



## Research paper

# Predicting the consequences of accidents involving dangerous substances using machine learning

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## ABSTRACT

A new dimension of learning lessons from the occurrence of hazardous events involving dangerous substances is considered relying on the availability of representative data and the significant evolution of a wide range of machine learning tools. The importance of such a dimension lies in the possibility of predicting the associated nature of damages without imposing any unrealistic simplifications or restrictions. To provide the best possible modeling framework, several implementations are tested using logistic regression, decision trees, neural networks, support vector machine, naive Bayes classifier and random forests to forecast the occurrence of the human, environmental and material consequences of industrial accidents based on the EU Major Accident Reporting System's records. Many performance metrics are estimated to select the most suitable model in each treated case. The obtained results show the distinctive ability of random forests and neural networks to predict the occurrence of specific consequences of accidents in the industrial installations, with an obvious exception concerning the performance of this latter algorithm when the involved datasets are highly unbalanced.

## 1. Introduction

Industrial safety has witnessed many important shifts during the past few decades as a result of the continuing increase in the occurrence rates of accidents along with their associated cruel impacts. Such accidents have repeatedly demonstrated a severe ability to cause heavy human, environmental and economic losses. Many unforgettable disasters can be stated in this context, from Seveso – 1976, Bhopal – 1984, Deepwater horizon – 2010, to recently, Lac-Mégantic – 2013, Tianjin – 2015, Philadelphia – 2019, etc. However, the experience-based learning from this kind of occurrence has contributed to the establishment and the reinforcement of many regulatory and normative frameworks in order to improve the existing practices in handling such a problem. Several approaches, methods and databases have also been created providing more trustful modeling and simulation settings of the phenomena and dynamics involved in quantitative risk assessments. This includes the involvement of the accidental scenarios, with what they hold of deviations, interactions and behavior of the safeguarding measures as well as many aspects related to the systematic nature of failures, uncertainty, resilience, security threats, etc. The Seveso Directive (OJ, 1982), the U.S. Chemical Safety and Hazard Investigation Board (CSB, 1998), and the leading and lagging process safety indicators (Baker et al., 2007) are examples of such milestones.

With a faster pace of evolution, machine learning has recently attracted a lot of attention. It is generally regarded as a branch of artificial intelligence, which aims to develop algorithms that can automatically and directly learn from data. This kind of learning is basically categorized as supervised, unsupervised and reinforcement. Taking advantage of the era of data explosion and the new computing technologies, machine learning has found a distinct space in almost all the areas with a huge number of remarkable applications. Dependability and safety were no exception, where for instance, k-means clustering is applied in (Shi and Zeng, 2014) to develop a new environmental risk zoning method of the chemical industrial areas by determining and categorizing the risk characteristics. Moreover, six supervised learning techniques are used in Goh et al. (2018) to evaluate the relative importance of different cognitive factors within the theory of reasoned action in influencing safety behavior. In (Rachman and Ratnayake, 2019), several machine learning techniques are applied to conduct risk-based inspection screening assessments with a comparative analysis between such an approach and the conventional assessments. 15,000 Incident reports of five different companies in Alberta's oil sands sector are exploited in (Kurian et al., 2020) to create a risk matrix with a consistent scale and an automation of the process of classifying and categorizing risks by utilizing supervised machine learning. Additionally, an improved deep learning-based approach is proposed in (Fang

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et al., 2020) to automatically classify near-miss information contained within safety reports using Bidirectional Transformers for Language Understanding. Prognostic and health management of systems has been extensively treated from different angles in the framework of machine learning. Deutsch and He (2018); Wu et al. (2018); Bektas et al. (2019); Rocchetta et al. (2019); Palazuelos et al. (2020) are examples of some recent contributions in such a context.

The main objective of this paper is to propose a prediction framework for the possible consequences of accidents involving dangerous substances through the exploitation of lessons learned from the occurrence of a wide range of chemical accidental events and the use of several trustworthy machine learning algorithms. For this, the EU Major Accident Reporting System (MARS) is considered because of its consistency to feed several binary classification models in purpose of foreseeing the possibility of facing human, environmental and/or material losses in the industrial facilities by taking into consideration some specific influential characteristics. Such a framework can offer a solid decision-making basis for the various policies of risk treatment.

