NUMERICAL SIMULATION OF OIL SPILLS: APPLICATION TO A COASTAL ZONE

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MASTER'S THESIS

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1. Introduction

Pollution in marine and coastal waters is dispersed on its surface due to the wind and currents dynamics prevailing in the area. When that occurs, it is important to establish the extent and scope of the pollution in order to prevent damaging coastal and marine ecosystems (Corral et al., 2012). With rapid economic growing around the world there are potential sources of contamination in high seas, marine and submarine transport. Those activities include shipping, storage, washing and cleaning tankers, discharges of coastal cities, and accidents during operations (e.g. marine pipeline ruptures or leaks, spills and ship accidents) (Cho et al., 2012; Corral et al., 2012; Wang et al., 2005).

There are certain conditions that affect any pollutant spilled in ocean waters such as wind, waving, currents, and ocean water turbulence. Large-scale advective processes linked to mass transport and dominated by currents, winds and waving can be separated from low-scale diffusive ones, which are responsible of modifying the contaminant concentration (Siguero-Guemes, 2010). Hydrocarbons for instance, are non-conservative pollutants, which indicate that once they are spilled in the ocean their physiochemical properties vary through time. This is called weathering, and consists in a sort of processes: (i) spreading, (ii) evaporation, (iii) vertical dispersion, (iv) photo-oxidation and (v) biodegradation, that lead to hydrocarbon degradation (Chen et al., 2007; Papadimitrakis et al., 2006; Siguero-Guemes, 2010).

Accurate prediction of behavior of the contaminants is very important in order to keep the marine system as intact as possible. The area of contaminant spreading can be predicted numerically by solving the equations that govern the flow and the associated mass transport phenomenon (Cho et al., 2012). For instance, oil spill risk assessments, designed to study the impact of a spill in marine environment, are based on the spill fate and transport models (Papadimitrakis et al., 2006). Numerical simulation is a transversal and versatile tool since and it can be applied in almost every field of study. Biology, ecology, economy, environmental sciences, engineering, nanotechnology, and social sciences are just a few ones, not to mention basic disciplines that support it (i.e. mathematics, statistics, physics, and computing sciences) (Cala-Vitery, 2010). The development of simulation models to control pollutant spills in the ocean is a high priority in order to help local authorities and governments to mitigate their harmful effects in coastal zones and marine ecosystems (Corral et al., 2012).
Coastal zones are among the highly productive, densely populated and valuable ecosystems on earth. They link land and marine ecosystems and cover a wide range of biophysical characteristics. More than 1 billion people live in coastal areas, that’s why it is important to keep the sustainability of those zones, since and they provide a lot of goods and services that represent valuable resources (Brown et al., 2012; Miller and Spoolman, 2011).

Coastal marine ecosystem’s goods and services, meaning the benefit that people obtain from them, offer a wide range of services to human beings. They include provisioning services such as supply of food, fuel, wood, energy resources, natural products, and bioprospecting. They also provide regulating services: shoreline stabilization, flood prevention, storm protection, climate regulation, hydrological services, nutrient regulation, carbon sequestration, detoxification of polluted waters and waste disposal. Other cultural and amenity services are culture, tourism and recreation, and supporting services such as habitat provision, nutrient cycling, primary productivity, and soil formation. These services are of high value not only to local communities that live in coastal zones, but also to national economies and global trade, meaning that there is a strong relationship between the status of marine ecosystems and human well being (UNEP, 2006).

Marine processes such as primary production occur on the upper meters of water column – also called the euphotic zone – covering approximately the first 200 meters of depth (Miller and Spoolman, 2011). Primary producers depend on nutrients availability and light in order to support photosynthesis, which regulates atmospheric carbon dioxide and oxygen concentrations and represent the main basis to ocean stability, as they are the first link in trophic chain. In fact, 25% of world’s primary production is done in coastal zones, and about 90% of marine organisms live in euphotic zone (Brown et al., 2012).

Based on the facts exposed above, keeping track of the constant pollution due to shipping and local ports that affects the marine coastal system is highly important, given the fact that affecting ecosystem’s stability definitely will affect its sustainability. Oil spills in shallow coastal zones are one of the most hazardous ways that can easily break ecosystems stability, since and they affect photosynthesis and severely alter the goods and services provided. Therefore the constant developing of coastal and shallow zones numerical models to predict contaminant’s behavior emerge as one of the most valuable tools in order to keep the marine environment’s integrity.
With the development of computer techniques, over the past decades the use of Shallow Water Models (SWM) has been increasing, particularly in wave modeling. However they also are applied to river and coastal dispersions, and spillways, bores, dam breaks, and even atmospheric modeling (Randall, 2006). Those applications of shallow water equations and models are coded in different programming software (e.g. Fortran, C++, among others), but it is important to develop a code for each specific application. It requires an additional effort because it contemplates every step in order to create and apply the code (and the model), as well as avoiding previous possible mistakes regarding used equations and adapt it to a specific need.
2. State of the art

Marine and coastal pollution goes back to the very beginning of history of human civilization. However this subject did not receive much attention until adverse consequences have been noted on ecosystems and organisms, and it has become a global concern. Nevertheless most of the countries, specially developing ones, are still producing huge loads of pollution and trends are expected to increase. The division of pollution in different categories (e.g. air, water, land, etc.) has been criticized and been suggested to be described as “one pollution”, since and every pollutant whether in air or land trends to end up in the ocean (Papadimitrakis et al., 2006; Pincinato et al., 2009).

Marine pollution knowledge gaps have been identified as one of the biggest problems in introducing effective management control strategies. Major pollutants include: fertilizers, pesticides, and agrochemicals; domestic, municipal wastes, and sewage sludge; heavy metals and trace elements; organic compounds; plastics; sediments; eutrophication and algal bloom; aquaculture activities; oil spills (Islam and Tanaka, 2004).

As for oil spills, they can be divided in 3 classes: 1) small oil spills, that are associated with berthing, bunkering and other terminal operations, and accidental discharges of oily water mixtures of machinery. This kind of spills occur at port and are the results of accidents, equipment failing or poor work practices. 2) Major shipping incidents (e.g. collisions, fires, undersea pipeline accidents, etc.) are potential sources of oil pollution. Those spills tend to produce intensive/large scale spill. 3) Refers to intended discharges, which dump waste oil into marine environment to save money or time (Gilbert, 1999). It is important to remark that while major shipping incidents refers to major oil spills that cause large and intensive scale damage, small oil spills such as described in class one tend to be slight to moderate in size but can still result in extensive environmental and economic damage. In coastline marine environments the tracking of oil spills, which are likely to impact the shoreline, is of high importance in order to deploy an oil spill response team to protect sensitive areas (Evans et al., 2014).

When a spill occurs in the marine environment the first concern is the fate of that slick, referring to direction, speed, movement, and spreading characteristics at sea to make...
a better response. In order to do that, it is important to understand the physical problem (e.g. movement) and weathering (e.g. chemical reactions) of oil when spilled.

2.1. The physical problem
Modeling oil spills and in general substances behavior in marine environment implies many physical variables intervention, which rule their transport and transformation processes. For this reason, in order to establish the evolution and concentration of those present substances through time it is necessary the use of transport equation, also called advection-diffusion equation, which is the main core in any numerical model of this kind (Sámano-Celorío, 2011; Siguero-Guemes, 2010).

When introduced in an aquatic media, a substance’s concentration evolution depends on the joint action of three processes: advection (or transport caused by existing currents), turbulent diffusion or dispersion (causing the substance’s spreading), and transformation processes (e.g. physical, chemical, or biological that act if the substance is not conservative). Contaminant’s concentration evolution depends not only on the substance’s properties, but also on hydrodynamics, meteorological, and environmental conditions that govern fate and transport in water bodies (Sámano-Celorío, 2011; Siguero-Guemes, 2010).

2.1.1. Advection
When simulating coastal oil spills, and in general any pollutant transport in shallow sea zones, advection movement is prevailing over the rest. Analyzing the principal forces that determine the transport of a pollutant in the sea, as well as their combined effect is of special interest (Siguero-Guemes, 2010; Wang et al., 2005).

Currents are one of the main forces that affect advective movement of a pollutant in the sea. About 10% of the water in the ocean is involved in surface currents, referring to water flowing horizontally in the upper 400 meters (Garrison, 2006). Since and this master’s work is focused on superficial oil spill transport, it is important to study which processes affect surface currents. Surface currents are driven largely by wind friction, and they patterns are determined by wind direction, Coriolis force, and the position of landforms that interact with currents. Other factors are the geostrophic currents, which involve density and pressure gradients closely related to temperature and salinity, and tidal currents that are affected by moon’s gravitational effect and they vary depending on the location of study (Garrison, 2006; Pidwirny, 2013).
Nevertheless wind friction will be the main force in advective movement in coastal zones and in the continental platform, where the effect of the other forces is relatively minor. Therefore the amount of displaced water – and the spilled oil trajectory – will depend mainly on wind intensity and direction (Garrison, 2006; Siguero-Guemes, 2010).

