**Machine Learning-based Decision Support Models for Performing Preliminary Hazard Analysis: An Application to an Atmospheric Distillation Unit**

July Macêdo, Márcio Moura, Isis Lins

Center for Risk Analysis and Environmental Modeling, Department of Industrial Engineering, Av. da Arquitetura, 211-351, 50740-550, Federal University of Pernambuco, Recife-PE, Brazil

Enrico Zio

Department of Energy, Polytechnic of Milan, Via Ponzio 34/3, 20133, Milan, Italy

MINES Paris Tech, PSL Research University, CRC, Sophia Antipolis, France

# ***Introduction***

Oil refineries are complex and expensive plants,whose main purpose isto separate the petroleum into valuable products. Three basic activities characterize the operation of these systems: separation, conversion and treatment [1]. In fact, the refining process starts in the atmospheric distillation unit (ADU). In a nutshell, the separation that takes place in ADU requires the application of heat and involves a series of evaporation and condensation of the liquid mixture and involves different hazardous materials chemical products, such as fuels and residues [2,3].

In fact, loss of containment of flammable and toxic materialsmay cause major accidents with severe effects to humans or environment. Particularly, these events entail the occurrence of fires, explosions and/or atmospheric dispersion of toxic products. Risk studies provides a basis for the implementation of measures to reduce potential risks and there are different qualitative techniques such asPHA that can be adopted[4–6] to analyze the risks involved withthe operation of an ADU in oil refinery.These methods are based on experts’ opinions and application of good engineering judgement to identify differentaccidental hypotheses, and then analyze and classify their expected frequency and severity.

Theserisk studies may be very costly and time-consuming [7] because they involve the evaluation of quantities of dense engineering documents, and often require experts’ knowledge and creativity to postulate several accidental scenarios that may not have happened in the past or have very low likelihood of occurrence and usually can take months depending on the dimension and complexity of the facilities and processes.

Besides that, eithernational/international standards or regulatory councils often require a periodical and/or compulsory review of PHA.These entities establish how often the update should be developed.The aim of these reviews is that the up-to-dated PHA represent the current state of the studied system.However, these studies usually start from scratch disregarding the past PHA versions that were done for the same system, which requires a rather high cognitive and time burden over the experts. Considering this, the development of models to assist the elaboration and review of these documents is certainly attractive.

At the best of the authors’ knowledge, there is a lack of works related to the application of machine learning (ML) to decrease the efforts involved in performing risk analysis (RA) aiming at preventing potential accidents.Moreover, the ability of ML techniques to deal with large volumes of data makes their application attractive for risk analysis. Indeed, to perform a PHA it is necessary to deal with several engineering documents that characterize the system to be analyzed. Next, a multidisciplinary teamof experts identify and analyze in-depth the potential accident scenarios. Finally, the risks are categorized by evaluating the likelihood of causes and severity of consequences of the possible accidental scenarios [8].

Recently, [9]used reports of aviation accidents to develop asupport vector machines (SVM) and deep learning-based hybrid model to predict the risk level associated with aviation incident outcomes, and also developed a rule to combine the prediction from the two machine learning algorithms. However, the predictions are related to accidents that have already occurred, which makes their model to respond reactively.[10] suggested a ML approach to perform risk assessment, where a deep neural network is used to predict the risk increase/decrease of well damage from wellhead frequency over time.Moreover, [11]developed a ML based-model to conduct risk-based inspection screening assessment that is used to identify equipment that makes major contribution to system’s total risk of failure, thus, allowing to prioritize high-risk systems. However, as the authors mentioned the risk category is obtained after the evaluation of the probability and consequence of failure, which are defined based on the knowledge of installation history, as well as engineering judgment.

Therefore, this paper proposes the use of ML for supporting automated PHA.To that end, we developed a model to execute the same reasoning used by expertsduring the elaboration of a PHA.Our idea is that knowledge about potential accidents, which can be extracted from previous PHA and/or engineering documents, is provided to an ML based method. Then, this model learns the relationships among the operating conditions, potential accident scenarios, their causes and consequences.Finally, the identified risks could be assessed with reduced efforts, using a trained ML classifier by predicting its consequence level and likelihood rating,that are combined to determine its risk class.The proposed method is here developed with reference to a specific ADU of a real oil refinery, which contains hazardous materials and is characterized by propitious conditions that may lead to catastrophic accidents.

