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JULY BIAS MACÊDO

A MACHINE LEARNING-BASED METHODOLOGY FOR AUTOMATED CLASSIFICATION OF RISKS IN AN OIL REFINERY

Recife
2019

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Dissertação apresentada ao Programa de Pós-Graduação em Engenharia de Produção da Universidade Federal de Pernambuco, como requisito parcial para a obtenção do título de Mestre em Engenharia de Produção.

Área de concentração: Pesquisa Operacional.

Orientador: Profº. Dr. Márcio José das Chagas Moura.

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BANCA EXAMINADORA

_____

Profº. Dr. Márcio José das Chagas Moura (Orientador)
Universidade Federal de Pernambuco

_____

Profª. Dra. Isis Didier Lins (Examinador Interno)
Universidade Federal de Pernambuco

_____

Prof. Dr. Savio Souza Venancio Vianna (Examinador Externo)
Universidade Estadual de Campinas

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ABSTRACT

Oil refineries process hazardous substances at extreme operational conditions to produce valuable products. The necessary and required risk assessment is generally rather time-consuming and involves a multidisciplinary group of experts to identify potential accidental hypotheses, and compute their frequency and severity. With respect to this context, in this work, we present a machine learning method to mine out useful knowledge and information from available data of past risk assessments. The aim is at automatically classifying possible accident scenarios that may occur in oil refinery processing units by using SVM (support vector machines). Data from a previous qualitative risk assessment of an ADU (atmospheric distillation unit) of a real oil refinery is used to demonstrate the applicability of the SVM-based approach. The test classification was made with an F1 score of 89.95%. In this way, the results obtained showed that the proposed method is promising for efficiently performing automated risk assessment of oil refineries.

Keywords: Risk assessment. Machine learning. Support vector machines. Oil refineries.

RESUMO

Refinarias de petróleo processam substâncias perigosas em condições operacionais extremas para produzir produtos valiosos. A execução da necessária e exigida avaliação de riscos é geralmente bastante demorada e envolve um grupo multidisciplinar de especialistas para identificar possíveis hipóteses acidentais e calcular suas frequências e a severidade de suas consequências. Com relação a este contexto, neste trabalho, apresenta-se um método de aprendizagem de máquina para extrair conhecimento e informações úteis a partir de avaliações anteriores de riscos. O objetivo é classificar automaticamente os possíveis cenários acidentais que possam ocorrer em unidades de processamento de refinaria de petróleo usando máquina de vetores de suporte. Os dados de uma avaliação de risco qualitativa previamente elaborada de uma ADU (unidade de destilação atmosférica) de uma refinaria de petróleo real são usados para demonstrar a aplicabilidade da abordagem baseada em SVM. A classificação dos dados de teste foi feita com um escore F1 de 89,95%. Os resultados obtidos demonstraram que o método proposto é promissor para realizar eficientemente avaliações automáticas de risco de refinarias de petróleo.

Palavras-chave: Avaliação de risco. Aprendizagem de ráquina. Máquina de vetores de suporte. Refinarias de petróleo.

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SUMMARY

1 INTRODUCTION

Petroleum has an impressive value to society. It is widely used as raw material to produce cosmetics, fuels, clothes, chemical for industry, and other useful materials. However, in its raw state, the crude oil does not have many useful applications. For this reason, it is essential to convert the crude oil into its products to explore all of its potential.

In this context, oil refineries are complex (and expensive) industrial systems whose main purpose is to separate the petroleum into more valuable and useful fractions to meet society needs (DEMIRBAS; BAMUFLEH, 2017). Three basic activities characterize the operation of petroleum refineries: separation, conversion and treatment. These activities involve handling hazardous materials, characterized by their explosiveness, flammability, and toxicity, which may cause catastrophic accidents.

Major accidents with severe effects to either humans or environment can be generated from the release of large amounts of energy or hazardous materials over a short lapse of time. In particular, they concern the occurrence of fires, explosions and atmospheric dispersion of toxic products. The consequences of these undesirable scenarios, then, depend on the nature of the released material and its physical state, and the conditions of the environment (CASAL, 2017; EL-HARBAWI et al., 2008; GEORGIADOU et al., 2010).

On one hand , the concern with human safety and the increasing complexity of industrial systems on the other, make indispensable the assessment of the risks of catastrophic accidents from industrial facilities. As a matter of fact, nowadays, national and international regulatory standards exist, that require organizations to adopt procedures to manage and minimize the potential risk related to the operation of industrial facilities (COX, 2009; HU et al., 2018; MURAKAMI, 2016).

Different techniques of risk analysis have been developed and applied, and they can be classified as qualitative, quantitative or semi-quantitative (KHAN; HASHEMI, 2017). Usually, qualitative methods are elaborated by means of good engineering judgement and know-how. In general, they are easy to apply, even though they can be very time-consuming (CCPS, 1992; SILVA et al., 2014). Amundrud and Aven (2015) pointed out that knowledge gain on risk takes time, but it is absolutely necessary to their prevention and mitigation. Besides, it composes the basis for the elaboration of emergency and safety measures.

In fact, to perform a qualitative risk analysis, a large number of documents should be consider, such as equipment and material lists, with the objective of characterizing the analyzed

system (CARRASQUILLA; MELKO, 2017). Next, it is necessary to identify the potential hazards, which is usually done through the application of some qualitative techniques by a multidisciplinary team. Then, the risks are categorized by analyzing the likelihood of causes and severity of consequences of the possible accidental scenarios (TNO, 2005a). This approach is often used to prioritize the risks, which allows efforts to be directed more effectively.

Silva and Jacinto (2012) pointed at the growing quantity of available data and information about industrial accidents and the need to explore novel techniques and statistical tools for mining knowledge from these data and information, with the aim at finding hidden details that could assist to understand the phenomena of interest. Ale (2016) also argued that the processing and analysis of the increasingly available information help predict accidents and allow for more founded decision making.

In this context, ML (machine learning) techniques have been successfully used to mine knowledge from information and data in different fields, such as, computer-vision, medicine, cyber security and so on (SINGH; ROY; MOHAN, 2017). For instance, Pang, Lee and Vaithyanathan (2002) analyzed the efficiency of different ML models to perform a sentiment classification, which usually involves intuition of experts, and thus pointed out that SVM (support vector machines) is effective to text categorization. Furthermore, Jiang and Chen (2014) indicated that there are well-established methods for chemical process risk management, such as HazOp, that can be adapted to supply chain networks, and then proposed an approach based on SVM to evaluate the supply chain's risk, transforming it into a risk rating problem. More recently, Liu et al. (2018) utilized and compared different ML methods for fault diagnosis of rotating machinery.

Indeed, the ability of ML to deal with large volumes of data, and to successfully identify and classify information makes the application of these techniques attractive to the risk assessment context in order to reduce necessary efforts to perform it. Therefore, this Master's dissertation proposes an SVM-based model for automated classification of risks. The proposed model is tailored for oil refining processes, which begin at the ADU (atmospheric distillation unit), where the crude oil is converted into more valuable products.

ADU contains different dangerous chemical products, such as fuels and residues from the process. Moreover, the separation that takes place in ADU requires the application of heat and involves a series of evaporation and condensation of the liquid mixture (KINSARA; DEMIRBAS, 2016). Thus, this dissertation presents a practical example, in order to illustrate the applicability of the developed SVM model to an ADU of an oil refinery, which contains

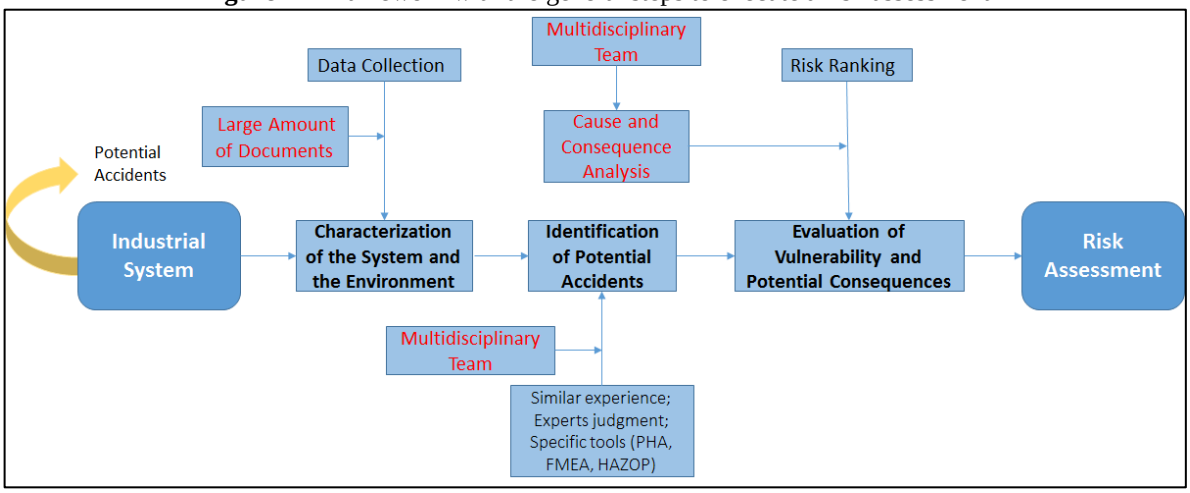
hazardous materials and is characterized by propitious conditions that may lead to catastrophic accidents.

1.1 JUSTIFICATION

Although the increasing efforts to prevent major accidents, they are far from being eradicate. Thus, it is indispensable to develop new methods to support risk studies. The framework showed in Figure 1 summarizes the general steps necessary to execute a qualitative risk assessment, which starts with the delimitation of the scope of the system to be analyzed.