To achieve this objective, Section 2 is dedicated to describing the employed materials through the study of the nature of information collected in the MARS database, which is essential for the presentation of the involved circumstances and features, and the selection of those that play an influential role in deviating from the safe state. Furthermore, the implementation methods of six different algorithms are described along with a set of different types of performance metrics. Detailed presentations of the obtained results, comparisons and discussions of the performance of the employed algorithms are provided in Section 3. Finally, some concluding remarks and perspectives are summarized in Section 4.

## 2. Materials and methods

In this section, the employed data, classification algorithms and performance metrics are presented.

### 2.1. The eMARS database

The Seveso III Directive (OJEU, 2012) explicitly obliges the Member States of the European Union to inform the Commission of major accidents meeting certain specified criteria, which have occurred within their territory as soon as practicable and at the latest within one year of the date of the accident for the purpose of prevention and mitigation of major accidents. In addition to the information associated with the occurrence place, date and operator, this includes descriptions of the accident, the involved dangerous substances, immediate effects on human health and the environment, the employed and the planned emergency measures, and the results and recommendations of the conducted analysis.

Created in 1982 by the EU's Seveso Directive 82/501/EEC (OJ, 1982), MARS (or eMARS after it has been put online), which is managed by the Major Accident Hazards Bureau (MAHB), represents currently a highly important support for learning lessons from the occurrence of a wide range of hazardous events involving dangerous substances. With 1015 records until the end of 2019, the database provides detailed descriptions regarding the various involved circumstances, covering legislation, causes, consequences, substances, installations, remedial measures, lessons learned, etc. In recent years, several studies have employed eMARS to extract different kinds of lessons. For instance, a statistical analysis is carried out in (Ahmad et al., 2015) of accidents that occurred between 1988 and 2012 reported to eMARS by focusing on human and organizational factors to provide a new approach for the quantitative integration of such factors in risk assessments. Along with many other European and American sources, eMARS is used in Moreno et al. (2018) to develop a database of 300 security-related accidents in chemical and process infrastructures. It is also employed to highlight many other issues associated to different kinds of risks and features,

including, domino effects (Abdolhamidzadeh et al., 2011), natural-technological (Natech) risks (Di Franco and Salvatori, 2015), involvement of contractors (Abdul Majid et al., 2015), biogas production (Moreno et al., 2016), and accidents in ports (Lecue and Darbra, 2019).

Certainly, the connection between the Seveso directive and eMARS as a database provides an important standardization of the employed terms, criteria, classifications and purposes. This can particularly contribute to the reduction of uncertainty associated with the process of adopting the lessons learned from the reported events to any other similar cases. It should be noted that location and company names are not included in eMARS reports for confidentiality purposes, but it is known that it covers the EU, EEA, OECD and UNECE countries.

The distribution of all the recorded events until the end of 2019 is given in Fig. 1, which shows some decrease in the number of major accidents in the last decade compared to the preceding one (a difference of more than 110 major accidents), with more manifestations of near misses. Among the reported 867 major accidents, 14 are associated to domino effects, 14 are classified as Natech, 6 have transboundary effects and 52 involve contractors. For the 44 near misses, the distribution of those special circumstances is 0, 1, 1 and 2, respectively. Lastly, the 104 other events include 1, 2, 0 and 14 special circumstances. Obviously, the involvement of contractors is a key factor in the three kinds of events.

Industry type is another critical feature as demonstrates Table 1, where the 44.7% coverage proportion highlights the dominance of the petrochemical sector, oil refineries and general chemicals manufacturing. The classification of establishments according to Seveso II is also considered revealing the high number of records in the upper-tier establishments compared to those categorized as lower-tier, which is expected due to the related risk level and requirements (e.g., safety reports, emergency plans and information to the public). The third division gathers events of installations that are not covered by the Seveso directive (mainly covered by the Organisation for Economic Co-operation and Development "OECD") or do not meet its categorization requirements or simply that are not known. Among the 402 events in the upper-tier category, 340 are major accidents, 26 are near misses and 36 belong to the other events' class. Also, 94, 13, 9 is the corresponding distribution of the 116 events in the lower-tier establishments. For the 497 cases in the not known/not applicable category, the distribution is 433, 5 and 59, respectively.

