool can be adapted to conduct Lagrangian simulations with any Lagrangian model for hydrocarbons or other pollutants in any region of the world. The tool provides automation for the entire cycle of an oil spill simulation request. It starts by reading the simulation and oil characteristics specified by the user. It then extracts the necessary hydrodynamic and atmospheric forcing data from the operational model specific to the study area. The tool creates the required files to run the Lagrangian model simulation and generates images representing the simulation for inclusion in the results report. The report itself is also generated by the tool, incorporating the simulation images and other relevant information. Finally, the tool sends the report to the requester's email address, which is collected through an entry form. With further improvements, this tool could serve as an early warning system to help reduce the impact of other pollutants and Hazard Noxious Substances (HNS) in the environment or support Search and Rescue Operations at sea. The tool has practical applications in supporting local authorities' response to oil spill incidents, allowing for rapid response and better decision-making, as well as helping oil spill companies assess the impact of accidents and implement mitigation measures. Its adaptability was demonstrated through simulations in different regions, showing its potential for global use with appropriate data.

The EWS Tool can be improved in several ways based on user feedback and system analysis. One potential improvement is to add additional types of hydrocarbons or hazardous substances to the system, which would require knowledge of their physical properties. The ADIOS database can be a useful resource for this, as it contains information on many commercially used hydrocarbons. However, it is important to ensure that the system's entry form is not overly complex. Another possible improvement is related to the execution time. If the number of simulation requests becomes excessive, it may be necessary to modify the code to process the simulations in parallel. This would require additional programming work and an increase in the computational capabilities of the server hosting the system. The decision to implement this change should be carefully considered based on the actual number of requests. Additionally, calibration and validation are essential for any modeling system. Calibration involves tuning empirical parameters based on a comparison of model results to field measurements. As hydrocarbon spills cannot be used for these measurements, similar materials that behave like hydrocarbons in water (usually biodegradable) are typically used. The current system uses parameters chosen by the development team based on prior experience with other response or test scenarios (Janeiro et al, 2017, Martins & Janeiro, 2018). However, these parameters were not specifically developed for Cartagena Bay. To improve the accuracy of the system, dedicated measurement campaigns using for example low-cost georeferenced drifting buoys would be required. Many of the errors detected in the EWS Tool might be fixed in the entry forms; unfortunately, Google Forms is fairly simple, and hence does not offer many options to prevent it. So, in the future, it might be prudent to investigate another type of entry form that provides more options for preventing user errors.

In addition to these specific improvements, it is important to consider the overall usability, user interface, and ethical implications of the modeling system. Ongoing feedback and input from experts and stakeholders can help ensure that the system remains up-to-date with the latest scientific understanding and best practices in spill response. Ultimately, continuous refinement of the system will be necessary to maximize its usefulness and impact in responding to spills in Cartagena Bay, Algarve and even beyond that.

REFERENCES

Allen, J. (1982). Sedimentary Structures: Their character and physical basis, vol.1. https://books.google.pt/books?hl=pt-PT&lr=&id=32G-x3wRWXwC&oi=fnd&pg=PP1&dq=Allen%27s+(1982)+particle+movement+turbulence&ots=dkhgrNKPlk&sig=Ysd5wEty6_QuqAIgAWsk9V7MXjE&redir_esc=y#v=onepage&q&f=false

Berry, A., Dabrowski, T., & Lyons, K. (2012). The oil spill model OILTRANS and its application to the Celtic Sea. Marine Pollution Bulletin, 64(11), 2489–2501. https://doi.org/10.1016/j.marpolbul.2012.07.036

Buchanan, I., & Hurford, N. (1988). Methods for predicting the physical changes in oil spilt at sea. Oil and Chemical Pollution, 4(4), 311-328. https://doi.org/10.1016/S0269-8579(88)80004-2

Caballero-Gallardo, K., Alcala-Orozco, M., Barraza-Quiroz, D., de la Rosa, J., & Olivero-Verbel, J. (2020). Environmental risks associated with trace elements in sediments from Cartagena Bay, an industrialized site in the Caribbean. Chemosphere, 242. https://doi.org/10.1016/j.chemosphere.2019.125173

Cohen, Y., Mackay, D., Shiu, W.Y. (1980). Mass transfer rates between oil slicks and water. The Canadian Journal of Chemical Engineering, 58(5), 569-575. https://doi.org/10.1002/cjce.5450580504

Daling, P. S., Brandvik, J., Mackay, D., & Johansen, O. (1990). Characterization of Crude Oils for Environmental Purposes. In Oil & Chemical Pollution 7(3), 199-224, https://doi.org/10.1016/S0269-8579(05)80027-9.

