Universidade de Évora - Instituto de Investigação e Formação Avançada

Programa de Doutoramento em Bioquímica

Tese de Doutoramento

Quality Management in Laboratories - Efficiency Prediction Models

Ana Teresa Moreirinha Vila Fernandes Mateus

Orientador(es) | Henrique Vicente

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A tese de doutoramento foi objeto de apreciação e discussão pública pelo seguinte júri nomeado pelo Diretor do Instituto de Investigação e Formação Avançada:

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Preface

Biochemistry is an essential area for contemporary societies as it deals with extremely important issues in several areas, such as health and the environment. It plays a decisive role in developing solutions to some of the biggest problems of our time (e.g., environmental pollution, food shortages, renewable energies, new diseases) and in establishing a sustainable society. This dissertation is the result of the author's experience as a teacher, auditor, consultant, and researcher in Quality and Environment in accredited laboratories and certified organizations. This work clearly describes a journey that started at the University of Évora in 1999 with a Degree in Physics and Chemistry Teaching and, in 2007, with a Masters Degree in Environmental Chemical Analysis. This training allowed the author to work as an analysis technician and quality manager in Water and Industrial Effluent Laboratories. The post-graduation in Safety, Health and Hygiene at Work and the various training courses in normative references in the areas of Audits, Chemistry, Microbiology, Sampling, Equipment Management, Calibrations and Laboratory Facilities allowed her to join a multinational certification body as a technical auditor, in addition to being a member of the Technical Commission for Health Information Systems of the Portuguese Institute of Quality.

Bearing in mind the multidisciplinarity that characterizes this dissertation, it is intended that its content be applied, not only to laboratories with a view to creating efficiency models, but also to other types of organizations. As a final purpose, it is hoped that, in some way, it will raise awareness to all those who assume responsibility and commitment to the urgency of building effective laboratory management models, in the certainty that only in this way will significant steps be taken in improving health, the environment and well-being of society.

Prefácio

A Bioquímica é uma área essencial para as sociedades contemporâneas uma vez que se debruça sobre questões de extrema importância, em diversas áreas, tais como a saúde e o ambiente. Tem um papel decisivo no desenvolvimento de soluções para alguns dos grandes problemas do nosso tempo (e.g., poluição ambiental, escassez de alimentos, energias renováveis, novas doenças) e no estabelecimento de uma sociedade sustentável. A presente dissertação é o resultado da experiência da autora como professora, auditora, consultora e investigadora nos domínios da Qualidade e do Ambiente em laboratórios acreditados e em organizações certificadas. Este trabalho descreve, de forma clara, um percurso que se iniciou na Universidade de Évora em 1999 com a Licenciatura em Ensino de Física e Química e, em 2007, com o Mestrado em Análises Químicas Ambientais. Esta formação permitiu-lhe exercer funções de técnica de análises e de gestora da qualidade em Laboratórios de Águas e de Efluentes Industriais. A pós-graduação em Segurança, Saúde e Higiene no Trabalho e as diversas formações em referenciais normativos nas áreas de Auditorias, Química, Microbiologia, Amostragem, Gestão de Equipamentos, Calibrações e Instalações Laboratoriais permitiram-lhe ingressar num organismo multinacional de certificação com a função de auditora técnica, para além de vogal na Comissão Técnica de Sistemas de Informação para a Saúde do Instituto Português da Qualidade.

Tendo em conta a multidisciplinaridade que carateriza a presente dissertação pretende-se que o seu conteúdo seja aplicado, não apenas a laboratórios com vista à criação de modelos de eficiência, mas também a outro tipo de organizações. Como último propósito, espera-se que ela, de algum modo, sensibilize todos quantos assumem a responsabilidade e o compromisso da urgência da construção de modelos eficazes de gestão laboratorial, na certeza que, só desta forma, se darão passos significativos na melhoria da saúde, ambiente e bem-estar da sociedade.

Abstract

In recent years, the choice of quality tools by laboratories has increased significantly. This fact contributed to the growth of competitiveness, requiring a new organizational posture to adapt to the new challenges. In order to obtain competitive advantages in the respective sectors of activity, laboratories have increasingly invested in innovation. In this context, the main objective of this study aims to develop efficiency models for laboratories using tools from the Scientific Area of Artificial Intelligence. Throughout this work, different studies will be presented, carried out in water analysis laboratories, stem cell cryopreservation laboratories and dialysis care clinics, in which innovative solutions and better resource control were sought, without compromising quality and promoting greater sustainability

This work can be seen as an investigation opportunity that can be applied not only in laboratories and clinics, but also in organizations from different sectors in order to seek to define prediction models, allowing the anticipation of future scenarios and the evaluation of ways of acting. The results show the feasibility of applying the models and that the normative references applied to laboratories and clinics can be a basis for structuring the systems.

Keywords: Laboratories; Artificial Intelligence; Quality Management; Decision Support Systems.

Gestão da Qualidade em Laboratórios
Modelos de Previsão de Eficiência

Resumo

Nos últimos anos, a adoção de ferramentas da qualidade por parte dos laboratórios tem aumentado significativamente. Este facto contribuiu para o crescimento da competitividade, exigindo uma nova postura organizacional de forma a se adaptarem aos novos desafios. Tendo em vista obter vantagens competitivas nos respetivos sectores de atividade, os laboratórios têm, cada vez mais, apostado em inovação. Neste contexto, o principal objetivo deste estudo visa o desenvolvimento de modelos de eficiência para laboratórios através do recurso a ferramentas da Área Científica da Inteligência Artificial. Ao longo deste trabalho irão ser apresentados diferentes estudos, realizados em laboratórios de análises de águas, laboratórios de criopreservação de células estaminais e clínicas de prestação de cuidados de diálise, nos quais se procuraram soluções inovadoras e um melhor controlo de recursos, sem comprometer a qualidade e promovendo uma maior sustentabilidade. Este trabalho pode ser encarado como uma oportunidade de investigação que pode ser aplicado não apenas em laboratórios e clínicas mas, também, em organizações de diversos sectores com o intuito de se procurar definir modelos de previsão, possibilitando a antecipação de cenários futuros e a avaliação de formas de atuação. Os resultados mostram a viabilidade da aplicação dos modelos e que os referenciais normativos aplicados aos laboratórios e às clínicas podem servir como base para estruturação dos sistemas.

Palavras-Chave: Laboratórios; Inteligência Artificial; Gestão da Qualidade; Sistemas de Apoio à Decisão.

List of Publications

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Acronyms, Initialisms and Abbreviations

AABB	American Association of Blood Banks
A-ECM-WS	Adjusted version of Eindhoven Classification Model for Water Sampling
AEMR-PS	Adverse Events Manager Reports for Public Services
AERF-PS	Adverse Event Reporting Forms for Public Services
AERLS-WS	Adverse Event Reporting and Learning System related to Water Sampling
AN	Anergy
ANNs	Artificial Neural Networks
BCS	Best Case Scenario
BOD	Biochemical Oxygen Demand
CBR	Case-Based Reasoning
CDRI – 4	Cleaning and Disinfection Related Items – Four Items
COD	Chemical Oxygen Demand
COVID-19	Coronavirus Disease 2019
CTs	Causal Trees
DM	Data Mining
DO	Dissolved Oxygen
DoC	Degree-of-Confidence
ECM	Eindhoven Classification Model
ECT	Extended Causal Tree
EFQM	The European Foundation for Quality Management
EFQM-EM	The European Foundation for Quality Management Excellence Model
ERSAR	Regulatory Entity for Water and Waste Services, from Portuguese "Entidade Reguladora dos Serviços de Águas e Resíduos"
ESA	Employee Satisfaction Assessment
EX	Exergy
GDPR	General Data Protection Regulation

HL7 PHR-S FM	Functional Model of HL7 Personal Health Record System
ICT	Information and Communication Technologies
IPAC	Portuguese Institute of Accreditation, from Portuguese “Instituto Português da ACreditação”
ISO	International Standard Organization
ISO/IEC	International Organization for Standardization/International Electrotechnical Commission
KDD	Knowledge Discovery in Databases
KMM	Knowledge Manager Module
LP	Logic Programming
MAE	Mean Absolute Error
MRM	Manager Reports Module
MSE	Mean Square Error
NP EN	Portuguese version of an European standard
NP EN ISO	Portuguese version of an European standard developed by the International Organization for Standardization
NP EN ISO/IEC	Portuguese version of an European standard developed by the International Organization for Standardization and the International Electrotechnical Commission
NPV	Negative Predictive Value
OQM	Overall Quality Management
PDCA	Plan, Do, Check and Act
PPV	Positive Predictive Value
PS	Public Services
QA	Quality Assurance
QC	Quality Control
QM	Quality Management
QMS	Quality Management System
QoI	Quality-of-Information
R^2	Determination Coefficient

RFM	Reporting Forms Module
RRI – 4	Resources Related Items – Four Items
SARS-COV-2	Severe Acute Respiratory Syndrome Coronavírus 2
SARS-COV-2	Severe Acute Respiratory Syndrome Coronavírus 2
SP	System Performance
TQM	Total Quality Management
TRI – 4	Training Related with COVID–19 Items – Four Items
VA	Vagueness
WCL	Water Consumption Literacy
WCS	Worst Case Scenario
WEKA	Waikato Environment for Knowledge Analysis
WHO	World Health Organization

Objectives

As Dreyfus et al. (1999) emphasise, organizations have been concerned with quality related issues for many years. Quickly this concern has been extended to several areas, including the laboratory area of analysis, test, and calibration. In addition to legal requirements, which lead to high costs, competitiveness between laboratories has also been increasingly frequent. Laboratories are increasingly asked to innovate, provide better products and/or services, enable product and/or service customization, meet deadlines, improve layouts, reduce accident rates, reduce waste/consumption, ensure compliance legal provisions, ensure the protection of information, improve working conditions, promote social responsibility policies, and above all, make a profit. In addition, current methods of quality control and management involve many technical and financial resources. Thus, it becomes necessary to find alternative solutions that allow to reduce costs, without compromising the quality of the services provided.

The **main goal** of this study is the development of efficiency models for laboratories using Artificial Intelligence based tools. To achieve this objective, studies with **specific goals** were outlined, which are presented in four of the chapters of this thesis.

Chapter I

Bearing in mind the idea that biochemistry is transversal, that its wide range of applications (e.g., in health and the environment) and its strong relationship with the quality area, it is important to frame the theme through an approach to the concept of quality, the presentation of the associated standards and the explanation of the importance of Artificial Intelligence as a vehicle to achieve excellence in laboratories.

Chapter II

In this chapter, two studies related to **Quality Control** are presented. In the first one, it is intended to build a model to prevent errors associated with the sampling process, while in the second it is intended to develop models to predict water quality parameters.

Chapter III

Quality Management is addressed through the presentation of three studies. The first one intends to develop a model for recording and analysing adverse events that may occur in daily work. In the second one, it is intended to develop a conceptual model that supports studies that aim to assess the literacy levels of the population, in relation to the theme of water and its relationship with health and sustainability. This study also applies the model developed to the clients of a water laboratory to assess their literacy in relation to water. Finally, the third study intends to characterize the psychosocial risks to which employees in a cryopreservation laboratory are exposed, to assess their awareness of these types of risks and, finally, to develop prediction models for their management.

Chapter IV

Three studies related to **Total Quality Management** are presented, with the idea of achieving the competitiveness and satisfaction of all the involved partners. The first one intends to evaluate the implementation of the general data protection regulation in a cryopreservation laboratory. The second one seeks to assess the satisfaction of employees in a water analysis laboratory, regarding the new procedures implemented to face the current pandemic scenario. Finally, in the third one, the intention is to assess customer satisfaction in a water analysis laboratory accredited according to the ISO/IEC 17025 standard, on one hand, and to develop models for predicting customer satisfaction, on the other hand.

Methodology

Throughout this work several methodologies for collecting and processing data were adopted. They were chosen according to the type and objectives of each of the studies. In this chapter, only general methodologies will be briefly mentioned. The detailed description will be presented in each of the studies.

Study Locations

The different studies were carried out in different locations of different dimensions, geographically differentiated (North zone, Central zone/metropolitan area of Lisbon and South zone) and of different contexts, (e.g., water analysis laboratories, stem cell cryopreservation laboratories and dialysis care clinics).

Data Collection

Data on water quality were collected in water analysis laboratories located in the south of Portugal (municipalities of Santiago do Cacém and Sines). About the literacy and satisfaction studies, it was decided to collect data that would allow us to obtain answers with some statistical validity, for the questions under study. Thus, the choice of the data-collecting instrument was the inquiry by questionnaire. This instrument has some advantages such as faster data collection, greater simplicity in the analysis and systematization of data, and the fact that it is cheap. The disadvantages include the difficulty of conception and the low rates of return (Carmo & Ferreira, 1998). The questionnaires were distributed during internal audits, in the context of the certification and/or accreditation audit cycle. The questionnaires were delivered to the heads of the laboratories to whom the objective of the study was explained. Those responsible people who agreed to participate provided a collaborator for the delivery and collection of the questionnaires. The referred employees were trained on the objectives and the type of questionnaire to be able to clarify any doubts that someone could have during its application. Finally, it should be noted that the participation in the study was voluntary and that the provisions of the general data protection regulation of 25th May 2018 were respected, the questionnaire was anonymous and confidential and the respondents were informed of the objectives of the study.

Data Processing

In the processing of the obtained data, tools from the Scientific Area of Artificial Intelligence (e.g., Artificial Neural Networks, Case-Based Reasoning) were used, in addition to the answer frequency analysis. The Knowledge Discovery in Databases was the strategy followed to treat the results. For this purpose, it was chosen the Waikato Environment for Knowledge Analysis (WEKA), a public-domain software. This tool offers several forms of data pre-processing, several data mining algorithms, and several methods for validating the results. It was developed in New Zealand, at the University of Waikato, and uses the facilities provided by object-oriented programming, in Java language. Regarding the data, they must be in a specific format (extension *arff*), which is done through the converter, made available by the software, applicable to files of *csv* or *tsv* type (Hall et al., 2009; Frank et al., 2016).

In some cases, the information collected is of a qualitative nature, so it necessary to convert it to a numerical scale. For this purpose, it was chosen the graphic method proposed by Fernandes et al. (2016a). In this method, for each dimension under study, a circle of radius $\sqrt{1/\pi}$ divided into a number of parts with an equal area, corresponding to the number of statements/questions to be considered. The answer alternatives were indicated in the axes, and the area corresponding to the selected option was drawn. The value corresponding to the dimension under study corresponds to the total area, i.e., the sum of the partial areas.

The coincidence matrixes were used to validate the classification models obtained. Based on the referred matrixes several metrics (e.g., sensitivity, specificity, accuracy, positive predictive value, negative predictive value) were computed (Souza et al., 2002; Florkowski, 2008; Vilhena et al., 2016). In the case of regression models, the errors or deviations were calculated from which the mean absolute error and the mean square error were obtained (McBride, 2005, Vicente et al., 2012b).

I.1. Overview

Despite that living beings are all macroscopically different, it has been noticed close similarities in their biochemistry and for that reason biochemistry is a subject that aims the global study of all beings and of life itself. Biochemistry has allowed (and it still moves forward) the understanding of mechanisms that characterize the cellular functioning of different tissues and organs, identifying the molecules that compose the cells (i.e., the biomolecules), as well as the chain reactions between them (metabolic pathways). In this way the biological phenomena can be explainable taking into account their chemical reactivity. These scientific breakthroughs are important because they allow that some of those phenomena can be observed in the laboratory, bringing endless advantages such as the development and the study of some medicines before being applied directly to living organisms. Nowadays biochemistry can be used in different areas, e.g., health science, industry, and analytical methods, due to its transversal nature. The contemporary society has shown more interest in this area because the environmental and health problems are quite often explained with a strong interaction between the biochemistry and the other knowledge areas, namely quality. Organizations have been increasingly facing external exposures. To deal with this challenge, the organizations should improve service quality, be more efficient, control costs, improve productivity rates, modernize, use new technologies and teach employees new skills. Excellent organizations continually design, manage, and improve their products, in order to satisfy their customers and stakeholders or, in other words, to add value. In this context, Artificial Intelligence can play a decisive role to improve products and services from different sectors of activity, such as information technologies, telecommunications, medical systems, nanotechnology, and biotechnology. The use of innovative biotechnologies has promoted a real revolution in the treatment of diseases (e.g., the use of new medicines for human and animal application), in the multiplication and reproduction of plant and animal species, in the development and improvement of food, in the sustainable use of biodiversity and in new waste treatments.

A laboratory equipped with a computational system that operationalizes its routines and acts as a data and information repository can be used as a tool of great utility to estimate costs and to manage other procedures that must be done. In Portugal, in the last decades, laboratories have been going through endless modifications, either to keep pace with the technological evolution, or to establish themselves in an increasingly competitive market. The standards created by the International Organization for Standardization help to comply with the legislation associated with this sector of activity and, allow to improve the quality of products and services worldwide.

I.2. Theoretical Perspectives

Quality is something connected to the human being, projecting itself in different acts, even in the most common and automatic ones of daily life. The consumer who on Saturdays walks around the market feeling and smelling pears and apples and questioning the sellers, seeks quality fruit, rejecting those that do not follow the standards defined and adopted by himself (António et al., 2016). The Portuguese Quality Institute the entity designated for quality issues in Portugal, through the Decree-Law no. 140/2004 of 8th June, presents quality as a set of attributes and characteristics of an entity or a product that define their ability to meet the needs and expectations of society. Quality is also defined in ISO 9000 standards: Quality Management Systems – Fundamentals and Vocabulary, as the degree of satisfaction of requirements, given by a set of intrinsic properties. Several definitions of quality could be mentioned from the most varied subjects and according to several authors. However, when analysed in detail, it is clear that this is a large set of concepts, all with connecting points and overlap, with their own relative importance (Hoyle, 2017; António et al., 2016). From a historical point of view, significant changes have occurred approximately every twenty years, in relation to the strategic approaches developed to achieve quality goals (Juran, 1995). This evolution, shown in Figure 1, includes six stages that will be briefly described below.

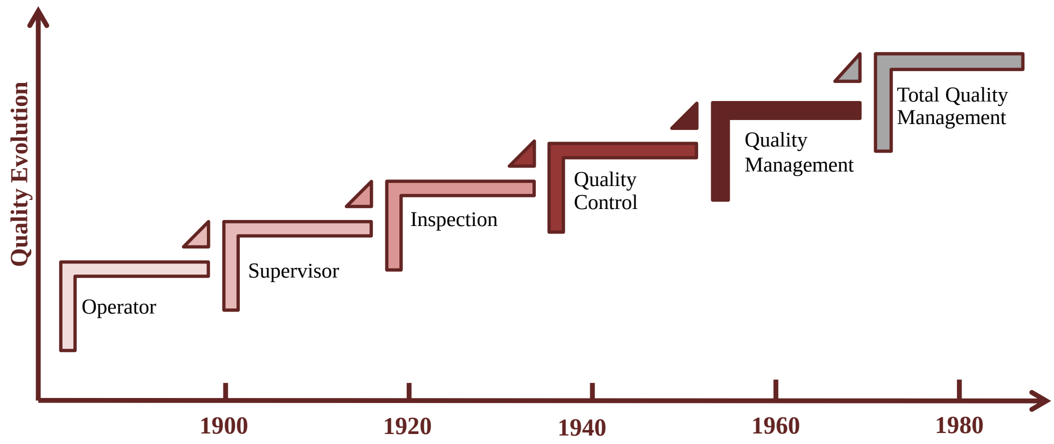

Figure 1 – Evolution of the strategic approaches to achieve quality.

Initially, the control of quality was done by the **Operator.** A worker or a small number of workers, called artisans, were responsible for all the stages of product manufacture, from conception to sale (Ganhão, 1992). The characteristics of the handmade model were low production and high-quality standards (Feigenbaum, 1994). At the beginning of the 20th century, with the Industrial Revolution and the emergence of large factories where workers were grouped into teams and directed by a supervisor, the control of quality was carried out by the **Supervisor** (Ganhão, 1992; Feigenbaum, 1994). However, it was easily shown that this type of quality control was not effective enough as it was highly dependent on the fact that supervisors give priority to meeting quantitative production targets. In this way, quality control started being done by **Inspection**. This new strategy passed through a central inspection department, led by a chief inspector (Ganhão, 1992; Feigenbaum, 1994). However, at the beginning of World War II, the demands of mass production triggered **Quality Control** based on sampling inspection and control charts. This type of control allowed the development of planning activities and the analysis of results, having raised the demand levels to much higher levels than those previously practiced by the inspection (Ganhão, 1992). However, as highlighted by Feigenbaum (1994), the quality control work remained restricted to the production areas, not covering other areas equally important regarding quality. According to Juran (1995), the end of the Second World War and the subsequent reconstruction of Japan allowed the development of unprecedented strategies, highlighting the role of a leader on top management process and the quality management came to be seen as a concern of all departments. The recognition of the positive results of quality assurance in the production area, allowed to extend quality improvement practices to all activities/sectors of the company, which led to **Quality Management** (Ross, 1999). However, it has been found that ensuring the quality of a specific product or service is not enough. The focus should be on the quality of a process as a whole, covering everything that happens in the company, being the customer satisfaction the final goal (Ross, 1999). This is the concept **Total Quality** or **Total Quality Management**, whose philosophy consists in the application of quality in all the branches of the company. The implementation of the concept of continuous improvement, aiming to obtain consumer satisfaction, is essential to achieve both competitiveness and quality management (Pires, 2016). This philosophy had a great impact on engineering practices, being at the basis of the evolution of current Quality Systems.

A System can be defined as a set of interdependent elements, which interact with common objectives, forming a whole. Each element behaves as if it was a system itself, contributing to an overall performance which is better than if the units operated independently. Each system transforms inputs into outputs, in a dynamic relationship with the environment, to achieve a common objective. A Quality Management System can be understood as a management philosophy, which presupposes the involvement and cooperation of all employees, aiming at providing products and services that satisfy the needs and expectations of customers (Pinto & Soares, 2018).

In the following sections, a reflection will be made on the concept of quality in laboratories since 1930, with the emergence of quality control, passing by quality management until today, where it is intended to achieve the satisfaction of both employees and customers through the total quality management.

I.3. Normative References

Analysis laboratories tend to rely almost entirely on tests to monitor and evaluate their performance. The Internal Quality Control, based on the analysis of standard samples whose reference values are known, and the External Quality Control, based on blind samples whose results are reported to the organizing laboratory, are examples of this (Kailner, 1998). However, it has become clearer that these tests are not enough to guarantee quality in the laboratories, and it is necessary to consider other ways. In this way, ISO 9000 standards created the basis for Quality Assurance Management with the Certification function. The NP EN 45001:1990 standard “Criteria for the operation of

Testing Laboratories", in turn, was the first benchmark aimed at guaranteeing and asserting the competence of laboratories in carrying out tests with the Accreditation function. In general, the NP EN 45001 standard focuses on the technical competence of testing laboratories to the detriment of quality management requirements, aimed at customer satisfaction (Kohl, 1998).

With the publication of the ISO/IEC 17025 standard, was made an attempt to cover topics from the Quality Management System (QMS) of a laboratory which were not covered in the previous standard. This one includes all the management requirements of the ISO 9001 standard relevant to the scope of the testing and calibration services covered by the laboratory management system (Kohl, 1998). The fulfil of the QMS requirements of ISO/IEC 17025, by a laboratory, means that it meets both the requirements of technical competence and management, which are necessary to guarantee consistent and technically valid results. However, it should be noted that laboratories with the ISO/IEC 17025 accreditation cannot claim that they automatically meet all the requirements of the ISO 9001 standard. To do that, they must apply for certification by the ISO 9001 standard, separately.

The 2005 version of the ISO/IEC 17025 standard used a comprehensive and transversal language, directed to any test and calibration laboratory. However, it was clear the need for a standard exclusively directed to clinical laboratories, due to the impact they have on the provision of services and the specificity of the samples used. Thus, in 2007, the ISO 15189 standard appeared. It was developed based on the ISO/IEC 17025 and ISO 9001 standards, which establish quality and competence requirements for clinical laboratories, with a language and structure appropriate to the sector, facilitating its understanding and implementation.

The standards NP EN ISO 15189 and NP EN ISO/IEC 17025 are structured in two types of requirements, i.e., Management Requirements and Technical Requirements. Notwithstanding the accreditation presupposes the fulfilment of all the requirements of the reference standard, according to Yanikkaya-Demirel (2009), the following requirements are considered as critical points for the implementation of the QMS in a laboratory:

- Facilities and environmental conditions;
- Laboratory equipment;
- Quality assurance of procedures and results, through measurement of uncertainties and participation in external quality assessment programs; and

- Presentation of results.

Concerning the facilities and environmental conditions requirement, there are some points to be taken into account with regard to the laboratory space, viz.,

- A design that allows efficient operation as well as risk reduction;
- Good lighting, ventilation, water supply, waste disposal and environmental conditions;
- An effective separation between areas where incompatible activities are carried out, such as microbiology, which must be apart from the other areas;
- Control of access to areas likely to affect the quality of the results; and
- The cleaning of work areas and their maintenance, through procedures and training of technicians and auxiliary staff (NP EN ISO 15189, 2014; NP EN ISO/IEC 17025, 2018).

Another important requirement includes all instruments, reference materials, consumables, reagents, and analytical systems. Laboratories must develop a programme that shows regular calibration and preventive maintenance of equipment. Instructions for selection, acquisition, calibration, validation and/or verification, maintenance, repair or decommissioning of the equipment must also be established (NP EN ISO 15189, 2014; NP EN ISO/IEC 17025, 2018).

The standard references above mentioned have been revised and/or updated over the years. In 2017 the ISO 17025 standard was revised leading to NP EN ISO/IEC 17025:2018. The latest updates of the NP EN ISO 15189 and NP EN ISO 9001 standards date from 2014 and 2015, respectively.

I.3.1. Laboratory Accreditation

The implementation of a QMS in the current scenario of the laboratories is a prerequisite for survival since it allows them to comply with the requirements imposed by the legislation in force, namely the accreditation. The accreditation process follows the international standard ISO/IEC 17011, and it is governed by the principles of openness, fairness, and non-discrimination. According to the Portuguese Institute of Accreditation (IPAC), accreditation is the procedure through which it is formally recognized that an entity is technically competent to perform a specific function, in accordance with international, European or national standards (IPAC, 2020). The accreditation activity was performed by the Portuguese Quality Institute, whose responsibility and competence were meanwhile attributed to the IPAC, which is now the regulator and conformity assessment agent. Regarding the certification function, there was greater decentralization, which can be carried out by entities accredited for the purpose. According to the Decree-Law No. 140/2004 of 8th June, certification is the procedure through which an accredited body gives a written guarantee that a product, process, service, or system follows specified requirements.

The accreditation aims to guarantee the technical competence to carry out a specific test or calibration. In addition, the incentive effect in promoting improvement within the laboratories is also relevant. The IPAC provides the brand – accreditation and this distinction must be used by accredited entities to benefit from national recognition and show that they give relevance to the quality issues, helping clients to have confidence in the results issued. Dugimont et al. (2006) list the advantages and disadvantages of implementing a QMS aiming the accreditation. Regarding the advantages, they highlight:

- The normalization of technical and administrative processes;
- Focus on customer satisfaction;
- The involvement of all employees and the guarantee of their technical competence;
- Greater credibility in the results;
- The comparability and reproducibility of the results issued;
- The increase of confidence between the parties involved;
- Ease of acquiring financing; and
- The continuous improvement of the service.

Regarding the disadvantages, the authors highlight the financial effort necessary to ensure effectiveness in the implementation of the QMS, as well as the problems that may arise from the constant updating of standards and equipment.

I.3.2. Quality Audits

In order to make an accurate assessment of the effectiveness of an organization management system, it is necessary to carry out audits (Pinto & Soares, 2018). According to the ISO 19011 standard, auditing is a systematic, independent, and documented process that aims to obtain evidence to carry out an objective assessment, against previously established criteria (NP EN ISO 19011, 2019). The audit involves the collection of data necessary for the correct analysis and assessment of compliance with the requirements of the benchmark, including the requirements associated with products, services and processes with a view to the timely detection of deficiencies, anomalies or non-conformities. In order to avoid the subjectivity that is common in all assessment, the following audit criteria should be taken into account:

- The criteria chosen to implement the system;
- The national legislation;
- The national and community standards;
- The regulations issued by reference bodies;
- The technical standards existing in each sector; and
- The specifications of products and services (Pinto & Soares, 2018).

The audit should be understood as a sampling process supported by objective evidences, aiming to help the organization in the identification of non-compliant situations and opportunities for improvement (NP EN ISO 19011, 2019). The audits are carried out by external and independent entities that lead to the formal recognition that the organization has a management system that complies with a certain reference standard, resulting in the issue of a certificate.

I.4. Artificial Intelligence in Laboratories

Accreditation is extremely important for laboratory activity. The balance between the quality requirements and the quick mutation of modern society is a challenge. In fact, it is necessary to balance the expectations of consumers and citizens regarding new products and services with the expectations about the requirements of safety, health, robustness, reliability (Saltzman, 2015). The laboratories, regardless of being autonomous or integrated into business groups, have already made their way along the line of digitization. Some sectors were pioneers in the systematic digital approach of their activity, highlighting those that operate in the context of clinical analyses, in testing areas associated with technologically demanding industries and in the ones where safety is a fundamental element. In the health sector the term eHealth came up to mention the tools and services of Information and Communication Technologies (ICT) for health (Silva, 2013; Saltzman, 2015). Health information network, electronic health records, telemedicine services, health portals and many other ICT-based tools can help citizens and health professionals in the prevention, diagnosis, and treatment of diseases, as well as monitoring health and lifestyles (Pereira et al., 2011). The requirements in some of these areas have allowed that, in many laboratories, there is now a perception of the way to follow in the digitization process, recognizing that this is a particularly sensitive activity to technological evolution, not only in the experimental context (instrumentation, knowledge and skills) but also by the intensive integration of technologies in the development of products and services. However, the future challenges are much more demanding. The development of smart cities must include testing, inspection and certification entities, i.e., the development of testing, inspection and certification sector in order to promote, in a broad sense, the confidence to citizens (Saltzman, 2015). Smart cities require effective and efficient links between resources, mobility, and services (i.e., technological components that guarantee lighting, traffic, transport management, communication, water supply, energy, just to name a few). Trust in systems and platforms requires testing, conformity assessment and data management (Dobner & Frede, 2016). The latter is essential for the future of laboratories. The existence of skills in new subjects, where data management or, in a general context, data science stand out is of utmost importance. Data science is a key element for the future. It is an interdisciplinary area that associates the analysis and understanding of data to the decision-making process. The recent revision of the ISO/IEC 17025:2017 standard brought an important update to the accreditation process. The standard includes a consistent approach that promotes the digital transition, allowing laboratories to build an activity model free of classical formal and documentary constraints. Furthermore, it adopts a linear organizational view, aiming an integrative perspective of resources and processes, more in line with the current organizational structures of companies and laboratories (ISO/IEC 17025, 2017). Indeed, the current version has a different view of laboratorial activity, perhaps due to the evolution of the classic idea of laboratory. It not only considers the high level of technical competence but also has started to include strategic and management elements. This review also allowed the standardization of the concepts shared with ISO 9001 and other standards. In order to respond to the challenges of the digital transition, the Portuguese laboratorial organizations have been developing skills aiming to give a positive answer, being at the forefront of the transition process, anticipating a successful adaption.

I.5. Knowledge Discovery from Databases

Technological means have provided an exponential growth, both in number of records and in complexity, regarding data storage. As a result of this effective increase in information, its processing through traditional methods has become increasingly difficult and complex. In this way, applications aimed to the task of knowledge discovery in databases have emerged, incorporating Data Mining (DM) tools (Han et al., 2012; Witten et al., 2017).

The concept Knowledge Discovery from Databases (KDD) appeared in 1989, as a reference to the broader concept of searching for knowledge in data, being a process that involves the identification and recognition of patterns or trends, in a database, in an autonomous and possibly automatic way (Han et al., 2012; Witten et al., 2017). As it can be seen in Figure 2, the KDD process depends on a new generation of data analysis tools and techniques that involves several steps, namely selection, data pre-processing, data transformation, data mining and interpretation (Han et al., 2012; Witten et al., 2017). Although Figure 2 may suggest the existence of a linear path, this is not always the case. At each stage, the need to return for each of the previous phases can be identified. For example, if in the DM phase it is concluded that the data are not fully coherent or the need to include a new data is verified, this can lead to the return to previous phases.

As previously mentioned, the DM stage is only one stage of the KDD process. It consists in choosing and using the methods and techniques that best fit the fulfilment of the established objectives. In general, objectives can be divided into two groups, i.e., prediction and description. In the case of prediction, it is intended to infer future behaviors based on past experiences, whereas in the description it is intended to describe compactly sets of data or variable associations (Han et al., 2012).

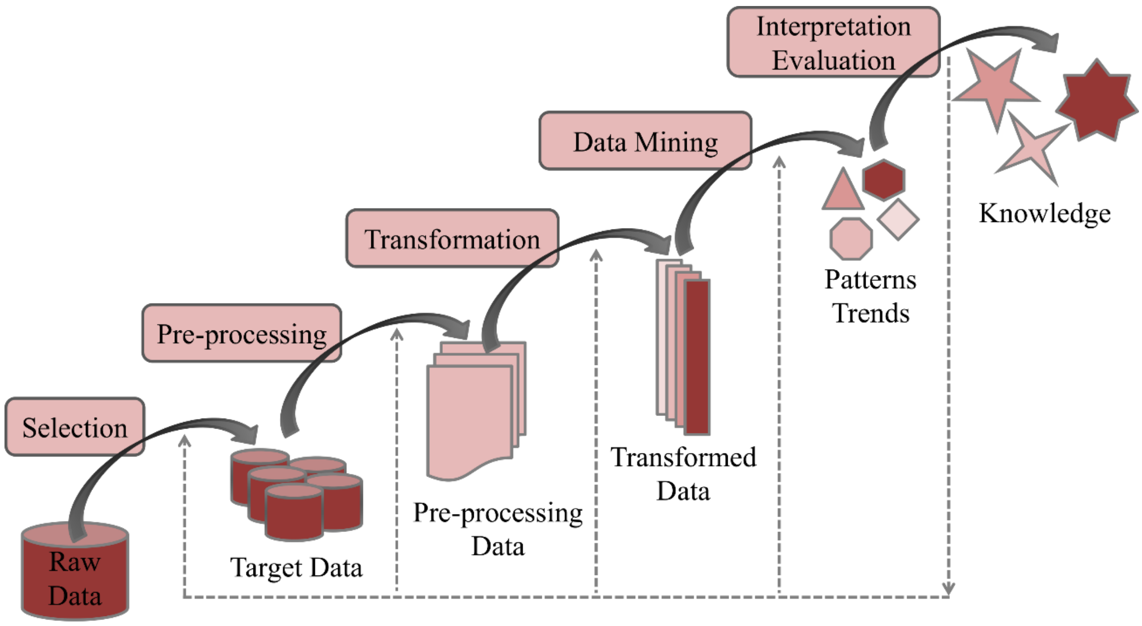

Figure 2 – The process of knowledge discovery in databases.

I.5.1. Artificial Neural Networks

Data analysis is not a recent subject. For several years it has been carried out using mainly statistical methods. However, from an early stage, it became clear that the human brain analyses data and treats information differently, using learning processes (Han et al., 2012). Artificial Neural Networks (ANNs) were inspired by the nervous system of living beings, particularly that of the human being (Haykin, 2009). An ANN is a set of simple processing elements, called artificial neurons or nodes, in a very interconnected parallel structure. They are similar to the behavior of the brain because, on one hand, knowledge is acquired from an environment through learning processes and, on the other hand, because knowledge is stored in the connections between the nodes (Haykin, 2009).

From a historical point of view, ANNs had their origin in the 40s of the 20th century, with the work of Warren McCulloch and Walter Pitts. These authors presented a simplified model of the neuron (called artificial neuron or node), based on the fact that the neuron or is active or inactive, at a given moment, which corresponds to the true/false of the proportional logic or the one/zero of the Boolean algebra (McCulloch & Pitts, 1943). Other contributions followed especially that of Rosenblatt (1958), who introduced the perceptron model, which originated the most used network architectures, called feed--forward neural network. These are organized by layers and the connections always propagate in one direction, with no cycles.

The artificial neuron, commonly called node, is the basic processing unit of an ANN. Although there are several types of nodes, in general, they all behave like comparators that produce an output when the cumulative effect of the inputs exceeds a given limit value. According to Haykin (2009), a node is made up of three fundamental elements:

- A set of connections (x_1, x_2, ..., x_n), each labelled by weight (w_{ij}), i.e., a real or binary number that has an excitatory or inhibitory effect depending on whether it has positive or negative values. Sometimes there is an additional node, called "*bias*", whose value is +1 that aims to establish the correct operational conditions for the network;
- An integrator, which reduces the input values to a single value (μ_i); and
- An activation function (f), which can condition the amplitude of the output signal (s_i), introducing a nonlinear component in the computational process.

With regard to activation functions, the Heaviside step function is normally used in McCulloch-Pitts nodes, where the output takes the value +1 only if the gain is non-negative, obeying a philosophy of all or nothing. The logistic activation and hyperbolic tangent functions, as well as the Gaussian and the square ones, introduce a nonlinear component to the computational process. The logistic function, also known as the sigmoid function, is the most used activation function in ANNs (Haykin, 2009).

Establishing the best network topology to respond to a given problem is a complex and crucial task. However, there are no clear rules for establishing either the number of intermediate layers or the number of nodes that constitute them. In most cases, the establishment of the best network topology is done by trial and error, starting with an initial structure that is selectively modified to minimize an error metric (Witten et al., 2017).

Regarding the training of neural networks, the backpropagation algorithm (Rumelhart et al., 1986) and its variants (Riedmiller, 1994) are reference algorithms, being efficient computational tools for the training of ANNs. They are based on gradient descent methods and seek to minimize the error function in the weight search space, in order to find the optimal set of weight values that, in an ideal situation, would result in the correct outputs for any input.

I.5.2. Case Base Reasoning

Case-Based Reasoning (CBR) is a problem-solving methodology, allowing to solve new problems by reusing knowledge acquired from past experiences. In fact, it can be described as the process of solving new problems based on solutions to similar previous problems (Aamodt & Plaza, 1994; Richter & Weber, 2013).

Any CBR system consists of four basic elements, namely the case repository (where previous cases are stored), a similarity measure (which allows comparing the new case with the stored cases), tools to adapt the previous case solutions to the new problem and learning ability, i.e., capability to integrate the case just solved in the repository (Richter & Weber, 2013).

The conventional CBR cycle (Figure 3) presents the sequence of steps that must be followed to obtain a consistent model. The first step is the initial description of the problem. Only after describing/understanding the problem is possible, using a similarity measure, to recover one or more cases from the repository. The number of recovered cases will vary depending on the similarity defined. High values of this measure lead to the recovery of cases with an extremely high degree of similarity. However, the number of recovered cases may be too low and compromise subsequent steps (Richter & Weber, 2013).

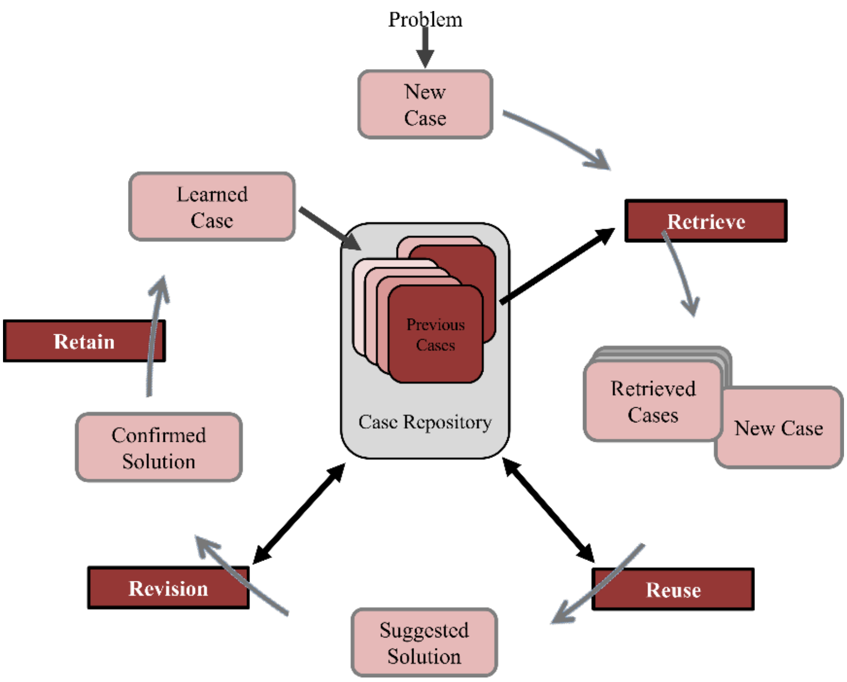

Figure 3 – The classical view of case-based reasoning cycle.