Initially, the facility is partitioned into smaller systems, whose boundaries are defined according to specific characteristics of the chemical products to be processed and the operational 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 postulate possible leakages. Next, the hazards and their possible causes and consequences are identified, which can be accomplished through different techniques such as PHA (preliminary hazard analysis). Finally, the risks are evaluated and classified.

Figure 1 – Framework with the general steps to execute a risk assessment

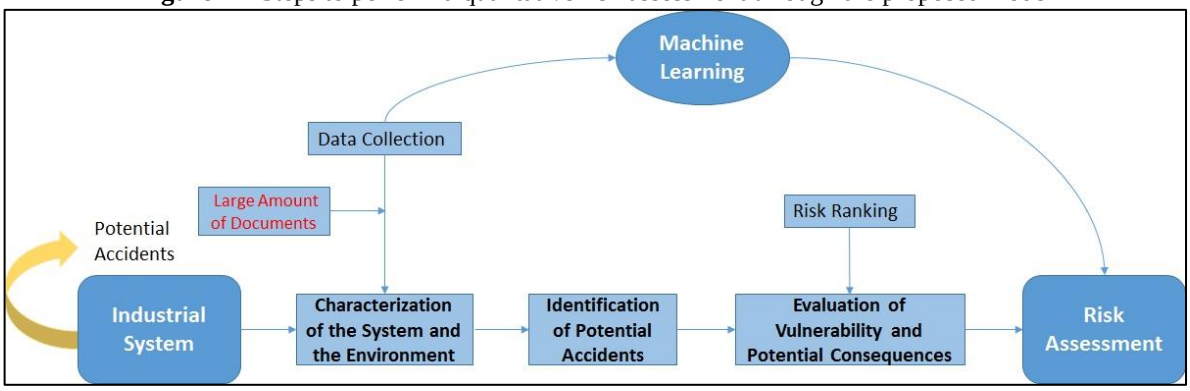


Source: This research (2018)

The process described in Figure 1 can be very time-consuming in practice, mainly depending on the complexity of the system analyzed and on the diverse backgrounds of the experts in the team that execute the risk assessment. In this context, the method here developed

aims at reducing the efforts required to perform risk assessments. Information about the potential accidents, which can be extracted from documents is provided to an ML model. Then, it learns the relationships among the operating conditions, potential accidents, their causes and consequences, and finally the identified risks could be automatically assessed by using the ML classifier. This procedure can be illustrated in Figure 2.

Figure 2 – Steps to perform a qualitative risk assessment through the proposed model



Source: This research (2018)

Comparing Figure 2 to Figure 1, the proposed model may reduce the time and manpower required to perform risk assessment. However, it is important to emphasize that the critical judgment of the risk analyst would still be necessary to evaluate the coherence of classifications obtained, the proposed model is not intended to replace the risk analyst, but to ease this process of risk assessment. Therefore, this dissertation proposes a method based on SVM to classify automatically the risks associated with an ADU from an oil refinery, which contains hazardous materials and is characterized by propitious conditions that may lead to fatal accidents.

1.2 OBJECTIVES

In this section the main objective of this dissertation is described and specific objectives related with this work are presented in the following sections.

1.2.1 General Objective

The main purpose of this study is to develop a method able to classify automatically risks related to an ADU, by means of the implementation of an SVM classifier model, which will be fed with information collected through the evaluation of previous elaborated PHA documents.

1.2.2 Specific Objectives

- Data collection: Previously prepared PHAs documents for the ADU were provided to this study. They were evaluated in order to extract information essential for the learning process;
- Characterization of the potential accidents: Identification of features relative to the potential accidents to build the set of input-output pairs to feed the SVM model;
- Algorithm implementation: Implementation of SVM classifiers;
- Hyper-parameters optimization: Attainment of the hyper-parameters that lead to the model with best accuracy;
- Risk classification: Provide test data as input to the classifier to obtain the related risk classification.

1.3 DISSERTATION STRUCTURE

The remainder of this research is organized as follows:

- Chapter 2 describes the process involved in the ADU, introduces important concepts used in risk analysis, and explains the theory that backs up SVM;
- Chapter 3 presents the SVM-based proposed methodology to classify automatically risks;
- Chapter 4 applies the proposed method to an ADU;
- Chapter 5 provides some concluding remarks.

2 THEORETICAL BACKGROUND AND LITERATURE REVIEW

In this chapter, we present the definitions and explanation about the key topics and concepts of this dissertation. Furthermore, a review of the current researches in the area is presented.

2.1 OIL AND GAS REFINERIES

Petroleum is a complex liquid mixture, whose composition varies according to its origin, but it consists basically of different hydrocarbons (over 80% of its composition), and a lower portion of contaminants, such as ammonia, sulfur, and some of their derivatives. Given that, the separation of the crude oil into pure compounds, or even into a mixture with exactly known composition, is almost impossible (SPEIGHT, 2015).

These products are more useful, and their value is higher than the value of the oil in its original state (AL-MUSLIM; DINCER, 2005). Table 1 shows these fractions and summarizes their composition, in terms of number of carbon atoms that represent the group of hydrocarbons, and typical boiling range, and the general applications of each fraction.

Table 1 - Petroleum fractions uses and characterization

Fraction	Boiling Point (°C)	Composition	Main Uses
Residual gas	-	C1 – C2	fuel
Liquefied petroleum gas	< 40	C3 – C4	bottled gas
Gasoline	40 – 175	C5 – C10	automobile fuel
Kerosene	175 – 235	C11 – C12	lamp oil, jet fuel
Light fuel oil	235 – 305	C13 - C17	diesel fuel
Heavy fuel oil	305 – 400	C18 - C25	fuel, lubricants production
Mineral oil	400 – 510	C26 - C38	lubricants
Residue	> 510	C38 +	asphalt, tar

Source: THOMAS et al. (2004)

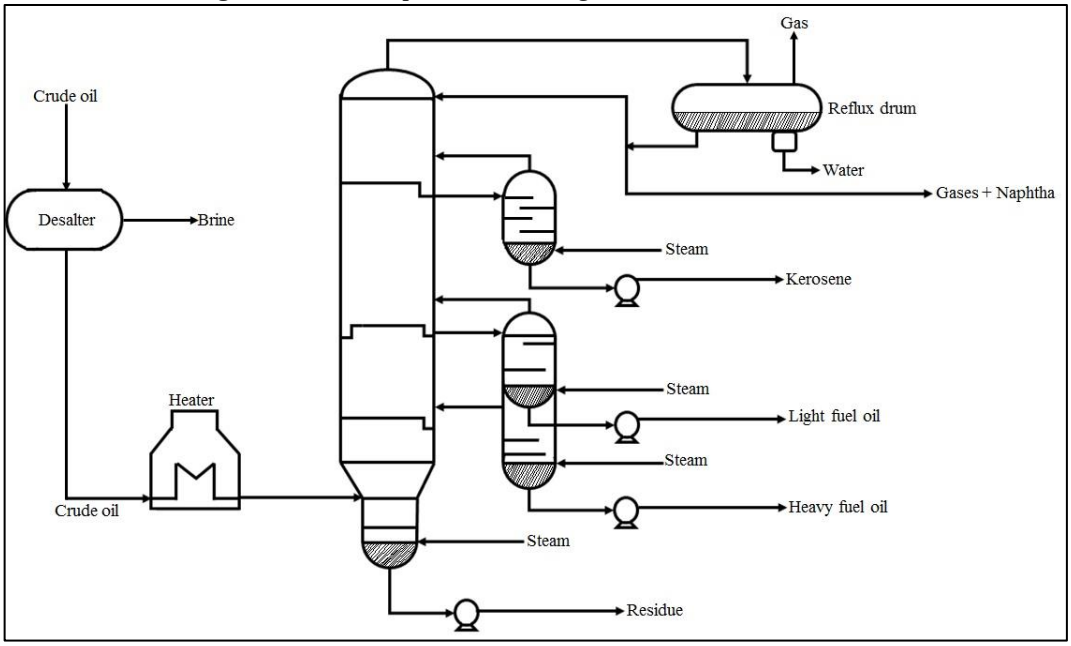
The refining process initiates in the ADU, which represents the main process in oil and gas refineries, where the raw oil is heated and transferred to distillation columns. Then, the

crude oil is converted into different fractions. Therefore, the products obtained in the ADU may be either treated as final products or they may be conducted to feed downstream units. Each fraction corresponds to a group composed of hydrocarbons, which are organic compounds consisting of carbon and hydrogen, with similar molecular weight and boiling points (OSUOLALE; ZHANG, 2017; SZKLO; ULLER; BONFÁ, 2012).

2.1.1 Atmospheric Distillation Unit (ADU)

The separation that takes place in the ADU, illustrated in Figure 3, involves petroleum's heating, vaporization, fractionation, condensation and cooling. Distillation is a physical separation process that involves heat and mass transfer, and it is based on the equilibrium between the liquid and vapor phases, which are obtained when a liquid mixture is heated, due to partial vaporization. The distillation towers usually work continuously, and it can be operated under hazardous conditions, i.e. very high/low temperature and/or pressure (SPEIGHT, 2015; AL-SAHHAF, ELKILANI; FAHIM, 2011).

