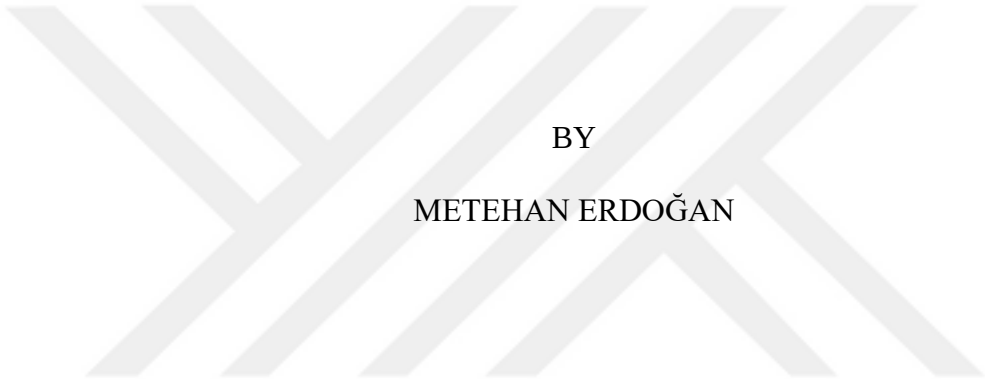


OIL SPILL SURFACE FATE MODEL THROUGH RANDOM WALK METHOD
WITH DRIFTED PARTICLES IN VORONOI DIAGRAM

A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
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METEHAN ERDOĞAN

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Approval of the thesis:

**OIL SPILL SURFACE FATE MODEL THROUGH RANDOM WALK
METHOD WITH DRIFTED PARTICLES IN VORONOI DIAGRAM**

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ABSTRACT

OIL SPILL SURFACE FATE MODEL THROUGH RANDOM WALK METHOD WITH DRIFTED PARTICLES IN VORONOI DIAGRAM

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Oil spilling is a hazardous case to the marine environment by increasing the risk of the destruction continually by flowing on the sea, expanding into sea and mixing into the air. Its potential threats can be prevented after the determination of its pathway. So, knowing the extent of oil contaminated sea as accurately as possible helps to decide the clean-up techniques like using skimmer, boom or dispersants and efficiently perform one of them. A well-defined models with the true reflection of the mechanisms behind the oil fate and transport can supply the oil extent to a great degree. Our main motivation in the study is to approach the oil surface processes with care and to numerically obtain the result from their equations in a good precision for instantaneously and continuously spilled oils. So, a numerical solution for oil spreading is provided by an algorithm already written and updated in this study. It is compared for many scenarios with an analytical solution, an experiment and another numerical solution applying finite element method. The numerical approach in the algorithm uses Nihoul's equation with the Gaussian random walk technique stepping the particles with a diffusive length for the spreading treated like diffusion. The oil surface contamination is demonstrated by Voronoi diagram. Also, the particles are drifted with a velocity of 3% wind speed for the advection in the algorithm.

The flexibility of the algorithm are checked through the slick parameters in this study. Besides, detailed analyzes on the slick shape, oil distribution on the surface and the contribution of the spreading regimes are carried out through the algorithm tried on the prescribed cases. Finally, the algorithm is evaluated with a software embodying the solution to the main oil spreading processes and proposing the clean-up techniques. This study will be evolved by the addition of dispersion, evaporation and other processes expanding the algorithm to three dimensional model in the future.

Keywords: Oil Spreading, Advection, Numerical Modeling, Voronoi Diagram, Random Walk Method

ÖZ

PETROL SIZINTISININ YÜZEYDEKİ AKİBETİNİN RASTGELE YÜRÜYÜŞ METHODU ARACILIĞIYLA PARÇACIKLARIN TAŞINMASIYLA BERABER VORONOİ DİYAGRAMI İÇİNDE MODELİ

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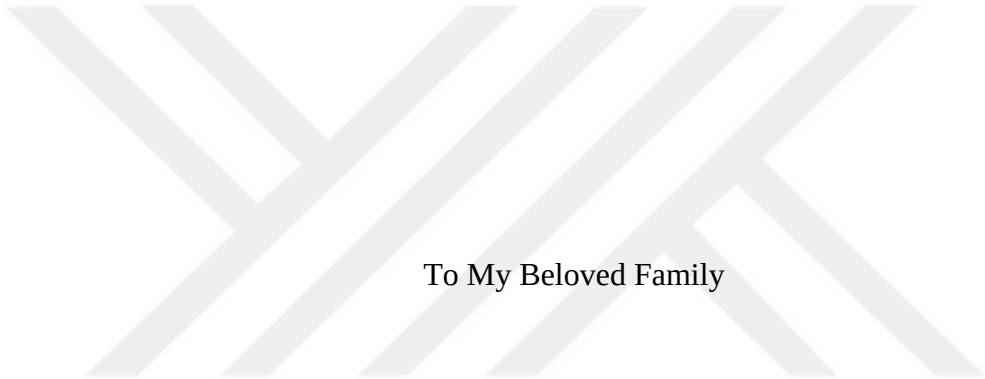
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Petrol sızıntısı deniz yüzeyinde yayılımıyla, denizin içine dağılmasıyla ve havaya karışmasıyla tahribat riskini sürekli arttıran deniz ortamına zararlı bir olaydır. Onun potansiyel tehditleri petrolün gidebileceği yerleri belirlemekle engellenebilir. Bu yüzden de petrol kirliliğinin denizde ulaşacağı boyutları mümkün olduğunca doğru bilebilmek hangi temizleme tekniğinin kullanılacağına karar vermede (bunlar sıyırıcı, muhafaza bomu veya dispersan kullanımı olabilir) ve onun etkili şekilde uygulanmasında yardımcı olacaktır. Petrolün akıbetinin ve taşınmasının ardındaki mekanizmaların doğru şekilde aktarılmasıyla beraber iyi tanımlanmış modeller bunu büyük bir oranda sağlayacaktır. Bizim de bu çalışmadaki temel motivasyonumuz, yüzeydeki petrolün süreçlerine dikkatle yaklaşmak ve onların denklemlerinden anlık ve sürekli sızıntıyla devam eden petroller için numerik bir şekilde yüksek oranda yakın sonuçlar elde etmektir. Bu doğrultuda petrol yüzey yayılımı için numerik bir çözüm, önceden hazırlanmış olan ve bu çalışmada da güncellenen bir algoritma tarafından temin edilir. Bu çözüm bir sürü senaryoda analitik bir çözümle, bir tane deneyle ve sonlu elemanlar yöntemini uygulanan bir numerik çözümle kıyaslanır. Algoritmadaki numerik yaklaşım, petrolün difüzyona benzeyen su yüzeyinde

yayılımı için Nihoul'un denklemini, parçacıkları nüfuz ettirici uzunluk ile hareket ettiren bir Gauss rastgele yürüyüş yöntemiyle beraber kullanır. Bu yüzey petrol kirliliği de Voronoi diyagramı tarafından gösterilir. Ayrıca petrolün yüzeydeki sürüklenmesi de parçacıkları rüzgar hızının %3ü bir hızla sürüklemesiyle olur.

Bu çalışmada algoritmanın esnekliği, petrol kirliliği parametreleri aracılığıyla kontrol edilir. Aynı zamanda kirliliğin yüzeydeki şekli, dağılımı ve yayılma rejimlerinin katkıları üzerine detaylı analizler algoritma aracılığıyla önceden hazırlanmış durumların denenmesiyle yapılır. Son olarak algoritma petrolün geçtiği önemli süreçleri barındıran ve onlara temizleme tekniklerini öneren bir yazılımla beraber değerlendirilir. Bu çalışmanın içeriği gelecekte algoritmanın petrolün denizin içine yayılımının, buharlaşmasının ve diğer olayların dahil edilmesiyle 3-D'ye genişletilmesiyle geliştirilecek.

Anahtar Kelimeler: Petrolün Yüzeyde Yayılımı, Petrolün Yüzeyde Taşınması, Numerik Modelleme, Voronoi Diyagramı, Rastgele Yürüyüş Yöntemi



To My Beloved Family

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LIST OF SYMBOLS

SYMBOLS

A_{slick}	slick area, m ²
$C(x)$	Concentration of a point along x axis, mol/cm ³
$D, D(h)$	diffusion coefficient, cm ² /sec
D_L	diffusive length (m)
$E(x)$	mean value of displacement of x
$E(x^2)$	mean value of square displacement
G	length along major axis of ellipse,m
g	gravitational acceleration, m/s ²
h	slick thickness, m
h_{max}	maximum slick thickness (m)
h_{mean}	mean slick thickness (m)
J	number of molecules passing from the unit area per second, mol/cm ² /sec
k	drag coefficient, kg/m ² s
L	length along minor axis of ellipse,m
l	step length
N	total step number
p	probability to move through one chosen direction
R	slick radius at time t (m)
r	radial distance from the center (m)
RN_i'	a normally distributed random number with mean and variance (dimensionless)

Q	term representing gain or loss of oil (m/s)
q	probability to move through the other reverse direction
t	time, sec
$t_{\min}$	time, min
$U_{advection}$	Advection velocity, m/s
U_{avg}	Average slick velocity, m/s
$U_{current}$	Current velocity, m/s
V	initial spill volume, m ³
W	wind speed, knots
x_i^n, y_i^n	current coordinates of i th particle at time t (m)
x_i^{n+1}, y_i^{n+1}	new coordinates of i th particle at next time step (m)
γ	surface tension difference, kg/s ²
$\gamma_{wa}, \gamma_{oa}^\circ$ and γ_{ow}°	water-air and, oil surface tensions-air and oil-water interfacial tensions, kg/s ²
λ, β	empirical constants for diffusive length (dimensionless)
ρ	oil density, kg/m ³
ρ_w	water density, kg/m ³
σ	variance of a probability distribution
τ_a	surface wind stress, kg/ms ²
ψ	function of surface tension variation from center to edges of the slick (dimensionless)
$\langle n \rangle$	mean value of steps to the reference direction

CHAPTER 1

INTRODUCTION

An oil spill is generally the leakage of liquid hydrocarbons from drilled wells and transportation systems like tankers and pipelines due to the blowouts, accidents, damages, etc. Although the term oil spill refers in general to leakages in both offshore and onshore locations, it is the term used mostly for the oil pollution in the offshore. As many of oil spills accidentally occurs, it is also possible to have the release of oil into the seawater on purpose. Controllable disposal of oil based mud used during drilling a well can be an example for oil spills deliberately. Nevertheless, the governments take actions about it by forbidding the usage of oil based muds in some countries and regulating the oil disposal into the specified areas.

Oil spill causes water pollution, harms to the living organisms in the sea and ruins the marine environment. When oil contamination is at high level in benthic environments, many of organisms like fishes, clams, limpets, periwinkles etc. die according to the investigations of seven spills by Teal & Howarth (1984). Even though the certain number of deaths is not known due to the possible migration of some organisms or the exact number of them not known before spilling, the study indicates that oil spills disturb the habitable zones with their toxicity in the sea. The egg and larvae survival is reduced leading to birth defects of some benthos, reducing reproduction success of fishes and planktons. Sensitive animals to oil like younger ones can easily disappear in oil contaminated seas. Oil slows down the evolution of the creatures in the sea, hinders the ability to move and rots the fish fins in the long-term. (Teal &Howarth, 1984)

Since oil spill is such a dangerous occurrence to the sea life, understanding of oil spill behavior, determining where the spilled oil goes and investigating which

dynamics and forces affect have become an important issue to explore since forty-five years. Its popularity has risen among researchers and governments in the last decades. They have paid attention for the marine transportation of oil and offshore oil wells. However, model-real case comparisons show that oil spill has been still not thoroughly explained because some oil properties, environmental conditions and oil-water dynamics are not considered or some assumptions which are made to approximate the models causes the inaccurate estimation of oil spill extent. (Brönner, 2018) Therefore, the researches should continue to observe the effects of the related parameters on the spill. More sophisticated models by the integration of findings from the investigations should be worked on to provide more realistic anticipation of fate and transport processes of oil.

Oil after spilling, experiences many processes which shape its fate on, below and above the surface of seawater. These processes are evaporation, dissolution and emulsification which weathers the some percentage of oil and changes the oil properties; turbulent diffusion, shear, buoyancy and breaking waves which disperses and mixes some of it into water; winds, currents and waves which transports remaining one on the surface; and gravity, inertia, viscous and surface tension forces which give rise to horizontal spreading of it. (Guo, 2009)

The horizontal movement of oil includes the advection with wind and current and expansion of oil spontaneously (spreading). If the hydrodynamic forces were not present, oil would spread by forming the circular shape. However, it is not a realistic case. Wind and current which are active on the sea orient the transportation of surface slick in the direction of these turbulences. Early methods such as the method introduced by Fay (1969) have not accounted the advection process. The advanced models have been modified to include advection by wind and current velocity and to revise the effects of oil dynamics on the spreading. In some models, horizontal movement of the spill is still independent of wind, current and wave only to simplify the models and examine the spill movement without external forces. Modeling the oil fate on the sea is an essential effort because knowing the extent of the spill with its thickness and area helps to take precautions for sea life and to prepare cleaning

methods before it devastates the marine life. In addition to them, if the area and thickness are precisely known, other processes like evaporation, entrainment and dissolution can be estimated precisely since oil lost through these processes are dependent on the thickness and area of the surface slick. The most erroneous estimation is faced during evaporative loss calculations with inaccurate thickness and area information, whereas dissolution is not highly dependent on them. (Berry et al., 2012)

In this study, an algorithm is developed to model oil spreading based on the data of continuous release experiment conducted by Brönner (2018). Actually, we presented our algorithm for instantaneous releases in Durgut et al. paper (2020). The algorithm uses the Gaussian random walk method representing the slick shape by Voronoi diagram which can be drawn through an available code written in C++. (Durgut & Reed, 2017 and 2020) In the algorithm, the spreading is treated like diffusion. This algorithm will be shown, discussed by the analytical solution and parametric analyzes. It will be finally expanded for continuous releases. To offer an algorithm for continuous releases, the algorithm created by Durgut (2020) for the instantaneous spill will be converted into a usable one for a continuous discharge through the guidance of COMSOL. COMSOL will be the intermediary model to ensure for our algorithm working well. It will accompany the algorithm for every scenarios of continuous releases. After transformation of it to a suitable algorithm for the continuous spills, advection processes under the impacts of wind and current will be added to see it on the surface more realistically.

CHAPTER 2

LITERATURE REVIEW AND THEORY

2.1 Oil Spill Types in Offshore

An oil spill can be categorized by two factors that are release type and release location. So, it can be instantaneous or continuous and surface or subsurface on the basis of them. These types of spills changing the fate of oil are differently handled. The different aspects of interactions between sea and oil due to the discharge conditions push to classify the spills in such ways especially for advection and spreading.

2.1.1 Continuous and Instantaneous Releases

The continuous release means that oil is discharged at a rate from a source for a certain period of time. The instantaneous release is the pouring of oil at a single time step with a random profile. (Brandeis, 1983) The instantaneous discharge only eases to treat the surface slick problems but it is not generally seen in the real world. So, idealization of continuous cases into instantaneous ones helps to find a solution in a quick way which is expected from the mathematical models for the combat actions. Also, validity of this assumption will be discussed in the Result and Discussion session. However, when the purpose is not to simplify the case, the terms of instantaneous and continuous releases can be interchangeably used for the massive slick at the beginning and continuing release at a very low rate because it does not change the distribution of oil in the large proportions. Another real example of instantaneous release is that oil spreading is tracked after the release ends.

2.1.2 Surface and Subsurface Releases

The surface release is the leakage of oil from the surface systems containing the oil sources such as the damaged tankers. This type of discharge was traditionally paid attention since it is more commonly encountered type. Many researches were conducted in this way. More empirical and numerical methods are available for the surface releases. On the other hand, a subsurface spill occurs when an accident at the subsurface system emerges like the damage of pipeline and blowout of wells. During the subsurface spill, gravity regime which is the critical stage of surface spill for spreading is not so effective. It gives place to other mechanisms like buoyancy flux to the surface. Besides, spill can be assumed to be surface release for oil leakages from the shallow waters. (Reed et al., 1999)

After the explanation of spill types, the processes which spill is exposed to are discussed to perceive how oil is transferred to the air, into the water and moves horizontally on the sea.

2.2 Deciding Processes to Oil Fate

The processes which oil spill undergoes can be classified as three groups. These are chemical, physical and biological processes. Almost all of them can be seen in Figure 2.1.

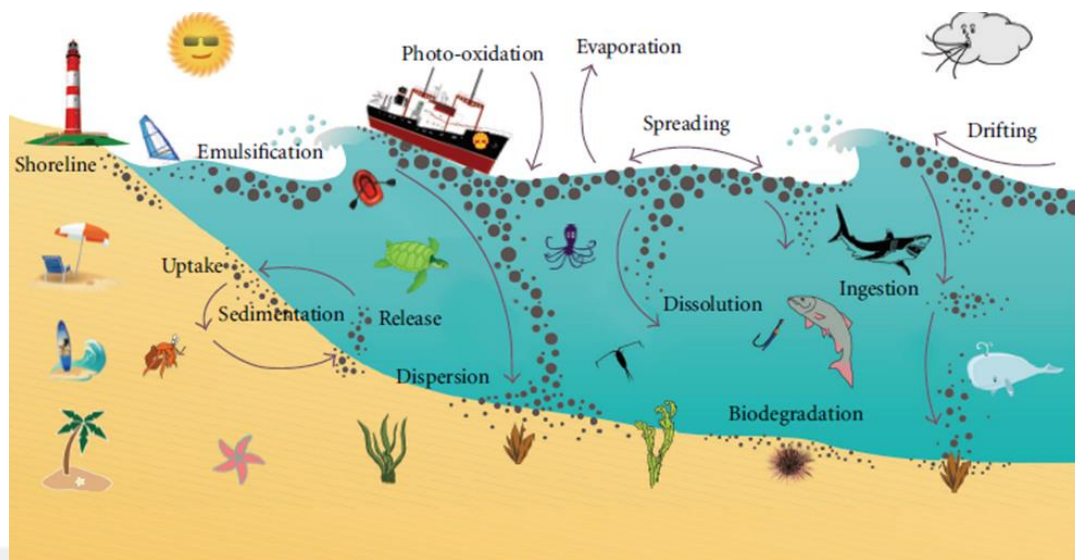


Figure 2.1: The processes oil spill undergoes (Zadeh, 2012)

2.2.1 Chemical Processes

Chemical processes are related to mass loss and change of oil properties. Oil can be weathered by the evaporation lost to the air, by the encapsulation of water molecules into the oil i.e. emulsification and by the dissolution of oil into the water. (Guo, 2009) The minor chemical processes like volatilization, chemical sedimentation and partitioning (McCay, 2004) have not explained in this work.

2.2.1.1 Evaporation

Evaporation take places in the beginning of the spill which affects the early fate of oil on the seawater. It starts with the transformation of most volatile elements in liquid phase into the gas phase and makes the surface slick heavier than before. It changes oil properties like viscosity, density and mass. Viscosity and density of surface slick increases while mass decreases due to the escape of light compounds (Fingas, 1995). National Research Council (2003) referred in Zanier (2014) has put forth that three quarters of the light oils is lost in the beginning of spilling whereas one tenth of heavy oils is lost during the early phase of spills. (Zanier, 2014) This

fact points out that heavy oils with non-volatile compounds almost maintains their properties and behavior on the sea.

Since oil can be heavy mixtures of hydrocarbons, it is characterized as pseudo-components that are used to define the boiling point and density of the heavy elements together hypothetically. Oil molecular weight is predicted as a function of these properties during modeling the evaporation in the high range of oil compounds. Therefore, the input parameters for evaporation algorithms are molar volumes, vapor pressures and molecular weights of each components forming the compound separately. With improvements, diffusivity becomes another input parameter. The number of components is increased to strengthen the identification of oil compounds in the recent models. Fingas (2011) has introduced an empirical method where oil can evaporate as a function of the time and ambient temperature while evaporation rates in previous approaches are function of slick coverage and thickness, wind speed and turbulent movements which are weakly related to evaporation according to him. However, Fingas method also contains some deficiencies like requiring rearrangements of it for different oil compositions, high dependence on the experimental conditions, etc. (Spaulding, 2017). Therefore, it needs to be paid attention for improvement of empirical methods.

2.2.1.2 Emulsification

Emulsification occurs when the sea is wavy by the strong winds and/or currents. Water in oil emulsions are commonly seen on the sea. The emulsion enlarges the surface slick up to five times greater than the actual volume. Also, oil becomes denser, heavier and more resistance to flow by the encapsulation of water within oil. So, the oil acts in a different manner during other processes as a result the emulsification. For example, the spreading of it is retarded with the low fluidity and higher density while it is accelerated by volume increase on the surface. However, in total, emulsified oil spreads more slowly. In addition, evaporation rate of oil with high water content reduces. Limitation of the emulsification on the oil evaporation

is formulated as a function of water content by Lehr (1994). It also complicates the combat actions against the spills having denser and more viscous characteristics on the sea (Xie, 2007) (Mishra, 2015)

For emulsification modeling, Mackay's (1982) numerical method has dominated the area for years. It had been modified slightly during the time. However, with the recent work of Fingas (2011), more advanced method whose stability index with a variety of oil properties is a measure of emulsion stability has been proposed (Spaulding, 2017).

2.2.1.3 Dissolution

Dissolution is the loss of soluble molecules of oil in the sea. These molecules are generally evaporative parts of oil. Since evaporation starts and finishes earlier than the dissolution, generally these molecules escape to the atmosphere without having enough time to dissolve inside water. However, the dissolution is hugely influential for the soluble components of subsurface slick since these molecules do not have any contact areas with the air to initiate the evaporation. Dissolution rate depends on the size of oil droplets under the sea. Finer oil droplets having greater ratio of contact area to volume exposes to the dissolution more. (Mccay, 2004)

The dissolution has been numerically schemed based on the ambient temperature and the solubility of oil by Mackay and Leionen (1977) whose model is still valid (Spaulding, 2017).

2.2.2 Physical Processes

Physical processes are ones which enlarge the spill extent by water-oil interactions, the effect of wind and current, the effect of turbulent diffusion, breaking waves, shear and buoyancy resulting in spreading, advection, vertical dispersion and mixing

respectively. Some physical processes like physical sedimentation, oil-shoreline interactions, etc. have not been touched upon in this work.

2.2.2.1 Advection

Advection is the drag of spill from one region to another by the turbulences on the sea. It is responsible for the progress of spill to the directions of current and wind significantly. The spill also moves to the other sides due to spreading forces horizontally. Therefore, the spreading and advection cooperate for horizontal movement of the spill. Strong wind and currents make the advection more pronounced and causes to deformation of slick shape on the sea. If the directions of turbulences especially wind direction changes, slick extends by tracing their path. In addition, Langmuir circulation due to surface turbulences can complicate the modeling of the surface slick where the slick deformation is severe. Oil is broken into the separate molecules that can expand in the distinct columns of streaks to the downwind. For the oil separation, the flow of adjacent Langmuir cells in the opposite directions should overcome the surface tensional interactions between sea and oil molecules (Debra Simecek-Beatty- 2017). So, hydrodynamic data should be continually monitored and recorded from the beginning of spilling until the clean-up to have the horizontal fate of slick realistically in the computational environment.

2.2.2.2 Spreading

The spreading of the slick is the horizontal propagation of the oil on the sea due to the mechanical forces which are inertia, gravity, viscosity and surface tension. The spreading exists in three stages that are (1) inertia-gravity, (2) gravity-viscous and (3) surface tension-viscous regimes under the interactions of two of the given forces. These two forces counteract to each other for the spreading. One force from gravity and surface tension promotes the spreading whereas the inertia or viscosity retards

it. (Chebbi, 2014) However, the remaining forces was or will be active during the other regimes.

In the first few minutes of the spill, inertial force works against the gravity in the spreading of gravity-inertial regime. Oil tends to go downward with the gravitational effect accelerating the oil spreading. On the other hand, inertia of oil tries to conserve the existing state of oil, so inertial force resists to spreading which changes the oil velocity at the moment of release. Since it is effective at the beginning corresponding to the spreading controlled by accident conditions like rate of leakage, velocity of oil molecules and spill position, gravity-inertia regime is not easily recognized. After a few minutes to almost one week, spreading is driven by the gravity-viscous phase in which viscous boundary layer between oil and water decelerates the oil spreading. (except for massive and very small spills) (Al Rabeh, 1989). Afterward, surface tension-viscous spreading takes place when the thin layer of oil covers the sea, which diminishes gravitational effect. It lasts until the end of spreading. Surface tension is the surface free energy to spread. Figure 2.2 shows the effects of regime forces separately on spilled oil.

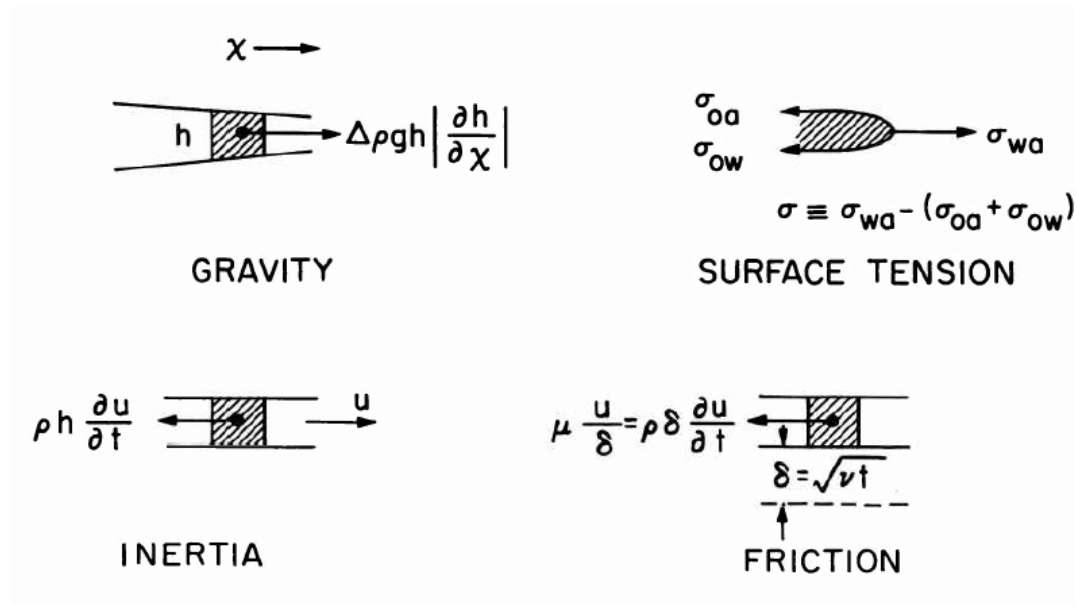


Figure 2.2: Forces of Oil Spreading Developing the Regimes (Fay, 1971)

The duration of influences of these forces can be seen for different spill volumes from Figure 2.3. Many models omit gravity inertial regime effective for a short period of time and surface tension regime governing the spreading in the long term. Generally, spreading continues at the gravity viscous regime before the cleaning-up the spill. However, small spills can undergo surface tension viscous regime in 1 day. Even they can spread only with surface tension regime. Modeling gravity and surface tension regimes together will eliminate the underestimation of slick area when the oil actually spreads in surface tension viscous regime.

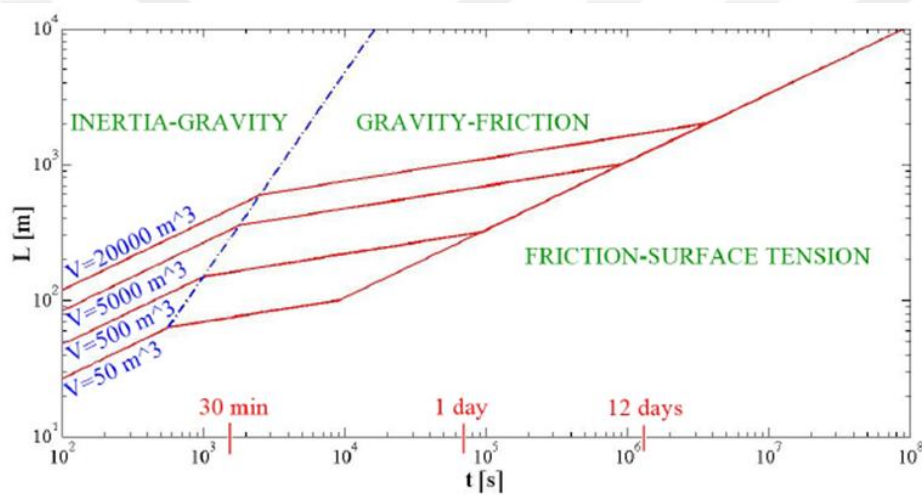


Figure 2.3: The spreading behavior in the regimes with the changing initial volume (Zanier 2014)

Fay (1969) has explained the dynamics of spreading on calm seawater, but the method with prescribed equations has been proven to be insufficient to accurately define it. Therefore, some modifications have been conducted onto this approach with the same descriptions about the spreading divided into three regimes with the given forces above.