Almost half of the registered entries involved release major occurrences, 314 of them are gas/vapor releases to air and 124 are fluid releases to ground/water. Among the 249 fire major occurrences, 82 are conflagrations and 63 are pool fires. Moreover, 76 out of the 198 explosions are vapor cloud explosions (VCE), 29 are associated to explosive decompositions, while the number of the boiling liquid expanding vapor explosions (BLEVE) does not exceed 7 cases. However, in most cases, off-site external interventions were necessary to control the situation.

Similarly, almost half of the total number of the records caused at least one injury or fatality. Such a toll has a predominant relationship to organizational and plant/equipment defects. The material consequences are present in 557 cases, mainly associated to direct material damages, response, cleanup and restoration costs. Lastly, the environment is affected in 158 events, more than 29 of them have a direct impact on freshwater.

### 2.2. Implementation

Aiming to select the best model for each type of consequence, several alternatives are implemented and compared using a variety of performance metrics. The considered features are: Seveso II status, industry type, implication of contractors, organizational, plant/equipment, external and other causes. Besides the conventional preprocessing treatment, some of the existing close industry type classes are merged into a single class (mainly, chemical installations). Consequently, the original 46 industry sectors are reduced to only 33. Moreover, k-fold

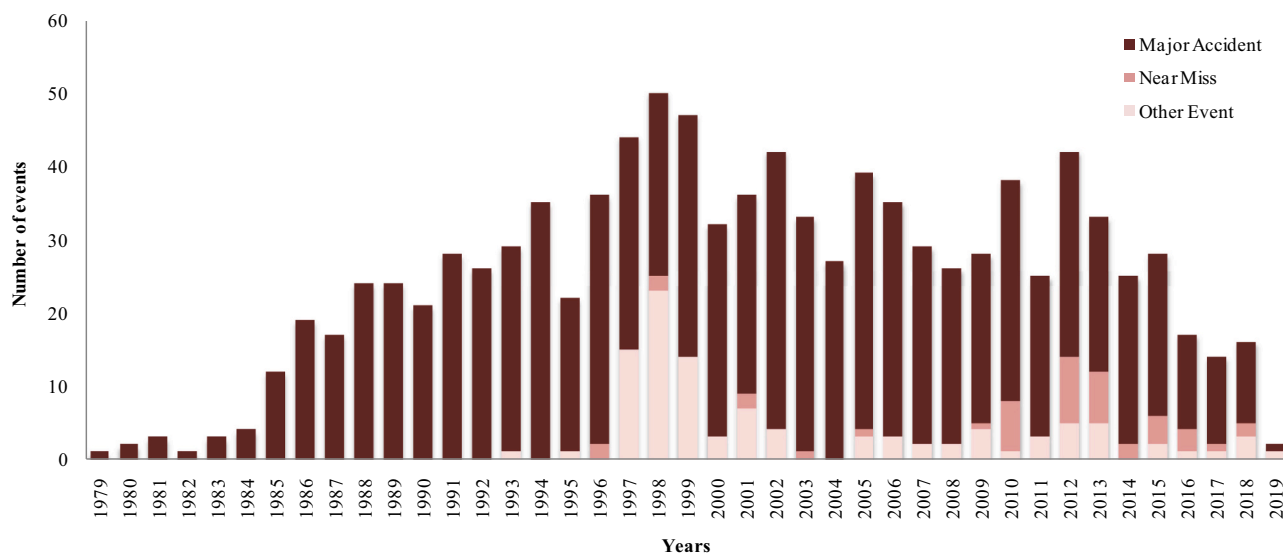


Fig. 1. Distribution of events between 1979 and 2019 according to their type.

cross-validation is employed to take advantage of the entire dataset for training and testing. A value of 10 is selected for “k” in all the implementations based on the iterative consideration of a large number of possible values.

The considered classification algorithms are: logistic regression (LR), decision trees (DT), neural networks (NN), support vector machine (SVM), naive Bayes (NB) and random forests (RF). These algorithms are fundamental in machine learning, which have a variety of applications in a large number of fields. Detailed presentations of the basic principles, applications and implementation guides of those employed algorithms in addition to many other associated concepts can be found in (Bonaccorso, 2017; Ayyadevara, 2018). However, the main involved hyperparameters in each developed model are cautiously tuned to obtain the best possible results within the framework of Scikit-learn.