Figure 3 - Generic process flow diagram from a distillation unit



Source: adapted from Al-sahhaf, Elkilani and Fahim (2011)

Part of the load vaporizes, and thus the light vapors move to the top of the column while the liquid content moves to the bottom. The liquid arrives by a downcomer in the tray and comes

in contact with the vapor that passes through holes, bubblers, or valves, that exist in the trays producing a foam. Then, the foam spread through the plate until it reaches another downcomer, where it coalesces and the liquid, without air, passes into the lower tray and the vapor remains on the tray. Thus, the distilled products are removed from the side of the column at different points, known as sidecuts, which are related to a boiling range. After the collection of fractions, they are condensed at different temperatures and, subsequently, processed in downstream units (AL-MUSLIM; DINCER, 2005; WAHEED et al., 2014).

2.2 BRIEF HISTORY OF ACCIDENTS IN OIL REFINERIES

Over the years there has been a growing demand of petroleum derivative products and a consequent increase of the amount of hazardous components stored, transported and processed, with also an increase in the risk of major accidents. (AMYOTTE et al., 2016; KHAN; HASHEMI, 2017). In the last years, diverse catastrophic industrial accidents have been occurred. In 1972, at REDUC (Duque de Caxias Refinery) occurred the explosion of three LPG (liquefied petroleum gas) storage tanks killing 42 people. These tanks contain valves to remove the liquid that forms inside. When the liquid is completely removed, the LPG starts to escape and the valve must be closed. The accident was caused by a worker that had opened the valve of one of the tanks and had gone for a break. When he returned, he could not close the valve because it was frozen. The gas spread quickly and, then, a fire started. As result, the LPG tanks exploded (COSTA, 2011).

In 1984, in Cubatão, Brazil, an operational failure caused the rupture of an oil pipeline spreading over 700,000 liters of gasoline through the mangrove. Then, a fire broke out a few hours later, leading to the death of 93 people (PORTO, 2016). In August 2012, an accident, involving an oil pipeline from ADU at Chevron Refinery, USA/California, occurred. As consequence of the high operating temperatures, the pipe suffered corrosion, leading to the leakage of diesel. A series of errors were committed in the attempt to stop the leakage without interrupting the production process, due to the lack of blocking valves between the leak and the valve. These mistakes led to the pipeline rupture. Then, a hydrocarbon vapor cloud was formed and rapidly expanded. Next, the cloud reached an ignition source. Although the accident did

not cause fatalities, more than 15,000 people went to the near hospitals with respiratory problems (LUSCHEK, 2012).

Early 2018, an explosion of tanks of the distillation column at Bayernoil Refinery, in Bavaria, Germany, injured 8 people and more than 1,800 had to be evacuated. After the explosions, a large fire erupted and the overpressure provoked by the explosions damaged the roofs and the windows of the houses in the residential area near the refinery (HÜSER; STARK, 2018). In addition, Table 2 lists a few more cases of recent fatal accidents that occurred in oil and gas refineries, their causes and number of deaths.

Table 2 – Fatal accidents in oil and gas industry

Deaths	Cause	Company	Year
1	Air compressor failure	PFB Energy	2015
2	Reboiler failure	CVR Refining	2013
2	Heat exchanger failure	ExxonMobil	2013
1	Furnace failure	Valero Energy Corp.	2013
7	Heat exchanger failure	Tesoro	2010
2	Welder failure within a tank	HollyFrontier	2010
2	Pipeline rupture	Delek Refining Ltd.	2008

Source: Malewitz et al. (2015)

2.3 RISK ANALYSIS

Khakzad, Khan and Paltrinieri (2014) described major accident as critical events that can lead to various fatalities and catastrophic impacts to people and environment or severe property damage. In the process industries, they can be defined as large-scale leakages, fires and explosions that may provoke multiple deaths and/or structural losses (AMYOTTE et al., 2016). The consequences and impacts of major accidents are directly related to the nature of the released material.

Indeed, when a flammable material gets in contact with an oxidant, they may react producing thermal energy and, then, a combustion process can result in either fire or explosion, where the latter occurs when there is a mixture of oxygen with the fuel gas in a certain proportion. This value is defined by the LFL (lower flammable limits) and UFL (upper flammable limits), where LFL represents the concentration value of the substance below which

the mixture is still not able to ignite, whereas above the UFL the mixture is excessively rich with the substance to lead to a combustion (HAUPTMANNS, 2015; DOBASHI, 2017).

Moreover, toxic emissions may also spread as clouds in the air, and the severity and extent of these clouds depend on the physicochemical and toxicological properties of the released substance, and on the atmospheric and geographical conditions. Then, there are possible different consequences of major accidents. Some of them are described as follows, according to Casal (2017), TNO (2005b) and CCPS (2010a, 2010b):

- Pool fire: Stable combustion of a vapor from a layer of flammable liquid;
- Vapor cloud explosion: Takes place when a flammable vapor cloud reaches an ignition source and the flames accelerate to sufficiently high velocities. Flame acceleration only occurs in the presence of congestion, a high-momentum release, or a combination of both;
- Flash fire: Combustion of a flammable vapor cloud in which there is no increase in combustion rate, i.e. the flame propagation occurs under near-laminar conditions and, thus, the flame speeds are not sufficient to produce significant blast effects;
- Toxic vapor cloud: Results from the release of toxic products into the atmosphere.

International and national regulatory standards, which demand the execution of RA (risk analysis) for hazardous facilities, such as oil and gas industry, have been required by several governments to prevent the aforementioned undesirable accidents (CAMERON et al., 2017; HAIMES, 2015).

Regulatory standards are established to provide information and develop scientific knowledge for decision-making, despite the uncertainties inherent in the risk assessment. Furthermore, these standards determine acceptance levels according to the tolerance for specific hazards (MURAKAMI, 2016; WILLIS, 2007). Then, the main purpose of the analysis consists in providing knowledge and information that aid to make decisions on layout changes, operation, maintenance, emergency preparation and risk management.

According to Aven (2012), risk assessment is the operative process of RA, where the accidental scenarios are characterized, through the methodical use of data and knowledge for describing and identifying accidents causes, probabilities and consequences, and the risk evaluation follows, where the risks are compared against given risk criteria. Weber et al. (2012) emphasized that risk assessment requires systematic research of accidental scenarios, and, in general, can be classified as qualitative, quantitative or semi-quantitative.

Generally, safety studies initiate with the detection of the possible hazards, and its main purpose can be achieved through a PHA (preliminary hazard analysis). This step is considered fundamental to risk assessment and risk management, for establishing effective safeguards (CAMERON et al., 2017; SILVA et al., 2014). PHA is applied early in the system life cycle, generally focusing on the hazardous materials present in the plant. This technique requires documents such as plant design, equipment and/or material specifications, and other sources of information (CCPS, 1992).

Generally, the final results of a PHA are given in the form of risk matrices, which are a methodical approach frequently used in qualitative risk assessment to categorize the different hazardous situations. The consideration of pre-defined categories of consequence and likelihood provides the risk ranking of a hazard (MARHAVILAS; KOULOURIOTIS; GEMENI, 2011). Thus, risk matrices are widely used to prioritize accidental scenarios in order to develop efficient measures to reduce or mitigate the risk. Also, the most critical scenarios can be further analyzed in detail by a quantitative method (BENEKOS; DIAMANTIDIS, 2017; Mannan et al., 2016).

However, the identification of hazards and their evaluation involves the analysis of numerous documents and the judgment of experts from different disciplines (TNO, 2005). This step usually represents an exhausting task in risk assessment studies. In fact, Cameron et al. (2017), Weber et al., (2012) and Pasman (2015) pointed at different methods that have been developed to automate the process of hazard identification and assessment, in an effort to reduce the time-consumption and labor required to perform PHA. For instance, Suokas, Heino and Karvonen (1990) developed a rule-based expert system, HAZOPEX, to support safety analysis. Srinivasan and Venkatasubramanian (1998) presented a method, which uses digraph-based models, dynamic mathematical approaches and fault tree methods to automate the processes during the execution of PHA for continuous processing in chemical industries. Then, the method was extended to batch processes (VISWANATHAN; SHAH; VENKATASUBRAMANIAN, 2002).

Lavasani et al. (2011) applied fuzzy risk assessment to quantify the risks levels related to hazardous events in offshore wells. Furthermore, Ifelebuegu et al. (2018) utilized generic data from different sources for a subsea gas compression system to improve the estimation of risk frequency through a Bayesian logic methodology. Markowski and Mannan (2008) developed a fuzzy logic approach to reduce the uncertainty and imprecision related with the application of risk matrices. Their methodology uses the estimated risk and efficacy indices (related to the

protective level of the system) as input data, which are mapped into a risk index through a fuzzy logic system. This methodology was applied to a distillation column unit aiming to obtain a more reliable result, compared to traditional risk assessment matrix. Further, Markowski and Siuta (2017) adopted the same methodology to select the representative accidental scenarios from a liquid petroleum gas (LPG) storage facility. However, these authors focused on eliminating the vagueness and subjectivity of the analysis, but did not take into account the efforts and the time consumption involved in the process. Tan, Ortiz-Gallardo and Perrons (2016) pointed at the fact that data analytics tools could help overcome persistent fatality and injury rates in the oil and gas industry, by revealing hidden patterns and trends that could lead to accidental scenarios.

In this context, the application of Artificial Intelligence (AI) techniques seems attractive to simplify and improve the process of risk assessment. As argued by Jordan and Mitchell (2015), developers of AI systems for diverse applications, it is simpler to train a system by providing it a set of instances that represent the desired behavior, and then, program it by predicting the response to new input, rather than building physical models. To that end, different Machine Learning (ML) techniques are applied, supervised learning methods being the most widely used, where instances are given with known labels (KOTSIANTIS; ZAHARAKIS; PINTELAS, 2006).

