An exploratory alternative approach to Potential Incident Simulation, Control, and Evaluation System Simulation for Prediction of Oil Spill Behavior through Supervised Machine Learning

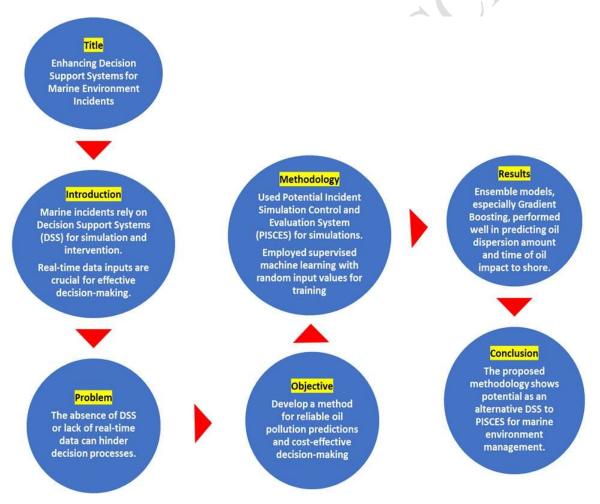
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GRAPHICAL ABSTRACT



ABSTRACT

The incidents occurring within the marine environment are supported by various Decision Support Systems (DSS), both in simulation and intervention. Accurate and real-time data inputs into these systems greatly contribute to the effective and prompt decision-making process. However, the absence of these systems in all situations or the inability to provide real-time data inputs can negatively impact the effectiveness of decision processes. This study aims to create a method that can enable reliable and accurate predictions regarding oil pollution and the cost-effective execution of certain decision processes. For this purpose, an exploratory study with various cases of ship-sourced oil pollution has been simulated using the Potential Incident Simulation Control and Evaluation System (PISCES). Random input values for each case have been utilized in PISCES simulation experiments. Afterward, supervised machine learning models were trained using the simulation experiments data set to predict oil dispersion amount and time of oil impact on shore. Model hyperparameters were optimized using cross-validated grid-searches. Through hyperparameter optimization using grid search, XGB, Random Forest, and Gradient Boosting emerged as the leading models for estimating oil dispersion. However, while Gradient Boosting yielded satisfactory outcomes, its performance could be further enhanced with additional data. Obtained results show that the proposed methodology has the potential for predicting the time of impact on shore, hence for rapid results for standard initial actions, they can be used as an alternative DSS to PISCES. **Keywords**: marine environment, machine learning, oil pollution, decision support system

1. Introduction

In interventions to incidents occurring in marine environment, the time factor is the primary criterion to be considered, both in search and rescue operations aimed at minimizing loss of life and property and in interventions to marine pollution. Changes occurring in the structures of chemicals after the interaction with seawater make intervention increasingly difficult over time. Therefore, prompt intervention in the disposal of polluting substances is crucial to minimizing harm to the ecological balance (Zeeshan et al., 2022), (Muhammad et al., 2024), (Muhammad et al., 2022). Considering the lessons learned from previous marine pollution incidents, technological capabilities such as predictive dispersion modeling to anticipate the possible movements of pollution, control, evaluation, and Decision Support Systems (DSS) have been developed to prevent similar events from occurring and to enable effective and rapid response once they occur.

DSS plays a crucial role in offering decision-makers a comprehensive understanding of incident areas during search and rescue and pollution response operations following maritime accidents. They achieve this by continuously monitoring and integrating real-time data about various sea surface, subsurface, and above-sea surface parameters. These parameters encompass a wide range of factors, such as oil evaporation, dispersion, degradation, and viscosity changes linked to pollution. Additionally, DSS incorporates information on meteorological conditions, sea state, surface currents, coastal geography, water depth, locations of ecological sensitivity, availability of intervention equipment, and other pertinent characteristics specific to the incident area. This holistic approach enables decision-makers to make informed choices and optimize their responses in maritime inputs, such as meteorological conditions, surface currents, sea conditions, and the presence of other vessels in the incident area, hold particular significance. These dynamic factors are instrumental in facilitating effective and prompt decision-making within the DSS. Their involvement ensures that decision-makers have access to continuously updated information, allowing them to make timely and well-informed decisions essential for managing maritime emergencies.

However, both cost and technological limitations make it not always possible to establish such a decision support system and achieve real-time integration of all static and dynamic data. This study aims to provide an alternative framework for decision support systems, using machine learning, to develop an intervention strategy for potential incidents at sea. Thus, an alternative methodology has been introduced, detached from the conventional decision support system paradigm, aimed at identifying two pivotal criteria essential for formulating intervention strategies in the context of marine pollution incidents. This innovative approach offers valuable insights and represents a departure from traditional methodologies. It serves as a foundation for more extensive and all-encompassing investigations within the realm of marine pollution management.

In the context of oil spill incidents, there exists a range of regulations designed to mitigate and prevent such occurrences. When a vessel adheres to these regulations, it can reasonably be assumed that all feasible preventive measures have been implemented to minimize the risk of spillage. However, in the unfortunate event of an oil spill, it is imperative to ensure a swift and effective response. The primary objective of this research is to develop a method capable of delivering reliable and precise predictions about oil pollution incidents while also facilitating cost-effective decision-making processes. Acquiring comprehensive datasets related to real-world oil spill events in marine environment is particularly challenging. Consequently, to circumvent this limitation, an exploratory approach has been adopted, wherein various scenarios of ship-induced oil pollution have been simulated using the Potential Incident Simulation Control and Evaluation System (PISCES). This approach offers a means to generate valuable insights and formulate strategies for managing oil spill incidents, even in cases where empirical data is limited. Utilizing PISCES enables sustainable dataset availability with high reliability. With the extracted data, to model the behaviors of oil spill, machine learning estimators have been trained using the simulation experiments data set for prediction of oil dispersion amount and time of oil impact on shore.