In this paper, six ML techniques were investigated in order to compare their performance, and select the most appropriate: AdaBoost (AB), SVM,random forest (RF),multilayer perceptron (MLP),k-nearest neighbors (KNN), andgradient boosting decision trees (GB); (ii) to develop anapproachto support risk analysts to evaluate accidental scenarios, aiming at preventing accidents, related to the operation of an industrial facility, by means of the reduction of efforts required to perform PHA. Thus, the trained model could be used as a practical tool to support risk analysts to perform PHA, and could be adopted as an alternative to speed up the review process of the risk study during the system life cycle.

# ***Theoretical background***

## **Risk Analysis**

Major accidents can be described as critical events that can lead to various fatalities and/or catastrophic impacts to people and environment or severe property damage[12,13]. In oil and gas industries, these eventsgenerally involve large-scale leakage of flammable and/or toxic materials that may result in fire, explosion and/or dispersion of toxic clouds [14].

The consequences and impacts of major accidents are directly related to the nature of the released material.Indeed, when flammable substances get in contact with an oxidant, they may react releasing thermal energyand,then,a combustion process thatresults in either fire or explosion, where the latter only occurs when there is a mixture of oxygen with fuel gas in a certain proportion, which is defined by the lower and upper flammable limits [15].Moreover, toxic emissions may also spread as clouds in the air, and theirseverity and extent depend on the physicochemical and toxicological properties of the released substance, and on the atmospheric and geographical conditions.In this context, risk assessment is theoperativeprocess of RA, where the accidental scenarios are characterized through the methodical use of data and knowledge for describing andidentifyingaccident causes, probabilities, and consequences. Then,the risks are compared against given risk criteria[16–18].

PHAis generally applied early in the facility life cycle.However, PHA is periodically and/or compulsorily reviewed when required by either national/international standards or regulatory councils, which establish how often PHA should be updated.Risk matricesare usually adopted in PHA to categorize the different hazardous situations. The consideration of consequence level and likelihood of occurrence provides the risk ranking for an accidental hypothesis[19]. Thus, risk matrices are widely used to prioritize accident scenarios, according to its effects and likelihood to occur, in order to develop efficient measures to reduce or mitigate the risk[20].

Initially, to execute a PHA, the experts determine the scope of the analysis, and generally divide the facility into smaller systems, whose boundaries are defined according to specific characteristics of the chemical products and operating conditions. Then, a large number of documents (e.g. process and operational flowcharts, equipment lists, material safety data sheets, etc.) are considered in order to gather relevant information to characterize the system and its environment. Next, the team of risk analysts evaluate and discuss these information to postulate possible leakages, identify the hazards and their possible causes and consequences. Finally, the team evaluate and classify the risks according to its effects and likelihood.

This process can be very time-consuming in practice, particularly depending on the complexity of the system analyzed and on the diverse backgrounds of the experts in the team,who execute the RA and must be periodically reviewed. In this context, the ML-based method here developed aims at reducing the efforts required to perform traditional PHA.

## **Machin e Learning**

In the context described so far, the application of artificial intelligence (AI) techniques seems attractive to simplify and improve the process of RA. Indeed, [21] pointed out that data analytic tools would help reduce fatality and injury rates in the oil and gas industry, by revealing hidden patterns and trends that could lead to accidental scenarios. Yet, as argued by [22], developers of AI systems acknowledge that, for diverse applications, it is simpler to train a system by providing a set of input-output pairs that represent the desired behavior and, then, use it for predicting the response to new input rather than building phenomenological models. [23] mentioned that AI has been developed to reproduce human abilities as perception, analysis, reasoning, learning, exchange information, and decision-making.