The ability of Support Vector Machine (SVM) to successfully solve classification problems makes this learning method interesting for risk analysis (HUANG et al., 2012). In fact, recent researches have already applied computer vision and ML techniques in this context to provide new tools to identify potential hazards through images extracted from webcams and surveillance cameras (MAIOR et al., 2017; MAIOR et al., 2018). However, these works were not focused in the efforts required to perform risk analysis. In this work, SVM is applied to replicate the process of qualitative risk assessment, aiming to reduce the efforts and time consumption involved. Thus, SVM will act as an aiding tool for decision-making purposes.

However, at the best of the authors' knowledge, there is a lack of works related to the application of ML to decrease the efforts involved in performing RA. Considering this, the development of an SVM-based model may provide a useful tool to support risk analysis, reducing the manpower and time required to execute the studies. Then, to next section introduces important definitions and concepts on SVM to provide essential knowledge for understanding the model proposed in this dissertation.

2.4 MACHINE LEARNING (ML)

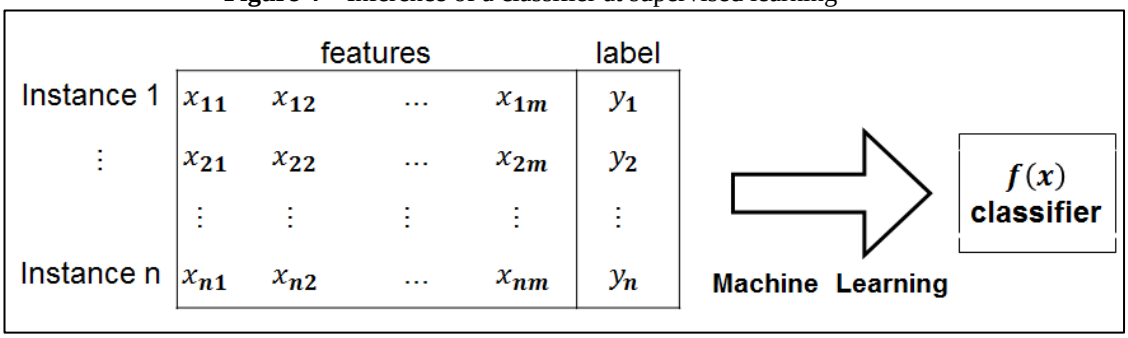
Kumar (2017) mentioned that AI techniques have been developed to reproduce human abilities as perception, analysis, reasoning, learning, exchange information, and decision-making. (LI; ZHANG, 2017). According to Jordan and Mitchell (2015), these techniques aim at improving a performance measure (e.g. the accuracy of a classifier) by means of any kind of training practice. In other words, ML detects and obtains knowledge from the real world through computers to reproduce the learning ability (PORTUGAL; ALENCAR; COWAN, 2018).

ML methods apply inductive inference to obtain knowledge from the environment from a set of examples, in general, they are classified as supervised or unsupervised learning. The first, uses set of n training examples, $D = \{(\boldsymbol{x_1}, y_1), (\boldsymbol{x_2}, y_2), \ldots, (\boldsymbol{x_n}, y_n)\}$, to infer a function f, through the mapping of the input values into the output value. Each example (or instance) is a pair consisting of an input, usually a vector of m features, $\boldsymbol{x}$, and an output value, y. (CHAPELLE et al., 2002; LINS et al., 2013). Moreover, the learning problem can be defined based on the type of the output y:

- Regression problems: y assumes real values.
- Classification problems: y assumes discrete values that represent categories. Moreover, they can be binary problems, where there are only two classes, or multi-classification cases.

In classification problems the supervised leaning algorithm extracts a classifier from a given set of examples, the inference process described and the concepts mentioned are illustrated in Figure 4.

Figure 4 – Inference of a classifier at supervised learning



Source: adapted from Lorena and Carvalho (2007)

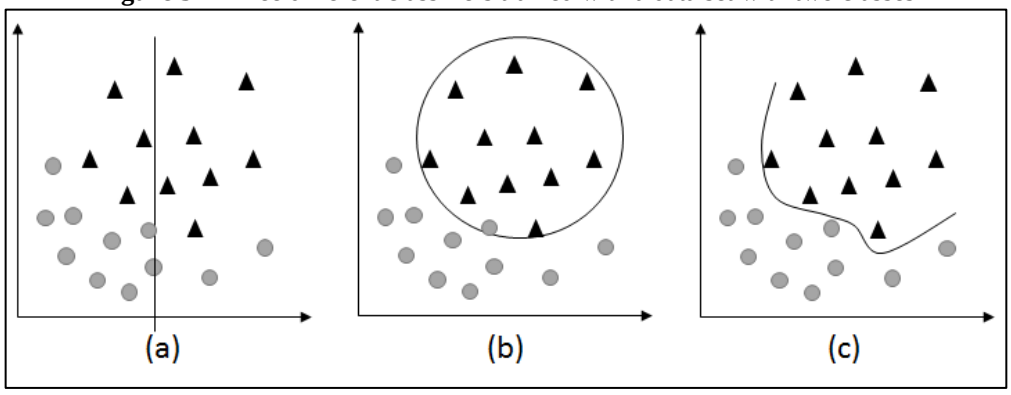
SVM is a supervised learning method trained with an algorithm of Mathematical Optimization and that implement a limit derived from Statistical Learning Theory (VAPNIK; IZMAILOV, 2017; VAPNIK, 1999). Thus, we have developed a method based on SVM classifiers to perform the automated qualitative risk assessment.

2.4.1 Support Vector Machines (SVM)

It is widely used to solve both classification and regression problems, as the proposed model in this dissertation uses support vector classifiers (SVC), this section describes the theory with an emphasis on classification problems.

As illustrated in Figure 5, the objective of the learning process is to find a classifier (decision surface) able to separate the different data classes, which are indicated by different symbols. It is possible to draw numerous lines to separate the two classes, this fact leads to an optimization problem that consists in determining which is the best line. The first classifier (Figure 5a) is not able adjust to fit the training data, thus it does not accurately separate the two classes. The second (Figure 5b), has an intermediate complexity and correctly classifies the most part of the training examples. The last (Figure 5c), does not make errors, however, it may not be able to correctly classify new (unseen) data due its high specificity.

Figure 5 – Three different classifiers trained with a data set with two classes



Source: adapted from Lorena and Carvalho (2007)

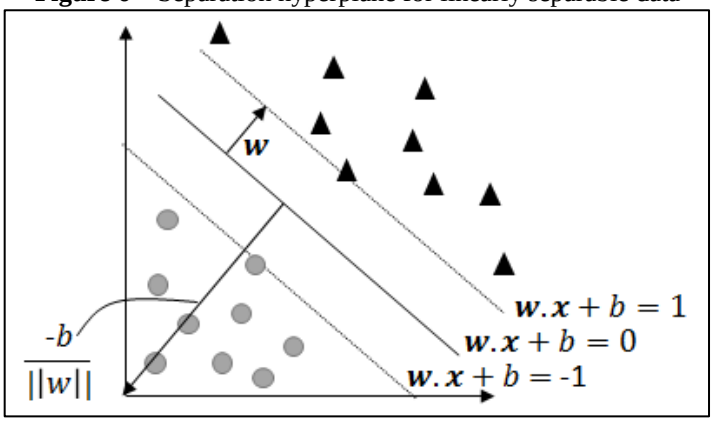
The Statistical Learning Theory (SLT) is a mathematical formulation of the general concept of learning, as defined by Steinwart and Christmann (2008), it establishes mathematical

conditions that support the selection of a particular classifier from a set of training data. It is not the aim of this research to go into details over SLT, for more information check Vapnik (2013).

In particular, SVM training involves the optimization of a quadratic convex function, which main purpose is to find a hyperplane able to separate different data classes by maximizing the distance between the hyperplane and the instances on both sides.

Figure 6 illustrates important concepts to define a linear classifier. Considering set of n training examples $D = \{(\boldsymbol{x_1}, y_1), (\boldsymbol{x_2}, y_2), \dots, (\boldsymbol{x_n}, y_n)\}$, each x_i belongs to one of the two classes, thus providing a label $y_i \in \{-1,1\}$. It is assumed that there is a hyperplane able to separate positive from negative instances. A hyperplane is defined by the set of $\boldsymbol{x}$ that satisfies $\boldsymbol{w}^T\boldsymbol{x} + b = 0$, these points are perpendicular to $\boldsymbol{w}$ and pass through the origin. Where $\boldsymbol{w}$ is the weight vector and $|b|/\|w\|$ is the perpendicular distance from the hyperplane to the origin (JIANG; CHEN, 2014; KOTSIANTIS; ZAHARAKIS; PINTELAS, 2006).