Supervised Machine Learning (SML) techniques, although a fairly new concept in the maritime domain, have been in use for the prediction of various systems whether it is on ship movement (Bassam et al., 2022; Nielsen et al., 2022), ship machinery (Guo et al., 2022; Hu et al., 2019; Lang et.al., 2022) onboard energy efficiency and sustainability (Erol et.al., 2020; Öztürk & Başar, 2022), decision making (Bal Beşikçi et al., 2016; Ozturk et.al., 2019) or marine pollution. There are two main modeling approaches for SML: regression and classification. Both prediction methods are available to use in the maritime domain. Regarding marine oil pollution, the utilization narrows down to considering the availability of data, which is the main component for accurate predictions. Hence, to evaluate the utilization of SML in oil spills, independent of the oil spill area, a systematic literature review has been carried out.

The systematic literature review approach enables rigorously reviewing several studies on SML applications on oil spills instead of an examination of independent studies while reducing the probability of carrying out a biased literature review. The systematic literature review methodology has been derived from the original guidelines set by (Kitchenham 2004).

An electronic search on the Web of Science Core Collection (WoSCC) database was performed for the systematic literature review. In the search process, AB= ("machine learn*") AND AB= ("oil* spil*" OR "mari* pollut*" OR PISCES) search code has been utilized for acquiring a wide range of studies on the main search subject. Instead of solely focusing on marine oil pollution, for evaluating the application of SML and best estimators, the cases have not been limited to a keyword. Initially, 94 studies resulted. To support the results' reliability, Science Citation Index- Expanded indexed journal articles have been extracted for search settings. After filtering and removing unrelated articles, 29 studies have been found. For this study, image processing has not been considered and only studies on regression and classification prediction models using numerical values have been included. With the inclusion-exclusion criteria set, 12 studies have been extracted for evaluation. The results of the systematic literature review are given in Table 1 below.

Table 1. Results of the systematic literature review.

Article	Reference	Publication	Machine	Oil Spill	Best Estimator
No	Kelerence	Year	Learning Model	Case	Dest Estimator

A1	(Khlongkhoi	2019	Regression	Marine	Deep Neural	
111	et.al., 2019)	2019	regression	Oil Spill	Network	
A2	(Li et al., 2021)	2021	Classification	Marine	Deep Neural	
AL	(Li et al., 2021)	2021	Classification	Oil Spill	Network	
A3	(M. Yang et al.,	2021	Regression	Marine	XGB Regressor	
AS	2021)	2021	Regression	Oil Spill	AOD Regressor	
A4	(Chen et al.,	2021	Classification	Marine	Random Forest	
A4	2021)	2021	Classification	Oil Spill	Classifier	
A5	(Mohammadiun	2022	Decreasion	Marine	Gaussian Process	
AJ	et al., 2022)	2022	Regression	Oil Spill	Regression	
	(Burmakova &			Cround	Adaptive Neural	
A6	Kalibatienė,	2022	Regression	Ground	Fuzzy Inference	
	2022)			Oil Spill	System	
A7	(Kaplan et al.,	2022	Regression	Ground	Convolutional	
A/	2022)	2022	Regression	Oil Spill	Neural Network	
				1	Subtractive	
	(Hafezi et al.,	2022	Classification	Marine Oil Spill	Clustering	
A8					Algorithm (SCA)	
	2022)				and Fuzzy C-Means	
					(FCM) Algorithm	
4.0	(Carvalho et al.,	2022	Classification	Marine	Artificial Neural	
A9	2022)	2022	Classification	Oil Spill	Network	
A 10	(J. Yang et al.,	2022	Classification	Marine	Convolutional	
A10	2023)	2023	Classification	Oil Spill	Neural Network	
A 1 1	(Wang et al.,	2022	Decreasies	Ground	Convolutional	
A11	2023)	2023	Regression	Oil Spill	Neural Network	
A12	(Genovez et al.,	2022	Classification	Marine	SVM	
A12	112 2023) 2023 C		Classification	Oil Spill	SVM	

According to the results of the systematic literature review, most of the studies have focused on marine oil spills. The percentage of utilization of machine learning models is found to be distributed evenly, where 50% of the studies are for regression and classification. Neural networks have been found to be the best estimators among utilized models in each study. Given that multi-layered

perceptron models are sensitive to the number of data and distribution of the data, it is unlikely to establish an estimator with reliable performance metric values based on neural networks.

It is also known that the performance of the estimator depends highly on the given data set and hyperparameters (Ozturk et al., 2019). To tackle the problem of data availability (Mohammadiun et al., 2022) utilized synthetic data, while (Ozturk et al., 2019) utilized expert opinions and fuzzy methodologies for compensating lack of data.

As argued in the previous chapter, when data acquisition is limited and reliable data is out of reach or costly, for maintaining a decision support system, alternatives are required. This study follows an exploratory approach for creating an alternative to a decision support system on marine oil spills by evaluating SML estimators on PISCES data.