In the reuse phase, a possible solution to the problem emerges based on the adaptation of the recovered cases to the new case. However, automatic adaptation is almost impossible, so the opinion of the user becomes essential. Thus, in the review phase, the solution suggested by the system is tested by the user, allowing for its correction, adaptation and/or modification, giving rise to the confirmed solution, i.e., the solution for the new case. This phase involves an iterative process as the solution must be tested, adapted and/or modified as many times as necessary to ensure the desired result. Finally, during the retention stage, the new case is learned, and the knowledge base updated with the new case (Aamodt & Plaza, 1994; Richter & Weber, 2013).

Despite the promising results, the current CBR systems are neither complete nor sufficiently adaptable to all domains. In some cases, they do not allow the user to choose the similarity function, which translates into a limitation. In addition, the existing CBR systems have limitations related to their ability to deal explicitly with unknown, incomplete, and/or contradictory information. In fact, this constraint is particularly compromising on real problems, where information is not always complete. In an attempt to solve the problems related to incomplete information, Fernandes et al. (2016a) introduced a new cycle for RBC (Figure 4) that includes a standardization phase where the *Quality-of-Information* and the *Degree-of-Confidence* of each case is taken into account, allowing to represent, in the Cartesian plane, the cases stored in the repository and, through unsupervised learning methods, reduce the search space and make the recovery process more effective. This methodology allows to deal explicitly with incomplete information, responding to one of the main limitations of the conventional CBR cycle. In addition to the above, this approach allows the optimization of recovered cases whenever the suggested solution is not in accordance with the intended objectives.

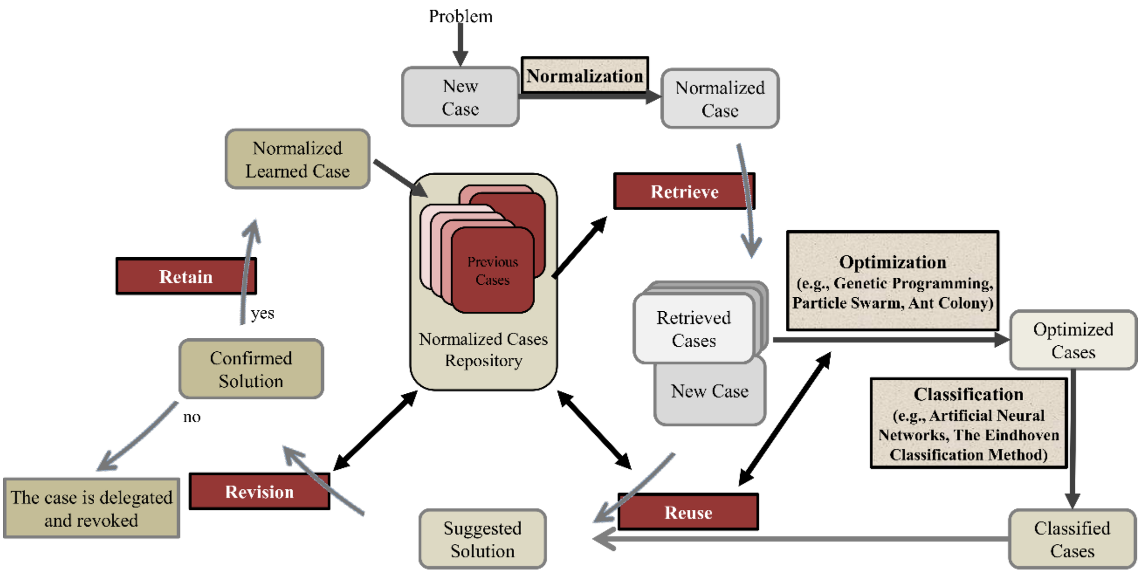

Figure 4 – The extended view of case-based reasoning cycle.

II.1. Overview

Nowadays the environment is experiencing serious problems, many of which are caused by excessive consumption and/or misuse of natural resources (e.g., water, oil, fishing). The direct or indirect impacts on the environment, which are often local, have, however, global repercussions. With regard to the predisposition of the Portuguese business in relation to environmental issues, the situation is much better than a decade ago, as evidenced by the growing number of organizations that obtain environmental certification, the number of laboratories that obtain accreditation and the application of computational techniques in the development of environmentally friendly solutions.

The importance of water, as a natural element indispensable to life, has been recognized since the beginning of the existence of Man on Earth. Throughout the ages, rivers have marked, in a decisive way, the settlement of populations and the evolution of great civilizations, whose culture and skills appear closely linked to the use of water (Serralheiro, 2001; Lehr & Keeley, 2005a; Haidvogl, 2018). However, it was only in the middle of the 20th century that Humanity became aware of the value of the renewable resource water as a basic factor of economic and social development, as a result of the increasing pressure related to the demographic growth, by the promotion of agricultural and industrial production and by the progressive urban concentration (Lehr & Keeley, 2005a; Lehr & Keeley, 2005b).

The problem of water, which includes the use and management of available water resources, is not a purely quantitative problem within its biogeochemical cycle, but it is mainly a qualitative problem (Mendes & Oliveira, 2004; Poppe et al., 2018). Water is not found in nature in its pure state, i.e., it does not appear as a colourless, odourless, and tasteless compound. On the contrary, it contains dissolved and/or suspended foreign substances that can condition its possible uses (Mendes & Oliveira, 2004; Bagchi, 2013). This fact originates the need to associate the quantification of water resources with the indication of their quality. In this context, water quality can be defined as a set of parameters and characteristics that will determine its adaptability to certain well-specified purposes (Mendes & Oliveira, 2004).

The need to guarantee the consumer a high-quality water presupposes its control not only at the point of consumption, but also in the collection. Thus, regulatory authorities establish quality standards for both raw water sources and distribution and consumption points. In Portugal, the Regulatory Entity for Water and Waste Services (ERSAR) is the competent authority for the inspection of the quality of water for human consumption (Vieira, 2018). This entity aims to comply with the legislation associated with water, in particular the Decree-Law No. 236/98, of 1 August. This legislation establishes quality standards, criteria and objectives for water intended to produce water for human consumption, transposing the Directive 75/440/EC into national law. The standards for the control of the quality of water for human consumption in Portugal have followed the modernization of the European regulatory framework. For example, the Directive 98/83/EC on the quality of water intended for human consumption, was transposed to the Decree--Law no. 306/2007 of 27 August, and subsequently revised by the Decree-Law no. 152/2017, of 7 December. This legal framework provides the use of EN ISO/IEC 17025 (or other internationally accepted standards) for the validation of analysis methods.

Although water supply systems can be contaminated by a wide variety of substances, only a limited number of them are a threat to human health (Serralheiro, 2001). National legislation on water intended for human consumption establishes acceptable values for microbiological, chemical and indicator parameters that resulted from the transposition of European directives into national law. However, pathogenic microorganisms are a priority in any monitoring program, as they represent a more serious risk to the safety of water intended for human consumption, considering their epidemiological relevance (Vieira, 2018). Chemical and radiological contamination can, in specific cases, cause harmful effects. However, this type of contamination is related to localized natural conditions or are the result of specific outbreaks of pollution due to anthropogenic action (Schäfer & Bundschuh, 2018).

The verification of the conformity of the quality of water for human consumption is carried out through the monitoring of microbiological, chemical parameters and indicators that are grouped into two types of control (i.e., routine control and inspection control). The first aims to provide regular information on the organoleptic and microbiological quality of the water, as well as on the effectiveness of treatments, particularly disinfection (Mendes & Oliveira, 2004). Inspection control aims to verify compliance with the parametric values stipulated by law. The minimum sampling frequency is determined by the priority given to the parameters to be monitored, considering the type of control. Sampling is a decisive step in the control of water quality, because the sample must represent, in a reliable way, the water situation at the time of collection (Relacre, 2017). After the samples arrive at the laboratory, a set of techniques and activities of an operational nature are triggered to meet the quality requirements (Relacre, 2017). Experience has shown that for most of the parameters analysed (especially the physical-chemical parameters), the concentrations present do not often violate the limit values (Vieira, 2018). In this way, considering the costs associated with monitoring parameters without much practical relevance, it is necessary to find alternative solutions that allow reducing costs without compromising water quality control. In this context, can be referred the introduction of flexible monitoring frequencies or the application of tools based on Artificial Intelligence, which have been applied with great success in several scientific areas (Pinto et al., 2009; Caldeira et.al, 2011; Vicente et al., 2012b; Couto et al., 2012; Martins et.al, 2015; Vicente et al., 2015; Ahmed, 2017; Loucks & Beek, 2017; Allawi et al., 2018; Ruben et al., 2018 Chen et al., 2019). In this way, management entities may be exempted from some of the provisions of the water quality control programs, provided that credible risk assessments are carried out, based on national guidelines or the World Health Organization (WHO) for the quality of the water for human consumption.

In this chapter we will address the issue related to water quality, presenting the following studies:

- **II.2 – Avoidance of Sampling Errors in Drinking Water Analysis – A Logical Approach to Programming**[1]
- **II.3 – Draw on Artificial Neural Networks to Assess and Predict Water Quality**[2]

In these studies, methodologies from the Artificial Intelligence scientific area were used, which can be applied in laboratories or in water management entities, in order to prevent errors associated with the sampling process (study II.2) and to predict some parameters (study II.3) without compromising water quality and protection of human health.

[1] Submitted to *Water Practice and Technology*.

[2] Published in *IOP Conference Series: Earth and Environmental Science*, 612: 012028, 2020.

II.2. Avoidance of Sampling Errors in Drinking Water Analysis – A Logical Approach to Programming

II.2.1. Introduction

Securing water quality for human consumption through a public supply system is an essential element of health policy. By the end of the 19th century, the assessment and control of the risks to human health from the transmission of diseases caused by water consumption was carried out empirically on the basis of the physical appearance of the water (Bagchi, 2013). The epidemiological studies conducted by John Snow showed the close association between the consumption of water with fecal contamination and a cholera outbreak in London (Snow, 1855). The discovery of the existence of microorganisms by Louis Pasteur in 1863 and the isolation of Vibrio cholera bacillus in 1883 by Robert Koch formed the crucial scientific basis for the association of water use with public health and served as a starting point for the establishment of practices and protocols to control water quality (Geison, 1995; Brock, 1999). Until the middle of the 20th century, the quality of water for human consumption was largely assessed based on its organoleptic characteristics, i.e. colorless, tasteless, and odorless (Baird et al., 2017). However, this type of assessment does not guarantee the protection of public health from pathogenic microorganisms and hazardous chemicals. It was therefore imperative to establish parametric standards that define the properties of water for human consumption in terms of microbiological, physical, chemical, and radiological parameters (ISO/IEC 17025, 2017). Current methods of controlling water quality are time consuming, complex, expensive, and have some known limitations. Indeed, the process of controlling water quality is complex and diverse and involves a large number of technical and financial resources (e.g. calibrated equipment, infrastructure, skilled technicians and reagents). With all this complexity, a large number of errors can occur (Byleveld et al., 2008). A failure can be defined as failure of a planned action, use of an incorrect plan and can be in connection with products, processes, and systems (Hommerson et al., 2008). The best way to prevent similar errors from happening again is to report them, i.e. create experiential learning systems to identify their causes. Although this approach is widely used in the water sector, it is important to note that classification systems work better when they are limited to a specific field/stage/phase (e.g. pre-analytical, analytical, and post-analytical phases). In this work, therefore, a system for reporting and learning errors is presented, with the aim of describing and preventing those that occur when sampling water for human consumption. Indeed, sampling is an important stage in a water quality control program as it can affect results if the sample is not representative of the water being controlled. The sampling of water for human consumption involves four main steps, i.e., collection, conditioning, preservation, and transport according Figure 5. The water samples are delivered to the laboratory for analysis, and the sampling technician is responsible for collecting a valid and representative sample (Li & Migliaccio, 2011).

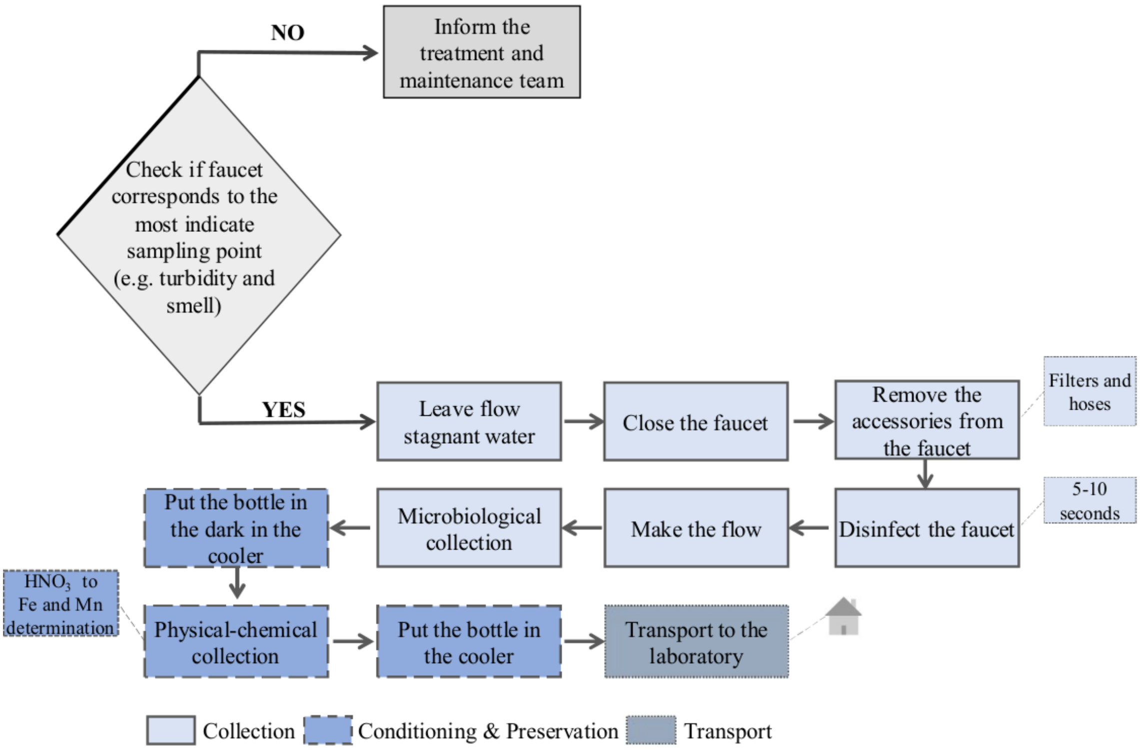

Figure 5 – The main steps in sampling water for human consumption.

Due to the increasing importance attributed to the representativeness of the sampling, greater emphasis was putted on the adequate collection, conditioning, preservation, and transport of the samples. Therefore, it is advisable that the laboratories help to plan a sampling program in partnership with the customers. This partnership is essential to ensure that the selection of samples is adequate to minimize errors and to correspond to the needs of the consumer (Nollet & Gelder, 2014). At this point it is important to reiterate that the main goal of water analysis is to aid the decision-making process.

Thus, the reliability of the decisions depends on the uncertainty of the experimental results. If the uncertainty is underestimated wrong decisions can occur with negative consequences for health, environment, and financial issues, just to name a few. Indeed, the errors that occur during the water analysis process are difficult to quantify. Inadequate training, reliance on automated systems and confusing software resources are some of the relevant issues behind the errors that may occur (Reason, 2000). Knowledge is crucial to solve the problems of the economy and society. In everyday situations, however, the information is often incomplete, inaccurate, uncertain, contradicting and even unknown. On the other hand, existing models are built based on some idealizations that remove these real-world properties. The result is a system that, due to its inability to model the world or universe of discourse, never delivers the expected answers (Parsons, 1996).

In the water sector, particularly regarding sampling errors, there are many situations where the information available on errors is insufficient or ambiguous. The system proposed in this work is based on the Eindhoven Classification Model (ECM) and focuses on avoiding the causes of errors by applying a model specially developed for the sampling phase. This system aims to record the nonconformities, errors, and adverse events. In addition, there should be a learning system that enables data analysis to ensure the continuous improvement of drinking water quality and the promotion of public health.

The ECM was set up to address human error in the chemical process industry and has then been applied in different areas like the steel industry, power generation, healthcare, water distribution or public administration (Henneman et al., 2006; Raab et al., 2006; Simmons & Graves, 2008; Rodrigues et al., 2011; Vicente et al., 2015; Fernandes et al., 2019). The ECM contains two types of errors, namely human or active errors and the latent ones. Regarding human error, the ECM incorporates Rasmussen's Skill-Rule-Knowledge framework, which includes three levels of behavior, i.e., the competence-based, the rule-based and the knowledge-based one (Rasmussen, 1976). In the case of latent errors, ECM differentiates between technical and organizational errors (van der Schaaf, 1995). The former one occurs when there is an obstacle associated with physical components (e.g. devices, physical installations), while the latter is associated with protocols, procedures, or knowledge transfers.

II.2.2. Related Work

The need for accurate predictions of water quality has encouraged researchers to develop new methods and improve the predictive capabilities of traditional ones. On the other hand, the potential of artificial intelligence based problem-solving methods has also been recognized significantly in the water industry. Several studies in the literature illustrate the application of these tools to quality water control, but very few relate to the drinking one. Indeed, water quality modeling is a powerful tool for studying, describing, and predicting the ecological status of an aquatic ecosystem. Wang et al. (2019) developed an artificial intelligence-based system called the *Integrated Long Short-Term Memory Network* that uses cross-correlation and association rules to identify the properties of water pollutants and track industrial point sources of pollutants.

Forio et al. (2017) analyze the effect of the major environmental variables on predicting ecological water quality, using fuzzy models. The optimal model was selected based on the predictive performance, ecological relevance, and interpretability. Morales-Torres et al. (2016) presented a study about the use of sustainable drainage systems to manage urban runoff, aiming to contribute to environmental and landscape improvement. The authors developed a tool to analyze the impact of storm water management in the urban environment and introduced energetic and environmental criteria in the decision-making process. Stefanovic et al. (2015) developed a web-based system to manage the Serbian reservoirs. The authors created a software that brings together all the pertinent actors, processes, data sources, and applications. The software allows to test different organizational scenarios, due to its flexibility, extensibility, and the fact that it could be customized. Allan et al. (2013) studied the effects of regulation, proprietorship, and business culture on the risk management within the water sector. The authors stress that a paradigm shift is necessary. The water sector should move from a reactive to a pro-active risk management culture based on knowledge. However, the authors state that there is a gap in the understanding of the drivers required to carry out such a change. Pearson et al. (2010) presented a decision support system to support managers in the urban water sector. The proposed system aims to shift the decision-making from the conventional standards to a sustainable, inclusive, and dynamic paradigm, anchored by social learning and commitment. The authors stressed the basic units of social learning, i.e., knowledge transfer for transformation, monitoring and evaluation of the decision process and stakeholder engagement.

II.2.3. Methods

An adjusted version of the ECM was conceived, with the extensions and adaptations for the water sampling scenarios, as well as the causal trees that describe the root causes of errors. The data used in this work were obtained during 1^{st} semester of 2019, in internal audits carried out at water laboratories within the scope of ISO/IEC 17025:2017 quality accreditation. Checklists were used to record the non-conformities. In the checklists, the verified observations are organized according to the general and specific requirements of the ISO/IEC 17025 standard. The non-conformities were classified into *major non-conformity*, *minor non-conformity*, and *opportunity for improvement*, and in terms of the ECM, are referred as adverse events or errors.

The formal approach of the proposed errors reporting system in water sampling is based on the Logic Programming (LP) paradigm for problem solving and set according to an extension to the LP language (Neves, 1984). Undeniably, there are many approaches to knowledge representation and reasoning using the epitome of LP, namely in the areas of model theory and proof theory. In this paper, the proof theoretical approach for problem solving was adopted and conveyed as an extension of the LP language. Indeed, an extended logic program is grounded on a specified ensemble of clauses in the form, viz.

$$\{$$

$$\neg p \leftarrow not\ p, not\ exception_p$$

$$p \leftarrow p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m$$

$$?\,(p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m)\ \ (n, m \geq 0)$$

$$exception_{p_1},\ \cdots\ , exception_{p_j}\ \ (0 \leq j \leq k),\ \ being\ k\ an\ integer\ number$$

$$\}$$

Program 1 – The archetype of an extended logic program.

The first clause denotes predicate's closure, "," designates "*logical and*", while "*?*" is a domain atom denoting "*falsity*", the p_i, q_j, and p are classical ground literals, i.e., either positive atoms or atoms preceded by the classical negation sign $\neg$. Indeed, $\neg$ stands for a strong declaration and speaks for itself, while not denotes *negation-by-*

failure, i.e., a failure in proving a certain statement since it was not declared in an explicit way. According to this way of thinking, a set of abducibles are present in every program (Neves, 1984). In this work are given in the form of exceptions to the extensions of the predicates that make the program, i.e., clauses of the form, viz.

$$exception_{p_1}, \ \cdots \ , exception_{p_j} \ (0 \leq j \leq k), \ \ being\ k\ an\ integer\ number$$

that denote data, information or knowledge that cannot be ruled out. On the other hand, clauses of the type, viz.

$$?\,(p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m) \ \ (n, m \geq 0)$$

are invariants that make it possible to specify the context under which the universe of discourse should be understood (Neves, 1984).

II.2.4. Results and Discussion

Table 1 lists the adverse events recorded during 1st semester of 2019, as well as the frequency of occurrence. A perusal of Table 1 reveals that 128 adverse events occurred. Considering the general requirements of the ISO/IEC 17025 standard, 28.9% of the occurrences are related *Resource Requirements*, 53.9% are associated with *Processes Requirements*, whereas 17.2% are linked to *Management System Requirements*. In terms of non-conformities, 81.2% were classified as *minor non-conformity* (*N*) and 18.8% corresponds to *major non-conformity* (*M*).

Considering the data presented in Table 1, it can be argued that the sample-related adverse events occur much more frequently than the others, which requires special attention.

II.2.4.1. The Adjusted version of the Eindhoven Classification Model for Water Sampling

In order to isolate a customized version of the ECM for a particular problem, it is of the utmost importance to identify all the causes that lead to such an undesirable event. To adapt the ECM to the problems related to the sampling of water for human consumption, new dimensions have been considered. These dimensions aim to adjust the original model to sampling context and supply a general view of the events that can happen. The

Adjusted version of ECM for Water Sampling (A-ECM-WS) follows the dimensions *Technical*, *Organizational*, *Human Behavior*, and *Other* presented in Table 2.

Table 1 – Frequency of occurrence of adverse events, during 1st semester of 2019.

General Requirements	Specific Requirements	Description	Classification	Frequency	Total
Resource requirements	Facilities and environmental conditions	Laboratory facilities are not adequate (e.g., no separation between incompatible testing areas.	M	2	7
		The laboratory did not formalize the facilities and environmental conditions.	N	5	
	Metrological traceability	The laboratory did not formalize the methodology for estimating uncertainties.	N	7	22
		The calculation of the uncertainty estimate for the temperature test was not shown.	N	9	
		The calculation of the uncertainty estimate for free and total residual chlorine was not shown.	N	6	
	Equipments	The laboratory did not show records of annual visual inspection of the volumetric glass material.	N	8	8
Process requirements	Nonconforming Work	The methodology for nonconforming work is not formalized.	M	10	10
	Selection, verification, and validation of methods	The laboratory has not formalized the requirement methods/procedures for testing and validating methods.	N	5	9
		The laboratory did not formalize the methodology for the implementation of the test methods.	N	4	
	Sampling	Sampling technician failures were found (e.g., failure in disinfection).	N	12	50
		It was found that in the procedure there were deficiencies in the location of the sampling point.	N	6	
		It was found that inappropriate bottles were being used to carry out the sampling.	N	12	
		It was found failures in preserving of samples.	N	10	
		Transport failures were noted (e.g. agitation during transport, time between collect, transport and testing)	N	10	
Management system requirements	Documentation	Documentation control is neither adequate nor formalized.	M	12	22
		The external documents to be controlled are not defined.	N	10	
Adverse Events Registered					128

M – Major Non-Conformity, N – Minor Non-Conformity

Table 2 – Categories of the adjusted Eindhoven classification model for water sampling and the corresponding codes.

Category	Description	Code
Technical Dimension		
External	Technical fault outside the control and responsibility of the company.	TEX
Design	Faults caused by inadequate design of equipments, software, tags, or templates.	TD
Construction	Construction faults regardless of a right design.	TC
Materials	Material deficiencies not categorized as TD or TC.	TM
Reagents	Faults caused by the lack or poor quality of chemicals.	TR
…	…	…
Organizational Dimension		
External	Faults at an organizational level outside the control of the company.	OEX
Transfer of Knowledge	Faults due to inadequate decisions that do not guarantee that the knowledge is shared with inexperienced employees.	OK
Protocols	Faults due to the quality/availability of the internal procedures (excessively intricate/simple, imprecise, or non-existent).	OP
Management Priorities	Internal choices in which safety is transferred to a lower position, given priority to production.	OM
Culture	Faults due to the collective attitude towards risk and behaviors within the company.	OC
…	…	…
Human Behavior Dimension		
External	Human faults that have its origins outside the control of the company.	HEX
Knowledge-Based Behavior		
Knowledge-Based Errors	The disability of a member to put in practice current knowledge in a new situation.	HKK
…	…	…
Rule-Based Behavior		
Qualifications	Inappropriate fit among the task to be performed and the employee's training, qualifications, or education.	HRQ
Coordination	Deficient task coordination (e.g., a fundamental task not fulfilled because the team was convinced that someone performed it).	HRC
Verification	Faults in the accurate and full assessment of the set of circumstances before starting the execution of a specific task, covering the conditions and materials and/or equipment to be used.	HRV
Intervention	Faults that arise from defective preparation of a task and/or bad implementation.	HRI
Monitoring	Faults that occur during the monitoring of an activity or process.	HRM
…	…	…
Skill-Based Behavior		
Slips	Fault in performing a task related with the operator's lack of fine motor skills.	HSS
…	…	…
Other		
Technicians Related Factor	Faults associated to physical and/or psychic conditions of the employee that affect the task execution and are outside the control of the company.	TRF
Consumers Related Factor	Faults associated to consumers' conduct that can affect the water quality and are outside the control of the company.	CRF
…	…	…
Unclassifiable	Faults that cannot be included in the previous categories.	X

Table 2 also shows the categories includes in each dimension, as well as a brief description and the corresponding codes. To illustrate the type of adverse events that can be included in each code, Table 3 presents a few examples. Thus, based on Table 2 and Table 3, the systematization of the causes that lead to an adverse event becomes straightforward and effective, being processed according to the flow chart presented in Figure 6. For instance, an adverse event assigned to the category *Organizational Dimension – Protocols* (*OP*) occur due to the quality/availability of the internal procedures. The events assigned to this category arise from difficulties in execution or interpretation of unclear protocols that can lead to adverse events such as non-flow of stagnant water or failure to remove the faucet accessories.

The ECM make use of Root Cause Analysis to classify the adverse events through codes established in advance (van der Schaaf, 1995). Thus, beyond the classification framework presented above, the Causal Trees (CTs) regarding each adverse event should be conceived. The CTs can be considered as a hierarchical representation of the adverse event, allowing to identify the circumstances that lead to its occurrence (van der Schaaf & Habraken, 2005). The original version of the ECM model just comprises cases for which the causes of adverse events are well known. This fact should be a limitation, since in many everyday situations, information about errors and adverse events can be incomplete, unknown, or even contradictory. To include the uncertainty that is always present in real situations, in the present work, the *unknown* and *forbidden* operators were considered in the conception of the extended causal trees.

Table 3 – An excerpt from the code set of the adjusted Eindhoven classification model for water sampling and examples of possible adverse events.

Code	**Extension to water sampling**	**Examples**
TR	Faults caused by the lack or poor quality of chemicals.	Use reagent out of date.
OP	Very complicated, inadequate, or missing protocols. Protocols not disclosed to the team.	Non-conformity of protocols with various negative effects (e.g., non-flow of stagnant water in the duct section, do not remove accessories outside the tap).
HEX	Human faults outside the control of the company.	Excessive time between sampling and delivery to the laboratory
HKK	Do not put on the preservative or choose the wrong preservative.	Do not add HNO_3 in the samples for the determination of iron and manganese.
HRI	Failure in task planning or during its execution.	Did not disinfect the hands before sampling, did not use gloves, did not use the blowtorch correctly, did not choose a tap under normal conditions of conservation and hygiene.
HRM	Faults that occurred during the monitoring of a task.	Failure to calibrate the data logger used inside the thermal bags.

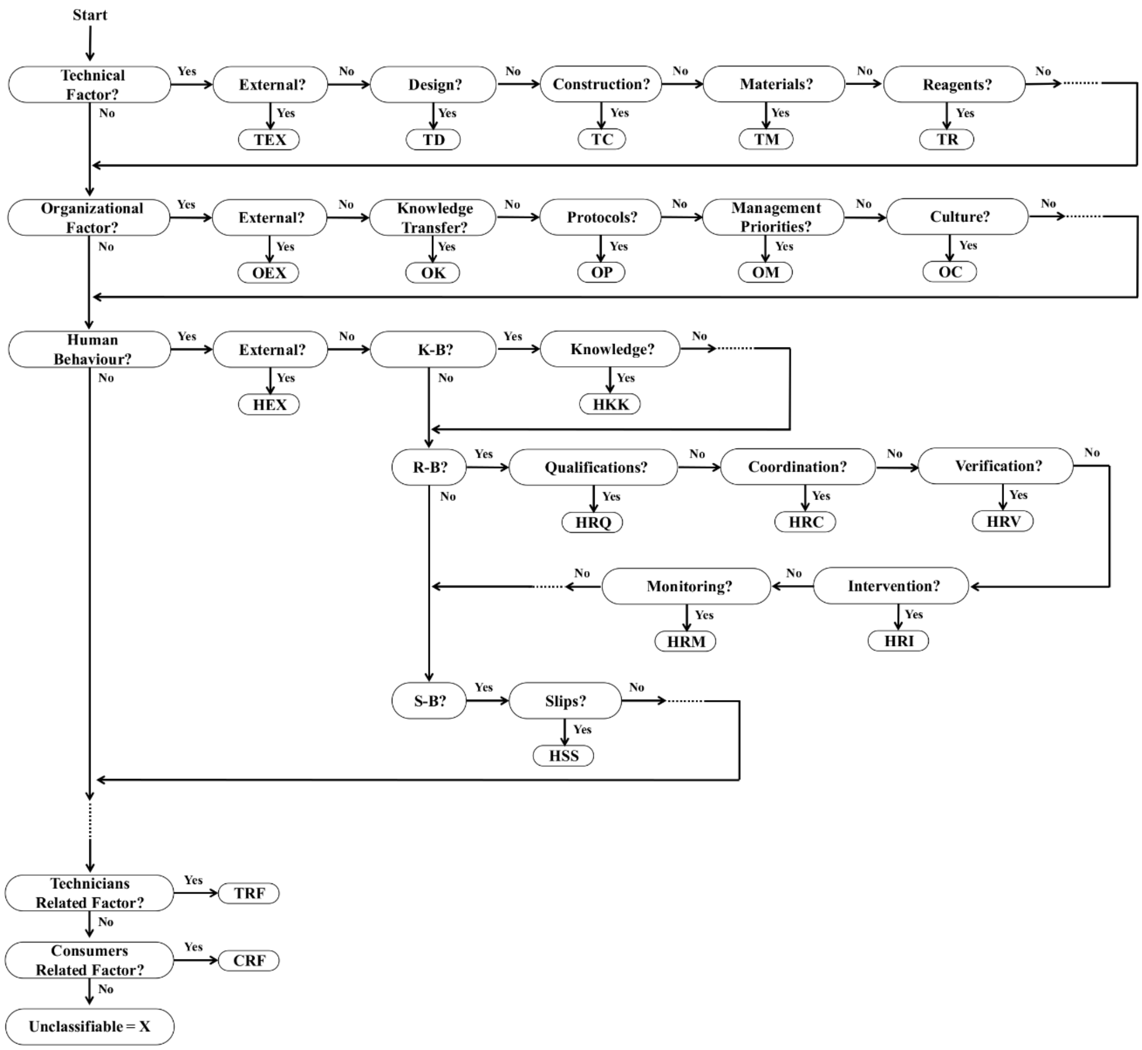

Figure 6 – The adverse event classification process.

From the non-conformities recorded during 1st semester of 2019 it is feasible to specify the actions and causes that contribute to the occurrence of the adverse event "*Failure in Sampling*". The Extended Causal Tree (ECT) presented in Figure 7 was established with collaboration of sampling technicians. The ECT was subject of an in-depth study before reaching the final structure. The ECT contain the feasible causes, being a symbolic depiction of the problem. Each branch of the ECT describes the causes of a particular adverse event.

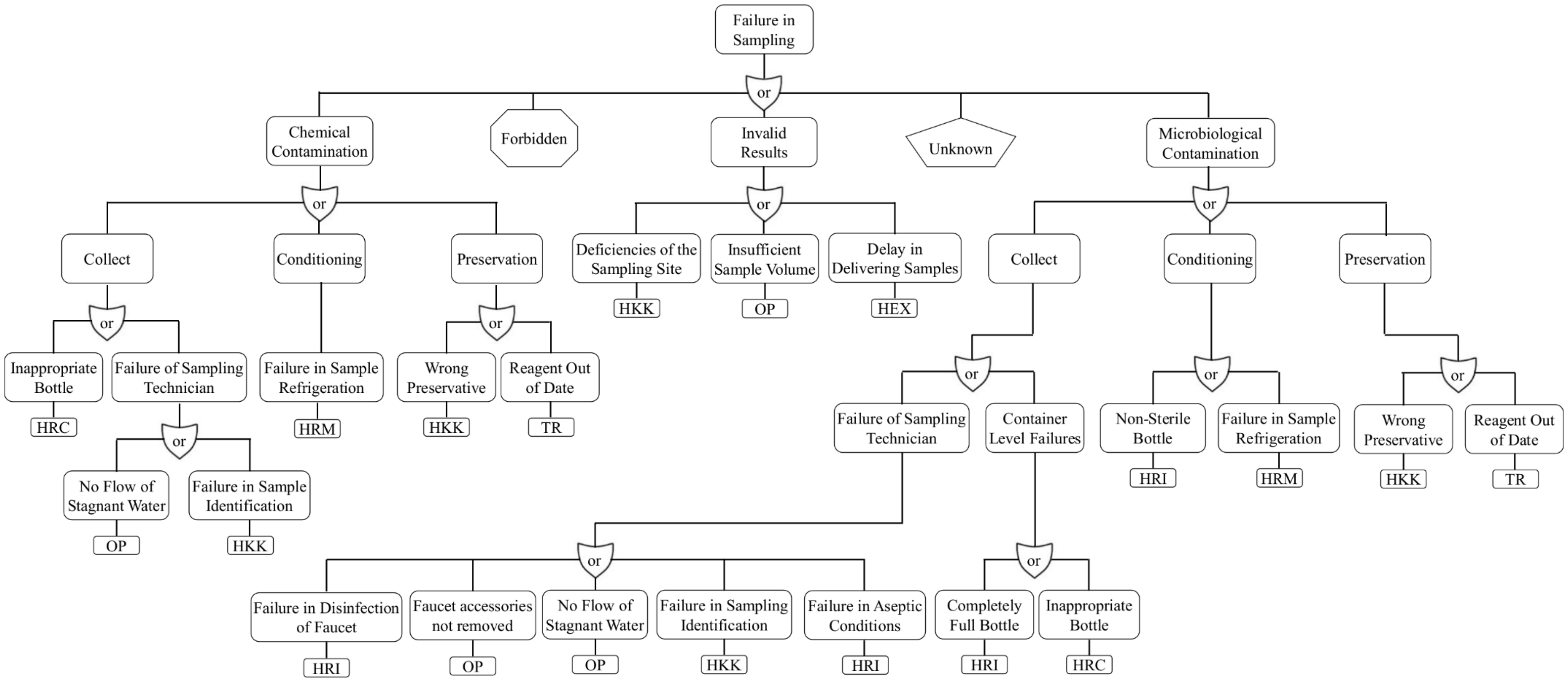

Figure 7 – The Extended Causal Tree regarding the adverse event “*Failure in Sampling*”.

II.2.4.2. The Computational System

To illustrate the operating mode of the A-ECM-WS, the undesired event "*Error in Sampling*" and the respective causal tree (Figure 7) are considered. Taking into account that the adverse event can emerge by several causes that should be considered simultaneously or separately, *AND/OR-nodes* were incorporated in the causal tree. Furthermore, the operators "unknown" and "forbidden" were also added to express events for which the causes are unknown, forbidden, or not permitted. Therefore, considering the information available in Figure 7, different scenarios can be examined, viz.

- Scenario *A* – The "Failure in Sampling" was due to microbiological contamination caused by the non-removal of the faucet accessories;
- Scenario *B* – The "Failure in Sampling" was due to chemical contamination caused by failure in sample preservation;
- Scenario *C* – A "Failure in Sampling" has occurred. The causes behind the event were not recorded; and
- Scenario *D* – A "Failure in Sampling" has occurred. The causes of the adverse event were not recorded due to internal rules of the company.

Regarding scenario *A*, the cause of the adverse event was recorded, corresponding to a known value. Scenario *B* corresponds to a situation in which the cause that led to the adverse event is unknown. However, it is possible to lay down a finite set of causes that can lead to its occurrence, configuring a situation of an unknown value in a finite set of values (two in the this example, wrong preservative or reagent out of data). In scenario *C* the occurrence of the adverse event was recorded but nothing is known about their causes, corresponding to an unknown value. Finally, scenario *D* involves a forbidden or a not allowed valued, since it is not permitted to know the causes of the adverse event.

The four scenarios described above can be depicted in Program 2, following the archetype presented in Program 1, in terms of the extent of predicate ***a****dverse_****e****vent_****c****ause* (*aec*), viz.