Methods based on AI and statistical techniques have been largely applied to different fields such as health care, finance, engineering and education [24]. Knowledge-based systems represent typical AI techniques, including ML, automatic speech recognition, natural language processing, and so on [23,24]. According to [22], ML techniques aim at improving a performance measure (e.g. the accuracy of a classifier) by means of training practice. In other words, ML detects and obtains knowledge from the real world to reproduce the learning ability [25]. To that end, different ML models have been established.Here,we compared the performance of six differenttechniques that are suitable for multiclass classification, available in scikit-learn [26]:KNN, SVM, MLP, AB, RF, and GB.

# ***Proposed Model***

The aim of the proposed model is of reducing the efforts made by multidisciplinary teams and time required during the development of PHAs. To that end, an ML based method has been developed by using information obtained through previous risk studies. Generally, during the elaboration of PHA, the potential risks are classified according to a risk matrix based on ISO 31000 [27] () as tolerable (T), moderate (M), or non-tolerable (NT). The risk category of an accidental hypothesis is determined by combining its consequence level () and likelihood rating ().

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Risk Matrix | | | | |
| Consequence level | Likelihood rating | | | |
| A | B | C | D |
| IV | T | M | M | NT |
| III | T | M | M | M |
| II | T | T | T | M |
| I | T | T | T | T |

Table 1. Risk matrix used in the preliminary risk assessment.

Source: adapted from [72]

| Consequence level | | |
| --- | --- | --- |
| Category | | Effects |
| I | low | without injuries or first aid cases |
| II | significant | serious injuries inside or mild injuries outside the facility |
| III | high | fatality inside or serious injuries outside the facility |
| IV | very high | multiple deaths inside or outside the facility |

Table 2. Description of the consequence level in terms of the effects to human life.

Source: adapted from [72]

| Likelihood rating | | |
| --- | --- | --- |
| Category | | Description |
| A | very rare | conceptually possible, but there are no records in the literature |
| B | rare | unlikely to occur in normal conditions |
| C | possible | may occur sometime |
| D | likely | expected to occur |

Table 3. Description of the likelihood categories. Source: adapted from [27]

Therefore, we here propose to develop two different ML classifiers, ML1 and ML2, to automatically classify the risks. In fact, the input,**,** contains useful information to characterize the hazards. In fact, the input,**,** contains useful information to characterize the hazards. Indeed, each instance registered in the input vector contains the operational conditions, besides features to characterize a hypothetical accident. As depicts, first, information about the accidental hypotheses, such as the material released and operating conditions, are extracted from past PHAs and analyzed in order to define a set of input-output data, where each pair is related to a potential accident scenario (pool fire, flash fire, explosion, or toxic cloud). Then, this information is provided to two different ML models that are implemented to classify both the likelihood rating (ML1) and the consequence level (ML2). Next, the categories are combined and the risk is classified as T, M or NT according toTable 1.