The systematic literature review on machine learning applications on oil spills shows that none of the studies followed such an approach and all of them presented a limitation on data availability on oil spills. The outcome of this study also presents an alternative for data acquisition and synthetic data utilization. Considering PISCES is a simulator on oil behavior, using extracted data from PISCES and creating machine learning models for predicting oil spill behavior based on specific requirements and cases have been explored to be a well-performing decision support system methodology without the usage of additional complementary methods.

2. Materials and Methods

The general approach to the problem at hand, generating data through PISCES and providing a viable alternative DSS to PISCES is given below in Figure 1. Simulator-based data acquisition is not a method explored much in maritime transportation studies regarding machine learning. As it is not conventional to utilize secondary data rather than actual data for SML models, the problem that was tackled in this study separates itself by trying to create an alternative for a decision support system, that is simulation software in the case of oil spills.

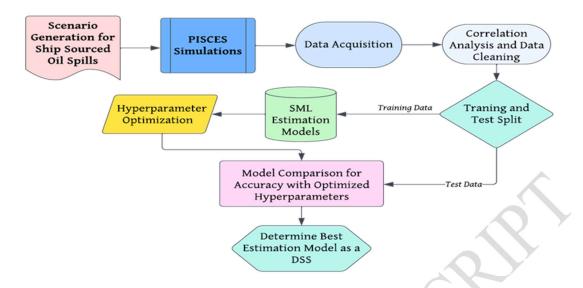


Figure 1. The general framework of the applied methodology.

For accessibility as a DSS alternative, conventional SML regression models have been utilized in this exploratory approach. As secondary data have been used from simulations, adding customized models or models with questionable reliability and validity has been avoided. As given in the framework, only hyperparameter tuning has been carried out to improve the accuracy of the estimators. The Scikit-Learn Library (Pedregosa et al., 2011) has been used for SML estimators with the addition of XGboost (Chen & Guestrin, 2016).

3. Results

3.1. Data Gathering

Following the framework, 110 scenarios have been generated for PISCES simulation runs. After generating scenarios for ship-sourced oil spills, utilizing PISCES the generated scenarios have been put into simulation runs and resulting data have been extracted from the software. The most significant obstacles to responding to marine pollution, specifically oil pollution, that leads to substantial damage, arise when the oil drops from the sea surface into the water intervening unattainable, and when it reaches the shoreline, significantly aggravating remediation efforts. The two above factors—the timing of oil dispersion and the onset of oil interaction to the coast—are meticulously assessed when developing pollution response plans, which encompass decisions about the timing of interventions, the locations of equipment deployment, and the methods of those

interventions. Therefore the simulation runs have been carried out considering two initial targets which are the time for oil to reach shore and the amount of oil dispersed in tonnes.

The outliers in the data distribution were primarily attributed to extreme scenarios in the PISCES simulations, such as prolonged spill durations or unusually high evaporation rates. These outliers can significantly affect predictive model performance, particularly in regression-based estimations. Furthermore, ensemble models like XGBoost and Random Forest, which are less sensitive to outliers due to their tree-based structure, were leveraged to achieve robust predictions.

The main simulation run has been carried out to find time for the oil to reach shore, where time stamps have been extracted for each 30 minutes. On the other hand, the amount of dispersion has been taken from the same simulation runs in which time has also been taken as a parameter. Overall, for the first rounds of simulation for time for oil to reach shore after evaluating the data extracted; speed of current (kts), speed of wind (kts), water temperature (°C), sea state (mt), water density (kg/m3), total amount of initial oil (t), oil density (kg/m3), surface tension (dyn/cm), viscosity (cSt), maximum water content and initial distance on shore (nm) selected as parameters and 110 simulation runs have been taken as data for SML models.

In the same manner, for the amount of oil dispersed; time passed (min), amount spilled (t), amount evaporated (t), amount stranded (t), amount floating mixture (t), max thickness (mm), slick area (km2), speed of current (kts), speed of wind (kts), water temperature (°C), sea state (mt), water density (kg/m³), oil density (kg/m³), surface tension (dyn/cm) initial viscosity (cSt), maximum water content, the initial distance of pollution to the coast (nm), viscosity change over time (cSt) have been considered as parameters. After the initial data acquisition, 1170 data points have been selected to be utilized in SML models. Figures 2 and 3 show the data distribution for the amount of dispersed and the time for oil to reach the shore respectively. For the amount of dispersed data, some outliers have been observed which are the results of longer simulations and for the time of impact, the data distribution although does not fit any conventional distribution gives a general idea of how the simulations resulted.

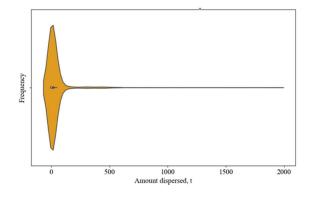
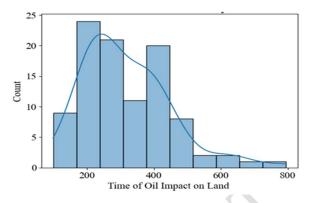
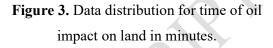


Figure 2. Data distribution for the amount of oil dispersion in tonnes.