Slick thickness and radius are the key objectives when methodizing and modeling the spreading process. Therefore, the accuracy of spreading methods and models is evaluated with respect to these parameters. The evolution of the spreading techniques will be discussed later in more detail.

2.2.2.3 Dispersion (Vertical Entrainment of Oil)

The dispersion of the oil means some oil droplets are separated from the oil body by turbulent actions and are pulled into the seawater. The main parameter that determines whether the oil droplets will be entrained in the water or not is the oil droplet size. If the droplets are large enough to escape from the water, they will be temporarily kept inside the water and immediately resurfaced. If the droplets are tiny, they will be permanently entrained by sea. The oil droplet whose size is lower than 20 nanometers stays in the sea while the size of oil droplet which has a tendency to rise is higher than 50 nanometers. (Fingas, 2015)

The dispersion depends on the droplet size, oil properties, sea conditions and slick thickness on the surface. For example, the breaking waves as a parameter of sea conditions partition the oil into the droplets and accelerate the entrainment of them. In another example, the rate of dispersion for the slick forming a thin layer, flowing with low viscosity and having lower interfacial tension with water is greater than it when the thick layer of slick is more viscous and creates higher adhesive forces with water molecules (Reed et al., 1999).

By considering the total duration of transportation of spill, what happens to the dispersed oil cannot be estimated accurately. Some fraction can be mixed into the sediments and precipitated to bottom. The other one can rise and tails the surface oil while remaining one can undergo into biological degradation by living organisms. (Fingas, 2015)

A popular and comprehensive method for oil dispersion had been claimed by Delvigne & Sweeney (1988). This empirical method has replaced the theoretical approach of Mackay (1980). (Spaulding, 2017)

2.2.3 Biological Processes

The living organisms under the sea decay some of dispersed oil through the biological activities. The decaying process is named as biodegradation. Photo-oxidation is also biochemical process decomposing the surface oil slowly by the sun light in the presence of oxygen. The oil properties are altered by these occurrences. Their effect on the oil fate is minor in most cases. (Shen, 1993) Also, it is difficult to model biological processes of oil since its severity cannot be known for every oil spill case.

As a conclusion, chemical, physical and biological processes interact with each other. All of them has direct/indirect and major/minor effects on themselves, deciding the fate of oil spill by affecting each other.

2.3 The Historical Evolution of Methods for Oil Surface Fate

Oil surface fate with “oil spreading” and “advection” phenomena has been discussed since 1969 when Fay has introduced a method which is milestone for spreading. In this section, the evolution of oil surface fate methods from the beginning has been explained by taking their contributions into consideration.

2.3.1 Fay’s Method (1969, 1971)

As mentioned in previous sections, Fay (1969) has explained the spreading occurring as a result of interactions of one retarding and one accelerating forces. In the context of energy, spill’s potential energy that diminishes with the progress of spill by being incentive for the accelerating force is exploited by the resisting forces and emitted from oil as heat and wave energy.

Four interactive forces (inertia, viscosity, gravity and surface tension) are responsible for the spreading. Inertia and viscosity inhibits the spreading, while gravity and surface tension support the spreading. Inertial force trying to keep oil

molecules together decreases during the oil spreading. After a point, it is replaced by frictional force of water (viscous force) increasing by larger oil contact area with water. In the same way, surface tension replaces the gravity force motivating the slick move downward. After passing to surface tension regime, spreading is supported by surface tension coefficient representing the net free energy at the slick edges, expressed as:

$$\gamma = \gamma_{wa} - \gamma_{oa} - \gamma_{ow} \quad (1)$$

A zero coefficient means that oil stops its spreading on the sea. That's why Fay (1971) linked the ultimate slick area to oil evaporation or dissolution by considering the remaining volume of spill on the surface. Besides, Fay emphasizes that even if four possible regimes of force interactions are available while oil spreading, surface tension-inertia interaction is negligibly effective on the spreading. Therefore, three regimes are examined, which are the gravity-inertia regime, the gravity-viscous regime and the surface tension-viscous regime. (Fay, 1971)

2.3.2 Hoult's Method (1972)

Hoult (1972) supported the idea of spreading developed in three regimes introduced by Fay. A theoretical work was performed and consistent results with the experimental study of Fay were found in the same study. It was claimed that spreading can be divided into two distinct processes which can be studied as slick propagations (1) naturally and (2) through the external forces later referred to as advection. As different from Fay, Hoult has explained wind and current effects moving the slick mass center as a vector summation. Accordingly, wind velocity includes the wave action and the least contributor to convective spreading is wave compared to wind and current. Hoult has integrated the similarity solution of boundary layer problems with oil edge velocity into the equations of regimes of spreading. The vertical movement of oil was assumed to be negligible compared to

horizontal extent of oil to approximate these equations by the similarity solution. It was also realized that oil moves horizontally in surface tension regime as not a function of slick volume. Like in Fay's study, it was discussed how oil will reach its ultimate area in the study. In this respect, the concentration of surfactants, the composition of oil, sea conditions like salinity, temperature and biological properties of the sea are considered as the parameters terminating the spreading, since they affect the surface tension coefficient. And then, Hoult evaluated two opinions for the final area with respect to these parameters. One of them is specifying a value for the thickness at the end of spreading belonged to Blokner (1964). Other one is loss of volatile and soluble parts of oil belonged to Fay (1971). Fay's approach was found to be more probable. (Hoult 1972, Zanier 2017)

2.3.3 Mackay's Method (1980a and b, 1982)

Mackay performed a series of studies in many processes of the spill. The oil properties and environmental factors like temperature, the salinity of water, etc. were focused in these studies to describe the fate processes of oil realistically. In this respect, Mackay tried to characterize the properties of oil on the sea surface like viscosity and density after evaporation, emulsification and dispersion by considering the sea conditions. After that, it is worthwhile talking about Mackay's method for spreading. The most important contribution in the method is that the thickness of oil varies in space, unlike Fay and Hoult methods where thickness of oil changes only as a function of time. The findings of Fay and Hoult about the spreading were combined with the phenomenon of thin-thick distribution of oil on the sea. Thin-thick distribution of oil refers that oil has thick central portion trailed by the thin oil film. Thin part of oil covers a significant part of the area (seven to eight out of ten) occupied by the oil slick. Furthermore, Mackay has created an algorithm by dividing the entire slick into many elements. These elements moving on the sea surface are expanded with time. Their expansion represents the increase in slick area. Such an algorithm written by Mackay laid the foundation for the spreading numerical

modeling and paved the way for describing the subsurface oil by the droplets. (McCay, 2004), (Berry, 2012), (Reed et al., 1999), (Al Rabeh, 1989) (Lehr, 2001)

2.3.4 Lehr's Method (1984a and b)

Lehr (1984a and b) observed the surface slick by the experiments in which three different amounts of oil spreads (13, 20 and 51 barrels). Thicknesses of these surface slicks are measured by a team and their areas are obtained by the taken pictures above the sea. The color differences of oil on the water are perceived as thick, transitional and thin portions of the slick and the areas between their margins are separately determined. Thickness, slick area and areas of thin, thick layers were interpreted together with the results obtained from Fay's and Blokker's formulas. The results from analytical equations do not agree with the experiments for their determination and the back calculation of initial volume of slick from area and thickness. In addition, 20 barrel of oil covers less area than 13 barrels of oil in these experiments, whereas the reverse case is expected in the spreading of oil. So, Lehr claimed that the reason of these two unusual findings is due to not accounting the environmental conditions. All spills will be additionally extended in the direction of winds and currents with the inclusion of these conditions into the spreading equations. Also, winds blow over the sea surface in different strengths and directions at the time of the release of these spills. So, wind and current effects on the surface fate can be comprehended from these experiments. These advective forces make the spill approximately elliptical from the top view unlike the equations estimating the circular distribution. Lehr (1984a and b) expressed it for the slick area with the equation of area of ellipse:

$$A_{slick} = \left(\frac{\pi}{4}\right) * L * G \quad (2)$$

L and G were found as functions of the oil volume, density difference and time at different degrees. In addition to them, R depends on the wind. After the combination of them, the equation is finalized as:

$$A_{slick} = 2.27 \left[\frac{\rho_w - \rho}{\rho} \right]^{\frac{2}{3}} V^{\frac{2}{3}} t_{min}^{-\frac{1}{2}} + 0.04 \left[\frac{\rho_w - \rho}{\rho} \right]^{\frac{1}{3}} V^{\frac{1}{3}} W^{\frac{4}{3}} t_{min} \quad (3)$$

2.3.5 Nihoul's Method (1984)

In Nihoul (1984) method, the thickness change with time is defined by the force balance between gravitational, frictional and surface tension forces applying the similarity solution method. The slick radius is found from an analytical solution or separate asymptotic equations of gravity and surface tension regimes as suggested by Deleersnijder (1992) for instantaneous spills. And then, radius is used to calculate maximum and average thickness of slick at the current time. A numerical approach is required to determine slick radius and thickness for continuous releases.

The important property of Nihoul's method is the expression of surface oil behavior as a simultaneous combination of regime forces. In addition, drag coefficient represents the viscous boundary layer effect between oil and water. In the numerical model of this study, Nihoul's model will be basis for our numerical solutions of both code and COMSOL solving the oil spreading problem, so it will be detailed in a separate section. (Nihoul, 1984)

2.3.6 Johansen (1984) and Elliot's (1986) Method

Elliot approached to the spreading of oil in three dimension by relating it with turbulences due to wind and current actions and dispersion. Their relationships were observed by the experiments of dye and oil. Dye sample is pumped onto the sea to find the diffusivity of a fluid horizontally and vertically on the sea. Like in Lehr's (1984) study, oil expands along the wind direction in oil experiment. On the contrary,

Elliot attributes this oil elongation to the dispersed particles and droplet size with an indirect contribution of wind and current to the oil spreading. Accordingly, large particles move to the downwind and dispersed small droplets but large enough to resurface follow the main slick from the closer region to the release site. So, Elliot created an algorithm of particle modeling by random walk and showed its compatibility with the experiments by advection-diffusion equation in three dimension. In the algorithm, the reason to prefer the application of random walk among the numerical solutions is to be able to assign particle properties. The number of large and small particles were adjusted through this feature in the study. Johansen also has noticed the relationship between dispersion and spreading of oil. Elliot has agreed with Johansen (1984) by confirming the Johansen's contribution and model with Eulerian approach.

2.3.7 Venkatesh's Method (1990)

A particular case which is the oil spill on the cold water, icy water and ice has been studied in Venkatesh's paper in 1990. The final thickness has been correlated with oil viscosity even if direct relation between them is not physically noticed. The final slick area on the cold, icy water or ice have been formulized by the simple volumetric equations. The sea temperature, the areal extent of ice of sea surface and ice fragmentation has been decisive on how oil extends. Low temperature drops the diffusivity of oil on the sea. Temperature terminates the spreading of oil on the cold water earlier than it on the warm water since the slick does not undergo the surface tension for oil on the cold water, icy water and ice according to the previous researches for oil with ice investigated by Venkatesh (1990). Ice formation up to 8/10 of ice to total surface ratio leads to increase of oil area when oil is poured from directly below the sea surface. For higher ice ratios to surface, oil cannot go up and needs to move laterally until it finds gap between the ices. So, oil area on the surface is lowered due to its some portion remaining under ice. If whole sea surface becomes icy, oil spreading starts and ends under the surface. However, spreading area is

greater than ice percentage of surface between %80 and %95 (percentage greater than 95% is accepted as total ice coverage of sea surface). In addition, ice fragmentation drops the final spreading area for the same ice percentages. Venkatesh (1990) provides a simple formulation for oil ice interactions placed in a software, OILBRICE and gives priority to comprehending the physics behind them. (Venkatesh, 1990)

2.3.8 Korinenko and Malinovsky's Method (2014)

Korinenko and Malinovsky (2014) sought the oil advection and oil spreading with a variety of hydrodynamic data by many experiments of vegetable oil with low volume maintaining its distribution without the strong external factors. The main inferences through the vegetable oil experiments are that small spills are treated by surface tension viscous regime (as indicated by Fay (1969)) and the horizontal slick dimensions are controlled by wind strength. These experiments have revealed that the circular shape of spreading still occurs under weak winds by investigating the horizontal axes of slick. Spreading shape turns into elliptical one elongated in the wind direction with stronger winds causing greater slick area. Korinenko and Malinovsky ensure that when wave is not accompanied by stronger winds, slick can preserve its distribution and circular shape. So, only wind driven waves affect the geometrical form of the slick. Korinenko and Malinovsky have contributed to confirm earlier advection studies through observations of slick in a variety of cases of turbulences. (Korinenko & Malinovsky, 2014)

Above researches help to understand the concept of oil spreading and advection and include the theoretical work about them. From this point, some examples of numerical modeling of oil surface fate will be introduced.

2.3.9 Examples of Lagrangian and Eulerian Modeling of Oil Surface Fate

The numerical models used for many research areas can be categorized as movement oriented-Lagrangian, the domain oriented-Eulerian models and combination of them. The oil spill mechanisms having the complex differential equations can be approached by applying one of these methods to a process separately and associated them in one solution. The choice of proper method for a process is as crucial as accurate implementation into the method. It will ease the model expandability for other mechanisms transmitting data to each other. A model can work with a problem well, but the same model can be failed with the addition of new terms representing new phenomenon due to the incompatibility of the equation type of the new phenomenon to the method. Therefore, some models of selected methods are illustrated to comprehend how they relate one process to another.

Al-Rabeh (1989) created an algorithm using the set of solutions for main processes of oil fate which are horizontal movement, entrainment and weathering due to evaporation and emulsification. The algorithm employs three dimensional advection-diffusion and Lehr's equations together for the horizontal and vertical movement of oil. The former equation is applied with random walk and hydrodynamic data obtained from a model. Oil is spread elliptically to the direction of wind by Lehr's equation. The model is initialized from the initial volume used for initial radius and thickness. The thickness distribution is layered without smooth passage in the profile and the layers are followed on the surface. The advection and spreading are linked to the evaporation and dispersion. The surface loss by weathering reduces surface elements to be considered for the horizontal movement.

Cekirge et al. (1997) also benefitted from the advection diffusion equation with random walk technique for the horizontal and vertical movements of a specific type of an oil emulsion formed from bitumen, water and surfactant fractions. However, they used the different Fay type equation dealing with oil spreading of surface tension regime in the algorithm. Initialization of algorithm for the fluid requires the oil fate without spreading since slick is initially not formed on the surface according

to the experiments. After surface molecules constitute a slick with a thin layer, it starts from the surface tension regime. Initialization contains the hydrodynamic information used for the divided elements and updated for the time. Number of elements are selected by the basis of 1 barrel corresponding to the 1 element in the algorithm. The evaporation of this type of fluid is not linked to the spreading resulted parameters, surface oil area and thickness.

Zhang et al. (1997) supplies a model of surface fate oil. They use two dimensional advection diffusion equation and implements a special type of random walk technique into it. Mass concentration of each particles are calculated from Gaussian kernel weighting after each particles are redistributed to their locations by Gaussian random walk. The reason for simulating the surface fate with this method is reducing the data scattering with lower number of particles. Their model takes into account the terrestrial obstacles to oil flow. It holds and frees the reaching particles to them randomly based on the prescribed times for the type of the land. The model can be worked with many possibilities of source geometry, moving release site, spilled oil instantaneously or continuously, etc.

Guo et al. (2014) examines the horizontal and vertical displacements of oil with a detailed advection data. Two hydrodynamic models transmitting data to each other help to contain the wave as well as wind and currents into the oil advection. The oil spill can be observed in the model when the terrestrial boundaries are close to the spilling site. Therefore, their model can describe the oil transport with change of daily sea elevation and the water flow direction around the coasts. A hybrid method coupling the particle tracking and the fixed region focusing in the model provides a solution for the oil spilling at the sea. Random walk method is implemented for the oil spreading. Oil spreading is considered like diffusion with a step length.

Tkalich et al. (2003) suggests to solve the fate equations by the application of Eulerian methods since most of the hydrodynamic models benefits from these methods. They claim that their compatibility will produce better solutions with easier data transmission and higher accuracy. In their model, two distinct finite difference

methods are used for spreading and advection to solve the Navier-Stokes equations after the confirmation of solution validity by Fay's spreading equation. Similar methodology is preferred for the entrained oil in water. After that, these equations in and on the sea are linked to each other and the oil passages in both directions are reflected in the modeling.

Martino (2007) presents a numerical approach to the oil spreading with the advection by converting the two separate equations into a form discretized by Galerkin method. The solution works in an open sea. However, it needs to be updated for the irregular slick progresses occurring when the terrestrial boundaries are defined since the structured meshes are used in the finite element solution. Another implementation to be required into the model is to specify the oil-water interactions on the slick edges.

Cho (2012) integrates a numerical solution into the model similar to the solution of Tkachik (2003) for the surface processes. The spreading and hydrodynamic equations are treated on the horizontal coordinates by the two types of finite difference technique. A converging method to the real data for advection is obtained, but only considered convective force is the current in the model. The daily change in sea elevation and flow directions of current can be projected into the model.

Arkhipov & Shapochkin (2019) performs a theoretical study of preliminary model tested against Fay's equations. They bring a numerical solution for oil spreading by using the characteristics method with a hybrid Lagrangian-Eulerian approach. The method admits two boundary conditions, but requires one more relation. Another boundary condition is determined by solving the force balance equation by self-similar solution for all of the spreading regimes separately. The regime changes are specified by the time and the discrete solutions are consecutively placed into the model.

The different studies show that oil spreading and advection can be described with both Lagrangian and Eulerian methods. It is integrated with other phenomena into the models in three dimensional workspace.

2.4 Theory of Our Modeling for Oil Spreading

2.4.1 Diffusion

Diffusion emerging from the excessive energy of a system is a potential based flux of heat, atoms and molecules to balance the forces of system. Diffusion due to the negative gradient of concentration with respect to the direction is realized by Fick explaining it in the first law.

$$J = -D * \frac{d(C(x))}{dx} \quad (4)$$

Like heat conduction, molecules move from one region to another by molecular unbalance of the system. Fick establishes an analogy of diffusion of molecules to heat conduction corresponding to Fick's second law. Similar type of heat conduction equation proposed by Fourier is used for concentration-driven diffusion and reduced to below equation. (Fick, 1995)

$$\frac{\partial C(x, t)}{\partial t} = - \frac{\partial J}{\partial x} \quad (5)$$

When species A goes to the voids of region of lower concentration, species B even air molecules diffuses in the reverse direction until the equilibrium is reached. Fick expresses the exchange of matter as a function of concentration and distances of molecules to each other. Higher the concentration difference between two environments and closer the molecules of same species, greater the diffusion of matter. This corresponds to Fick's second law. Later, the driving forces of diffusion are generalized as chemical potential, thermal disequilibrium and electric potential. Chemical potential can replace the concentration. In the case where the part of

system has lower concentration of a matter, but higher chemical potential compared to the surrounding, some molecules are transferred to the surrounding. Therefore, chemical potential corresponding to the electrical potential in heat equations is a better analog than concentration to heat conduction as diffusive forces for self-diffusion (Islam, 2004). In addition, Fick's laws describe the diffusion in macroscopic level. Einstein (1905) investigates the probabilistic diffusion of particles in microscopic level which is the subject of our modeling. This atomic diffusion is specified by the Brownian motions referring to random movement of particles.

2.4.2 Random Walk Approach

Random walk is a mathematical technique inspired by the random movements of tiny particles/molecules in nature and used to predict the future state of randomly occurring events in many research areas. For our modeling, it helps to numerically solve the complex ordinary and partial differential equations. It considers the fluid as aggregation of small particles moving randomly.

Hunter (1987) emphasizes on the similarity of the movement of small particles to molecular diffusion of Fick, as investigated by Einstein (1905). Therefore, the particle movement of random walk is modeled with the diffusion coefficient. The random walk method is suggested for oil processes occurring horizontally and vertically. Hunter claims that random walk will outperform finite element and difference methods for 2 or 3 dimensional problems due to the insufficiency of latter methods to describe the advection into the models. Hunter declares that the probability distribution of a random walk in one dimensional is binomial transformed into Gaussian with many steps (N). Number of steps required for the transformation is 10 in this study.

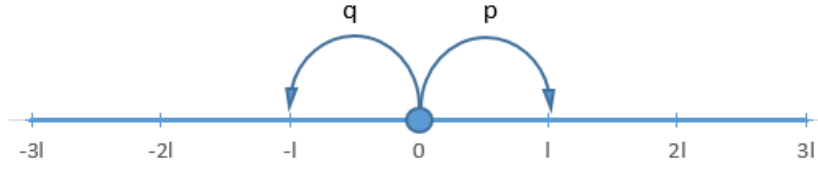


Figure 2.4: 1-D Random Walk with step length of l and particle stepping from origin

In 1-D binomial or Gaussian random walk, the mean value of x (position of particle with respect to origin) corresponds to the first moment with probability of p to move through one chosen direction. It can be found by:

$$E(x) = (2 \langle n \rangle - N)l \quad (6)$$

Where

$$\langle n \rangle = Np \quad (7)$$

$\langle n \rangle$ is mean value of steps in the chosen direction and l is step length meaning the taken path in a step. Mean value of displacement is given as:

$$E(x) = (2Np - N)l \quad (8)$$

The probability of going to the opposite direction is assigned as q . $E(x^2)$ (mean-square displacement) can be expressed as:

$$E(x^2) = \langle [(2n - N)l]^2 \rangle \quad (9)$$

$$E(x^2) = (4 \langle n^2 \rangle - 4 \langle n \rangle N + N^2)l^2 \quad (10)$$

where

$$\langle n^2 \rangle = (Np)^2 + Npq \quad (11)$$

$$E(x^2) = (4(Np)^2 + 4Npq - 4.N^2p + N^2)l^2 \quad (12)$$

The second moment gives the variance as:

$$\sigma^2 = E(x^2) - E^2(x) \quad (13)$$

$$\sigma^2 = (4(Np)^2 + 4Npq - 4N^2p + N^2)l^2 - (4(Np)^2 - 4N^2p + N^2)l^2 \quad (14)$$

$$\sigma^2 = (4Npq)l^2 \quad (15)$$

Total step number (N) is the ratio of the time range of observation to time step.

$$\sigma^2 = \left(\frac{4t}{\Delta t}pq\right)l^2 \quad (16)$$

Diffusivity can be implemented by substituting $D = \frac{l^2}{2\Delta t}$ as suggested by Hunter (1987) into the above equation:

$$\sigma^2 = 8Dpqt \quad (17)$$

So, the standard deviation of the probability distribution of the random walk will be in general form without specifying the probability of going to one direction as:

$$\sigma = \sqrt{8Dpqt} \quad (18)$$

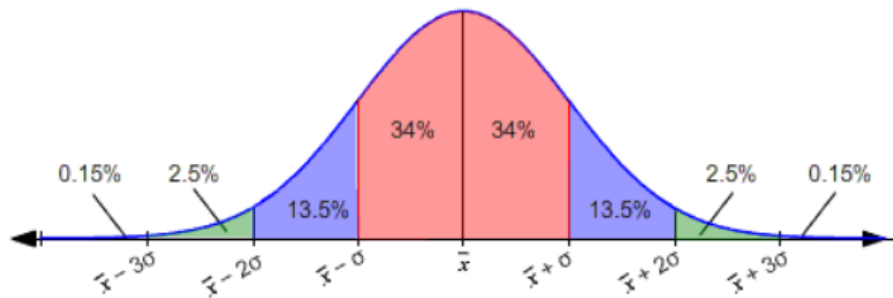


Figure 2.5: Gaussian Distribution with $\langle x \rangle$ (mean)=0 and σ (variance) (varsitytutors.com)

Figure 2.5 depicts the Gaussian distribution with zero mean and one standard deviation. A particle can be transported to a new point as far as one standard deviation with the probability of 0.68 at the next time step. It is crucial to see that probability distribution limits the chance of particle going further.

The random walk described above is the 1-D random walk with one particle. Expanding it into simple 2 or 3-D random walk for more particles, it is restricted by some simple specifications. The first rule is that particles forget the route they travel. It means that a step does not affect the next step, or is not affected from previous step. Secondly, in the treatment of 2-D or 3-D random walk, the jump in one dimension is not related to jump in another dimension. Thus, the standard deviation in any axis is equal to $\sqrt{8Dpqt}$. Thirdly, the particles are free of interactions among each other during the movement. (Berg, 1993)

The isotropic random walk holds true when the probabilities of particle walk are equal in each direction with the above specifications. It is the form of most simplified random walk. In such a random walk, diffusion is not accompanied by a drift. The probability distribution of isotropic random walk obeys Central Limit Theorem. Central Limit Theorem (CLT) states that a large sample taken from data cluster follows Gaussian distribution regardless of the distribution type of all data. Diffusion is categorized into normal diffusion and anomalous diffusion based on complying with CLT or not. In the random walk of normal diffusion, CLT is approached after many steps. In anomalous diffusion, CLT is ruined by probability distribution with a significant skewness or kurtosis, not identical steps and particle interactions, steps' dependency to each other which make random walk complex.

2.4.3 Nihoul's Method (1984)

Nihoul's method provides an equation analogous to advection-diffusion equation describing oil spreading and advection on the quiescent water. Surface tension dominated regime becomes as crucial as the gravity-friction regime in Nihoul's

method. Surface tension is expressed with free energy of sea surface remained after some of the energy is consumed by the tensional stress created on the sea by the floating spill. This free energy accelerating the oil spreading is zero at the center and linearly increases to its maximum at the edge. The force interactions between inertia, friction, gravity and surface tension are brought together in an equation.

In Nihoul's method, both the boundaries of upper side and lower side of oil are considered for the thickness variation of whole oil patch. And then, their integration from bottom to top are combined with hydrodynamic equations. The main equation is given as:

$$\frac{\partial(hU_{avg})}{\partial t} + \nabla(hU_{avg}^2) = -g'h\nabla h + \frac{k}{\rho}U_{advection} + \frac{k\gamma}{\rho k}\nabla\varphi^2 - \frac{k}{\rho}U_{avg} \quad (19)$$

$$U_{advection} = \frac{\tau_a}{k} + U_{current} \quad (20)$$

$$\gamma = \gamma_{wa} - \gamma_{oa}^\circ - \gamma_{ow}^\circ \quad (21)$$

$$g' = g \frac{\rho_{water} - \rho}{\rho} \quad (22)$$

Left-hand side of Eqn. 19 represents the force actions of inertia. Even though gravity inertia regime is available in the equation, it is not investigated like gravity-viscous and surface-viscous regimes in Nihoul's work (1984) and Deleersnijder's works (1985 and 1992) emphasizing on the similarity solution of Nihoul's method. Nihoul suggests to modelers of oil spreading to eliminate the gravity-inertia regime lasting for short periods initially. So, it is neglected in Eqn. 19.

First, second, third and fourth terms of RHS of Eqn. 19 represent gravity, advection, surface tension and friction respectively. Ultimately, mass balance equation (23) with the substitution of average oil velocity (U_{avg}) from Eqn. 19 provides Nihoul's equation simultaneously interacting force with each other (24):

$$\frac{\partial h}{\partial t} + \nabla(hU_{avg}) = Q \quad (23)$$

$$\frac{\partial h}{\partial t} + \nabla(hU_{advection}) = Q + \nabla \left(\frac{g'\rho}{k} h^2 \nabla h - \frac{\gamma}{k} h \nabla \varphi^2 \right) \quad (24)$$

In the polar coordinate system, it will be in the form of Eqn. 25 with the assumptions of advection-free environment and negligible mass change in the system.

$$\frac{\partial h}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(\frac{g'\rho}{k} h^2 \frac{\partial h}{\partial r} - \frac{\gamma}{k} h \frac{\partial \varphi^2}{\partial r} \right) \right] \quad (25)$$

To find a solution to this complicated partial differential equation, Nihoul (1984) applied the similarity solution as suggested by Hoult (1972) by writing the thickness as:

$$h(\varphi, t) = m(t)n(\varphi) \quad (26)$$

Thickness looks like depending only on the time and surface tension variation from Eqn. 26. However, it is also space dependent parameter, since surface tension variation (φ) is expressed with ratio of radial distance in slick to slick radius (r/R).