Figure 6 – Separation hyperplane for linearly separable data



Source: adapted from Lorena and Carvalho (2007)

The decision boundary of the classifier is the boundary between the two regions separated by the hyperplane. To extend this idea to generate nonlinear decision boundaries, a nonlinear function ϕ in used to map $\boldsymbol{x}$ into a vector of feature space, F, of higher dimension. Thus, the discriminant function in F is defined as in Equation 2.3.1.

$$f(\boldsymbol{x}) = \boldsymbol{w}^T\emptyset(\boldsymbol{x}) + b \tag{2.3.1}$$

However, the determination of the adequate mapping can be difficult. Moreover, the increase of dimensionality may be computationally demanding. This problem is solved by Kernel methods, which avoid the explicit mapping of the data to F. Firstly, assume that the weight vector can be expressed by linear combination of the training examples (Equation 2.3.2), where α is the dual representation of the decision boundary.

$$w = \sum_{i=1}^{n} \alpha_i x_i \tag{2.3.2}$$

Then, considering the kernel function (Equation 2.3.3), which is defined in the input space, the inner product in feature space is calculated directly through $k(x_i, x_j)$ and, thus, it can be efficiently computed.

$$k(x_i, x_j) = \emptyset(x_i)^T \emptyset(x_j) \tag{2.3.3}$$

Finally, f can be written in terms of the kernel function as

$$f(\boldsymbol{x}) = \sum_{i,j=1}^{n} \alpha_i k(x_i, x_j) + b \tag{2.3.4}$$

The maximum margin is determined by solving the dual Lagrangian problem formulated as follows in Equations 2.3.7, subject to the constrains represented in Equations 2.3.5 and 2.3.7 (AL-YASEEN; OTHMAN; NAZRI, 2017):

$$max\ L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i\, \alpha_j y_i y_j k(x_i, x_j) \tag{2.3.5}$$

subject to

$$\sum_{i=1}^{n} \alpha_i y_i = 0, \tag{2.3.6}$$

$$0 \leq \alpha_i \leq C, \forall i \tag{2.3.7}$$

where α is the dual variable, C is the soft margin parameter, n is the number of training instances, and $k(x_i, x_j)$ is the kernel function, responsible for separating the data's instances into different classes. The RBF (radial basis function) kernel is given as Equation 2.3.8:

$$k(x_i, x_j) = exp\left[-\gamma(x_i - x_j)^2\right] \tag{2.3.8}$$

where $\gamma > 0$ is the kernel parameter. According to Kotsiantis, Zaharakis, and Pintelas (2006), the selection of the adequate kernel function and the tuning of its parameters are fundamental, since they determine the feature space, where the training data instance will be classified.

To automatically classify the risks associated with an ADU two different SVM classifiers were developed, SVC_1 and SVC_2. The input, $\boldsymbol{x}$, contain useful information to characterize the hazards. Indeed, each instance registered in the input vector contains the operational conditions, besides features to characterize a hypothetical accidental scenario. Both SVC_1 and SVC_2, were feed with the same input vector. While the output for SVC_1, y_1, is the likelihood rating, and for SVC_2, y_2, is the consequence level. Then, the predictions were combined to provide the risk classification according to a risk matrix (that is further described under Chapter 3).

2.4.2 Model Selection

It is widely known that the hyper-parameters, C and γ, represent a key factor to the SVM performance (CHAPELLE, 2002). A common problem, considering these models, is that they can present satisfactory results on training set, at the same time they might also not classify unseen data correctly. The tuning of SVM hyper-parameters is known as model selection problem, as Lins (2009) stated. Then, it is essential to select C and γ meticulously.

The most common and reliable procedure is to perform an exhaustive GS (grid search) over the entire search space. However, it can be unpractical and time consuming if there are several parameters and/or possible combinations. To execute GS, it is necessary to select a finite set of values for C and γ, considering the fact they are continuous. Next, an SVM is trained with all pairs that resulted from the combination of both parameters and, then, GS returns the set relative to the highest scores obtained during the validation (WITTEN et al., 2016).

Usually, CV (cross-validation) is used to estimate the performance of the model, aiming to find the best approach appropriate for the available data. There are different methods to achieve this purpose. For instance, k-fold CV consists in splitting the data into k equal parts and, then, the training is proceeded on k-1 parts and the test is done in the part that is left out. Next, this process is repeated alternating the testing portion until all k parts has been tested (YADAV; SHUKLA, 2016). In this research, we applied a 10-fold-cross-validation method to select the best pair of hyper-parameters for each SVC model. Next Chapter describes the details of the proposed method.

3 METHODOLOGY

The aim of the classification model is to reduce the efforts made by the multidisciplinary teams during the development of PHAs. To that end, a method based on the supervised machine learning technique, SVM, has been developed by using information obtained through previous PHAs.

Generally, during the elaboration of PHA, the potential risks are classified according to a risk matrix based on ISO 31000 (2018) (Table 3) as moderate (M), tolerable (T) and non-tolerable (NT). The risk category of a possible accident is determined by combining its consequence level (Table 4) with its likelihood rating (Table 5), which respectively represent the expected severity of the effects related to a respective scenario and the expected frequency of occurrence of the causes of the accident.

Table 3 - Risk matrix used in the preliminary risk assessment

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

Source: ISO 31000 (2018)

Table 4 - Description of the consequence level in terms of the effects to human life

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

Source: ISO 31000 (2018)

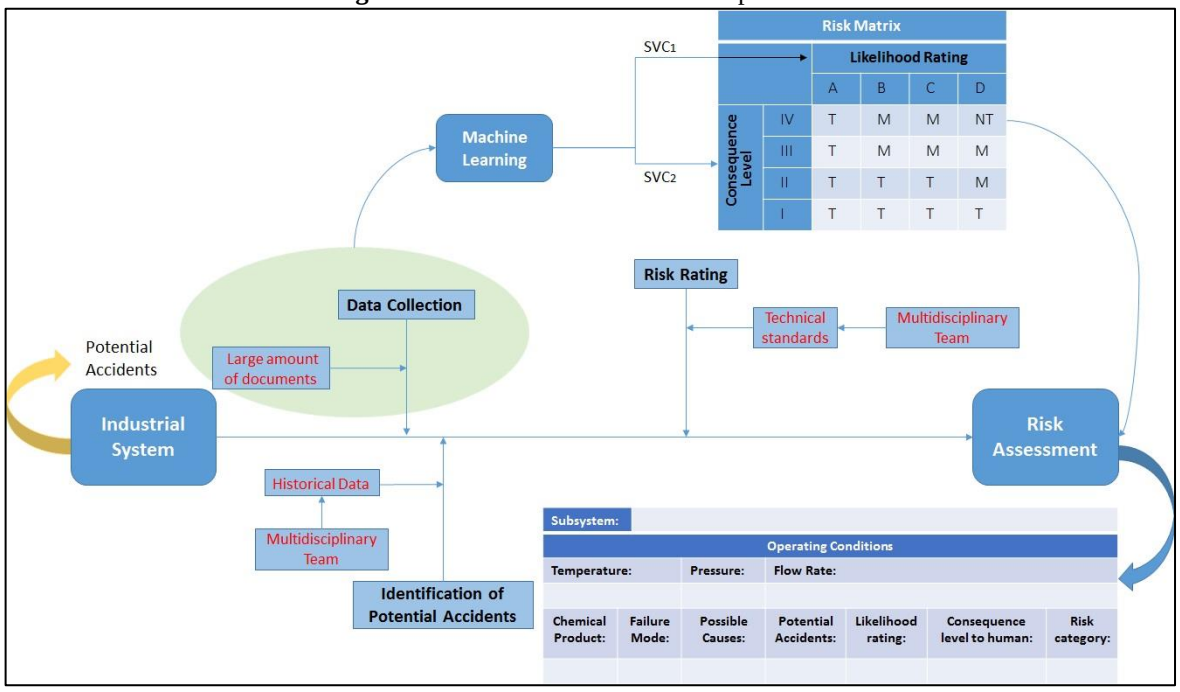
Table 5 - Description of the likelihood categories

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

Source: ISO 31000 (2018)

Firstly, as depicts in Figure 7, information about the accidental scenarios, such as the material released and operating conditions, are extracted from PHAs elaborated for an ADU of an oil refinery and analyzed in order to define a set of input-output data, where each pair is related to a potential accident. Then, this information is provided to two different SVM models that are implemented to classify both the likelihood rating (SVC_1) and the consequence level (SVC_2). Next, the categories are combined and the risk is classified as T, M or NT according to Table 3. In this way, the proposed model represents a shorter path to perform risk assessment. Thus, the SVM-based models are able to perform the classification of the risks associated to potential accidents in a more efficient way.

Figure 7 - General view of the developed model



Source: This research (2018)

Next, Section 3.1 describes the process executed to collect information for the SVM models construction. Then, Section 3.2 defines how these data are organized and provided as input to the SVM. Finally, Section 3.3 explains the implementation of the SVM classifier to assign the risk categories to the identified hazards.

3.1 DATA COLLETION

The SVM learning process requires a reasonable quantity of good quality input data to comprehend the reasoning adopted to classify the risks during PHA by the multidisciplinary group, composed by engineers and technicians from different fields. Thus, PHA documents of an ADU of petroleum refinery were evaluated to extracted information to build the data set used in this study. For example, Table 6 contains the description of potential accidents, associated to the release of petroleum from a pipeline, which were taken into account by the experts during PHA. The pipe is located on the exit of the desalters and a mass flow rate of $760{,}000\ kg.h^{-1}$ passes through it at $160°C$ and $5.0\ kgf.cm^{-2}$ under normal conditions.

Small and large leakages were considered to occur and their causes were either human failure, abnormal operating conditions or corrosion, where the former is expected to occur (D) and the latter is very rare (A); see Table 5. In this case, each failure mode might lead to three potential accidents (pool fire, flash fire or toxic vapor cloud), which have different impacts to human life. For example, in these operating conditions, the severity of the consequences of a pool fire caused by a small leakage was categorized as significant (II), while the ones associated to a large leakage as high (III); see Table 4. Finally, the risk of these possible accidents were respectively classified as M and T according to Table 3.