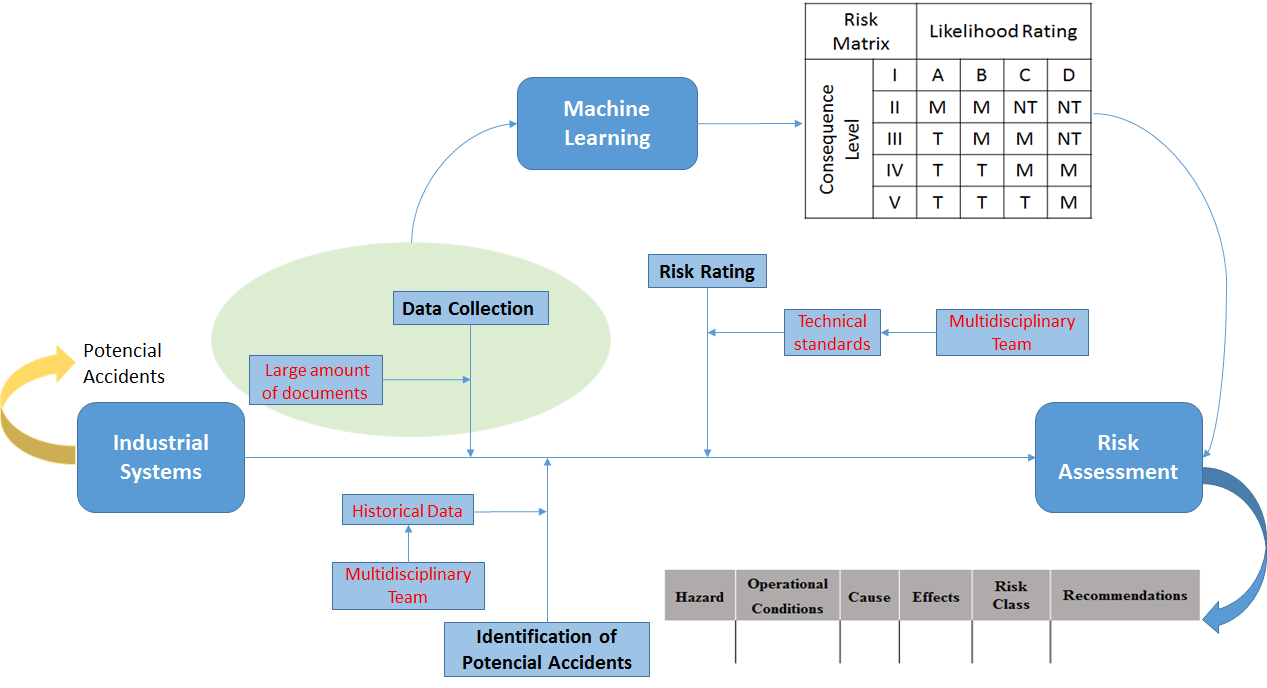


Figure 1. General steps to perform a qualitative risk assessment through the proposed model

In this way, the proposed model represents a less costly path to perform RA since it does not require that experts interpret the engineering data in order to indicate which are the categories of likelihood and consequence that are more appropriate to a given accidental scenario. This characteristic makes the ML-based model even more useful when national or international regulators demand revisions of a PHA. In these situations, experts usually have to assess new accidental hypotheses that had not been analyzed in previous studies. Thus, the ML-based models would be able to perform the classification of the risks in a more efficient way.

Moreover, it is important to emphasize that the critical judgment of the risk analyst would still be necessary to evaluate the coherence of classifications provided by the ML models. Thus, the proposed model is not intended to replace the risk experts. In contrast, our aim is at easing and reducing the efforts and time involved in this process of risk assessment.Our aim is at selecting the ML classifier that provides the best results. To that end, we compared a set of six well-established ML classifiers, which are briefly introduced in Section 4.3that also explains the whole modeling process.

## **Information available in past PHA**

The training of a ML model requires a reasonable quantity of good quality input data to comprehendthe reasoning adopted to classify the risks during PHA by the multidisciplinary group, which is composed by experts from different fields.Thus,PHApreviously conducted for an ADU of an oil refinerywas evaluated and importantinformation was extracted to build the dataset used in this study.Experts assume small leakages and ruptures are, respectively, expected to occur (likelihood rating () - D) and very rare (A), their causes may be either human failure, abnormal operating conditions or corrosion, and then lead to three potential accident scenarios (AS): pool fire, flash fire or toxic vapor cloud that in turn have different impacts. For instance, in these operating conditions, the severity of the effects of a pool fire caused by a small leakage was categorized as significant (consequence level - II), while ruptures are classified as high (III); see .

Finally, the risk of these hypotheses were respectively classified as M and T according to . Given that, PHA allowedfor extracting important information related to the events of interest. Now, it is necessary to select which information to use as input variables, . This step is called feature selection and is described in next Section.

## **Feature selection**

We have analyzed two initiating events: i) small leakages through a hole in the pipeline, valves, etc., and, ii) ruptures that contemplates situations where a large quantity spills. These assumptions were represented by including in the input data a binary variable (IE), where 0 and 1 mean small holes and ruptures respectively. Thus, IE directly determines the surface area of the leaked product, which in turn influences the rate of evaporation, along with the environment conditions. The assessment of two different IE for the same subsystem implies diverse accidental scenarios,andthen different risk classes. For instance, when a material is released through a small hole, if the release rate is lower than the rate of evaporation, it would not result in a pool[28].

The effects of an uncontrollable leakage depend on the nature of the material and its physical state, determined by the operational conditions and the presence of adverse situations, e.g. ignition sources and contaminants. In this context, it is important to have in mind the influence of some variables, such as temperature (T), pressure (P) and mass flow rate (FR), on the physical effects produced. All variables considered in ML1 and ML2.