Thickness at any position can be found from Eqn. 25, 26 and the expression of $\varphi=r/R$ as:

$$h = \frac{3V}{2\pi R^2} \left[1 - \left(\frac{r}{R} \right)^2 \right]^{1/2} \quad (27)$$

Same thickness of oil forms at the equal radial distances ($r_1=r_2$). It means that oil spreads in a circular pattern with the assumptions of no advection and no mass loss.

Since φ is r/R ,

$$\varphi = \left[1 - \left(\frac{2\pi}{3V} R^2 h \right)^2 \right]^{1/2} \quad (28)$$

To find the radius of slick, equation 25 is transformed into 29 by adding equation 28:

$$\frac{\partial h}{\partial t} = \left[\frac{g'\rho}{k} + 2 \frac{\gamma}{k} \left(\frac{2\pi}{3V} \right)^2 R^4 \right] \frac{1}{r} \frac{\partial}{\partial r} \left(r h^2 \frac{\partial h}{\partial r} \right) \quad (29)$$

Now, equation 29 is in a desired form for the determination of radius of slick. Putting 27 into equation 29 and solving the radius with respect to the time as suggested by Deleersnijder and Loffet (1985), the analytical solution for the slick radius of instantaneous release is obtained as:

$$R^2 - \frac{1}{a} \arctan(aR^2) = \frac{4\gamma}{k} t \quad (30)$$

$$a = \frac{2\pi}{3V} \left(\frac{2\gamma}{g'\rho} \right) \quad (31)$$

The average thickness is calculated from the volume equation of circle:

$$h_{avg} = \frac{V}{\pi R^2} \quad (32)$$

The maximum thickness is observed at the center of slick. It has a relation with average thickness for instantaneous releases like Eqn. 33:

$$h_{max} = \frac{3V}{2\pi R^2} = \frac{3h_{avg}}{2} \quad (33)$$

Then, the radius of slick is found asymptotically for gravity and surface tension dominated regimes. When the thick layer of oil extending by the gravity viscous regime spreads on the sea, the criterion is taken as $aR^2 < 1$ radius of slick is:

$$R = \left[\frac{27V^2}{2\pi^2} \frac{g'\rho}{k} t \right]^{1/6} \quad (34)$$

After oil extends by the gravity viscous regime forming very thin oil layer ($aR^2 > 1$), surface tension takes place for the spreading. In surface tension-viscous regime, slick has different spreading rate (radius change per time) determined from:

$$R = 2 \left(\frac{\gamma}{k} t \right)^{1/2} \quad (35)$$

Deleersnijder (1985, 1992) rearranges Eqn.24 by Eqn. 33. The coefficients of regime forces are grouped into one coefficient named as diffusion coefficient of spreading related to diffusion. It makes easier to use the advection-spreading equation for numerical solutions. Such an expression gives the main equation in the form of:

$$\frac{\partial h}{\partial t} + \partial(hU_{advection}) = Q + \nabla \left(\left(\frac{g'\rho}{k} + \frac{2\gamma}{kh_{max}^2} \right) h^2 \nabla h \right) \quad (36)$$

Combining all forces in one equation for the fate of slick on the surface is the distinguishing feature of Nihoul's model from preceding ones. For asymptotic solutions of instantaneous releases, these forces are taken as active or passive based on the valid regime (Eqn. 34 and 35). For analytical solution, they are in combination without neglecting any of them. So, change in magnitude of the regime forces with time establishes the current regime (Eqn. 30). For numerical solutions, one way that we preferred in this study is to consider all of the forces as active and their magnitude determines the current regime. We will compare all of the solutions and another numerical solution used in COMSOL to check our solution's accuracy. In COMSOL software, advection will be defined like Eqn. 36. In our code, oil particles will advect by assigning a wind velocity to them.

2.4.4 Arkhipov's Approach (2007)

Arkhipov (2007) explained how advection-diffusion type oil spreading equation can be applied to a numerical algorithm for only gravity-viscous regime. Gaussian

random walk of discrete particles was used and introduced with a description of steps in Arkhipov's study. The reason to prefer the random walk for spreading of slick is that oil boundaries expand at every time step with the sharp end at the edges. For movable and sharp front boundaries of oil, random walk is simpler to implement than Eulerian numerical solutions according to Arkhipov. Moreover, regular grids depict the progress of slick in Arkhipov's numerical solution.

In the model, the surface tension term of Eqn. 24 is dropped for gravity dominated regime with no wind or current action. The equation is reduced to Eqn. 37 with the same assumptions used to obtain Eqn.25 from Eqn.24.

$$\frac{\partial h}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(\frac{g' \rho}{k} h^2 \frac{\partial h}{\partial r} \right) \right] \quad (37)$$

The diffusion coefficient is the coefficient of thickness gradient in Eqn. 37 as:

$$D(h) = \frac{g' \rho}{k} h^2 \quad (38)$$

As it can be noticed, the diffusion coefficient of spreading is a function of square of thickness, diffusion coefficient of oil molecules spatially differs due to thickness change at positions of oil molecules.

As discussed in the random walk section, a large subset of a data cluster approaches to Gaussian distribution regardless of the population's probability distribution when Central Limit Theorem is followed. So, the distribution of random numbers above does not need to be Gaussian distribution in order to obey CLT. However, as it is explained in the same paragraph, a step's dependency to previous route and interactions of the particle between each other will break CLT theorem. It results in a time and space dependent random walk of particles. CLT is broken in the spreading process of oil spill due to given reasons. To treat the process by the random walk in a simple manner, Gaussian distribution of random numbers was chosen in

Arkhipov's study (2007). Again in random walk section, their standard deviation of Gaussian random with time and space independent particles is given in Eqn 18. In this case, the random walk is assumed to be isotropic one and the standard deviation (diffusive length) is updated for each step due to the step dependency of particles resulting in variable diffusion coefficient for every time steps. So, it turns into the equation of:

$$\sigma = \sqrt{8D(h)pq\Delta t} = \sqrt{2D(h)\Delta t} \quad (39)$$

However, assumption of Gaussian distribution for random walk was not enough to have oil particle distribution properly. Particles were scattered, disturbing normal distribution with high variance after starting the process in the numerical solution. The solution to this problem is to define a new parameter “ λ ” whose value is 0.34 into diffusive length equation for each time step in order to fit the distribution of particles into Gaussian one. Standard deviation (diffusive length) becomes:

$$\sigma = \sqrt{2\lambda D(h)\Delta t} = \sqrt{2\lambda \frac{g'\rho}{k} h^2 \Delta t} \quad (40)$$

Arkhipov has assigned λ as 0.34 by the trial-error method by comparing with the similarity solution of Nihoul's method (Eqn. 34) for instantaneous release and solution of the finite difference method of Eqn. 37. Also, Arkhipov has proven that when 0.34 is a selected value of λ for continuous release of slick, results of Gaussian random walk and finite difference method of Eqn 37 are consistent with each one.

For random walk of spreading, oil was split into N particles going to the new location updated after every time step with a random number of Gaussian distribution by the equation of:

$$x_i^{n+1} = x_i^n + U_{xi}\Delta t + RN_i'\sigma \quad (41)$$

or

$$y_i^{n+1} = y_i^n + U_{yi}\Delta t + RN_i'\sigma \quad (42)$$

2.4.5 Voronoi Diagram Representing Oil Spreading

Voronoi diagram used in our modeling of oil spreading will be explained with its properties in this section. It will be discussed with mathematical approach to oil spreading and the integration into Durgut Model (2017 & 2020). Voro++ which is background code in the model will be introduced.

2.4.5.1 Voronoi Diagram and Delaunay Triangulation

Voronoi diagram is a kind of visualization of spatial members surrounded by polygons called as Voronoi cells with their vertices and edges. The edges connecting the vertices emerge at the middle point of closest neighbor members as perpendicular to a straight line drawn between these members. The vertices, the junctions of three or more edges, are taken as the center of circle which passes through these members. Any spatial members are not located inside this circle. So, one member has same number of neighbors with vertices. With placements of vertices and edges, cells are formed and every cells become to be belonged to only one member. Cells enclosed by other ones are shaped as convex. Remaining of them are open-sided when they represent the outermost members of the Voronoi diagram. All of the arguments can be checked against Figure 2.6a.

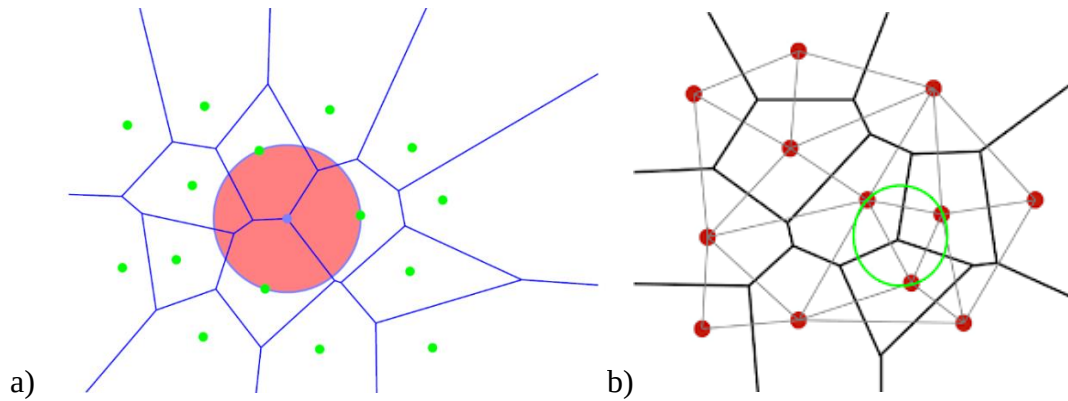


Figure 2.6: Illustration of the Voronoi Diagram (a) and Voronoi Diagram-Delaunay Triangulation together (b) (stackoverflow.com, 2017)

The straight lines drawn between the members becomes the edges in Delaunay tessellation. The vertices in Delaunay tessellation are directly spatial members. Thus, Delaunay tessellation with the Voronoi diagram provides a dual representation of the same region. The elements of Delaunay tessellation have triangular shapes unless four closest members can create a circle. So, the tessellation can be also named as Delaunay triangulation. The outermost edges of Delaunay tessellation actually correspond to the convex hull of the cluster. In Figure 2.6b, the dual graph of the Voronoi diagram and Delaunay triangulation can be considered with above information. In order to ensure the edges, vertices and regions of Voronoi and Delaunay tessellations are put correctly, the generalized rule about the numbers of them can be checked. Number of cells are equal to the number of members (n), number of edges must be equal to or lower than $3n-6$ while the number of vertices must be equal to or lower than $2n-5$ for Voronoi diagram. Number of Delaunay elements must be equal to or lower than $2n-5$, number of edges must be equal to or lower than $3n-6$ whereas the number of vertices are equal to the number of members (n) for Delaunay tessellation. (Okabe, 2000)

In spreading of oil patch on the sea, Voronoi diagram, Delaunay triangulation or their combination can be used as an alternative method to gridding preferred by Arkhipov (2007) to represent the particles of the random walk for oil spreading. It is discussed

with advantages, drawbacks and solution to drawbacks mentioned in Durgut's (2017) paper.

2.4.5.2 Durgut and Reed's Model (2017 & 2020)

Durgut and Reed model (2017) benefitted from the combination of Nihoul method and Arkhipov numerical model with the empirical constant " λ ". The main difference of Durgut from Arkhipov models is the integration of the Voronoi diagram to spread the instantaneously released oil instead of grids. The reason to prefer the Voronoi diagram is to describe oil spreading with lower dependencies on the particle and time step. Gridding the oil distributed area of sea in numerical algorithm requires more number of particles to reach the similar precision of algorithm employing Voronoi diagram. Furthermore, it is proven in the Durgut's paper (2020) that the simulation is not required to start at the beginning of the release. Such a numerical approach does not disturb the stability of solution to oil spreading with the numerical parameters. Also, Durgut's model allows observing particle distribution step by step clearly. It becomes an innovative representation of spreading. So, to elucidate Durgut's model briefly, the spreading of instantaneous spill in gravity-viscous regime is realized by an algorithm applying Gaussian random walk of particles to update their positions by diffusive length (Eqn. 40) proposed for Nihoul's evolution equation (Eqn. 24). The algorithm uses Voronoi diagram with hexagonal Voronoi cells to place the particles in their updated positions. The numerical model of Durgut was tested against Nihoul's analytical (Eqn. 30) and asymptotic solution (Eqn. 34) with sensitivity analysis of the slick properties. Its suitability to visualize the spreading of oil on the sea surface was proven.

It is worth talking about integration of Voronoi diagram into Durgut's model and the difficulties which are faced with and solved. Durgut created an algorithm based on Voro++, an open source library of C++ [38]. Voro++ gives a chance to assign size and shape of Voronoi cells. Such an implementation actually solves the main drawback about open-sided cells for spreading process. The open-sided Voronoi

cells normally go to infinity in graphs of them. They can be limited by Delaunay edges, that are convex hull, but it restricts the outermost particles of slick to the lower area than their original areas and irregular slicks cannot be represented well. In Vorop++, the outermost particles will be also put in an enclosed polygon by assigning cell radius. So, the cell radius assignment supplies the possibility of having concave slick. It helps to reflect the slick shape more realistically. In addition, the overlapping cell problem is solved by Vorop++. It rearranges the overlapping adjacent cells by adding new edges after placement of cells with the pre-assigned sizes. Another issue is about spacing among cells. Cell radius is arbitrarily selected, but it should be properly adjusted to prevent the cavities among the cells and the excess movement of particles.

Similar study by Durgut et al. (2020) has been released to observe the slick extent in the surface tension regime as well as gravity viscous regime with same methodology of Gaussian random walk of the particles. Main difference of new study from earlier one is to rearrange the diffusion coefficient from Eqn. 36 including the surface tension regime. So, new diffusive length defining both gravity-viscous and surface tension-viscous regimes is expressed as:

$$\sigma = \sqrt{2\lambda D(h)\Delta t} = \sqrt{(2\lambda \frac{g'\rho}{k} + 2\beta \frac{2\gamma}{kh_{max}^2})h^2\Delta t} \quad (43)$$

Durgut et al. (2020) proposed a constant, $\beta=0.31$ for surface tension regime term to reduce the scattering of particles as Arkhipov proposed $\lambda=0.34$ for gravity regime term. The solution with new diffusive length produces similar results obtained through Nihoul's asymptotic (Eqn. 34 and 35) and analytical solutions (Eqn. 30).

2.4.5.3 Vorop++ for 2-D Distributions

Vorop++ has a capacity to define almost 17 million members in a region. It constitutes the region of problem from many small pieces which are Voronoi cells. So, it takes

these cells as a basis for the description of region. Cells are primarily formed and placed into Voronoi diagram. A single cell can be possibly analyzed without organizing Voronoi diagram for a region in Voro++. Voro++ consists of header and source files specifying the errors, code lines for opening and closing the files and cell constraints like maximum number of vertices of Voronoi diagram. These are fundamentally compulsory parts of Voro++ to open, process and close the files of simulations. For cell construction, another header and source files are written. Voro++ provides both convex and concave cells through these files. Convex cells are built in rectangular or hexagonal shapes, vertex positions are regulated and their edges are connected. On the other hand, concave cells are built by introducing the vertex positions and their nonconvex edges are specified for plane cut if adjacent cells are overlapped by these edges. The cells having neighboring relations are noticed by concentric shells enlarging until twice times greater than the cell size. When these cells overlap by their edges, these cells are reorganized by deleting the overlapping edges and adding new edges. To do this, plane cuts are performed. The excess area of cell into other cell are eliminated. The points lying in the plane are searched. So, Voro++ takes these points as new vertices of overlapping cells. The new edges with other vertices are drawn through the plane cut function. For concave cells, the convex edges are treated in a same way at the edges of convex cells. However, nonconvex edges are cut out by half plane function considering their irregularity.

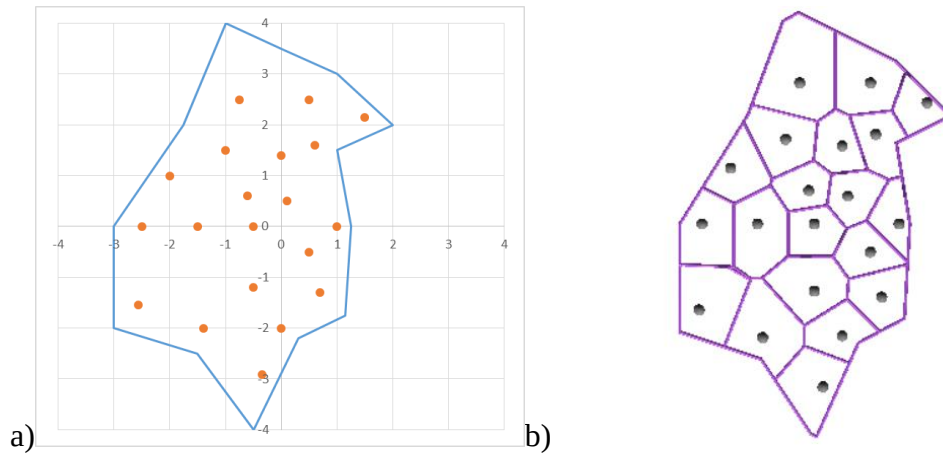


Figure 2.7: a) Particle Coordinates and Irregular Domain b) Voronoi Diagram of the Domain

Like nonconvex cells, nonconvex domain can be also defined in Voro++. The combinations of convex and concave cells in an irregular domain can be depicted in Figure 2.7. Cells are located into the domain consisting of the blocks of specified number of cells with the loops. Looping of blocks makes the treatment of problem easier. It starts with first block and continues in an order. The corresponding blocks where the particles are embodied are ensured by the code functions. As a special case, periodicity of domain can be implemented by the code if the domain boundary in a direction is repetitive such as cylindrical or spherical domains. Particle coordinates are redefined with periodic domains. After specifying all features of cells and domain, cells are placed onto the domain. The cell radii, particle ID and 2-D coordinates, vertex positions, vertex numbers per a cell and edge numbers are recorded in Voro++ at the end of member placement. The neighboring particle IDs to the current particle are specified. Boundary and spiky cells are marked. Many cell based calculations and statistical analyzes are possible from vertex, edge and particle positions. Cell area, perimeter and centroid can be determined, the distance from farthest vertex of cell to particle can be known and mean distances among adjacent particles can be found. All of these information can be taken from output files.

Voro++ being open source C++ library can be developed for oil spreading modeling. It can be converted into time dependent solution with the definition of new functions.

It is selected in our modeling, since it supplies enclosed cells for outermost particles, rearranges overlapping cells and eliminates cavities among cells as discussed in previous section. In addition, it helps to define the boundary cells, neighboring relations among particles are taken into account and cell based analyzes easily provide the slick area, thickness and oil distribution.

2.5 COMSOL

COMSOL, a software of finite element method contains separate interfaces for general scientific and engineering problems like fluid flow, heat conduction and optics with the already arranged equations. However, it is also applicable to the specific problems by reducing the given ordinary or partial differential equations in a desired form. COMSOL follows the general numerical structure of a finite element method shown in Figure 2.8. Firstly, its preprocessor corresponds to building a model including the information required for the process. The global parameters in the process can be defined as constants and functional variables implemented by the curves. One can add properties of the material that system is made of, and material components searched in the problem. The domain where components are located is constructed with its shapes and sizes. After that, equations of physical phenomenon can be built or be already available. Boundary conditions, initial conditions, constraints and loads need to be specified to complete the problem definition. The final and critical stage of preprocessor is to decide how the problem domain will be meshed. In COMSOL, domain meshing can be done in two different ways. One of them is to implement physics controlled meshing where COMSOL suggest a gridding of the region by considering the local changes of tracked parameter with restrictions, regional flows of fluid, heat, current and boundaries etc. On the other hand, user can identify the locations where fine elements are required with the selection of user controlled meshing. The latter meshing type can be better for preventing the solution from manipulating whenever the solution is not as precise as it is accepted. Secondly, processor uses the problem specifications, and produces the

dependent value in space. Type of study which can be stationary, time dependent, eigenvalue or their combinations determines the solution. For example, the solver of COMSOL can arrange time steps taken to solve the time dependent problem by taking into account the error tolerance, but we need to state output intervals and start and end times of simulation in time dependent problem. Analysis of an independent parameter, geometric and material properties and different studies in one file are allowed. Output is obtained at the end of processor. Then, COMSOL generates variation plots of the dependent variable in dimensions at the postprocessor. We can do additional analysis on the solution by taking integral over the entire geometry, cutting the system through cross section lines, showing the change of dependent variable along these lines, etc.

COMSOL will be used in our study for the comparison purposes with our numerical solution. The main reason to prefer COMSOL is its unstructured grids to easily define the moving boundary of the slick contacting with the underlying sea where thickness change is rapid.

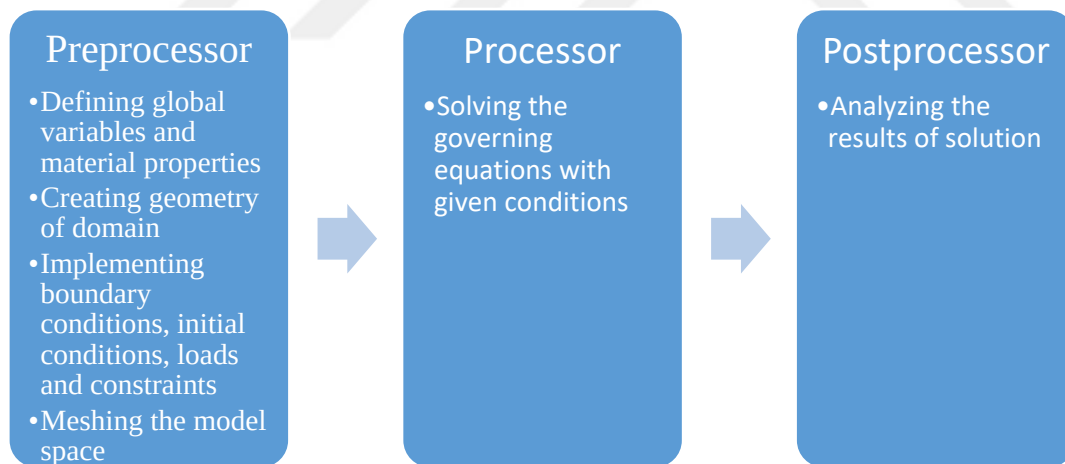


Figure 2.8: General steps of Finite Element Models

2.6 Waxy Oil Findings

Brönner et al. (2018) made a series of experiments in the laboratory with Marine Gas Oil (MGO), Wide Range Diesel (WRD) and mixtures of WRD with artificially weathered Norne Crude in different percentages. These fluids are chosen since values of their densities are close to each other to eliminate other factors except high viscosity associated with wax content. MGO resembles Newtonian fluid, while WRD and mixtures of WRD and Norne Crude are non-Newtonian fluids. The non-Newtonian ones expose to the significant, additional resisting force apart from the viscous forces during gravity-viscous regime due to their yield stresses. The spreading rate is decreased by the yield stress causing earlier end of the spreading. Brönner utilizes an empirical equation for waxy oils compatible with spreading data of WRD and the mixtures.

In the experiments, the continuous release is preferred rather than the instantaneous release because continuously released spill undergoes from gravity-inertia regime to gravity-viscous regime in a shorter period of time. Brönner states that continuous release leads to more oil accumulated at the center than the instantaneous release which creates a slick profile defined by Nihoul in Eqn. 32 and 33. So, relation between Eqn. 32 and 33 does not hold true for continuously released oil profiles.

In this study, radial extent of MGO having almost zero yield stress will be used to check applicability of our numerical solution and COMSOL for continuous releases. Also, spreading described in Nihoul's method without additional term for waxy oils is tried to match with non-Newtonian fluid spreading by higher drag coefficients to reflect the yield stress in the viscous term.

CHAPTER 3

STATEMENT OF PROBLEM

Our one of the objective is to present an algorithm describing accurately the spreading of instantaneous and continuous releases based on Nihoul's model. Instantaneous release simulations of the algorithm promise the oil spreading under both gravity and surface tension regimes. Continuous release simulations of oil spreading contain only gravity-viscous regime due to the slick profile complexity to arrange the surface tension term for continuous releases. We introduce the available algorithm created by Durgut (2020) for instantaneous spills and update it by changing the release type from instantaneous to continuous spill to generate the experimental conditions of waxy oil paper in simulation for comparison purpose. To seek curve fit to waxy oil findings, we try to find numerical solutions with the drag coefficient. The algorithm employs Gaussian random walk for particles representing oil slick in order to move them from a position to another based on diffusive length relating diffusion process to spreading process. Thickness and radius for any point in slick are presented by Nihoul's slick evolution equation. At the end of the run of the algorithm, particles are distributed in the Voronoi diagram drawn through Voro++ (an open source library of C++).

After confirming the code compatibility for both instantaneous and continuous spill cases, we analyze the slick progress with sensitivity analysis of parameters to investigate the flexibility of the code with a great range of parameters. COMSOL offering finite element solution to advection-diffusion process accompanies to our numerical solution to check the accuracy of our model for all cases.

Our another objective is to describe a complete model of oil surface fate through the implementation of advection and spreading together. Advection is defined into the model by assigning the wind velocities to the particles. The effect of advection is observed through different wind strengths.

CHAPTER 4

METHODOLOGY

Oil spreading is modeled with three different modules in our study. It is shown in Figure 4.1. Main algorithm places particles through Gaussian random walk, calculates slick radius and transmit the coordinates of particles and the slick radius to Voropp. Voropp considers the location of particles, specifies neighboring particles and rearranges cell edges among these particles by plane cutting. It constructs Voronoi diagram restricted by slick radius. It records the coordinates of cell vertices, determines boundary cells, calculates cell area and sends processed data to main algorithm. Main algorithm uses cell area for the thickness calculations of each particle and slick radius. The slick radius and thickness which are main output of oil spreading are converted into text file. MATLAB module takes the coordinates of particles, cell vertex positions and specified boundary cells from main algorithm and visualizes the slick from top view with Voronoi diagram.

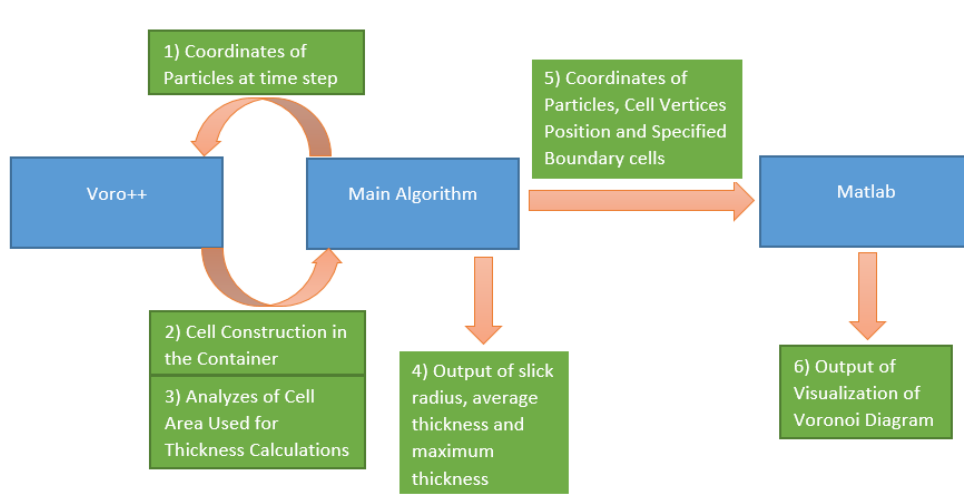


Figure 4.1: Flow Chart of Integration of Three Different Modules

4.1 Voro++ Implementation of Oil Spreading

Voro++ with 2-D configuration creates the particle distribution of oil spreading in our modeling. Durgut and Reed (2017) have developed such a model for instantaneous releases. It is improved for continuous releases in this study. The main advantage of Voro++ is being an open source giving the chance of introduction of new functions, so the particles can be redistributed through some Voro++ functions and new functions added for time dependent problems. It supplies to resize the domain if it is required. Therefore, it is preferred for our problem.

In our modeling, each particle represents the same volume of oil. We calculated cell radius by dividing the slick radius from Eqn. 30 by an arbitrary number. The cell radius calculated in this way is assigned to all cells for every time steps and fits to our solution for a variety of spills.

First, oil and water properties, initial spill volume, frictional and surface tensional parameters are defined in model. Particles are placed at the mass center into the circular domain with the slick radius from Eqn. 30 at $t=0.1$ seconds. They are distributed randomly. After random initialization, they are redistributed step by step with their diffusive lengths multiplied by Gaussian random number (Eqn. 40 or 43). New particles are introduced from the slick center as we do at the initialization step when oil is continuously released. The thicknesses assigned to each particle are averagely determined from the summation of volumes of current and neighboring cells divided by total area of them. Such a calculation reduces the fluctuations of the assigned thickness to a cell. Figure 4.2 briefly demonstrates the steps of the simulation as a flow chart.