Table 6 - Example of PHA representing the data that is used to feed the SVM model

Subsystem	Petroleum pipeline on the exit of the desalters					
Operating Conditions	**Temperature**		**Pressure**		**Flow Rate**	
	$160\ °C$		$5.0\ kgf.cm^{-2}$		$760{,}000\ kg.h^{-1}$	
Chemical Product	**Failure Mode**	**Possible Causes**	**Potential Accidents**	Likelihood rating	Consequence level to human	Risk category
Petroleum	Small leakage	- Human failure - Abnormal operating conditions - Corrosion	Pool fire	D	II	M
			Flash fire	D	II	M
			Toxic vapor	D	I	T
	Large leakage		Pool fire	A	III	T
			Flash fire	A	IV	T
			Toxic vapor	A	IV	T

Source: This research (2018)

Taking into account the given example, PHA allowed for extracting important information related to the events of interest. Then, it is necessary to select which information

to use as the SVM model input variables. Next Section describes these variables and the relations among them.

3.2 FEATURE SELECTION

In this study, four hypothetical accidental scenarios (AS) were considered: pool fire, flash fire, vapor cloud explosion and toxic vapor cloud. For each one, there is a respective combination of likelihood rating (LR) and consequence level (CL), which are dependent on different variables, such as chemical materials and/or thermodynamic parameters. These conditions are considered by the experts for classifying LR and CL, and for this reason, are also included in the SVM models.

We have analyzed two initiating events (IE): 1) when a small amount of chemical product leaks, e.g. through a hole in the pipeline, valves, etc., and, 2) the other IE contemplates situations where a large quantity escapes, such as due to rupture of a pipeline. These assumptions were represented by including in the input data a binary variable (IE), where 0 means small holes and 1 indicates ruptures. Thus, IE qualitatively represents the amount of the material that escapes. This characteristic directly affects the surface area of the leaked product, which in turn determines the rate of evaporation. The assessment of two different IE for the same subsystem implies diverse accidental scenarios and, consequently, 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 fire.

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 by major accidents. In fact, T and P play an important role to determine if the chemical product (CP) is liquid or gaseous. Additionally, combined with FR, they are necessary to determine the vaporizing rate and the pool area or vapor cloud (TNO, 2005; TNO, 2005b). Moreover, T and P determine the UFL and LFL values, which are fundamental to characterize fires and explosions (TNO, 2005).

Thus, these variables are necessary to evaluate which accidental scenarios may occur and, thus, to classify the potential risks. For this reason, T, P and FR were included as continuous variables in the input data. In addition, it was also considered contamination (CT), a binary variable associated with CP (e.g. diesel contaminated with H_2S, which is a toxic substance) that represents the presence of toxic substances (in small amount) in the sub-system analyzed.

Yet, the release of a material that is both flammable and toxic could lead to different scenarios. Thus, the risk analysts can assume that if the product reaches an ignition source, this leads to an accident in the fire category; otherwise, if the released material evaporates, it would disperse as a toxic cloud. Due to this fact, providing information about operational conditions is not sufficient to classify risks. Thus, the proposed model also considers a categorical variable, PA, to distinguish the potential accidents: pool fire, flash fire, vapor cloud explosion and toxic cloud.

Finally, integrating the features with the different accidental scenarios considered in the PHA the associated risk can be categorized through the combination of the LR and CL, which are respectively here provided by two different SVM classifiers, SVC_1 and SVC_2. All variables considered in the model, and their possible values and types are summarized in Table 7.

Table 7 - Variables considered in the proposed model

Variables		**Range/Categories**	**Type**
Input Variables ($\boldsymbol{x}$)	Temperature (T)	25 – 300 °C	Continuous
	Pressure (P)	1 – 35 atm	Continuous
	Mass Flow Rate (FR)	79 – 765,000 kg/h	Continuous
	Chemical Product (CP)	Petroleum	Categorical
		Natural gas	
		Atmospheric residue	
		Diesel	
		Naphtha	
		Kerosene	
		LPG	
	Contamination (CT)	0	Binary
		1	
	Failure Mode (FM)	0	Binary
		1	
	PA	Pool fire	Categorical
		Flash fire	
		Toxic cloud	
		Vapor cloud explosion	
SVC_1 (y)	LR	A	Categorical
		B	
		C	
		D	
SVC_2 (y)	CL	I	Categorical
		II	
		III	
		IV	

Source: This research (2018)

3.3 MODELING PROCESS

For the implementation of both SVCs, a free machine learning library, scikit-learn (PEDREGOSA et al., 2011), was adopted. Both SVC_1 and SVC_2 take the same 7-order vector as input $\boldsymbol{x}$ and return y (either LR for SVC_1 or CL for SVC_2) as output. Both $\boldsymbol{x}$ and y are n-sized, where n represents the number of training samples. Then, the information extracted from previous PHA was used to train both classifiers, and an example of how these data were structured to feed the models is presented in Table 8, which shows the codification of the PHA contained in Table 6.

Table 8 - An example of the data provided to the model

Input							Output	
CP	CT	T	P	FR	IE	AS	SVC_1	SVC_2
							LR	CL
1	0	0.30569	0.170787	1	0	1	D	II
1	0	0.30569	0.170787	1	0	2	D	II
1	0	0.30569	0.170787	1	0	3	D	I
1	0	0.30569	0.170787	1	1	1	A	III
1	0	0.30569	0.170787	1	1	2	A	IV
1	0	0.30569	0.170787	1	1	3	A	IV

Source: This research (2018)

The SVM functions require that categorical variables are transformed into dummies. To that end, CP and AS were respectively converted to 5 and 3 dummy variables, where the resulting number of dummies is related to the number of categories of each variable minus 1. Notice that we have normalized the real-valued variables T and P.

RBF was adopted as the non-linear SVM kernel. Next, a 10-fold cross-validation 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 portion of the data and, then, test the model on the remaining part of the data set. In the 10-fold cross-validation, the data is equally divided into 10 parts, where 9 are used for training and 1 for validation purposes. Then, this process is executed 10 times, changing the validation portion, until all data has been used (YADAV; SHUKLA, 2016).

Thus, the metrics provided by this method are the averages of the values 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 F_1 score (Equation 3.3.1), which is the harmonic average between two other measures (precision and recall), calculated,

respectively, by Equations 3.3.2, that take into account false negative rate, and Equations 3.3.3, that consider the false (see FLACH; KULL, 2015):

$$F_1 = 2 \times \{(Precision \times Recall)/(Precision + Recall)\} \quad (3.3.1)$$

$$Precision = \frac{CCj}{Pj}, \forall j \quad (3.3.2)$$

$$Recall = \frac{CCj}{Oj}, \forall j \quad (3.3.3)$$

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

Thus, the F_1 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 3.3.4, 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.

$$Accuracy = \frac{\sum CCj}{\sum Oj} \times 100, \forall j \quad (3.3.4)$$

After the selection of the hyper-parameters, 80% of the samples were used for learning purposes, while the rest was adopted for testing evaluation. Then, the trained SVC functions were used to give the risk label for the remaining samples. This classification is performed by both methods, SVC_1 and SVC_2, and thus the risk label is obtained through the risk matrix given in Table 3. The results are discussed in next Chapter.

4 RESULTS AND DISCUSSION

Firstly, we divided ADU into subsystems, which are characterized by different chemical products and operating conditions and, thus, they might lead to different accidental scenarios. 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 data set composed of 151 samples was provided to the model, and it is presented in Appendix A. To achieve a good performance, SVM hyper-parameters C and δ were obtained by adopting a 10-fold cross-validation and using 80% of the data set (PEDREGOSA et al., 2011).

Tables 9 and 10 present F_1 scores achieved by SVC_1 and SVC_2 with different pairs of C and δ. Other values were also tested, but we here present only some of them for sake of illustration. Then, we selected the hyper-parameters that yield the best results (the highest F_1 score), which are highlighted in the tables.

Table 9 - Mean F_1 score achieved by SVC_1

	C				
		100	1,000	10,000	100,000
δ	0.1	0.720	0.720	0.720	0.720
	0.01	0.843	0.785	0.785	0.785
	0.001	0.755	0.808	0.867	0.805
	0.0001	0.735	0.780	0.808	0.794

Source: This research (2018)

Table 10 - Mean F_1 score achieved by SVC_2

	C				
		100	1,000	10,000	100,000
δ	0.1	0.688	0.679	0.679	0.653
	0.01	0.679	0.691	0.680	0.666
	0.001	0.610	0.588	0.689	0.700
	0.0001	0.570	0.610	0.638	0.605

Source: This research (2018)

For SVC_1 the test predictions were obtained with an accuracy of 83.87%, while the training accuracy was 96.67%. As expected, the training score was higher, but the results for testing are still considered satisfactory. The performance of the SVC_1 on test data was evaluated trough F_1 score, precision and recall, the results are presented in Table 11. Note that the average F_1 score was influenced by the lower recall for categories A and D, and the lower precision to predict C. Despite that, the model presented better scores to predict B, which alone made up

42.38% of all instances. Thus, as expected, the higher number of samples provided to the model clearly benefited the learning process of that respective category.