Several metrics are employed to assess the performance of those developed models, namely, Accuracy, Precision, Recall, F1 score, Cohen’s kappa score, Area under the Receiver Operating Characteristics (ROC) curve (AUC), Log loss (cross entropy) and Brier score (squared error). Accuracy is a basic qualitative measure relying on specific thresholds to measure the final outcome of a model. It represents the number of all the correct predictions divided by the total number of the tested samples. Recall (aka, sensitivity, true positive rate) and precision (aka, positive predictive value) belong also to the qualitative category representing the number of the correctly predicted positives divided by the total number of real positive samples in the former and by the number of the predicted as positives in the latter. Obviously, recall favors the model’s ability to avoid the false negative predictions while precision favors its ability to avoid the false positive predictions. F1 score is used as combination of these two metrics by estimating the associated harmonic mean. Cohen’s kappa can be used to measure the agreement between reality and prediction considering the effect of randomness in such a consensus. In a more general context, AUC is a widely used performance metric for binary problems measuring the area under the ROC curve, which shows the variation of recall and fall-out (false positive rate) over various discrimination thresholds. Belonging to the probabilistic category, Log loss is another popular measure that considers the divergence of the predicted probability distribution based on the concept of entropy. Furthermore, Brier score measures the mean squared difference between the predicted probability distribution and the real observation. Detailed descriptions and comparisons of a wide range performance metrics can be found in (Ferri et al., 2009; Luque et al., 2019).

### 3. Results and discussions

The obtained results for the human, environmental and material consequences are described and discussed subsequently.

#### 3.1. Human consequences

Health and safety of human beings, both inside and outside the concerned facility, represent a primary threat of accidents regardless of their occurrence likelihood. Ranging from minor illnesses, disabilities to more serious injuries and even deaths in the worst-case scenarios, such a type of loss has a decisive impact in risk assessment studies. This subsection is devoted to the prediction of casualties, which are characterized by the occurrence of at least one injury or fatality, using the various discussed classification algorithms. The obtained performance metrics for each developed model are summarized in Table 2, while the associated ROC curves are shown in Fig. 2.

In spite of the obvious convergence between the results of the various developed models, the eight estimated measures demonstrate the superiority of the RF implementation, in which 102 trees are considered. An 80% score is approximately reached for all of the accuracy, F1 and AUC. With the exception of the precision’s classification that favored NB, NN networks provided the second best ability to treat such a problem. Clearly, the lowest performance is associated to DT except for the case of recall, which has a score similar to that of RF. However, it should be noted that from a safety perspective false negatives represent a key issue what aligns the consideration of recall. On the other hand, precision is important for other operational, financial and complexity related aspects.

#### 3.2. Environmental consequences

The effects of accidents on the natural environment represent another critical matter due to the involvement of several factors related to its sensitive and multidimensional nature. Such effects can have an immediate massive brutality but also a sustainable contribution to an irreversible distortion of the existing diversity and equilibrium conducting to other regenerative impacts that can directly and indirectly threaten many vital aspects. In this context, the associated accidental events are mainly related to the direct release and spillage of hazardous materials as well as outcomes of the related fires and explosions causing different kinds of pollution.

Referring always to eMARS, the main trait in this part is the

**Table 1**  
Distribution of events according to the industry type and Seveso II status.

Industry Type	Number of events			
	Not known/not applicable	Lower tier	Upper tier	Total
Chemical installations – carbon oxides		1		1
Waste storage, treatment and disposal			1	1
Chemical installations – nitrogen oxides		1		1
Chemical installations			1	1
Manufacture of glass			1	1
Building and works of engineering construction	1			1
Power generation, supply and distribution			1	1
Mining activities (tailings and physicochemical processes)			2	2
Chemical installations – inorganic acids		1	1	2
LNG storage and distribution			2	2
General engineering, manufacturing and assembly	2			2
Chemical installations – sulfur oxides, oleum		2		2
Electronics and electrical engineering	1	1		2
Water and sewage (collection, supply, treatment)		2		2
Textiles manufacturing and treatment	2			2
Processing of non-ferrous metals (foundries, smelting, etc.)			2	2
Chemical installations – Industrial gases		1	2	3
Chemical installations – chlorine			3	3
Ceramics (bricks, pottery, glass, cement, etc.)	2		2	4
Production of pharmaceuticals	2	2		4
LPG production, bottling and bulk distribution	1		3	4
Production and storage of fertilizers		1	3	4
Chemical installations – ammonia			4	4
Wood treatment and furniture	4	1		5
Leisure activities	5			5
Production and storage of fireworks		4	3	7
Not known / not applicable	3	1	4	8
Processing of ferrous metals (foundries, smelting, etc.)			9	9
Agriculture	10			10
Handling and transportation centers (ports, airports, lorry, etc.)	7	1	3	11
Fuel storage (including heating, retail sale, etc.)	2	1	11	14
Production of basic organic chemicals		5	10	15
Processing of metals using electrolytic or chemical processes		7	8	15
Chemical installations – other fine chemicals	2	5	10	17
Production and manufacturing of pulp and paper	13	4	1	18
Power supply and distribution	9	6	6	21
Production and storage of explosives	1	3	18	22
Waste treatment, disposal	17	4	4	25
Manufacture of food products and beverages	28	4	1	33
Plastic and rubber manufacture	19	3	17	39
	38	4	9	51