Figure 4.2: Main Steps of Simulation of Oil Spreading

4.2 MATLAB Code for Output

Normally, Voropp output files are opened from Gnuplot and POV-Ray software to visualize the distribution. However, they are benefitted for the time-stationary solutions. Durgut wrote a code in MATLAB to visualize the progressive distribution for our case reflecting the slick contamination step by step. The code uses the output file from C++ and takes the particle and vertex positions and slick radius for the current time. Particles are surrounded by cells with the position info. It draws a red line by the slick radius from Eqn. 30 to recognize the distribution accuracy for instantaneous releases. Since Eqn. 30 is not derived for continuous releases, the red line will be removed for their cases. Since outermost particles are known, they are differentiated as blue cells whereas other cells are colored with the black. Figure 4.3 exemplifies the plot from MATLAB.

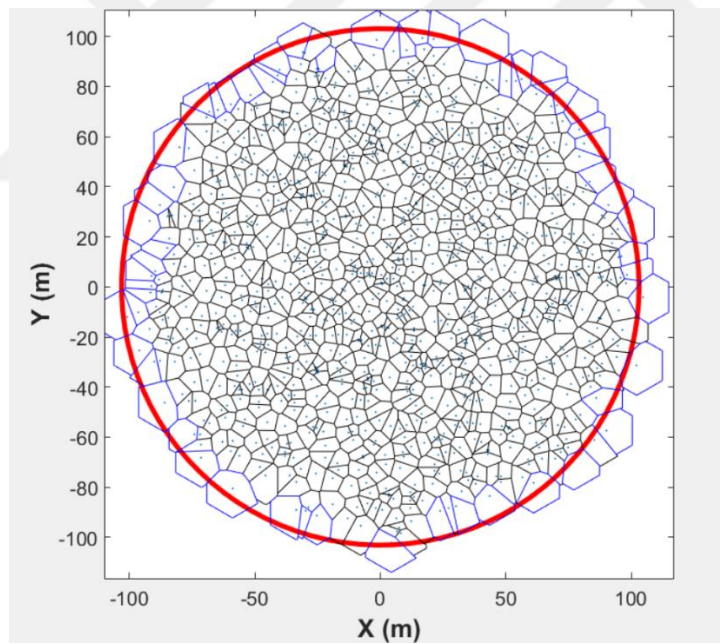


Figure 4.3: Voronoi Distribution of Oil Particles

4.3 COMSOL Implementation of Oil Spreading

COMSOL supplies many interfaces of both specific problems and general equation forms converted into different problem equations. Oil spreading equation is advection-diffusion type PDE. Therefore, we decided to use the interface of Coefficient Form PDE in 2-D workspace of COMSOL reduced to advection-diffusion equation with the time dependent study. The equation in this interface is given as:

$$e_a \frac{\partial^2 h}{\partial t^2} + d_a \frac{\partial h}{\partial t} + \nabla(-c \nabla h - \alpha h + \gamma) + \beta \nabla h + \alpha h = f \quad (44)$$

$e_a, \alpha, a, \gamma = 0, d_a = 1$ and c is selected as coefficient inside the gradient in Eqn. 36. β is assigned as %3 of wind speed or zero and f is oil addition onto or escape from the surface. As it can be interpreted from the comparison of Eqn. 36 and 44, Eqn. 44 can be converted into advection-diffusion equation with these assumptions. So, generalized form of the spreading advection equation for our cases will be written as:

$$\frac{\partial h}{\partial t} + \beta \partial h = f + \nabla \left(\left(\frac{g' \rho}{k} + \frac{2\gamma}{k h_{max}^2} \right) h^2 \nabla h \right) \quad (45)$$

4.3.1 Source Term Definition

In COMSOL, f is also taken as zero in Eqn. 45 for instantaneous and continuous releases. Normally, it is a true assumption for instantaneous spills with the elimination of weathering processes. However, for continuous spills, we need a source term. If f was not zero for the continuous releases, it would add oil into system from the beginning to the end of simulation. However, we want to add oil for limited time periods to observe the long-term spreading after the end of release. Therefore, an additional source function is defined and limited by demanded periods of time in

COMSOL as it can be illustrated in Figure 4.4 for 600 seconds leakage from the beginning of simulation. The triangular function represents the varying rate of oil leakage whereas rectangular function corresponds to the constant rate of oil leakage on the sea. The functions are expressed as thickness change because the unit of every term in Eqn. 45 is m/s. The area under the curves becomes equal to the total spill volume per source area represented as the thickness change. For example, $1 \text{ m}^3/\text{s}$ oil leaks for 10 min from a source having 2 m^2 area. Total spill volume is 600 m^3 at the end of leakage, but it is implemented into the model as thickness increase of 0.5 m/s .

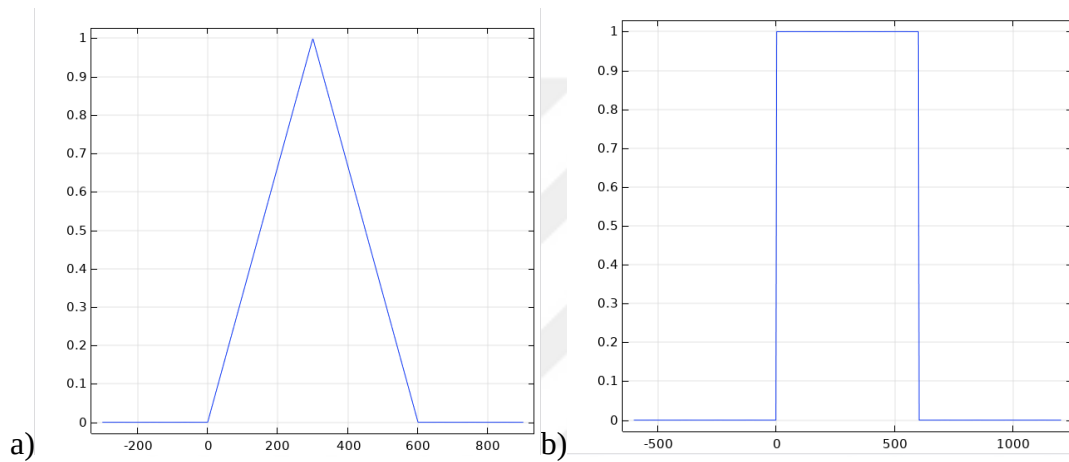


Figure 4.4: a) Triangular and b) Rectangular Functions of Source Term for Continuous Spills

4.3.2 Initial and Boundary Conditions

Describing the moving boundaries of oil can be only possible by creating a large and fixed container (sea) in an Eulerian model instead of limiting the domain to initial oil contaminated area. So, rectangular problem domain is created as a piece of sea surface in COMSOL. Oil leaks from a circular source placed to the center of workspace. Circle radius is computed from Eqn. 30 at $t=0.1$ sec. The configuration of region can be seen in Figure 4.5a. For finite element model, initial and boundary conditions must be given. Initial condition is specified as initial thickness from Eqn. 32. In addition, whole problem domain (sea surface) has four boundaries required to

be specified. For this reason, these boundaries are specified as zero flux-Neumann boundaries since oil inlet or outlet is not encountered around the sea boundaries. The region can be meshed by COMSOL with only selection of element size by physics controlled mesh. The region after applying the mesh can be seen from Figure 4.5b. The suitability of this meshing and element size determination with modeling data will be discussed in Result and Discussion part.

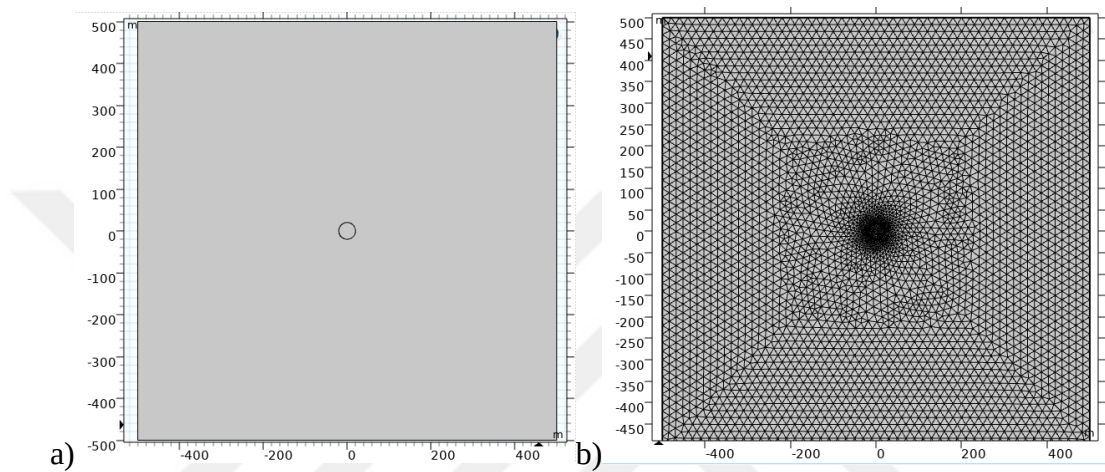


Figure 4.5: a) A Part of Sea with Leaking Oil Source and b) Meshed Appearance of the Region

CHAPTER 5

RESULTS AND DISCUSSION

The section starts with analysis of element size of COMSOL and validity check of COMSOL by an instantaneous release case. And then, results of COMSOL and our code are checked against the exact solution (Eqn.30) and asymptotic solutions(Eqn.34 and 35) of instantaneous spills. The suitability of numerical solutions for continuous releases is ensured by an experiment of oil with non-waxy content, conducted in SINTEF. The study also contains experiments of waxy oils which we try to match in our models with high drag coefficients. Besides, parametric analyzes for continuous and instantaneous oils spreading are conducted with a series of scenarios. After that, the slick behavior with convective forces is analyzed to observe the complete fate of horizontal oil displacement on the surface. Thereafter, we see how our model performs compared to a software created by SINTEF. At the end of the section, the pros and cons of code are discussed.

5.1 COMSOL Numerical Parameter and Validity Check for Oil Spreading

Domain meshing in COMSOL is done by the physics controlled mesh suggesting a structure computed by the elements. Only mesh size is assigned by user in this type of mesh. COMSOL benefits from the triangular elements for our problem. The analysis of element size assignment is demonstrated in Figure 5.1 for spreading of instantaneous oil spill under gravity and surface tension viscous regimes. The case parameters are given in Table 5.1. Greater the element size, greater the spreading of oil than forecasted by Nihoul method (Eqn.30). This can be explained based on the numerical diffusion creating additional spreading of data. The domain meshing with normal or coarser elements causes to difficulty of catching the drastic thickness changes around the oil boundaries. In addition, numerical diffusion periodically

emerges with the coarser elements in COMSOL. It can be interpreted as numerical diffusion occurs prominently when the oil edges step into the next element. The increasing distortion of slick circular shape with increasing element size can be comprehended from Figure 5.2. Instead of physics controlled mesh, user controlled mesh can be used to have locally fine elements for boundaries to accelerate the computation time of model with accurate results. However, since the model of extremely fine elements is accurate enough for oil spreading and computation time is not too much, we preferred physics controlled meshing with extremely fine elements and implemented for the remaining analyzes.

Table 5.1: Used Parameter Values for Instantaneous Spill

Input Parameters (symbol)	Values (unit)
Initial spill Volume (V_o)	150 (m^3)
Oil Density (ρ_o)	890 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.003 ($kg/(m^2 s)$)
Surface Tension Parameter (γ)	0.03 (kg/s^2)

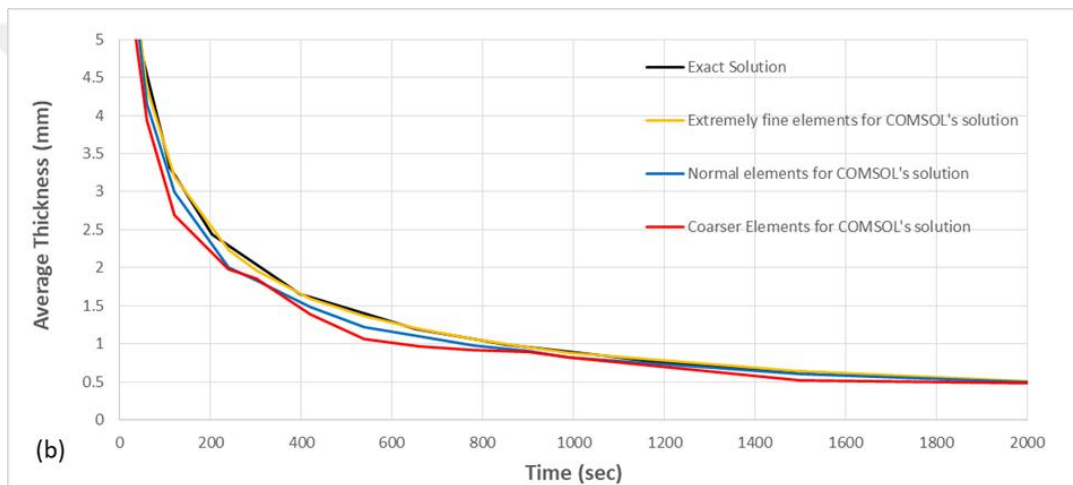
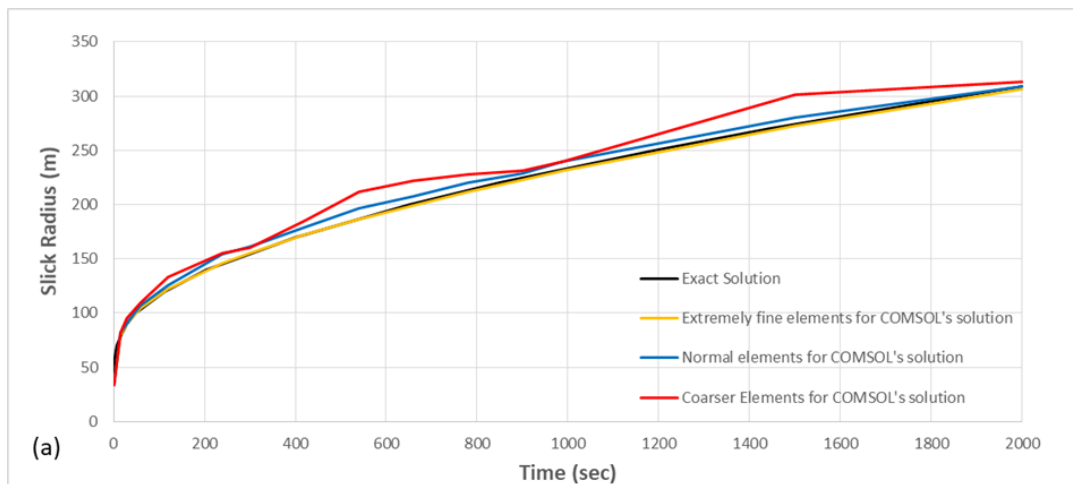
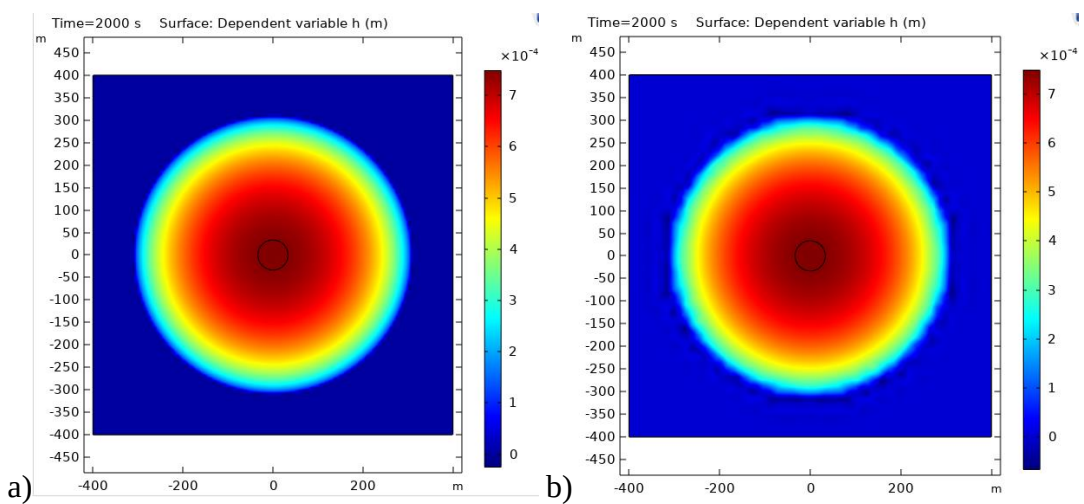


Figure 5.1: a) Slick Radius and b) Average Thickness Progresses in Time



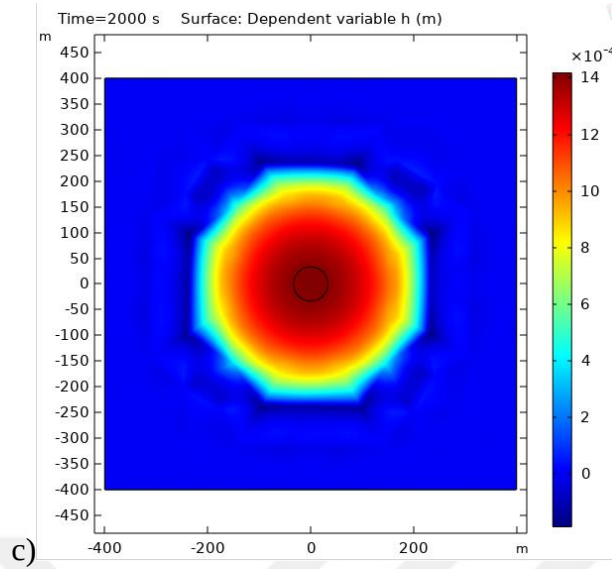


Figure 5.2: Oil Contaminated area at $t=2000$ sec a) Extremely fine elements b) Normal elements c) Coarser Elements

5.2 Instantaneous Spill Spreading with Gravity and Surface Tension Viscous Regimes

Same case stated in Table 5.1 is studied for the instantaneous release of oil with our algorithm employing 1000 particles and time steps of 0.1 seconds increasing to 100 seconds. Asymptotic solutions (Eqn. 34 and Eqn. 35) are added to the analysis. They help to observe the transition between the gravity and surface tension-viscous regimes, and to see the spreading rate difference under the regimes by considering the slopes of asymptotic solutions. It is easy to notice the rate difference with log-log plot of radius vs time shown in Figure 5.3. Oil spreads more rapidly under the surface tension regime compared to the gravity viscous regime. It can be confirmed by a quantitative comparison of the slopes of asymptotic solutions. The slope of first asymptotic solution for gravity viscous regime is calculated as 0.265 m/sec while the slope of second asymptotic solution for surface tension regime is found as 0.41 m/sec. There is a transition zone between the asymptotic solutions. Using these solutions with their intersection leads to the underestimation of the radius in the transition interval. However, it provides a good prediction with enough accuracy for

the slick behavior at most of the time. Our algorithm results match with all of other solutions well. So, the case confirms that COMSOL and our code solutions can successfully carry out the cases of instantaneous spill. With implementation of surface tension regime to Durgut's algorithm (2017), oil spreading is precisely estimated in the long-term. Figure 5.4a and 5.4b of numerical solutions clearly show that oil spreads by forming the circular shape and the oil distributions put by COMSOL and our code are similar. The particle intensity around the center in code and the red color at the same locations in COMSOL express that the mass center of oil is not moved under the advection-free environment. It can be said that COMSOL and code reflect the instantaneous spill behavior on the sea well, defined in Nihoul's method. In addition, the distribution of oil particles with decreasing intensity from the center agrees with the oil spreading related to diffusion. So, particles are moved from higher intensity to lower ones with normal distribution. The Gaussian random distribution of particles can be seen at 90 seconds as shown in Figure 5.5. COMSOL and exact solutions coincide. The particle distribution of our code fits the profile defined by these solutions. Some significant fluctuations in particle elevations are observed. However, they are within acceptable range ensured by the solution accuracy for the time development comparisons of thickness and radius demonstrated in Figure 5.3. Here, it is important to declare that the fluctuations were greater and are reduced by assigning the cell thickness as area weighted average of thickness from current and surrounding cells.

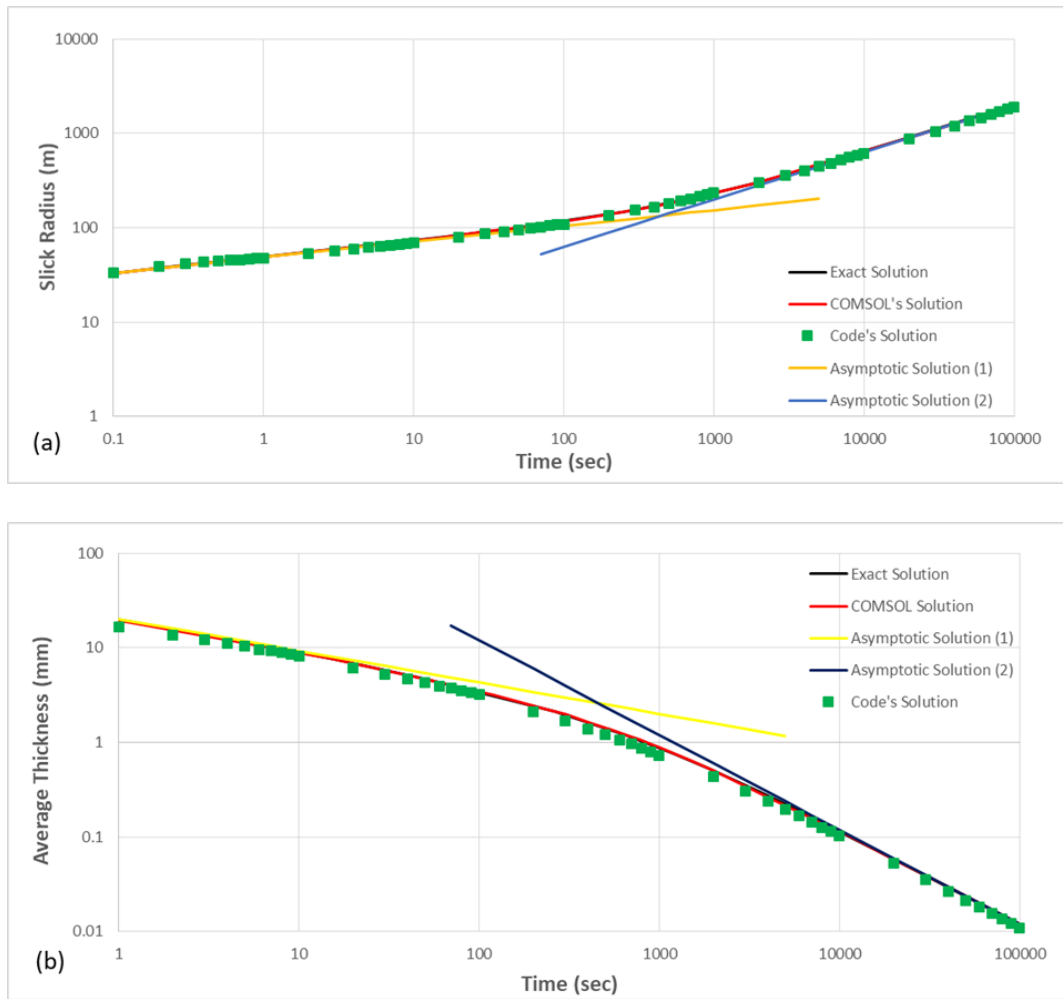


Figure 5.3: a) Slick Radius and b) Average Thickness Progresses in Time

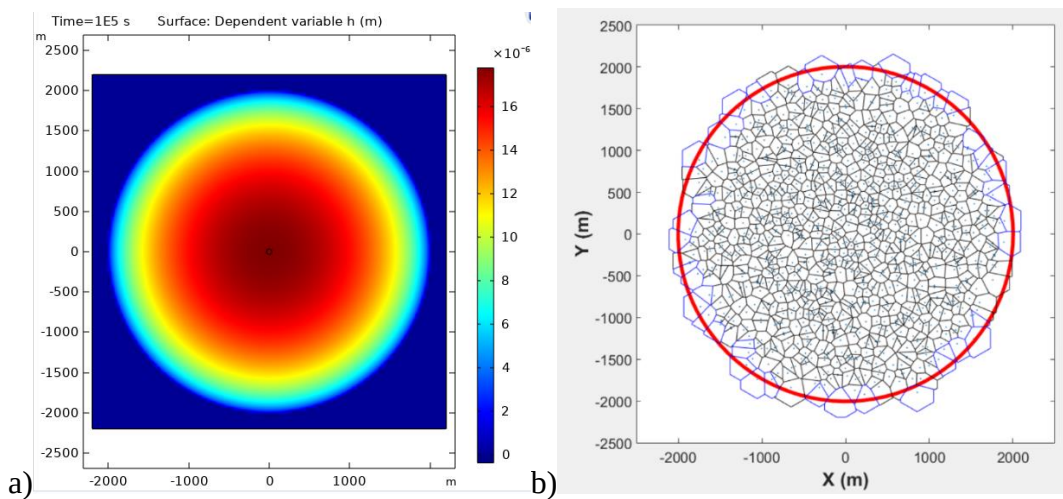


Figure 5.4: Oil Contaminated Area at 100000 seconds in a) COMSOL b) code

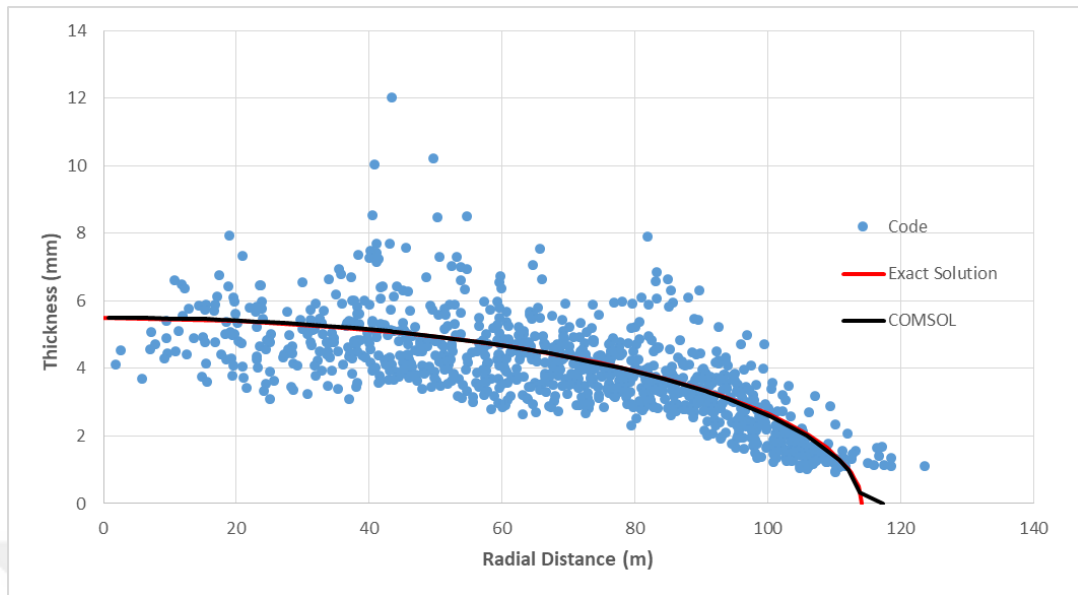


Figure 5.5: Particle Distribution of Solution in Code Compared with COMSOL's and Exact Solutions at 90 seconds

The slick profile can be investigated from Figure 5.6 which is the output of COMSOL. As time progresses, slick spreads and becomes thinner and thinner on the surface. It conserves its circular shape and its distribution of thick portion at the center tracked by thin portion of oil. A visual investigation of oil spreading in Figure 5.6 can reveal which force regime takes place for oil spreading at a time. The examination of Figure 5.3 and 5.6 together states that oil spreading continues with gravity viscous regime at 200 sec. Slick is highly concentrated around the center. It makes the surface tension interactions negligible since cohesive forces of oil molecules closer to each other are stronger. Oil tends to go to downward due to gravitational effect. Also, oil spreads under the surface tension regime at 2000 sec. Slick has a flatter distribution on the surface. Surface tension effect becomes effective with negligible gravity effects on the very thin oil. Oil spreads with the surface tension attractions driving to reduce the thickness spatial variations.