In fact, T and P play an important role to determine if the chemical product (CP) is liquid or gaseous. In the ADU, the CPs that are somehow processed are: petroleum, natural gas, atmospheric residue, diesel, naphtha, kerosene, and LPG. Additionally, combined with FR, they are necessary to determine the rate of evaporation and the pool area or vapor cloud [8,29]. Moreover, T and P determine the lower and upper flammablelimits, which are fundamental to influence the occurrence of fire or explosion [8]. Thus, these variables are necessary to condition which scenarios may occur and, thus, to classify the potential risks. For this reason, T, P and FR were included as continuous variables in the features dataset. In addition, it was also considered contamination (CT), a binary variable associated with CP (e.g. diesel contaminated with H2S) that represents the presence of toxic substances (in smaller amount) that may spread toxic clouds.

Yet, the release of a material that is both flammable and toxic could lead to different scenarios. Thus, the risk analysts can assume loss of containment (IE) may lead to fire if the product reaches an ignition source; otherwise, it would disperse as a toxic cloud if the released material evaporates. In this way, four types of effects (scenarios – AS) were considered: pool fire, flash fire, vapor cloud explosion and toxic vapor cloud. For each one, there is a respective risk, which is classified as T, M or NT, according to its likelihood rating (LR) and consequence level (CL); see . Finally, the risk associated to an accidental scenario is categorized through the combination of the LR and CL.

## **Modeling process**

For the ML classifiers’ implementation,a free machine learning library, scikit-learn[26], was adopted.Then, the information extracted from previous PHA was used to train both classifiers. Next, a 10-fold cross-validation (CV) was performed to select the hyper-parameters of the SVM models. The idea is to partition the data in order to train the model with one part and, then, test it on the remaining portions of the dataset. Then, the data was equally divided into 10 parts, where 9 are used for training and 1 for test purposes in each CV run.

Thus, this process is executed 10 times, changing the test portion, until all data has been used (Yadav & Shukla, 2016). Finally, the model adequateness metrics are estimated as the averages over 10 runs and the hyper-parameters that lead to the highest mean score were selected.In this work, the performance of the model on the test set was evaluated through the F1 score (Equation 1), which is the harmonic average between two other measures (precision and recall), that take into account false negative rate and the false positives (see Flach & Kull, 2015):

(1)

where , and are the number of correct classifications, the total number of predictions and the number of observed instances with label respectively.

In this way, F1 score represents how precise and robust the model is (Pedregosa et al., 2011) by measuring both how many instances are correctly classified and how many classifications the model does not miss. The accuracy, equation 2, which represents the percentage of correct classification, was also used to compare the results obtained during the training and test in order to detect possible overfitting.

(2)

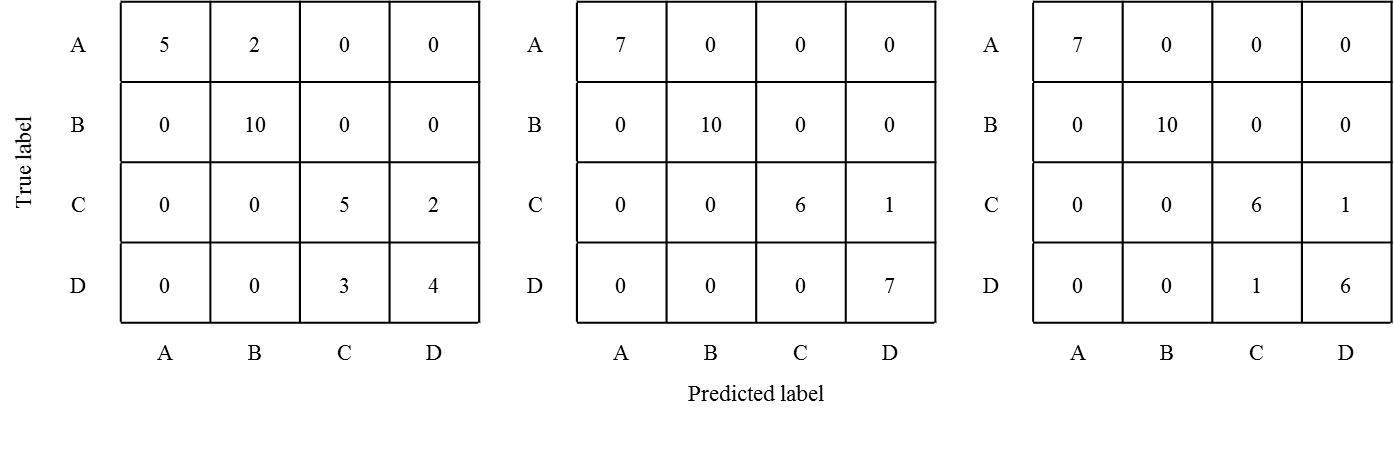
After the selection of the hyper-parameters, the classifiers were fitted. Then, the results of the 10-CV to predict CL and LR were evaluated. Thus, the ML classifiers that showed the best F1 score were used to construct the combined model (as illustrated in ). The results were summarized through the F1 score mean and standard deviation, for each classifier. Finally, the combined model were used to estimate the risk label () for the remaining samples. The results are discussed in next Section.