2.1.2. Diffusion
Diffusion transport processes refer to turbulent diffusion and pure diffusion by contaminant concentration differences. They are characterized by having a much lower time and space scale compared to advective ones. It is hard to resolve horizontal diffusion for all scales simultaneously, so it must be focused on a determined space-time scale (Siguero-Guemes, 2010).

Modeling turbulence in the ocean is a complex process that requires complicated computer simulations. Most oil spill models use simplified formulas to simulate mixing. A common approach is to represent turbulence using a constant diffusion coefficient, but there are other options. However most of spill models assume constant and uniform dispersion coefficients based on historical measurements. The appropriate coefficient is dependent on the scale of the spill and the location of the release (Wang and Stout, 2010).

Depending on the scenario where the study is taken, ocean surface transport hydrodynamic modeling is close more or less to the real transport. When implementing a Stochastic Langragian Model (SLM) more precision can be achieved, and will eventually lead to a better approximation of all physical processes that intervene in particle movement (Sámano-Celorío, 2011; Siguero-Guemes, 2010). The oil spill modeler may adjust the turbulent mixing term if the model output does not completely match the observations of the oil distribution (Wang and Stout, 2010).

2.2. Oil weathering
As mentioned before, advection and diffusion are two of the main processes involved in movement of a pollutant, but hydrocarbons mixtures spilled in the sea also are subjected to weathering processes, such as spreading, evaporation, emulsification, dissolution, biodegradation, photo-oxidation, vertical dispersion, sedimentation, etc. All these processes occur simultaneously, so if there is a spill it will: 1) move by advection and turbulent diffusion, 2) spread to form a thin film, 3) lighter compounds will evaporate, 4) non-soluble compounds will become emulsified and dispersed in the water column, 5) degradation and photo-oxidation will occur depending on the
contaminant (Figure 1) (Corral et al., 2012; Sámano-Celorío, 2011; Siguero-Guemes, 2010; Wang et al., 2005).

Once analyzed advective and diffusive components that affect oil spilled in the sea it is important as well to know about the physicochemical processes that interfere in weathering. In general they have a particular behavior once spilled in marine environment. Their compositions vary through time and external agents alter its physical properties (Figure 2).

![Figure 1](image.png)

**Figure 1.** Major weathering and natural processes that can affect spilled oil on water. Once oil interacts with the shoreline, some of these processes will no longer apply. There are computer models that can forecast most or all of these processes (Evans et al., 2014).

### 2.2.1. Spreading

When a lighter liquid is spilled over other one, a sort of physical and chemical phenomena produces a natural spreading. After an oil spill in the sea, those products rapidly spread on the surface, reaching extensive areas even in calmed sea conditions. Spreading is caused by an imbalance of internal and external forces and is called mechanical spreading, to distinguish it from extensive diffusion (Siguero-Guemes, 2010). Spreading and drifting of the oil occurs immediately after oil mixes with water and occurs as a result of interacting forces including gravity, wind and surface tension. This process is also directly influenced by the viscosity or fluidity of the oil. The rate of
spreading is influenced by many other factors as well, which involve weather conditions (Wang and Stout, 2010). Spills have been known to spread hundreds of kilometers in a matter of days due in part to high currents (Ramakrishna, 2012). The less viscous the oil, the more it will spread and increase the area of water covered by an oil slick.

![Figure 2. Time scale for oil weathering (and hydrocarbons in general) (Project-MEDESS-4MS, 2015).](image)

Spreading evolves temporarily until reaching a state in which the thickness of the spill reaches to what is called minimum thickness, and afterwards mechanical spreading stops. Minimum thickness will vary depending on the hydrocarbon-type spilled and depends on its viscosity and density. Once reached minimum thickness, caused by weathering processes or strong water turbulence, the slick in surface can fragment to form small sub-slicks (Siguero-Guemes, 2010).

Spreading has a relative relevance in open sea but in sheltered waters it represents principal expansion of oil, because minimum thickness can be reached in less than one day. Spill researches have attempted to model spreading by two separate approaches. One deterministic approach balances spreading and retarding forces in a fluidic application of Newton’s law. The most widely used such deterministic model was developed by James Fay in 1969, which labeled spreading in three phases: gravity-inertial, gravity-viscous, and surface tension-viscous. As alternative approach, researchers have attempted to model slick spreading as strictly a water turbulence phenomenon with the oil acting as a neutral tracer (Ramakrishna, 2012; Siguero-Guemes, 2010; Wang and Stout, 2010).

### 2.2.2. Evaporation

One of the most important mechanisms that intervene in oil elimination is evaporation. The amount of evaporated hydrocarbons mainly depends on the spilled oil properties
(lighter or heavier), wind speed (enhanced dragging effect and fluid-gas mass transfer, resulting in high evaporation), and temperature (higher temperatures will speed up evaporation). Lighter refined products, such as gasoline or aviation fuels, will evaporate faster than heavier products like heavy oils. Evaporation affects spilled oil as it increases viscosity and density (it can even sink, making it more likeable to emulsification). As viscosity and density increases, solubility decreases, which result in a reduction of total spilled product’s toxicity. Environmental conditions also affect evaporation. If spilled oil thickness is lower, evaporation rates will be higher (Hernández-Montes, 2009).

Evaporation occurs immediately after the spill and will endure depending on the product’s composition from a few hours to a few days. As mentioned before, evaporation rates of lighter products will be close to 100% and in the case of heavier products will barely reach 10%. To compute the rate of oil evaporation Mackay in 1981 developed a multi-component theory (Chao et al., 2001; Siguero-Guemes, 2010).

A good knowledge on evaporation will be essential to make a good management when a spill occurs, specially the first few hours afterwards since and in that precise moment it is important to know how much product will evaporate and how much will remain in the sea. Also, evaporation itself interacts with other physicochemical reactions (of weathering), causing rheology changes in the spilled oil (Siguero-Guemes, 2010).

2.2.3. Emulsification

Waving energy spontaneously mixes oil and seawater, occasionally forming a water-oil emulsion, a process called emulsification. This results due to wave breaking and sea surface turbulence. Sea surface disturbance entrains seawater into the oil slick. As slick viscosity increases with time, higher amount of water is trapped in the slick. Therefore, the formation of emulsion increases water content of oil. This further impedes the rate of evaporation (Mishra and Kumar, 2015). Mousse can range in color from dark brown to nearly red or tan, and typically has a thickened or pudding-like consistency compared with fresh oil. The water can bulk up the oil to increase the apparent volume of oil by up to four times. This process affects heavier products and it is practically nonexistent in lighter ones (Evans et al., 2014).

This is considered a critical process regarding final recovery, since and emulsification increases drastically viscosity, and bombing is very difficult. In certain cases, up to 80% proportion of water in oil is achieved, multiplying contaminant’s initial volume.
Emulsification also reduces the possibility of treating oil-water mix with dispersants or other products, making it more resistant to biodegradation. It is important to take into account that oil-water surface mix will incorporate other particles along its trajectory (e.g. objects, sediments) until reaching coastal zone, where it will be mixed with sand. In this way, from the moment that oil is spilled until it reaches the coastal/sandy zone total residue volume may be increased by ten times (Siguero-Guemes, 2010).

2.2.4. Photo-oxidation

Solar UV radiation generates photo-oxidation, depending on solar radiation’s intensity. This alters the properties of oil mixtures modifying their chemical structures. Chemical combination of oil with atmospheric oxygen contributes to oil degradation (Siguero-Guemes, 2010). Therefore photo-oxidation is a potentially significant process in spilled crude oil degradation at sea, and depends on the sun incidence and the thickness of the oil slick. Photochemical degradation yields a variety of oxidized compounds including alcohols, aldehydes, ketones, and acids, which are more soluble in water than starting compounds (Wang and Stout, 2010).

A fundamental understanding of the effect of photochemical degradation is a prerequisite for providing an accurate description of the potential spilled oil in a marine environment. Compared with biodegradation, the phenomenon of photo-oxidation is less well understood and affects oil composition differently than microbial degradation, but may provide and opportunity for the introduction of remediation techniques (Garrett et al., 1998). As those last three processes occur simultaneously, oil composition can be altered and transformed into a viscous tarry mass (Figure 3).

2.2.5. Biodegradation

Biodegradation is a natural process in which microorganisms are responsible of degrading hydrocarbons into lighter and simpler compounds. Oil is a natural resource, then it is expected that some bacteria, fungi and other marine organisms will use them as food source. However, this is a slow process because it depends on nutrients and oxygen availability, and can be limited by the presence of toxic pollutants (Siguero-Guemes, 2010).

Biodegradation rate depends on many factors: nutrients content (mainly nitrates, phosphates, and iron) is critical. To foment biodegradation, an adequate supply of nutrients is essential when large quantities of hydrocarbons are released in the marine environment. For example, during the Exxon Valdez spill, fertilizers containing nitrogen were added to speed up oil biodegradation (Atlas and Hazen, 2011). Other factors
include dissolved oxygen (most of petroleum hydrocarbons are biodegradable under aerobic conditions), salinity, temperature, superficial area of spill, and specific characteristics of microbial community (Atlas and Hazen, 2011; Gertler et al., 2012; Siguero-Guemes, 2010).