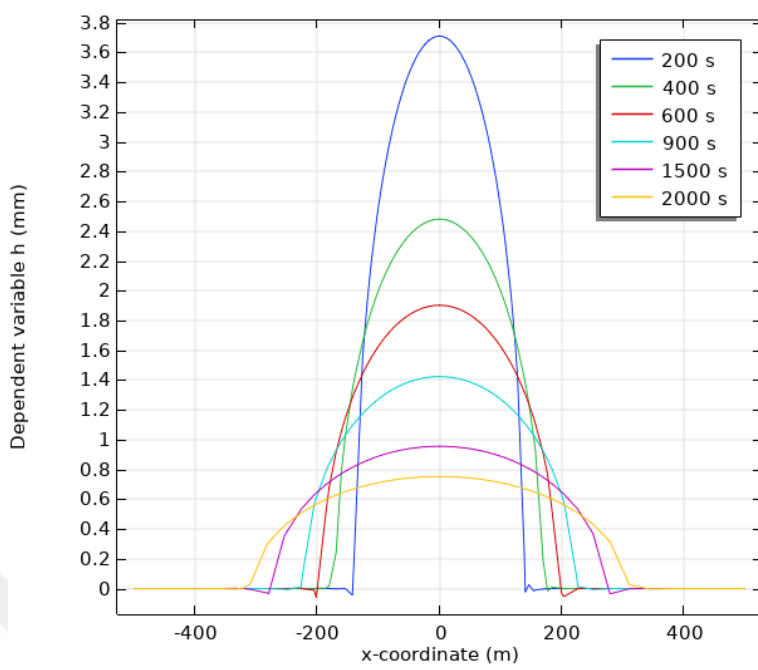


Figure 5.6: Slick Distribution on the Sea @ t=200, 400, 600, 900, 1500, 2000 Seconds

The analysis on the number of particles indicates from Durgut (2017) study that optimum results are gained with 1000 particles in the contexts of computational time and errors. So, same number of particles is run for instantaneous spills in the study. Time steps are gradually increased from 0.1 seconds to 100 seconds for the simulation time of 100000 seconds again based on Durgut (2017) study.

5.3 Continuous Spill Spreading with Gravity Viscous Regimes

Continuous oil spreading in Nihoul's method is not defined by any analytical or asymptotic solutions. The omission of sink/source term for Nihoul's analytical solution makes the solutions merely appropriate for instantaneous spills. Therefore, we decided to confirm our numerical solutions through the experiments conducted by Brönner et al. (2018). Brönner et al. claimed that slick experiences only gravity-viscous spreading during the observation. So, their experimental cases are suitable for the comparison, since our algorithm works with only gravity-viscous spreading of continuously released oil.

Actually, only the experiment of non-waxy oil (Marine Gas Oil) can be used for the solutions of classical models since other waxy oils require a new term for the retarding effect of yield stress of waxy compounds into the force balance of gravity and viscosity. Nevertheless, we think it is better to see spreading of the waxy oils with our model. The retarding effect of yield stress will be reflected in the viscous term of the numerical models. Viscous forces are expressed as the frictional forces by a parameter of drag coefficient in Nihoul's model. Therefore, we tried to find the solutions for these fluids by trial error method to assign proper drag coefficient.

The exhaustive analysis are presented for Marine Gas Oil starting with Figure 5.7. The case parameters are given in Table 5.2. 20 particles are released for every second with totally 2400 particles. COMSOL and the algorithm provide a good solution for the slick radial extent for most of the time, but some deviations among the numerical solutions and experimental study appear during the leakage. The modeling conditions can be one of the possible reasons of the deviations. Oil leaks from a source close to the surface in the experiment. However, COMSOL and code allows only oil leakage from the surface with their 2D workspace. Furthermore, the deviations can occur due to the model itself. A mathematical model can describe a real process with some acceptable errors. These errors can arise from the limitations of our numerical models or Nihoul's model while handling continuous or small spills. Other reason can be related to the leakage rate. Equal amount of oil is added into the system for every second in the numerical solutions, but it is not claimed in the experiments. The rate can fluctuate during the release for a real case. As another factor, slick radius is not measured in the experiments. They find it by an assumed thickness profile correlated to the measured radial extents where 0.5, 1 and 2 mm oil thicknesses are observed. As a result, the curves can differ in some points due to one or more of the above factors. However, spreading of a continuously released oil is sufficiently reflected in our models.

The average thickness progress in time is not observed in Brönner et al.'s study. Therefore, we only compared our numerical models with each other. Figure 5.8 shows that code similarly estimates the thickness with COMSOL. However, the code

takes a time to stabilize the data due to the initial condition of randomness of particle locations and scantiness of particles in the first times of oil leakage. Therefore, some fluctuated data is initially observed. It can be inferred that COMSOL initially provides more stable solution than the code does. In addition, same figure reveals that slick average thickness on the surface is conserved during the oil leakage. Slick thickness is reduced while spreading, but the oil flux into the system increases the slick thickness. In total, slick thickness is conserved. It can be the indication of the slick build up around the center. So, the gradual increase in central thickness during the release supports the idea from Figure 5.9. It can be more comprehensive when we look at Figure 5.10. The central thickness increases, and then decrease, beginning from the end of leakage. The slick profile looks different than the profile for the instantaneous spill case. The peaks at the center and ridges close to the slick edges are observed during the release. The distribution resembles the instantaneous distribution after release. The central peak is flattened. The ridges disappear with smooth distributions.

Maximum thickness is calculated with the average thickness data of code as a function of the time and average thickness during leakage. Eqn. 33 can be implemented after the leakage, since the spill resembles to instantaneous spills.

Table 5.2: Used Parameter Values for Continuous Spill

Input Parameters (symbol)	Values (unit)
Total Spill Volume (V_o)	0.004 (m^3)
Spill Duration	120 (s)
Density of MGO (ρ_o)	846 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.07 ($kg/(m^2 s)$)
Total number of particles	2400

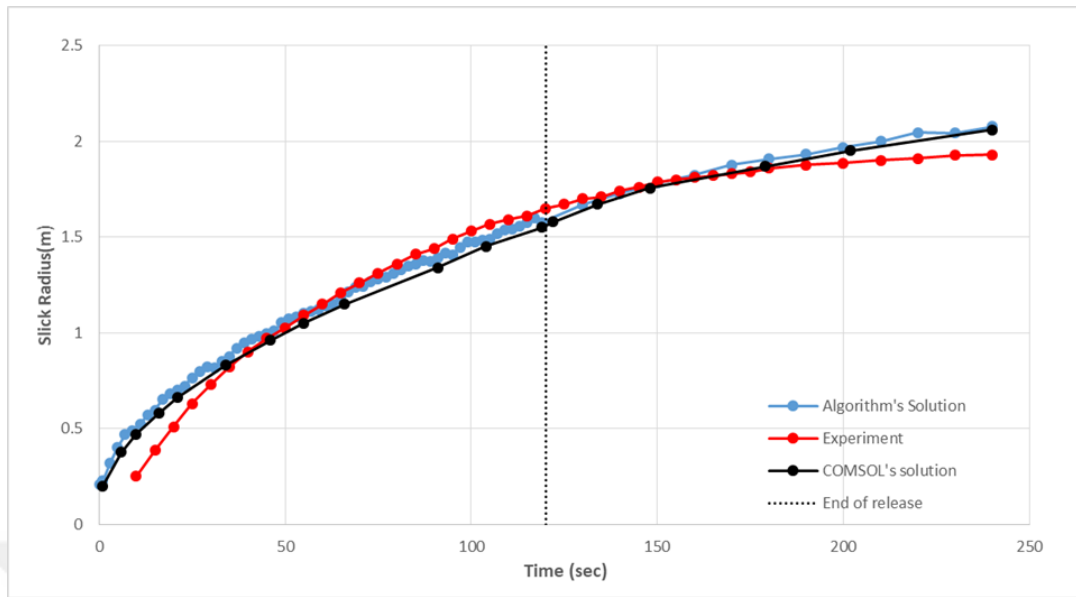


Figure 5.7: Slick Radius Progress in Time

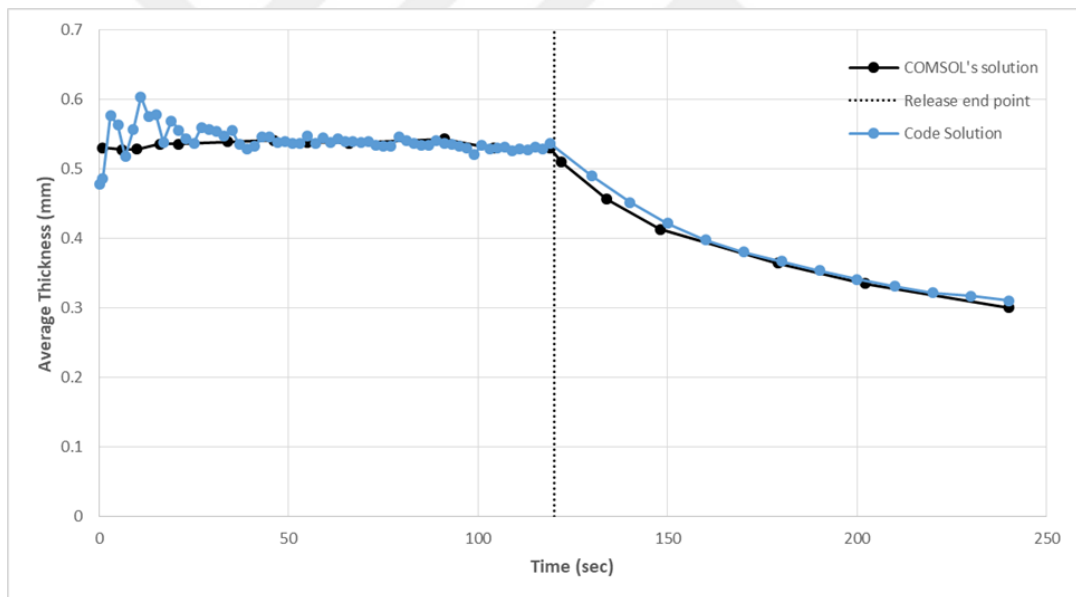


Figure 5.8: Average Thickness Progress in Time

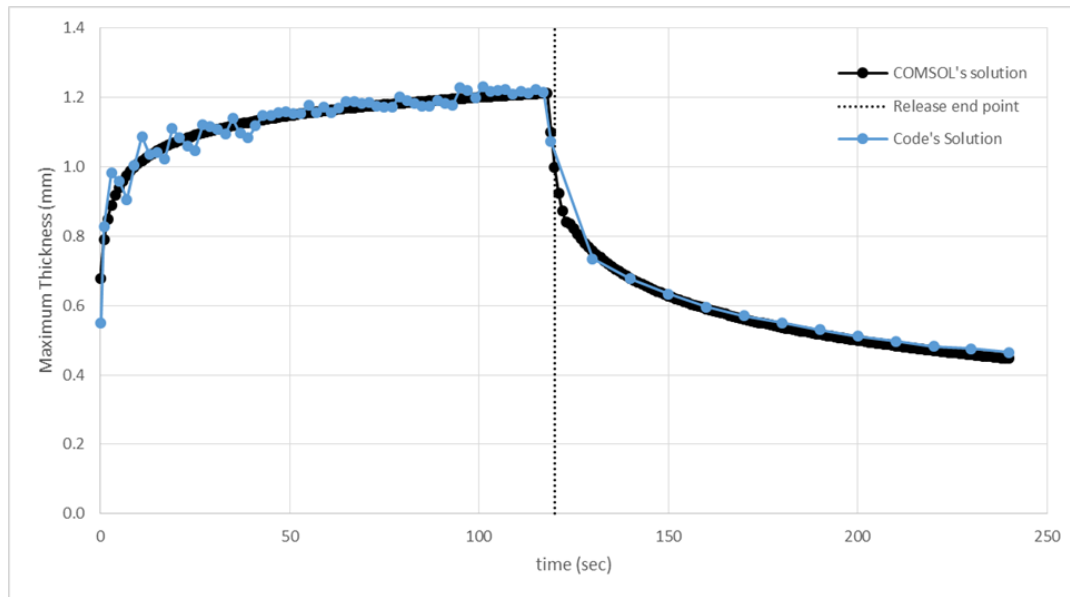


Figure 5.9: Maximum Thickness Progress in Time

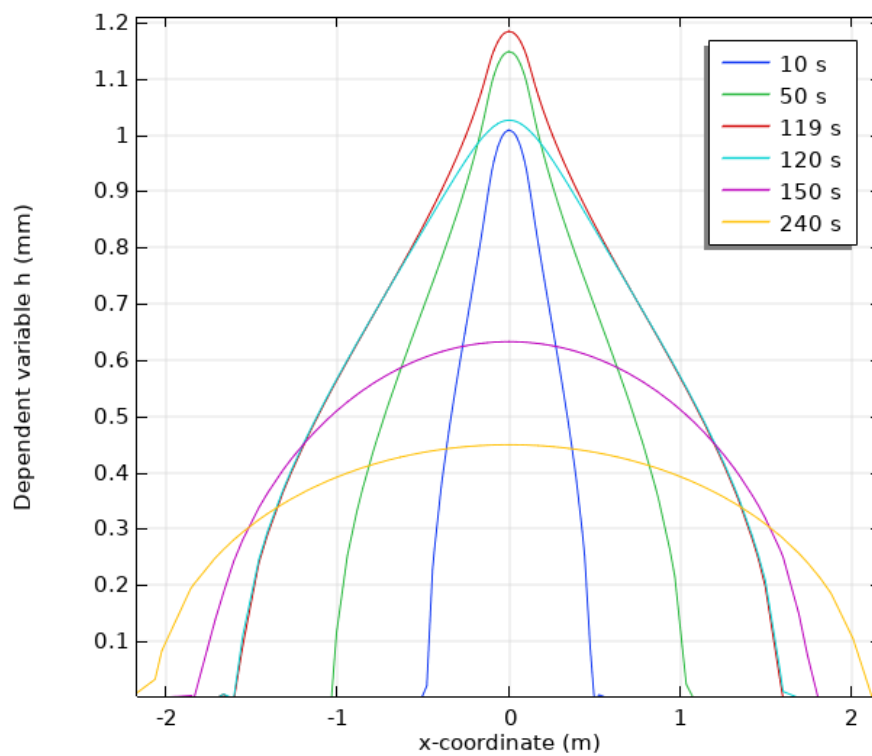


Figure 5.10: Slick Distribution from Cross-Sectional View on the Sea @ $t=10, 50, 119, 120, 150, 240$ Seconds

The prediction of slick oil distribution is shown in Figure 5.11 belonging to the end of simulation. High intensity of particles and red color is followed by the reduced number of particles and blue color close to edges in code and COMSOL respectively. They indicate that the central thick oil is trailed by thinner layer. According to the particle distribution presented in Figure 5.12, the particles follow the trend of COMSOL solution at 95 seconds. The ridge towards to slick edges, flat part observed in the middle section and the peak close to the center are prominent in the code. The transition among the regions is perceived by the changing trends of particle distributions in the figure.

Figure 5.13 illustrates the snapshots of oil distribution at the intermittent times in the code. The scale and boundary of workspaces are kept same to help notice the slick evolution in time. New particles are produced at the center while oil spreads to the greater surface area. The introduction of new particles stops at 120 seconds, end of leakage. The oil flux can be observed through the increase of number of particles during the leakage in the figure. The particles are only spread for the remaining times.

We tried to find the solution to the waxy oils in Figure 5.14. The retarding effect of yield stress is expected to be compensated by higher drag coefficients. But higher wax content creates pronounced ridges on the curves which cannot be satisfied by the classical models. A new term is required in the force balance equation as Brönner et al. (2018) stated. For future, we want to add a suitable term substituting the yield stress effect. Our criterion for the term will be obtaining the approximate results to the experiments. We will try to transform the term expressing yield stress in Brönner et al. study to the proper form in Nihoul's model.

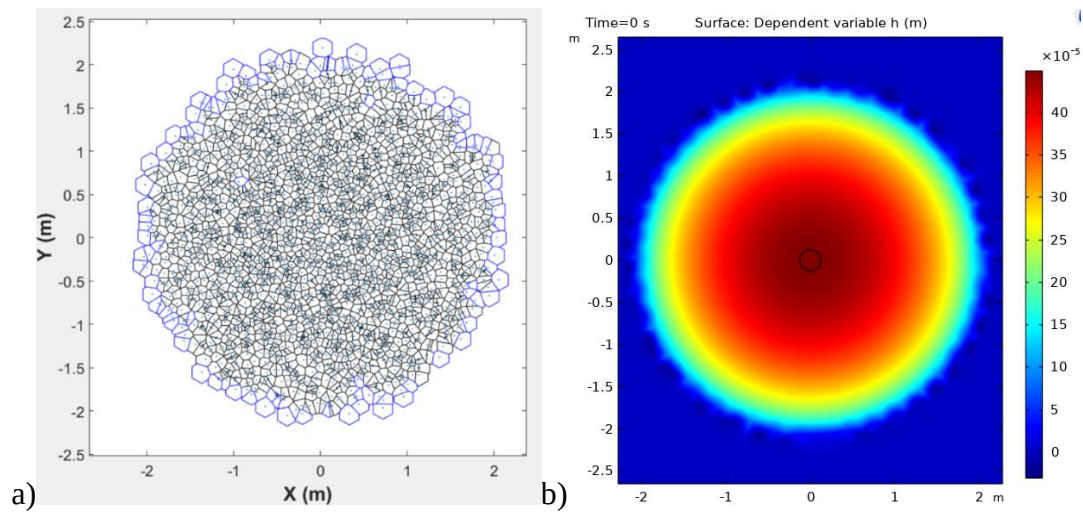


Figure 5.11: Oil Contaminated Area at t= 240 Seconds in a) Algorithm b) COMSOL

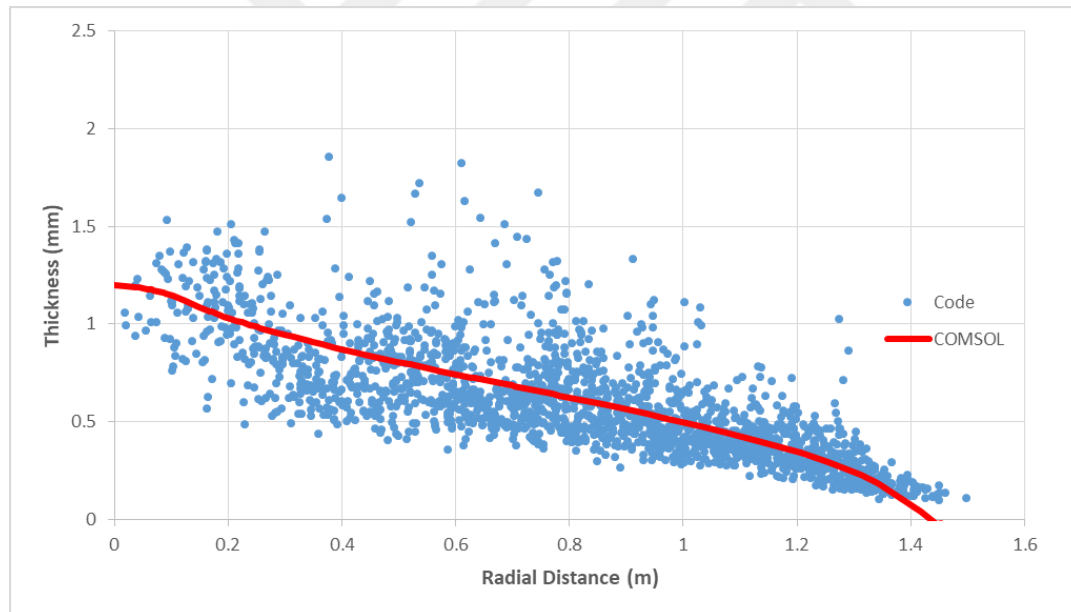


Figure 5.12: Particle Distribution in Code Compared with COMSOL's Solution at 95 sec during the leakage period

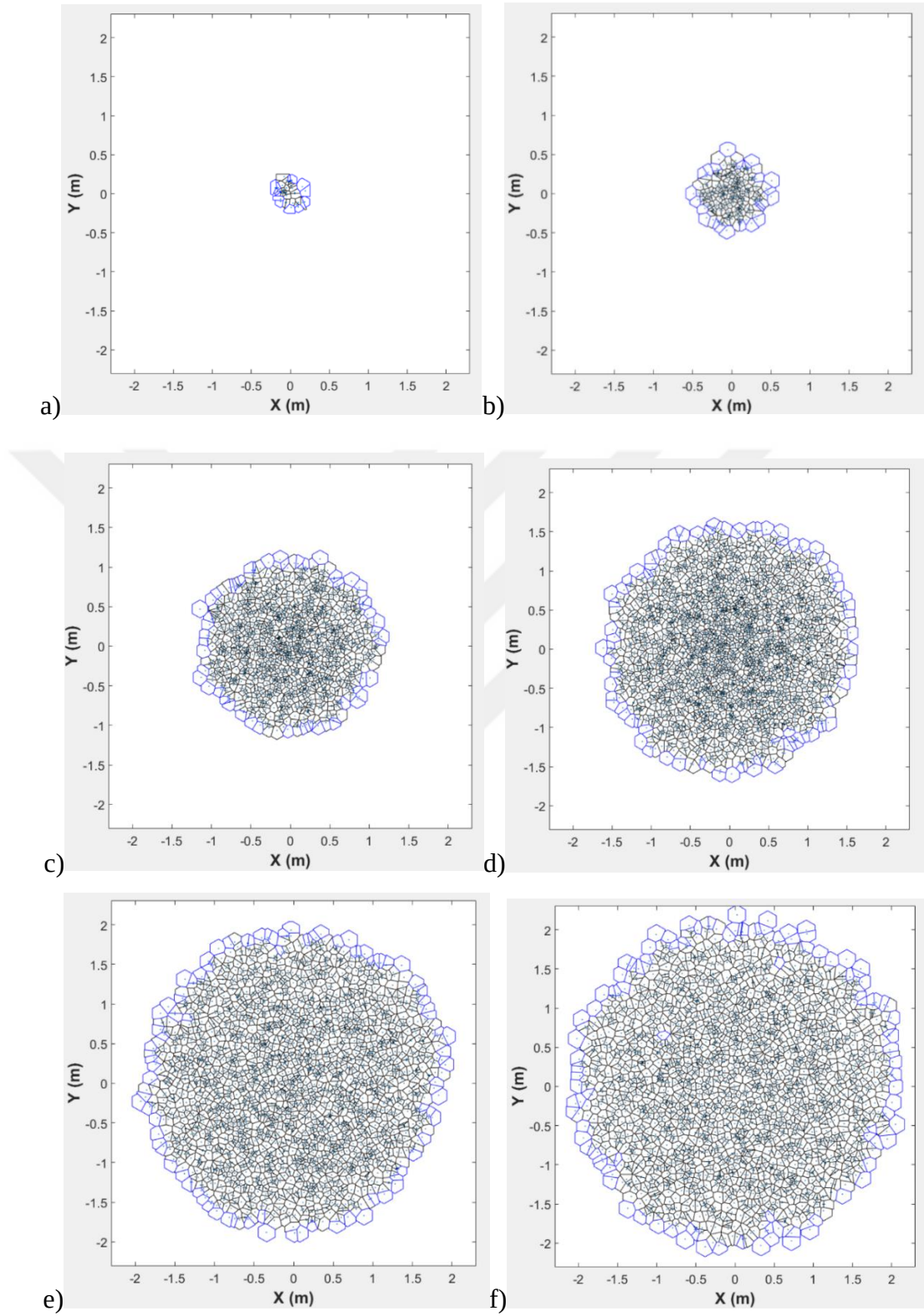


Figure 5.13: Slick Evolution Observed at a) $t=1$, b) 10, c) 60, d) 120, e) 180 and f) 240 seconds

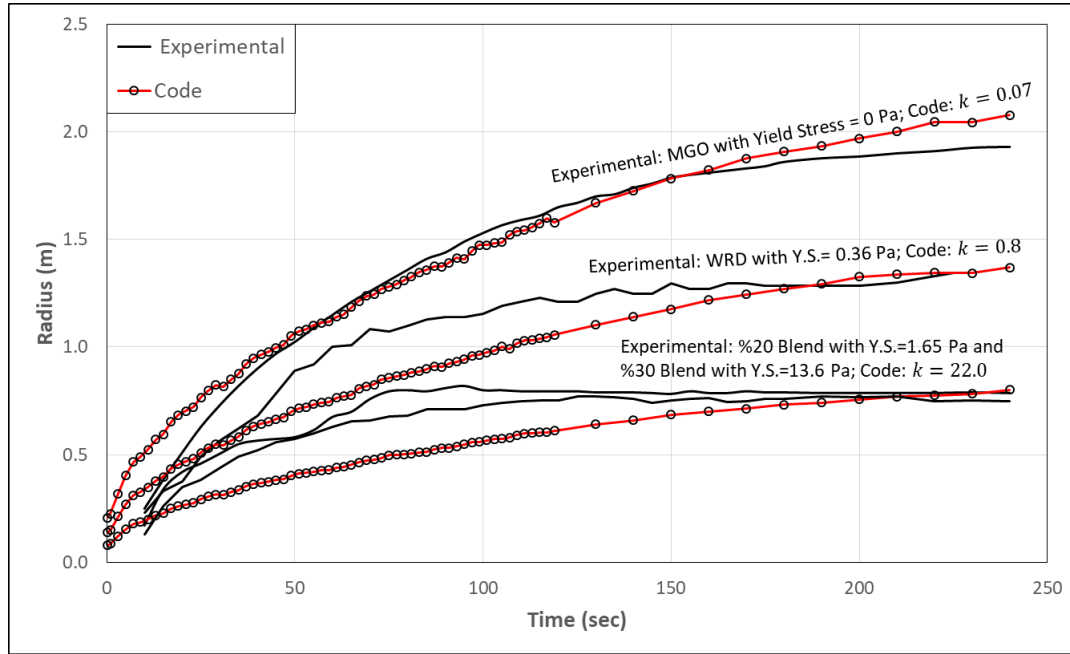


Figure 5.14: The Prediction of Waxy Oil Radius Progress in Time (Yield stresses of waxy oils were measured from oscillating rheometer by Brönner et al. (2018))

5.4 Selection Methodology of Radius, Average & Maximum Thicknesses and Numerical Parameters in the Algorithm

Durgut (2017 and 2020) suggests some selection criteria for radius and thickness of instantaneous spills for the random walk based algorithm. Accordingly, radius is determined by the arithmetic mean of the radial distances of outermost particles. Average thickness is found from the total spill volume divided by the total cell area. And then, Nihoul's relation of average and maximum thicknesses (Eqn. 33) is applied to estimate maximum thickness. These selection methods perform very well for instantaneous spills. They are tried for continuous spills and compared with other possible methods in this section.

The algorithm with the earlier method suggested by Durgut (2017 and 2020) underestimates the radius of continuous spills in Figure 5.15a with parameters in Table 5.3. However, it is acceptable with only %5 deviation from the radii estimation of COMSOL. New methodology is the calculation of slick radius as the summation

of average outermost cell radii and the average radial distance of outermost particles at the simulation time. It provides solution closer to COMSOL solution in Figure 5.15a. The usage of new methodology is reasonable because whole Voronoi diagram is taken into account by considering the outermost particles and their cells for radial extent instead of only the outermost particles. Although it is not certainly required, it is preferred in this study.

Average thickness calculation is examined with previous and new criteria in Figure 5.15b. The solution with earlier method significantly deviates from COMSOL's solution during the release period. The gradual increase of average thickness in code with the method can be the sign of the solution trying to catch the stabilized real thickness by the data. Underestimation of average thickness arises from the estimation of slick radius with slight differences, randomness of particles and low number of them in the beginning. The insignificant differences in estimated slick radius lead to great changes in thickness. In addition, new particles are randomly introduced into the system without having a pattern. It reduces solution accuracy of the code until data is stabilized. Furthermore, we add five particles per second that is very low to initially define the spreading for this case. The initial cell radii becomes too high with low number of particles for outer cells, causing predicted thickness to be lower. So, we can observe errors for the thickness determination with old methodology. Increasing the number of particles per second to reduce the errors will cause high computational time. Therefore, we excluded outermost cells for the thickness calculation in the new methodology. Hence, the average thickness is computed through the total interior cells' volume divided by the total area of these cells. The numerical solutions by it produce similar output with COMSOL. As another methodology, average thickness can be directly calculated from Eqn. 32 after finding radius, but we want to utilize from the features of our code for every calculations, so former new methodology will be preferred.