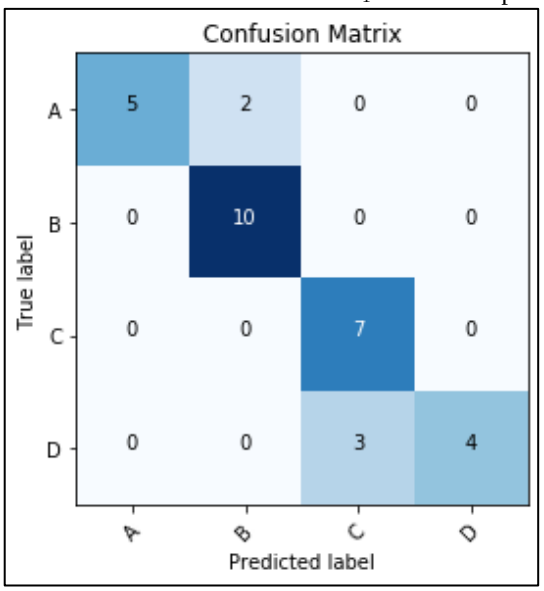
Table 11 - Classification report for SVC_1

	Number of Observations		Precision (%)	Recall (%)	F_1 score (%)
	Training Set	Test Set			
A	15	7	100.00	71.43	83.33
B	54	10	83.33	100.00	90.91
C	20	7	70.00	100.00	82.36
D	31	7	100.00	57.14	72.72
Total/Average	120	31	88.33	82.14	82.33

Source: This research (2018)

Figure 8 shows the SVC_1 confusion 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 SVC_1 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 (Table 5), that makes it difficult even in traditional evaluation to make a distinction between these classes. Despite that, the model did not classify very rare/rare scenarios as possible/likely and vice versa.

Figure 8 - Confusion matrix relative to SVC_1 for test samples prediction



Source: This research (2018)

SVC_2, in turn, presented an accuracy of 95.00% and 74.19% for training and test, respectively. The classification report is given in Table 12 and the confusion matrix for SVC_2 is shown in

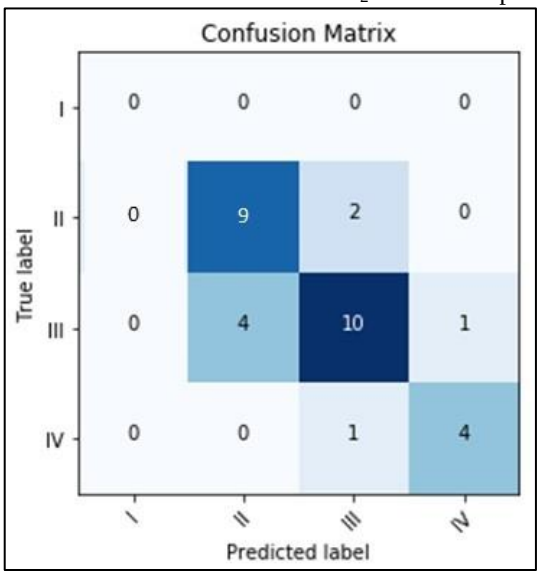
Figure 9. It is possible to notice that SVC_2 presented difficulties to distinguish class III, among II and IV, which in fact represent subtle differences of meaning (Table 4). The scores were lower for classes II and III, which may indicate the necessity of adding other pieces of information (attributes and/or instances) to improve the learning process for the consequence level. SVC_2 also showed consistency in the predictions, there were no accidental scenarios associated with consequence level II (injuries without deaths) classified as IV (multiple deaths) and vice versa. Moreover, there were no instances containing severity level I and, thus, SVC_2 was not able to predict class I during the test phase.

Table 12 - Classification report for SVC_2

	Number of Observations		Precision (%)	Recall (%)	F_1 score (%)
	Training Set	Test Set			
I	0	0	-	-	-
II	44	11	69.23	81.82	75.00
III	57	15	76.92	66.67	71.43
IV	19	5	80.00	80.00	80.00
Total/Average	120	31	75.38	76.16	75.48

Source: This research (2018)

Figure 9 - Confusion matrix relative to SVC_2 for test samples prediction



Source: This research (2018)

Finally, the combination of the outputs of SVC_1 and SVC_2 provided the risk label following the rules presented in Table 3. Then, Table 13 shows the predictions achieved through this method as compared with the actual risk labels for the test data. The estimated F_1 scores were 88.00% for T and 91.9% for M. Given that, a mean F_1 score of 89.95% was obtained. There were neither training nor test instances containing the risk label NT and expectedly the model never classified risks as NT, which yields a precision of 100% for this class, once the combination of the predictions obtained with SVC_1 and SVC_2 could lead to this class label. The values for precision and recall are also reported in Table 13.

Table 13 - Test scores of the method using SVC_1 and SVC_2 to classify risk categories

Label	Observed Risk Labels	Predictions	Correct Predictions	Precision (%)	Recall (%)	F_1 score (%)
T	11	14	11	78.57	100.00	88.00
M	20	17	17	100.00	85.00	91.90
NT	0	0	0	100.00	-	-
Total/Average	31	31	28	92.86	92.50	89.95

Source: This research (2018)

We also considered a third model, SVC_3, which aims at directly predicting the risk label instead of using SVC_1 and SVC_2 for the intermediate evaluation of likelihood and consequences. In other words, the output vector, y, for SVC_3 is the risk label, while $\boldsymbol{x}$ is the same as that of SVC_1 and SVC_2. The hyper-parameters, C and δ, were selected with the same procedure as SVC_1 and SVC_2, and the values adopted were 1,000 and 0.1 respectively. The results are shown in Table 14. The F_1 score relative to each risk label was 80% for T and 90.47% for M.

Table 14 - Accuracy of the method using SVC_3 to classify the risk labels

Label	Observed Risk Labels	Predictions	Correct Predictions	Precision (%)	Recall (%)	F_1 score (%)
T	11	9	8	88.89	71.73	80.00
M	20	22	19	86.36	95.00	90.47
NT	0	0	0	-	-	-
Total/Average	31	31	25	87.62	83.36	85.23

Source: This research (2018)

The mean F_1 score of SVC_3 was 85.23%, which is lower than the results obtained by using both SVC_1 and SVC_2. This performance decrease indicates that SVC_3 model is not fed with enough information to learn the subtleties of the risk evaluation and, thus, the prediction of likelihood and severity categories through SVC_1 and SVC_2 are essential. Moreover, apart from

the lower precision and recall to classify some categories through SVC_1 and SVC_2, the joint model replicates, with satisfactory scores, the same reasoning executed during PHAs by the risk experts, who postulate the likelihood and consequence categories, and not directly the risk category as SVC_3 does.

5 CONCLUSIONS

Risk studies are fundamental and, thus, required to prevent catastrophic accidents and avoid economic losses and fatalities that could result from their occurrence. However, it is a rather resource-expensive and time-consuming activity that requires multidisciplinary expertise and the application of different tools and methodologies. In this context, there are different AI techniques that could be allied to these objectives and would help to create a solution to perform effectively the assessment.

In this research, we have developed an SVM model based on data related to hypothetical accidents postulated in previous PRA. ML methods can, thus, learn the attributes of potential accidental scenarios of an industrial system for performing a risk assessment, with reduced efforts. However, we emphasize that the utilization of these methods can never completely replace the reasoning of risk experts, since it will always be necessary to analyze and review the results obtained by the automated approaches. Indeed, the idea is that the ML models can be a practical tool to support risk analysts, providing a starting point for more elaborated studies.

Information on the process, such as the operational conditions and chemical products, were considered as inputs to characterize the potential accident scenarios. The selected features allowed for feeding the SVM model with knowledge about the identified hazards, and then evaluate their consequences and likelihood, providing as output the classification of the risk as tolerable, moderate or non-tolerable. In further studies different ML models can be applied in order to compare with the performance obtained with the proposed model.

The approach was applied for the automated classification of the potential accidental scenarios of a complex industrial system, known as ADU, where different hazardous chemical products are manipulated and processed. In the application, we combined two SVM models to classify likelihood and severity categories, and then map them into risk labels, according to a risk matrix rule.

The information was extracted manually and exclusively from PRA related to a particular ADU, but different documents can be analyzed to provide additional information to the SVM, increasing the dimension of the data set. 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 manual feature

extraction, allowing computer to automatically build complex features (GOODFELLOW, 2016). Thus, the learning process can be improved in further studies.

To conclude, ML methods can, thus, learn the attributes of potential accidental scenarios related to an industrial system for performing a risk assessment, with reduced efforts. However, we emphasize that the utilization of these methods can never completely replace the reasoning of risk experts, since it will always be necessary to analyze and review the results obtained by the automated approaches. Indeed, the idea is that the ML models can be a practical tool to support risk analysts, providing a starting point for more elaborated studies.