It is important to remark that although slow, biodegradation is economically highly competitive compared to traditional techniques of bioremediation (e.g. manual cleanup, dispersant application, in situ burning) (Gertler et al., 2012).

Figure 3. Evaporation, emulsification, and oxidation convert oil to a viscous tarry mass (Santa Barbara County, California) (Copyright: American Geosciences Institute, 2015).

2.2.6. Dissolution

This process involves the dissolution of soluble fractions of oil spilled in the water. Dissolution time depends on the composition, spreading rate, water temperature, turbulence, and dispersion rate. Although the process starts immediately, it can be seen more clearly in the long term, and continues during whole hydrocarbon degrading process. Lighter and water-soluble compounds will dissolve rapidly and increase water media toxicity, since and they incorporate to water column instantaneously. However since and evaporation is faster compared to dissolution most of those chemicals will evaporate quickly. The amount of crude oil dissolved in seawater, is therefore typically
small (less than 5%) or even nonexistent in certain cases (Mishra and Kumar, 2015; Siguero-Gumes, 2010).

### 2.2.7. Shoreline deposition

When oil in marine environment reaches the coastal zone it can be deposited in beaches, rocks, wave breakers, cliffs, or can just be in the coast until sea conditions change and return it back to open sea (Siguero-Gumes, 2010). Coastal stretches that are highly affected by oil spilled are defined on “Shoreline Exposure Index (SEI)”. SEI is used to evaluate the impact based on the oil level on sea surface, consists on 5 degrees of exposure (ranging from A1: very low to A5: very high) and each one corresponds to shoreline oil accumulation (El-Fadel et al., 2012; Hayes, 1996).

### 2.2.8. Sedimentation

Refers to the process by which oil is deposited on the bottom of the sea (e.g. hydrocarbon adheres to denser-than-water particles and sinks to the bottom). Once oil in on the bottom, it is usually covered by additional sediments and degraded very slowly. Oil-mineral aggregates (OMA) result from interactions among oil residues, fine material particles, and seawater. OMA formation has been identified as an important process that facilitates the natural removal of oil in coastal sediments. OMA formation is enhanced by physical processes such as waving, tides, and currents (Corral et al., 2012; Wang and Stout, 2010).

Sedimentation may occur by two mechanisms: the first one is defined as oil is degraded, resulting in increased density. The second one occurs when oil adheres to suspended particles in the water column. In both circumstances oil precipitates, as it incorporates more and more sediments and other suspended particles (Siguero-Gumes, 2010).

### 2.2.9. Vertical dispersion

Vertical dispersion is about intrusion of a contaminant in the water column, forming what is called water-oil emulsion. This is made starting from contaminant fractioning in different size particles that will be dispersed in the water column because of specially ocean turbulence, wind, and marine currents. This process could be very important, since and in certain cases dispersed volume in the water column can reach up to 60 % (Siguero-Gumes, 2010).

Hydrocarbons in general are usually non-soluble and lighter than seawater. Some drops of spilled oil that were dispersed could eventually return to the original spill or
could form a new one. However part of the oil will stay dispersed in particulate form that can mix up with other particles or sediments. Vertical dispersion can occur in natural form (e.g. turbulence, waving) or induced form (e.g. use of chemical products that stabilize smaller particles spilled). The induced form has been controversial given their highly toxicity – in certain cases even higher than the spilled oil – leading to a very restricted use of them. Currently induced dispersion is applied in offshore oil spills, but it is important to take into account that the products used may incorporate to trophic chain or accumulate on the bottom by sedimentation. Dispersed oil volume can affect directly on marine organisms that live in water column, or even those who live in the bottom if it precipitates. (Comerma-Piña, 2010; Siguero-Guemes, 2010).

It is important to compute the natural dispersion in order to evaluate the lifetime of an oil spill. As mentioned before, this dispersion depends on environmental parameters, but is also influenced by oil-related parameters such as oil thickness and its properties (e.g. density, surface tension, and viscosity). Emulsification will also contribute to persistence of oil spilled, mainly due to increased viscosity and slick thickness, causing retarded spreading, increasing volume, that will reduce natural dispersion (Reed et al., 1999). The facts exposed show that environmental conditions are critical factors to vertical dispersion.

Table 1 shows a summary of the dominant oil spill processes, their importance, operative times, and dependence:
Table 1. Prevailing and most important processes during and after an oil spill (Sebastião and Guedes Soares, 1995).

<table>
<thead>
<tr>
<th>PROCESS</th>
<th>IMPORTANCE</th>
<th>OPERATIVE TIME</th>
<th>DEPENDENCE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spreading</td>
<td>Area extent.</td>
<td>Hours to weeks.</td>
<td>Gravity, surface tension, inertia, viscosity and/or droplet size.</td>
</tr>
<tr>
<td>Evaporation</td>
<td>Loss of 20-40% mass. Increases density and viscosity.</td>
<td>Hours to days.</td>
<td>Spill area, slick thickness, oil vapor pressure, mass transfer coefficient.</td>
</tr>
<tr>
<td>Emulsification or mousse formation</td>
<td>Uptake of up to 80% water into oil. Increases viscosity and volume; Densities become similar to seawater.</td>
<td>Hours to days.</td>
<td>Turbulence, temperature and oil composition (e.g. constituents that favor mousse formation).</td>
</tr>
<tr>
<td>Biodegradation</td>
<td>It may be the ultimate fate of much of the dissolved and dispersed oil.</td>
<td>Weeks to years.</td>
<td>Hydrocarbon dilution and degradability, water contents of nutrients and oxygen, location of the spill (coastal vs. open sea).</td>
</tr>
<tr>
<td>Photo-oxidation</td>
<td>Slow formation of oxygenated polar water-soluble species, which affect spreading and mousse formation and may contribute to the toxic burden of oil in water column.</td>
<td>Hours to weeks.</td>
<td>Incidence and intensity of sunlight or clouds, interrupted by nights.</td>
</tr>
<tr>
<td>Dissolution</td>
<td>Loss of aprox.1% of mass; important from toxicological view.</td>
<td>Hours to days.</td>
<td>Dissolution mass transfer coefficient, solubility.</td>
</tr>
<tr>
<td>Sedimentation</td>
<td>Rarely expected through weathering alone in cold waters. Temporary submergence in the top meters may occur in consequence of high seas and over-washing by waves. It may occur if oil associates with suspended matter.</td>
<td>Days to months.</td>
<td>Increased density as a result of weathering, association with suspended particulate matter or local pellets.</td>
</tr>
<tr>
<td>Shoreline deposition</td>
<td>Beaches can hold up certain amount of oil.</td>
<td>---</td>
<td>Distance of the spill to shore, currents, waves, sea conditions in general.</td>
</tr>
<tr>
<td>Vertical dispersion</td>
<td>Up to 2 mg L⁻¹ in the top 10 meters of water column.</td>
<td>Hours to days.</td>
<td>Sea state (wind shear and breaking waves).</td>
</tr>
</tbody>
</table>
2.3. Modeling an oil spill

Several oil spills models have been developed to forecast its fate and transport, and some others also were developed to simulate weathering processes once the spill occurs. They can range from a simple vector calculation to current modern and sophisticated computer ones of fate and transport of oil in three dimensions along with predictions of the change in properties as the oil weathers (ITOPF, 2011).

The model should include oil’s characteristics: quantity, type and amount of product spilled. Other key input data include environmental conditions, such as wind and sea currents speed and direction, but also can include temperature and tides. Currently there are models that can simulate almost each weathering process along with fate and transport at the same time. A model would be more accurate as they include more variables and oil’s characteristics and real data of environmental variables (however data availability is often an issue). More than one model can be used because a particular one may perform better in certain situations. A model’s performance varies because mathematical equations that describe oil movement are complex, and it’s almost impossible to make an analytical solution that includes all of them. That's why every model can be applied to certain situations only, by making assumptions in some inputs. For instance, one model can be good at modeling fate and transport behavior, but it can be weaker in other aspects (Samuels et al., 2013; Wang and Stout, 2010).

El-Fadel et al., 2012 stated regarding simulating oil spills:

“For this purpose, numerical models have been developed and applied to simulate the fate and transport of oil spills mainly based on known physiochemical principles or experimental interactions (Fay, 1971; Ahlstrom, 1975; MacKay and Leinonen, 1977; Mackay et al., 1980, 1983; Mackay and Paterson, 1980; Darras, 1982; Aravamudan et al., 1982; Beer et al., 1983; CSE, 1986; Al-Rabeh et al., 1989, 2000; Spaulding et al., 1993; Reed and AAmo, 1994; Sebastiao and Soares, 1995; ASCE, 1996; French, 1998; Lonin, 1999; Riazi and Al Enezi, 1999; Garcia-Martinez and Flores-Tovar, 1999; Reed et al., 1999; Lardner, 2004; Baruque et al., 2010). These models often represent the oil behavior characteristics that affect the fate and transport of the oil in the marine environment including advection, spreading, evaporation, dispersion, dissolution, emulsification, sedimentation, oil shoreline interactions, photo and bio-degradation (EPA, 2006). Typically, such models are driven by winds and currents denoted by atmospheric and ocean circulation algorithms”.
Oil spill models have been widely used for incident planning and often are helpful for decision makers. By modeling a series of most likely spill scenarios, decisions concerning a suitable response can be made on time, and the most vulnerable locations identified to place a response team properly. However, making an effective use of a model during a real spill is very challenging, since numerous variables are required to make it accurate and real-time data are not always available at the exact moment of the spill (ITOPF, 2011).