The new methodologies for radius and average thickness are also tried with instantaneous spills. The accuracy of solution reduces compared to earlier

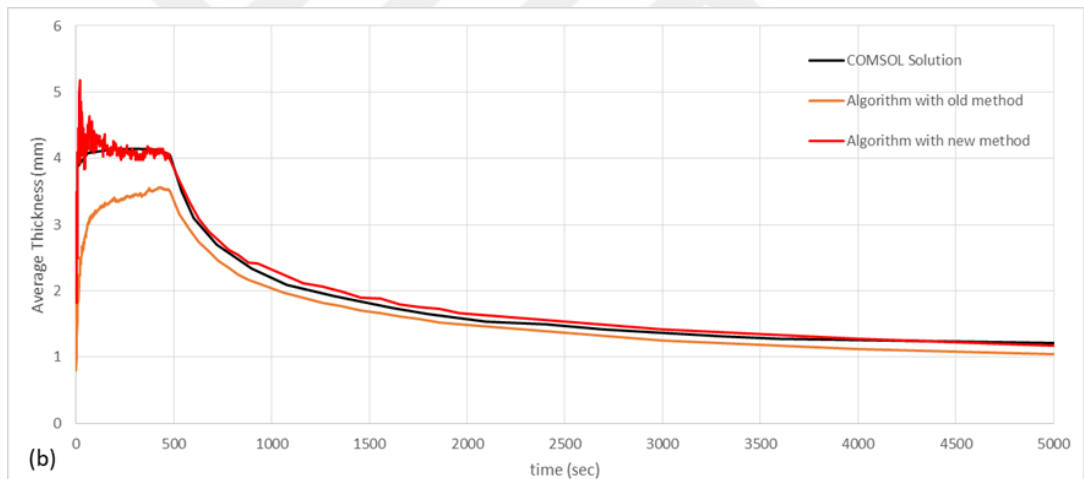
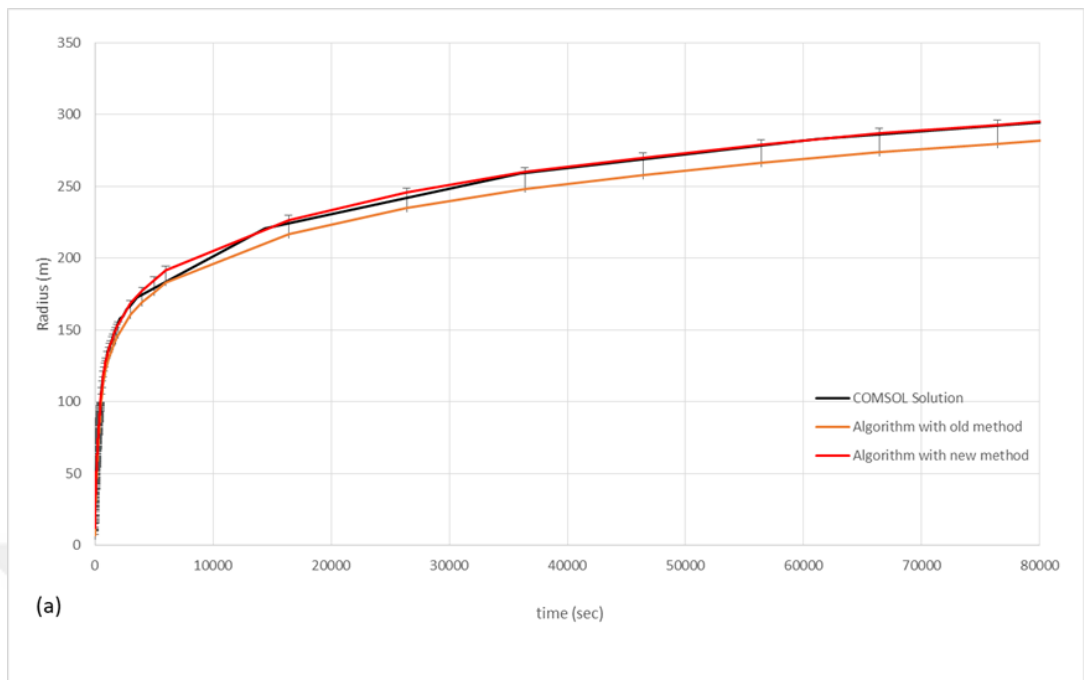
methodologies suggested by Durgut. However, they are in acceptable ranges with the errors lower than ten percent.

Maximum thickness cannot be obtained from Eqn. 33 for continuous spills having unique profiles as a function of the oil rate. Eqn. 33 is proposed for instantaneous spills. It can be applied for continuous spills after release interval because continuous spills start to turn into instantaneous one at that moment.

Our future methodology will be proposing an empirical equation determining the maximum thickness based on the comparisons with COMSOL for a variety of cases. It is actually required for the implementation of surface tension regime to the algorithm using the maximum thickness in diffusive length (Eqn. 43). For this case, the multiplier of average thickness is gradually increased from 1.8 to 2.3 in the leakage interval seen in Figure 5.15c. Eqn. 33 with the multiplier of 1.5 is used for the remaining part.

Table 5.3: Used Parameters for the Test Case of Continuous Spill

Input Parameters (symbol)	Values (unit)
Total Spill Volume (V_o)	120 (m^3)
Spill Duration	480 (s)
Density of MGO (ρ_o)	890 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.003 ($kg/(m^2 s)$)
Total number of particles	2400



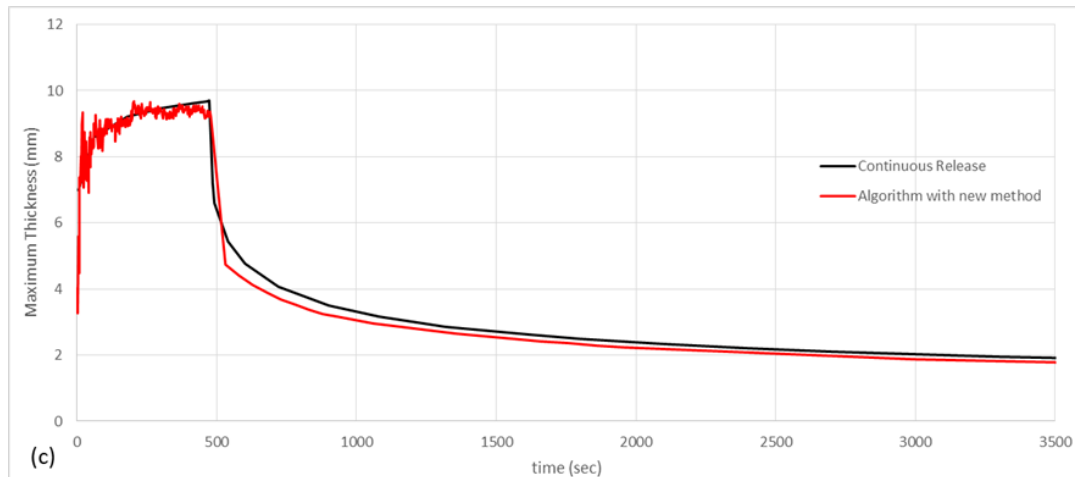


Figure 5.15: a) Radius ($\bar{r}$): Error Bar with the Range of 6% Percent), b) Average Thickness c) Maximum Thickness Progresses in Time

5.5 Effects of Slick Parameters on Spreading of Instantaneous and Continuous Spills

The oil properties, oil-water interactions and discharge type change the spreading area and thickness profiles. The increment or decrement of these parameters can create the similar trends in the series plots of thickness and radius on a log-log scale. However, these parameters can lead to the different spreading behavior by causing the different oil contaminated area. In addition, parameters can shorten or lengthen the intervals of a regime. Parametric analyzes carried out for the instantaneous and continuous releases can give an insight for above issues.

5.5.1 Relationship between Initial Spill Volume and Oil Spreading

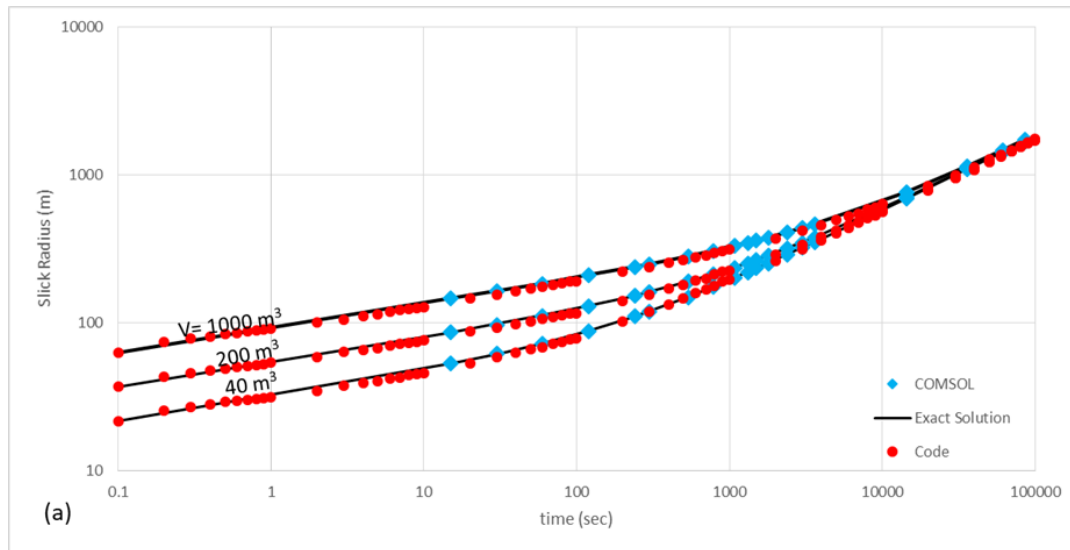
Initial spill volume is an important parameter especially for gravity-viscous regime spreading. We explained the gravitational effect on earlier sections. Oil tends to go towards slick edges due to gravity resulting in the slick spreading under gravity-viscous regime. Gravitational spreading will last until the thin oil layer on the surface is insignificantly affected from the gravitational force. So, massive oil spills can experience the gravity-viscous spreading for longer periods of time demonstrated in

Figure 5.16a with benchmark parameters of Table 5.4 for instantaneous releases. However, small spills with thin layers can pass to the surface tension regime earlier. Since spreading is faster in surface tension regime than gravity-viscous regime and is realized at the same rate in surface tension regime for all amount of oils, the coverage of these small spills can approach to coverage of the massive slicks after a while when both of them spreads under surface tension regime. In addition, slick behaves differently in gravity viscous regime having different radii, but the slick follows similar pattern with spreading rate having similar power of time in gravity viscous regime. The pattern similarity is realized by the parallel lines on it with almost same slopes. Also, the spill volume affects the gravity viscous regime. Its effect diminishes in surface tension regime. Lower volume of the oil has increasing spreading rate quickly in the latter regime.

When we volumetrically consider the coverage of same area of oils with different volumes, the thickness of greater amount of oil should be higher. It is shown in Figure 5.16b. The numerical solutions provide an accurate radius and thickness for instantaneous releases. Important conclusion from Figure 5.16 is that oils extend to the same ultimate area with different volumes under the surface tension regime when other parameters are kept constant. It can be confirmed from the asymptotic solutions (Eqn. 34 and 35). These solutions give the relation between the volume and spreading in gravity and surface tension regimes. Volume is not the driving parameter for surface tension regime. That information explains why the spreading rates of all volumes approaches to the same value in surface tension.

Table 5.4: Benchmark Parameters for Instantaneous Spill

Input Parameters (symbol)	Values (unit)
Initial spill Volume (V_o)	200 (m^3)
Oil Density (ρ_o)	890 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.003 ($\text{kg}/(\text{m}^2 \text{ s})$)
Surface Tension Parameter (γ)	0.025 (kg/s^2)



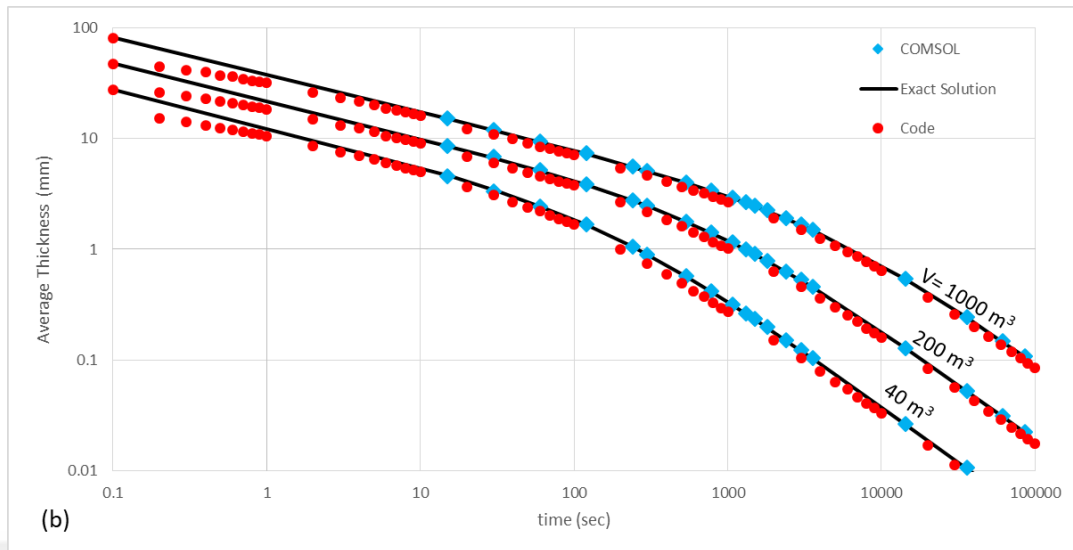


Figure 5.16: The Relationship between Initial Oil Volume and a)Radius b) Average Thickness Progresses of Instantaneous Spills in Time

The spreading pattern similarity of oils with different volumes is obtained in continuous spill cases with only gravity-viscous regime shown in Figure 5.17a. The benchmark parameters are shown in Table 5.5. The spreading rate is reduced at the end of leakage. So, oil leakage onto the surface creates additional spreading apart from the gravity effect. The average layer on the surface is conserved during the leakage for a variety of volumes in Figure 5.17b.

Table 5.5: Benchmark Parameters for Continuous Spill

Input Parameters (symbol)	Values (unit)
Total Spill Volume (V_o)	120 (m^3)
Spill Duration	240 (s)
Density of MGO (ρ_o)	890 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.003 ($kg/(m^2 s)$)
Total number of particles	2400

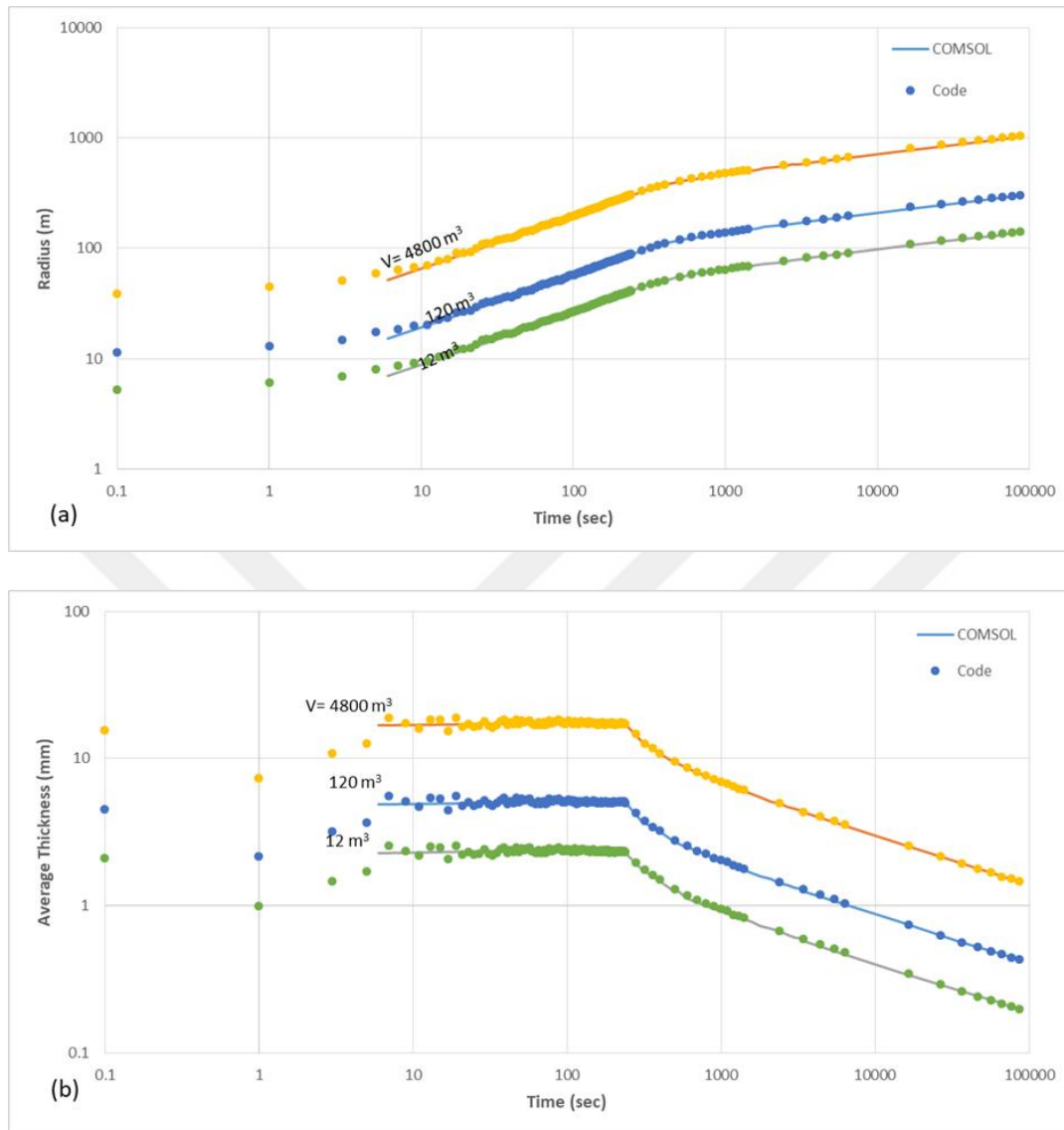
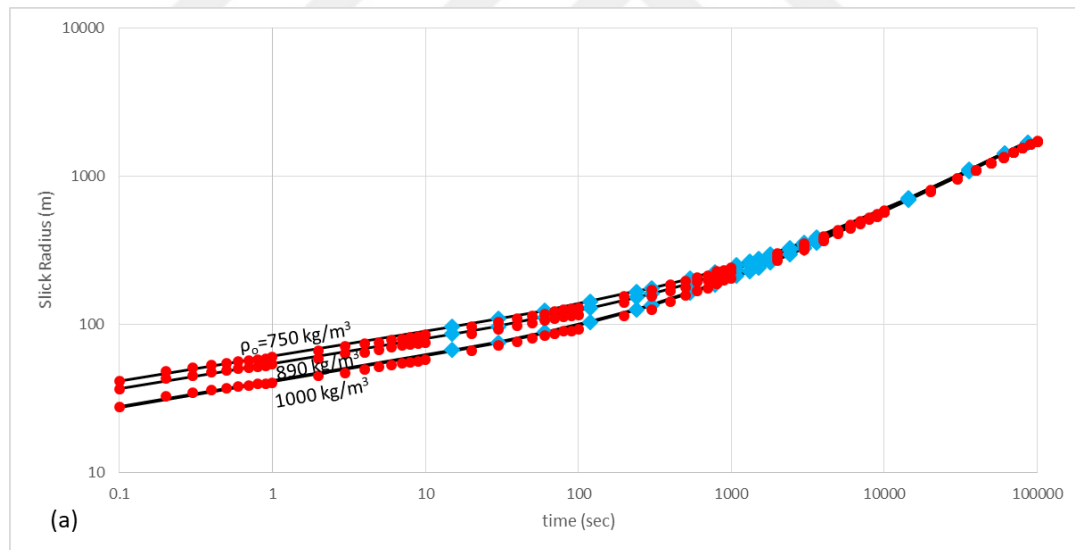


Figure 5.17: The Relationship between Initial Oil Volume and a)Radius b) Average Thickness Progresses of Continuous Spills in Time

5.5.2 Relationship between Density of Oil and Oil Spreading

Oil density is another parameter to be analyzed. It expresses the lighter and heavier fractions of an oil. When heavier components constitute a greater percentage of oil, it generally brings the more viscous and denser oils moving on the surface with retarded spreading. In addition, many researchers like Tkalic (2003), Fingas (2011) emphasize that denser fluids have higher oil-water interfacial tension with lower

surface free energy. So, frictional force and interfacial tension interactions could be changed with density change. Nevertheless, we want to conduct sensitivity analysis for only oil density in Figure 5.18a and other parameters used as Table 5.4 are kept constant. For instantaneous spills, as oil volume does, density affects the spreading, but its effect is limited with the limited change in density of oil. Lighter oils have the thinner layer on the surface in gravity viscous regime due to the greater spreading, but reaches to the same ultimate area and thickness in surface tension spreading regime. We can say that oil properties or leakage conditions alone are not as effective as oil-water interactions like friction and interfacial tension while oil spreading in the surface tension regime. It can be approved from the asymptotic expansions of Nihoul model (Eqn. 34 and 35). For continuous releases, oil density changes the slick radii and thickness during and after the leakage in gravity viscous regime in Figure 5.19. Again, average thickness is balanced by the oil flux and spreading in leakage periods.



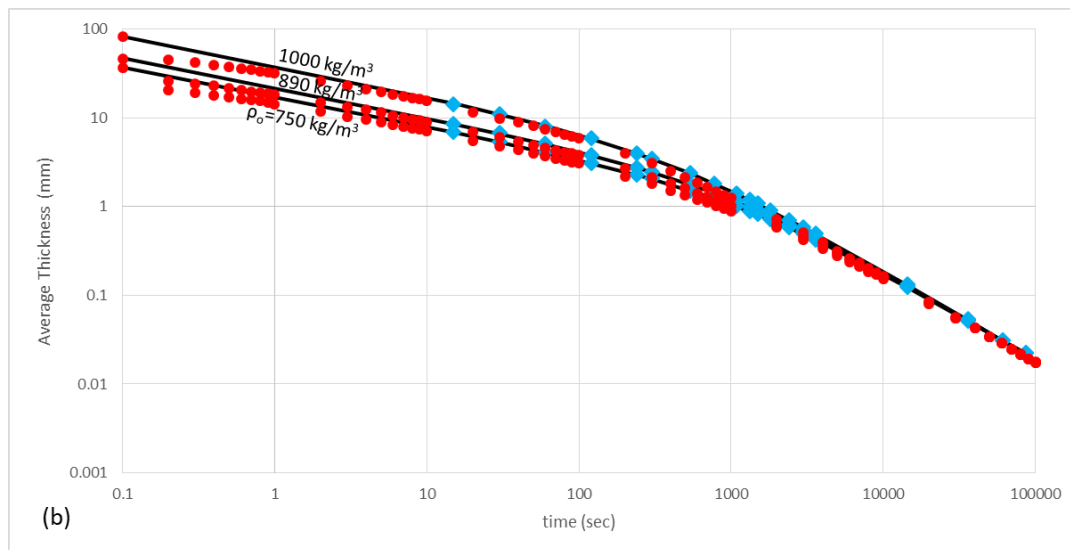
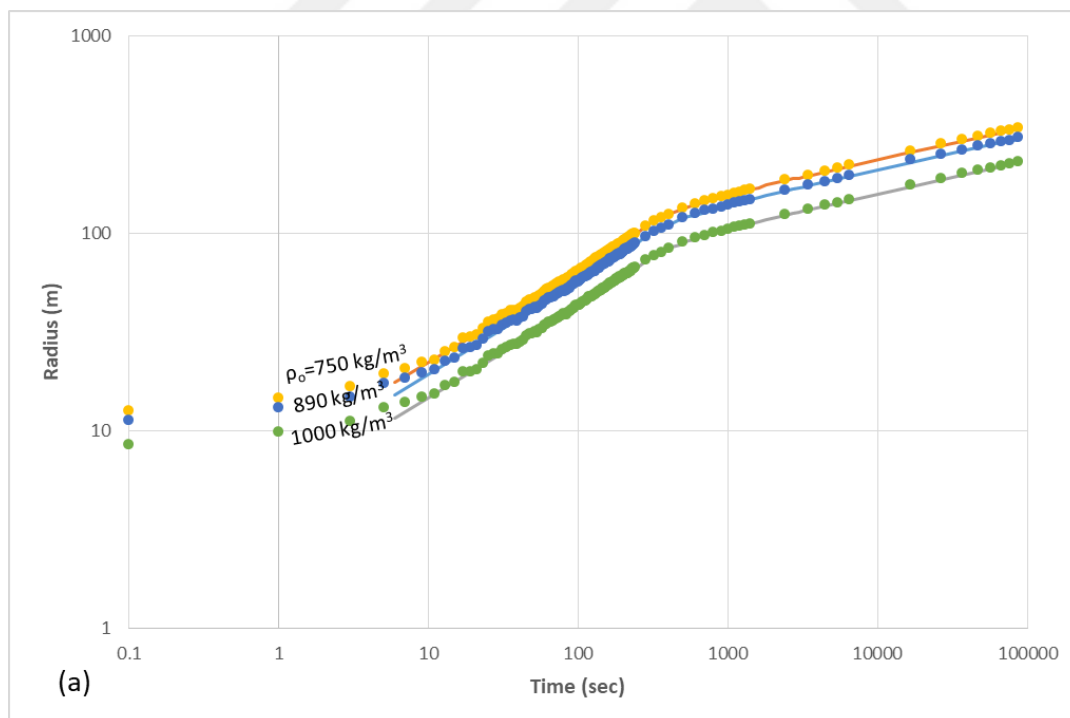


Figure 5.18: The Relationship between Oil Density and a)Radius b) Average Thickness Progresses of Instantaneous Spills in Time



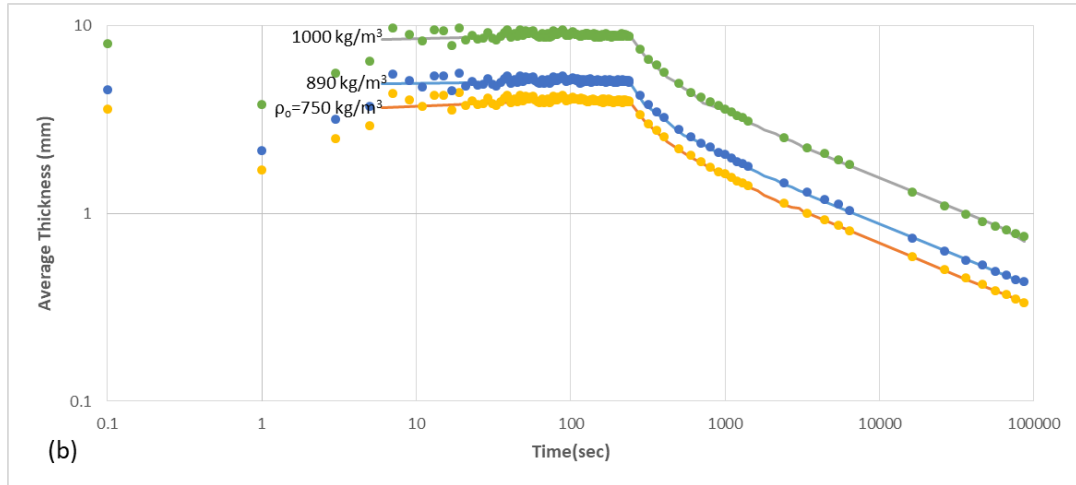


Figure 5.19: The Relationship between Oil Density and a) Radius b) Average Thickness Progresses of Continuous Spills in Time

5.5.3 Relationship between Drag Coefficient and Oil Spreading

Drag coefficient corresponding to the parameter of viscous force in Nihoul's model retards the spreading in gravity and surface tension viscous regimes. Asymptotic solutions (Eqn. 34 and 35) admit the relationship between drag coefficient and oil spreading in both regimes. Therefore, increasing the drag coefficient, increasing the frictional forces, lowering the spreading potential of slick and increasing the oil layer thickness for the entire time of simulation. Figure 5.20a and 5.20b clearly demonstrates these effects on the radius and thickness for instantaneous releases. Similar results for continuous spills under gravity viscous regime are obtained in Figure 5.21a and Figure 5.21b.