{

{

/ The following sentence denotes that the extent of the predicate $aec_{scenario\ A}$ is based on the explicitly specified clauses and those that cannot be dropped, i.e., the exceptions */*

$$\neg\ aec_{scenario\ A}\ (X) \leftarrow not\ aec_{scenario\ A}\ (X),$$

$$not\ exception_{aec_{scenario\ A}}\ (X).$$

/ The following sentence stands for an axiom of $aec_{scenario\ A}$ */*

$$aec_{scenario\ A}\ \ (failure\ in\ desinfection\ of\ faucet).$$

}

{

/ The following sentence denotes that the extent of the predicate $aec_{scenario\ B}$ is based on the explicitly specified clauses and those that cannot be dropped, i.e., the exceptions */*

$$\neg\ aec_{scenario\ B}\ (X) \leftarrow not\ aec_{scenario\ B}\ (X),$$

$$not\ exception_{aec_{scenario\ B}}\ (X).$$

/ The following sentence stands for adbucible axioms of $aec_{scenario\ B}$ */*

$$exception_{aec_{scenario\ B}}\ \ (wrong\ preservative).$$

$$exception_{aec_{scenario\ B}}\ \ (reagent\ out\ of\ data).$$

}

{

/ The following sentence denotes that the extent of the predicate $aec_{scenario\ C}$ is based on the explicitly specified clauses and those that cannot be dropped, i.e., the exceptions */*

$$\neg\ aec_{scenario\ C}\ (X) \leftarrow not\ aec_{scenario\ C}\ (X),$$

$$not\ exception_{aec_{scenario\ C}}\ (X).$$

/ The following sentence stands for an adbucible axiom of $aec_{scenario\ C}$ */*

$$exception_{aec_{scenario\ C}}\ \ (unknow).$$

}

{

/ The following sentence denotes that the extent of the predicate aec*$_{scenario\ D}$ *is based on the explicitly specified clauses and those that cannot be dropped, i.e., the exceptions */*

$$\neg\, aec_{scenario\ D}\ (X) \leftarrow not\ aec_{scenario\ D}\ (X),$$
$$not\ exception_{aec_{scenario\ D}}\ (X).$$

/ The following sentence stands for an invariant with respect to predicate aec*$_{scenario\ D}$ **/*

$$?\ aec_{scenario\ D}\ (X), not\ null_{scenario\ D}(X).$$

/ The following sentence denotes that the extent of the predicate null is based on the explicitly specified clauses and those that cannot be dropped, i.e., the exceptions */*

$$\neg\, null_{scenario\ D}\ (X) \leftarrow not\ null_{scenario\ D}\ (X),$$
$$not\ exception_{null_{scenario\ D}}\ (X).$$

/ The following sentence stands for an axiom of null's predicate */*

$$null_{scenario\ D}\ (forbidden).$$

}

}

Program 2 – Structure of the logic program in relation to scenarios *A*, *B*, *C* and *D*.

In decision-making processes, it is necessary to consider only the most promising answers. Thus, each answer must be tested in terms of its ability to adapt to dynamic environments (i.e., environments that are constantly updated) to choose the most appropriate action from a wide range of alternatives. The optimal response, in terms of LP paradigm, is a logic program or theory that models the universe of discourse, maximizing the Quality of Information (Vilhena et al., 2016; Coelho et al., 2017). The Quality of Information (*QoI*) with respect to a generic predicate *p* can be analyzed in four situations and can be measured in the interval [0, 1]. Regarding cases in which the information is known the *QoI* for the extension of predicate *p* is 1. For occurrences where the information is unknown, the *QoI* is given by, viz.

$$QoI_p = \lim_{N\to\infty} \frac{1}{N} = 0, \qquad (N \gg 0)$$

where *N* stands for the number of terms or clauses of the extension of predicate *p*. For cases in which the information is unknown but can be selected from a set of possible values, although only one can be considered, the *QoI* is given by, viz.

$$QoI_p = {}^{1}/_{Card}$$

being *Card* the the cardinality of the set of exceptions of *p*. If more than one value can be considered, the *QoI* is given by, viz.

$$QoI_p = {}^{1}/_{(C_1^{Card} + C_2^{Card} + \cdots + C_{Card}^{Card})}$$

where C_{Card}^{Card} is a card-combination subset, with *Card* elements (Vilhena et al., 2016; Coelho et al., 2017).

The information included in ECT was depicted in terms of LP paradigm through the extensions of a predicate set (Program 2), which make possible to evaluate the *QoI* regarding each of the scenarios described above. In the case of scenario *A* there is no doubt about the cause of the adverse event. The sampling failure was caused by the non-removal of the faucet accessories, being *QoI* equal to 1 (one). In the scenario *B* the cardinality of the set of exceptions of the predicate is 2 (two), i.e., the usage of a wrong preservative or an out of data reagent, being the *QoI* is equal to 1/2. Finally, in the scenarios *C* and *D* it is known that the adverse event took place, but its causes are unavailable. Any value presented in ECT can be assumed as a feasible solution and the *QoI* is 0 (zero).

Using the formal approach based on the LP paradigm mentioned above, an Adverse Event Reporting and Learning System related to Water Sampling (AERLS-WS) was developed. In addition to recording adverse events, the AERLS-WS is an information management system that provides a knowledge base where it is possible to use data mining tools. Thus, the AERLS-WS includes three main modules as shown in Figure 8. The Reporting Forms Module (RFM) allocate the web interface that allows the registration of the adverse events. The record can be carried out by any laboratory employee, regardless of the department, by way of pre-defined forms adapted to each user profile (e.g., sampling technicians, chemical/microbiological technicians, technical managers, management team). Bearing in mind what just been mentioned, the focus in the development of this interface was its usability.

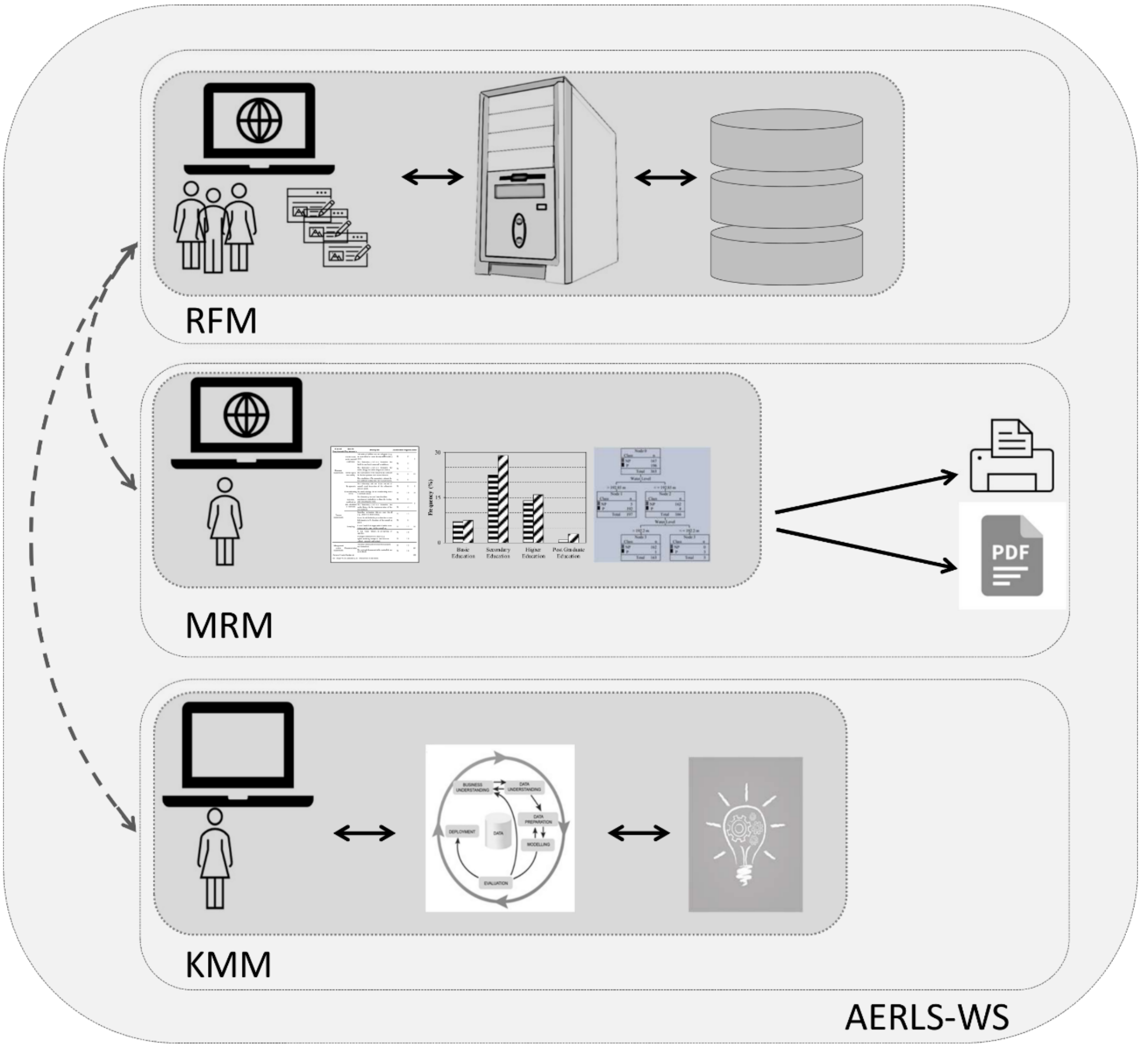

Figure 8 – A global view of the Adverse Event Reporting and Learning System related to Water Sampling (AERLS-WS).

The Manager Reports Module (MRM) is equally a web interface. It intends to make possible the analyse the adverse events previously recorded in the RFM, having subjacent the A-ECM-WS. The A-ECM-WS allows that the system provide suggestions for improvements to minimize/eliminate the organization failures. Thus, the system can issue automatically individual reports for the adverse events recorded, as well as its details in terms of branches of the ECT. The improvement suggestions contained in the reports are due to the methodology followed that combines adjusted version of ECM for water sampling and LP to knowledge representation and support the reasoning mechanisms. The central point of these reports are the event causes. The system's reports are essential to ensure quality to laboratory results, since the time and resources required to study the causes of the events, to make inferences, and to establish patterns and trends are substantially reduced. In this way, this task (which is usually time consuming) can be performed timely contributing to avoid/mitigate failures. In addition, once the data are stored in the same database, they are always available for further studies. The MRM can provide updated information about the impact, occurrence, and type of events recorded. The user can choose how the information is displayed (e.g., bar charts, pie charts, tables, tree diagrams). Based on the system's reports the user can have information about the contribution of each possible action/cause to the adverse event. It should be noted that the actions/causes were identified by the system automatically, considering the A-ECM-WS and the ECTs.

Lastly, the Knowledge Manager Module (KMM) is a Java application. This module makes use of the records stored in the database to generate a knowledge base, from which other relevant studies (e.g., through the use of data mining tools) aiming to optimize the sampling procedures.

II.2.5. Conclusions

To achieve accurate results in water analysis is essential that the sampling stage is carried out correctly. Thus, this work presents an adverse event reporting and learning system, developed specifically for the sampling phase, that aims to improve the quality of drinking water and therefore contribute to the promotion of public health. The key contribution of this work is related with the quantification of the Quality of Information imbedded in Causal Trees and to address the issues regarding incomplete information using the Logic Programming paradigm. The proposed approach allows to identify in advance the causes that lead to adverse events, enabling the establishment of action plans to avoid or, at least, minimize them. The construction of the causal tree for a particular event be often time-consuming and difficult, once it requires the development of the branches regarding to each possible cause. However, after this stage being overcomed, the process of classification and analysis of adverse events becomes very fast and easy. The computation of the Quality of Information enables the ranking of possible causes and, therefore, to identify the ones that should be prioritized. Consequently, in the construction of the causal tree, it is mandatory to look for all possible causes, not only the most probable or the usual ones.

The adverse event reporting and learning system presented allows knowledge extraction, i.e., the identification of the main failure causes, possible trends, areas requiring improvement plans or changes in procedures. The automatic reports generated by the system are reliable. In fact, the quantification on-the-fly of the Quality of Information of the logic terms used in the process of judgement (given in terms of a theorem to be proved) minimizes user participation, which is only necessary to approve the recommendations. One of the main advantages of the proposed system has to do with its modularity. This feature allows one to update the system at any time (e.g., add new categories, subcategories and/or causal trees) without changing its structure or way of functioning.

II.3. Draw on Artificial Neural Networks to Assess and Predict Water Quality

II.3.1. Introduction

Water management is not only a quantitative problem that is embedded in its biogeochemical cycle, but also a qualitative one. Water is important to ensure the sustainability of life, and given its meaning for health, it is mandatory to ensure its quality. The quality assessment of water bodies implies the knowledge of a large set of parameters used to indicate its suitability for different purposes (e.g., drinking water production, irrigation). Water quality can be expressed by indicating the condition (i.e. dissolved or particulate) and the concentration of inorganic and organic substances present as well as some water-physical properties (Bagchi, 2013). The water quality is assessed using analysis methods carried out in situ and in the laboratory. This process involves several steps, such as taking, preserving, and transporting samples. In addition, it is still necessary to consider the time that has elapsed since the time of sampling and the completion of the laboratory analyzes as well as the financial resources expended. To maintain water quality in real time, developing computational models grounded on methodologies from Artificial Intelligence scientific area can be an alternative to water quality assessment. The Chemical Oxygen Demand (COD) and the Biochemical Oxygen Demand (BOD) enable to quantify the organic matter present in water. Some organic substances can be directly responsible for unpleasant colors and aromas or for the development of organisms from which they originate (Alley, 2000). Organic matter can be of biological origin (e.g. proteins, fats, and sugars) and/or due to anthropogenic activities. COD and BOD are criteria for controlling pollution and indicators of chemical and/or bacteriological contamination that can pose a threat to water consumers. COD can be defined as the amount of a particular oxidizer that reacts with the sample under controlled conditions. The BOD in turn measures the molecular oxygen consumption in a certain incubation period (five days) for the biochemical degradation of organic material (Alley, 2000). This work aims the development of models grounded on artificial intelligence techniques for problem solving, particularly ANNs (Haykin, 2009), to predict BOD and COD based on pH, Dissolved Oxygen (DO), conductivity and water temperature.

In last decades, several studies have been published demonstrating the effectiveness of ANNs in the prediction of surface water quality variables. In this context Maier & Dandy (2000) present several case studies published in literature from 1992 to 1998. Chen et al. (2019) compared the types and the use of ANNs taking into account the direction of the information flux, classifying them into feed-forward, recurrent and hybrid networks, and discussing the pros and cons of each different types of ANNs. Regarding the problems addressed, the prediction of salinity (Maier & Dandy, 1996; 2000), oxidability, total suspended solids (Vicente et al., 2012a), nitrate, manganese (Vicente et al., 2012b), dissolved oxygen (Palani et al., 2008; Sing et al., 2009; Ahmed, 2017), BOD (Sing et al., 2009) or COD (Ruben et al., 2018) stand out.

This paper is divided into four sections. After the introduction, a new section is presented that describes the materials and methods used in this study. Section II.3.3 shows how data is processed and the results obtained are discussed. The last section draws conclusions and outlines future work.

II.3.2. Materials and Methods

This study was conducted at four dams located in the south of the district of Setúbal (southern Portugal). The Dams of Daroeira (37º 54' 20.2" N, 8º 19' 27.0" W), Fonte Serne (37º 52' 54.0" N, 8º 29' 51.4" W) and Campilhas (37º 50' 37.4" N, 8º 37' 8.9" W) are located at the municipality of Santiago do Cacém while Morgavel dam (37º 54' 8.8" N, 8º 45' 49.3" W) is in the municipality of Sines (Figure 9).

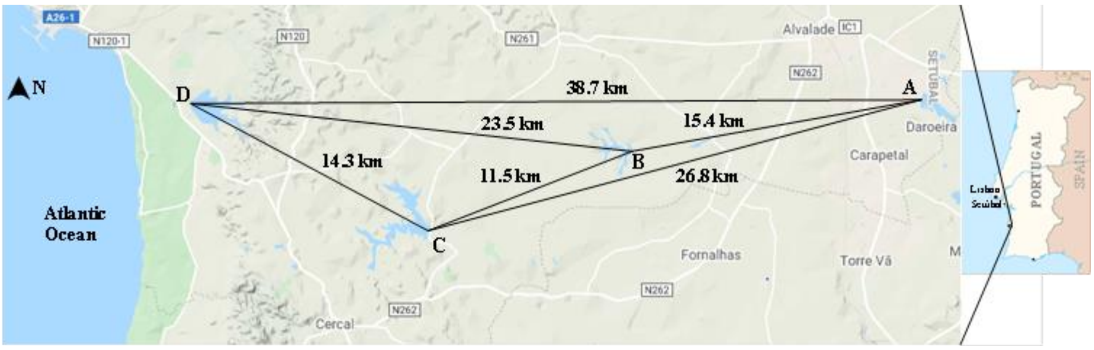

Figure 9 – Geographical localization and distances between the dams where this study was conducted. **A** – Daroeira, **B** – Fonte Serne, **C** – Campilhas and **D** – Morgavel dams. Source: *Google maps*

Sampling was carried out between September 2005 and December 2017. Water Temperature, pH, DO, and Conductivity were evaluated in situ while BOD and COD were analyzed in lab.

II.3.2.1. Sample Collection and Preservation

The analytical control of water quality begins with sampling once a month (12 times a year) in the morning. The sampling procedures were conducted taking into account the recommendations presented in Standard Methods for the Examination of Water and Waste Water (SMEWW) (Baird et al., 2017). For in situ determinations 50 cm^3 wide-mouth polyethylene flasks were used, while 100 cm^3 polyethylene flasks were used to collect the samples for COD analysis. Sulphuric acid (until $pH<2$) were added as preserving agent. Finally, for the BOD determination 1000 cm^3 polyethylene flasks were used. The samples were transported in thermal bags containing ice accumulators. To ensure that the samples were not exposed to temperatures higher than those in the collection, a Data Logger, programmed to take minute-by-minute measurements, was placed in the pouch to record the temperature during transportation.

II.3.2.2. Analytical Procedures

The water analyzes were carried out in a water laboratory accredited according to the ISO/IEC 17025. The pH, DO, Conductivity, Water Temperature, BOD and COD evaluation were carried out in accordance with SMEWW 4500-H+ B, SMEWW 4500-O B, Portuguese version of European Standard 27888: 1996, SMEWW 2550 B, SMEWW 5210 B and SMEWW 5220 B (Baird et al., 2017).

II.3.2.3. Artificial Neural Networks

ANNs are computing tools designed to mimic the human brain and nervous system procedures. The multilayer perceptron is one of the most widespread ANNs architectures, in which neurons are disposed in layers, connected through forward connections (Haykin, 2009). In order to implement ANNs the software WEKA was used, maintaining unchanged the software set of parameters (Hall, et al., 2009; Frank, et al., 2016). Aiming to guarantee the statistical significance of the experiments, 25 replicates were realized. In each replicate the dataset was randomly split into two mutually exclusive sets. The training one, used to build the model, includes approximately two thirds of the cases. The remaining examples form the test set, used to assess the model performance.

II.3.3. Results and Discussion

II.3.3.1. Database

The database contained 605 records and 6 fields (i.e., pH, Conductivity, Water Temperature, DO, COD, and BOD). Table 4 provides a statistical view of the variables recorded in the database. A review of Table 4 allows to state that all variables, except pH, exhibit large dispersion with variation coefficients that range from 25.4% to 84.8%. Such variability may be due to the large geographical area, differences in climate, seasonal effects and the numerous water sources. The pH, in turns, shows the lowest dispersion and this fact can be justified taking into account the buffering capacity of water bodies. Nonetheless, the values presented in Table 4 are in accordance with the ones reported in several similar studies (Palani et al., 2008; Sing et al., 2009).

Table 4 – A statistical view of the database that supports this study.

Variable	Minimum	Maximum	Mean	Standard Deviation	Coefficient of Variation (%)
pH (Sørensen scale)	6.5	9.9	7.8	0.7	9.0
Dissolved Oxygen (%)	40.3	184.5	91.4	23.2	25.4
Conductivity (µS/cm)	97.9	667.9	201.2	75.9	37.7
Water Temperature (ºC)	6.2	28.7	16.0	4.7	29.3
Biochemical Oxygen Demand (mg/dm^3)	0.0	13.4	2.9	2.4	84.8
Chemical Oxygen Demand (mg/dm^3)	9.2	48.9	19.4	6.1	31.3

To evaluate the interrelationships between the variables, the Pearson correlation coefficients between the input variables (pH, DO, Water Temperature and Conductivity) and the output variables (COD and BOD) were computed (Table 5). A review of Table 5 reveals that the values of the coefficients are small and are all in the range from 0.08 to 0.43, which shows that there is no direct relationship among them.

Table 5 – Pearson correlation coefficients among variables.

Input Variables \ Output Variables	Biochemical Oxygen Demand (BOD)	Chemical Oxygen Demand (COD)
pH	0.11	0.21
Dissolved Oxygen	0.14	0.12
Conductivity	0.08	0.43
Water Temperature	0.13	0.32

II.3.3.2. Artificial Neural Networks Models

To achieve the best prediction of the variables COD and BOD, various network structures have been developed and evaluated. To assess the performance of the different networks, the Mean Absolute Error (MAE) and the Mean Square Error (MSE) were estimated. Such metrics compute the mean error but do not give any sign about the type of error. Thus, aiming to fulfil this lack of information, i.e., to estimate whether the COD and BOD values were overestimated or underestimated the average of all individual errors, known as Bias, was computed. The results obtained are present in Table 6 for the networks tested. A review of Table 6 reveals that the 4-6-5-2 ANN minimizes MAD, MSE and has a near zero Bias for both sets.

Table 6 – Mean Absolute Error (MAE), Mean Square Error (MSE) and Bias for the ANN topologies tested.

ANN Topology	Training Set						Test Set					
	MAE[a]		MSE[b]		Bias[c]		MAE[a]		MSE[b]		Bias[c]	
	BOD	COD	BOD	COD	BOD	COD	BOD	COD	BOD	COD	BOD	COD
4-15-2	1.637	5.783	50.80	6.137	0.432	-0.214	1.712	5.996	7.511	58.22	-0.523	-0.278
4-6-5-2	0.284	2.415	0.132	8.083	-0.258	0.021	0.324	2.643	0.148	9.859	0.036	0.037
4-8-5-2	1.701	7.258	6.699	82.46	0.352	-0.103	1.728	7.567	7.596	84.24	-0.367	0.201
4-10-7-2	0.523	3.925	0.561	22.78	-0.502	0.118	0.685	4.487	0.616	27.25	0.048	-0.023
4-11-10-2	1.586	5.094	5.814	38.48	0.232	0.654	1.590	5.291	5.887	46.46	0.432	-0.752
4-16-12-2	1.464	7.203	4.234	60.97	-0.298	-0.016	2.285	9.623	8.189	76.99	-0.196	0.007

[a] $MAE = \frac{\sum_{i=1}^{N}|A'_i - A_i|}{N}$; [b] $MSE = \frac{\sum_{i=1}^{N}(A'_i - A_i)^2}{N}$; [c] $bias = \frac{\sum_{i=1}^{N}(A'_i - A_i)}{N}$

where A and A' stand for measured and predict values, while N indicates the number of cases.

The ANN, which was selected to predict COD and BOD based on pH, Water Temperature, Conductivity and Oxygen Content includes a four nodes input layer, six and five nodes hidden layers and an output layer with two nodes (Figure 10).

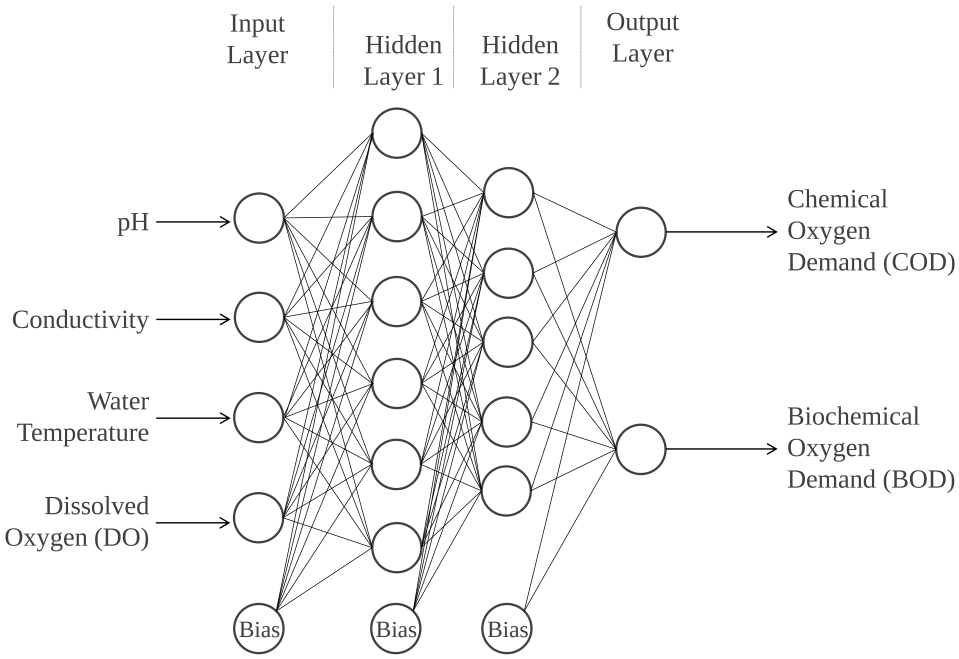

Figure 10 – Structure of the ANN selected to predict COD and BOD.

Figure 11 shows the diagrams between experimental and predicted BOD and COD values for training and test sets. The Determination Coefficient (R^2) regarding training set were 0.975 and 0.813 for BOD and COD, respectively, while they were 0.979 and 0.822 for the test set. The accordance among measured and predict values for COD and BOD, R^2, MAE and MSE (Figure 11 and Table 6) allows to state that the model fits well to the data being useful to predict the COD and BOD.

To reinforce the previous statements, Figure 12 presents the plot errors versus the ANN responses for both output variables and training and test sets. A review of Figure 12 allows to state that the relationship among errors and ANN responses shows complete independence and a random distribution for both COD and BOD. The previous statement is supported by the small values of the determination coefficients between 0.013 and 0.138. The points are well distributed above and below of the correct prediction line, i.e. the horizontal line of the ordinate zero. This type of display provides very useful information on model adaptation. Thus, when the distribution of errors is random, it indicates that the model performs well. Conversely, if a non-random distribution is discernible, the model performance is not satisfactory (McBride, 2005).

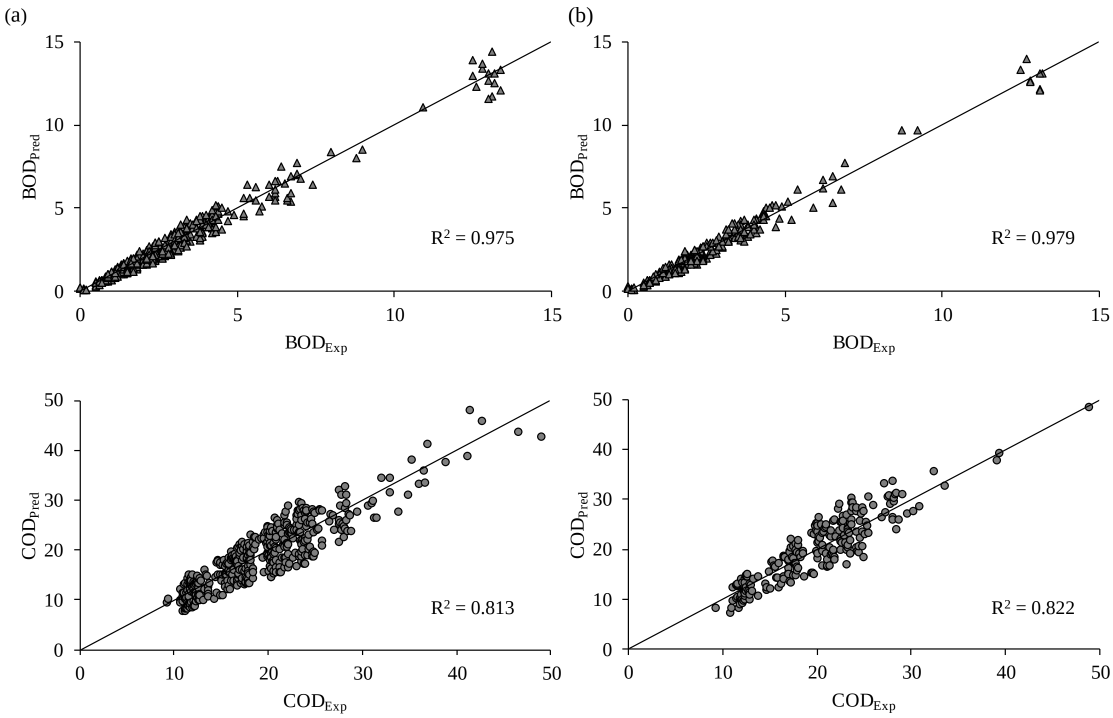

Figure 11 – Graphical representation of *ANN* responses versus measured values regarding *BOD* and *COD*. (a) Training data, (b) test data.

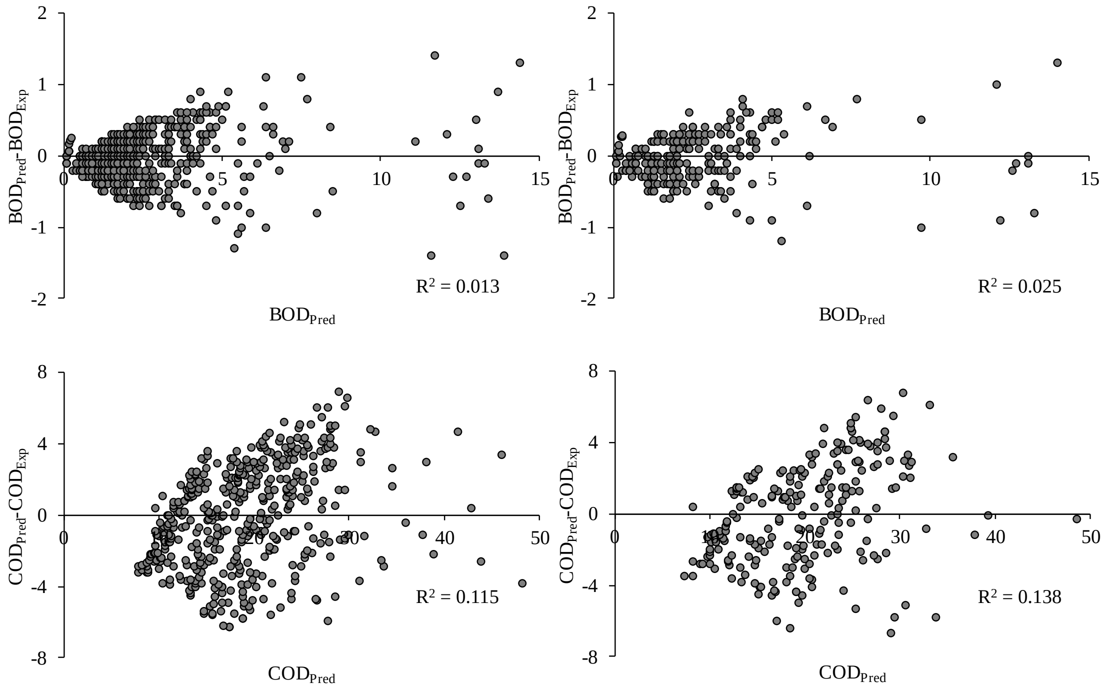

Figure 12 – Graphical representation of errors versus *ANN* responses regarding BOD and COD. (a) Training data, (b) test data.

II.3.3.3. Sensitivity Analysis

Sensitivity analysis is a process that can be used to assess the model response when the input values are changed. In the present study, the sensitivity based on variance (Maier et al., 1996; Kewley et al., 2000) was followed to evaluate the effects of each input variable on the ANN outputs. The outcomes are displayed in Figure 13 and suggest that ANN outputs are influenced in a similar way by the inputs, although the water temperature and pH have a slightly higher influence.

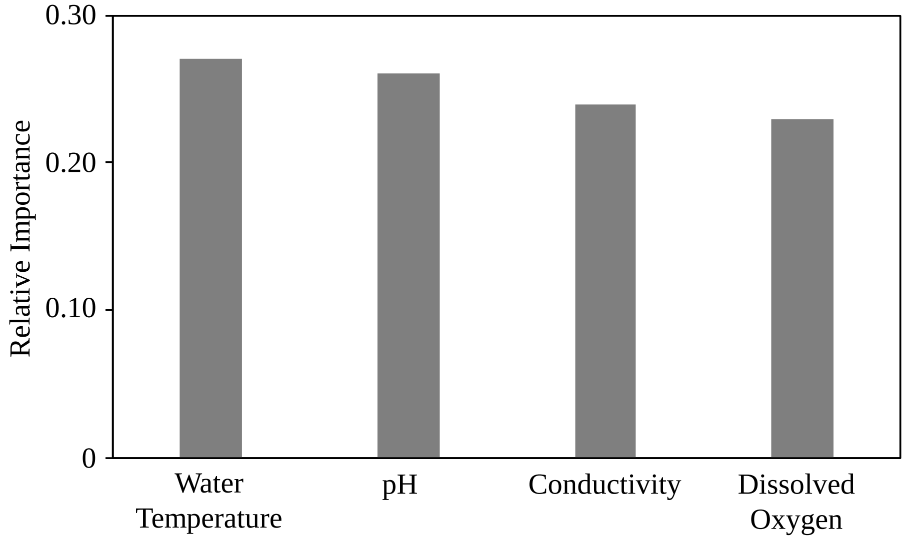

Figure 13 – Influence of each input variable on the *ANN* outputs.

II.3.4. Conclusions

This work presents an ANN model to forecast the BOD and the COD in superficial waters. Various ANNs architectures have been developed and evaluated using data collected from an accredited water laboratory in southern Portugal over a period of 17 years (from September 2005 to December 2017). The feedforward network with back propagation learning algorithm was used. The selected network exhibits a good performance in predicting of BOD and COD based on pH, Water Temperature, Conductivity and Oxygen levels and showed no overfitting. The promising results obtained in this study demonstrate the usefulness of ANNs as tools to predict water quality parameters, contributing to improve the management of the reservoirs as well as to preserve the quality of the water.

II.4. Synopsis

This chapter focused on the study of water quality control for human consumption. Water laboratories play an essential role in the health system and many decisions regarding the treatment of raw water are made considering laboratory results. In this context, failures, errors and/or bad practices can lead to serious problems that can often be devastating. The traditional form of quality control still remains in many laboratories, but increasingly, the right path seems to be to understand the process as a whole, each step and its function, in order to identify, correct and prevent adverse events. Current methods of quality control involve a large number of technical and financial resources (e.g., calibrated equipment, infrastructure, qualified technicians and reagents). Due to all this complexity, a large number of errors can occur from sampling to obtaining the final results. In this context, in the study **"Avoidance of Sampling Errors in Drinking Water Analysis – A Logical Approach to Programming"** a system was proposed that aims to avoid the main causes of errors, applying a model developed specifically for the sampling period. This system aimed to record non-conformities, errors and adverse events that occur during the collection of a sample of water for human consumption. An adjusted version of the Eindhoven classification model was designed, with extensions and adaptations for the referred scenario, as well as the causal tree associated with the adverse event "*sampling failure*". Due to the modularity of the proposed system, other types of adverse events can be explored and added whenever justified.

In addition to the sampling stage, the analytical control of water was also addressed through the study **"Draw on Artificial Neural Networks to Assess and Predict Water Quality"**. This paper presents the training and evaluation of artificial neural networks to predict, simultaneously, the biochemical and chemical oxygen demand based on the values of pH, dissolved oxygen, conductivity, and water temperature. The models were trained and tested using experimental data obtained from surface water samples used to produce water for public use and/or irrigation. The promising results of this study showed that this methodology can be particularly useful for improving water resource management and maintaining water quality.

Chapter III. Quality Management

III.1. Overview

Quality Assurance (QA) corresponds to the set of activities planned and carried out in a systematic way by companies, to demonstrate that the products/services meet the quality requirements. This can be ensured either through laboratory tests or through the evaluation of consumer satisfaction (Vieira, 2018). QA includes all activities from design, development, production, installation, maintenance, and documentation. QA cannot fully guarantee the production of quality products, but it makes it more likely. Montegomery (2019) distinguishes between the concepts of Quality Control (QC) and Quality Assurance. While the first emphasizes testing and blocking the release of defective products, QA is concerned with improving and stabilizing production to avoid or at least minimize issues that could lead to defective products. Quality Management (QM) and Quality Assurance are two associated concepts, the first being a way to guarantee quality. The second comprises the set of coordinated activities to manage and control an organization about quality (ISO 9001, 2015). QM can have three components, namely control, guarantee and quality improvement, focusing itself not only in the quality of the product but also in the ways to achieve it.

There are many methods to manage and improve quality, from continuous improvement of the product and process, to the continuous training of employees. One of the most used strategies is the Deming cycle, also known as the PDCA cycle, which incorporates the Plan, Do, Check and Act steps (Deming, 1982). Although it was developed in the 1930s by the American Shewhart, its main promoter was Deming. It is a systematic and disciplined approach to identify opportunities for improving quality and implementing lasting solutions. In the context of a quality management system and considering its dynamic character, the PDCA cycle can be applied both in each of the processes and in the organization as a whole. In addition to the above, it is also considered a problem-solving method, as each improvement goal originates from a problem that must be solved (Berlitz & Haussen, 2011). Thus, it is strongly associated with the planning, implementation, control, and continuous improvement of product realization, processes, and quality management systems. In fact, the referred cycle has some characteristics such as simplicity, operational ease, the valuation of facts, the analysis of the global problem, and the identification of the real causes of the problem. The success achieved comes from a wide applicability, as it can be used in all activities of an organization, whatever its area of intervention. This methodology has been adapted and implemented in the health area, and it is often used as a process of continuous improvement in the quality of both health care and health systems, and it can also be used in other areas (Plebani, 2006).

Considering the fundamental role that water plays in disease prevention and health promotion, issues concerning literacy in relation to the water issue relate to health literacy. Thus, citizens must have a level of knowledge and skills to support conscious decision-making, leading to changes in behaviour and ways of life, with a view to improving health both from an individual and a public perspective. As a reflection of this process, in the last decades the water sector has undergone transformations that required laboratories to restructure the business management models (Bossuyt et al, 2007). In addition to the water industry, other sectors in the health context (such as the blood and pathological anatomy sector) had to readjust and seek refuge in alliances, mergers, and partnerships, aiming at reducing the cost of analysis and optimization of efficiency indicators (Dollard et. al., 2019). In particular, the cryopreservation sector, which aims to conserve biological cells or tissues for long periods at low temperatures without losing cell viability, had to readjust itself and look for new methodologies. This technique allows stem cells (isolated from blood and umbilical cord tissue, harvested on the day of delivery), to be preserved for later clinical application. In terms of scientific credibility, stem cell treatments are still in the maturation stage, especially in the sense of achieving comparable results, even though there is already evidence of their effectiveness, namely in the treatment of haemato-oncological diseases (Slack, 2018). Over the next decade, it is expected that some stem cell therapy protocols (currently undergoing clinical trials) will become treatments for currently unresponsive diseases. The fact that these techniques show to be very promising leads to the existence of a strong pressure on workers in the sector, which can lead to the appearance of psychosocial risks that need to be studied.

This chapter aims to address quality management by presenting the following studies:

- **III.2 – Fully Informed Classification Systems – Simpler, Maybe Better[3]**
- **III.3 – A Conceptual Model to Assess the Literacy of Water Consumers[4]**

[3] Published in *Communications in Computer and Information Science*, 1038: 3–16, 2019.

[4] Submitted to *Journal of Water and Health*.

- **III.4 – Psychosocial Risks Assessment in Cryopreservation Laboratories**[5]

These studies were designed with the aim of supporting quality management departments in preventing adverse events that may occur in daily work (study III.2), checking the level of knowledge of consumers regarding water quality control (study III.3) and, finally, the assessment of the psychosocial risks to which laboratory employees are exposed, who increasingly prioritize speed, efficiency and effectiveness at the lowest possible cost (study III.4).

[5] Published in *Safety and Health at Work*, 11: 431–442, 2020.