**Table 1 (continued)**

Industry Type	Number of events			
	Not known/not applicable	Lower tier	Upper tier	Total
Production and storage of pesticides, biocides, fungicides				
Processing of metals	36	2	17	55
Other activity (not included above)	25	15	20	60
Wholesale and retail storage and distribution (excluding LPG)	47	5	18	70
Petrochemical / Oil Refineries	71	11	104	186
General chemicals manufacture (not included above)	149	18	101	268
<b>Total</b>	<b>497</b>	<b>116</b>	<b>402</b>	<b>1015</b>

unbalanced nature of the associated dataset, where 158 of the existing 1015 reports conducted to environmental damages. To handle this matter, the synthetic minority over-sampling technique (SMOTE) (Chawla et al., 2002) is employed using Imblearn to adjust the under-represented class “1” by generating new synthetic samples. The obtained results are given in Table 3.

It can be seen that all the obtained scores are less powerful than the previous case, which is due to the unbalanced nature of the linked dataset. However, an AUC of 71% is reached with an associated accuracy of 77%, once again by means of RF. Without employing the over-sampling technique, such values arrive to 50% and 82% respectively, with a zero value for all of the precision, recall, F1 and Cohen's kappa. The associated confusion matrices are shown in Fig. 3.

However, DT achieved the second best performance according to all the estimated metrics excepting recall, which takes the only different value. LR comes in the last order with a slightly lesser performance than NN, SVM and NB.

### 3.3. Material consequences

This category assembles the various economic losses, which mainly implies the costs of the affected equipment, buildings and vehicles in addition to the released materials. It also takes into consideration the costs of production loss, response, cleanup, restoration, repair, decontamination, etc. The results of modeling this type of consequences are presented in Table 4.

For this type of consequence, NN yielded the best modeling ability with an AUC value of 73% and an accuracy of order of 77%, where 78 cases were correctly classified, 18 false positive samples and other 5 ones that fell in the false negative category. Nevertheless, DT provides a slightly higher score for precision. The gap between the results of NN and those of all the other alternatives is observable with a relative proximity of RF and LR, and clear weakness of NB.