# ***Results and Discussion***

Firstly, we divided ADU into a number of subsystems, which are characterized by different chemical products and operating conditions, and thus they might cause diverse types of accidents. Each sample extracted from previous PHA is composed by a pair input-output that represents an accidental scenario with respective LR and CL. Then, a dataset made up of 151samples.The classes are considerably unbalanced, and that there were no instances classified as consequence level I or risk category NT. The information provided to the classifiers is exclusively from a specific ADU. Moreover, the dataset is relatively small and unbalanced. For this reason, it is important to be careful when generalizing the results obtained. Despite that, the outcomes could be cautiously applied for supporting the update/review of PHA of ADU from the same oil refinery.

Next, the classifiers were fitted and we assessed their performance to predict LR and CL through ML1 and ML2 respectively. All classifiers have provided lower F1 scores to predict the CL.Moreover, they presented larger standard deviation to predict CL. This could be due to the fact that there are a considerably inferior number of instances classified as IV, which might have disrupted the learning process for this class.Thus, MLP, GB and RF will be evaluated in deeper details. To that end, these classifiers were used to predict the CL and LR from the test data.

All classifiers had good performance to predict LR, MLP showed the lowest precision, recall and F1 score average: 86%, 82% and 83%, respectively, while GB and RF classifiers scored above 90% in all metrics.

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|  |  |  |
| --- | --- | --- |
| *(a)* | *(b)* | *(c)* |

*Figure 2. Confusion matrix relative to LR prediction with test datasetwith (a) MLP, (b) RF and (c) GB*

shows the classifiersconfusion matrix for prediction of test samples, where the rows and columns indicate the actual and predicted likelihood categories respectively. Then, the number of correct predictions is shown in the main diagonal. It is clear that classifiers have made mistakes between classes A and B, and between C and D, which is acceptable considering the subtle difference of meaning of these categories that makes it difficult for experts even in traditional PHA to distinct between these classes that makes it difficult for experts even in traditional PHA to distinct between these classes (see Table 3). Despite that, the models did not classify very rare/rare scenarios as possible/likely and vice versa. Moreover, MLP showed inferior performance. Yet, the confusion matrix allows to identify more easily that RF provides the best results.

|  |  |  |  |
| --- | --- | --- | --- |
|  | | | |
| *(a)* | *(b)* | *(c)* |

*Figure 3. Confusion matrix relative to CL prediction with test datasetwith (a) MLP, (b) RF and (c) GB*

Considering CL prediction, shows that RF and GB classifiers have misclassified 3 out of 5 scenarios that should be categorized as IV, while MLP misinterpreted only 1. Moreover, the models also made mistakes when predicting classes II and III. However, MLP did not classify instances belonging to III as II, and, as mentioned, only one instance belonging to IV was classified as III, in contrast to the other classifiers that classified 4 scenarios as a less severe class. As it can be seen, RF and GB classifiers showed the same results, emphasizing the poor performance to classify the severity category IV, which represents the most critical scenarios (see ). Moreover, the precision, recall and F1 score averages for MLP classifier were 89%, 88% and 88% respectively, whereas for GB and RF scored below 80%.This MLP’s characteristic is rather important, particularly for prioritizing the allocation of resources to mitigate the impact of scenarios with the highest potential consequences.