III.2. Fully Informed Classification Systems – Simpler, Maybe Better

III.2.1. Introduction

Citizens are better informed and increasingly demanding in terms of the quality of the Public Services (PS) on offer. The development of quality management systems in compliance with the ISO 9001 guidelines ensures their efficiency and helps to increase inner and outer satisfaction (George, 2003; Chong-Fong, 2015; ISO 9001, 2015). An adverse event in this context means failure to perform a prescribed action or the use of a false plan to achieve an intended objective. The most efficient strategy for avoiding adverse events is recognizing their sources, i.e., avoiding the causes can in particular improve the quality of PS. Such causes can be related to practical problems, human relationships, policies, action plans, products, strategies, and/or leaders. People continue to learn from their own mistakes rather than from their successes. However, they do not share the appearance of glitches or what they have learned with them. So, similar mistakes can occur repeatedly, and citizens can be harmed by avoidable mistakes. Some studies have suggested that reporting may be a possible solution to this problem. The basic idea of reporting is based on the learning process based on experience. However, it is important to emphasize that the registration of errors is not sufficient to ensure the quality of the services provided. Collecting data is not enough to improve the process. Only an efficient response to adverse events may affect the change. A technical review of the data is essential to identify trends and patterns (van der Schaaf, 1995; World Alliance for Patient Safety, 2005). One answer to this limitation is the combination of an adverse event reporting system and machine learning methods to identify hazards and risks (Vicente et al., 2015). Using models to identify causes of adverse events is extremely important to ensuring the exchange of knowledge and experience. Thus, in this paper it is set the formal basis of an adverse event reporting and learning system. It will focus on preventing the causes of adverse events, therefore ensuring performance benchmarking of the organization against a standard, whether absolute or relative to others (Cowper & Samuels, 1979).

III.2.2. Computational Model

In order to avoid the occurrence of adverse events, the study of the main causes is obligatory. In order to develop systems that can be used in the PS, special attention should be given to those who describe adverse events, seek to identify their root causes and assess the outcome of the preventive measures taken. The Eindhoven Classification Model (ECM) (van der Schaaf, 1995) was chosen once it uses root cause analysis methods to classify causes based on previously defined codes. The ECM includes two types of errors, human or active and latent ones. Concerning active faults, the ECM adopts Rasmussen’s Skill-Rule-Knowledge framework, which includes three levels of behavior i.e., the skills-based, the rules-based and the knowledge-based (Rasmussen, 1976). With respect to latent errors, ECM differentiates between technical and organizational ones (van der Schaaf, 1995). The former one occurs when there are problems with physical components (e.g., equipment, physical installations), while the latter is related to protocols, procedures, or knowledge transfer operations. The starting point in the development of ECM based systems is the recognizing of the sources of a particular adverse event. Thus, in order to attain this end a causal tree was built and root cause analysis techniques applied (Figure 14), viz.

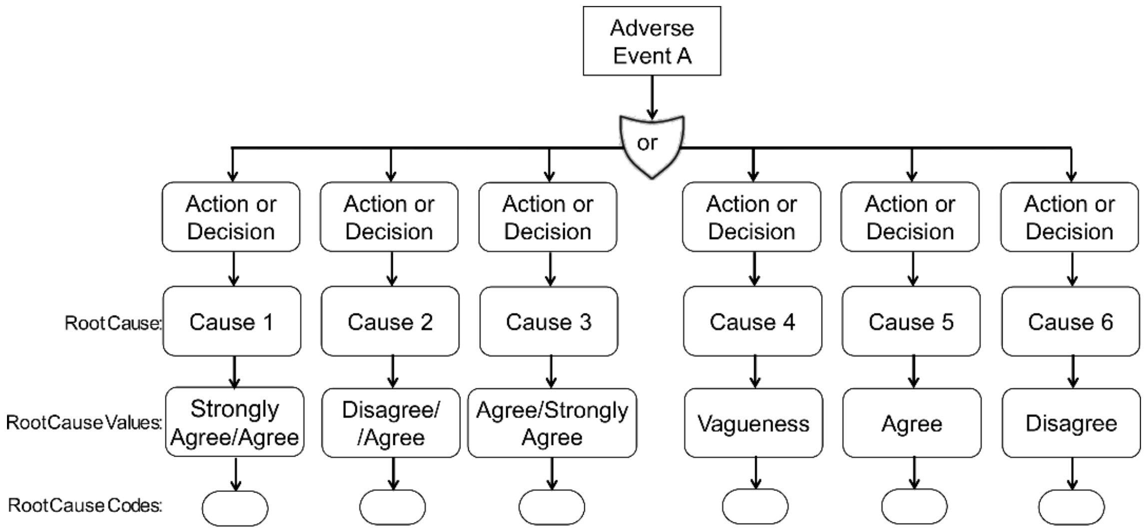

Figure 14– General structure of the causal tree for the adverse event *A*.

Once the root causes have been identified, it is possible to obtain a global picture of the functioning of the system under a hierarchical structure and put useful and long-term solutions into practice. In Figure 14 the adverse event *A* has six possible grounds. It is known that the contribution of causes 5 and 6 to the undesired event are *agree* and *disagree*, respectively (known values), while the contribution of the remaining causes is *unknown*, which sets two different types of unknown values. With regard to causes 1, 2 and 3, it is not possible to determine their precise values, but it is known that their domains are given by the sets {*strongly agree*, *agree*}, {*disagree*, *agree*} and {*agree*, *strongly agree*}, respectively, i.e., an *unknown* value in a finite set of values. With regard to cause 4, it is not possible to assert its contribution to the undesirable event, all values are plausible, i.e., an *unknown* value (not necessarily from a finite set of values).

III.2.2.1. Knowledge Representation and Reasoning

The *Knowledge Representation and Reasoning* practices in use are to be understood as a process of energy devaluation (Wenterodt & Herwig, 2014), i.e., a data item is to be understood as being in a given moment at a given entropic state as untainted energy that, according to the *First Law of Thermodynamics*, is a quantity well-preserved that cannot be consumed in the sense of destruction but may be consumed in the sense of devaluation. This new understanding may be introduced by splitting a given amount of energy into its parts, viz.

- **Exergy**, that stands for a measure of the energy that is transferred to the internal energy of a working environment and consumed, i.e., it also stands for a relevant physical factor, its entropy (In Figure 15 it is given by the dark colored areas);
- **Vagueness**, i.e., the corresponding energy values that may or may not have been transferred and consumed (In Figure 15 it is given by the gray colored areas); and
- **Anergy**, that stands for an energetic potential that was not yet transferred, being therefore available (In Figure 15 it is given by the white areas and stands for an energetic potential that may be available to be transferred and consumed).

which denote all possible energy's transfer operations as pure *energy*. Aiming at the quantification of the qualitative information contained in the causal tree presented in Figure 14, and in order to make the process comprehensible, it will be presented in a graphical form (Figure 15). Taking as an example a group of 6 (six) items that make the Citizen's Charter-Six-Items (Luhtanen & Crocker, 1992), viz.

C1 – Standards;

C2 – Information and openness;

C3 – Choice and consultation;

C4 – Courtesy and helpfulness;

C5 – Putting things right; and

C6 – Value for money.

which aims to raise the standard of public services and to make them more responsive. In order to achieve this goal, it will be used the scale (Rosenberg, 1965; Baumeister et al., 2003), viz.

strongly agree (4), agree (3), disagree (2), strongly disagree (1),
disagree (2), agree (3), strongly agree (4)

and the question "*How easy would you say **agree**?*", leading to Table 7 and Figure 15.

Table 7 – The single citizen answers to Citizen's Charter-Six-Items.

Items	Scale						
	(4)	(3)	(2)	(1)	(2)	(3)	(4)
C1	×	×					
C2					×	×	
C3						×	×
C4				*unknown*			
C5			×				
C6						×	

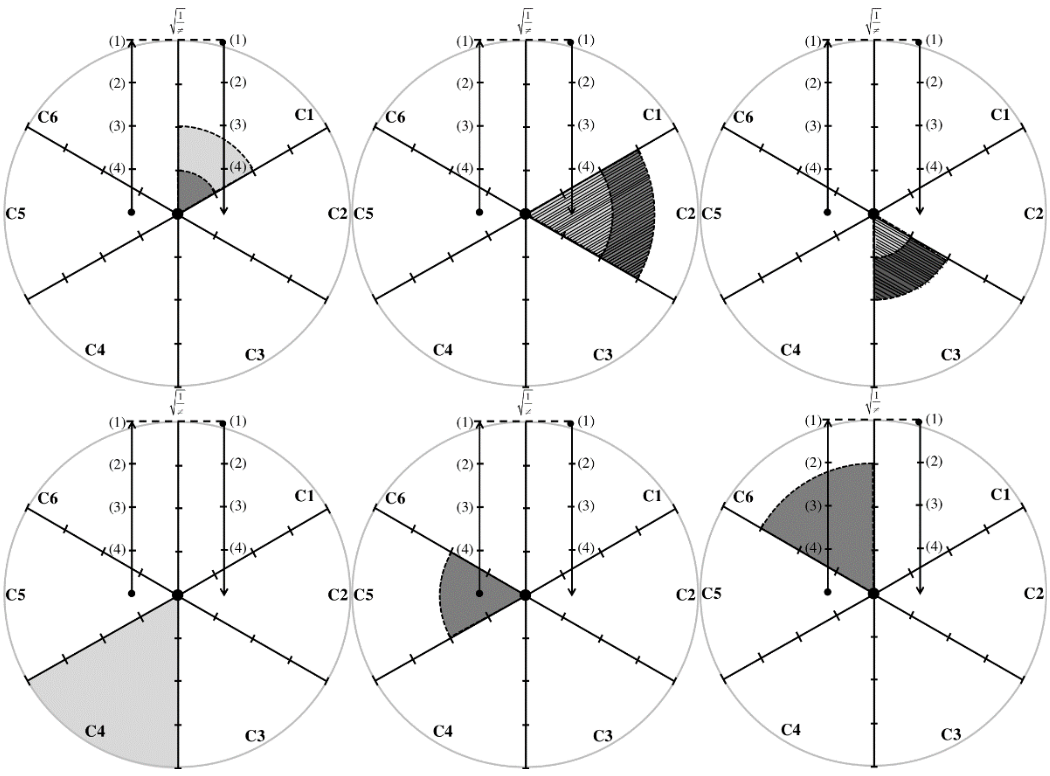

Figure 15 – An assessment of the attained energy with respect to a single citizen answer to Citizen's Charter-Six-Items.

Considering that the markers on the axis correspond to any of the possible scale options, which may be used from *bottom* → *top* (i.e., from *strongly disagree (1)* to *strongly agree (4)*), meaning that the system will work better once its entropy decreases, or is used from *top* → *bottom* (i.e., from *strongly agree (4)* to *strongly disagree (1)*), indicating that the performance of the system decreases as entropy increases), which is the case with respect to *C1*. The entropic states as untainted energy are evaluated as follows, for *C1*, *C2* and *C3*.

$$exergy_{C1} = \frac{1}{6}\pi r^2\Big]_0^{\frac{1}{4}\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\frac{1}{4}\sqrt{\frac{1}{\pi}}\right)^2 - 0 = [0.01,\ 0.01]$$

$$vagueness_{C1} = \frac{1}{6}\pi r^2\Big]_{\frac{1}{4}\sqrt{\frac{1}{\pi}}}^{\frac{1}{2}\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\frac{1}{2}\sqrt{\frac{1}{\pi}}\right)^2 - \frac{1}{6}\pi\left(\frac{1}{4}\sqrt{\frac{1}{\pi}}\right)^2 = [0.03,\ 0.03]$$

$$anergy_{C1} = \frac{1}{6}\pi r^2\Big]_{\frac{1}{2}\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\sqrt{\frac{1}{\pi}}\right)^2 - \frac{1}{6}\pi\left(\frac{1}{2}\sqrt{\frac{1}{\pi}}\right)^2 = [0.13,\ 0.13]$$

$$exergy_{C2} = \frac{1}{6}\pi r^2\Big]_0^{\frac{3}{4}\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\frac{3}{4}\sqrt{\frac{1}{\pi}}\right)^2 - 0 = [0.09,\ 0.09]$$

$$vagueness_{C2} = \frac{1}{6}\pi r^2\Big]_0^{\frac{1}{2}\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\frac{1}{2}\sqrt{\frac{1}{\pi}}\right)^2 - 0 = [0.04,\ 0.04]$$

$$anergy_{C2} = \frac{1}{6}\pi r^2\Big]_{\frac{3}{4}\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\sqrt{\frac{1}{\pi}}\right)^2 - \frac{1}{6}\pi\left(\frac{3}{4}\sqrt{\frac{1}{\pi}}\right)^2 = [0.07,\ 0.07]$$

$$exergy_{C3} = \frac{1}{6}\pi r^2\Big]_0^{\frac{1}{2}\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\frac{1}{2}\sqrt{\frac{1}{\pi}}\right)^2 - 0 = [0.04,\ 0.04]$$

$$vagueness_{C3} = \frac{1}{6}\pi r^2\Big]_0^{\frac{1}{4}\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\frac{1}{4}\sqrt{\frac{1}{\pi}}\right)^2 - 0 = [0.01,\ 0.01]$$

$$anergy_{C3} = \frac{1}{6}\pi r^2\Big]_{\frac{1}{2}\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = \frac{1}{6}\pi\left(\sqrt{\frac{1}{\pi}}\right)^2 - \frac{1}{6}\pi\left(\frac{1}{2}\sqrt{\frac{1}{\pi}}\right)^2 = [0.13,\ 0.13]$$

To C_4, C_5 and C_6 the procedures are the same. On the other hand, once a system's performance is a function of its entropic state, the data collected above may be structured in terms of the extent of the so-called ***citizen's charter (cc)*** predicate, viz.

$$cc: EXergy, VAgueness, System's\ Performance, Quality\text{-}of\text{-}Information \rightarrow \{True, False\}$$

whose graphical and formal descriptions are given in Figure 16 and
Table 8.

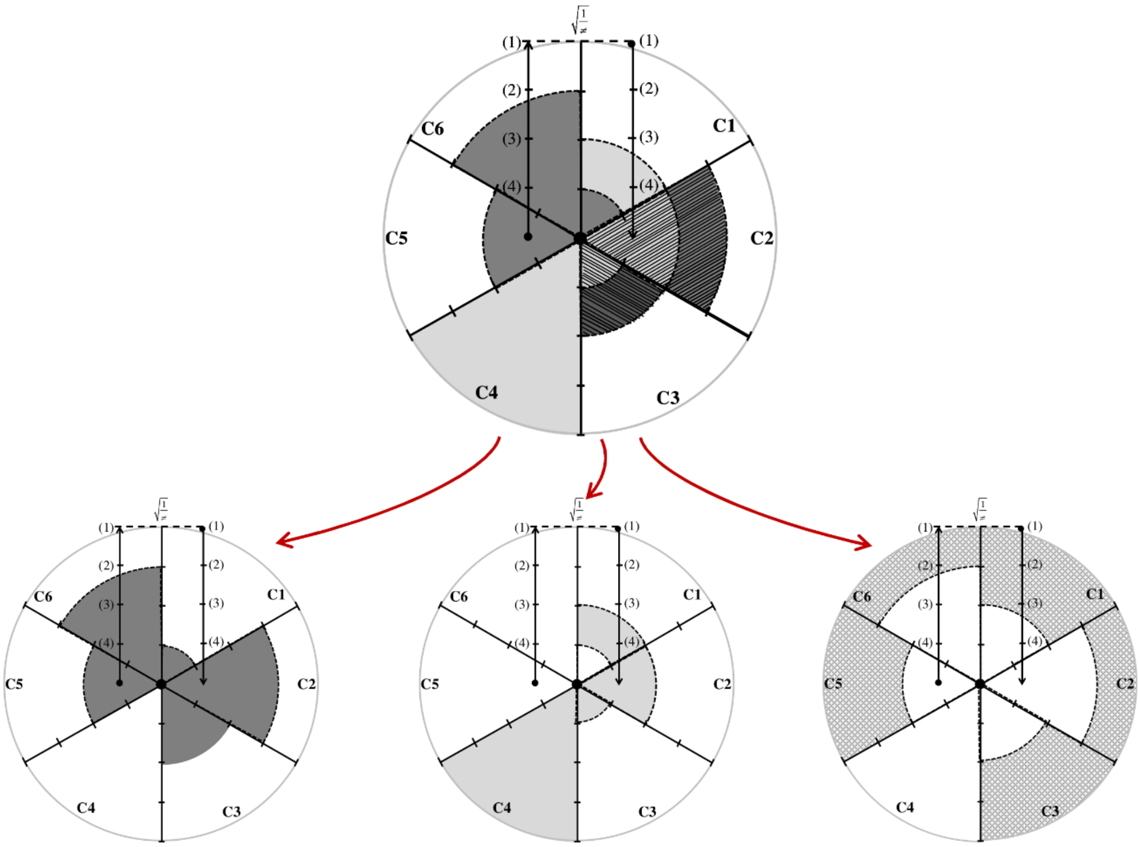

Figure 16 – A graphical view of the *citizen's charter* predicate's extent obtained according to the answers of a single citizen to the Citizen's Charter-Six-Items.

Table 8 – The *citizen's charter* predicate's extent obtained according to the answers of a single citizen to the Citizen's Charter-Six-Items.

Exergy	Vagueness	System's Performance	Quality-of-Information
0.32	0.29	0.79	0.52

which may now be depicted in terms of the Logical Program 3, in accordance with the template given in Program 4 (Neves, 1984).

$\{$

$\neg\, cc\,(EX,\, VA,\, SP,\, QoI) \leftarrow not\ cc(EX,\, VA,\, SP,\, QoI),$

$not\ exception_{cc}(EX,\, VA,\, SP,\, QoI)$

$cc\,(0.32, 0.29, 0.79, 0.52).$

$\}$

Program 3 – Structure of the logic program in relation to the answers of a single citizen to the Citizen's Charter-Six-Items.

$\{$

$\neg\, p \leftarrow not\ p, not\ exception_p$

$p \leftarrow p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m.$

$?\,(p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m).\ \ (n,\ m\ \geq 0)$

$exception_{p_1},\ \cdots,\ exception_{p_j}\quad (0 \leq j\ \leq k), being\ k\ an\ integer\ number$

$\}$

Program 4 – The archetype of an extended logic program.

where *EX*, *VA*, *AN*, *SP* and *QoI* stand for *EXergy*, *VAgueness*, *ANergy*, *System's Performance* and *Quality-of -Information*, respectively. The evaluation of *SP* and *QoI* for the different items that make the *CC – 6* are given in the form, viz.

- *System's Performance* is figured out using $SP = \sqrt{1 - (exergy + vagueness)^2}$, a value that ranges in the interval [0, 1] (Figure 17).

  $SP = \sqrt{1 - (0.32 + 0.29)^2} = 0.79$

- *Quality-of -Information* is evaluated in the form, viz.

  $QoI\ = exergy/(exergy + vagueness) = 0.32/(0.32 + 0.29) = 0.52$

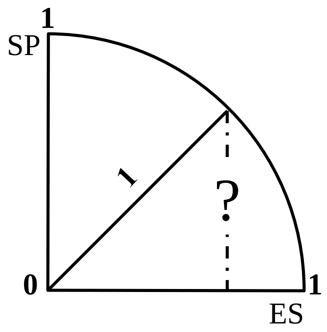

Figure 17 – System’s performance evaluation.

III.2.3. Case Study

A new version of the ECM with the extensions and adaptations for the PS was conceived, as well as the causal trees for the classification of the adverse events’ root causes. Such extensions and adaptations allowed to adequate each category to PS occurrences making the classification easier and more effective. The flow chart of the classification process is depicted in Figure 18, as well as the codes assigned to classify each type of the adverse events. For instance, the adverse events classified as “*Organizational – Protocols*” (code OP) occur due to failures related to the quality or availability of the internal protocols (e.g., too complex, too simple, unclear, nonexistent).

As an example, let one consider the adverse event “*deadline to respond to the request exceeded*” and the correspondent causal tree (Figure 19). Once this adverse event can arise due to various causes that should be taken simultaneously or separately, *AND/OR*-nodes are used to include such features in the causal tree. In addition, it was used the “*unknown*” and “*forbidden*” operators to describe events for which the event’s causes are *unknown/forbidden/not permitted* (e.g., due to internal policies). Thus, considering the information presented in Figure 19 it is possible to identify all the possible situations, viz.

- Situation A – The adverse event “deadline to respond to the request exceeded” presents as cause a “**r**equirement for **a**dditional **p**rocedures”, i.e., its value is known;
- Situation B – The adverse event “deadline to respond to the request exceeded” denotes that the “report is not ready”. It is not possible to be clear about the cause to bear in mind, but it is known that it can only be “**r**eport **n**ot **w**ritten”, “**r**eport **n**ot **r**evised” or “**r**eport **n**ot **v**alidated”, whose domain values are {strongly

disagree, disagree}, {disagree, agree} and {agree, strongly agree}, respectively, that as a matter of interpretation are assumed to be disjoint; and

- Situation C – It is only known that the adverse event stands for "deadline to respond to the request exceeded". Here all assumptions are plausible, i.e., one is faced with an "**u**nknown or a **f**orbidden **v**alue".

Thus, the logic program depicted below (Program 5), built in terms of the extents of predicates *action_or_situation_A*, *action_or_situation_B*, *action_or_situation_C* stands for itself, i.e., it denotes a formal description of *Situations A*, *B* and *C* referred to above. It will allow the use of benchmarking in public organizations, trying to explain the background of the approaches used, providing details on the methods used to solve the problems, alerting to problems and problems encountered, and examining the extent to which benchmarking results were used in decision-making.

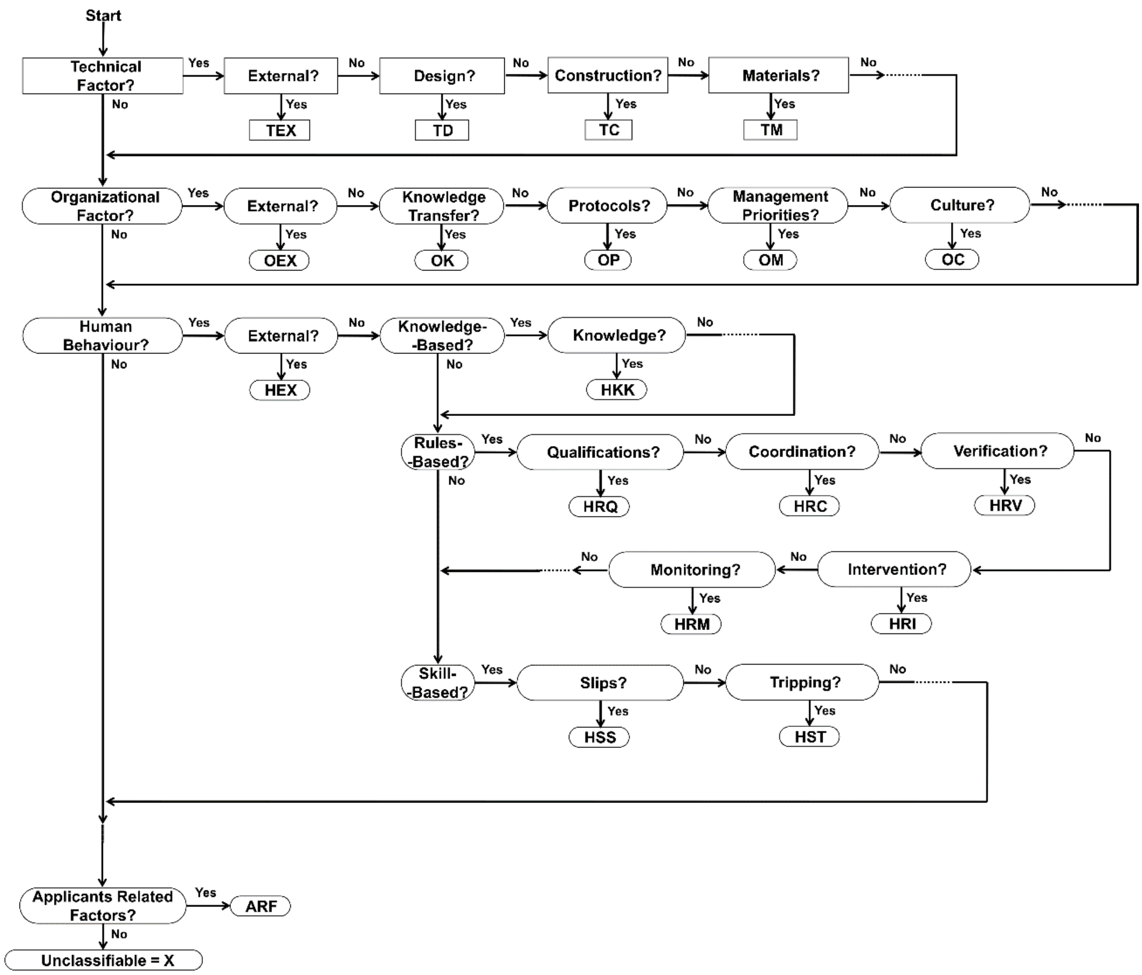

Figure 18 – Flow chart of the Eindhoven classification model for the public services.

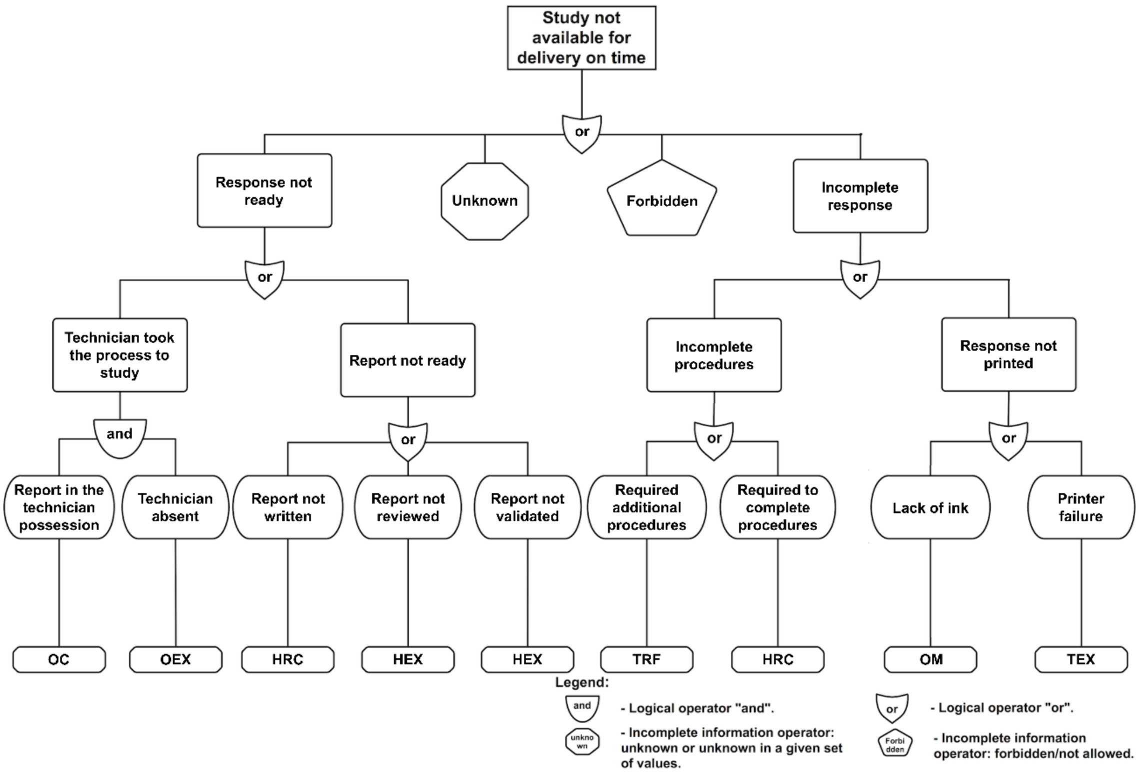

Figure 19 – The adverse event "*deadline to respond to the request exceeded*" in terms of an extended causal tree.

The logic program that sets A Full Informed Classification System leading to the excellence in the provision of public services

$$\{$$

$$\{$$

$$action\_or\_situation\_A: \ EXergy, \ VAgueness, \ System's \ Performance,$$

$$Quality\text{-}of\text{-}Information \rightarrow \{True, \ False\}$$

$$\neg \ action\_or\_situation\_A \ (EX, \ VA, \ SP, \ QoI) \ \leftarrow$$

$$not \ action\_or\_situation\_A \ (EX, \ VA, \ SP, \ QoI)$$

$$not \ exception_{action\_or\_situation\_A}(EX, \ VA, \ SP, \ QoI)$$

$$action\_or\_situation\_A(1, \ 0, \ 0, \ 1)$$

$$\}$$

$\{$

$action\_or\_situation\_B: EXergy, VAgueness, System's\ Performance,$

$Quality\text{-}of\text{-}Information \rightarrow \{True, False\}$

$\neg\, action\_or\_situation\_B\ (EX, VA, SP, QoI) \leftarrow$

$not\ action\_or\_situation\_B\ (EX, VA, SP, QoI)$

$not\ exception_{action\_or\_situation\_B}(EX, VA, SP, QoI)$

$exception_{action\_or\_situation\_B}(0.02, 0.06, 0.99, 0.20)$

$exception_{action\_or\_situation\_B}(0.08, 0.11, 0.98, 0.42)$

$exception_{action\_or\_situation\_B}(0.19, 0.14, 0.94, 0.58)$

$\}$

$\{$

$action\_or\_situation\_A: EXergy, VAgueness, System's\ Performance,$

$Quality\text{-}of\text{-}Information \rightarrow \{True, False\}$

$\neg\, action\_or\_situation\_C\ (EX, VA, SP, QoI) \leftarrow$

$not\ action\_or\_situation\_C\ (EX, VA, SP, QoI)$

$not\ exception_{action\_or\_situation\_C}(EX, VA, SP, QoI)$

$action\_or\_situation\_C(0, 1, 0, 0)$

$\}$

$\}$

Program 5 – Structure of the logic program in relation to situations *A*, *B*, and *C*.

III.2.4. Conclusions and Future Work

The fully informed classification system is simpler, maybe better, when compared with others. It may be used to assess performance objectively, expose areas where improvement is needed, identify other organizations with processes resulting in superior performance, with a view to their adoption, and to test whether improvement programs have been successful. On the other hand, once it has its root in the Language of Logic

Programming where the system's querying is set as theorems to be proved, the answers are object of formal proof. Another advantage is in its modularity, i.e., it offers the possibility of adding new categories and/or sub-categories at any time, without changing the structure or its working mode.

Future work encompasses the development of the *Adverse Events Manager Reports for Public Services* (*AEMR-PS*) module. Such component aims at the analysis of the adverse events recorded by the *Adverse Event Reporting Forms for Public Services* (*AERF-PS*). The *AEMR-PS* will provide automatic reports of the adverse events complemented with charts and statistical information about the events recorded and will contribute to identify trends.

III.3. A Conceptual Model to Assess the Literacy of Water Consumers

III.3.1. Introduction

The water that exists in nature contains microorganisms that may be pathogenic for humans (Bagchi, 2013). Considering the key role that water plays in disease prevention and health promotion, the issues related with water literacy can be related to health literacy. The World Health Organization (WHO) defines health literacy as the set of cognitive and social skills that determine individual motivation and skills, and enable access, understanding and use of information in health promotion. In this way, citizens should have a level of knowledge and skills to support conscious decision-making, leading to changes in behavior and ways of living, with a view to improving health from an individual or public perspective (WHO, 1998). For this reason, the concern with the determination of the parameters of water quality for human consumption has been growing in Portugal. The number of accredited laboratories is increasing, and the existence of Quality Management Systems can contribute to raise the level of services provided and to enhance customers' satisfaction which, on the other hand, may be aware of, viz.

- To know the diseases that can arise from untreated water consumption;
- To understand the importance of using public water;
- To know how and where to find information on public water quality;
- To identify situations that may affect the water quality;
- To understand the need to carry out analyzes of water withdrawals; and
- To recognize the importance of choosing a laboratory that meets legal and technical standards.

In order to do justice to these aspects, the literature was revised. The aim of this review is to assess the relevance of consumer literacy in relation to water quality control. A conceptual model is presented and used to develop a questionnaire to examine the level of knowledge of water consumers about their quality. In addition, this study establishes the connection between the conceptual model and the Deming's PDCA one.

III.3.2. Methods

III.3.2.1. Study Design

A literature search was carried out to identify key concepts, theories, sources of evidence and knowledge gaps. The five steps described by Arksey & O'Malley (2005), (i.e., identifying the research question, identifying relevant studies, selecting studies, plotting the data and finally, group, summarize and report the results) were followed.

III.3.2.2. Electronic Search Strategy

A bibliographic search was carried out for the period between January 2015 and January 2020 using the *ScienceDirect* and *B-On* platforms using keywords like literacy, awareness, water, water for human consumption, drinking water, the environment, disease prevention and public health.

III.3.3. Results

The search for the term literacy gave 304.319 results (Figure 20). The studies related to consumer literacy in the areas of finance (Cameron et al., 2014; Kramer, 2016) and health (Amoah, 2018; Balmer et al., 2020) are more frequent than the ones concerning environment and water. A study carried out by Amoah (2018) demonstrated that participation in social activities (religious, voluntary and in groups) and health literacy have positive effects on health well-being. Data were collected through the application of 779 questionnaires to rural and urban residents in the Ashanti region of Ghana, from June 2015 to October 2015. Balmer et al. (2020) studied the connection between the literacy level of nursing students over the years of their training in 4 regions of the world. The data were collected between 2014 and 2016, enrolling 845 nursing students. In all regions, the results show significant changes in health literacy profiles according to the training year, namely in the ability to find good health information.

The association of the terms "*literacy*" + "*environment*" and "*literacy*" + "*water*" allowed to identify thirteen works (Figure 20). After discarding the duplications, twelve papers were considered. Their analysis shows that five of them are related with environment, but in a perspective different from the one intended in this study.

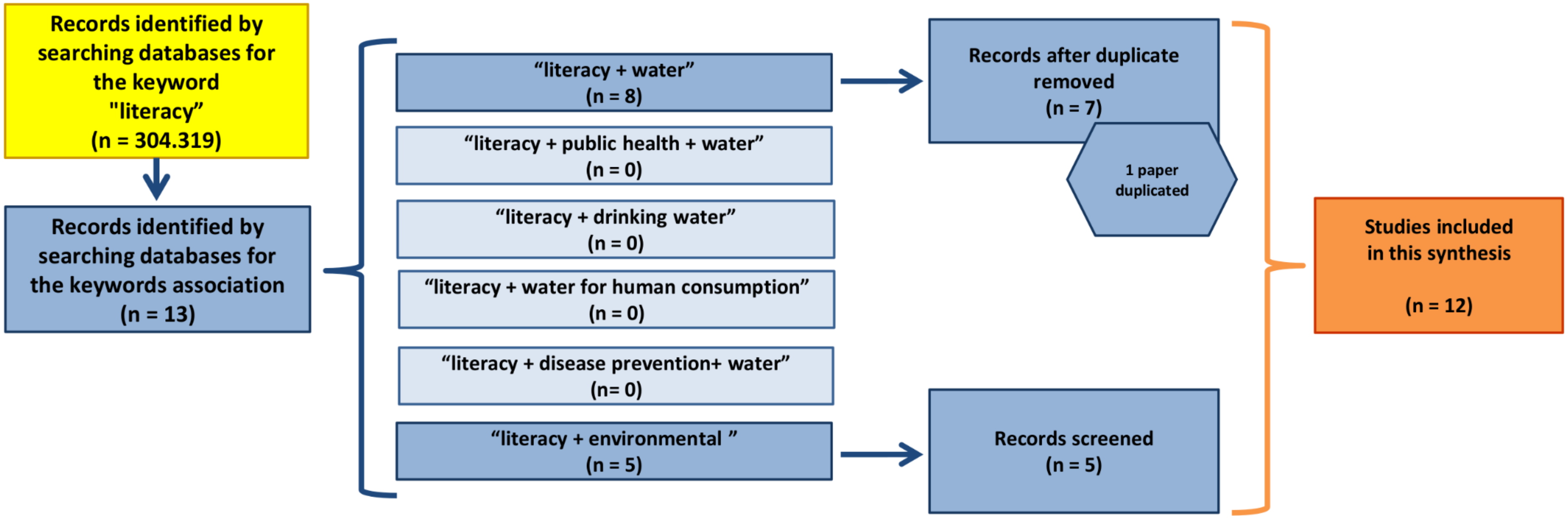

Figure 20 – Flow chart of papers selection process.

Ramdas & Mohamed (2014) define the concept of environmental literacy not only as the knowledge about the environment and its problems, but also related to attitudes, sensitivity, and motivation. Having this in mind, the authors addressed the problematic of tax application to tourists to change their environmental behavior. The study shows strong associations between tourists' level of environmental literacy and willingness to pay for environmental conservation (Ramdas & Mohamed, 2014). Broek (2019) studied the household energy literacy. The author highlighted that consumers with positive environmental attitudes and with higher education demonstrate greater levels of energy saving literacy. Craig & Allen (2015) studied students' environmental literacy and energy saving behaviors. Goldman et al. (2018) investigated the environmental literacy of students and the environmental performance of schools with certification. Sovacool & Blyth (2015) studied the Danish consumer literacy in issues related with affordability of electricity and gasoline, climate change and their preferences for alternative energies.

From the set of selected papers, only seven associate the terms literacy and water. However, only one presents a study regarding water quality literacy. Irvin et al. (2019) studied the level of knowledge of well owners about the risks associated with the use of water from private sources. In particular, regarding environmental pollution or the presence of contaminants. The rest of the work deals with the term's literacy and water from a different perspective than this study. He (2018) analyzed the Chinese literacy regarding the use of water as a resource that must be preserved. The author evaluated the current status of water literacy across different geographic areas of China, in order to develop a methodology to establish reasonable water-using policies. Roldan et al. (2019) investigate students' climatic literacy to identify relationship between the problem of water and the climate crisis. Simonds et al. (2019) studied the literacy of the risks associated with the consumption of contaminated water in some rural communities in the USA. Seelen et al. (2019) carried out a study on the level of knowledge regarding the factors that can threaten water quality (agriculture, industry, and climate change). Su et al. (2011) studied the level of literacy related to the impacts on public health resulting from catastrophes associated with intense rain phenomenon. Finally, Bhardwaj et al. (2017) investigated the percentage of people in India who practice defecation in the open sky. The authors investigated the different factors which were responsible for the non-usage of toilets in India and explore the drainage system and sanitation conditions in public places. According to the authors the low education levels (particularly of women) and the lack of awareness regarding the ill-effects of open defecation are the main responsible for the no-use of toilets in India.

III.3.4. Discussion

Considering the importance of water quality for health and the paucity of literature on this topic, a conceptual model for the study of Water Consumption Literacy (WCL) was developed and presented in this paper (Figure 21). In this model the main dimensions of the WCL (i.e., *Water Quality*, *Disease Prevention* and *Public Health Promotion*) are presented within the pentagon. These dimensions evolve from an individual-centred perspective (inner pentagon) to a population-focused one (outer pentagon). In each dimension four competencies should be investigated, i.e., *Access*, *Understand*, *Appraise* and *Apply* information related to water consumption. *Access* is related to the ability to seek, find, and obtain information. *Understand* refers to the ability to cognize the information found. *Appraise* is linked with the individual's ability to interpret, filter, judge, and evaluate information. Finally, *apply* refers to how information is used and shared (Sørensen et al., 2012). The factors that can influence the dimensions described above are the literacy of consumers on the subject, the recognition of the need of consume controlled water, the existence of accredited laboratories and the existence of a water treatment services. Such factors go forward from a person-centred perspective to a community-focused one. Thus, the proposed conceptual model considers literacy for water consumption in a broader perspective aiming to contribute for global sustainability.

The model presented aims at human well-being and the promotion of quality of life of citizens. Indeed, the concept of quality is inherent to the human being, and it is implicit in the daily life acts (Hoyle, 2017). During the 50s and 60s of the last century the concept of total quality management was developed. According to this philosophy, quality became to be seen as a problem of the company and not exclusively of the production or the product. This paradigm shift took Deming, in the 80s, to propose the PDCA Model (*Plan*, *Do*, *Check* and *Act*). This model, also known as the Deming Cycle, consists of a sequence of four repetitive steps of improvement and learning, i.e., *Planning*, *Do*, *Check*, and *Act* as shown in Figure 22. *Plan* consists in identifying and analyzing the problem. *Do* includes the development and testing of the potential solutions. *Check* consists in assessing the effectiveness of the solutions and analyzing the improvements. Finally, *Act* refers to the implementation of the improved solutions (Hoyle, 2017).