Despite the challenging task of simulating oil spills in real time, some efforts have been made to make it possible. For example, the *Ocean Global Oil Spill Modeling System* could be a useful tool to make a real-time incident approach as it integrates oil spill modeling tools with forecast of datasets available on the Internet. One of its most overwhelming characteristics is that the model is not limited to coastal and open seas zones, but also can be applied on rivers. The system uses the models and data available and hydrological range from surface runoff to stream and river flows, tidal estuaries, bays, coastal regions and oceans. It can be used for real time, forecast and probabilistic applications. The system has been successfully applied on all continents. Even some individual components of the model have been used to evaluate radioactive fallout for surface runoff and stream flow from the Fukushima nuclear plant accident (2011) and ocean and wind currents for modeling the Deepwater Horizon oil spill (2010) (Samuels et al., 2013).

NOAA’s Office of Response and Restoration has also developed some other software for spill response and planning. The most important of them are:

- **GNOME** (General NOAA Operational Modeling Environment), a trajectory-forecasting tool that predict how wind, currents, and other processes might move and spread oil on the water. This software finally shows a “spill movie” showing the predicted trajectory of the oil spilled.
- **ADIOS** (Automated Data Inquiry of Oil Spills) is an oil weathering’s model software. This tool models how different type of oils change in the marine and coastal environment. It works with a database of more than a thousand different crude oils and refined products, so it allows estimating quickly the expected characteristics and behavior of oil spilled.
- **Environmental Sensitivity Index (ESI) Maps**, which is focused in the coastal resources that are in risk if an oil spill occurs nearby. It includes biological resources (e.g. birds, shellfish beds), sensitive shorelines (e.g. tidal flats,
swamps), and human resources (e.g. beaches, parks). ESI maps can help
decision makers in reducing environmental consequences of the spill and clean
up efforts. Also it can help to identify vulnerable locations and establish
protection priorities before the spill occurs.

- **ERMA** (Environmental Response Management Application) is an online
  mapping tool that integrates static and real-time data such as ship locations,
  weather, and ocean currents. The data can be manipulated as will and
  represents an easy-to-use format for decision makers.

  (NOAA, 2015)

However it is important to keep in mind that even the models are good and the
software developed is of a high-level performance, it never will replace real
observations (e.g. aerial/oceanic/shoreline monitoring). Real time observations along
with a model specifically developed to a spill issue are the more reliable sources in
order to predict correctly an oil spill.
3. Objectives

The main purpose of this master’s thesis is to write a numerical code which will allow simulating pollutants transport in coastal/shallow waters (particularly oil spills), keeping in mind the various processes a substance may pass through when spilled in seawater. It is expected that the resulting model will constitute a supporting tool to oil spills research and mitigation given the harmful effects of spills on human and marine environment. The resulting model will then be applied to a coastal environment, in order to simulate a simple oil spill.

Code writing to achieve the main objective will be done as following:

- Transport equation development (advection-diffusion-reaction) in 1D and 2D, which will set the initial conditions for the model.
- Use of Finite Differences Method (FDM) and Finite Volumes Method (FVM) in 1D and 2D.
- Application of the numerical model written, validating the resulting model and applying it on a simple case of oil spill simulation.
4. Numerical method

A numerical model should represent a tool to understand, interpret, and reproduce an oil spill behavior. Therefore a model must be: 1) robust and versatile in order to comprise accurately the causes of an oil spill, 2) easy to simplify data processing volume and 3) be able to incorporate real-time data to readjust or rectify a prevision. All of these are achieved by two separated modules mentioned before: fate and transport, and weathering (Siguero-Guemes, 2010).

In order to simulate oil spills it is necessary develop a numerical method that will represent as accurate as possible the fate and transport of the product spilled. The great variety of oil spills and in general contaminants behavior makes almost mandatory to develop a particular algorithm that can describe in detail the modeling process to a specific case. This implies either a time-step concentration equation (Eulerian models) or a tracking particles monitoring (Lagrangian models). A numerical scheme is more effective in certain circumstances. For instance Eulerian models may cause excessive numerical diffusion regarding advection, but it’s not a problem with Lagrangian ones. However, the use of Lagrangian models require the use of a great particles number that can assure sufficient retention of particles in each cell to properly represent the oil concentration (Sámano-Celorio, 2011). For the desired application of this research work, the Lagrangian method is not considered, since and they are more complex and demands more calculation resources.

4.1. Eulerian methods

Eulerian numerical methods have a fixed framework, which means that the calculations are simple and demands less computational resources. However the main weakness is regarding advection movement. According to Sámano-Celorio, 2011 schemes based on 1st order approximations for advection result in a stable algorithm, but artificial dispersion is introduced. Upwind schemes for example, present excessive numerical diffusion but are the easiest finite differences method: stable, free of numeric oscillation, and their implementation in numerical codes is simple. It is important to know that numerical diffusion derived from the use of upwind schemes is minor than the real diffusion, therefore the resulting error will not be only as a consequence of its use, but also will be a result of other sources derived from approximations and suppositions that must be done during modeling. Nevertheless, many authors believe that upwind schemes efficiently solve the advective fraction of the derivative equations of the fate and transport equation.
In hydrodynamic modeling is imperative the development of equations that represent the physical behavior of water (e.g. mass conservation and movement equations), and mass transport equations (e.g. advection-diffusion-reaction of substances in the water). To make a correct simulation of contaminants dissolved and spilled in water is crucial to know the velocity fields in each point of the area of study (Sámano-Celorío, 2011).

Hydrodynamic modeling includes a variety of approximations that are commonly used in several studies. In all of them, basic equations that support the model are well known and there are multiple ways to resolve them. That makes necessary to count on with a wide variety of modeling techniques in order to meet the diverse applications that can arise (Sámano-Celorío, 2011).

4.2. Finite differences method (FDM)

FDM consists in approximating Partial Differential Equations (PDE) by algebraic expressions with dependent variable values in a limited number of selected points. Basically it replaces derivatives in a differential equation with algebraic approximations of the derivatives. Those algebraic equations are then solved to get an exact solution to the original PDE. As a result of the approximation, the PDE that describes the problem is replaced by a finite number of algebraic equations in the selected nodes. The values of the selected nodes are then the unknown. The algebraic system must be solved and are related to grid points. The accuracy of FDM strongly depends upon the mesh size and its properties (Chen, 1961).

A FDM scheme involves three steps (Chen, 1961):

- Dividing the solution into grids of nodes.
- Approximating the given differential equation by finite difference equivalence that relates the solutions to grid points.
- Solving the difference equations subject to the prescribed boundary conditions and/or initial conditions.

4.3. Finite volume method (FVM)

Finite Volume Methods (FVM) are mainly employed for numerical solution of problems regarding fluid mechanics as they were introduced in the 1970’s. Still, the current application is not limited to flow problems. FVM is perhaps the most successful class of numerical methods for solving PDEs. These methods are closely related to FDM.
However, FVM are derived on the basis of the integral form of the conservation law. Contrasting with FDM, in which looks for an approximation values of different points, FVM seeks for approximations to integral averages of the solution in control volumes (Figure 5 and Figure 6).

In general FVM involves the following steps (Schäfer, 2006):

1. Decomposition of the problem domain into control volumes. The domain is discretized into a finite number of subdomains or Control Volumes (CVs) (e.g. \( i=1, i=2, \ldots N \)) and the nodes connecting between them are computed. The union of all CVs must cover the whole problem domain.

2. Formulation of integral balance equations for each control volume. After defining the CVs the balance equations that describe the problem are formulated in integral form for each CV.

3. Approximation of the integrals by numerical integration. Usually applying the “midpoint rule” is the simplest way for numerical integration, although higher order can be applied (Gaussian ones) but in this case the computational cost increases. For a cell-centered variable is carried out in 2 steps:
   3.1. Approximation of convective and diffusive fluxes by values on the CV faces (up, down, left, and right). They are also known as physical fluxes. It will calculate the fluxes only in the CV of interest, regardless of CVs near it.
   3.2. Approximation of the variable at the CV faces by node values. In the nodes it is necessary to define a unique value of the flux. The most common fluxes are Lax-Wendroff, Lax-Friedrichs, and Force (also called numerical fluxes). The adjacent CVs are taken into account and the fluxes of the adjacent volumes are combined. Force flux represents the arithmetic mean of Lax-Wendroff and Lax-Friedrichs. The diffusive flux is usually obtained using an arithmetic mean between CV faces fluxes.