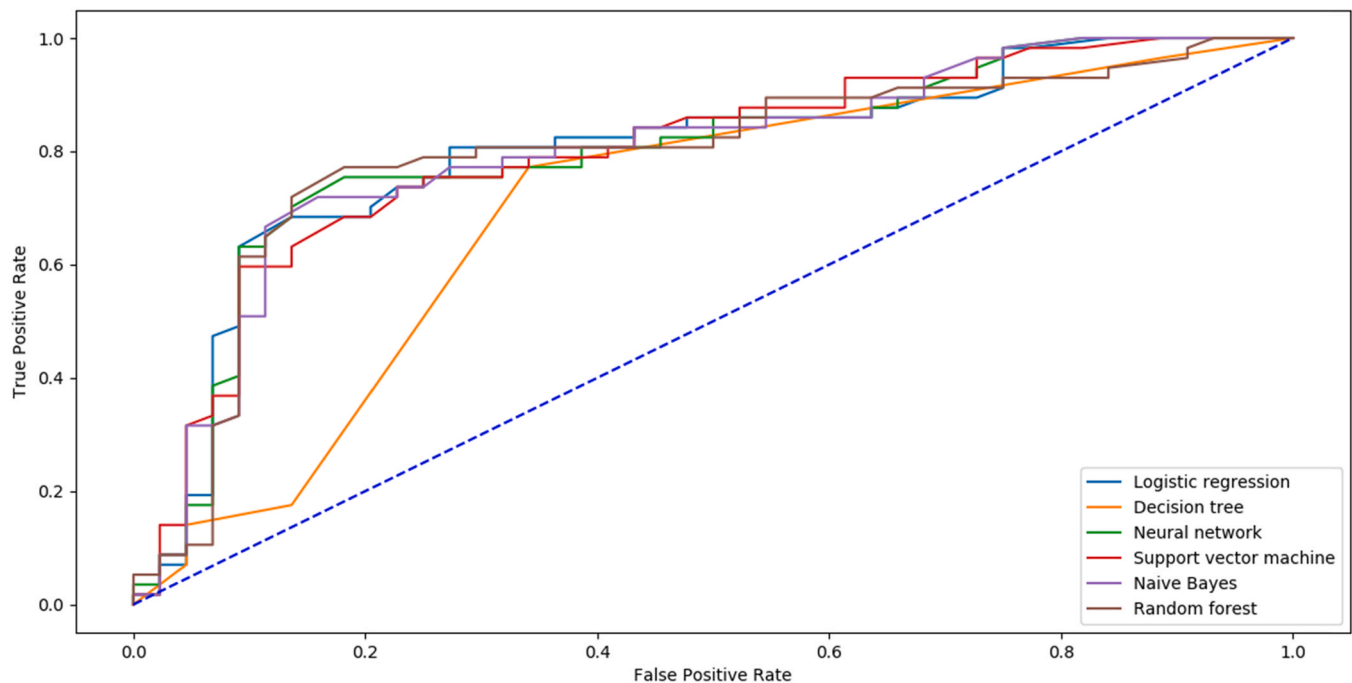
It can be extracted that RF and NN provided the best prediction frameworks for the two types of consequences in which the datasets are balanced. RF has a similar effectiveness for the unbalanced case as well. Moreover, in the first two cases, there was complete correspondence between the different measures regarding the classification of the performance of the various models. Some exceptions are associated to precision, recall, and slightly F1. In the last case, the level of discrepancy was higher affecting some other metrics. Fortunately, such a matter has no effects on the top-ranked model in each category. Relying on accuracy, precision and/or recall requires a clear definition of the implied conditions and objectives.

## 4. Conclusion and perspectives

Ensuring the safe operation of the industrial facilities and processes that deal with hazardous materials is a necessity that enfolds many

**Table 2**  
Comparative analysis for the human consequences.

	Accuracy	Precision	Recall	F1	Cohen kappa	AUC	Log loss	Brier
LR	0.733	0.813	0.684	0.743	0.469	0.740	9.233	0.267
DT	0.723	0.746	0.772	0.759	0.433	0.716	9.575	0.277
NN	0.772	0.827	0.754	0.789	0.543	0.775	7.865	0.228
SVM	0.752	0.796	0.754	0.775	0.500	0.752	8.549	0.248
NB	0.762	0.837	0.719	0.774	0.527	0.769	8.207	0.238
RF	0.792	0.846	0.772	0.807	0.583	0.795	7.181	0.208



**Fig. 2.** ROC curves for the human consequences.

**Table 3**  
Comparative analysis for the environmental consequences.

	Accuracy	Precision	Recall	F1	Cohen kappa	AUC	Log loss	Brier
LR	0.693	0.314	0.611	0.415	0.235	0.661	10.601	0.307
DT	0.752	0.370	0.556	0.444	0.293	0.675	8.549	0.248
NN	0.703	0.324	0.611	0.423	0.248	0.667	10.259	0.297
SVM	0.713	0.333	0.611	0.431	0.261	0.673	9.917	0.287
NB	0.713	0.333	0.611	0.431	0.261	0.673	9.917	0.287
RF	0.772	0.407	0.611	0.489	0.350	0.709	7.865	0.228

convoluted challenges. Such a necessity is following an escalating tendency due to the reached levels of climate sensitivity in addition to the demographic and economic notable changes. Away from the traditional risk assessment practices, which are generally founded on scenario-based decomposition analysis techniques, machine learning has opened up new horizons to exploit the acquired experience in order to handle new situations and to extract new knowledge.

Six different binary classification algorithms are employed to predict the possible occurrence of specific consequences of accidents in the industrial installations using the eMARS database. The considered features are chosen to cover the nature of involved activities, circumstances and management procedures in addition to the potential causes of accidents. Referring to the various utilized performance metrics, which matched most often, RF showed certain superiority for the human and environmental consequences, while NN provided the best results for the material consequences. However, excepting the case of the unbalanced datasets using NN, both implementations can handle the entire problem,

where a 70% AUC score can approximately be ensured.