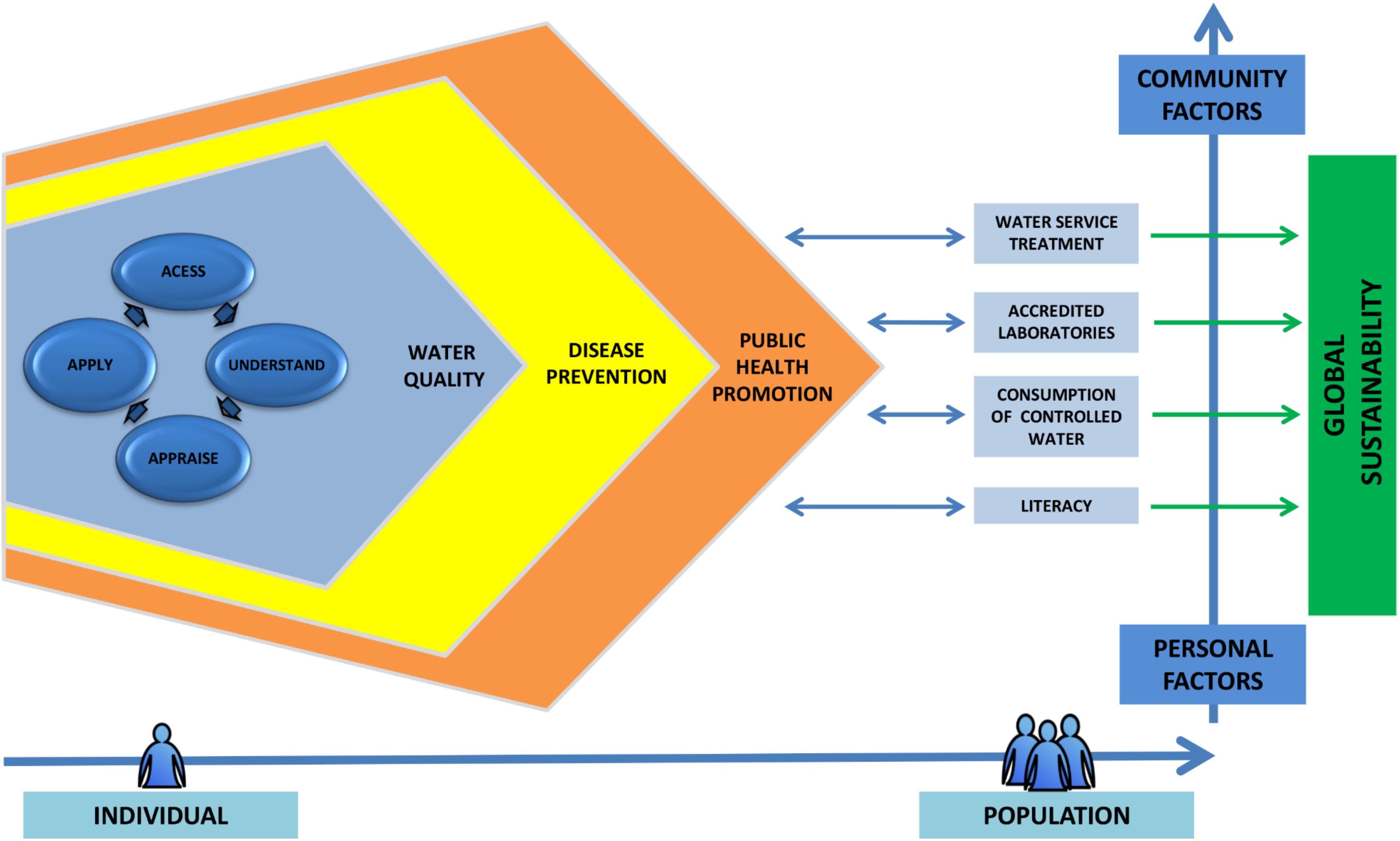

Figure 21 – Conceptual model for the planning and operationalizing studies on water consumption literacy.

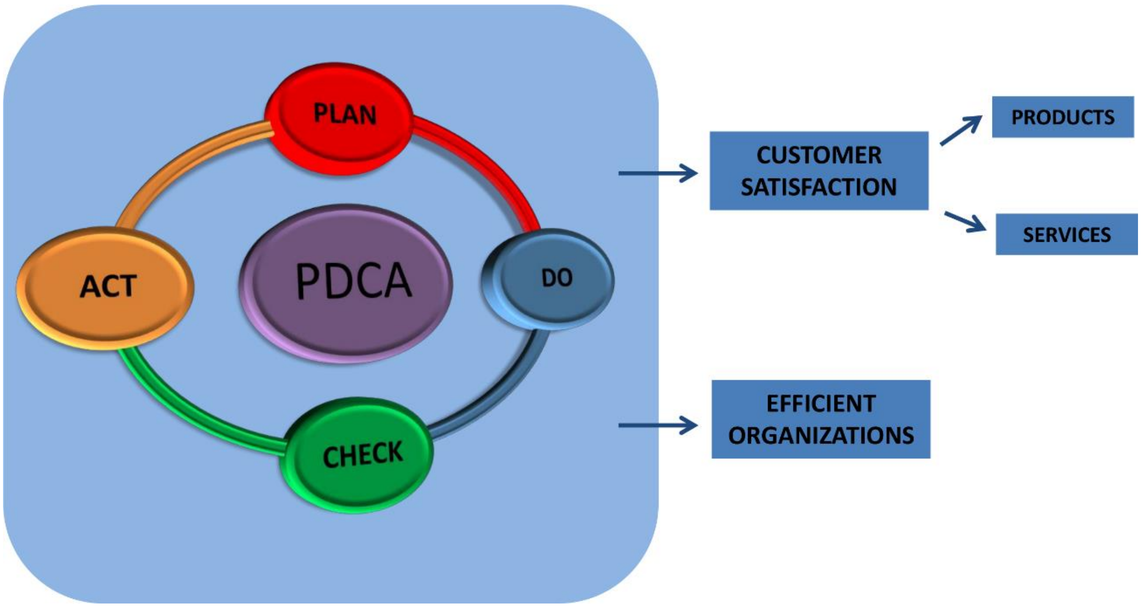

Figure 22 – PDCA Model.

The PDCA Model is a management tool widely used by companies around the world, aiming to ensure business success, regardless company, area, or department (e.g., sales, purchasing, engineering, industry, laboratories, services). It is a model of continuous improvements that allows for a clearer and more agile management process. In this cycle, the input information (used for defining and planning the quality system) is the reality of the organization and its context, the requirements of customers and the needs/expectations of stakeholders (i.e., suppliers and regulatory bodies). The results, i.e., the outputs from the quality system, are customer satisfaction about the products/services provided and the efficiency of the processes that make the day by day of the organization.

The PDCA model (Figure 22) and the conceptual model for WCL (Figure 21) aim to achieve excellence, through the evaluation of the current reality and, from there, to identify new solutions that lead to processes improvements. Thus, it is possible to interrelate them matching the competencies *Access* and *Understand* to the *Plan* and *Do* phases, the competency *Appraise* to the *Check* stage and, finally, the competence *Apply* to the *Act* step (Figure 23). Indeed, both models aim to promote organizational efficiency and customer satisfaction through the reinforcement of their literacy. The knowledge acquired by them can lead to good practices and to contribute to the desired global sustainability.

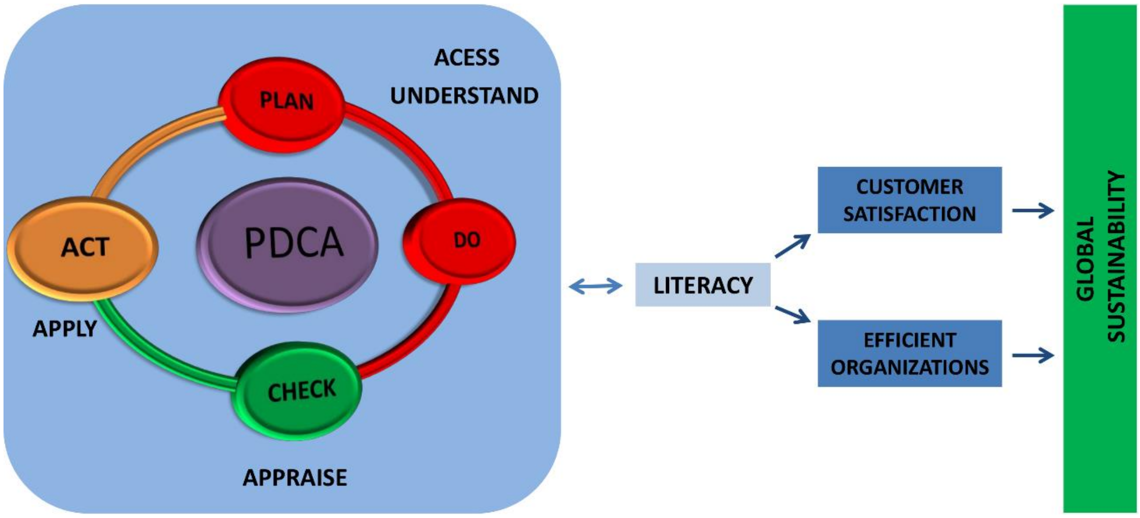

Figure 23 – Interrelationships between PDCA and WCL Models.

The articulation of the WCL and PDCA models will support future studies related with consumers (e.g., assessing literacy levels in relation to water issues), organizations operating in this sector (efficiency studies) as well as public policy formulation and/or implementation. In fact, the global management of water resources should be regarded in a holistic perspective, taking into account different viewpoints, ranging from water quality to the multiple dimensions of water governance (e.g., integrated management (Claassen 2013; Wang et al. 2018), evaluation/implementation of water guidelines (Akinsete et al. 2019; Apostolaki et al. 2019; Giakoumis et al. 2019), stressing conditions (Hartley et al. 2018; Horne et al. 2018; Tortajada et al. 2019), water reuse (Hartley et al. 2019; Rebelo et al. 2020; Takeuchi & Tanaka 2020)), including the connection water – health.

III.3.4.1. WCL Model in Practice

Aiming to exemplify the use of WCL model, a questionnaire to evaluate the literacy of the consumers regarding the quality of the water consumed was conceived and applied individually to a cohort of 147 participants, in person, by the researcher (section III.3.6). The study was carried out in the Municipality of Santiago do Cacém. This is one of the largest municipalities in Portugal located in the Alentejo Litoral, belonging to the district of Setúbal. The questionnaire covers the three dimensions referred in the WCL model and, in each of them, the four competencies were investigated, i.e., *Access*, *Understand*, *Appraise* and *Apply* information. It was organized into two sections, where the former one includes general questions (e.g., age, gender, academic qualifications). The second one comprises statements related with water literacy. In the first section the answers are descriptive, whereas in the second one a Likert scale with four levels (i.e., *very easy*, *easy*, *difficult*, and *very difficult*) was used.

The age of the participants ranged from 18 to 82 years of age (average age 41 ± 23 years), with 57.8% women and 42.2% men. Participants' age was categorized into age groups, i.e., under the age of 25, 26-50, 51-70 and above the age of 70. 38.1% of participants are aged between 26 and 50 years of age, 29.2% between 51 and 70 years of age, 19.8% are under 25 years of age, whereas 12.9% are above 70 years of age. Concerning academic qualification, 14.3% of the respondents expressed to have only basic education, 55.1% declared to have concluded secondary education, 25.8% stated to have finished a degree and 4.8% affirmed to have a post graduate education.

Figure 24 displays the frequency of answering to the second section of the questionnaire, where respondents expressed their opinion on the groups of questions regarding each WCL dimension. The questions Q1 to Q6 refer to the *Water Quality*, Q7 to Q11 are related to *Disease Prevention*, and Q12 to Q16 are relative to *Public Health Promotion*. Concerning *Water Quality*, the analysis of the frequency of answers (Figure 24(A)) shows that the overwhelming majority of respondents, varying among 75.0% and 97.5%, tick the options *difficult* or *very difficult*. These results revel the low literacy level of the respondents about water quality topics, regardless of the competence investigated (i.e., *Access*, *Understand*, *Appraise* or *Apply*). The results related with *Disease Prevention* (Figure 24(B)) reveal a slightly higher level of literacy than that obtained in the previous dimension. Indeed, in all questions of this group (except Q10) the options *very easy* or *easy* were selected by a percentage of respondents ranging between 29.5% and 72.5%. With respect to Q10, related with the appraising if a particular symptom is related to the use of untreated water, the overwhelming majority of respondents ticked the options *difficult* or *very difficult* (96.0%). Finally, regarding *Public Health Promotion* (Figure 24(C)) the options ticked by the respondents reveal a higher level of literacy. In fact, the percentage of respondents that choose the options *very easy* or *easy* vary between 60.5% and 83.0%, except in Q16, where this percentage was lower (36.0%). Despite the fact that the respondents state to be able to apprise if their lifestyle contributes to sustainable water use (Q15) they reveal ineffectiveness to apply actions to save water in their daily life (Q16).

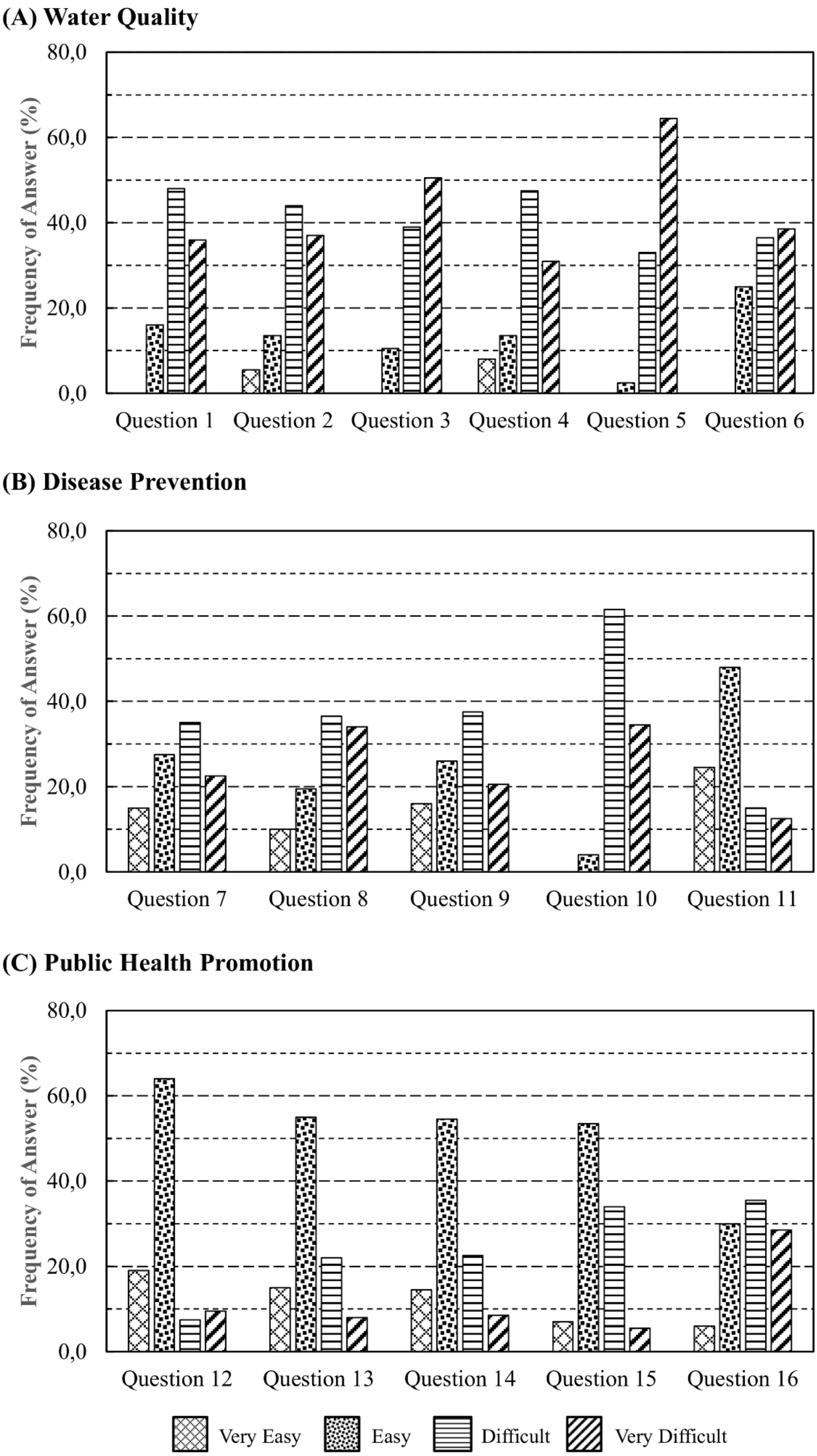

Figure 24 – Frequency of answer regarding each WCL dimension. (A) Water quality; (B) Disease Prevention; and (C) Public Health Promotion.

A global analysis of the results presented in Figure 24 allows to state that in *Water Quality* and *Disease Prevention* dimensions, the competence where the respondents reveal the greatest difficulties is *Appraise*, which, according to what was presented previously, matches the step *Check* in the PDCA model. In other words, respondents reveal difficulties in assessing the effectiveness of the solutions/information. Regarding the remaining dimension (i.e., *Public Health Promotion*) the respondents reveal the greatest difficulties in the competence *Apply*, which corresponds to the step *Act* in the PDCA model, i.e., the implementation of the solutions/information.

III.3.5. Conclusions

Despite the high number of papers on literacy, this work identified a paucity of papers on literacy studies related to the quality of water for human consumption. Considering the risks to health associated with the consumption of inappropriate water it is mandatory to evaluate the population's literacy levels on these issues. Thus, the scarcity of information on the topic and the importance of water quality for health have led to the development of the conceptual model presented in this study. Such model can be of utmost importance to support studies aiming to assess water consumers' literacy. The articulation of the developed model (WCL) and the PDCA model allowed to build a questionnaire that was applied to a cohort of 147 respondents in order to evaluate the literacy of the consumers regarding the quality of the water issues. The questionnaire can be extended to include other questions in future literacy studies by water laboratories and/or by the water management entities. The main contribution of this work is to present a methodology that can contribute to access/promote water literacy, organizational efficiency, and consumer satisfaction, leading to good practices that contribute to public health and global sustainability. In fact, the articulation of the WCL model and an organizational tool like the PDCA model aims to achieve excellence through the evaluation of the current reality to promote improvement solutions, in a global perspective that leads to a sustainable water management.

III.3.6. Questionnaire on Water Quality and Health

QUESTIONNAIRE ON WATER QUALITY AND ITS RELATIONS WITH HEALTH

In order to develop strategies to improve health and well-being levels, a study is being carried out to analyze literacy related to water quality and its relations with health.

Your collaboration in answering these questions will help us to better understand the importance of this topic in health promotion.

Note: The Laboratory protects your privacy. The personal data collected will be processed by computer and will not be transferred to any other institution not used for any purpose other than the support to the Internal Quality Management System.

PART I

CUSTOMER DATA

Tick the box that corresponds to your case or fill the blanks.

Gender	Feminine ☐	Masculine ☐		
Academic Qualifications	Basic Education ☐	Secondary Education ☐	Higher Education ☐	Post Graduate Education ☐
Age	______________ **years old**			

QUESTIONNAIRE ON WATER QUALITY AND ITS RELATIONS WITH HEALTH

PART II

On a scale from *very easy* to *very difficult*, how easy would you say it is to …

WATER QUALITY

	Very Easy	Easy	Difficult	Very Difficult
Q1 ... access information about the results of the water analysis of the public network in your area of residence?	☐	☐	☐	☐
Q2 ... access information on where to do the water quality control of private water abstractions?	☐	☐	☐	☐
Q3 ... understand the information regarding the results of the water analysis of the public network in your area of residence?	☐	☐	☐	☐
Q4 ... understand the need to carry out the water quality control of private water abstractions?	☐	☐	☐	☐
Q5... appraise the need to analyze the water of a private abstraction?	☐	☐	☐	☐
Q6 ... apply the instructions given by the competent authorities regarding the use of water from private abstractions?	☐	☐	☐	☐

DISEASE PREVENTION

	Very Easy	Easy	Difficult	Very Difficult
Q7 ... access information about the health risks associated with the use of untreated water?	☐	☐	☐	☐
Q8 ... access information about symptoms of diseases associated with the use of untreated water?	☐	☐	☐	☐
Q9 ... understand the health risks associated with the use of untreated water?	☐	☐	☐	☐
Q10 ... appraise whether a particular symptom is related to the use of untreated water?	☐	☐	☐	☐
Q11 ... apply the instructions given by health professionals in the face of symptoms due to the use of untreated water?	☐	☐	☐	☐

PUBLIC HEALTH PROMOTION

	Very Easy	Easy	Difficult	Very Difficult
Q12 ... access information on water saving measures?	☐	☐	☐	☐
Q13 ... access information on how to protect water resources?	☐	☐	☐	☐
Q14 ... understand the correct behaviors for the sustainable use of water?	☐	☐	☐	☐
Q15 ... appraise whether your lifestyle contributes to sustainable water use?	☐	☐	☐	☐
Q16 ... apply actions that save water in your daily life?	☐	☐	☐	☐

Thank you for your cooperation!

III.4. Psychosocial Risks Assessment in Cryopreservation Laboratories

III.4.1. Introduction

According to the Portuguese general, Labor Law the employers should identify the riskiness to which workers are exposed and perform the risk assessment. Thus, it is of utmost importance to understand this phenomenon in terms of occurrence, prevalence, and prevention in various professional activities (EU-OSHA, 2012). Beyond the physical, chemical, and biological risks, due to the significant changes that have taken place in the working world, in recent years the psychosocial risks have emerged, with negative consequences for society, businesses, and workers (EU-OSHA, 2007; 2012; Leka & Jain, 2010). Psychosocial risks derive from deficiencies in work design, organization, and management, as well as from a problematic social working context and may have psychological, physical, and social effects such as work-related stress, burnout, or depression (Leka & Jain, 2010).

The study of this theme began to develop in 1950, when the psychological aspects of the work became an object of research. Attention to this phenomenon became more pronounced in 2000, after an increase in serious accidents at work was noted. However, psychosocial risks are still identified today as a major challenge for occupational health and safety professionals (Leka & Jain, 2010; Lerouge, 2017).

III.4.2. State of Art

III.4.2.1. Psychosocial Risks

Psychosocial risks are a relatively recent concept and refer to conditions present in work situations, related to work organization, hierarchy, performance of the task, and the work environment, which may favor or impair work activity, as well as the quality of life, well-being, and health of workers (Dollard et al., 2019). These conditions, when favorable, foster the personal development of individuals. Conversely, when unfavorable, undermine the health and well-being, becoming a source of occupational stress with potential to cause psychological, physical, or social harm to individuals (Lerouge, 2017).

Psychosocial risks can be caused by a diversity of factors. Some may be intuitive, whereas others require detailed analysis to be identified as underlying causal factors. As a result, there are usually no quick fixes at hand, that is, a continuous and effective management process is required. To achieve this level, it is important to understand the most important underlying causal factors before selecting solutions (Dollard et al., 2019). The factors that may lead to psychosocial risks are related to content of the work, workload and work rate, working hours, control, environment and equipment, culture and organizational function, interpersonal relationships at work, organization role, development of career, and work–home interaction, as shown in Figure 25A.

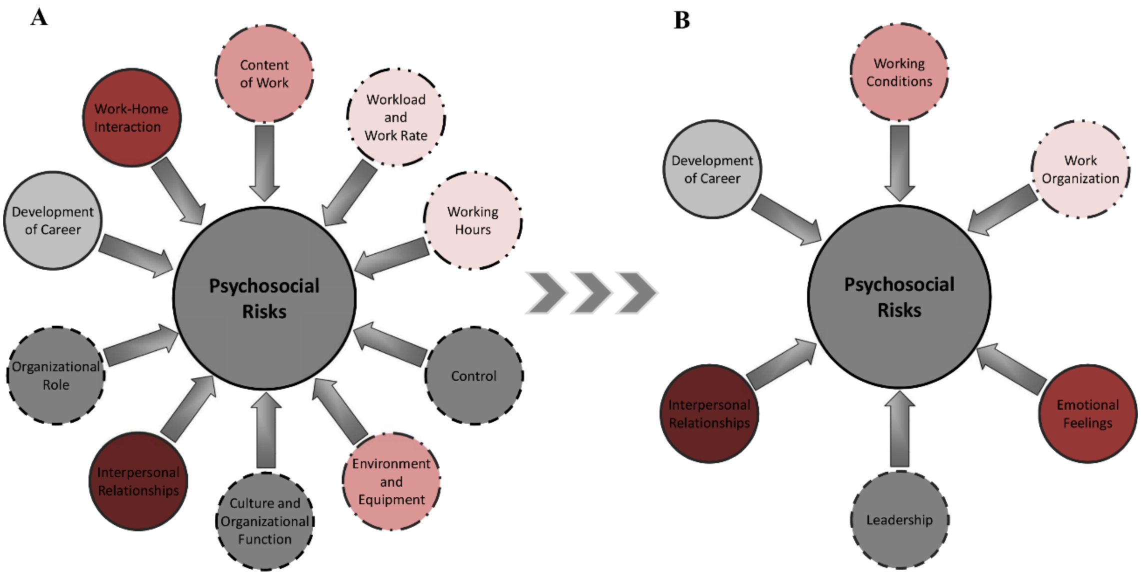

Figure 25 – (A) Psychosocial risks factors. (B) Categories of psychosocial risks factors.

- **Content of the work** refers to the lack of short work cycles, to the automatic or meaningless work, and to the under/over use of worker's skills (i.e., skills do not correspond to the tasks assigned). The lack of variety and complexity of tasks and the consequent monotony or repeatability can also be a source of suffering at work (Eurofound & EU-OSHA, 2014; Lerouge, 2017).
- **Workload and work rate** is related to the inability to cope with the demands of the profession (e.g., when the worker feels that the demands of the job are excessive and cannot cope with them or the lack of sufficient requirements). This item is also associated to high levels of emotional pressure and mental burden, as well as the continued existence of difficult deadlines (Eurofound & EU-OSHA, 2014).
- **Working hours** is related to working hours (e.g., shift work, night shifts, Sunday work, rigid and inflexible work hours, unpredictable hours, and long hours or those

that do not allow socialization). These issues are seen as being inconsistent with the preservation of the well-being and influence temporal and emotional availability for personal and family relationships (Eurofound & EU-OSHA, 2014).

- **Control** refers to the person's stress level that can be influenced by the person's level of control over workload and work rate, as well as other risk factors (Eurofound & EU-OSHA, 2014). When a worker has control and influence over how his work is planned and carries out, it helps him cope with challenges ahead. Conversely, if the worker does not have the expected control, whether other people determine the pace or the way of work, the worker can feel stress. Lack of flexibility, as well as low participation in decision–making, contribute to stress and prevent a person from developing and using new skills (Eurofound & EU-OSHA, 2014).
- **Environment and equipment** refer to inadequate availability, adequacy, or maintenance of equipment as well as precariousness and job insecurity. This item also stresses the poor environmental conditions, such as lack of space, poor lighting, excessive noise, or high temperatures, which may hinder workers' ability to concentrate (Eurofound & EU-OSHA, 2014).
- **Culture and organizational function** relate to the levels of support and encouragement for problem–solving and personal development (Eurofound & EU-OSHA, 2014). Positive support and feedback (from colleagues, from leaders, social support, or direct support for the profession) can help people overcome difficulties and lead to job satisfaction. This item is also related to communication, definition of organizational objectives, structural variables, hierarchical structure, leadership style, recognition at work, employees' freedom of expression, and changes within organization (Lerouge, 2017).
- **Interpersonal relationships at work** are related to differences of opinion in a work environment. Work relationships can cause stress when people suffer discrimination, have poor relationships with superiors, colleagues, face interpersonal conflict, or lack social support (Eurofound & EU-OSHA, 2014). In addition, inadequate, incomprehensible, or unbearable supervision should be included in this item. Another factor that cannot be overlooked and causes stress is bullying/mobbing (Dollard et al., 2019). Bullying may involve violence (physical, verbal, or psychological), intimidation, sexual harassment, and subtler acts such as physical or social isolation, excessive supervision, unfounded criticism, the impoverishment of tasks, evasion of information, or persecution at work (Lerouge, 2017).

- **Organization role** refers to stress that arises from the lack of clarity about the roles and responsibilities that people have or when the roles and responsibilities give rise to conflict with colleagues, superiors, or customers. This factor also covers the stress that arises from the feeling that his role is incompatible with his skills and abilities (Eurofound & EU-OSHA, 2014).
- **Career development** refers to the stress due to career stagnation, under-promotion, over-promotion, low compensation, or low commission. Career development also encompasses issues linked to job insecurity, career uncertainty, and low social value to work (Lerouge, 2017).
- **Work–home interaction** is related with the conflict between work and family demands which can lead to conflicts of time, commitment, and support. In addition, it encompasses the stress that arises because of low home support and from dual career problems (Eurofound & EU-OSHA, 2014).

Some of aforementioned factors can be grouped into generic categories, namely *Work Conditions*, *Work Organization*, and *Leadership*. The former one includes the factors *Environment and Equipment* and *Content of Work*, whereas the second comprises *Workload and Work Rate* and *Working Hours*. Finally, the third category groups the factors *Culture and Organizational Function*, *Control* and *Organizational Role* (Figure 25B).

Recent studies show that psychosocial risk analysis in organizations is increasingly common in the industrial sector (Joensuu et al., 2010; Ferguson et al., 2012; Metzler et al., 2019) and less frequent in the laboratory sector. Ferguson et al. (2012) studied the psychosocial and biomechanical factors in furniture distribution workers, involving 454 participants at nine furniture distribution facilities for 6 months. The authors developed a multivariate logistic regression model that includes baseline functional performance probability, facility, perceived workload, intermediated reach distance number of exertions above threshold limit values, job tenure manual material handling, and age combined. The model sensitivity and specificity were of 68.5% and 71.9%, respectively.

Joensuu et al. (2010) examined associations between job control, social support, and mental ill health in a multinational forest industry corporation. The 13,868 employees of a Finnish forest company with no previous hospital admissions for mental disorders responded to questionnaires on decision authority, skill discretion, co–worker, and supervisor support. The results show that high skill discretion was related with reduced risks of hospital admission for mental disorders, whereas high decision authority was connected with an elevated risk. Furthermore, the authors concluded that high decision authority was a risk factor for alcohol-related and depressive disorders, whereas good co–worker support was linked with a reduced risk of non–depressive non–alcohol–related mental disorders. Supervisor support, in turns, was not associated with any mental disorders.

Metzler et al. (2019) compared different methods for evaluating psychosocial hazards in the scope of risk assessment in a sample of 549 blast furnace workers of a German steel manufacturing. The authors highlighted that the risk management was strongly influenced by the choice of risk evaluation method because the measures to minimize the risks are directed only to the ones identified and in accordance with their level of priority.

In analysis laboratories, regardless of the sector of activity, the excessive pace of work, monotony, routine, as well as problems of interpersonal relationships, are examples of psychological risks for the workers. Bronkhorst (2015) realized a hierarchical linear modeling of physical safety behavior to examine the relationship between job demands, job resources, safety climate, and safety behavior among employees working in health care. The author used a sample of 6230 health–care employees of 52 different Dutch organizations. Regardless of the focus (i.e., physical, or psychological safety), this study shows that the consolidation of the safety climate increases employees' safety behavior. In addition, the authors point out that the organization's safety climate is an ideal target of intervention to avert and enhance negative physical and psychological health and safety outcomes, mainly in times of doubt and change.

Aiming to estimate the association between psychosocial risk factors in the workplace and musculoskeletal disorders in nurses and aides Bernal et al. (2015) examined 17 papers. Despite the low heterogeneity of cohorts, the authors identified associations between high psychosocial demands and low job control with prevalent and incident low back pain, prevalent shoulder pain, prevalent knee pain, and prevalent pain at any anatomical site.

All these studies show the main role of the psychosocial risk in organizations to minimize possible damage to the health of employees. In addition, the foregoing demonstrates the relevance of the development of models aiming to predict the level of psychosocial risks based on employees' experiences. In the present work, a predictive model based on Artificial Neural Networks (ANNs) will be presented.

III.4.2.2. Artificial Neural Networks

ANNs are computational tools that aim to simulate the human brain and nervous system. The multilayer perceptron is one of the utmost common ANN architectures, in which neurons are assembled in layers and only forward connections exist (Haykin, 2009). ANNs are increasingly applied in data mining because of their good performance in prediction (Mitra et al., 2002). In last decades, several studies have been published showing the usefulness of ANNs to apprehend complex relationships between variables, in various areas of application, e.g., environment (Allawi et al., 2018; Ruben et al., 2018), health (Vicente et al., 2016; Neves et al., 2018a), and law (Stranieri & Zeleznikow, 2012; Neves et al., 2016; Nguyen et al., 2018) just to name a few.

III.4.3. Methods

III.4.3.1. Place of Study

This study took place in a cryopreservation laboratory and in dialysis care clinics located in the north of Portugal. In Portugal, the quality and safety requirements for human tissues and cells are set by the Portuguese Ministry of Health (Law No.12/2009). However, the criteria implemented by the laboratory under study are even stricter. The laboratory participates in external quality assays, where national and international entities test and certify the reliability of the stored sample quality control tests. Furthermore, the laboratory has the accreditation of the American Association of Blood Banks (AABB), which sets the most stringent quality criteria in the industry worldwide (AABB, 2020). The cryopreservation laboratories were chosen because the work performed in them requires immediate results, confidentiality, and secrecy and deals with large volumes of information. The pressure associated to these requirements can create conditions for the appearance of psychosocial risks in the workers, and it is important to study these risks.

III.4.3.2. Participants

This study included 200 participants aged between 17 and 80 years, with an average of 41 ± 23 years old. The gender distribution was 44.5% and 55.5% for male and female participants, respectively. The participants belong to different departmental areas in the laboratory (i.e., quality management, human resources, finance, administrative, commercial, and technical).

III.4.3.3. Data Collection

Aiming to perform the purposes defined before, a versatile tool to data collection was used. After taking into consideration, the advantages and limitations intrinsic to possible techniques, the inquiry by the questionnaire was chosen because it has a well-defined structure and enables the conversion of the qualitative information into a quantitative (McMillan & Schumacher, 2009; DeKetele & Roegiers, 2016; Cohen et al., 2017).

A questionnaire aiming to evaluate the perception of psychosocial risks in the workplace was designed specifically for this study and applied to a cohort of 200 employees. The questionnaire was organized into three sections, where the former one includes the general questions related with workers' age, gender, academic qualifications, and departmental areas. The second one comprises statements related with the work conditions, organization, leadership, career development, interpersonal relationships, and emotional feelings. Finally, the third section comprises issues related with the workers' opinions about the psychosocial risks. In the first part of the questionnaire the answers are descriptive, whereas in the second one the Likert scale with four levels (*strongly disagree*, *disagree*, *agree*, and *strongly agree*) was used. In the third section, the respondents choose five terms (the ones that they consider more relevant) from a list of 12 terms, ranking them in accordance with their relevance, using a numeric scale that varies from 1 to 5 (section III.4.7).

The validation of the questionnaire follows practices of Bell (Bell, 2010). Thus, the questionnaire was evaluated by a group of experts (i.e., a group of auditors) that suggested some corrections. After expert analysis, the questionnaire was modified and applied to a restrict group of employees, not included in the sample, to assess it validity and to identify difficulties in the interpretation of the questionnaire. The updated version was applied individually to the entire sample, in person, by the researcher. The return rate was 90.9% (200 inquiries received in 220 delivered).

III.4.3.4. Qualitative Data Processing

Aiming the conversion of qualitative information into quantitative information followed the method proposed by Fernandes et al. (2016b). As per this method, a set of *n* issues regarding a particular subject is itemized into a unitary area circle split into *n* slices, where the marks in the axis correspond to each one of the possible answers, as described in the section III.4.4.3.

III.4.3.5. Artificial Neural Networks

The software used to implement ANNs was the Waikato Environment for Knowledge Analysis (WEKA), keeping the default software parameters (Hall et al., 2009; Frank et al., 2016). Aiming to guarantee statistical significance of the results, 30 experiments were applied in all tests. In each simulation, the database was randomly split into two mutually exclusive partitions, i.e., the training set, with 2/3 of the data, used to build up the model, and the test set, with the remaining examples to evaluate its performance (Souza et al., 2002).

III.4.3.6. Ethical Aspects of the Study

The respondents took notice of the goals of the study participate voluntarily, without any pressure or coercion and were informed that their grades would not be affected. The participants gave an informed consent to participate in the study. The study was conducted in compliance with the relevant laws and institutional guidelines and was approved by the relevant authorities.

III.4.4. Results and Discussion

III.4.4.1. Sample Characterization

Respondents were organized into age groups (i.e., 17-20, 21-30, 31-50, 51-70 and higher than 70 years old). 79.5% of participants are aged between 21 and 50 years. In all age groups the percentage of female participants is higher, except in the group 31-50 where 22.5% of respondents are male and 20.5% are female (Figure 26A). Regarding academic qualification, 14.5% of the cohort stated to have basic education, 51.5% declared to finish secondary education, 30.0% affirmed to have a degree, and 4.0% declared to have post graduate education (Figure 26B). Figure 26B also shows that the distribution of respondents by gender is very similar for the different types of academic qualifications. Concerning departmental areas to which respondents belong, 7.5% are allocated to the quality management department, 4.0% to the human resources department, 11.5% to the finance department, 10.5% to the administrative department, 21.0% to the commercial department, and 45.5% to the technical department (Figure 26C). Figure 26C also shows that in all the departments the percentage of female respondents is higher, except in the administrative department where 5.5% of respondents are male and 5.0% female.

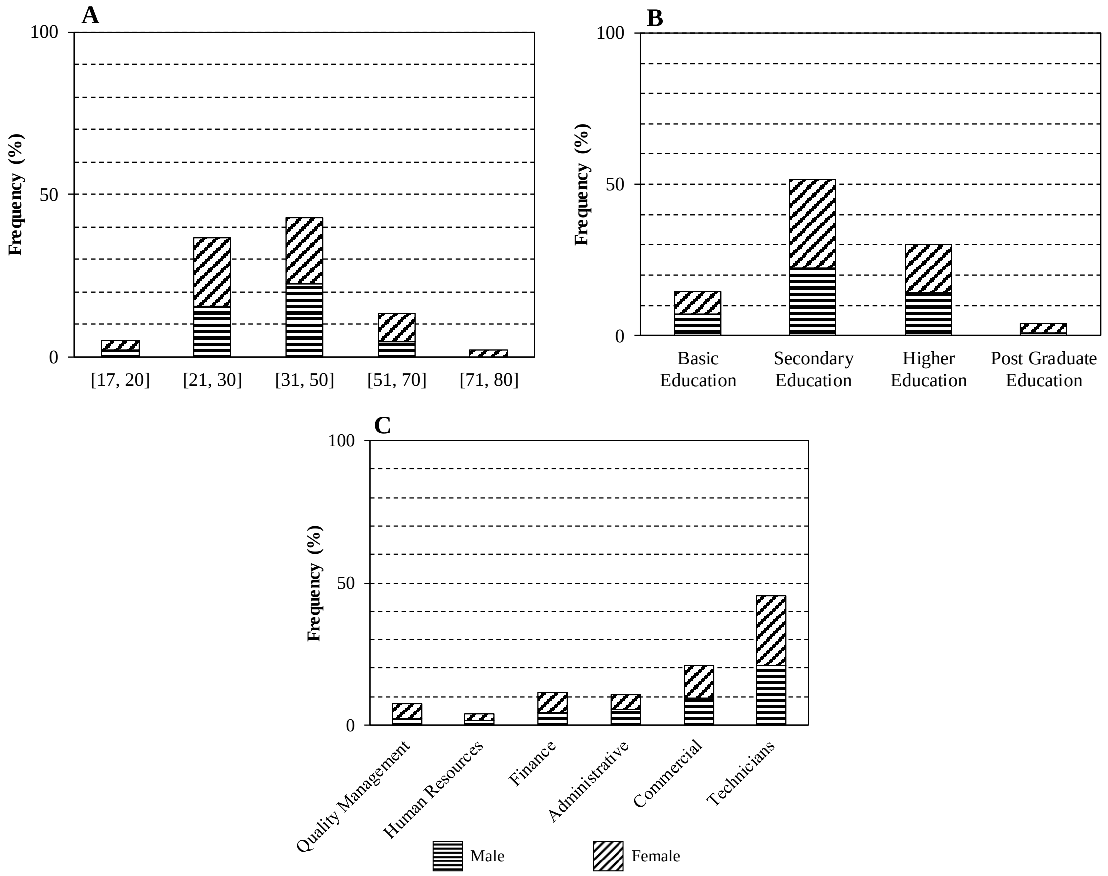

Figure 26 – (A) Sample characterization in terms of age groups. (B) Sample characterization in terms of academic qualifications. (C) Sample characterization in terms of departmental areas.