4. Approximation of function values and derivatives by interpolation with nodal values (cell centered CV).

5. Assembling and solution of discrete algebraic system.
Figure 4. Finite volume method scheme (1D), which integrates a given function of a particular control volume. The rectangle’s area is equal to the area under the function.

\[ \int_{x_1}^{x_2} f(x) \, dx \]

Figure 5. 2D-Finite difference method, which will calculate the solution at the nodes of the grid.
Shallow water equations have been extensively used for a wide variety of coastal and environmental engineering phenomena such as periodic (e.g. tides), flow, transient wave phenomena (e.g. tsunami or shock waves), transient pollutant transport (e.g. oil spills), etc. It is well known that current flow in estuaries and coastal seas can be described by the shallow water equations (Navon, 1988).

Shallow water equations are derived from the principles of conservation of mass and momentum. In general the shallow water equations model and describe the propagation of disturbances in water and other incompressible fluids, being the dam break one of them (Figure 7). The underlying assumption is that the depth of the fluid is small compared to the wavelength of the disturbance, as occurs in a coastal zone,

**Figure 6.** 2D finite volume method, which will calculate cell averages at the control volume.

### 4.4. Shallow water equations

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implying that the vertical velocity of the fluid is small. Given this situation the shallow water approximation provides a reasonable model for a real scenario. More realistic models of oceans and tsunamis include terms that describe the topography of the ocean floor, the Coriolis force resulting from the earth’s rotation, and possibly other external forces (Moler, 2011). Basically a SW scheme will serve as an application of a FVM that will be applied to a problem with a known and the numerical results can be compared.

**Figure 7.** 1D Shallow Water Scheme. In the dam break situation it is important to mention that it represents a non-realistic situation, since and the solution calculated is based on the abrupt removal of the dam.

### 4.5. Other simulation parameters

#### 4.5.1. Boundary conditions (BCs)

One delicate aspect of the model is the Boundary Conditions (BCs), especially if the intention is to apply it to a real-world geometry. The simplest way to make it work is to define a reflective boundary condition (for instance $u=0$ and $v=0$), which will make the spilled oil that reaches the boundary to reflect back into the domain.

In that case different BCs can be applied (e.g. Dirichlet, Neumann, Robin, absorbing, among others) depending on the physical problem. In FVM the incorporation of BCs is not as straightforward as in FDM and FEM and the use of ghost cells is required. The cell averages for these cells are computed from cell averages in the real domain depending on the BCs considered. The number of ghost cells depends on the order of the scheme.
4.5.2. Ghost cells
As mentioned before, a ghost cell is a fictitious – or auxiliary – grid point that is used to deal with the boundary conditions, but it is not part of the final solution. In order to implement the behavior of the fluid at boundaries, and also to allow the connection of several grid blocks, each array has an additional layer (called ghost cell). Ghost cells can be used as boundary conditions as well, as showed in Figure 8.

![Ghost cells as supplementary cells to deal with boundary conditions of the grid (2D).](image)

**Figure 8.** Ghost cells as supplementary cells to deal with boundary conditions of the grid (2D).

4.5.3. Courant, alpha, and Peclet numbers
Courant, alpha, and Peclet numbers are important as they determine the stability of a numerical scheme. However if they reach some critical limit, the numerical solution will oscillate in space and time. The oscillatory solution is non-physical and grows rapidly, providing numerical overflow. They are used in the advection-diffusion-reaction equation.

- **Courant-Friedrichs-Lewy condition (CFL)**
CFL condition, also known as Courant’s number, is a necessary condition for convergence and stability while solving certain PDEs, but it is not a sufficient condition, so in order to establish convergence it is necessary to use other methods. As a result of this condition, the time step must be controlled and less than a certain time; otherwise the simulation will produce incorrect results (Weisstein, 2015).

However, even with stability, convergence is not guaranteed. It is important to take into account consistency, which occurs when \( \Delta x \) and \( \Delta y \) tend to zero, and the error will tend
to disappear, remaining the original equation. This is an obligatory situation in order to obtain a consistent scheme. When refining the mesh in space and time, the error will diminish, and the method will be closer to the real solution. When a linear scheme is consistent and stable, then it is convergent (according to Lax theorem) and the CFL condition is met (Figure 9).

A scheme will be consistent when the difference between the numeric solution $(u)$ and the exact solution $(U)$ tend to be zero, as the following:

$$\lim_{\Delta x \to 0, \Delta t \to 0} |u - U| = 0$$

Courant number can be in $[0-1]$ range, usually close to 1, and it is expressed as follows:

$$C_0 = \frac{v \cdot \Delta t}{\Delta x}$$

Where:
$v$: substance velocity.
$\Delta t$: time step.
$\Delta x$: space interval.

- **Alpha ($\alpha$)**

Alpha, also called diffusion number, is used to guarantee also the stability of the method when a diffusion term is used. Courant number is applicable when there is only an advective term. Then, it is necessary a combination of Courant and Alpha to obtain the so desired scheme’s stability.

Subsequently, to guarantee stability time step must be the smaller one of them, as the following equation states:

$$\Delta t = \text{min} \left( \frac{\Delta x}{v} \cdot \frac{\Delta x^2}{D}, \alpha \cdot \frac{\Delta x^2}{D} \right)$$

Where:
$v$: velocity term (advection).
$D$: diffusion coefficient.
Generally Alpha primes over Courant since and it has a smaller time step, but when the ratio between velocity and diffusion is higher then CFL primes. On the other hand, when the ratio between them is small then the alpha primes. Finally when there are similar or equal conditions, Alpha number primes (Table 2).

Alpha number is calculated as shown next:

\[ \alpha = D \cdot \frac{\Delta t}{\Delta x^2} \]

Where:

D: diffusion coefficient.

**Table 2.** CFL condition and Alpha number comparison. This will be crucial to guarantee the method’s consistency.

<table>
<thead>
<tr>
<th></th>
<th>Time step</th>
<th>v/D relationship</th>
<th>Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFL condition</td>
<td>Higher</td>
<td>Higher</td>
<td>Primes when velocity is minor compared to diffusion.</td>
</tr>
<tr>
<td>Alpha number</td>
<td>Smaller</td>
<td>Smaller</td>
<td>Alpha primes when similar conditions, since and alpha usually has lower time step.</td>
</tr>
</tbody>
</table>

**Figure 9.** To obtain convergence there are two main requirements: consistency and stability.
- **Peclet number**

The Peclet number is a dimensionless number that relates the effectiveness of mass transport by advection to the effectiveness of mass transport by either dispersion of diffusion. In literature is easy to find up to 10 different Peclet numbers that are used in particular cases, leading to very diverse Peclet number values. Some studies often evaluate the different Peclet number definitions and estimate their ability to determine the relative importance of transport by advection and transport by diffusion (Huysmans and Dassargues, 2005).

Summarizing, the proportion on which advection and diffusion of a substance contribute to the transport equation is quantified in terms of Peclet’s number. Thus, if Peclet > 1 advection is more dominant than diffusion. Peclet number is obtained as shown in the following term:

\[
Peclet = \frac{v}{D} \times \Delta x
\]

### 4.6. **Numerical coding and simulation**

To perform the numerical simulation of shallow water’s oil transport the software MATLAB® 2013a was used. This high level–programming software is one of the most widely used tools across engineering departments worldwide. Its extensive demand relies on its interactive environment with hundreds of functions and programs written in similar programming languages, such as C, C++, Java, Fortran, and Python (EE Times, 2004).

MATLAB® allows analyzing data, algorithm development and models creation. There is no wonder why it has more than 1 million users – from backgrounds in engineering, sciences and economics – across the industry and academia (The MathWorks Inc, 2012).
5. Mathematical problem

To perform the simulation a model successfully developed in previous works and proven trustworthy in Prestige’s oil spill near Galicia’s coastal zone in 2002 was used. The model, developed after the spill, showed that its estimations fit with the real spill evolution when compared with satellite, mathematical, and historical data (Alavani et al., 2010; Gomez et al., 2015, 2011; Ivorra et al., 2015). The same model was also used to predict the Oleg Naydenov oil spill near Canary Islands in 2015, which currently is a research in progress by the University Complutense of Madrid’s Department of Applied Mathematics and its final results are not published yet (Benjamín Ivorra, personal communication, September 24th of 2015). It is based on a second order finite-volume approximation of an advection-diffusion-reaction equation, and has considered the motion of oil spots resulting from combined effects of diffusion and transport by wind and sea currents (Gomez et al., 2015).

Data used in this master’s work regarding the oil spill were assumed to verify and calibrate the parameters and the model in general, along with essays with known speed and wind currents. Then the simulation of a hypothetical oil spill was made with wind and currents data obtained from Colombian’s oil company OCENSA and Copernicus Marine Environment Monitoring Service (http://marine.copernicus.eu). Because of the good results shown in previous oil spills, it is expected the resulting model will also predict oil spills evolution reasonably well in this research.