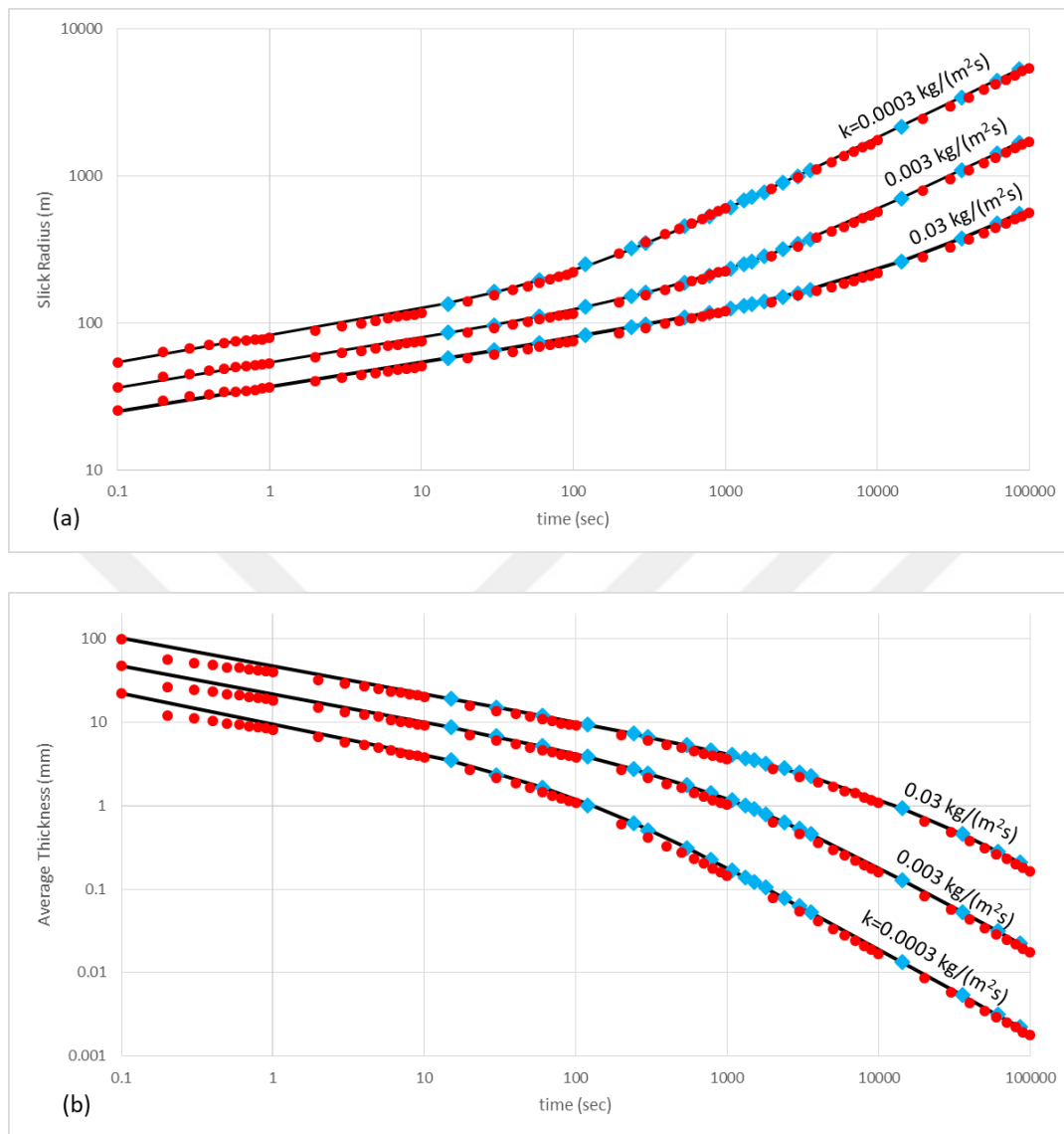


Figure 5.20: The Relationship between Drag Coefficient and a)Radius b) Average Thickness Progresses of Instantaneous Spills in Time

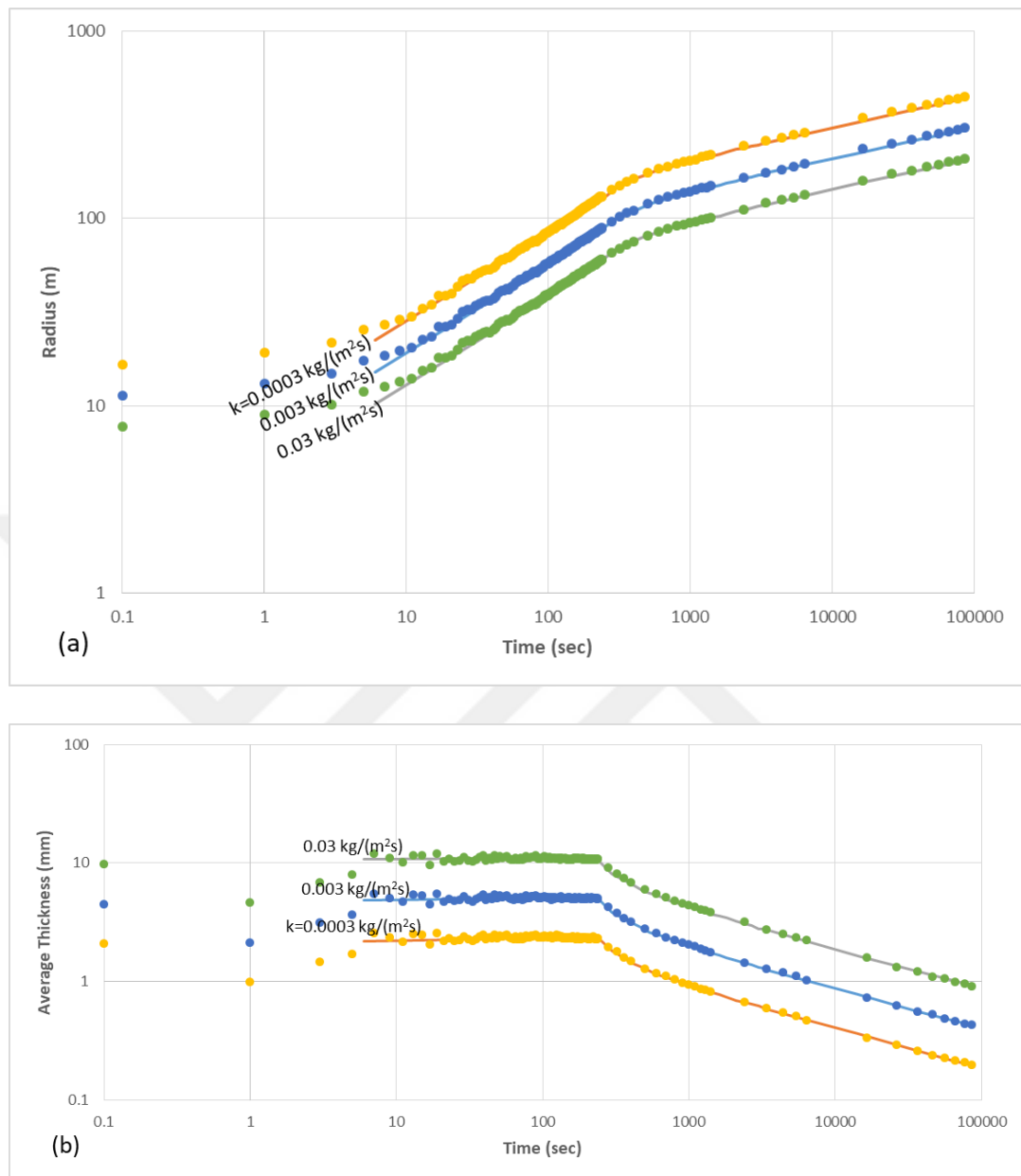
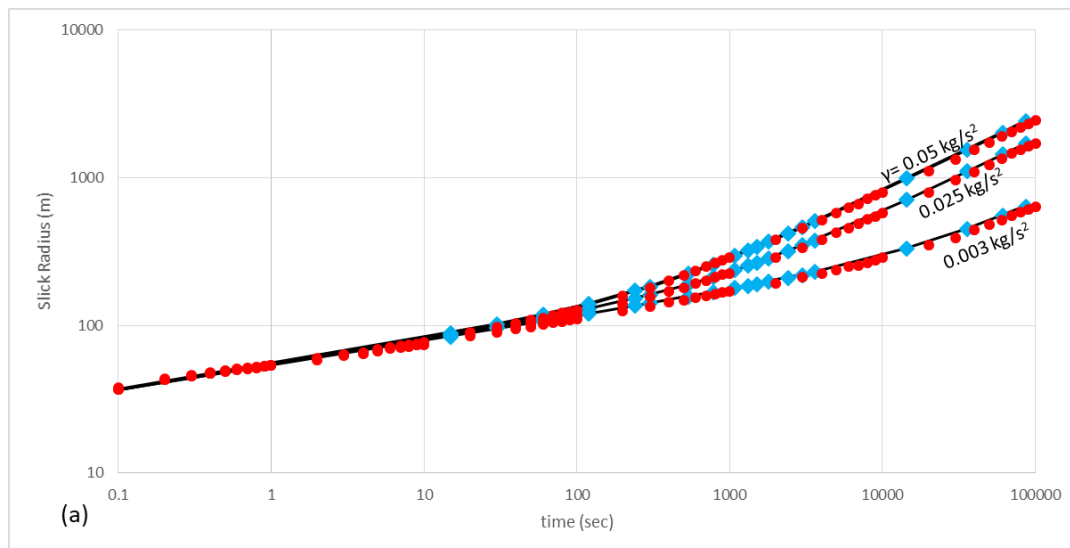


Figure 5.21: The Relationship between Drag Coefficient and a)Radius b) Average Thickness Progresses of Continuous Spills in Time

5.5.4 Relationship between Surface Tension Parameter and Oil Spreading

Surface tension parameter (γ) represents the surface free energy on the sea surface driving the spreading when oil is spread as a very thin layer with the negligible gravity forces. Higher surface free energy causes oil to spread more in the surface tension regime compared to the lower surface free energy. Increased spreading rate of oil is observed in surface tension regime. Figure 5.22a and 5.22b depict these effects for instantaneous spills. Gravity-viscous regime itself is not affected from this parameter, but its effective duration is reduced with higher surface tension parameter. So, it is possible to say that surface tension spreading of slick having greater surface free energy causes the greater slick area. Ultimate thickness is reduced. As a result of this analysis, unlike many model assumptions, neglected surface tension regime causes to estimation of slick radius lower than the actual one according to Nihoul's model. It should be noted that our continuous release model requires the containment of surface tension regime for long term predictions to be more accurate. It precisely guesses the spreading of high volume of spills in the short to medium terms, but it can always produce erroneous results for the spreading of low amount of oils beginning from surface tension regime.



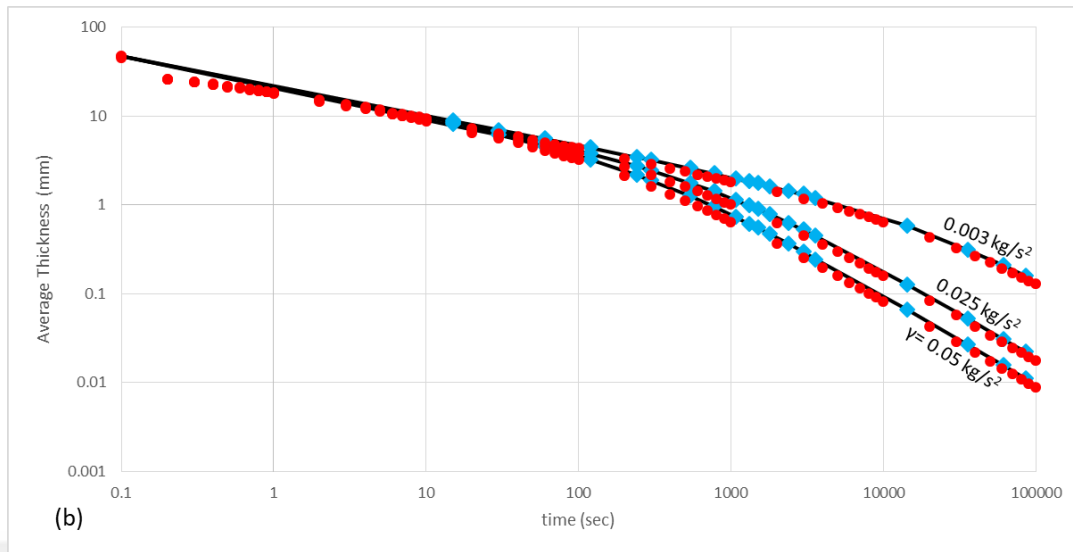


Figure 5.22: The Relationship between Surface Tension and a) Radius b) Average Thickness Progresses of Instantaneous Spills in Time

5.5.5 Relationship between Discharge Type of Oil and Continuous Oil Spreading

The oil leakage continuously can have same or changing rates for a discharge period. Up to now, all of the cases of continuous spills was presented at the constant rate. For this reason, average thickness was conserved. Another case with oil leakage at changing rate is designed with the parameters in Table 5.6. The average thickness change during the release can be examined in Figure 5.23. The rate increase in first 60 seconds increases the average thickness while the rate decrease in remaining leakage section lowers the average thickness. So, rate changes will affect the average thickness in the same manner compared to the constant rate case. Also, code solution underestimates the thickness lower than %10 percent of COMSOL's thickness prediction. It is an acceptable deviation and the algorithm supplies better prediction for the slick radius in Figure 5.24.

Table 5.6: The Parameters Used for the Case of Changing and Constant Discharges

Input Parameters (symbol)	Values (unit)
Total Spill Volume (V_o)	300 (m^3)
Spill Duration	120 (s)
Density of MGO (ρ_o)	890 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.003 ($kg/(m^2 s)$)
Total number of particles	6000

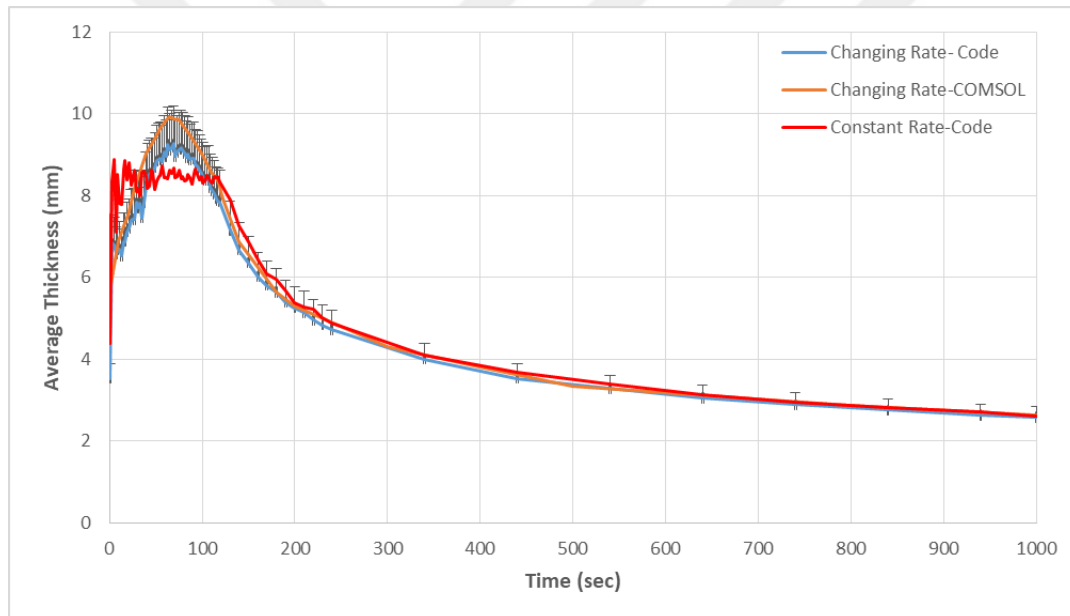


Figure 5.23: Average Thickness Progress with Time for the Different Discharge Types

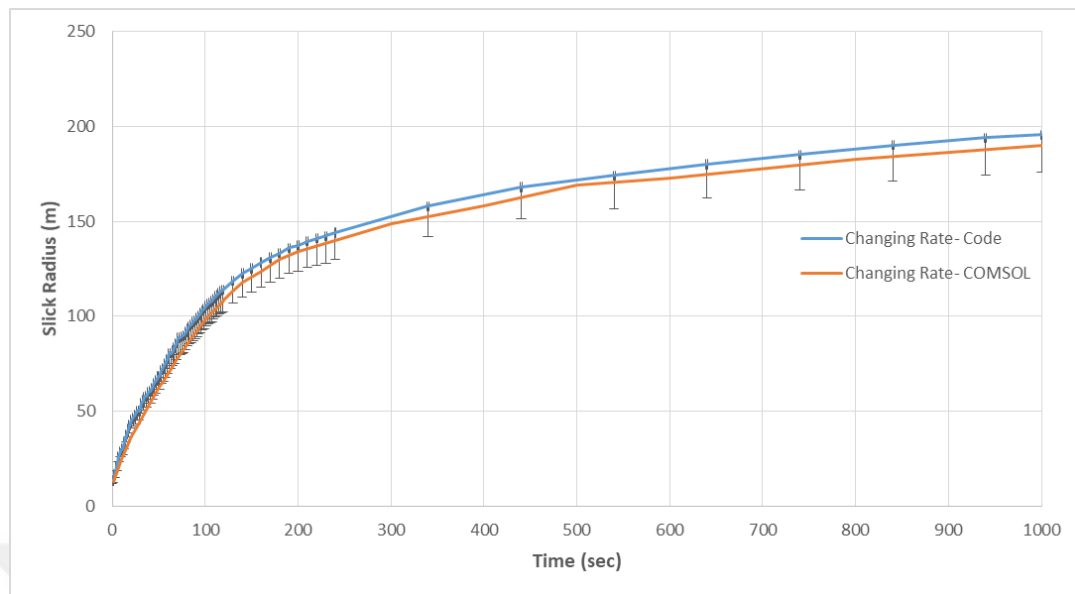


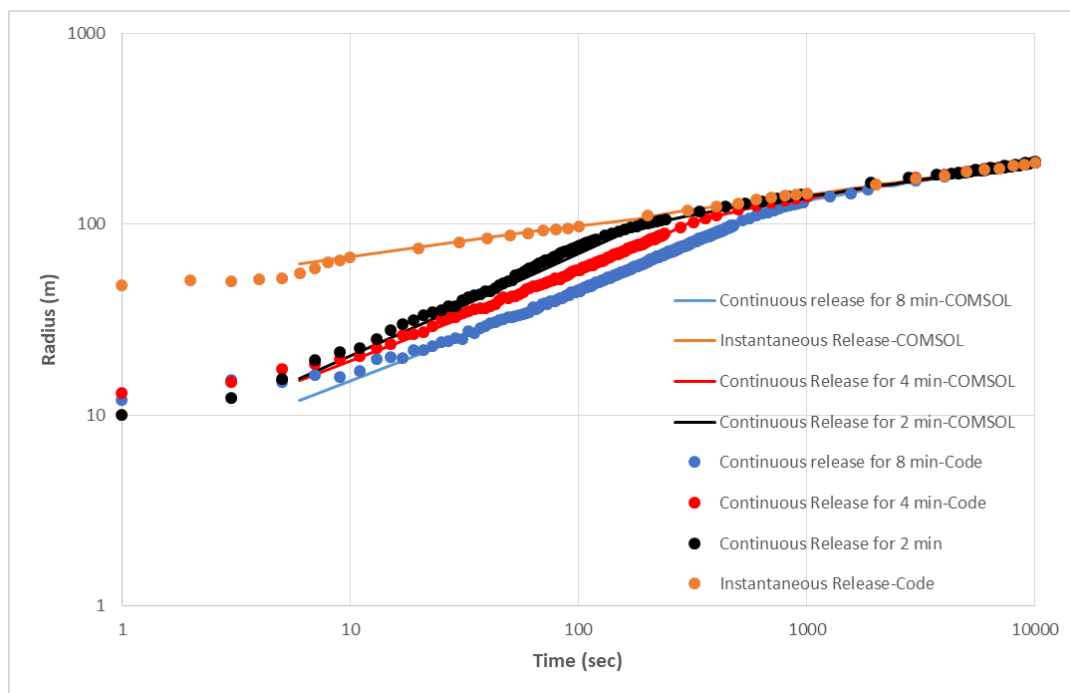
Figure 5.24: Radius Progress in Time with the Case of Changing Rate

5.5.6 Comparisons of Same Amount of Oil Leakage Instantaneously and Continuously

A case of instantaneous and continuous releases are examined in the gravity viscous regime with the data in Table 5.7. Continuous release for 2 minutes is performed at changing rate while other continuous spills are observed with constant rate. Figure 5.25 shows that the spills with same amount of oil spreads to the same extent after a while. It highlights that continuous spills start to resemble instantaneous spills after the leakage regardless of the leakage duration and constant or changing rate. Leakage duration and discharge type (constant/changing rate) specify the time period required for the complete transformation of continuous spill to the instantaneous one. So, continuous spills can be assumed as it is instantaneously leaked to simplify the modeling of surface slicks for the long-term predictions of slick behavior.

Table 5.7: Common Parameters Used in the Case of Spilling Type

Input Parameters (symbol)	Values (unit)
Initial spill Volume (V_o)	120 (m^3)
Oil Density (ρ_o)	890 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.003 ($kg/(m^2 s)$)

**Figure 5.25:** The Radius Progress in Time with Spilling Types

5.6 Wind Effect for Oil Horizontal Movement

The wind driven advection of oil is observed with wind speed of 1 m/s, 6 m/s and 12 m/s respectively in the direction of positive y coordinate (see Figure 5.26, 5.27 and 5.28). Other parameters are given in Table 5.8. For the wind speed of 1 m/s, the advection velocity of slick is 0.03 m/s and slick mass center moves through y+ axis. At the end of simulation, the slick extends to y=-115 m, y+=211 m, x+=158 m and

$x = -159$ m along the axes from the algorithm. The maximum values along the axes are $y = -110$ m, $y = 210$ m, $x = 151$ m and $x = -150$ m from COMSOL. The irregularities at the edges and drifting oil particles with some remaining oil fractions at the previous positions in COMSOL solution are observed. They arise from the hyperbolic nature of advection-spreading equation. Also, it can be said from the results that slick insignificantly expands in the direction of y compared to x coordinate by taking the average of y coordinates found as 163 m. The elongation along the y axis is almost 3.7%. It is not easily recognized by visually checking. Horizontal movement of slick on the sea with the wind speed of 6 m/s becomes more elongated depicted in Figure 5.27. The average elongation along y axis is almost 19 m corresponding to 12.5% with respect to x axis. Slick mass center is more directed to y axis with the extensions of $y = 455$ m and $y = -112$ m from the algorithm. Slick radii along X axes are unremarkably shrunk with new coordinates of $x = 150$ m and $x = -155$ m. The strong wind causes the much prominent elongation to the downwind shown in Figure 5.28. The elongation amount is approximately 24%. The slick moves away the leakage point at $x = 0$ and $y = 0$. The slick contraction increases from the x directions with $x = 143$ m and $x = -146$ m. COMSOL solution gets more disrupted with increasing wind speed at the end of simulation. Some regions around the edges become no flow zones with zero thickness values. They are surrounded by other regions with negative thickness values.

It is obviously realized that slick expands more towards to the downwind with the increasing velocity of wind by comparing Figure 5.26, 5.27 and 5.28. So, our results are compatible with the findings of Korinenko & Malinovsky (2014). The authors emphasize that weak wind does not reshape the slick to elliptical one. Moderate to strong winds advect the oil molecules more, leading to the elliptical shape of slick.

Another analysis with wind effect demonstrated in Figure 5.29 involves the continuous spill of same amount of oil released in different intervals. The slick elongation increases with increasing interval of leakage. The higher leakage duration results in the greater distances between the oil molecules added at the beginning and at the end of leakage. Former molecule moves with the wind before latter molecule

is introduced into the system. So, more elongated slick can be comprehended with the idea of particle introduction in greater time interval into the system of algorithm. It can be inferred from this perspective that the wind only moves the mass center of instantaneous spills. Noticing the correlation between the leakage interval and slick elongation helps to broaden the idea proposed Johansen (1984) and Elliot (1986). They claim that slick elongation is possible with the rejoining of dispersed oil molecules to the others on the surface. So, the wind is indirectly effective for slick expansion along the wind direction because surface oil molecules take some distance with the wind while dispersed oil moves less with the reduction of wind driven advection in the sea. Our contribution to the idea of Johansen and Elliot can be the oil increase on the surface by rejoining of dispersed oil or oil leakage onto the surface can cause the slick elongation. Otherwise, slick shape remains as circular with instantaneous spills with the convective forces. Our argument idealizes the advection by ignoring the local changes of the wind driven effect on the sea. If the advection local changes is paid attention, some elongations can be possibly seen. In addition, the presence of terrestrial obstacles to drifted oil particles causes the asymmetrical slick progress which is not considered in our cases.

Long duration of simulation and moderate to strong wind speed produce abnormal oil intrusions from sea boundaries in COMSOL. It can be checked from Figure 5.30. It is ensured that oil is not introduced from the boundaries in the cases. COMSOL's solution with wind speed of 6 m/s starts to be failed later than 600 minutes. So, the spreading and advection together can create the problems due to the usage of hyperbolic equation with the inclusion of advection velocity as mentioned. Hunter (1987) actually informs about the insufficiency of finite element solutions to describe the advection. This problem is the one of the reasons of addition of advection term. In above cases, the advection velocity is independent of space and time. COMSOL's solution can get worse for describing the oil horizontal movement if the space dependent advection velocity is applied, but it is not considered in this study. Nevertheless, the solution looks like similar with the solution of algorithm at earlier steps and at the end of simulation.