To characterize the laboratory, the graph shown in Figure 27 presents the distribution of the academic qualifications of the respondents by department. A perusal of Figure 27 reveals that only in quality management and human resources departments the percentage of respondents that claim to have higher education are greater than the percentage of respondents that declare to have basic/secondary education. The remaining departments show an inverse trend, being the administrative, commercial, and technical departments those that present differences higher than 7.5% between respondents with basic/secondary and higher education.

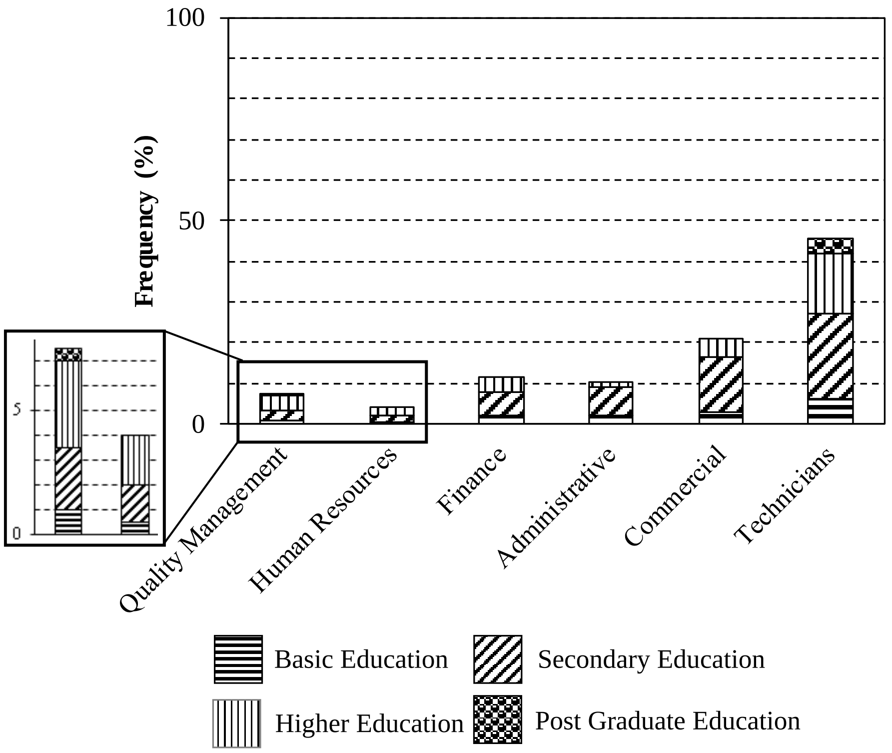

Figure 27 – Distribution of academic qualifications of the respondents by department.

III.4.4.2. Answer Frequency Analysis

Figure 28 presents the results obtained in the second part of the questionnaire, where respondents expressed their opinion on the sets of statements regarding each of the psychosocial risk factors. The graphs show the frequency of answering to each factor statement (Table 9).

Table 9 – Correspondence between the statements included in the questionnaire and the psychosocial risk factors.

Factor	Working conditions	Work organization	Leadership	Career development	Interpersonal relationships	Emotional feelings
Statements	S1 – S4	S5 – S7	S8 – S10	S11 – S13	S14 – S16	S17 – S20

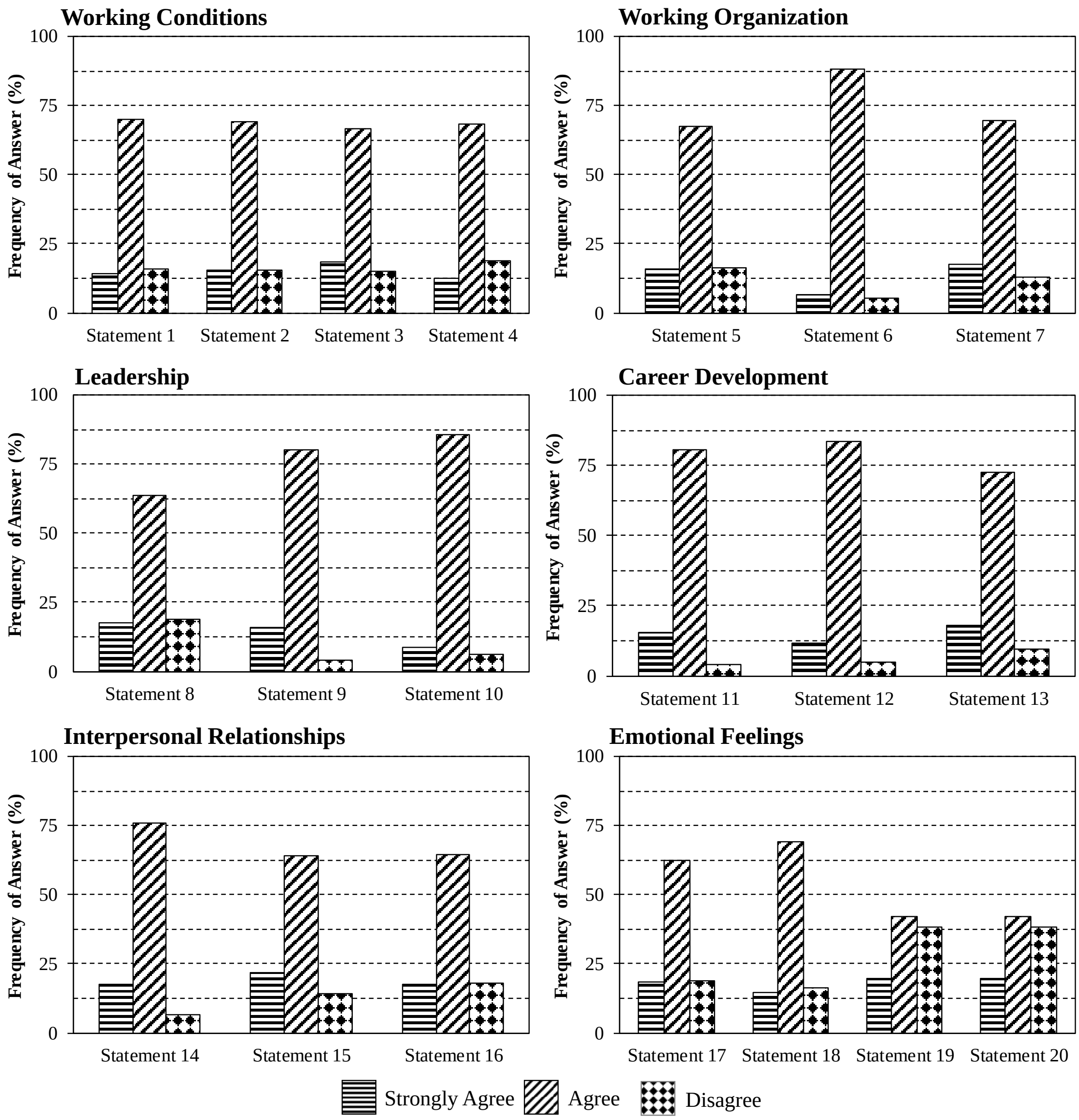

Figure 28 – Respondents' agreement/disagreement with the statements regarding each factor.

Regarding *Working Conditions*, the analysis of results shows that a percentage of respondents ranging between 66.5% and 70.0% consider they have good working conditions (S1), resources and equipment adequate to perform the work (S2). Furthermore, they consider that the work is not monotonous and routine (S3) and need learning and ongoing updates (S4). However, a percentage ranging from 15.0% to 19.0% has an opposite opinion, which may point out a need for improvement. With regard to *Work Organization*, the overwhelming majority of respondents consider that decision making and goal setting take into account the workers' opinions (S6). Taking a glance to the answers related to goal setting (S5) and the service distribution (S7) shows that the majority of the participants declare they are clear and evenly, respectively. However, a percentage of about 10% disagree, which may suggest that leaders should pay attention to these points. The results related to *Leadership* show that most respondents claim that their work is recognized (S10) and has a favorable opinion about leadership (S9). Nevertheless, 19.0% state that the guidelines and priorities are unclear (S8), being an issue that should be improved. Concerning *Career Development*, the overwhelming majority of participants have a very positive opinion. Only a percentage less than 10% is dissatisfied with the expectations of career development. The graphs related with *Interpersonal Relationships* (S14 to S16) show that more than 80% of respondents consider that there is a good relationship between colleagues. However, 14.0% and 18.0% of respondents have a negative opinion regarding communication and information sharing (S15) and mutual help/support (S16), respectively. These relatively high values of unfavorable opinions indicate that this is a point where improvements are needed. Finally, with regard to *Emotional Feelings* (S17 to S20), most participants have a favorable opinion, which ranges between 61.5% (S19, S20) and 83.5% (S18). In fact, the statements related with professional life/personal life overlapping (S19) and time available/tasks to perform (S20) collected the highest number of negative responses.

The statements included in the questionnaire were elaborated so that a higher percentage of positive answers correspond to a lower psychosocial risk. Thus, the overall analysis of the results shown in Figure 28 suggests that the factors *Interpersonal Relationships* and *Emotional Feelings* are the ones that more contribute to psychosocial risk in the organization under study. Conversely, *Leadership* and *Career Development* seem to have a minor contribution.

These results are in agreement with those obtained by Ando et al. (2000) and MacDonald et al. (2001). The authors refer that a strong association between psychosocial risk factors in the workplace and musculoskeletal disorders exists, identifying the working conditions (e.g., monotony, routine and repetitive movements) as the main cause.

Figure 29 presents the results obtained in the third part of the questionnaire, where respondents select and classify, based on their opinion, the five more relevant terms related with psychosocial risks. The frequency of term selection is presented in the bar chart and may be read on the left side scales. The frequency of term priority (scale on the right side) was computed considering only the respondents that chose that term. The analysis of the frequencies of term selection allows identifying three groups. The first one includes the terms *Lack of Resources*, *Stress*, and *Concentration* that were selected by more than 40% of respondents. The second group comprises the terms *Working Hours*, *Control*, *Lab Equipment*, and *Precariousness* that were chosen by 30.0% to 36.0% of respondents. Finally, the third group is formed by the terms *Trials*, *Violence*, *Insecurity*, *Rhythm*, and *Routine*, chosen by less than 20% of respondents.

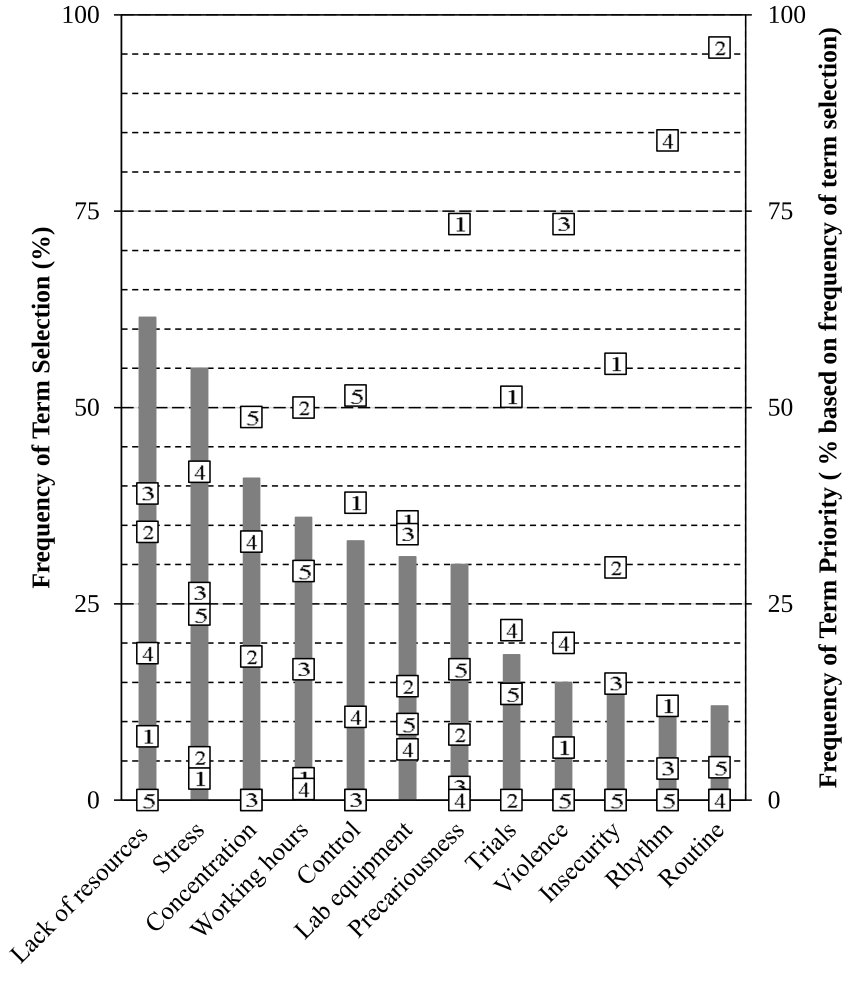

Figure 29 – Frequency of term selection versus term priority (considering only the respondents that choose the term).

Regarding the priority given to the selected terms, only a small percentage of participants who chose terms of group 1, classified them as the first priority (ranging from 0.0% to 8.0%) or as the second priority (varying between 5.4% and 34.1%). *Lack of Resources*, *Stress*, and *Concentration* were mainly chosen as the third, fourth and fifth priority, respectively (Figure 29). Despite the fact that they were selected by more than 40% of respondents, the terms of group 1 are not considered as the ones that best describe psychosocial risks. As regards to the terms of the second group, it should be emphasized that *Precariousness*, *Control*, and *Lab Equipment* were classified as the first priority by, respectively, 73.3%, 37.9%, and 35.5% of the participants who selected them. Furthermore, it should be highlighted that *Working Hours* was classified as the second priority by 50.0% of the respondents who selected it. Finally, in the third group there was a similar trend. *Insecurity* and *Trials* were classified as the first priority, respectively by 55.6% and 51.3% of the participants who selected them, whereas *Routine* was classified as the second priority by 95.8%. These results suggest that the terms of second and third groups, although chosen by a smaller number of respondents, were considered by them as the best to describe the psychosocial risks.

The graph presented in Figure 30 shows the relative frequency of binary associations between terms selected by more than 30% of participants. Their analysis shows that any possible combination of terms of group 1 (*Lack of Resources*, *Stress*, and *Concentration*) was chosen by at least 33% of participants. Regarding associations between terms of group 1 and group 2, only the combination between *Stress* and *Working Hours* was selected by more than 33% of participants. The associations *Stress* and *Precariousness*, *Concentration* and *Precariousness*, *Concentration* and *Working Hours* and all possible combinations between *Lack of Resources* and terms of group 2 (*Working Hours*, *Control*, *Lab Equipment* and *Precariousness*) were chosen by a percentage of participants ranging between 20.0% and 33.3%. The remaining binary associations were selected by less than 20% of participants.

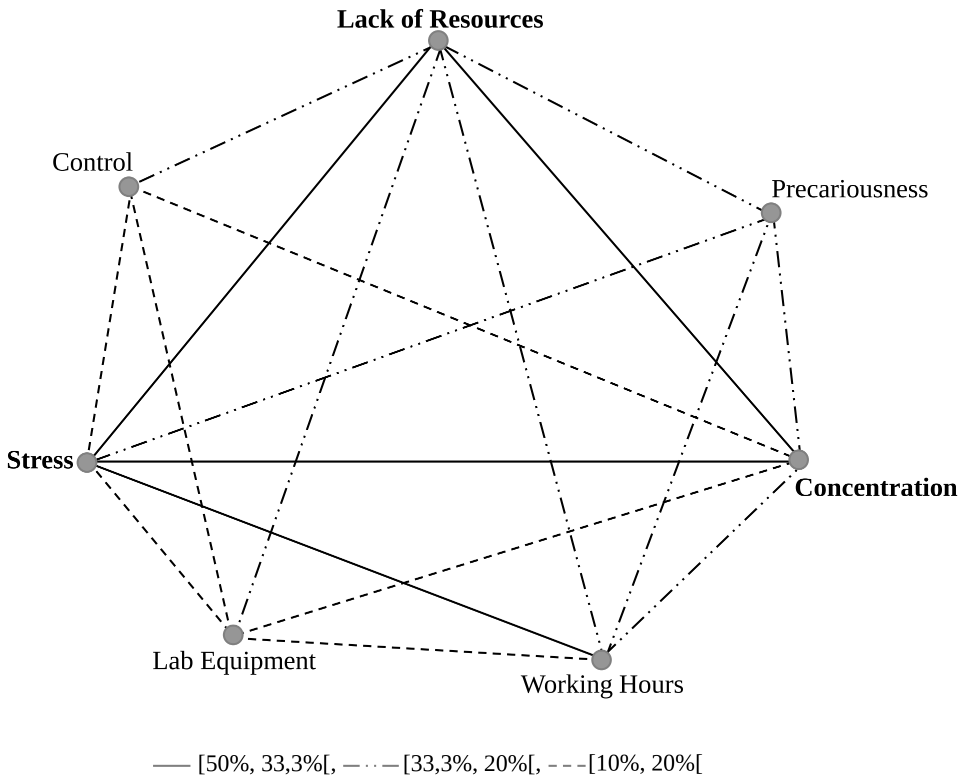

Figure 30 – Binary associations between terms selected by more than 30% of respondents. (Bold stands for terms of first group and no-bold denotes terms of second group).

The frequency of association between sets of three terms was also studied (Figure 31). It was found that the terms of the group 1 were simultaneously selected by a percentage of participants ranging between 25.0% and 33.3%, as well as all ternary associations between *Precariousness* and terms of first group. Sets of three terms containing *Working Hours* and terms of first group were selected by at least 15% of respondents. To finish the analysis of Figure 31, it also noted that a percentage between 10.0% and 15.0% of respondents set associations between *Rhythm*, *Lack of Resources* and *Stress*; *Routine*, *Lack of Resources* and *Stress*; and *Trials*, *Lack of Resources* and *Concentration*.

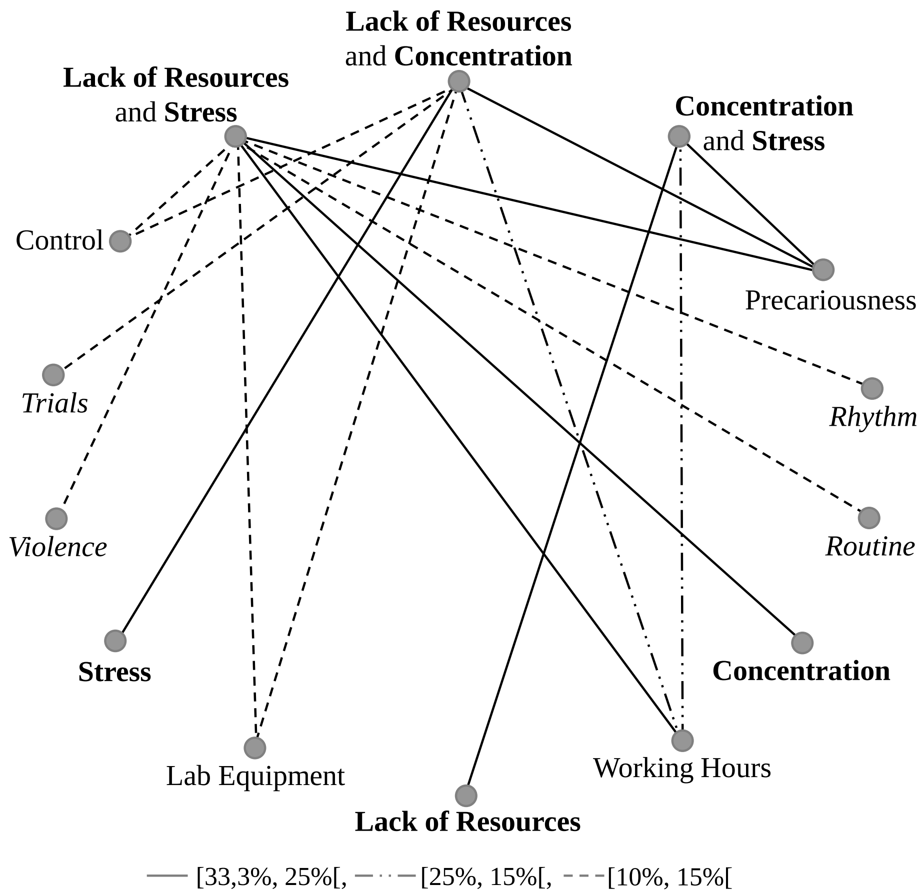

Figure 31 – Ternary associations between terms. (Bold stands for terms of first group, no-bold denotes terms of second group, and italics indicate terms of third group).

The graph depicted in Figure 32 shows the frequency of quaternary associations between terms selected by the participants. Its analysis shows that *Lack of Resources*, *Concentration*, and *Stress* were chosen simultaneously with *Precariousness* by 23.0% of participants and with *Working Hours* by 19%. Quaternary associations between terms of group 1 and the remaining terms of group 2, i.e., *Control* and *Lab Equipment*, exhibit frequencies less than 5%. Regarding terms of third group, only *Violence* and *Insecurity* were selected together with the terms of group 1.

In addition, this analysis enables to identify, among the less selected factors, the ones that present a strong association with the most chosen by the respondents. A perusal to Figure 29 and Figure 32 reveals that *Precariousness* (selected by only 30% of respondents) was associated in 23% of cases with the terms of group 1, being ticked as first priority by 73.3% of those who chose it. A similar result was obtained for *Working Hours*, selected by 36% of respondents, but linked in 19% of cases to the terms of group 1, being ticked as second priority by 50.0% of those who chose it.

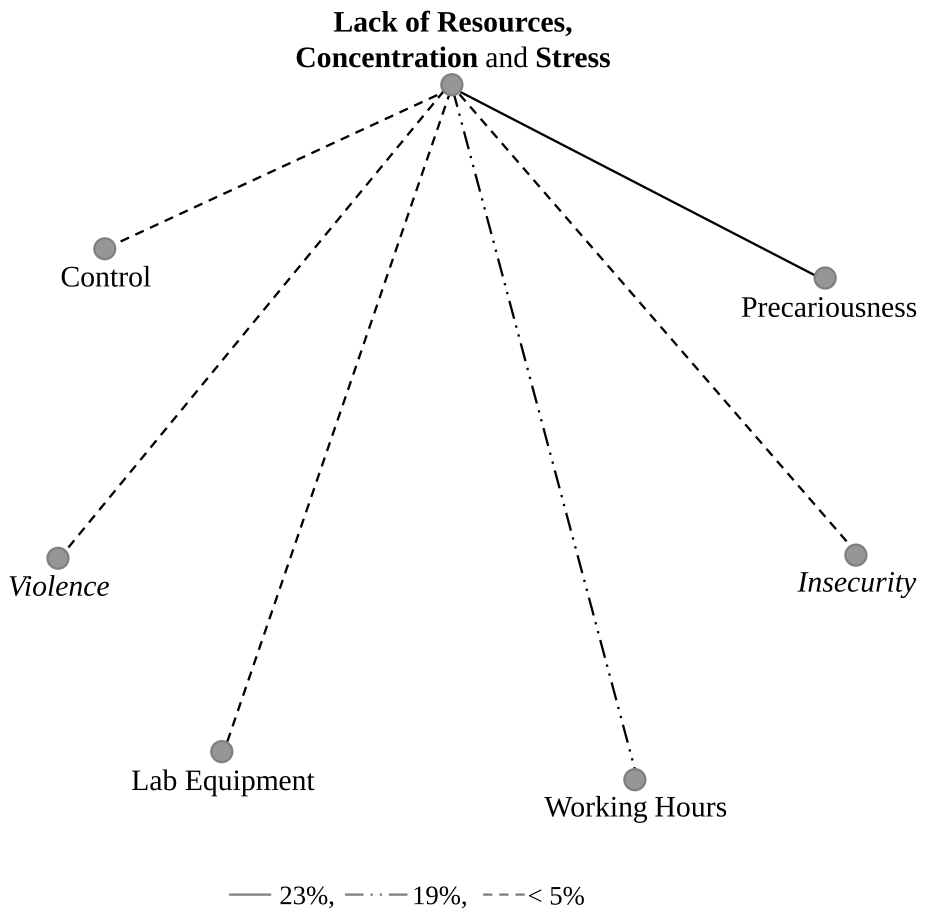

Figure 32 – Quaternary associations between terms. (Bold stands for terms of first group, no-bold denotes terms of second group, and italics indicate terms of third group).

III.4.4.3. Psychosocial Risk Assessment

Aiming to gather information about psychosocial risk factors, the second section of the questionnaire comprises statements related to work conditions, organization, leadership, career development, interpersonal relationships, and emotional feelings. Figure 33 shows the answers of respondent #1 to the second part of the questionnaire.

PSYCHOSOCIAL RISKS QUESTIONNAIRE

PART II

For each statement tick the option that best reflects your opinion.

Working Conditions	Strongly Agree	Agree	Disagree	Strongly Disagree
S1. There are good working conditions.	☒	☐	☐	☐
S2. There are resources and equipment needed to perform the work.	☐	☒	☐	☐
S3. The work done isn't monotonous and routine.	☐	☐	☒	☐
S4. Work requires learning and ongoing updates.	☐	☐	☒	☐

Work Organization	Strongly Agree	Agree	Disagree	Strongly Disagree
S5. There is a clear definition of objectives.	☐	☒	☐	☐
S6. There is involvement in decision making and goal setting.	☐	☒	☐	☐
S7. The service is distributed evenly.	☐	☒	☐	☐

Leadership	Strongly Agree	Agree	Disagree	Strongly Disagree
S8. The leader gives clear guidelines and sets priorities for the team	☐	☐	☒	☐
S9. The leader knows when to support and advise or give autonomy.	☐	☒	☐	☐
S10. The leader recognizes your work.	☐	☒	☐	☐

Career Development	Strongly Agree	Agree	Disagree	Strongly Disagree
S11. Employees aren't professionally stagnant.	☒	☐	☐	☐
S12. Prospects for career progression are good.	☒	☐	☐	☐
S13. The training and knowledge gained are valued for career progression.	☐	☒	☐	☐

Interpersonal Relationships	Strongly Agree	Agree	Disagree	Strongly Disagree
S14. There is a good relationship with your colleagues.	☐	☒	☐	☐
S15. There is good communication and sharing of information between colleagues.	☐	☐	☒	☐
S16. The help and support of the colleagues are frequent.	☐	☐	☒	☐

Emotional Feelings	Strongly Agree	Agree	Disagree	Strongly Disagree
S17. The situations of verbal violence aren't recurrent.	☐	☒	☐	☐
S18. There is flexibility and understanding for family life.	☐	☐	☒	☐
S19. Work sometimes overlaps with social and family life.	☐	☐	☒	☐
S20. The time you have is enough to accomplish your tasks.	☐	☐	☒	☐

Figure 33 – The answers of respondent #1 to the second part of the questionnaire.

To quantify the qualitative information presented in Figure 33 the method proposed by Fernandes et al. (2016b) was followed. For each dimension (i.e., work conditions, organization, leadership, career development, interpersonal relationships, and emotional feelings) the correspondent answers were itemized into a unitary area circle. The marks in the axis correspond to the possible answer, i.e., *strongly agree*, *agree*, *disagree*, and *strongly disagree*. Taking as an example the dimension *work conditions*, the answer of respondent #1 to statement 1 (S1) was *strongly agree*, and the correspondent area is computed as $\frac{1}{4} \times \pi \times \left(\frac{1}{\sqrt{\pi}}\right)^2 = 0.25$; the answer to the statement 2 (S2) was the alternative *agree* and the area is $\frac{1}{4} \times \pi \times \left(\frac{3}{4} \times \frac{1}{\sqrt{\pi}}\right)^2 = 0.14$. Finally, for the statements 3 and 4 (S3 and S4), the answers were d*isagree* and the areas are $\frac{1}{4} \times \pi \times \left(\frac{2}{4} \times \frac{1}{\sqrt{\pi}}\right)^2 = 0.06$. The total area (i.e., 0.51) is the sum of the partial ones, being the quantitative value regarding the dimension *work conditions* for respondent #1 (Figure 34). For the remaining dimensions, the procedure is similar, and the results are shown in Table 10.

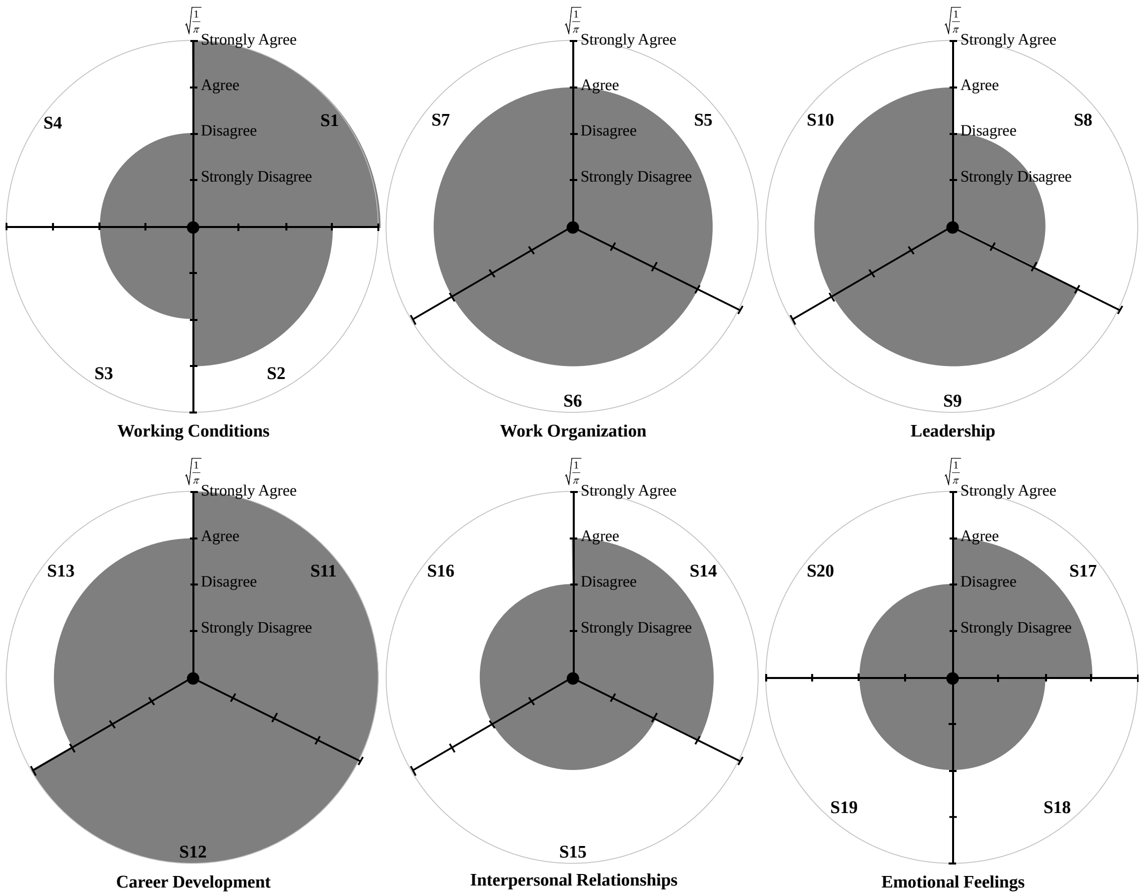

Figure 34 – A view of the qualitative data processing.

Table 10 – A fragment of the knowledge base for psychosocial risk assessment.

#	Working conditions	Work organization	Leadership	Career development	Interpersonal relationships	Emotional feelings
1	0.51	0.57	0.46	0.85	0.35	0.19
2	0.67	0.71	0.35	0.57	0.46	0.40
…	…	…	…	…	…	…
200	0.70	0.60	0.85	0.71	0.57	0.48

The performance of the ANN model can be assessed through the confusion matrix. Table 11 presents the confusion matrix for the ANN model shown in Figure 35 (The values indicate the average of the 30 experiments). The values presented in Table 11 allow computing the model accuracy for training set (93.4%, i.e., 127 well classified in 136) and for test set (90.6%, i.e., 58 well classified in 64).

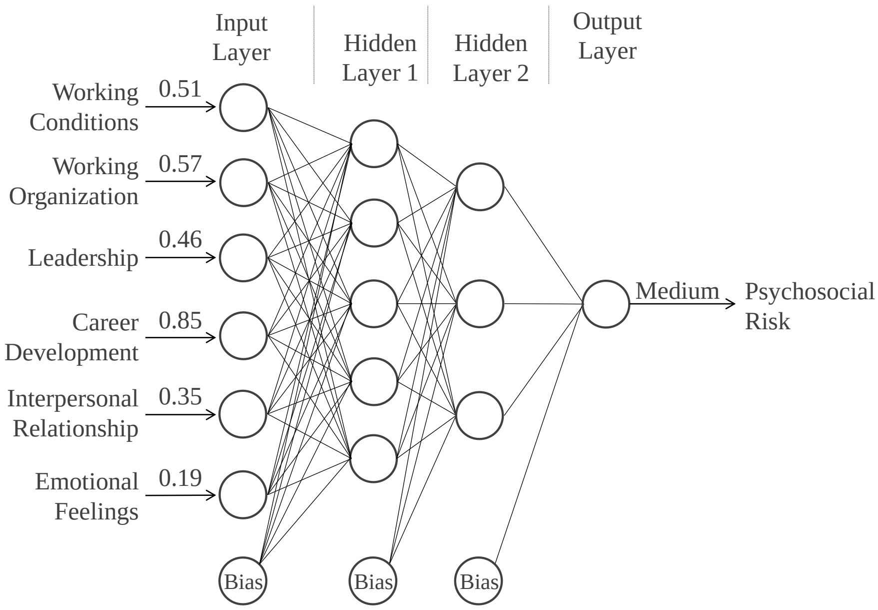

Figure 35 – The ANN model for psychosocial risks assessment.

Table 11 – Confusion Matrix regarding ANN model for psychosocial risks assessment.

Target	Predictive					
	Training set			Test set		
	Low	Medium	High	Low	Medium	High
Low	15	2	1	4	1	0
Medium	1	98	4	0	48	5
High	0	1	14	0	0	6

To compute the sensitivity, specificity, Positive Predictive Value (PPV), and Negative Predictive Value (NPV) of the model, the confusion matrixes regarding each possible output were conceived (Table 12). Sensitivity evaluates the proportion of positives cases (i.e., *Low*, *Medium*, or *High*) that are correctly identified as such, whereas specificity translates the proportion of negative ones that are correctly identified (i.e., *No-Low*, *No-Medium*, or *No-High*). PPV stands for the proportion of *Low*, *Medium*, or *High* cases well classified, whereas NPV denotes the proportion of *No-Low*, *No-Medium*, or *No-High* cases well labeled (Florkowski, 2008; Vilhena et al., 2016). Table 13 presents the values obtained for those metrics. Sensitivity and specificity exhibit high values, from 0.80 to 0.99, indicating that the model exhibits a good performance in the evaluation of psychosocial risks. Regarding PPV and NPV, the values range between 0.94 and 0.99, except for $PPV_{output\text{-}High}$ and $NPV_{output\text{-}Medium}$ (0.74, 0.54 and 0.86, 0.67, respectively, for training and test). Those results show that the confidence that can be placed when the model classifies a case as *High* or *No-Medium* is lower. Despite those weaknesses, the overall performance of the model is not affected. In fact, the model should avoid classifying the *High* cases as *Low* or *Medium*, to identify all the problematic cases, i.e., workers at high psychosocial risk.

III.4.5. Study Limitations

The results obtained in this study were very interesting. However, it is important to mention some limitations that prevented a more detailed assessment of the psychosocial risks to which workers in this type of laboratory are exposed. The main limitation is related to the sample size. The reduced number of workers in some departmental areas did not allow a more detailed analysis (i.e., department by department) of the psychosocial risks associated with the performance of different tasks with workloads differentiated. With a larger sample, it would also be possible to study the influence of other variables such as age, gender, or academic qualifications.

The questionnaire used to collect the data was conceived to be general, i.e., to be applied to all employees, regardless of the sector of the laboratory to which they belong. However, with a larger sample, differentiated data collection tools could be designed specifically for each departmental area.

Table 12 – Confusion matrix regarding each output classes of the ANN model for psychosocial risks assessment.

Target	Predictive			
	Training set		Test set	
	Low	No-low	Low	No-low
Low	15	3	4	1
No-low	1	117	0	59

Target	Predictive			
	Training set		Test set	
	Medium	No-medium	Medium	No-medium
Medium	98	5	48	5
No-medium	3	30	1	10

Target	Predictive			
	Training set		Test set	
	High	No-high	High	No-high
High	14	1	6	0
No-high	5	116	5	53

Table 13 – Sensitivity, specificity, Positive Predictive Value (PPV) and Negative Predictive Value (NPV) for each output classes of the ANN model, split by training and test.

Output	Training set				Test set			
	Sensitivity	Specificity	PPV	NPV	Sensitivity	Specificity	PPV	NPV
Low	0.83	0.99	0.94	0.97	0.80	1	1	0.98
Medium	0.95	0.90	0.97	0.86	0.91	0.91	0.98	0.67
High	0.93	0.96	0.74	0.99	1	0.91	0.54	1

III.4.6. Conclusions

Nowadays, psychosocial risk assessment has been left to the discretion of each organization. However, the standards used (i.e., OHSAS 18001 and ISO 9001) are not clear as to how these risks should be measured. The certifications based on these standards do not guarantee that psychosocial risks are, in fact, controlled. This study showed that *Interpersonal Relationships* and *Emotional Feelings* are the factors that more contribute to psychosocial risks, particularly the issues related with the overlapping of working and personal lives, the lack of time to accomplish some tasks, the sharing of information, and peer support. This study also revealed that the concept of psychosocial risks is generally present among most respondents. Despite respondents having ticked the terms *Lack of Resources*, *Stress*, and *Concentration* as the ones that better describe the psychosocial risks, the terms *Precariousness*, *Control*, and *Lab Equipment* were the ones most often marked as first priority. Moreover, the terms *Lack of Resources*, *Working Hours*, and *Lab Equipment* were chosen simultaneously by a great number of respondents, as well as the terms *Stress*, *Working Hours*, and *Precariousness*. In addition, this work presents an intelligent decision support system that stands for a new approach to this problem using the ANN paradigm to assess psychosocial risks. The presented approach presents a worthy performance exhibiting sensitivities and specificities higher than 80%. This approach focuses on the processing of information, collected through inquiry by questionnaire, and aims to prevent recurrent events and to enhance the psychosocial risks management. Beyond the possibility of identifying the weakness of the organization, this system allows to concept and to design future improvement actions to promote the employees' quality of life. The results of this study cannot be generalized to all organizations because the employees are exposed to different risks depending on the sector and the type of activity in which they operate. However, these kinds of models can be used in any organization. For this, it is necessary to carry out an assessment of the risks to which employees are exposed and adjust the data collection tools (i.e., questionnaires).

III.4.7. Psychosocial Risks Questionnaire

PSYCHOSOCIAL RISKS QUESTIONNAIRE

The work environment and the nature of work significantly influence health.

In recent decades, there have been significant changes (closely linked to the nature, organization and management of work) that have resulted in emerging risks and new challenges in the field of occupational health and safety, including known as psychosocial risks that can lead to a serious deterioration in the physical and mental health of workers.