5.1. Transport equation

As the final model is based on advection-diffusion-reaction equation (or transport equation), in order to write the entire code the starting point was one-dimensional pure advection equation [1], then adding a dispersion term [2], and completing it with a reaction and time parameters.

\[
\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} (v \star u) = 0
\]

[1]

Where:
- \( u \): concentration of a substance.
- \( t \): time.
- \( v \): substance velocity.
\[ \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( v \ast u - D \frac{\partial u}{\partial x} \right) = 0 \]  

[2]

Where:

D: diffusion coefficient.

Finally, adding a reaction term the equation is “completed”. It corresponds to one-dimensional advection-diffusion-reaction equation, also called “transport equation” [3]. Reaction effect generates loss of matter – which is really transformed by the mentioned mechanisms of weathering – altering contaminant’s concentration and making it more accurate to a real scenario.

\[ \frac{\partial u}{\partial t} - D \frac{\partial^2 u}{\partial x^2} + v \frac{\partial u}{\partial x} + q \ast u = f \]  

[3]

Where:

q: reaction coefficient.

A two-dimensional form of the transport equation will describe the variation of a substance concentration in time and space, taking into account the contribution of each earlier process [4] where constant coefficients have been considered.

\[ \frac{\partial u}{\partial t} - D_x \frac{\partial^2 u}{\partial x^2} - D_y \frac{\partial^2 u}{\partial y^2} + v_x \frac{\partial u}{\partial x} + v_y \frac{\partial u}{\partial y} + q \ast u = f \]  

[4]

Where:

Dx and Dy: diffusion coefficient in x-axis and y-axis respectively.

vx and vy: substance velocity in x-axis and y-axis respectively.

As for grid parameters, closed boundary conditions were used \((x_0=0 \ y_0=0 \text{ and } x_1=10 \ y_1=10)\), and the source contamination concentration was set to 1 (Dirichlet conditions).

This last equation [4] can be applied to any substance present in the water column, which can be characterized by its concentration and reacting processes that it can experience in the water. Many of those processes, which can include some toxic substances, may be approached by a first order kinetics (Sámano-Celorío, 2011).
5.2. Finite differences scheme
Starting from the transport equation, the objective is to seek for an algebraic expression that will describe the distribution of a substance in space and time.

Before running the simulation it is important to set the initial conditions, mainly when applying a time derivative. Subsequently, in this non-stationary scheme the substance’s concentration (in this case oil) will change along time. The same Dirichlet conditions that were applied to the transport equation were used for this scheme. An initial distribution function of concentration was assumed on 1.

5.2.1. 1D Finite differences scheme
Starting from the 1D transport equation [3], the next algebraic expression will describe the evolution of a substance’s concentration in 1D [5].

\[
\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} - D \frac{u_{i+1}^{n} - 2u_{i}^{n} + u_{i-1}^{n}}{\Delta x^2} + v \frac{u_{i}^{n} - u_{i-1}^{n}}{\Delta x} + q * u_{i}^{n} = f_{i}^{n+1}
\]

[5]

Where:
\( u_{i}^{n+1} \): Concentration of the substance in the next time step.
\( u_{i}^{n} \): Concentration of the substance in the present time step.

The equation above [5] is an upwind approximation. It works only if the velocity is positive. Thus, the information flux is considered from left to right. In order to take into account the different possible scenarios a simple modification is applied, so the scheme will work fine when velocities are negative. Furthermore a “centered” approximation is included, which will work fine if there is diffusion, but is unstable when no diffusion applied [5.1].

\[
\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} - D \frac{u_{i+1}^{n} - 2u_{i}^{n} + u_{i-1}^{n}}{\Delta x^2} + \rho v \frac{u_{i}^{n} - u_{i-1}^{n}}{\Delta x} + v(1 - \rho) \frac{u_{i+1}^{n} - u_{i}^{n}}{\Delta x} + q * u_{i}^{n} = f_{i}^{n+1}
\]

[5.1]

With \( \rho = \frac{\nu + |\nu|}{2|\nu|} \).

Then, solving [5] to find the substance concentration in the next time step will result as follows [5.1]:

Donaldo Augusto Juvinao Barrios
\[ u_i^{n+1} = u_i^n + D \frac{\Delta t}{\Delta x^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) - v \frac{\Delta t}{\Delta x} (u_i^n - u_{i-1}^n) + q * u_i^n * \Delta t + f_i^{n+1} \Delta t \]

\[ \text{[5.1]} \]

### 5.2.2. 2D Finite differences scheme

The 2D scheme is more elaborated than the 1D as it will be take into account both x and y axis for calculations. As showed in Figure 6 both velocities in x-axis and y-axis are positive. The algebraic expression that describes the evolution of a contaminant’s concentration in 2D is [6]:

\[
\begin{align*}
\frac{u_{ij}^{n+1} - u_{ij}^n}{\Delta t} - D_x \frac{u_{ij+1}^n - u_{ij-1}^n}{\Delta x^2} - D_y \frac{u_{ij+1}^n - 2u_{ij}^n + u_{ij-1}^n}{\Delta y^2} + v_x \frac{u_{ij}^n - u_{ij-1}^n}{\Delta x} + v_y \frac{u_{ij}^n - u_{ij}^{n-1}}{\Delta y} = f_{ij}^{n+1}
\end{align*}
\]

\[ \text{[6]} \]

Solving [6], the evolution of a substance’s concentration using a 2D finite differences scheme will be a the following equation [6.1]:

\[
\begin{align*}
&u_{ij}^{n+1} = u_{ij}^n + D_x \frac{\Delta t}{\Delta x^2} (u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n) + D_y \frac{\Delta t}{\Delta y^2} (u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n) \\
&- v_x \frac{\Delta t}{\Delta x^2} (u_{i,j}^n - u_{i-1,j}^n) - v_y \frac{\Delta t}{\Delta y^2} (u_{i,j}^n - u_{i,j-1}^n) + q_{ij}^n * u_{ij}^n * \Delta t + f_{ij}^{n+1} \Delta t
\end{align*}
\]

\[ \text{[6.1]} \]

### 5.3. Finite volume scheme

As mentioned before, although FDM and FVM are quite similar the latter one seeks for approximations to integral averages instead of algebraic expressions in each control volume. The same Dirichlet conditions used above were applied in this scheme as well. The equation that served as starting point to build a finite volume scheme was [7]:
$$\begin{aligned}
\text{PDE :} & \quad \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} + \frac{\partial g(u)}{\partial y} = 0 \\
\text{IC :} & \quad u(x, y, 0) = u^0(x, y) \\
\text{BCs :} & \quad u(a, t) = u(a(t)) \\
& \quad u(b, t) = u(b(t)) \\
\text{With :} & \quad f = v_x \ast u - D_x \frac{\partial u}{\partial x} \\
& \quad g = v_y \ast u - D_y \frac{\partial u}{\partial y}
\end{aligned}$$

Where PDE is the partial differential equation. The initial condition (IC) at time $t=0$, and BCs are the boundary conditions. The aim is to construct a FVM numerical method to solve it. As mentioned before the numerical solution of this problem requires the discretization of the domain in a finite number of volumes (CVs, also called cells).

### 5.3.1. Slope calculation

In order to obtain fluxes at cell interfaces, a reconstruction procedure is followed. In this work we have used piecewise linear reconstruction where slopes are chosen according to [7.1] and [7.2]:

$$\Delta_i = \begin{cases} 
\frac{u^n_{i,j} - u^n_{i-1,j}}{\Delta x} \equiv Sx1 \\
\frac{u^n_{i+1,j} - u^n_{i,j}}{\Delta x} \equiv Sx2
\end{cases}$$

[7.1]

$$\Delta_j = \begin{cases} 
\frac{u^n_{i,j} - u^n_{i,j-1}}{\Delta y} \equiv Sy1 \\
\frac{u^n_{i,j+1} - u^n_{i,j}}{\Delta y} \equiv Sy2
\end{cases}$$

[7.2]

Where Sx and Sy corresponds to the calculated slope in each axis. There are two for each axis since and the chosen slopes would be the smallest absolute values of $\Delta_i$ and $\Delta_j$ in order to attenuate the solution. This is also called an Essentially Non Oscillatory (ENO) scheme.
5.3.2. Physical and numerical fluxes

Each cell also has four boundaries (in 2D simulation) and to each one corresponds a numerical flux. Two kinds of fluxes were used in the simulation, the physical fluxes (in each face of the evaluated CV), and the numerical fluxes (taking into account the adjacent CVs).

a. Physical fluxes

The physical fluxes correspond to advective and diffusive ones. Physical fluxes are achieved by Fourier’s law – used when dealing with transfer of energy (e.g. heat) – or Fick’s Law – when working with mass transport –. In both cases, advective flux (AF) and diffusive flux (DF) are expressed as [7.3] and [7.4] shows:

\[ AF = v * u \]

\[ DF = -D \frac{\partial u}{\partial x} \]

b. Numerical fluxes

Numerical fluxes are introduced to obtain a unique value of the flux at each cell interface. Among the wide variety of fluxes that can be used we have opted for those defined in formulae [7.5], [7.6], and [7.7].