Table 5.8: Parameters Used for the Simulations of Code Compared for Advection

Input Parameters (symbol)	Values (unit)
Total Spill Volume (V_o)	120 (m^3)
Spill Duration	120 (s)
Density of MGO (ρ_o)	890 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.003 ($\text{kg}/(\text{m}^2 \text{ s})$)
Total number of particles	2400

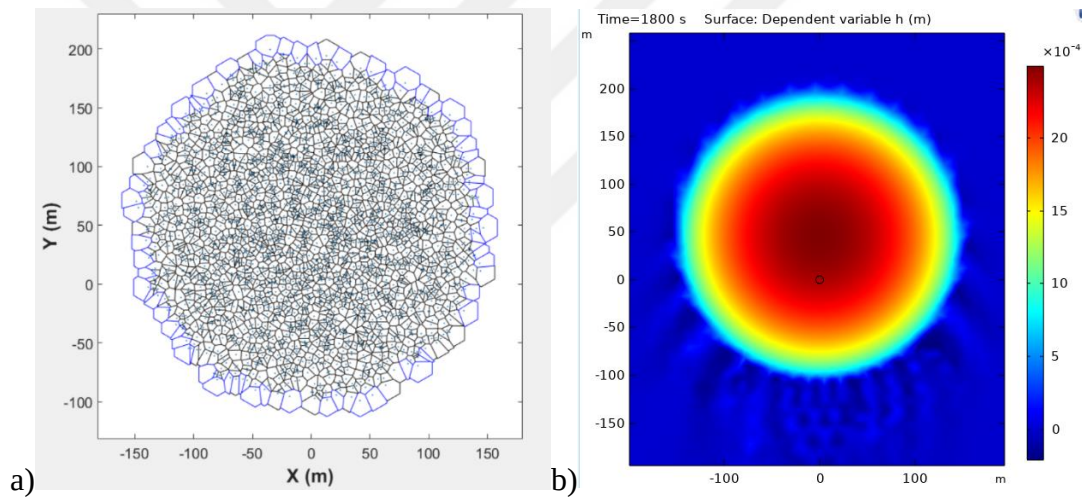


Figure 5.26: Oil Horizontal Movement along y Direction with $V_{\text{wind}}=1$ m/s at the End of Simulation in Solutions of a) Algorithm b) COMSOL

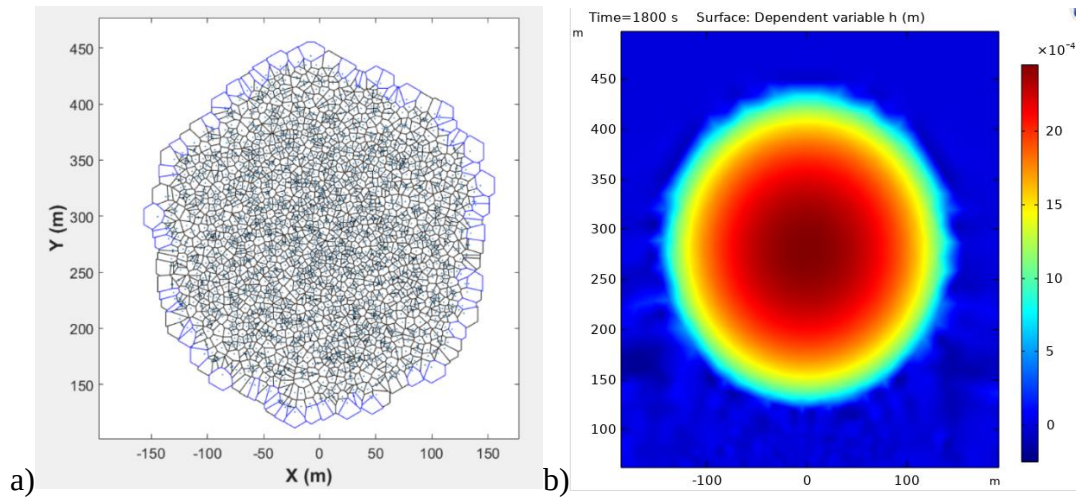


Figure 5.27: Oil Horizontal Movement along y Direction with $V_{wind}=6$ m/s at the End of Simulation in Solutions of a) Algorithm b) COMSOL

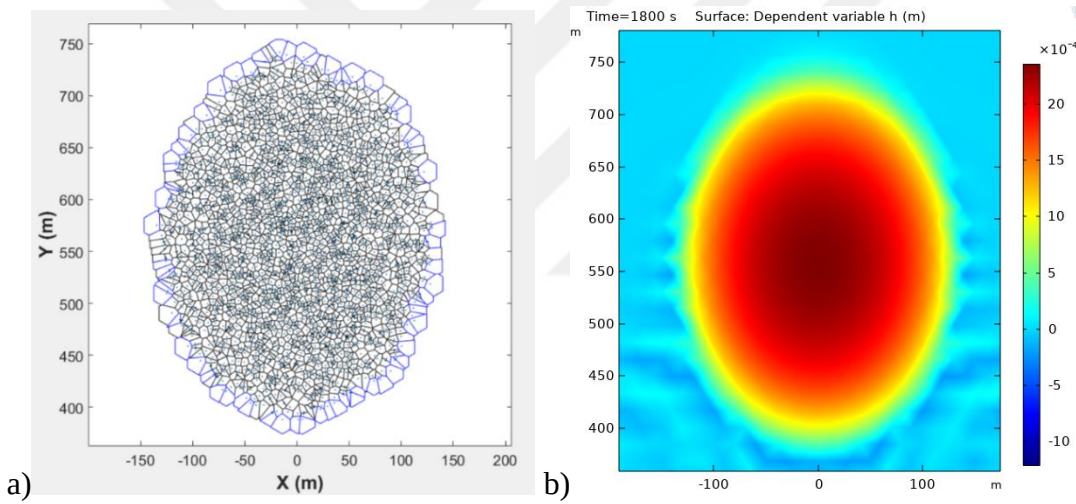


Figure 5.28: Oil Horizontal Movement along y Direction with $V_{wind}=12$ m/s at the End of Simulation in Solutions of a) Algorithm b) COMSOL

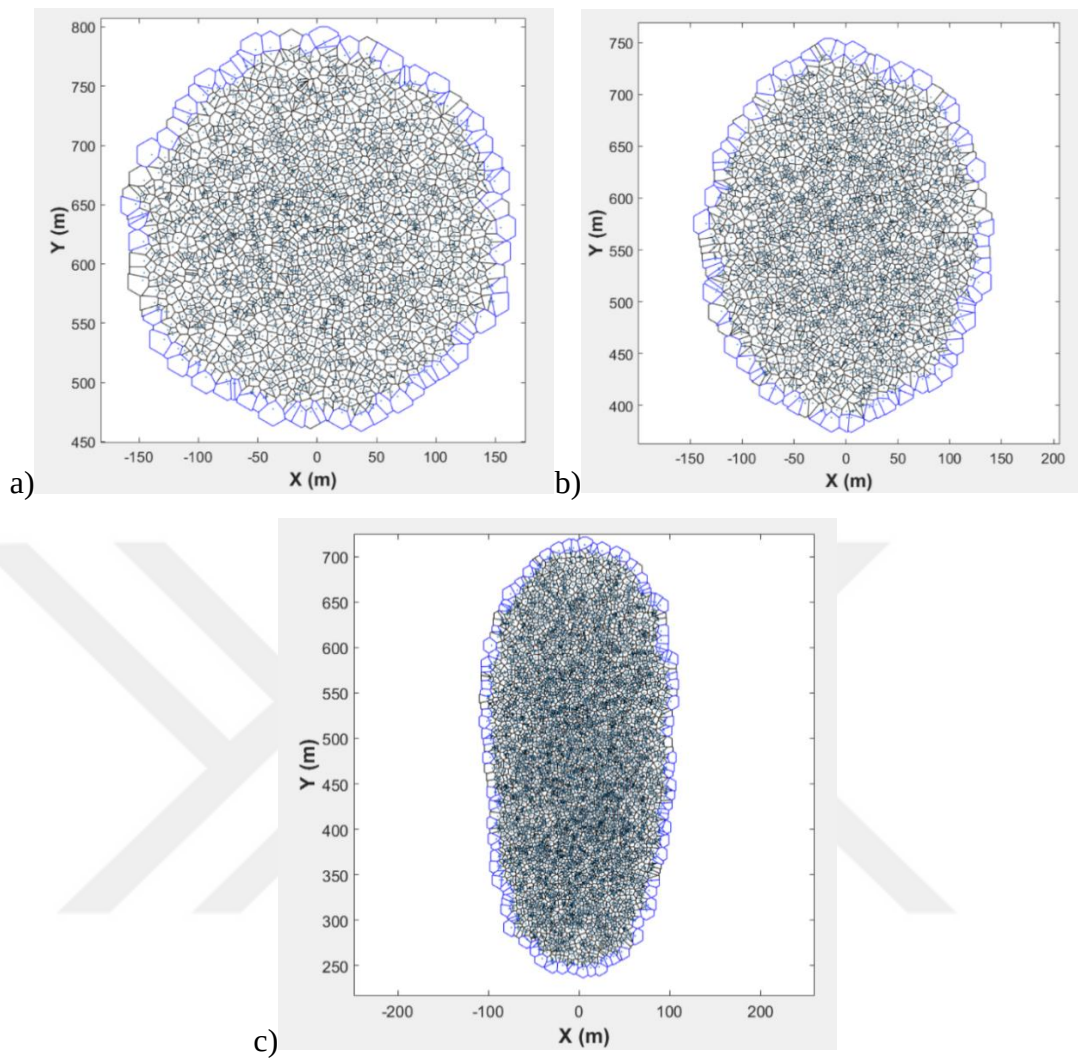


Figure 5.29: Elongation of 120 m³ Oil Leaked in a) 2 Minutes, b) 8 Minutes and c) 16 Minutes

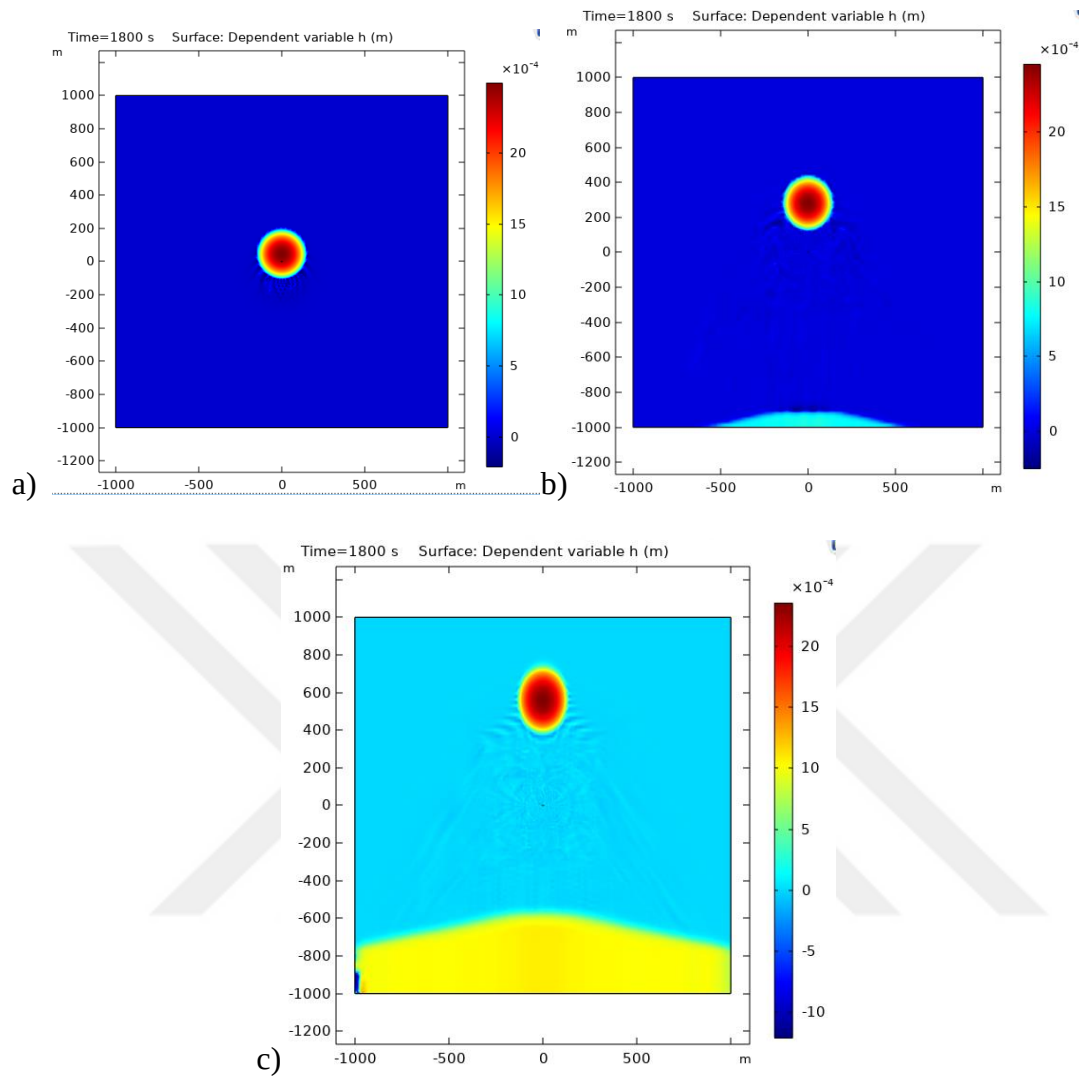


Figure 5.30: The Gradual Distortion of COMSOL's Solution with the Hyperbolic Advection term for a) Weak Winds ($V_{wind}=1$ m/s) b) Moderate Winds ($V_{wind}=6$ m/s) and c) Strong Winds ($V_{wind}=12$ m/s)

5.7 Comparison of the Numerical Model with a Software Created for the Estimation of Oil Fate

In the final analyzes, our algorithm and Marine Environmental Modelling Workbench (MEMW) developed by SINTEF are compared for a scenario designed for continuous oil spreading with the parameters presented in Table 5.9. The advection is not involved in the case. Figure 5.31 reveals the spreading of a light oil

estimated in MEMW with only radial extension of 15 m whereas slick radius is almost 300 m after 4 hours from the beginning in the algorithm. Surface slick thickness from MEMW is very high with central thickness of almost 2 m at the same time. The numerical solution predicts the maximum thickness in-between 1.5-2 mm. These thicknesses with the slick profiles are depicted in Figure 5.32. MEMW and the algorithm solutions excessively differ for the description of oil spreading and slick profile on the sea. The horizontal movement of oil with same parameters is examined in Figure 5.33 with changing wind speed for 4 hours. Wind speed is assigned as 1.81 m/s blowing from 211.5° for first 2 hours, 1.67 m/s from the direction of 221.12° for second 1 hour and 1.73 m/s from 231.54° for the remaining time. So, oil is drifted to the north-east direction obtained in both simulations. However, slick elongation occurs with the weak wind during the simulation in MEMW while the algorithm proposes a solution with circular shape dominated by the spreading in gravity viscous regime. Oil major and minor axes in MEMW increase as %167 and %40 respectively by wind effect. They insignificantly change in the code. It can be interpreted from looking at Figure 5.31 and 5.33 that MEMW slightly considers the oil spreading contribution to the horizontal movement of oil compared to the advection. Oil spreading is as effective as advection in the numerical solution of Nihoul's model. Therefore, circular slick contaminates the area in the north-east side of oil source. If the contribution of spreading was similar in both solutions, similar shapes would be observed. MEMW is modeled for instantaneous spills as a final scenario in Figure 5.34 with the same hydrodynamic conditions of above case. The slick elongation is very low at the end of simulation. These can be due to grid stepping and/or consideration of local changes of wind effect. However, the extended simulation time with same direction of wind (231.26°) shows that slick tries to turn into circular shape, pointing out that grid stepping is probable reason of elongation. So, MEMW contributes our argument referred in previous section about instantaneous spills. These spills are moved by the advection as a circle to north-east direction when the wind is independent of space.

Table 5.9: Parameters Used for the Simulations of Code Compared with MEMW

Input Parameters (symbol)	Values (unit)
Total Spill Volume (V_o)	300 (m^3)
Spill Duration	600 (s)
Density of MGO (ρ_o)	890 (kg/m^3)
Water Density (ρ_w)	1025 (kg/m^3)
Drag coefficient (k)	0.003 ($kg/(m^2 s)$)
Total number of particles	3000

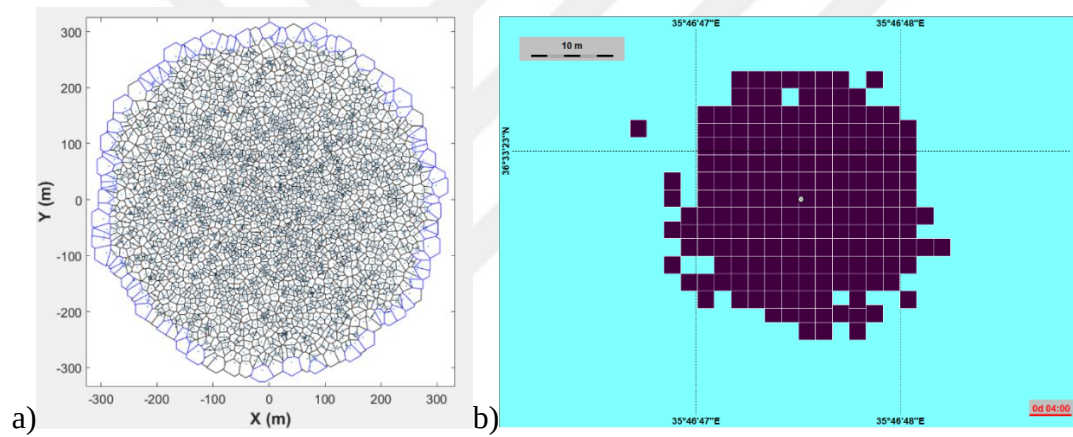
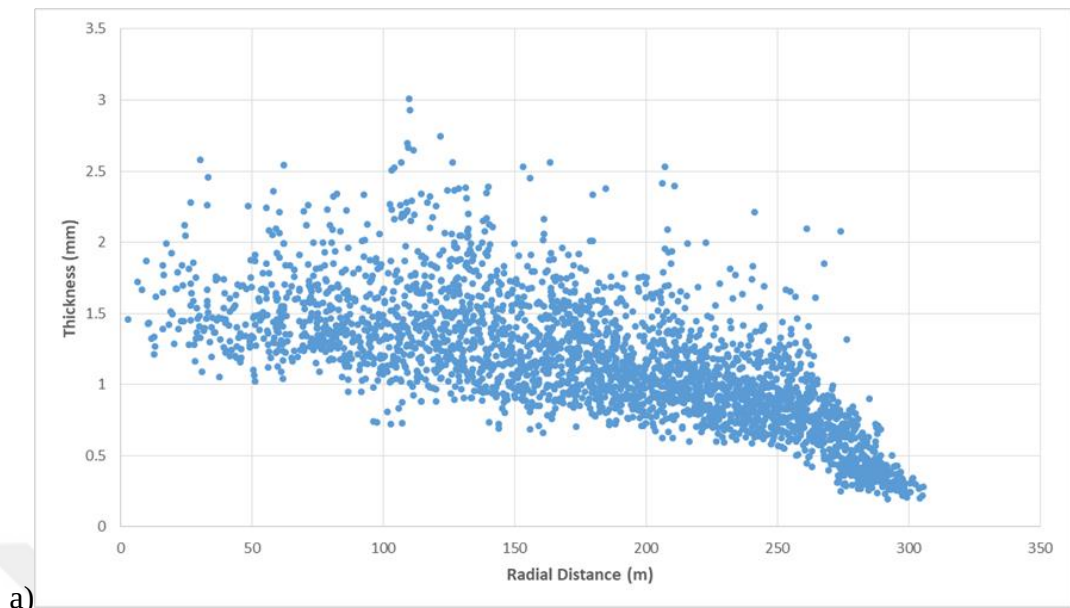
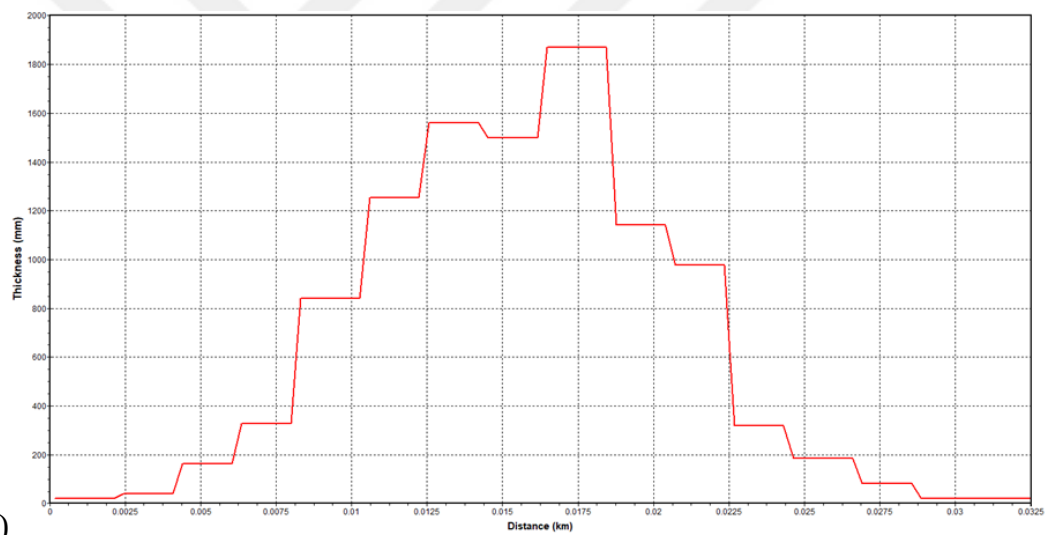


Figure 5.31: Slick Coverage on the Surface at the End of Simulations in a) the Algorithm and b) MEMW



a)



b)

Figure 5.32: Slick Distribution on the Surface at the End of Simulations in a) the Algorithm and b) MEMW

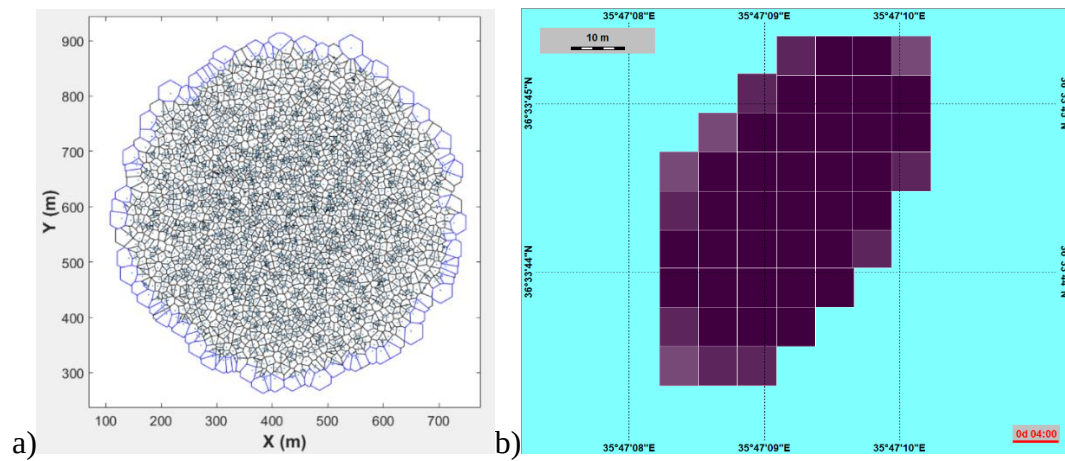
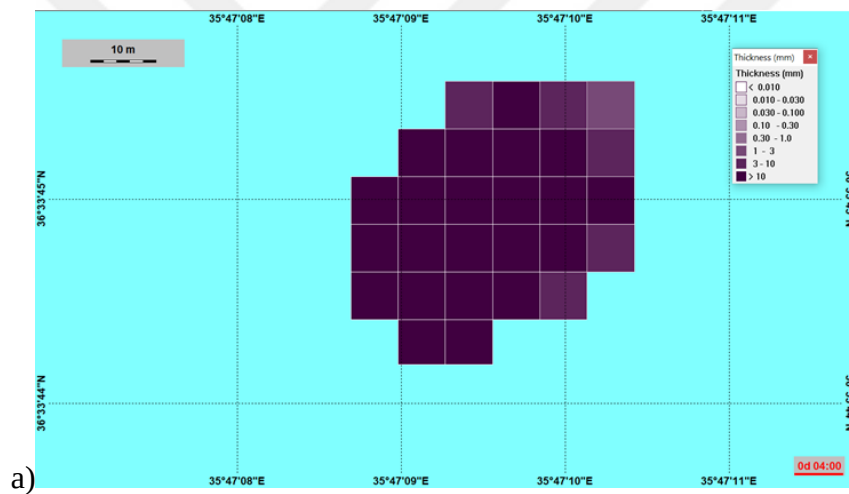


Figure 5.33: Slick Coverage on the Surface at the End of Simulations (4 hours) in
a) the Algorithm and b) MEMW with the Wind Blowing from South-East
Direction



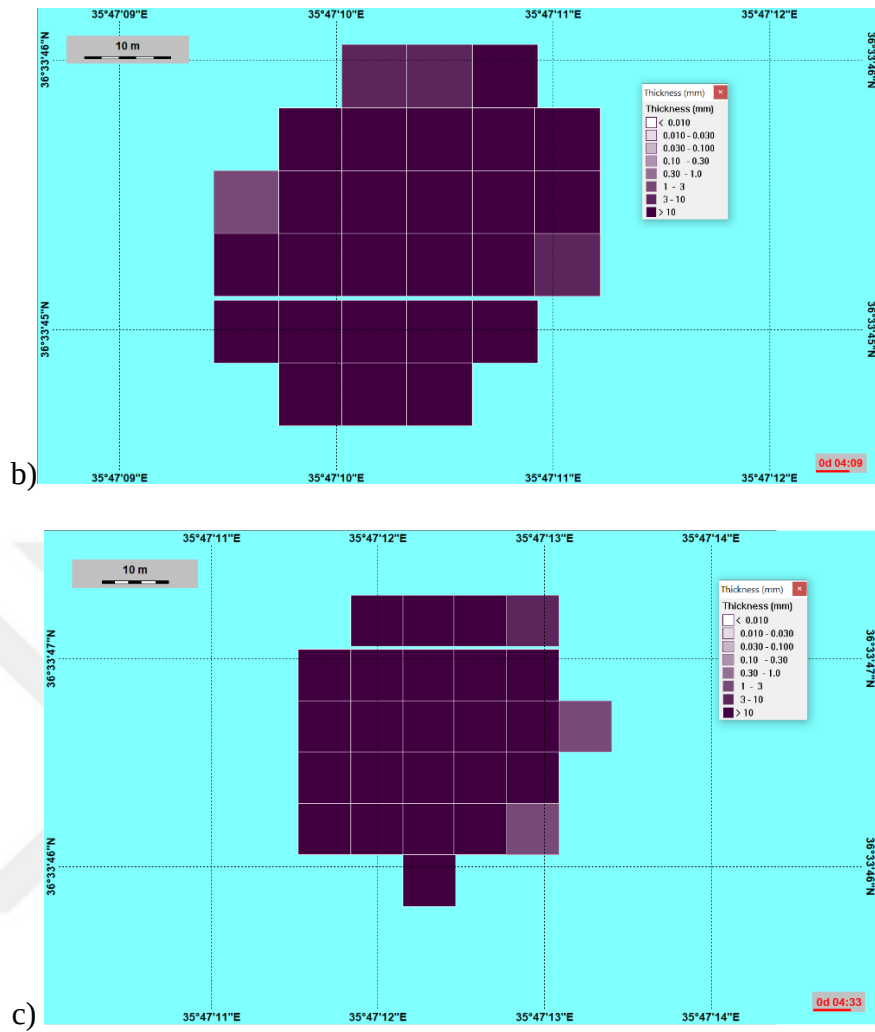


Figure 5.34: Instantaneous Spill Movement through the Wind in MEMW a) at 4 Hours and b) at 4 Hours and 9 Minutes c) 4 Hours and 33 Minutes

5.8 The Pros and Cons of the Algorithm

First favorable side of our model are the easy usage with acceptable computational time and low number of particles for the accurate results with the errors lower than %10 percent. Secondly, it presents many opportunities to investigate the slick from many perspectives. In the study, radius and thickness progresses are obtained, slick evolution are observed, surface oil distributions from the top and the cross-sectional views are showed, the slick center movement and elongation by the wind is put. Also,

in the future, easy computation of separate cells through Vorop++ can help to observe the special cases like disengaged oil molecules and the irregular slicks encountering with Langmuir circulations, terrestrial obstacles, etc. Also, the algorithm by converting the problem workspace into three dimension can be easily cooperated with the dispersion and turbulent diffusions in the sea.

One deficiency of our modeling emerges from the thickness depending on the cell area. The calculations in the algorithm are performed by the edge and vertex positions of cell with the features of Vorop++. The thickness of a cell is not estimated directly. The cell area is found in the algorithm and the thickness is determined by the volumetric calculations. Therefore, the cell area actually affects the step length for next time step due to the thickness dependency of the step length (Eqn. 40 and 43). The small changes in radius can create enormous thickness changes, so some fluctuations can be observed while modeling. Other efficiency is to not investigate continuous releases with surface tension regime in this study since the slick profile is not easily put like Eqn. 33. For such a case, maximum and average thickness relation changes in time. Modeling the surface tension regime is not an easy task without direct computation of thickness. Another deficiency having minor effect on the solution is stepping the particles for continuous releases. Equal steps while releasing makes the solution more accurate. So, the dependency on time steps is initially high. Also, the solution takes time to have data balance after random initialization with low number of particles at the beginning. To optimize the solution, these disadvantages can be treated for the future improvements. The maximum and average thickness relation can be empirically obtained by the surveillance of COMSOL's solution. In addition, special numerical techniques like kernel weighting as suggested by Zhang (1997) can be used to minimize the data scattering and numerical dependency of the solution especially at the beginning of the continuous spills.

CHAPTER 6

CONCLUSION

An algorithm providing a numerical solution to the oil surface processes has been proposed to observe the oil surface processes. It benefits from Gaussian random walk method based on Brownian motion of particles through a diffusive length because the spreading and advection have the same type of partial differential equation with advection-diffusion equation. It visualizes the slick on the sea water through Voronoi diagram with the cells assigned to the each particle. Another numerical model solving the equation through finite element method is used for the improvements of the algorithm by comparing in every cases of oil spreading process. The selection criteria of radius and thickness in the algorithm is updated for continuous spills through the FEM based model. Nihoul's analytical solution and its asymptotic expansions are considered as the benchmark to check these numerical models for instantaneous spills while an experiment helps to check them for continuous releases. Their accuracy proves the applicability of these models to the oil spreading. After that, the flexibility of the models are ensured by using a great range of the parameters. The analyzes of initial spill volume, oil density, drag coefficient, surface tension parameter and discharge type of same amount of oil for both instantaneous and continuous releases emphasize that slick can behave similarly in one of the regimes while their spreading can be changed in another regime according to the degree of the importance of a parameter for a regime. The introduction of advection into the models indicates that the wind can cause the elongation and mass center movement of a slick in the cases of increase in oil amount for long durations. Otherwise, only mass center will be shifted towards the downwind direction. In addition, finite element method is shown to be not sufficient for inclusion of the convective forces to oil surface fate due to the hyperbolic nature of the advection term. Finally, the algorithm is evaluated with a software designed for the whole oil spill processes.

Accordingly, the spreading contribution in the software is very low compared to the algorithm. Therefore, the slick elongation is realized even with the weak winds in it whereas the algorithm outputs an axisymmetric slick with them. Based on the all analyzes, the algorithm can be improved for implication of the surface tension with an empirical equation for the central thickness in continuous spill cases. It can contain a new term for the waxy oils based on the experiment. Later, it can be extended to the three dimensional numerical solution cooperated with dispersion, evaporation and other significant oil fate processes.



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APPENDIX

Publication

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