De Kerf, T., Gladines, J., Sels, S., & Vanlanduit, S. (2020). Oil spill detection using machine learning and infrared images. In *Remote Sensing* (Vol. 12, Issue 24, pp. 1–13). MDPI AG. https://doi.org/10.3390/rs12244090

Delvigne, G. A. L., & Sweeney, C. E. (1988). Natural Dispersion of Oil. In Oil & Chemical Pollution (Vol. 4, Issue 4, pp. 281-310), https://doi.org/10.1016/S0269-8579(88)80003-0.

Fay, J. (1969). The Spread of Oil Slicks on a Calm Sea. Oil on the Sea, pp 53–63. https://link.springer.com/chapter/10.1007/978-1-4684-9019-0_5

Fingas, M. F. (2004). Modeling evaporation using models that are not boundary-layer regulated. Journal of Hazardous Materials, 107(1–2), 27–36. https://doi.org/10.1016/j.jhazmat.2003.11.007

Fingas, M., & Brown, C. E. (2018). A review of oil spill remote sensing. In *Sensors (Switzerland)* (Vol. 18, Issue 1). MDPI AG. https://doi.org/10.3390/s18010091

Frazão Santos, C., Carvalho, R., & Andrade, F. (2013). Quantitative assessment of the differential coastal vulnerability associated to oil spills. *Journal of Coastal Conservation*, *17*(1), 25–36. https://doi.org/10.1007/s11852-012-0215-2

Giannaros, T. M., Melas, D., Daglis, I. A., & Keramitsoglou, I. (2014). Development of an operational modeling system for urban heat islands: An application to Athens, Greece. Natural Hazards and Earth System Sciences, 14(2), 347–358. https://doi.org/10.5194/nhess-14-347-2014

Graça, R., Rebelo, E., & Martins, F. (2016). Vulnerability Identity (V.ID) for the Algarve coastal municipalities subjected to coastal oil spill accidents. ICUR2016 - International Conference on Urban Risks. Atas de Conferência Internacional. https://hdl.handle.net/10216/107340

Huang, J. C. (1983). A REVIEW OF THE STATE-OF-THE-ART OF OIL SPILL FATE/BEHAVIOR MODELS. International Oil Spill Conference Proceedings, 1983(1), 313-322. https://doi.org/10.7901/2169-3358-1983-1-313

Janeiro, J. (2014). Development of an operational tool for oil spill forecast: Application to oil exposed regions, http://hdl.handle.net/10400.1/6865.

Janeiro, j., Neves, A., Martins, F., & Relves, P. (2017) Integrating technologies for oil spill response in the SW iberian coast. Journal of Marine Systems, 173, 31-42. https://doi.org/10.1016/j.jmarsys.2017.04.005

Keramea, P., Spanoudaki, K., Zodiatis, G., Gikas, G., & Sylaios, G. (2021). Oil spill modeling: A critical review on current trends, perspectives, and challenges. In Journal of Marine Science and Engineering (Vol. 9, Issue 2, pp. 1–41). MDPI AG. https://doi.org/10.3390/jmse9020181

Lehr, W., Jones, R., Evans, M., Simecek-Beatty, D., & Overstreet, R. (2002). Revisions of the ADIOS oil spill model. In Environmental Modelling & Software 17(2), 189-197, https://doi.org/10.1016/S1364-8152(01)00064-0.

Mackay, D., & Mcauliffe, C. D. (1988). Fate of Hydrocarbons Discharged at Sea. In Oil & Chemical Pollution 5(1), 1-20, https://doi.org/10.1016/S0269-8579(89)80002-4.

Malan, N., Durgadoo, J. v., Biastoch, A., Reason, C., & Hermes, J. (2019). Multidecadal Wind Variability Drives Temperature Shifts on the Agulhas Bank. *Journal of Geophysical Research: Oceans*, *124*(5), 3021–3035. https://doi.org/10.1029/2018JC014614

Mendonça, F. (2020). A PYTHON BASED SYSTEM TO MANAGE SIMULATIONS OF COASTAL OPERATIONAL MODELS, Universidade do Algarve, http://hdl.handle.net/10400.1/15472.

Parga-Lozano, C. H., Marrugo-Gonz, A. J., & Fern A Andez-Maestre, R. (2002). Baseline Hydrocarbon contamination in Cartagena Bay, Colombia, 44(1), 4-71, http://dx.doi.org/10.1016/S0025-326X(01)00201-6.