In Figures 4 and 5, correlation heatmaps have been created to visualize the pairwise correlations between all features across the data set. A reasonable correlation rate has been determined as ~0.5 and the highly correlated feature pairs have been identified and addressed, while features with weak correlation to the target variable have been kept even though they may not contribute significantly to the predictions. Hence, a feature selection process was carried out according to the heat map that was created. The features are selected based on the domain knowledge and statistical analysis that are used in the study. A correlation threshold set forth identified the features related meaningfully to the target variables: oil dispersion and time of impact on shore. A threshold of ~0.5 was selected to balance between features having a moderate to strong correlation, and at the same time avoid risks from overfitting due to multicollinearity.

Minutes -	1	-0.1	0.15	0.25	0.054	0.15	-0.21	-0.22	0.049	-0.11	-0.048	0.022	-0.1	0.056	0.13	0.15	0.37	-0.038		1.0
Amount spilled, t	-0.1	1	0.03	0.072	0.045	0.34	0.062	0.32	0.38	0.53	0.13	-0.08	0.13	-0.033	-0.34	0.081	-0.08	0.55		
Amount evaporated, t	0.15	0.03	1	0.0047	0.0037	0.13	-0.026	-0.14	0.25	-0.046	-0.24	0.042	0.12	-0.075	0.15	-0.096	-0.045	-0.042		0.8
Amount stranded, t	0.25	0.072	0.0047	1	0.43	0.071	0.096	0.024	0.014	0.079	0.0025	0.031	0.087	-0.049	-0.065	0.032	0.021	0.1		
Max thickness, mm-	0.054	0.045	0.0037	0.43	1	-0.026	0.084	-0.0044	-0.00047	0.043	-0.046	0.06	-0.0078	-0.024	0.037	-0.043	0.016	0.023		0.6
Slick area, km2 -	0.15	0.34	0.13	0.071	-0.026		0.098	0.24	0.34	0.46	-0.056	-0.018	0.14	-0.093	-0.086	0.039	0.1	0.35		
Speed of Current (kts)		0.062	-0.026	0.096	0.084	0.098	1	0.011	0.06	0.11	0.16	0.09	0.21	-0.07		0.16	-0.17	-0.11		0.4
Speed of Wind (kts)	-0.22	0.32	-0.14	0.024	-0.0044	0.24	0.011	1	0.22	0.51	0.12	-0.13	0.14			-0.029	-0.046	0.43		0.4
Water Temparature (°C)	0.049	0.38	0.25	0.014	-0.00047	0.34	0.06	0.22	1	0.28	0.11	-0.062	0.11	-0.15	-0.054	0.18		0.23		
Sea State (mt)	-0.11	0.53	-0.046	0.079	0.043	0.46	0.11	0.51	0.28	1	0.044	-0.15	0.21		-0.16	-0.072	0.0049	0.38		0.2
Water Density (kg/m ³)	-0.048	0.13	-0.24	0.0025	-0.046	-0.056	0.16	0.12	0.11	0.044	1	0.015	-0.011	0.062	-0.11	0.25	0.034	0.096		
Density (kg/m ³) -	0.022	-0.08	0.042	0.031	0.06	-0.018	0.09	-0.13	-0.062	-0.15	0.015		-0.54	0.36	0.19	0.45	0.22	-0.1		0.0
Surface Tension (dyn/cm) -	-0.1	0.13	0.12	0.087	-0.0078	0.14	0.21	0.14	0.11	0.21	-0.011	-0.54	1	-0.14	-0.39	-0.24		0.14		
Initial Viscosity (cSt)	0.056	-0.033	-0.075	-0.049	-0.024	-0.093	-0.07		-0.15		0.062	0.36	-0.14	1	0.031	0.25	0.52	-0.031		-0.2
Max. Water Content (%) -	0.13	-0.34	0.15	-0.065	0.037	-0.086	-0.23		-0.054	-0.16	-0.11	0.19	-0.39	0.031	1	0.017	0.22	-0.35		
Initial Distance of Pollution to the Coast (nm)	0.15	0.081	-0.096	0.032	-0.043	0.039	0.16	-0.029	0.18	-0.072	0.25	0.45		0.25	0.017	1	0.17	-0.086		
Viscosity Delta, cSt	0.37	-0.08	-0.045	0.021	0.016	0.1	-0.17	-0.046	-0.24	0.0049	0.034	0.22	-0.2	0.52	0.22	0.17	1	-0.085		-0.4
Amount dispersed, t			-0.042	0.1	0.023	0.35	-0.11	0.43	0.23	0.38	0.096	-0.1	0.14	-0.031			-0.085			
	Minutes	Amount spilled, t	Amount evaporated, t	Amount stranded, t	Max thickness, mm	Slick area, km2	Speed of Current (kts)	Speed of Wind (kts)	Water Temparature (°C)	Sea State (mt)	Water Density (kg/m')	Density (kg/m')	Surface Tension (dyn/cm)	Initial Viscosity (cSt)	Max. Water Content (%)	Initial Distance of Pollution to the Coast (nm)	Viscosity Delta, cSt	Amount dispersed, t		
		1																		

Figure 4. Correlation heat map for all variables for predicting the amount of oil dispersion.