- Lax-Friedrichs flux [7.5]

\[ LF_{i+1/2} = \frac{1}{2} \left[ FC_{R(i)} + FC_{L(i+1)} + \frac{\Delta x}{2 * \Delta t} \left( u_{R(i)} - u_{L(i+1)} \right) \right] \]

With

\[ FC_{R(i)} = v(x_{i+1/2}) * u_{R(i)} \]
\[ FC_{L(i+1)} = v(x_{i+1/2}) * u_{R(i+1)} \]

[7.5.1]

Where:

- \( FC_{R(i)} \): Convective flux at the right side of the CV.
- \( FC_{L(i+1)} \): Convective flux at the left side of the nearby CV.
- \( u_{R(i)} \): Substance concentration at the right side of the CV.
- \( u_{L(i+1)} \): Substance concentration at the left side of the nearby CV.
• **Lax-Wenroff flux** [7.6]

\[
LW_{i+1/2} = \frac{1}{2} \left[ u_{R(i)} + u_{L(i+1)} + \frac{\Delta t}{2 \Delta x} FC_{R(i)} + FC_{L(i+1)} \right]
\]

\[
\downarrow
\]

\[
LW_{i+1/2} = v(x_{i+1/2}) * u_{R(i+1/2)}
\]

[7.6]

• **FORCE flux** [7.7]:

\[
FF_{i+1/2} = \frac{1}{2} \left[ LF_{i+1/2} + LW_{i+1/2} \right]
\]

[7.7]

### 5.3.3. Numerical scheme

In order to calculate the evolution of the concentration in the following time step, the code will compute the resulting concentration as the initial one at the next time step. The \(\Delta t\) has been chosen to ensure the numerical method’s stability. Integrating [7], the concentration in the next time step will be as follows [8]:

\[
\left\{ \begin{array}{l}
\frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial u}{\partial t} \, dx + \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial f(u)}{\partial x} \, dx = 0 \\
\frac{d}{dt} \left( \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} u \, dx \right) + \frac{1}{\Delta x} \left[ f(u_{i+1/2}) - f(u_{i-1/2}) \right] = 0 \\
\frac{d\bar{u}}{dt} + \frac{1}{\Delta x} \left[ f(u_{i+1/2}) - f(u_{i-1/2}) \right] = 0 \\
\frac{d\bar{u}}{dt}|_{t_i} \approx \frac{\bar{u}^{n+1} - \bar{u}^n}{\Delta t} \\
\frac{\bar{u}^{n+1} - \bar{u}^n}{\Delta t} + \frac{1}{\Delta x} \left[ f(u^n_{i+1/2}) - f(u^n_{i-1/2}) \right] = 0 \\
\bar{u}^{n+1} = \bar{u}^n - \frac{\Delta t}{\Delta x} \left[ f(u^n_{i+1/2}) - f(u^n_{i-1/2}) \right]
\end{array} \right.
\]

[8]

However, integration of [8] corresponds to 1D FVM. As for 2D FVM, the result will be [9]:

---

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\[
\bar{u}_{ij}^{n+1} = \bar{u}_{ij}^n - \frac{\Delta t}{\Delta x \Delta y} \left[ \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i+1/2}}^{x_{i-1/2}} \left( f(x_{i+1/2}, y, t^n) - f(x_{i-1/2}, y, t^n) \right) dy + \int_{x_{i-1/2}}^{x_{i+1/2}} \left( g(x, y_{j+1/2}, t^n) - g(x, y_{j-1/2}, t^n) \right) dx \right] \]

Where [9.1] is the cell average of \( u \) in the CV \((i,j)\).

\[
\bar{u}_{ij} = \frac{1}{\Delta x \Delta y} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} u \ dy \ dx
\]

### 5.4. Shallow water equations

After a FVM 2D scheme was done, a 1D Shallow Water Model (SWM) was developed. Shallow Water Equations (SWE) are derived from Navier-Stokes equations (which describe fluids motion by conservation of mass and momentum) and they are described in [10] and [11]. The independent variables are time \( (t) \), and a one-space coordinate \( (x) \). The dependent variables are the fluid height or depth \( (h) \), and the two-dimensional fluid velocity field \( (u \text{ and } v) \). With the proper choice of units, the conserved quantities are mass, which is proportional to \( h \), and momentum, which is proportional to \( uh \) and \( vh \). The force acting on the fluid is gravity, represented by the gravitational constant \( (g) \).

**Continuity equation**

\[
\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = 0
\]

**X-momentum equation**

\[
\frac{\partial q}{\partial t} + \frac{\partial}{\partial x} \left( \frac{q^2}{h} + \frac{gh^2}{2} - \frac{h}{\rho} \tau_{xx} \right) = -gh \frac{\partial Z_b}{\partial x} - \frac{\tau_{bx}}{\rho}
\]

Where:
- \( q \): \( x \)-component of specific flow.
- \( Z_b \): bottom elevation.
- \( \tau_{bx} \): bottom shear stress.
\( \rho \): density of fluid.
\( T_{ii} \): turbulent normal stresses.
\( T_{ij} \): turbulent shear stresses.

### 5.5. Model application

As mentioned before, the model used was developed by University Complutense of Madrid’s Applied Mathematics Department. Although the model has proven reliable, it has certain limitations:

1. The model is designed to consider low or moderate wind speed velocities (lower than 50 km h\(^{-1}\)). Thus, in case of storm there is no guarantee of validity of the model results.
2. This model does not take into account possible cleaning methods. Some models developed by Ivorra’s team include them (e.g. skimmer ships).
3. In most cases there is no exact data of amount of oil spilled in the sea, so the model will consider a coarse approximation.
4. Because the model’s objective is to forecast the oil spill, it is important to keep in mind that satellite images and data may not be available in real-time spill.

The model used to simulate the evolution of oil spots concentration, due to effects of the sea current, wind velocity fields and the pumping process during a time interval is given by [12].

The considerations of the model are the following:

1. The model is a 2D spatial computational domain (\( \Omega \)), and land domain is not included.
2. Two boundary conditions: one for the open sea and another one as a boundary in the coast.
3. The density of the pollutant spilled (oil) is smaller than sea water (remaining in the surface), and layer thickness (h) is considered to be constant. In fact, h depends on the color of the oil in the water.
4. Superficial contaminant concentration is denoted by \( u(x,t) \), measured as the amount of pollutant per surface area in the domain. The evolution of c is governed by a source of contaminant, taken as a circle of radius (R\(_s\)) that follows a trajectory (\( \zeta \)), and spills an amount of oil per unit of time (S(t)), by the diffusion effect of the pollutant, and by transport due wind and sea currents.
5. To avoid undesired diffusion effect, velocity of diffusion propagation is controlled using a nonlinear diffusion term. A BC with appropriate absorbing properties is included as well, in order to simulate the behavior of the computed solution near the boundary of the computational domain.

\[
\begin{aligned}
\frac{\partial u}{\partial t} - \nabla \cdot \left( \frac{u_k}{u_{k,\text{ref}}} \nabla u \right) + \nabla \cdot (u_w + \nabla \cdot u_s) &= \frac{S}{2\pi R_s} \chi B(\varsigma(t), R_s) & \text{in } \Omega \times (0, T) \\
\text{BC open sea: } L \frac{\partial u}{\partial t} + \left[ -(w + s + P_{\text{tol}})u + \frac{u_k}{u_{k,\text{ref}}} \nabla u \right] \cdot n &= 0 & \text{in } \partial \Omega_0 \times (0, T) \\
\text{BC coast: } \left( \frac{u_k}{u_{k,\text{ref}}} \nabla u \right) \cdot n &= 0 & \text{in } \partial \Omega_c \times (0, T) \\
\end{aligned}
\]

\[u(0) = u_0\]

[12]

Where:

\(u_k\): substance concentration (it will introduce non-linear diffusion, but will give a more realistic view of the phenomena).

\(u_{k,\text{ref}}\): referent pollutant concentration (here, \(u_{k,\text{ref}} = 1\)), and \(k > 0\) (typical values are 1, 2, and 3).

\(D\): diffusion coefficient.

\(w\): horizontal component of the wind velocities multiplied by a suitable drag factor.

\(s\): sea current velocity.

\(L = \sqrt{(x_{\text{max}} - x_{\text{min}})^2 + (y_{\text{max}} - y_{\text{min}})^2}\) is characteristic size of the domain (\(\Omega\)).

\(P_{\text{tol}}\): Related to pumping speed and does not apply in this work.
6. Numerical results

Several runs were conducted in 1D, 2D, and 3D geometries, in order to calibrate and evaluate each method’s stability. The transport equation developed at the beginning of the methodology was applied to finite differences scheme and finite volume method.

6.1. Finite Differences Method

We solve the advection-diffusion reaction equation in 1D using the finite differences method as described in section 5. Results are shown in Figure 10.

Figure 10. 1D finite differences method simulation.