The present questionnaire addresses a number of issues relating to how employees perceive the organization in order to assess the existence of psychosocial risks in the workplace.

Note: The Laboratory protects your privacy. The personal data collected will be processed by computer and will not be transferred to any other institution not used for any purpose other than the support to the Internal Quality Management System.

PART I

Tick the box that corresponds to your case.

Gender	Feminine ☐	Masculine ☐		

Academic Qualifications	Basic Education ☐	Secondary Education ☐	Higher Education ☐	Post Graduate Education ☐

Age	Less than 20 ☐	From 21 to 30 ☐	From 31 to 50 ☐	From 51 to 70 ☐	More than 70 ☐

Departmental Areas	Quality Management ☐	Human Resources ☐	Finance ☐	Administrative ☐	Commercial ☐	Technical ☐

PSYCHOSOCIAL RISKS QUESTIONNAIRE

PART II

For each statement tick the option that best reflects your opinion.

Working Conditions

	Strongly Agree	Agree	Disagree	Strongly Disagree
S1. There are good working conditions.	☐	☐	☐	☐
S2. There are resources and equipment needed to perform the work.	☐	☐	☐	☐
S3. The work done isn't monotonous and routine.	☐	☐	☐	☐
S4. Work requires learning and ongoing updates.	☐	☐	☐	☐

Work Organization

	Strongly Agree	Agree	Disagree	Strongly Disagree
S5. There is a clear definition of objectives.	☐	☐	☐	☐
S6. There is involvement in decision making and goal setting.	☐	☐	☐	☐
S7. The service is distributed evenly.	☐	☐	☐	☐

Leadership

	Strongly Agree	Agree	Disagree	Strongly Disagree
S8. The leader gives clear guidelines and sets priorities for the team.	☐	☐	☐	☐
S9. The leader knows when to support and advise or give autonomy.	☐	☐	☐	☐
S10. The leader recognizes your work.	☐	☐	☐	☐

Career Development

	Strongly Agree	Agree	Disagree	Strongly Disagree
S11. Employees aren't professionally stagnant.	☐	☐	☐	☐
S12. Prospects for career progression are good.	☐	☐	☐	☐
S13. The training and knowledge gained are valued for career progression.	☐	☐	☐	☐

PSYCHOSOCIAL RISKS QUESTIONNAIRE

Interpersonal Relationships	Strongly Agree	Agree	Disagree	Strongly Disagree
S14. There is a good relationship with your colleagues.	☐	☐	☐	☐
S15. There is good communication and sharing of information between colleagues.	☐	☐	☐	☐
S16. The help and support of the colleagues are frequent.	☐	☐	☐	☐

Emotional Feelings	Strongly Agree	Agree	Disagree	Strongly Disagree
S17. The situations of verbal violence aren't recurrent.	☐	☐	☐	☐
S18. There is flexibility and understanding for family life.	☐	☐	☐	☐
S19. Work sometimes overlaps with social and family life.	☐	☐	☐	☐
S20. The time you have is enough to accomplish your tasks.	☐	☐	☐	☐

PART III

From the 12 terms presented, select 5 which in your opinion best describe the psychosocial risks, classifying them from 1 to 5 where 1 is the most important and 5 is the least important.

Rhythm	☐	Routine	☐	Working hours	☐	Concentration	☐
Control	☐	Insecurity	☐	Lab equipment	☐	Stress	☐
Precariousness	☐	Violence	☐	Lack of resources	☐	Trials	☐

Thank you for your cooperation!

III.5. Synopsis

In addition to quality control, laboratories also need adequate management. The costs associated with poor quality are as high or higher than the costs associated with maintaining high quality standards. Currently, all organizations in general, and laboratories in particular, are asked to innovate, provide better products/services, enable the customization of products/services, meet deadlines, improve layouts, reduce accident rates, reduce waste/consumption, ensure compliance with legal provisions, ensure the protection of information, improve working conditions, promote social responsibility policies and, above all, make a profit. Within the scope of this chapter, the study **"Fully Informed Classification Systems Simpler, Maybe Better"** was presented in which it was shown how important the failure prediction in public service organizations is. In spite of being a complex topic, a model was proposed to prevent unfavorable events (adverse events) using the Eindhoven classification method. The adverse event "*deadline to respond to the request exceeded*" was chosen and the respective causal tree was built, which includes causes that can be considered simultaneously or separately. The model presented allows describing events for which the causes are unknown/prohibited/not allowed. It also allows the use of benchmarking in public organizations by providing details to resolve and alert about problems found.

In addition to the importance of predicting failures in the management of an organization, the quality of services will also be higher if customers' demands are also higher. The study **"A Conceptual Model to Assess the Literacy of Water Consumers"** sought to develop a methodology to assess literacy on the theme of water. A conceptual model was proposed, and its articulation with the PDCA cycle was demonstrated. In addition, a literature review was carried out and it was found that, despite the high number of studies on literacy, there are very few on the quality of water for human consumption. To fill this gap, a questionnaire was created and applied to consumers of the municipality of Santiago do Cacém. The results point out to a low literacy level of the respondents about water quality topics, regardless of the competence investigated (i.e., *Access*, *Understand*, *Appraise* or *Apply*). In fact, respondents revealed greatest difficulties in assessing the effectiveness of the solutions/information, as well as in its implementation.

The demand for service quality and competitiveness can lead to deteriorating working conditions and the appearance of psychosocial risks. The study **“Psychosocial Risks Assessment in Cryopreservation Laboratories”** aimed to characterize psychosocial risks in laboratories and to develop a predictive model for their management. The methodology used to collect the information was the inquiry by questionnaire, applied to a sample of 200 employees. The results show that most respondents are aware of psychosocial risks, identifying interpersonal relationships and the emotional component as the main factors that lead to this type of risk. In addition, terms/expressions such as *lack of resources*, *working hours*, *laboratory equipment*, *stress* and *precariousness* showed a strong correlation with psychosocial risks. The model presented in this study, based on artificial neural networks, worked well in predicting this type of risk.

Chapter IV. Total Quality Management

IV.1. Overview

Following the evolution of the Quality Management concept, the Total Quality Management (TQM) concept appeared. According to the Quality Management concept, work is understood to belong to everyone and such thinking must cover all stages of the process, giving rise to an organizational policy that provides synergies between all sectors of the organization (Pohlmann, 2005; Alves, 2009). For its part, TQM does not only focus on organization, but mainly on customers and employees. TQM is a philosophy guided by the principles mentioned below (Westcott, 2013), like the quality management principles contained in the ISO 9001 standard (Neves et al., 2015), viz.

- **Customer focus** – The customer is the one who ultimately determines the quality level of a product or service. If quality is not perceived by the customer, the product or service has no value;
- **Total employee involvement** – TQM encourages teamwork. A favourable environment should be created, without intimidation and promoting decentralization, in order to give workers greater autonomy and decision-making power;
- **Process-centric** – Processes must be managed and improved. For this, it is necessary to define the activities that constitute them and to measure their performance through indicators;
- **Integrated system** – The organizational system must be integrated, so that the processes are interconnected. The work culture must be transversal to the entire organization so that excellence is achieved;
- **Strategic and systematic approach** – The strategic planning of an organization must be guided according to its vision, mission and objectives, with quality as a central element;
- **Continuous improvement** – The organization must seek to continuously improve its processes and critically analyse the problems, in order to propose solutions to reinforce its competitiveness and promote the satisfaction of all interested parties;
- **Making decisions based on facts** – Decisions must be made based on analysis and data collection. Historical data recording may be useful for future forecasts; and

- **Effective communication** – Communication between workers must be effective, as this has a significant impact on their motivation.

TQM currently represents the main quality guideline (Han et al., 2007), where more and more technologies are used and that contribute to the free circulation of personal data. In the health sector, given the extremely sensitive nature of data, the protection of personal data has gained increasing relevance after the mandatory implementation of the General Data Protection Regulation (GDPR). Within the scope of the provision of cryopreservation and storage of stem cells, both of blood and umbilical cord tissue, it is necessary to collect and process personal data of patients related to physical or mental health, information about their past health status or present, information obtained from analysis or examination of a body part or biological samples, information about a disease, disability, medical history or clinical treatment. Thus, it is necessary to process and maintain this data in accordance with the GDPR, to ensure due security and confidentiality.

In the context of the current pandemic situation, organizations have had to adopt strategies to maintain productivity, the satisfaction of employees and customers. The exceptional situation that the world is going through, facing the pandemic crisis caused by COVID-19, transformed the world of work, and brought big and fast changes in organizations, business models and work management. COVID-19 is a disease caused by the new coronavirus SARS-COV-2, which can cause severe respiratory infection such as pneumonia. This virus can be transmitted through the respiratory droplets of the infected person when he speaks, coughs or sneezes. On the other hand, the contact of the hands with infectious respiratory secretions existing in the material components of the work (e.g., tools, machines, or equipment) and subsequent transfer to the mucous membranes (from the mouth, nose or eyes) is also a form of transmission of the COVID-19 in the workplace. Therefore, it is necessary that each organization (re)assesses the risks and adopts the necessary measures to prevent and protect against infection by SARS-COV-2, in order to protect work about conditions of hygiene, safety and health to all workers, as recommended by the Constitution of the Portuguese Republic, the Labour Code and the Basic Health Law (Decree-Law No. 10-A/2020).

In this context, the studies presented in this chapter aim to contribute to the effective functioning of an organization, namely:

- **IV.2 – An Assessment of Data Guidelines in Cryopreservation Laboratories[6];**
- **IV.3 – A Case-Based Approach to Assess Employees' Satisfaction with Work Guidelines in Times of the Pandemic[7];**
- **IV.4 – Customers' Satisfaction Assessment in Water Laboratories[8]**

The study IV.2 was designed to support the cryopreservation laboratory in the implementation of the GDPR, to guarantee the safety and confidentiality of genetic data, analysis, and information on diseases.

According to Fernandes et al., (2016a; 2016b; 2019) evaluating satisfaction is essential for companies that seek competitive advantage in the market. With the study IV.3 it was intended to know the satisfaction of the collaborators regarding the implementation of the new processes and methodologies imposed in the scope of the pandemic COVID-19. Finally, the study IV.4 aimed to assess customer satisfaction considering the technical and management requirements of the ISO/IEC 17025 standard in a water laboratory.

[6] Published, in *Proceedings of the 2021 International Symposium on Electrical, Electronics and Information Engineering (ISEEIE 2021)*. ISBN: 978-1-4503-8983-9

[7] Published in *Communications in Computer and Information Science*, 1277: 183–196, 2020.

[8] Submitted to *AQUA – Water Infrastructure, Ecosystems and Society*.

IV.2. An Assessment of Data Guidelines in Cryopreservation Laboratories

IV.2.1. Introduction

New technologies have changed the economy and social life and facilitated the free flow of personal data. The collection and dissemination of such data has increased significantly in all areas of society, not only because people are increasingly making their personal data available, but also because the new technologies enable the use/dissemination of personal data by private/public institutions. Loss of control over personal data can cause physical, material, or immaterial damage to citizens. Therefore, the issues of data protection have become increasingly important, and the General Data Protection Regulation (GDPR) in force in the European Union since May 25, 2018 was the last step in the direction of data protection (European Parliament, 2016). In the health sector, given the extremely sensitive nature of the data, the application of this regulation is compulsory in order to ensure proper security and confidentiality (Sørensen et al., 2012). In this sector, personal data can be associated with physical or mental health; past, present or future state of health; information from analyzes or examinations of a part of the body or samples; genetic data; Information about an illness, disability or risk of illness; anamnesis, treatments; or physiological/biomedical status. Indeed, the GDPR is still a controversial issue in the health sector and has been the subject of various studies and debates around the world (McCall, 2018; Morriss-Roberts et al., 2018). Demotes--Mainard et al. (2019) discuss the problem of transparency and data sharing (i.e., the foundations of open science), the potential of big data analytics, and the reuse of hospital data and health databases in the face of GDPR restrictions. The authors stress that European countries should avoid poorly interoperable regulatory systems and make the necessary adjustments to protect users' data while streamlining clinical research. To this end, they emphasize the need to define in the context of health what is understood as anonymous data, pseudonym data as well as the public interest. In addition, the authors emphasize the importance of the patient's initial consent encompassing future research, and express how the data will be accessed, rather than restricting its use in future research. They also underscore the need for a technology infrastructure that enables researchers to access repositories and stores to reuse data (Demotes-Mainard et al., 2019). Flaumenhaft & Ben-Assuli (2018) discuss the main barriers that have led to relatively low acceptance of personal health records and avoided their widespread use. The authors state that concerns about the security and privacy of this sensitive data are one of the main obstacles. The study examines in detail the more relevant characteristics related to the security and privacy of health data in five jurisdictions. The authors point out that the revised legislation needs to highlight the GDPR as it is the most understanding and strictest data protection measures (Flaumenhaft & Ben-Assuli, 2018). In some key areas, however, there are still different interpretations and show a certain ambiguity (e.g. the introduction of the term pseudonymization) (Mourby et al., 2018). Mense & Blobel (2017) compare the key features of the GDPR and the functional model of the HL7 Personal Health Record System (HL7 PHR-S FM). According to the authors, the security and data protection standards HL7 PHR-S FM enable the efficient implementation of the GDPR, i.e., meeting the goals of the legislature and clearly defining the steps organizations should follow to ensure adequate data protection (Mense & Blobel, 2017). This study was performed in cryopreservation laboratories, which deal with the storage of stem cells from both blood and umbilical cord tissue. In this type of activity, it is necessary to collect and process personal data from customers or potential customers. The aim of this study is therefore to check whether the laboratory can implement and comply with the GDPR. This paper consists of five sections. After a brief introduction to the problem, the basics used in this work are discussed, namely the Knowledge Discovery in Databases (KDD) process (Han et al., 2012; Witten et al., 2017) and a computer approach based on Artificial Neural Networks (ANNs) (Haykin, 2009). Section IV.2.3 presents the methodology, whereas in section IV.2.4 the results are presented and discussed. Finally, conclusions are drawn and future work is outlined.

IV.2.2. Fundamentals

Technological means have provided an exponential growth, both in number of records and in complexity, regarding data storage. As a result of this effective increase in information, its processing through traditional methods has become increasingly difficult and complex. In this way, applications aimed to the task of KDD have emerged, incorporating Data Mining (DM) tools (Han et al., 2012; Witten et al., 2017). The KDD process involves several steps, namely selection, data pre-processing, data transformation, data mining and interpretation (Han et al., 2012; Witten et al., 2017). The DM stage consists in choosing and using the methods and techniques that best fit the fulfilment of the established objectives (Han et al., 2012).

IV.2.2.1. Artificial Neural Networks

Data analysis is not a recent subject. For several years it has been carried out using mainly statistical methods. However, from an early stage, it became clear that the human brain analyses data and treats information differently, using learning processes (Han et al., 2012). ANNs were inspired by the nervous system of the human being and have been progressively applied in DM (Haykin, 2009). An ANN is a set of simple processing elements, called artificial neurons or nodes, organized in a highly interconnected parallel structure. They are similar to the behavior of the brain because, on one hand, knowledge is acquired from an environment through learning processes and, on the other hand, because knowledge is stored in the connections between the nodes (Haykin, 2009).

From a historical point of view, ANNs had their origin in the 40s of the 20th century, with the work of Warren McCulloch and Walter Pitts. These authors presented a simplified model of the neuron (called an artificial neuron or node), based on the fact that the neuron or is active or inactive, at a given moment, which corresponds to the true/false of the proportional logic or the one/zero of the Boolean algebra (McCulloch & Pitts, 1943). Other contributions followed, especially that of Rosenblatt (1958), who introduced the perceptron model, which originated the multi-layer perceptron. These are organized by layers and the connections always propagate in one direction, with no cycles. During the last few years the architecture mentioned above were used to capture no-linear relationships among variables, in different areas, such as law (Nguyen, 2018), water quality (Ruben et al., 2018; Fernandes et al., 2020a), psychosocial risks management (Fernandes et al., 2020b), or health (Ghosh et al., 2019; Shahid et al., 2019).

IV.2.3. Methods

This study was carried out in cryopreservation laboratories and in dialysis care clinics located in the north of Portugal. The age of the participants ranged from 22 to 69 years (average age 41 ± 19 years), with 57% women and 43% men. A questionnaire to assess the implementation of GDPR in cryopreservation laboratories was created and used for a cohort of 156 employees. To avoid the potential hidden errors associated to ostensibly random sampling methods that can lead to biased results (Shang, 2019), the questionnaires were applied to all employees of the laboratories. The questionnaire was divided into two sections, the first containing general questions (e.g., age, gender, academic qualifications and departmental areas of employees), while in the second the participants were asked to mark the option that best complete each statement according to their opinion. In the first section the answers are descriptive, whereas in the second one a Likert scale with four levels (i.e., *very reduced*, *reduced*, *medium* and *high*) was used.

The statements under consideration were organized into three groups, namely *Awareness Related Statements*, *Priority Related Statements*, and *Processes and Technologies Related Statements*. The former one comprises the statements, viz.

S1 The awareness of the laboratory on the guarantees of the rights of the holders of personal data is …;

S2 The awareness of the laboratory on the obligations and principles of the GDPR is …;

S3 The awareness of the laboratory on the general impact of the GDPR is …; and

S4 The awareness of the laboratory regarding the implications of non-compliance with the GDPR is ….

The second group encompasses the statements, viz.

S5 The management's priority in triggering the resources needed to implement the GDPR are …;

S6 The priority of the information management department regarding the implementation of a data protection system is …; and

S7 The priority of the group to which the laboratory belongs in unleashing the necessary resources for the implementation of the GDPR is ….

Finally, the third one includes the statements, viz.

S8 The processes and technologies that guarantee the exercise of all the rights of data holders are …;

S9 The information security management system that ensures a level of security appropriate to the data holders is …; and

S10 The competence and training of the person who performs the functions of data protection officer are ….

Pursuing the transformation of the qualitative data (collected using the questionnaire) into a quantitative one, the method suggested by Fernandes et al. (2016b) was adopted.

Thus the set of *n* statements respecting to a particular theme is itemized into a unitary area circle split into *n* slices, where the marks in the axis correspond to each one of the possible options, corresponding the quantitative value to the total area, as specified below (section IV.2.4.3).

The Waikato Environment for Knowledge Analysis (WEKA) was used to implement ANNs, maintaining the standard software parameters (Frank et al., 2016). In each simulation, the database was randomly divided into two mutually exclusive partitions, i.e., the training and test sets.

IV.2.4. Results and Discussion

IV.2.4.1. Sample Characterization

Applicants' age was categorized into age groups, i.e., less than 20 years of age, 20-30, 31-50, 51-65 and higher than 65 years of age. 64.8% of applicants are aged between 31 and 65 years old, 33.3% are lesser than 30 years of age, while 1.9% are higher than 65 years of age. Concerning academic qualification, 25.6% of the applicants expressed to have basic education, 23.7% declared that concluded secondary education, 40.4% stated to have finished a degree and 10.3% affirmed to have post graduate education.

IV.2.4.2. Answer Frequency Analysis

Figure 36 displays the frequency of answering to the second part of the questionnaire, where applicants selected the option that best complete each statement according to their opinion. The statements S1 to S4 refer to the *Awareness*, S5 to S7 are related to *Priority*, and S8 to S10 are relative to *Processes and Technologies*. The analysis of results presented in Figure 36 shows that for all the statements, regardless the dimension considered (i.e., *Awareness*, *Priority* and *Processes and Technologies*), most of the applicants (ranging between 89.1% and 94.2%) ticked the options *Medium* or *High* considering that the commitment of the laboratory regarding the implementation and fulfill of the GDPR is appropriate. In fact, only a small percentage of applicants, ranged between 5.8% and 10.9%, considers the efforts in the implementation of the mentioned guidelines unsatisfactory.

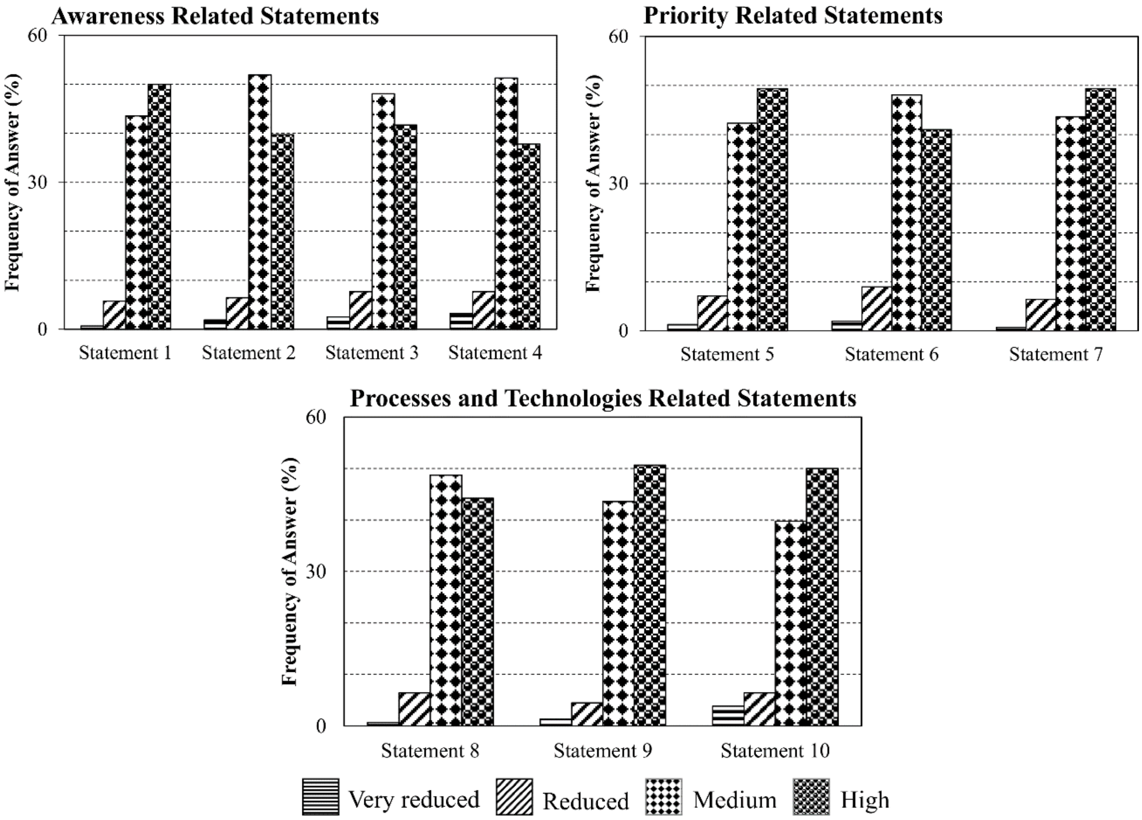

Figure 36 – Frequency of answer to the statements included in the second section of the questionnaire.

Bearing in mind the percentage of applicants which stated that the implementation of the GDPR is deficient, it would be interesting to apply a new questionnaire in order to clarify which are the main barriers to the effective implementation of the guidelines. Such study would allow to compare the results obtained in the studied laboratories with the results published in the literature (Mense & Blobel, 2017; Flaumenhaft & Ben-Assuli, 2018; Mourby et al., 2018).

IV.2.4.3. GDPR Implementation Assessment

To create a decision support system to assess the implementation of the GDPR, the results obtained in the second section of the questionnaire were used to train and test an ANN. Bearing in mind that the data collected has a qualitative nature, it was necessary to quantify them. For this purpose, the method suggested by Fernandes et al. (2016b) was chosen. Aiming to exemplify the procedures, Figure 37 presents the answers of applicant 1 to the mentioned section of the questionnaire.

IMPLEMENTATION OF THE GENERAL DATA PROTECTION REGULATION (GDPR) QUESTIONNAIRE

PART II

Tick the option that best complete each statement according to your opinion.

1. Awareness Related Statements	Very Reduced	Reduced	Medium	High
S1. The awareness of the laboratory on the guarantees of the rights of the holders of personal data is …	☐	☐	☐	☒
S2. The awareness of the laboratory on the obligations and principles of the GDPR is …	☐	☐	☒	☐
S3. The awareness of the laboratory on the general impact of the GDPR is …	☐	☒	☐	☐
S4. The awareness of the laboratory regarding the implications of non-compliance with the GDPR is …	☐	☐	☒	☐

2. Priority Related Statements	Very Reduced	Reduced	Medium	High
S5. The management's priority in triggering the resources needed to implement the GDPR are …	☐	☐	☒	☐
S6. The priority of the information management department regarding the implementation of a data protection system is …	☐	☐	☐	☒
S7. The priority of the group to which the laboratory belongs in unleashing the necessary resources for the implementation of the GDPR is …	☐	☐	☒	☐

3. Processes and Technologies Related Statements	Very Reduced	Reduced	Medium	High
S8. The processes and technologies that guarantee the exercise of all the rights of data holders are …	☐	☒	☐	☐
S9. The information security management system that ensures a level of security appropriate to the data holders is …	☒	☐	☐	☐
S10. The competence and training of the person who performs the functions of data protection officer are …	☐	☐	☒	☐

Figure 37 – The answers of applicant 1 to the second section of the GDPR questionnaire.

For each statement group (i.e., *awareness*, *priority*, and *processes and technologies*) the answers were itemized into a unitary area circle. The marks in the axis correspond to each alternative, i.e., *very reduced*, *reduced*, *medium* and *high*. Exemplifying with the group of statements regarding *awareness*, the answer to S1 was *high* and the correspondent area is given by $\frac{1}{4} \times \pi \times \left(\frac{1}{\sqrt{\pi}}\right)^2 = 0.25$, in S2 and S4 were marked the option *medium* and the areas are $\frac{1}{4} \times \pi \times \left(\frac{3}{4} \times \frac{1}{\sqrt{\pi}}\right)^2 = 0.14$. Finally, for S3 the answer was *reduced*, and the area is $\frac{1}{4} \times \pi \times \left(\frac{2}{4} \times \frac{1}{\sqrt{\pi}}\right)^2 = 0.06$. The total area (i.e., 0.59) is the sum of the partial ones, being the quantitative value regarding the *awareness* group for applicant 1 (Figure 38). Proceeding in a similar way for the remaining statements groups and for each of the 156 applicants, the results displayed in Table 14 were obtained.

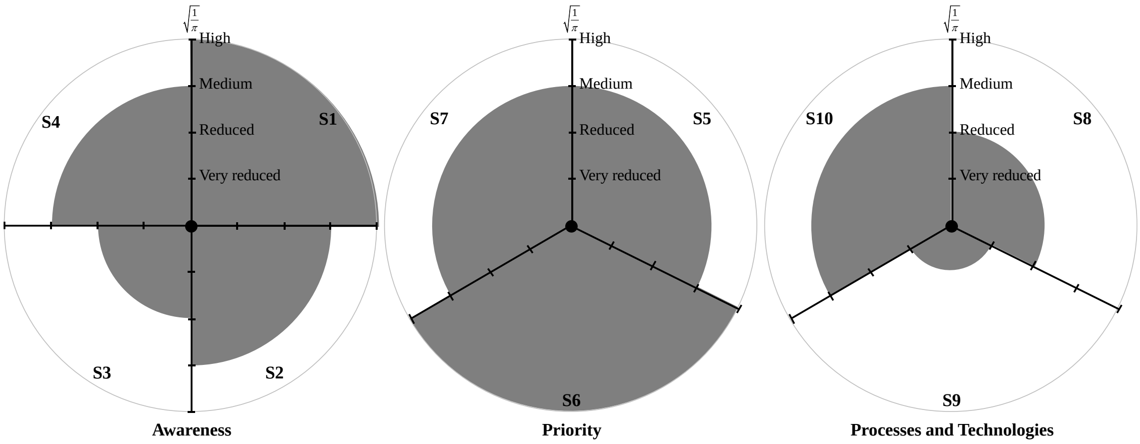

Figure 38 – The quantification process of the qualitative information collected in the second section of the GDPR questionnaire for applicant 1.

Table 14 – A fragment of the knowledge base for the GDPR implementation assessment.

Applicant	Awareness	Priority	Processes and Technologies
1	0.59	0.71	0.29
2	0.78	0.56	0.50
…	…	…	…
156	0.81	1.0	0.42

To obtain the best ANN model to assess the GDPR implementation different network structures have been elaborated and evaluated. The performance of ANN models was compared using the confusion matrixes (Vilhena et al., 2017). The 3-3-2-1 topology (Figure 39) was the one that presented the best performance in terms of accuracy and was selected to evaluate the implementation of the GDPR. The correspondent confusion matrix is shown in Table 15 (the values displayed are the average ones, based on 25 experiments). Thus, it is possible to calculate the model accuracy for training set (92.5%, i.e., 99 correctly labeled in 107) and for test set (89.8%, i.e., 44 correctly labeled in 49). In this way, the assessment of GDPR implementation with the proposed ANN model is satisfactory, reaching accuracies of around 90%.

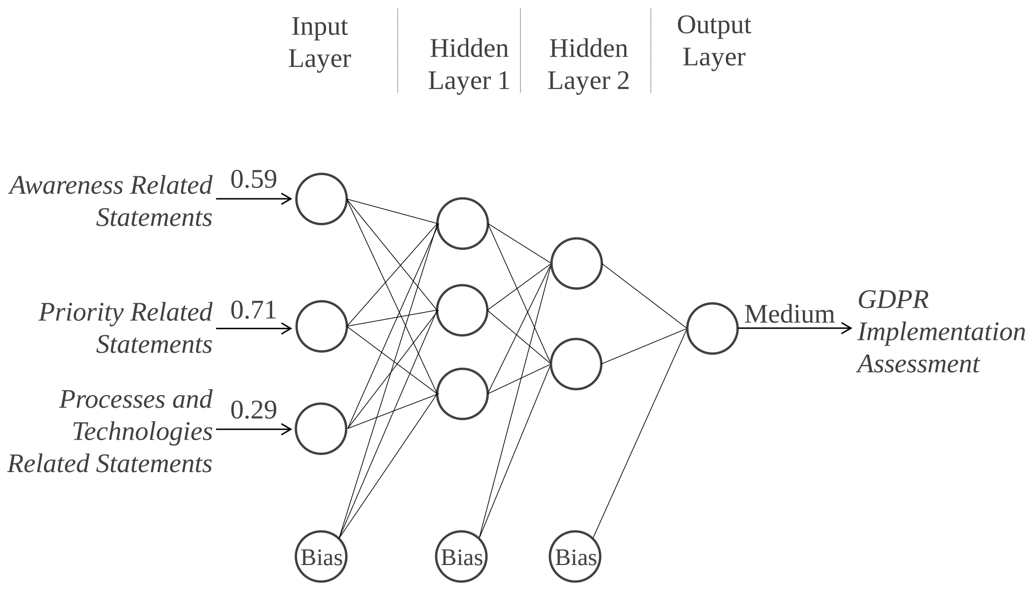

Figure 39 – A schematic view of the *ANN* selected for GDPR implementation assessment.

Table 15 – Confusion matrix to ANN model for the GDPR implementation assessment.

Target	Predictive					
	Training Set			Test Set		
	Reduced	Medium	High	Reduced	Medium	High
Reduced	11	0	0	5	0	0
Medium	5	67	0	3	31	0
High	0	3	21	0	2	8

The focus on data acquisition should be concentrated on the more important variables, considering the model accuracy, depreciating or setting aside the matter least ones. Sensitivity analysis is related with model output response to variations in its input variables. It is a basic procedure that may be carried out after the modelling phase and examines the model responses when the inputs are modified. Sensitivity according to variance (Kewley et al., 2000) was used to compute the relative importance of the input variables. The results are shown in Figure 40 and seem to indicate that ANN inputs affect the outputs in an analogous way, although the fluctuations on *Processes and Technologies Related Statements* show a slightly more pronounced effect. Thus, the organization should pay attention to all these factors for an effective implementation of the GDPR. These outcomes are corroborated by the results shown in Figure 38. In fact, the 3 groups of statements show a similar frequency of negative responses (i.e., *very reduced* and *reduced*) and, consequently, a small variation in this type of answers should have impact on the output.

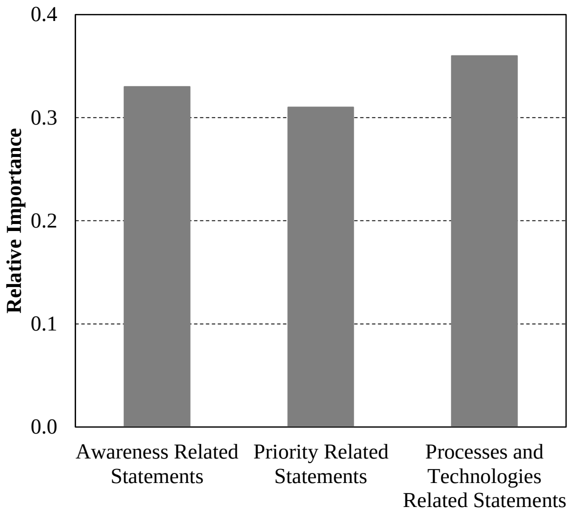

Figure 40 – Relative importance of the input variables of the *ANN* selected for GDPR implementation assessment.

IV.2.5. Conclusions and Future Work

Privacy and data protection are a very old topic, but at the same time very current, being the subject of recent developments that promise to have a significant impact on the provision of health services with the entry into force of the GDPR. Ensuring data protection should be the responsibility not only of citizens, but also of health professionals/technicians in the course of their activities. However, it is difficult to assess the level of GDPR implementation since it is a matter that deals with different variables with complex relationships among them. Therefore, and in order to assess the level of implementation of the GDPR in a cryopreservation laboratory, a data acquisition and evaluation framework was developed and experienced in practice. The emphasis was putted on processing of information, being the data gathered using inquiry by questionnaire. Complementary, this paper also proposes an intelligent decision support system to appraise the level of GDPR implementation based on the ANN paradigm. This approach exhibits a satisfactory effectiveness, showing an accuracy of about 90%. Furthermore, it allows to recognize the fragilities of the laboratory, and help the decision makers to promote future improvements to ensure high levels of data protection. Future work will consider new factors, namely the training given to the employees on this matter or the volume of information processed. In addition, it is intended to extend the study to a larger sample to study the influence of other variables such as age, gender, or academic qualifications of employees on their perception about the GDPR implementation.

IV.3. A Case-Based Approach to Assess Employees' Satisfaction with Work Guidelines in Times of the Pandemic

IV.3.1. Introduction

The health sector is central to the well-being of society, and people become gradually more important to the proper functioning of such area. Indeed, the COVID–19 pandemics are a major challenge for health, for organizations and for society. On the other hand, work activities are potential sources of exposure to the virus due to the closeness of employees and customers when acting according to their obligations (Decree-Law No. 10-A/2020). Maintaining the health of professionals who continue to work is therefore essential to control the spread of the disease. Last but not least, and according to the guidelines announced by the World Health Organization (WHO), all organizations had to introduce new operating procedures such as social distance in order to avoid the spread of the virus (WHO, 2020a). In order to maintain the productivity and satisfaction of customers and employees, all new processes and working measures must be understood and accepted by each one (WHO, 2020b). The entire team should be satisfied, as employee satisfaction is highly linked to productivity, personal fulfillment, and customer satisfaction. However, assessing employee satisfaction is a difficult task that comprises a variety of issues that depend on both the employee and the organization (Petrescu & Simmons, 2008; Alfes et al., 2013; Berman et al., 2020). The present work aims to assess the satisfaction of the employees of water analysis laboratories with the new working methods in connection with the pandemic crisis.

The paper is composed by five sections. Afterwards to a brief introduction to the problem, the basics used in the study are discussed, specifically the notion of *Entropy*, the procedures of *Logic Programming* for *Knowledge Representation and Reasoning* (Neves, 1984; Fernandes et al., 2020c; Figueiredo et al., 2020) and a computer-based approach to *Case-Based Reasoning* (Aamodt & Plaza, 1994; Richter & Weber, 2013). Sections IV.3.3 presents the methodology and data processing, whereas in Section IV.3.4 the results are presented and discussed taking into account the notion of *Entropy* (Wenterodt & Herwig, 2014). Finally, in Section IV.3.5, the main conclusions pointed out and future work are delineated.

IV.3.2. Literature Review

IV.3.2.1. Thermodynamics and Knowledge Representation and Reasoning

The methodology used in this article is grounded on thermodynamics and aims to present the practices of *Knowledge Representation and Reasoning* as an energy conversion process (Wenterodt & Herwig, 2014, Neves et al, 2019; Figueiredo et al., 2020). In order to illustrate the basics of the method, the first two laws of thermodynamics were taken into account, attending that one is faced to a dynamic system, i.e., that moves continuously from state to state. The *First Law* or the *Energy Saving Law* establishes that the total energy of an isolated system is constant, although it can take different forms. The *Second Law* is concerned with *Entropy*, i.e., the state of order of a system, establishing that in an isolated system the entropy never decreases. These qualities meet one's viewpoint of *Knowledge Representation and Reasoning* practices. In fact, such does are inspired by the processes of energy degradation in an isolated system, which can be described as, viz.

- *exergy*, also denominated as energy ready for use or work ready for use, and corresponds to the energy fraction that may be used in an arbitrary way by a system, providing a measurement of its entropy, being figured by the dark zones (Figure 42, section IV.3.3.2);
- *vagueness*, i.e., that corresponds to the energy values that were or were not used, being represented by the dark regions with circles (Figure 42, section IV.3.3.2); and
- *anergy*, that can be set as an available energetic potential, i.e., the energy that was not consumed at moment, being denoted in Figure 42 (section IV.3.3.2) by the dark surfaces with asterisks (Wenterodt & Herwig, 2014, Neves et al, 2019; Figueiredo et al., 2020).

Several advances to *Knowledge Representation and Reasoning* are based on the *Logic Programming* architype, namely in *Model* and *Proof Theory*. The problem-solving method used in this work is based on *Proof Theory* and is applied to logic programs that use an extension of the *Logic Programming* language (Neves, 1984) in the form of a finite summative of clauses, as shown in Program 6.

$$\{$$

$$\neg p \leftarrow not\ p, not\ exception_p$$

$$p \leftarrow p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m$$

$$?\,(p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m)\ \ (n, m \geq 0)$$

$$exception_{p_1}, \ \cdots \ , exception_{p_j}\ \ (0 \leq j \leq k), \ \ being\ k\ an\ integer\ number$$

$$\}$$

Program 6 – A generic example of a *Logic Program*.

The former clause stands for the closure of the predicate, "," symbolizes the "*logical and*", whereas "?" is a domain atom indicating "*falsity*". Finally, p_i, q_j, and p are positive atoms or atoms preceded by the classical negation sign ¬ (Neves, 1984). Indeed, ¬ is used for strong negation, whereas *not* represents *negation-by-failure*, i.e., a failure in proving a declaration that was not expressed explicitly. Following this this line of thought, each program contains a number of abducibles expressed as exceptions to the extensions of the predicates included in the program, viz.

$$exception_{p_1}, \ \cdots \ , exception_{p_j}\ \ (0 \leq j \leq k), \ \ being\ k\ an\ integer\ number$$

designating data/information/knowledge that cannot be discarded. Clauses of the type, viz.

$$?\,(p_1, \cdots, p_n, not\ q_1, \cdots, not\ q_m)\ \ (n, m \geq 0)$$

stand for invariants, i.e., terms or expressions that determine the context and guide the understanding of the universe of discourse (Neves et al., 2019; Fernandes et al., 2020c).

IV.3.2.2. Case-Based Reasoning

In the broadest sense, *Case-Based Reasoning* (*CBR*) can be labelled as the practice of solving new problems centered on solutions to parallel ones by reusing and adapting their solutions (Aamodt & Plaza, 1994; Richter & Weber, 2013). In fact, the basic postulate that serves as the basis for *CBR* is *analog problems can be solved with analog solutions*. Various descriptions of this methodology can be found in the literature that converge to a model that includes the steps knowledge representation, retrieving, reusing, repairing, and maintaining. (Ferraz et al., 2016; Vilhena et al., 2016; Neves et al., 2018b) presents an extended *CBR* cycle that includes a case optimization process, taking two new metrics into account, i.e., the *Quality-of-Information* (*QoI*) and the *Degree-of-Confidence* (*DoC*) on the solution so far obtained. The similarity measure is calculated using *QoI* and *DoC*, which allows the search space for similar cases to be narrowed.