													1.0
Speed of Current (kts)	1	-0.027	-0.0031	0.13	0.16	0.076	0.12	0.2	-0.06	-0.22	0.18	-0.41	1.0
Speed of Wind (kts) -	-0.027		0.21	0.51	0.083	0.3		0.16			-0.08	-0.38	- 0.8
Water Temparature (°C) -	-0.0031	0.21	1	0.3	0.18	0.44	-0.054	0.089	-0.11	-0.11	0.25	0.14	
Sea State (mt)	0.13	0.51	0.3	1	0.031	0.55	-0.17	0.23			-0.042		- 0.6
Water Density (kg/m ³) -	0.16	0.083	0.18	0.031	1	0.18	-0.028	-0.015	0.069	-0.11	0.27	0.0051	- 0.4
Total Amount (t) -	0.076	0.3	0.44	0.55	0.18	1	-0.089	0.15	-0.013	-0.38	0.17		
Density (kg/m ¹) -	0.12		-0.054	-0.17	-0.028	-0.089	1	-0.53	0.34	0.22	0.38	0.014	- 0.2
Surface Tension (dyn/cm) -	0.2	0.16	0.089	0.23	-0.015	0.15	-0.53		-0.14	-0.44		-0.16	- 0.0
Viscosity (cSt)	-0.06		-0.11	-0.18	0.069	-0.013	0.34	-0.14	1	0.033	0.27	0.11	
Max. Water Content (%)			-0.11		-0.11	-0.38	0.22	-0.44	0.033	1	-0.01	0.25	0.2
Initial Distance of Pollution to the Coast (nm) -	0.18	-0.08	0.25	-0.042	0.27	0.17	0.38	-0.18	0.27	-0.01	1	0.33	
Time of Oil Impact on Land	-0.41	-0.38	0.14		0.0051	-0.19	0.014	-0.16	0.11	0.25	0.33	1	0.4
	Speed of Current (kts) -	Speed of Wind (kts) -	Water Temparature (°C) -	Sca State (mt) -	Water Density (kg/m ³) -	Total Amount (t) -	Density (kg/m²) -	Surface Tension (dyn/cm) -	Viscosity (cSt) -	Max. Water Content (%) -	Initial Distance of Pollution to the Coast (nm) -	Time of Oil Impact on Land	-

Figure 5. Correlation heat map for all variables for predicting the time of oil impact on land.

3.2. Hyperparameter Tuning

Grid Search has been used for hyperparameter tuning to determine the optimal values of a model when applicable (Yang et al., 2023), (Pedregosa et al., 2011). For each estimator, a range of hyperparameters has been defined for Grid Search to look for the best combination as given in Table 2 and Table 3. Regarding hyperparameter ranges, a wide range has been tried, and as the range increased the performance decreased. Hence, the limited range has been presented in the below tables and vast granularity has been avoided for convenience. For all grid search applications, negative MSE is used for scoring and 5 folds have been used for splitting the data set for cross-validation. The significance of Grid Search, although computationally expensive, it ensures the models do not only work with given data but are generalized well into new unseen data.

Grid Search Hyperparameters for each estimator	Parameter Ranges
Decision Tree	
Max Depth	[3, 4, 5, 8, 10, 20, 30, 40, 50]
Min Samples Split	[2, 3, 4, 6, 8, 10]
Min Samples Leaf	[1, 2, 3, 4]
Random Forest	
Number of Estimators	[400, 800, 1000, 1500]
Max Depth	[3, 4, 5, 8, 10, 20, 30, 40, 50]
Min Samples Split	[2, 3, 4, 6, 8, 10]
Min Samples Leaf	[1, 3, 5, 10]
Max Features	[Auto, Square root]
Gradient Boosting Regressor	
Number of Estimators	[500, 1000, 1500]
Learning Rate	[0.01, 0.05, 0.1]
Max Depth	[3, 4, 5, 8, 10, 20, 30, 40, 50]
Loss Function	[Absolute error, quantile, squared
	error, huber]
Min Samples Leaf	[50, 100, 150]
XGBoost Regressor	
Number of Estimators	[500, 1000, 1500]
Learning Rate	[0.01, 0.05, 0.1]
Subsample	[0.5, 0.7, 1]
Booster	[GBTree, GBLinear]
Max Depth	[3, 4, 5, 8, 10, 20, 30, 40, 50]
Min Child Weight	[1, 2, 3]
Base Score	[0.25, 0.5, 0.75, 1]
SVR	
С	[10, 100, 200]
Epsilon	[0.01, 0.1, 1]
Kernel	[Poly, RBF, Sigmoid]

Table 2. Grid Search hyperparameter options for predicting the amount of oil dispersion.

Grid Search Hyperparameters for Each Estimator	Parameter Ranges
Decision Tree	
Max Depth	[3, 4, 5, 10, 20, 30, 40, 50]
Min Samples Split	[2, 3, 4, 6, 8, 10]
Min Samples Leaf	[1, 2, 3, 4]
Random Forest	
Number of Estimators	[400, 800, 1000, 1500]
Max Depth	[5, 10, 20, 40, 50]
Min Samples Split	[2, 3, 6, 8, 10]
Min Samples Leaf	[3, 4, 5, 10]
Max Features	[Auto, Square root]
Gradient Boosting Regressor	
Number of Estimators	[50, 100, 500, 1000]
Learning Rate	[0.1, 0.15, 0.2]
Max Depth	[3, 4, 5, 8, 10, 20, 30, 40, 50]
Loss Function	[Absolute error, quantile,
	squared error, huber]
Min Samples Leaf	[1, 3, 5, 10]
Min Samples Split	[2, 4, 6, 8]
Subsample	[0.5, 0.7, 1.0]
XGBoost Regressor	
Number of Estimators	[50, 100, 500, 1000]
Learning Rate	[0.01, 0.05, 0.1, 0.2]
Subsample	[0.5, 0.7, 1]
Colsample by tree	[0.5, 0.7, 1]
Booster	[GBTree, GBLinear]
Max Depth	[3, 4, 5, 8, 10, 20, 30, 40, 50]
Min Child Weight	[1, 2, 3]
Base Score	[0.25, 0.5, 0.75, 1]
SVR	1
C	[10, 100, 200]
Epsilon	[0.01, 0.1, 1]
Kernel	[Poly, RBF, Sigmoid]

Table 3. Grid Search hyperparameter options for predicting the time of oil impact on land.