Simulation results in 2D of transport equation when applying 0.005 diffusion coefficients (all simulations were made with this diffusion coefficient) for each axis showed clearly the contaminant’s dispersion over the grid. There is high concentration and no diffusion of oil in the starting spill point, but as time passes by it starts to spread until reaching equilibrium in the domain (homogenization) (Figure 11). It is important to note that at this situation only diffusion is taken into account, leaving out the advection movement and reaction.
When adding the advection and reaction term in both axes the simulation shows not only the diffusion but also oil slick’s movement and its reaction. Advection term is the sum of x-axis and y-axis vectors, and the movement will be determined by it. In this case the resulting vector (vx=1 and vy=1) caused the movement to be in northeast direction. On the other hand the reaction catalyzes contaminant’s depletion and in consequence less concentration over time, which can be attributed to weathering processes described above (Figure 12).

These results can be considered as valid ones, because the contaminant’s diffusion occurred as expected, with lower concentrations as time passes by. Advection movement was validated as well, since and the slick moved along the domain as anticipated. The results of the reaction term are harder to observe exactly, but since and lower concentrations were observed when it was introduced, it is possible to say that behaved as estimated.

Figure 11. 2D simulation with diffusion coefficient, showing homogenization of the spill.
Figure 12. Adding an advection term, the spill will also move while spreading.

Figure 13. 3D simulation with diffusion and advection coefficients.
6.2. Finite Volume Method

In this section we solve pure advection 1D by the finite volume method. In Figure 14 a Courant number equal to one has been taken, therefore no numerical diffusion appears.

![Figure 14. 1D simulation with advection coefficient only.](image)

Regarding advection plus diffusion 1D scheme, the method shows consistency since and the concentration of the oil starts diminishing – which means that spreads – and the slick moves along the domain simultaneously. Advective movement and spreading are uniform and demonstrate reliability during the simulation, which represent properly the expected oil movement and dispersion during a spill (Figure 15).

![Figure 14. 1D simulation with advection coefficient only.](image)

As for 2D advective movement the velocities vx and vy were set to 1 and the simulations illustrate the anticipated movement of the spill – just like the 1D scheme – which provides reasonable results and postulates a good structure for the further simulations in this work (Figure 16). For 2D and 3D advection-diffusion ones, the velocities were vx and vy -1, in order to test the simulation. Results showed that the slick moves in the southwest direction, concordant with the expected ones (Figure 17; Figure 18).
Figure 15. FVM 1D simulation with diffusion and advection coefficients. Oil concentration will be reduced and move through the domain as time passes by.

Figure 16. FVM 2D advective simulation.
Figure 17. FVM 2D simulation with diffusion and advection, showing the movement of the spill as it spreads.

Figure 18. FVM 3D simulation with diffusion and advection coefficients.
FVM were originally invented to solve hyperbolic problems but they are actually used to solve any kind of problems, and the results obtained from applying this method shows an accurately representation of a real spill. In general, the numerical experiments carried out in this section in two-dimensional and three-dimensional test cases demonstrate the accuracy, computational efficiency, and overall stability of the method.

6.3. 1D Shallow water

As for 1D shallow water model, the equations were solved using the Lax-Friedrichs and Lax-Wendroff schemes. 1D shallow waters works well with dam breaks problem, in which the vertical velocity is neglected and horizontal velocity is assumed constant. The model’s validity can be done by simulating a hypothetical dam break, in which some assumptions are made: 1) initial height (at the left of the dam is 1, and at the right of it is 0.1) and flow velocity is known (in this case was constant); 2) the dam fails instantaneously and completely; 3) there is no friction; and 4) the horizontal advection term is much more wider than the vertical one.

To validate the results there are exact solutions to a dam break problem. The results are considered valid because the resulting model behaves similarly to the exact solution given found in literature (Toro, 2001). The difference between them relies on numerical diffusion mainly, and artificial viscosity, which attenuates the curves of the results making an approximation to the exact solution (Figure 19).
**Figure 19.** Comparison between the exact solution and the resulting 1D shallow water model.
6.4. **Validation of results**

To evaluate the model’s performance, it is important to apply known conditions so the model will work as expected. The simulation was performed with controlled velocities and directions of the oil spill. The domain was divided in 10 CVs with the following conditions: while the oil spill was between a [4-6] range in the domain the velocities in both axis were vx=1 and vy=1, meaning that the spill should move in the northeast direction. When the spill moves and leaves that range the velocities would change to vx=-1 and vy=-1, implying that the spill should change its trajectory and move in the southeast direction.

![Simulation images](image)

**Figure 20.** Oil spill simulations with known conditions, in this case the advective term, which will serve as a validation method for the model.

The simulation results show that when applying different known conditions the spill moves as expected, meaning that there is a positive relationship between the projected movement and behavior of the oil spill with what really happens.

Still, the current model has been validated and published with other oil spills in Spain, including the Prestige’s oil spill (2002) and most recently the Oleg Naydenov oil spill.
Also the model was used to simulate the evolution of oil spots in open sea and the effect of a skimmer ship pumping oil out of the spots.

### 6.5. Simulation of an oil spill

The resulting model was used to predict the fate of a hypothetical oil spill caused by a marine pipeline rupture at the marine terminal of Coveñas, located in Morrosquillo Gulf, Colombia.

#### Figure 21. Location of the proposed zone to make an oil spill simulation. Morrosquillo Gulf is the primary oil export terminal in Colombia.

This location was selected because it is main oil-export area in Colombia. 96% of total exported Colombian oil is through Coveñas marine terminal (total oil production is around 1 million barrels per day) (ElMeridianoDeCordoba, 2014; Portafolio.co, 2015). In the coastal zone there are 3 TLUs (Tanker Loading Unit) with a storage capacity of more than 7 million barrels, and are operated by 3 companies: the national and largest oil company Ecopetrol S.A, and the private ones Oleoducto de Colombia (ODC), and Oleoducto Central S.A (OCENSA). For instance, a single TLU can load up 40000 barrels per hour and can receive up to 15 oil tankers per month. Due to increasing oil
production and demand a 4th pipeline, Oleoducto Bicentenario, is under construction. This new 970 km pipeline will have transport capacity of 450000 barrels/day, and a new TLU will be needed for its operation (UPME, 2013).

Because of the increasing oil activity in the zone and the probability of oil leaks, accidents, and discharges during loading/unloading operations this location appears to be ideal to evaluate and validate the resulting model.

![Red de principales oleoductos de Colombia](image)

**Figure 22.** Main pipelines for oil transport across Colombia. There is a new pipeline under construction, which eventually will rise the amount of transported oil through the coastal zone (Copyright: Oleoducto Central – OCENSA (2015)).

Using the model written and taking into account the considerations mentioned before, a final simulation was made using marine data from December 1st 2015 to December 31st 2015 in order to evaluate the fate of an oil spill in said gulf.

The results of the simulation shows that and hypothetical oil spill will spread and be dispersed for about 150 km along the whole south Caribbean basin, and eventually will affect some coastal zones at the southwest and close to Panama-Colombia borderline. However it is important to remark that the method used normally introduces some numerical diffusion, meaning that dispersion and extent of the oil spill could be overestimated.
Figure 23. Simulation results of a hypothetical oil spill in the southwest Caribbean basin. The spill’s movement is mainly affected by the wind and sea current regime at the time of the simulation.

Nevertheless the simulation shows rational results due to the wind and currents regime over the zone. Sea currents in the gulf are subjected to seasonal changes of winds in the Caribbean Sea and area morphology. During the “dry season” – which goes from December to April – strong trade winds from the northeast dominate (up to 42 km/h), conducting to a unique current stream that goes along the whole Colombian’s Caribbean coast from northeast to southwest. As the simulation was made with marine data corresponding to dry season, it is expected the oil spill to move by advection to the southwest (INVEMAR, 2002). This is exactly what the simulations results show: an oil spill moving by advection to the southwest. The oil spill then is projected to move differently during the “wet season”.

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7. Conclusions

- This master’s work presents a mathematical model for oil spill movement simulation in marine environment, taking into account diffusion, and the source of contamination. It reproduces well the movement of an oil spill as shown by the simulations carried out.

- The code written is reliable and can be used for oil spill simulations not only in coastal zones but also in open sea simulations.

- To verify its real performance it should be compared with a real spill scenario. However the equations and the numerical model applied suggests that the exposed model is a trustworthy one.
8. Recommendations

The following recommendations are suggested for related and further research in this particular work and in general numerical simulation field in coastal and marine zones.

- Most of spilled oil will keep to the water surface, but some of it will sink. Therefore it is important to take into account not only the ocean surface (2D) but also is imperative to evaluate the spill along the water column, specially when water currents will transport it back to surface by upwelling, thus is recommended for further works to make a 3D simulation.

- An Adaptive Mesh Refinement (AMR) is recommended as it implementation will adapt the accuracy of the solution in certain nodes of the grid, so simulations in the critical area would be more exact, and the real spill evolution more accurate.

- To adjust and delimitate the coastal zone better, it is recommended to do a mesh refinement at the coastal zone particularly, such as triangles shapes that will provide a better simulation of the oil spill when contacting the coast.

- Oil spill risk assessments are considered essential to assess danger for human health and ecosystems, so it is recommended for further research their application to complement oil spill simulation as they have been implemented in some studies.
9. References


ElMeridianoDeCordoba, 2014. Por Coveñas sale el petróleo colombiano.