Therefore, RF and MLP classifiers were selected as ML1 and ML2 respectively.Finally, the combination of the outputs of ML1 and ML2 provided the risk label following the rules presented in . Then, the combined model achieved an accuracy of 96.77%,Table 4 shows the predictions achieved through this method as compared with the actual risk labels for the test data. The estimated F1 scoreswere 95.24% for T and 97.56% for M, which provided a mean F1 score of 96.40%. There were neither training nor test instances containing the risk label NT and expectedly the model never classified risks as NT.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Label** | **Observed Risk Labels** | **Predictions** | **Correct Predictions** | **Precision** | **Recall** | **F1 score** |
| **T** | 11 | 10 | 10 | 100.00 | 90.91 | 95.24 |
| **M** | 20 | 21 | 20 | 95.24 | 100.00 | 97.56 |
| **NT** | 0 | 0 | 0 | - | - | - |
| **Total/Average** | 31 | 31 | 30 | 97.62 | 95.46 | 96.4 |

Table 4. Results of the classification report of risk label by the combined model

The results obtained was extremely satisfactory. In fact, all instances labeled as M were correctly classified, besides that only one T were classified as M, that can be explained due to the errors committed by ML1 and ML2,that mostly led to more critical CL and LR, consequently resulting in more a critical risk category, which is acceptable considering that the most critical scenarios shall be further evaluated by the experts.

# ***Conclusions***

We have here developed anML model based ondata related tohypothetical accidents postulatedin previous PHA.An ML-based method was developed and could, thus, learn the attributes of potential accident scenarios of an industrial system for performing a risk analysis with reduced efforts. Information on the process, such as the operational conditions and chemical products, were considered asfeatures to characterize the potential accidentscenarios. The selected variables allowed for feeding the ML models with knowledge about the identified hazards, andthen evaluate their consequences and likelihood, providing as output the classification of the risk as T, M or NT.

The approach was applied for the automated classification of the potential accident scenarios of a complex industrial system, known as ADU, where different hazardous chemical products are manipulated and processed. In the application example, we combined two ML models, RF and MLP classifiers, to classify likelihood and severity categoriesrespectively, and then map them into risk labels, according to a risk matrix rule. It is important to emphasize that the generalization of the results should be carefully analyzed since a relatively small dataset, collected from a specific ADU, was used. Then, risk analysts must evaluate to what extent these outcomes could be adopted for supporting the update/review of PHA of different ADUs. It is also important to highlight that scenarios with variables, whose values/categories are out of the model training range, may arise when updating PHA. In this case, the model would not be able to infer about them.

The information was extracted manually and exclusively from pastPHA related to a particular ADU.Even though the manual extraction is one limitation addressed in our work, a subroutine is under development and as soon as it is implemented the automatic extraction of information from the PHA spreadsheets will be feasible. Moreover,PHA from similar ADUs and/or different units can be analyzed to provide additional information to the classifiers, increasing the dimension of the dataset. Moreover, the addition of information related to different processing units may be useful to generalize the proposed method for the whole oil refinery. In this situation, deep learning methods could be applied to avoid the manual feature extraction performed in Section 4.2, allowing computer to automatically extract and build complex features [31]. Thus, the learning process can be improved in further studies.

Moreover, it is important to emphasize the joint ML1 and ML2 model exactly replicates the very same reasoning executed by the experts, who postulate the likelihood and consequence categories. We showed the results obtained indicate that the developed model was able to learn the subtleties of the risk evaluation.However, we highlight that the utilization of such method does not aim to completely replace the reasoning of risk experts, who will always be necessary to analyze and review the outcomes obtained by the automated approaches. Indeed, the idea is that the ML-based models can be a practical tool to support risk analysts, allowing a faster update of the PHA with new operating conditions, and also providing a starting point for more elaborated studies.

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