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APPENDIX A – DADOS UTILIZADOS NO MODELO

CP	CT	T	P	FR	FM	PA	LR	CL	Risk Label
1	0	0.687204	0.208825	0.380134	0	1	II	D	M
1	0	0.687204	0.208825	0.380134	1	1	III	B	M
1	0	0.687204	0.208825	0.380134	1	2	III	B	M
1	0	1	0.452263	0.087715	0	1	II	D	M
1	0	1	0.452263	0.087715	1	1	III	B	M
1	0	1	0.452263	0.087715	1	2	III	B	M
1	0	0.57109	0.433245	0.108821	0	1	II	D	M
1	0	0.57109	0.433245	0.108821	1	1	III	B	M
1	0	0.57109	0.433245	0.108821	1	2	III	B	M
1	0	0.57109	0.463674	0.337486	0	1	II	D	M
1	0	0.57109	0.463674	0.337486	1	1	III	B	M
1	0	0.57109	0.463674	0.337486	1	2	III	B	M
2	0	0.412322	0.395207	0.043317	0	1	II	D	M
2	0	0.412322	0.395207	0.043317	1	1	III	B	M
2	0	0.412322	0.395207	0.043317	1	2	III	B	M
2	0	0.436019	0.018638	0.037788	0	1	II	C	T
2	0	0.436019	0.018638	0.037788	1	1	III	A	T
3	1	0	0.817421	0.003884	0	2	II	C	T
3	1	0	0.817421	0.003884	0	3	II	C	T
3	1	0	0.817421	0.003884	1	2	IV	B	M
3	1	0	0.817421	0.003884	1	3	III	B	M
3	1	0	0.817421	0.003884	1	4	III	B	M
3	1	0.028436	0.383796	0.004388	0	2	II	C	T
3	1	0.028436	0.383796	0.004388	0	3	II	C	T
3	1	0.028436	0.383796	0.004388	1	2	IV	B	M
3	1	0.028436	0.383796	0.004388	1	3	III	B	M
3	1	0.028436	0.383796	0.004388	1	4	III	B	M
3	1	0	0.832636	0.000395	0	2	II	C	T
3	1	0	0.832636	0.000395	1	2	IV	B	T
3	1	0	0.832636	0.000395	1	3	III	B	T

CP	CT	T	P	FR	FM	PA	LR	CL	Risk Label
3	1	0	0.832636	0.000395	1	4	III	B	M
4	0	0.331754	0.303918	0.605058	0	1	II	D	M
4	0	0.331754	0.303918	0.605058	0	2	II	D	M
4	0	0.331754	0.303918	0.605058	1	1	III	B	M
4	0	0.331754	0.303918	0.605058	1	2	III	B	M
4	0	0.331754	0.303918	0.605058	1	4	IV	B	M
4	1	0.28673	0.011031	0.1709	0	2	III	C	M
4	1	0.28673	0.011031	0.1709	0	3	III	C	M
4	1	0.28673	0.011031	0.1709	1	3	IV	B	M
4	1	0.28673	0.011031	0.1709	1	2	III	B	M
4	1	0.28673	0.011031	0.1709	1	4	III	B	M
4	1	0.182464	0.231647	0.074088	0	2	II	D	M
4	1	0.182464	0.231647	0.07409	0	3	II	D	M
4	1	0.182464	0.231647	0.074091	1	4	III	B	M
4	1	0.182464	0.231647	0.074092	1	3	III	B	M
4	1	0.182464	0	0.096463	0	2	III	C	M
4	1	0.182464	0	0.096463	0	3	III	C	M
4	1	0.182464	0	0.096463	1	4	IV	B	M
4	1	0.182464	0	0.096463	1	3	III	B	M
4	1	0.182464	0	0.096463	1	2	III	B	M
4	1	0.028436	0.61202	0.053753	0	2	II	D	M
4	1	0.028436	0.61202	0.053755	0	3	II	D	M
4	1	0.028436	0.61202	0.053756	1	2	III	B	M
4	1	0.028436	0.61202	0.053757	1	3	III	B	M
4	1	0.028436	0.61202	0.053759	1	4	IV	B	M
4	0	0.481043	0.391404	0.076133	0	2	II	C	T
4	0	0.481043	0.391404	0.076133	1	2	III	B	M
4	0	0.481043	0.391404	0.076133	1	4	III	B	M
4	0	0.481043	0.391404	0.052528	0	2	II	C	T
4	0	0.481043	0.391404	0.052528	1	2	III	B	M
4	0	0.481043	0.391404	0.052528	1	4	III	B	M
5	1	0.274882	0.011031	0.186277	0	1	II	C	T
5	1	0.274882	0.011031	0.186277	0	2	II	C	T

CP	CT	T	P	FR	FM	PA	LR	CL	Risk Label
5	1	0.274882	0.011031	0.186277	0	3	III	C	M
5	1	0.274882	0.011031	0.186277	1	1	III	B	M
5	1	0.274882	0.011031	0.186277	1	2	III	B	M
5	1	0.274882	0.011031	0.186277	1	3	III	B	M
5	1	0.274882	0.011031	0.186277	1	4	IV	B	M
5	1	0.13981	0.075694	0.002135	0	2	II	C	T
5	1	0.13981	0.075694	0.002135	0	3	III	C	M
5	1	0.13981	0.075694	0.002135	1	2	III	B	M
5	1	0.13981	0.075694	0.002135	1	3	III	B	M
5	1	0.13981	0.075694	0.002135	1	4	IV	B	M
5	1	0.274882	0.011031	0.186277	0	2	II	D	M
5	1	0.274882	0.011031	0.186277	0	1	II	D	M
5	1	0.274882	0.011031	0.186277	0	3	III	D	M
5	1	0.274882	0.011031	0.186277	1	2	III	B	M
5	1	0.274882	0.011031	0.186277	1	1	III	B	M
5	1	0.274882	0.011031	0.186277	1	3	III	B	M
5	1	0.274882	0.011031	0.186277	1	4	IV	B	M
5	1	0.13981	0.075694	0.002181	0	2	III	C	M
5	1	0.13981	0.075694	0.002181	0	3	III	C	M
5	1	0.13981	0.075694	0.002181	1	2	IV	B	M
5	1	0.13981	0.075694	0.002181	1	3	IV	B	M
5	1	0.13981	0.075694	0.002181	1	4	IV	B	M
5	1	0	0.368581	0	0	2	II	C	T
5	1	0	0.368581	0	0	3	II	C	T
5	1	0	0.368581	0	1	2	IV	B	M
5	1	0	0.368581	0	1	3	III	B	M
5	1	0	0.368581	0	1	4	III	B	M
5	0	0.253555	1	1	0	1	II	D	M
5	0	0.253555	1	1	0	3	II	D	M
5	0	0.253555	1	1	1	1	III	A	T
5	0	0.253555	1	1	1	3	III	A	T
5	0	0.305687	0.136554	1	0	1	II	D	M
5	0	0.305687	0.136554	1	0	2	II	D	M

CP	CT	T	P	FR	FM	PA	LR	CL	Risk Label
5	0	0.305687	0.136554	1	0	3	II	D	M
5	0	0.305687	0.136554	1	1	1	III	A	T
5	0	0.305687	0.136554	1	1	2	IV	A	T
5	0	0.305687	0.136554	1	1	3	IV	A	T
5	0	0.305687	0.151769	1	0	1	II	D	M
5	0	0.305687	0.151769	1	0	2	II	D	M
5	0	0.305687	0.151769	1	0	3	II	D	M
5	0	0.305687	0.151769	1	1	1	III	A	T
5	0	0.305687	0.151769	1	1	2	IV	A	T
5	0	0.305687	0.151769	1	1	3	IV	A	T
5	0	0.632701	0.562571	1	0	1	II	D	M
5	0	0.632701	0.562571	1	0	2	II	D	M
5	0	0.632701	0.562571	1	0	3	II	D	M
5	0	0.632701	0.562571	1	1	1	III	A	T
5	0	0.632701	0.562571	1	1	2	IV	A	T
5	0	0.632701	0.562571	1	1	3	IV	A	T
5	0	0.222749	0.003423	0.186277	0	1	II	D	M
5	0	0.222749	0.003423	0.186279	0	3	II	D	M
5	0	0.222749	0.003423	0.18628	1	1	III	A	T
5	0	0.222749	0.003423	0.186281	1	3	III	A	T
5	0	0.305687	0.170787	0.95449	0	1	II	D	M
5	0	0.305687	0.170787	0.95449	1	1	III	A	T
5	1	0.317536	0.121339	0.011538	0	1	II	D	M
5	1	0.317536	0.121339	0.011538	0	2	II	D	M
5	1	0.317536	0.121339	0.011538	0	3	II	D	M
5	1	0.317536	0.121339	0.011538	1	1	III	B	M
5	1	0.317536	0.121339	0.011538	1	2	IV	B	M
5	1	0.317536	0.121339	0.011538	1	3	III	B	M
5	0	0.632701	0.790795	0.939593	0	1	II	D	M
5	0	0.632701	0.790795	0.939593	0	2	II	D	M
5	0	0.632701	0.790795	0.939593	1	1	III	B	M
5	0	0.632701	0.790795	0.939593	1	2	III	B	M
5	0	0.632701	0.790795	0.939593	1	4	IV	B	M

CP	CT	T	P	FR	FM	PA	LR	CL	Risk Label
5	1	0.819905	0.052872	0.951504	0	1	II	C	T
5	1	0.819905	0.052872	0.951504	0	2	III	C	M
5	1	0.819905	0.052872	0.951504	0	3	II	C	T
5	1	0.819905	0.052872	0.951504	1	1	III	A	T
5	1	0.819905	0.052872	0.951504	1	4	III	A	T
5	1	0.819905	0.052872	0.951504	1	3	III	A	T
5	0	0.751185	0.144161	0.073429	0	1	II	D	M
5	0	0.751185	0.144161	0.073429	1	1	III	A	T
6	0	0.765403	0.532141	0.654075	0	2	II	D	M
6	0	0.765403	0.532141	0.654075	0	1	II	D	M
6	0	0.765403	0.532141	0.654075	0	3	II	D	M
6	0	0.765403	0.532141	0.654075	1	2	IV	B	M
6	0	0.765403	0.532141	0.654075	1	1	III	B	M
6	0	0.765403	0.532141	0.654075	1	3	III	B	M
6	0	0.549763	0.170787	0.654075	0	2	II	C	T
6	0	0.549763	0.170787	0.654075	0	1	II	C	T
6	0	0.549763	0.170787	0.654075	0	3	II	C	T
6	0	0.549763	0.170787	0.654075	1	2	IV	A	T
6	0	0.549763	0.170787	0.654075	1	1	III	A	T
6	0	0.549763	0.170787	0.654075	1	3	III	A	T
6	0	0.765403	0.657665	0.653995	0	1	II	D	M
6	0	0.765403	0.657665	0.653995	1	1	III	B	M