From a risk assessment viewpoint, the developed prediction study can provide a helpful support for predicting the nature of the involved risks and judging their acceptability, which is crucial for the definition of the various allocation, prevention and mitigation strategies of risk management. Nevertheless, further improvements can be made in future research through the consideration and combination of other datasets with a wider feature space. Integrating and validating such a dimension in the traditional risk assessment frameworks represent also an important perspective.

#### CRediT authorship contribution statement

**Mourad Chebila:** Conceptualization, Methodology, Software, Validation, Data Curation, Writing - Original Draft.



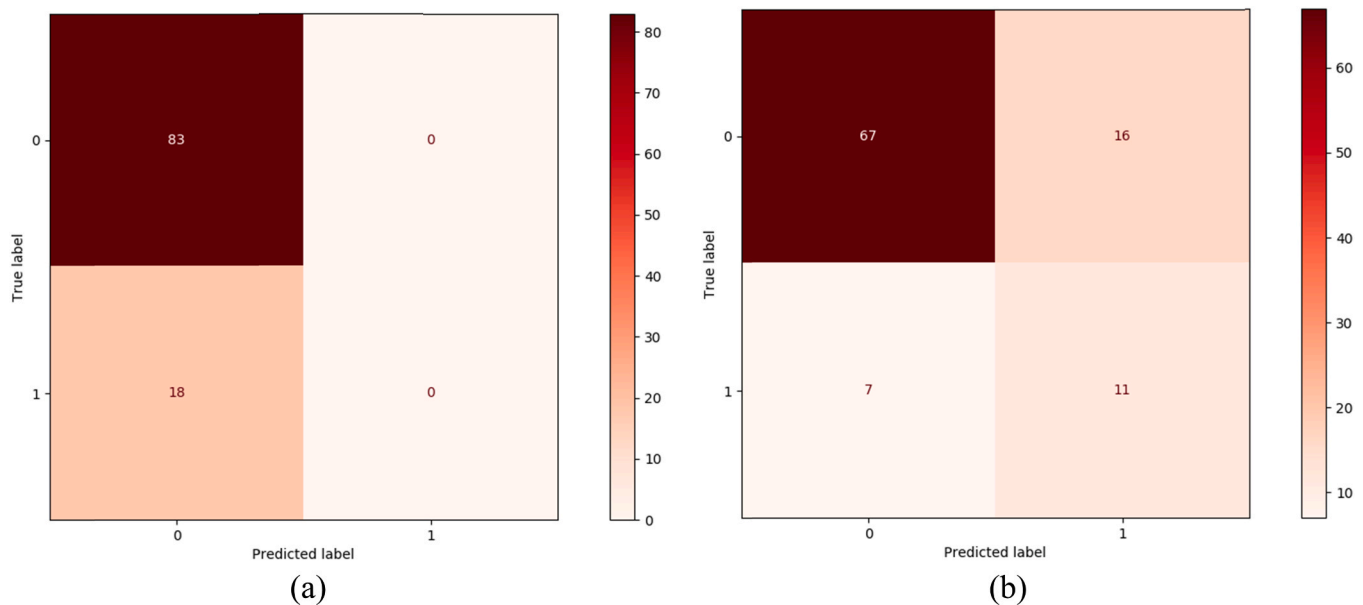


Fig. 3. RF confusion matrices (a) without, and (b) with over-sampling .

Table 4

Comparative analysis for the material consequences.

	Accuracy	Precision	Recall	F1	Cohen kappa	AUC	Log loss	Brier
LR	0.703	0.731	0.803	0.766	0.363	0.677	10.259	0.297
DT	0.673	0.759	0.672	0.713	0.337	0.674	11.285	0.327
NN	0.772	0.757	0.918	0.830	0.496	0.734	7.865	0.228
SVM	0.673	0.700	0.803	0.748	0.289	0.639	11.285	0.327
NB	0.634	0.676	0.754	0.713	0.210	0.602	12.653	0.366
RF	0.713	0.716	0.869	0.785	0.364	0.672	9.917	0.287

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.ecoenv.2020.111470](https://doi.org/10.1016/j.ecoenv.2020.111470).

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