4. Discussion

SML models have been compared with mean squared error (MSE), coefficient of determination $(0 \le R^2 \le 1)$ and mean absolute error (MAE) performance metrics. MSE measures the average squared distance between actual and predicted values, R2 is used for assessing the quality of model predictions and MAE compares the absolute error between the actual and predicted values. After model fits, *for the amount of oil dispersion*, the best hyperparameters obtained from the Grid Search are given in Table 4, performance metric scores for each SML are given in Table 5, and the performance comparisons are given in Figures 6, 7, and 8.

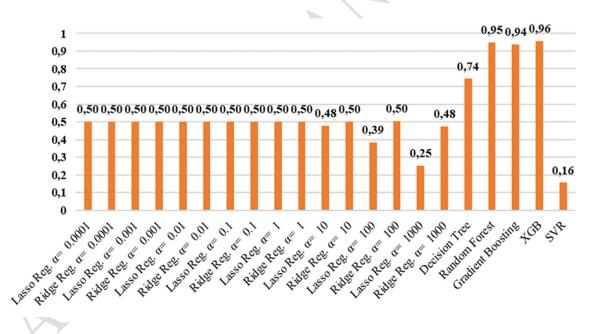
SML Regression Model	Optimized Hyperparameters after Grid Search
SVR	C=200; epsilon=0.1; kernel = RBF
Decision Tree	Max depth=5; min samples leaf=1; min samples split=3
Random Forest	Estimators=400; Max depth=10; min samples leaf=1; min samples split=3; max features= square root
Gradient Boosting	Estimators=1500; learning rate= 0.1; loss function=squared error; max depth=5; min samples leaf=100
XGB	Estimators= 1500; learning rate=0.05; max depth=3; min child weight=1; subsample=1; booster=gbtree; base score=1

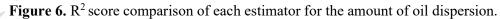
Table 4. Grid Search results for estimators for the amount of oil dispersion

Table 5. Performance metric scores for each SML model for the amount of oil dispersion

SML Regression Model	MSE	R ²	MAE
Linear Regression	11822,14	-0.086847	52,483630
Polynomial Regression degree 2	16726,19	-61,254360	100,052274
Lasso Regression α= 0,0001	9409,278	0.499493	49,33748
Ridge Regression α = 0,0001	9409,284	0.499492	49,33757
Lasso Regression α= 0,001	9409,216	0.499496	49,33664
Ridge Regression $\alpha = 0,001$	9409,283	0.499493	49,33755
Lasso Regression $\alpha = 0,01$	9408,602	0.499529	49,32826
Ridge Regression $\alpha = 0,01$	9409,265	0.499493	49,33733
Lasso Regression $\alpha = 0,1$	9402,631	0.499846	49,24441

Ridge Regression $\alpha = 0, 1$	9409,093	0.499503	49,33509
Lasso Regression α= 1	9369,238	0.501623	48,54825
Ridge Regression $\alpha = 1$	9407,389	0.499593	49,31275
Lasso Regression α= 10	9842,174	0.476466	43,82178
Ridge Regression $\alpha = 10$	9392,214	0.5004	49,09507
Lasso Regression α= 100	11561,68	0.385	39,97093
Ridge Regression α = 100	9344,653	0.50293	47,4382
Lasso Regression α= 1000	14044	0.252958	44,34885
Ridge Regression α = 1000	9863,075	0.475354	44,67469
SVR	15883,71	0.155098	38,501
Decision Tree	4822,661	0.743468	13,90511
Random Forest	949,599	0.949488	7,517505
Gradient Boosting	1191,176	0.936638	17,24098
XGB	828,707	0.955919	6,777389
	1		





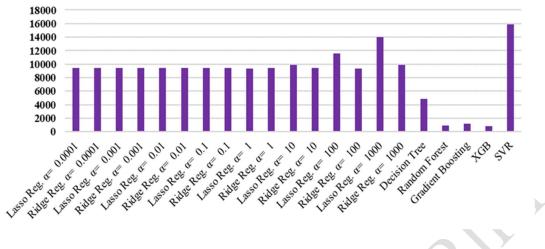


Figure 7. MSE comparison of each estimator for the amount of oil dispersion.

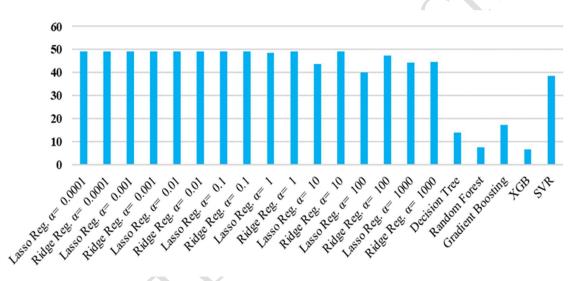


Figure 8. MAE comparison of each estimator for the amount of oil dispersion.