Rosas, E., Martins, F., & janeiro, J. (2021). Marine Litter on the Coast of the Algarve: Main Sources and Distribution Using a Modeling Approach. Journal of Marine Science and Engineering, 9(4), 412. https://doi.org/10.3390/jmse9040412

Sánchez Catalán, F., Mayo Mancebo, G., Rivero Hernandez, J., Mercado Páez, J. P., & Johnson Restrepo, B. G. (2021). CARACTERIZACIÓN FISICOQUÍMICA, DETERMINACIÓN DE MERCURIO TOTAL E HIDROCARBUROS DISUELTOS Y DISPERSOS EN AGUAS Y SEDIMENTOS DE LA BAHÍA DE CARTAGENA, OLOMBIA. Boletín Científico CIOH, 39(2). https://doi.org/10.26640/22159045.2020.505

Santos, C. F., & Andrade, F. (2009). Environmental Sensitivity of the Portuguese Coast in the Scope of Oil Spill Events — Comparing Different Assessment Approaches. In *Source: Journal of Coastal Research: Vol. I* (Issue 56). https://about.jstor.org/terms

Sebastiao, P., & Soares, C. G. (1995). Modeling the Fate of Oil Spills at Sea. In Spill Science & TechnoIogr Bdelin 2(2-3), 121-131, https://doi.org/10.1016/S1353-2561(96)00009-6.

Semmendinger, K., Lee, D., Fry, L., & Steinschneider, S. (2022). Establishing Opportunities and Limitations of Forecast Use in the Operational Management of Highly Constrained Multiobjective Water Systems. Journal of Water Resources Planning and Management, 148(8). https://doi.org/10.1061/(ASCE)WR.1943-5452.0001585

She, J., Meier, H. E. M., Darecki, M., Gorringe, P., Huess, V., Kouts, T., Reissmann, J. H., & Tuomi, L. (2020). Baltic Sea Operational Oceanography—A Stimulant for Regional Earth System Research. In *Frontiers in Earth Science* (Vol. 8). Frontiers Media S.A. https://doi.org/10.3389/feart.2020.00007

Singh, U., Acharya, D., & Mishra, S. (2022). Oil Spill Detection & Monitoring with Artificial Intelligence: A Futuristic Approach. Proceedings of the Workshop on Control and Embedded Systems (WCES 2022), Chennai, India, April 22 - 24, 2022.

https://www.researchgate.net/publication/367309457_Oil_Spill_Detection_Monitoring_with_Artificial_Intelligence_A_Futuristic_Approach

Sotillo, M. G. (2022). Ocean Modelling in Support of Operational Ocean and Coastal Services. In Journal of Marine Science and Engineering (Vol. 10, Issue 10). MDPI. https://doi.org/10.3390/jmse10101482

Spaulding, M. L. (2017). State of the art review and future directions in oil spill modeling. In Marine Pollution Bulletin (Vol. 115, Issues 1–2, pp. 7–19). Elsevier Ltd. https://doi.org/10.1016/j.marpolbul.2017.01.001

Stiver, W., & Mackay, D. (1984). Evaporation rate of spills of hydrocarbons and petroleum mixtures. Environmental Scinece and Tecnhnology, 18(11), 834-840. https://doi.org/10.1021/es00129a006

Suh, S. W. (2006). A hybrid approach to particle tracking and Eulerian-Lagrangian models in the simulation of coastal dispersion. Environmental Modelling and Software, 21(2), 234–242. https://doi.org/10.1016/j.envsoft.2004.04.015

Tosic, M., Martins, F., Lonin, S., Izquierdo, A., & Restrepo, J. D. (2019a). Hydrodynamic modeling of a polluted tropical bay: Assessment of anthropogenic impacts on freshwater runoff and estuarine water renewal. Journal of Environmental Management, 236, 695–714. https://doi.org/10.1016/j.jenvman.2019.01.104

Tosic, M., Restrepo, J. D., Izquierdo, A., Lonin, S., Martins, F., & Escobar, R. (2018). An integrated approach for the assessment of land-based pollution loads in the coastal zone. Estuarine, Coastal and Shelf Science, 211, 217–226. https://doi.org/10.1016/j.ecss.2017.08.035

Tosic, M., Restrepo, J. D., Lonin, S., Izquierdo, A., & Martins, F. (2019b). Water and sediment quality in Cartagena Bay, Colombia: Seasonal variability and potential impacts of pollution. Estuarine, Coastal and Shelf Science, 216, 187–203. https://doi.org/10.1016/j.ecss.2017.08.013

Wang, Z., Fingas, M., & Page, D. S. (1999). PII: S0021-9673(99)00120-X. In Journal of Chromatography A 843(1-2), 369-411, http://dx.doi.org/10.1016/S0021-9673(99)00120-X.