For the amount of oil dispersion, XGB, Random Forest, and Gradient Boosting have been observed to be the top performers among all models considered with R_XGB^2=0.96, R_RF^2=0.95, and R_GB^2=0.94 values respectively as well as having the lowest MSE and MAE values. All three top performers are ensemble models that leverage multiple learning algorithms to improve prediction performance. Even though the Decision Tree performed well enough, it was outperformed by ensemble models. Among others, XGBoost allows the processing of high-dimensional datasets with efficiency and easily embedded feature interactions without preselection bias, thus avoiding overfitting by a set of regularization techniques. The XGBoost algorithm is appropriate, especially for datasets with complicated relationships among input features, because of its iteratively minimized

prediction error through the optimization of residuals in its gradient boosting mechanism. Grid-search hyperparameter tuning ensures optimal parameter selection to improve its predictive capability further. Such characteristics enable XGBoost to model nonlinear relationships that are innate in the oil spill dataset: viscosity changes and interaction among environmental factors, such as sea state and oil density. With high-performance results, ensemble models can be considered to be a candidate DSS as an alternative to PISCES simulations for rapid prediction with reliability for predicting oil dispersion.

For the time of oil impact on shore, the best hyperparameters obtained from the Grid Search are given in Table 6, performance metric scores for each SML are given in Table 7, and the performance comparisons are given in Figures 9, 10, and 11.

SML Regression Model	Optimized Hyperparameters after Grid Search				
SVRC=200; epsilon=0.1; kernel = RBF					
Decision TreeMax depth=3; min samples leaf=4; min samples split=2					
Random Forest	Estimators=1000; Max depth=5; min samples leaf=4; min samples				
	split=2; max features= auto				
Gradient Boosting	Estimators=50; learning rate= 0.2; loss function=huber; max				
	depth=3; min samples leaf=10; min samples split=2; subsample= 1				
	Estimators= 50; learning rate=0.1; max depth=5; min child				
XGB	weight=3; subsample=0.5; booster=gbtree; base score=1;				
	colsamlpe bytree=1				

Table 6. Grid Search results for estimators for the time of oil impact on shore.

Table 7. Performance metric scores for each SML model for the time of oil impact on shore.

SML Regression Model	MSE	R ²	MAE
Linear Regression	58740,882286	-20,655910	138,343622
Lasso Regression $\alpha = 0,0001$	9660,976163	0.421533	75,071723
Ridge Regression $\alpha = 0,0001$	9660,982922	0.421533	75,071873
Lasso Regression $\alpha = 0,001$	9660,876227	0.421539	75,069761
Ridge Regression $\alpha = 0,001$	9660,949639	0.421535	75,071230
Lasso Regression $\alpha = 0,01$	9659,945540	0.421595	75,050049

Ridge Regression $\alpha = 0.01$	9660,617279	0.421555	75,064800
Lasso Regression $\alpha = 0,1$	9651,792903	0.422083	74,861490
Ridge Regression $\alpha = 0, 1$	9657,340705	0.421751	75,000713
Lasso Regression $\alpha = 1$	9602,074530	0.425060	73,711481
Ridge Regression $\alpha = 1$	9628,941944	0.423452	74,380531
Lasso Regression $\alpha = 10$	9708,940289	0.418661	77,001600
Ridge Regression $\alpha = 10$	9590,047414	0.425780	73,825956
Lasso Regression α= 100	17123,963067	-0.025325	108,279747
Ridge Regression α = 100	11522,261521	0.310086	85,268750
Lasso Regression α = 1000	17123,963067	-0.025325	108,279747
Ridge Regression α = 1000	15745,280553	0.057226	103,575249
Decision Tree	10476,396063	0.372709	73,988470
Random Forest	9173,914970	0.450697	71,717453
Gradient Boosting	5107,329803	0.704190	49,573632
XGB	5963,364088	0.642934	51,573956
SVR	8422,224413	0.495706	63,193655
Linear Regression	58740,882286	-20,655910	138,343622

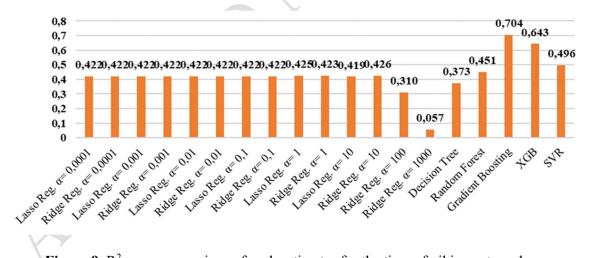


Figure 9. R² score comparison of each estimator for the time of oil impact on shore.

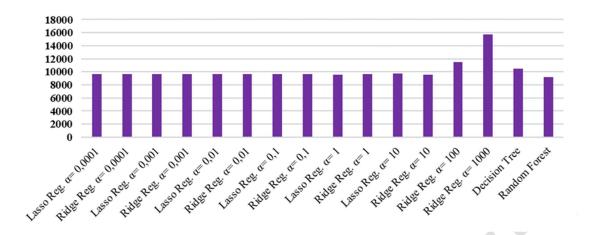


Figure 10. MSE comparison of each estimator for the time of oil impact on shore.

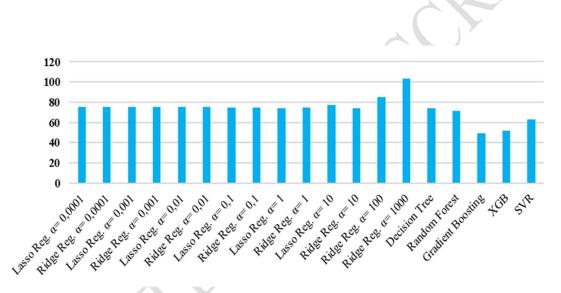


Figure 11. MAE comparison of each estimator for the time of oil impact on shore.

Time of oil impact on shore research has been carried out with a small data sample as mentioned before. Hence the results obtained are subject to improvement. Only Gradient Boosting has been observed to perform well with given data with R_GB^2=0.704. Although the performance score is lower than expected, it is indicative of a strong fit to data with the lowest MSE and MAE scores as well. Ensemble models showed promising results for predicting the time of oil impact on shore same as the amount of oil dispersion prediction with the exclusion of Random Forest.

It can be discussed that for oil spill behavior prediction, tree-based models outperform linear and polynomial regression models as well as SVR. Regularization also did not benefit regarding performance since a wide range of α values have been tested with none of them performing well.

Tree-based ensemble models, mainly Gradient Boosting and/or XGB, can serve as quick and effective DSS as an alternative to PISCES. While the PISCES serves as a valuable tool for visually simulating oil spill scenarios, it is worth noting that this simulation process can be time-consuming. In situations requiring swift and immediate response, the utilization of Gradient Boosting emerges as a highly valuable approach for expeditious decision-making and the prediction of oil spill behavior.

5. Conclusions

The potential impacts of oil spills can escalate into severe environmental disasters if prompt and wellinformed decisions are not implemented. The Oil Spill Contingency and Response (OSCAR) system, developed by the Environmental Technology Department of the Norwegian IKU Petroleum Research Institute, the Search and Rescue and Emergency Response Automation System (YAKAMOS) developed by the Scientific and Technological Research Council of Türkiye (TÜBİTAK), the Potential Incident Simulation Control and Evaluation System (PISCES), and the GNOME (General NOAA Operational Modeling Environment) system developed by the National Oceanic and Atmospheric Administration (NOAA), among others, provide critical support to decision-makers for the effective and execution of maritime emergency response. These systems utilize meteorological data (e.g., wind, air and sea temperature), oceanographic data (e.g., seawater density, surface currents, wave conditions, depth), maritime traffic dynamics, and pollutant and response equipment data (e.g., viscosity, density, barrier height, skimmer capacity). The integration of static data, which must be preloaded and regularly updated, alongside real-time dynamic data is vital for accurately representing the incident scene. Therefore, it is essential for institutions and organizations that provide such data (e.g., meteorological offices, oceanographic/hydrographic agencies, coast guard radars, vessel traffic service radars/AIS, police radars, satellite surveillance systems) to ensure seamless real-time data integration into decision-support systems. This extensive data input and the necessity for its real-time processing demand substantial organizational effort and time. While the Potential Incident Simulation Control and Evaluation System (PISCES) serves as an effective Decision Support System (DSS) for addressing oil spill incidents at sea, it's important to acknowledge that the duration required to obtain

simulation results can be impractical in certain urgent situations. This study introduces an alternative approach by employing supervised machine learning techniques as a means to expedite the estimation of critical parameters such as the extent of oil dispersion and the time it takes for oil to reach coastal areas. Unlike PISCES, which excels in scenario-specific customization and in-depth application, machine learning models offer the distinct advantage of providing rapid results for standard initial actions and adaptability to a wide range of scenarios. This approach aims to strike a balance between precision and expeditious decision-making in managing oil spill incidents.

With hyperparameters optimized with Grid Search, for estimating the amount of oil dispersion, XGB ($R^2=0.96$), Random Forest ($R^2=0.95$), and Gradient Boosting ($R^2=0.94$) have been observed to be top performers and for estimating time for oil to reach shore, Gradients Boosting ($R^2=0.704$) gave satisfactory results, with room to improve on with more data. The findings of this study demonstrate the superiority of tree-based models over other models, with ensemble models surpassing individual decision trees in terms of prediction performance.

While ensemble learning approaches, such as XGBoost and Gradients Boosting, performed extremely well, further applications of these techniques might still be limited due to computational resources and sizeable datasets, especially for real-time applications or less number of datasets. Moreover, reliance on synthetic data based on simulations may limit the validity of the results under field conditions. While the performance of ensemble models was good, their interpretability is lower compared to the simpler models, which may present some challenges for decision-makers who seek clear explanations of predictions. These limitations point toward avenues of future research involving the development of interpretable ensemble methods and validation with real-world datasets.

In conclusion, while PISCES offers valuable capabilities for visually simulating oil spill scenarios, it's important to acknowledge its inherent time-consuming nature. In contrast, ensemble models, which emerged as the top-performing techniques in this research, stand out as powerful alternatives for expedited decision-making and prediction of oil spill behaviors. As a foundational study, this exploratory research showcased that supervised machine learning models can be trained as complete decision-making tools for immediate and efficient responses to critical incidents such as oil spills in the near future with sufficient.

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Disclosure statement

The author declares no potential conflicts of interest

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