IV.3.3. Case Study

IV.3.3.1. Methods

The study was performed in a water laboratory in southern Portugal. The participants' ages varied between 18 to 60 years (mean age 38 ± 20 years old), with 61% female and 39% male. A questionnaire to assess employee satisfaction with the new pandemic crisis procedures was created and used for a cohort of 64 personnel. The questionnaire was formed by into two segments, the initial one containing common questions (such as age, gender, educational qualifications, seniority and department within the organization), while the second covered points for assessing employees' satisfaction with the current restrictions.

IV.3.3.2. Data Processing

Aiming to gather evidences related with the satisfaction of the employees concerning the new procedures related with the pandemic crisis, the participants were requested to mark the alternative(s) that best reflect their feelings concerning each item. In the case of the participant mark more than one alternative, he/she is also requested to specify the tendency of his/her answer, i.e., growing tendency (*Very Dissatisfied* → *Very Satisfied*) or the opposite (*Very Satisfied* → *Very Dissatisfied*) as displayed in Figure 41. Taking into account the cohort dimension, the answer alternatives were given in a four items Likert scale, *viz.*

(4) Very Satisfied, (3) Satisfied, (2) Dissatisfied, (1) Very Dissatisfied

The answer alternatives are in accordance a four items Likert type scale with the *decreasing tendency*, to be in terms with the *First Law of Thermodynamics*, i.e. *from (4) Very Satisfied, (3) Satisfied, (2) Dissatisfied*, to *(1) Very Dissatisfied*, and from *(1) Very Dissatisfied), (2) Dissatisfied, (3) Satisfied*, to *(4) Very Satisfied* with the *increasing tendency*, to be in terms with the *Second Law of Thermodynamics*.

QUESTIONNAIRE ABOUT EMPLOYEES' SATISFACTION IN PANDEMIC TIMES

PART II

For each statement tick the option(s) that best reflects your opinion. If you tick more than one option please indicate the meaning for the organization of your answer in terms of its evolution, i.e., increasing trend (Very Dissatisfied → Very Satisfied) or the decreasing trend Very Satisfied → Very Dissatisfied).

TRAINING (RELATED WITH COVID–19) ITEMS							
	Very Satisfied	Satisfied	Dissatisfied	Very Dissatisfied		Decreasing Trend	Increasing Trend
S1. The syllabus of COVID–19 training actions.	☐	☒	☐	☐		☐	☐
S2. The usefulness of COVID–19 training in the context of the organization.	☒	☒	☐	☐		☐	☒
S3. The usefulness of COVID–19 training in a personal context.	☐	☐	☐	☐		☐	☐
S4. The applicability of COVID–19 training in daily tasks.	☒	☒	☐	☐		☐	☒

Figure 41 – A fragment of employee # 1's answers to COVID–19 training items included in the second part of the questionnaire.

The items to be considered were structured in three distinct groups, i.e., *Training Related with COVID–19 Items – Four Items* (*TRI – 4*), *Resources Related Items – Four Items* (*RRI – 4*), and *Cleaning and Disinfection Related Items – Four Items* (*CDRI – 4*). The former one contains the items, viz.

I1 The syllabus of COVID–19 in individual training actions;

I2 The usefulness of COVID–19 training in the context of the organization;

I3 The usefulness of COVID–19 training in a personal context; and

I4 The applicability of COVID–19 training in daily tasks.

The second group was built according to the particulars, viz.

I5 Implementation of distance measures of at least 2 meters (signal lines on the ground) between employees;

I6 The suitability of personal protection equipment during chemical tests;

I7 The suitability of personal protection equipment during microbiological tests; and

I8 The suitability of personal protection equipment during sample collection.

Finally, the third one comprises the specifics, viz.

I9 Disinfectant gel availability at the entrance to the rooms;

I10 Disinfection of contact surfaces with the employees between each use;

I11 *Disinfection of hands with alcohol at 70º or alcohol-based solution, between each service/employee;* and

I12 *Cleaning of common spaces (e.g. bar; WC; service rooms data holders).*

To transpose the qualitative information into a quantitative one all calculation details for *Training Related Items – Four Items* (*TRI – 4*) are presented, in order to illustrate the process. The answers of the employee #1 to the *TRI – 4* group are present in Table 16. Considering that the answers to *I2* and *I4* were *Satisfied (3)* → *Very Satisfied (4)*, it reveals an increase tendency on the employee's satisfaction, corresponding to a decrease in entropy. For *I1* the answer was *medium (3)*; a fact that is self-explanatory, while for *I3* no alternative were marked, configuring an ambiguous situation, i.e., vague, where the energy expended is unknown, but ranging between 0 and 1.

Regarding the different types of energy, *exergy* corresponds to the well-defined answers, i.e. the cases where only one alternative was marked. Indeterminacy (i.e., *vagueness*) occurs when no alternatives or more than one alternative have been marked and *anergy* corresponds to the energy not yet used. Figure 42 and Figure 43 show the conversion of the information contained in Table 16 into the diverse types of energy described above (*exergy*, *vagueness* and *anergy*). Taking into consideration that the marks on the axis match to each one of the possible scale alternatives, the employees' opinion is encouraging in the cases where occur a decrease of entropy (*I2* and *I4*), as presented in Table 17.

Table 16– Answers of the employee # 1 to *TRI – 4*.

Items	*Scale*							
	entropy → *increasing tendency*				*entropy* → *decreasing tendency*			
	(4)	(3)	(2)	(1)	(2)	(3)	(4)	*vagueness*
I1		×						
I2						×	×	
I3								×
I4						×	×	

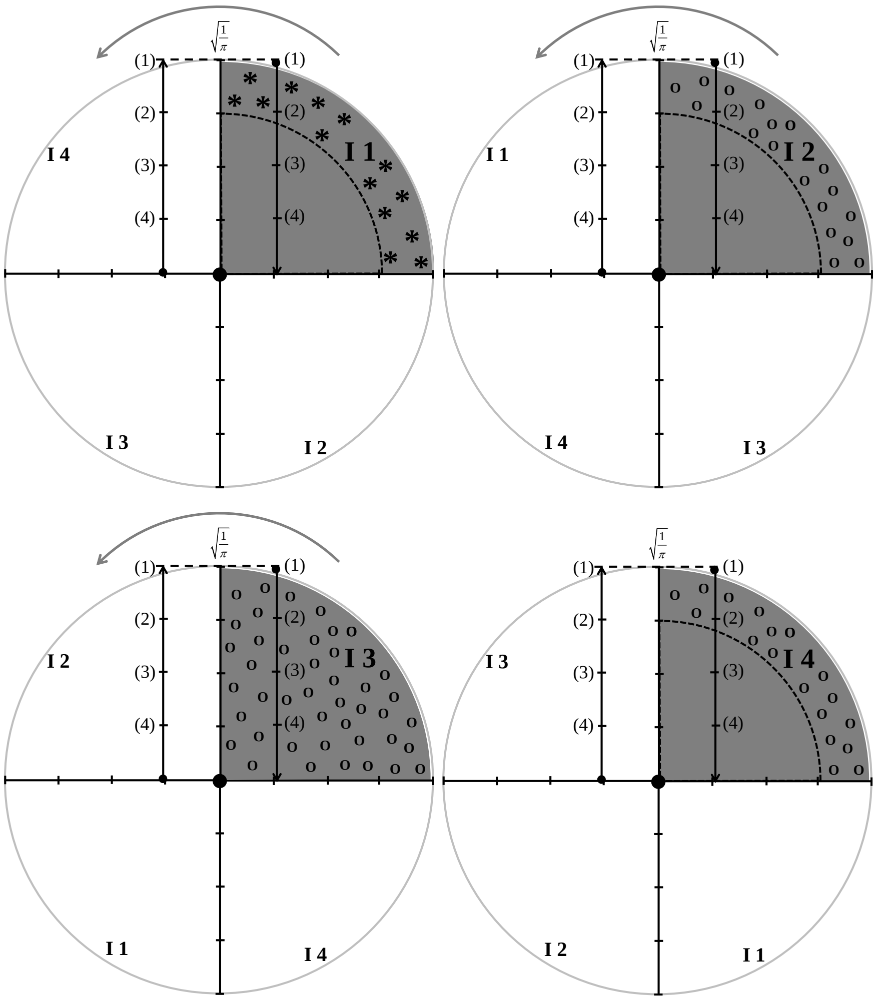

Figure 42 – Estimation of energy types for the diverse items respecting to the answers of employee # 1 to the *TRI – 4*. The dark zones stand for *exergy*, dark areas with circles denote *vagueness* and dark regions with asterisks characterize *anergy*.

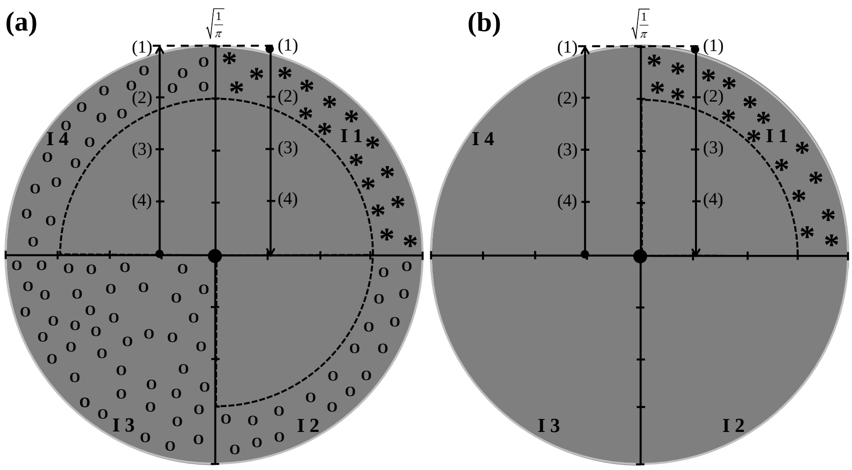

Figure 43 – The global evaluation of the contribution of employee # 1 to the team's satisfaction in answering *TRI – 4* in the *Best* (a) and in the *Worst* (b) *Case Scenarios*.

Table 17 – Assess the employee's contribution to evaluating the team's satisfaction in responding to *TRI – 4* for the *Best* and *Worst Case Scenarios*.

Items	*Best Case Scenario (BCS)*	*Worst Case Scenario (WCS)*
I1	$exergy_{I_1} = \frac{1}{4}\pi r^2\Big]_0^{\frac{3}{4}\sqrt{\frac{1}{\pi}}} = \; = \left(\frac{1}{4}\pi\left(\left(\frac{3}{4}\sqrt{\frac{1}{\pi}}\right)^2 - 0\right)\right) = 0.14$	$exergy_{I_1} = \frac{1}{4}\pi r^2\Big]_0^{\frac{3}{4}\sqrt{\frac{1}{\pi}}} = 0.14$
	$vagueness_{I_1} = \frac{1}{4}\pi r^2\Big]_{\frac{3}{4}\sqrt{\frac{1}{\pi}}}^{\frac{3}{4}\sqrt{\frac{1}{\pi}}} = 0$	$vagueness_{I_1} = \frac{1}{4}\pi r^2\Big]_{\frac{3}{4}\sqrt{\frac{1}{\pi}}}^{\frac{3}{4}\sqrt{\frac{1}{\pi}}} = 0$
	$anergy_{I_1} = \frac{1}{4}\pi r^2\Big]_{\frac{3}{4}\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0.11$	$anergy_{I_1} = \frac{1}{4}\pi r^2\Big]_{\frac{3}{4}\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0.11$
I2	$exergy_{I_2} = \frac{1}{4}\pi r^2\Big]_0^{\frac{3}{4}\sqrt{\frac{1}{\pi}}} = 0.14$	$exergy_{I_2} = \frac{1}{4}\pi r^2\Big]_0^{\sqrt{\frac{1}{\pi}}} = 0.25$
	$vagueness_{I_2} = \frac{1}{4}\pi r^2\Big]_{\frac{3}{4}\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0.11$	$vagueness_{I_2} = -\frac{1}{4}\pi r^2\Big]_{\frac{4}{4}\sqrt{\frac{1}{\pi}}}^{\frac{4}{4}\sqrt{\frac{1}{\pi}}} = 0$
	$anergy_{I_2} = \frac{1}{4}\pi r^2\Big]_{\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0$	$anergy_{I_2} = -\frac{1}{4}\pi r^2\Big]_{\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0$
I3	$exergy_{I_3} = \frac{1}{4}\pi r^2\Big]_0^{0} = 0$	$exergy_{I_3} = \frac{1}{4}\pi r^2\Big]_0^{\sqrt{\frac{1}{\pi}}} = 0.25$
	$vagueness_{I_3} = \frac{1}{4}\pi r^2\Big]_0^{\sqrt{\frac{1}{\pi}}} = 0.25$	$vagueness_{I_3} = \frac{1}{4}\pi r^2\Big]_{\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0$
	$anergy_{I_3} = \frac{1}{4}\pi r^2\Big]_{\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0$	$anergy_{I_3} = \frac{1}{4}\pi r^2\Big]_{\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0$
I4	$exergy_{I_4} = \frac{1}{4}\pi r^2\Big]_0^{\frac{3}{4}\sqrt{\frac{1}{\pi}}} = 0.14$	$exergy_{I_4} = \frac{1}{4}\pi r^2\Big]_0^{\sqrt{\frac{1}{\pi}}} = 0.25$
	$vagueness_{I_4} = \frac{1}{4}\pi r^2\Big]_{\frac{3}{4}\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0.11$	$vagueness_{I_4} = \frac{1}{4}\pi r^2\Big]_{\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0$
	$anergy_{I_4} = \frac{1}{4}\pi r^2\Big]_{\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0$	$anergy_{I_4} = \frac{1}{4}\pi r^2\Big]_{\sqrt{\frac{1}{\pi}}}^{\sqrt{\frac{1}{\pi}}} = 0$

IV.3.4. Results and Discussion

The data presented in Table 17 can be organized in terms of the extent of the predicate ***t**raining **r**elated **i**tems* (*tri – 4*) in the form, *viz*.

$$tri - 4: \boldsymbol{EX}ergy,\ \boldsymbol{VA}gueness, \boldsymbol{AN}ergy,\ \boldsymbol{E}mployee\ \boldsymbol{S}atisfaction\ \boldsymbol{A}ssessment,$$

$$\boldsymbol{Q}uality\text{-}\boldsymbol{o}f\text{-}\boldsymbol{I}nformation \rightarrow \{True, False\}$$

The scope and formal description of the predicate *tri – 4* are present in Table 18 and in Program 7.

Table 18 – The extent of the predicate *tri – 4,* obtained using the answers of the employee # 1 to *TRI – 4.*

Group	*EX BCS*	*VA BCS*	*AN BCS*	*ESA BCS*	*QoI BCS*	*EX WCS*	*VA WCS*	*AN WCS*	*ESA WCS*	*QoI WCS*
TRI – 4	0.42	0.47	0.11	0.91	0.58	0.89	0	0.11	0.46	0.11

The calculation of *Employee Satisfaction Assessment* (*ESA*) and the *Quality-of-Information truth values (QoI truth values)* for the different terms or clauses that make the *tri* – 4 predicate's extent are now given in the form, *viz*.

- ESA is found as $\sqrt{1 - Exergy^2}$ (Figure 44), which leads to, viz.

  $ESA_{BCS} = \sqrt{1 - (0.42)^2} = 0.91$; and

  $ESA_{WCS} = \sqrt{1 - (0.89)^2} = 0.46$

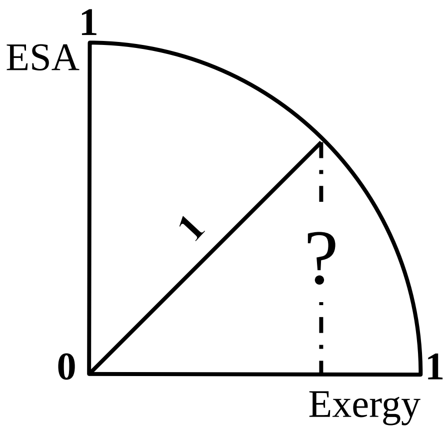

Figure 44 – Employee Satisfaction Assessment (ESA) evaluation.

- The *QoI* truth values are evaluated as $(1 - Exergy/Interval\ length)$ (Neves et al., 2019), leading to, viz.

  $QoI\ truth\ values_{BCS} = 1 - 0.42 = 0.58$

  $QoI\ truth\ values_{WCS} = 1 - 0.89 = 0.11$

$\{$

$\neg\ tri - 4\ (EX,\ VA,\ AN,\ ESA,\ QoI\ truth\ values)$

$\leftarrow not\ tri - 4\ (EX,\ VA,\ AN,\ ESA,\ QoI\ truth\ values),$

$not\ exception_{tri-4}\ (EX,\ VA,\ AN,\ ESA,\ QoI\ truth\ values)$

$tri - 4\ \ (0.42,\ 0.47,\ 0.11,\ \ 0.91,\ 0.58).$

$\}$

Program 7 – The extent of the *tri – 4* predicate for the *Best Case Scenario.*

In addition to Table 16, Table 19 and Table 20 show employee # 1's answers to the *RRI – 4* and *CDRI – 4* groups.

Table 19 – Answers from employee # 1 to *RRI – 4* and *CDRI – 4.*

Group	Items	*Scale*							
		entropy increasing tendency →				*entropy decreasing tendency* →			
		(4)	(3)	(2)	(1)	(2)	(3)	(4)	*vagueness*
RRI – 4	I5	×							
	I6						×	×	
	I7					×			
	I7								×
CDRI – 4	I9					×	×		
	I10		×						
	I11								
	I12								×

Table 20 – The *tri – 4, rri – 4* and *cdri – 4* predicates' scopes computed in conformity with the answers of the employee # 1 to *TRI – 4, RRI – 4* and *CDRI – 4.*

Groups	*EX BCS*	*VA BCS*	*AN BCS*	*ESA BCS*	*QoI BCS*	*EX WCS*	*VA WCS*	*AN WCS*	*ESA WCS*	*QoI WCS*
TRI – 4	0.42	0.47	0.11	0.91	0.58	0.89	0	0.11	0.46	0.11
RRI – 4	0.45	0.26	0.19	0.89	0.55	0.81	0	0.19	0.59	0.19
CDRI – 4	0.40	0.30	0.30	0.92	0.60	0.70	0	0.30	0.71	0.30

IV.3.4.1. A Symbolic, Logic Method to Evaluate Employee's Satisfaction

Computational Logic can be understood in the broadest sense as a problem-solving methodology, in which the problems and the respective solutions are expressed in logic terms so that a computer can execute them using deductive/inductive interpretations methods. This section presents the logic program that takes into account employee opinions regarding their satisfaction with the new procedures related to the coronavirus crisis (Program 8). This framework brings into being the basis for an assessment of the level of the *Employee's Satisfaction Assessment* (*ESA*) and a measure of its *Sustainability* (*QoI truth values*), an assembly of *truth values* belonging to the interval $0 \ldots 1$.

$\{$

/ The subsequent sentence specifies that the extent of predicate tri – 4 is based on the explicitly itemized clauses and the ones that cannot be dropped */*

$$\neg\, tri - 4\,(EX,\, VA,\, AN,\, ESA,\, QoI\ truth\ values)$$

$$\leftarrow not\ tri - 4\,(EX,\, VA,\, AN,\, ESA,\, QoI\ truth\ values),$$

$$not\ exception_{tri-4}\,(EX,\, VA,\, AN,\, ESA,\, QoI\ truth\ values)$$

/ The following sentence stands for an axiom of tri – 4*/*

$$tri - 4\ (0.42,\ 0.47,\ 0.11,\ 0.91,\ 0.58).$$

/ The subsequent sentence specifies that the extent of predicate rri – 4 is based on the explicitly itemized clauses and the ones that cannot be dropped */*

$$\neg\, rri - 4\,(EX,\, VA,\, AN,\, ESA,\, QoI\ truth\ values)$$

$$\leftarrow not\ rri - 4\,(EX,\, VA,\, AN,\, ESA,\, QoI\ truth\ values),$$

$$not\ exception_{rri-4}\,(EX,\, VA,\, AN,\, ESA,\, QoI\ truth\ values)$$

/ The following sentence stands for an axiom of rri – 4*/*

$$rri - 4\,(0.45,\ 0.26,\ 0.19,\ 0.89,\ 0.55).$$

/ The subsequent sentence specifies that the extent of predicate cdri – 4 is based on the explicitly itemized clauses and the ones that cannot be dropped */*

$$\neg\, cdri - 4\ (EX,\ VA,\ AN,\ ESA,\ QoI\ truth\ values)$$

$$\leftarrow not\ cdri - 4\ (EX,\ VA,\ AN,\ ESA,\ QoI\ truth\ values),$$

$$not\ exception_{cdri - 4}\ (EX,\ VA,\ AN,\ ESA,\ QoI\ truth\ values)$$

/ The following sentence stands for an axiom of cdri – 4*/*

$$cdri - 4\ (0.40,\ 0.30,\ 0.30,\ \ 0.92,\ 0.60).$$

}

Program 8 – The make-up of the *Logic Programming* for assessing the contribution of employee #1's in the evaluation of the team's satisfaction for the *Best Case Scenario.*

IV.3.4.2. A Case-Based Approach to Process Employee's Satisfaction

In this study a cohort of 64 employees was involved. The *Database*/*Knowledge Base*/*Case Base* is now obtained by validating the theorem, viz.

$$\forall\ (EX_1, VA_1, AN_1,\ ESA_1, QoI\ truth\ values_1,\ \cdots,$$

$$\cdots,\ EX_3, VA_3, AN_3,\ ESA_3, QoI\ truth\ values_3),$$

$$(tri\text{–}\ 4\ (EX_1, VA_1, AN_1,\ ESA_1, QoI\ truth\ values_1),$$

$$rri - 4\ (EX_2,\ VA_2,\ AN_2,\ ESA_2,\ QoI\ truth\ values_2),$$

$$cdri\text{–}\ 4\ (EX_3,\ VA_3,\ AN_3,\ ESA_3, QoI\ truth\ values_3))$$

---

in all possible ways, i.e., generating every possible sequencing of the terms/clauses of the extents of predicates *tri – 4*, *rri – 4* and *cdri – 4*, viz.

$$\{\{tri\!-4\ (EX_1, VA_1, AN_1,\ ESA_1, QoI\ truth\ values_1),$$
$$rri-4\ (EX_2,\ VA_2,\ AN_2,\ ESA_2,\ QoI\ truth\ values_2),$$
$$cdri\!-4\ (EX_3,\ VA_3,\ AN_3,\ ESA_3, QoI\ truth\ values_3)\}, \cdots\} \approx$$
$$\approx \{\{tri\!-4\ (0.42,\ 0.47,\ 0.11,\ \ 0.91,\ 0.58),\ rri\!-4\ (0.45,\ 0.26,\ 0.19,\ \ 0.89,\ 0.55),$$
$$cdri-4\ \ (0.40,\ 0.30,\ 0.30,\ \ 0.92,\ 0.60)\},\ \cdots\}$$

Regardless of encouraging results, the current *CBR* systems don't be versatile enough to be used in all domains. Often, users are forced to adopt the similarity methods imposed by the system, despite they do not completely adjusted to their needs (Richter & Weber, 2013; Vilhena et al., 2016). To meet this challenge, the alternative *CBR* cycle suggested by Vilhena et al. (2016) was adjusted taking into account the global *Employee Satisfaction Assessment* (*ESA*) and the employees *QoI truth values*. For the *Best-Case Scenario*, they can be calculated in the form, viz.

$$\{\{(ESA_{tri-4}+ESA_{rri-4} + ESA_{cdri-4})/3\},\ \cdots\}_{BCS} \approx$$
$$\approx \{\{(0.91 + 0.89 + 0.92)/3 = 0.90\},\ \cdots\}_{BCS}$$

$$\{\{(QoI\ truth\ values_{tri-4} +\ QoI\ truth\ values_{rri-4} +$$
$$+QoI\ truth\ values_{cdri-4})/3\ \},\ \cdots\}_{BCS} \approx$$
$$\approx \{\{(0.58 +\ 0.55 + 0.60)/3 = 0.58\},\ \cdots\}_{BCS}$$

Thus, when handled with a new occurrence, the system is search and retrieve the cases that match in certain degree the new case specifications, and act accordingly (Ferraz et al., 2016; Vilhena et al., 2016; Neves et al., 2018b).

IV.3.5. Conclusions and Future Work

Employees' satisfaction is an old topic, but simultaneously a very current one, since it is closely related to productivity. The actual pandemic crisis brought new challenges to organizations, which had to adjust themselves to new requirements to avoid contagion. From this perspective the *Employee Satisfaction Assessment* is of utmost importance. Despite to be a challenging task, it is very hard to achieve since imply to manipulate distinct variables with numerous and multifaceted interconnections among them. In this study, the development of a Case-Based Reasoning model is presented, with which the satisfaction of employees with the new work guidelines due to the actual pandemic crisis is assessed. It takes the advantages of the synergies between Logic Programming and the Laws of Thermodynamics for Knowledge Representation and Reasoning, together with a computational approach that uses Case-Based Reasoning. The model was tested with real data collected through questionnaires exhibiting an overall accuracy of 85,9%. On the other hand, the weights of the case attributes can be defined so that the bandwidth of the search space can be selected for comparable cases at runtime. Regarding subsequent work, it will take new factors into account, namely issues relating to occupational medicine or the organizational climate. In addition, the study is to be extended to a larger sample in order to examine the role of additional variables like age, gender or the academic and social training of employees on their emotions and feelings.

IV.4. Customers' Satisfaction Assessment in Water Laboratories

IV.4.1. Introduction

In the last years, water quality issues as been framed in public health thematic. Thus, it is in this context that the importance that water laboratories began to achieve in terms of the issuance of credible and reliable results for the community should be understood. Water quality is a set of physical, chemical, and biological characteristics defined according to water use (e.g., human consumption, industrial and agricultural). The parameters evaluated can reveal physical, chemical, and biological threats, when reaching values higher than those established for a particular use. The concern with the evaluation of the water quality parameters has been growing in Portugal and, more and more, there are accredited laboratories. Accreditation by ISO/IEC 17025 aims to improve employee performance in determining water quality parameters and help in complying with the current Portuguese regulation (Decree-Law 152/2017, 2017), which establishes the drinking water quality regime in accordance with European legislation, promotes human health from the effect's harmful of water contamination and ensures the availability of clean and balanced water. According to this law the water laboratories are required to have accreditation in accordance with ISO/IEC 17025 (ISO/IEC 17025, 2017). In other words, all Portuguese laboratories that perform water analyses must work in accordance with internationally approved procedures and use validated methods. In fact, quality is the main factor that differentiates organizations, being considered a fundamental aspect that can influence the survival of the organization in an increasingly competitive market. Quality defines the service level of the organization and determines customer satisfaction.

IV.4.1.1. Quality Concept

The quality's perception is inherent in humans and extends us to different politic domains, including the most common and automatic actions in our daily life (Christian & Drilling, 2010). Quality is the set of attributes and characteristics of a product or service that affect the ability to meet a person's needs. If the main characteristic of quality is, on the one hand, the continuous improvement of company processes and, on the other hand, the intention to satisfy the customer and everyone involved in the functioning of the organizations, then the concept of Overall Quality Management (OQM) arises (Hoyle, 2017). Quality management was of the utmost importance as it included efforts to maintain and improve quality in all areas of the company and to create products and services with the greatest possible savings (Kotler et al., 2016). The OQM aims to continuously improve all processes, products, and services (Kotler et al., 2016). It is a philosophy that came up in the 1950s and 1960s that led to a change in attitudes where quality became a business problem (Hoyle, 2017). The basic requirement of OQM is based on the fact that the success of the company is based on the quality level that it offers the customer by integrating the production and all processes that support the quality processes (Hoyle, 2017). In the context of organizations, there are various definitions of quality, all of which relate to customer satisfaction with the products or services offered by companies (Kotler et al., 2016). The European Foundation for Quality Management (EFQM) claims that the model of excellence is not a requirement, for the reason that there are many ways to achieve organizational excellence (Protzman et al., 2015). The EFQM Excellence Model (EFQM-EM) is based on nine criteria, five of which are enablers and four results. Activation criteria include what an organization does and how it does it. The criteria of the results cover what an organization achieves. The model assumes that excellent organizations achieve superior performance results in a sustainable manner and thus meet or exceed the expectations of all stakeholders (EFQM, 2020). According to EFQM-EM, leadership outcomes that motivate employees, develop strategies and guidelines, build partnerships with their suppliers and analyse the organization as a process can help to remove (or at least minimize) obstacles between different departments (EFQM, 2020). The activators cover what an organization does and how it happens, while the results cover what an organization achieves. The results are caused by the enablers and the enablers are improved by the feedback of the results (Figure 45). The arrows in Figure 45 illustrate the dynamics of the model and also show that learning and innovation support the improvement of enablers, which in turn leads to better results (EFQM, 2020). Regarding the criteria shown in Figure 45 , it is important to highlight some aspects, viz.

- **Leadership** – Excellent organizations have leaders who build trust in others. A good leader is flexible, creates trust and ensures the continued success of the organization;

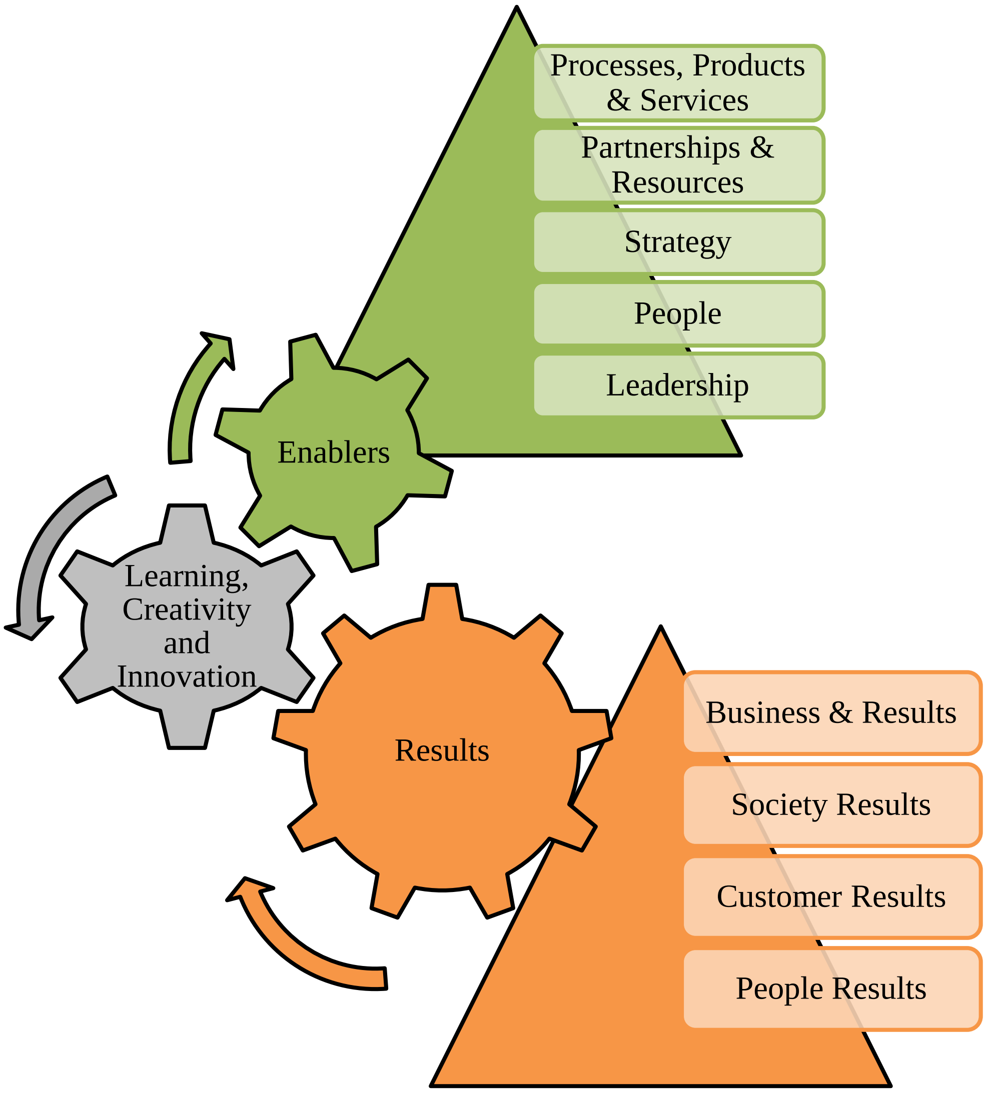

Figure 45 – The European Foundation for Quality Management Excellence Model.

- **Strategy** – Excellent organizations implement their mission and vision by developing a strategy that is geared towards the interest groups. The guidelines, plans, goals, and processes are developed and implemented considering the previously defined strategy. Companies that want excellent service appreciate people and create a culture that enables them to achieve personal and organizational goals that are mutually beneficial. This type of organization develops the skills of the employees and promotes fairness and equality through communication, reward, and recognition. It also motivates and develops a very beneficial compromise for the organization; and
- **Partnerships** – Excellent organizations build good partnerships with suppliers and have good resources to ensure that they work properly. Good management of processes, products and services enables the generation of added value for

customers and other stakeholders. Companies that focus on their customers can achieve excellent results and respond to customers' needs and expectations. In addition, focusing on the company's employees is critical to get good results. Only through measures that make it possible to exceed the needs and expectations of stakeholders can an organization be viewed as effective and achieve good results both in society and in the economy itself.

IV.4.1.2. Accreditation

Portuguese organizations, as well as their international counterparts, seek success in an increasingly globalized market. One of the most efficient ways to achieve that goal is undoubtedly the accreditation. The definition of accreditation according to ISO/IEC 17000 standard is the *"claim of third party concerning a body for conformity assessment, which is a formal recognition of their competence to carry out specific activities of conformity assessment"* (ISO 17000, 2020). Accreditation is the formal recognition by an independent official entity that an organization has technical competence to exercise, with credibility, the activities of conformity assessment (e.g., calibration, testing, certification and/or inspection), in accordance with certain requirements (ISO 17000, 2020). The ISO/IEC 17025 defines a harmonized methodology, specifying the general requirements for the competence, impartiality and consistent operation of laboratories and it is applicable to all organizations performing laboratory activities. Indeed, accreditation to ISO/IEC 17025 allows recognizing the competence of the laboratories and offers competitive advantages in submitting proposals to clients that require independent and reliable laboratories. Any calibration or test certificate issued by a laboratory that is accredited by an accreditation body is accepted in any country (ISO 17025, 2017). According to Squirrell (2001) this is one of the main advantages of accreditation. Beyond confirming that the calibration/testing is based on written procedures, accreditation also attests the technical competence to perform the respective calibration (Jimenez et al., 2015). For laboratories interested in demonstrating their technical competence supported by a quality system, the appropriate reference is the ISO/IEC 17025 (ISO 17025, 2017).

IV.4.1.3. Study Aims

Assessing customer satisfaction is critical for companies looking to gain competitive advantage in the market. Therefore, customer satisfaction is tied to the standards that apply to different areas of activity, including chemical analysis laboratories. The present work aims to assess the satisfaction of the customers of water analysis laboratories on the basis of parameters that influence the management requirements and the technical requirements of the ISO/IEC 17025 standard. To achieve this general goal, artificial intelligence methods and techniques have been used to develop a decision support system. for this reason, this article introduces a formal method of customer satisfaction assessment that is based on a logical programming approach for knowledge representation and reasoning (Neves, 1984; Neves et al., 2019; Fernandes et al., 2020c) leading to a computational system geared towards artificial neural networks (Haykin, 2009; Vicente et al., 2012b).

IV.4.2. Related Work

In the literature, employee satisfaction studies are more common than customer satisfaction studies. These were carried out in areas such as health (Allen 2013; Boev et al., 2015; Borishad et al., 2018; Liu et al., 2019), tourism (Francesco et al., 2019; Gerdt et al., 2019) and call centers (Walsh et al., 2012; Chicu et al., 2019). To our knowledge, no customer satisfaction studies have been published in water laboratories. Regarding healthcare, Boev et al. (2015) examined the relationship between occupational satisfaction in care and health-related infections in intensive care unit in adults. Wage inequality, dissatisfaction with the salary and lack of recognition are the most important aspects. Allen (2013) examined the effects of the introduction of a quality management system based on ISO 15189 on the improvement of security and customer satisfaction. The author emphasized that the implementation of such systems led to an improvement in quality and an increase in customer security. Borishad et al. (2018) examined the relationship between customer experience and customer satisfaction in four private hospitals in Nigeria. The data were recorded on a questionnaire with a 5-point Likert scale and a total of 365 participants were registered. The authors developed a model that describes customer satisfaction as a function of the reliability of services, the correct diagnosis of diseases, the correct treatment of diseases, the effectiveness of verbal communication and non-verbal communication. The model was able to explain 43.1% of the observed variance in customer satisfaction (Borishad et al., 2018). Liu et al. (2019) examined the relationship between workplace violence and patient safety. A questionnaire was conducted in 23 Chinese hospitals in Guangdong Province, with 1502 nurses participating. The data were collected between December 2013 and August 2014. According to this study, workplace violence was associated with a higher incidence of burnout, lower job satisfaction and lower patient safety. The authors also found strong associations between nursing staff burnout and less patient safety. Conversely, a higher level of job satisfaction among nursing staff was directly linked to greater patient safety. The authors also point out that burnout and job satisfaction among nurses played a mediating role in workplace violence and patient safety (Liu et al., 2019).

IV.4.3. Materials and Methods

IV.4.3.1. Place of Study

This study was carried out in the Water Laboratory of Santiago do Cacém Municipality, located in southern Portugal. This laboratory is accredited according to the ISO/IEC 17025 standard. It is known for its technical know-how in sampling and analytical tests. The water laboratory offers services for the collection, transport, physical-chemical and microbiological analysis of samples of treated and non-treated water (e.g. wells, boreholes, pool water and whirlpools) for private and municipalities customers. The laboratory team consists of 1 laboratory manager, 1 quality manager, 1 administration employee, 4 sample technicians, 5 microbiology technicians, and 6 physic-chemical technicians.

IV.4.3.2. Participants

This study included 253 participants (lab customers) aged between 23 and 76 with an average age of 43. The gender distribution was 46% for men and 54% for women. 87.6% of the participants came from rural areas, 12.4% from urban ones.

IV.4.3.3. Data Collection

A versatile data collection tool was used to achieve the previously defined goals (DeKetele & Roegiers, 2016; Cohen et al., 2017). Considering the advantages and disadvantages of the possible techniques (McMillan & Schumacher, 2009), the survey was selected using a questionnaire. The reasons for this choice are related to the fact that this tool has a clearly defined structure and makes it possible to convert the qualitative information provided by the respondents into quantitative one. For this study, a customer satisfaction questionnaire was created that was used for a cohort of 253 customers. The questionnaire was divided into three sections, the first of which contained general questions (e.g. age, gender, location, academic qualifications, and type of acquaintance with the laboratory). The second contains statements on the services provided, namely customer service, the quality of the services, documentation of the support and handling complaints. Finally, in the third section, respondents are asked to express their worldwide satisfaction with the services provided by the laboratory. In the first part of the questionnaire the answers are descriptive, while in the others the Likert scale was used with four levels, i.e., *very dissatisfied*, *slightly dissatisfied*, *satisfied* and *very satisfied* (section IV.4.6). The questionnaire is validated according to the rules of Bell (2010). Therefore, the questionnaire was evaluated by a group of experts (i.e., a group of accountants) who suggested some corrections. After an expert analysis, the questionnaire was modified and applied to a limited group of customers who were not included in the sample to assess its validity and identify difficulties in interpreting the questionnaire. The response rate was 86.1% (253 inquiries were received in 294 endorsed).

IV.4.3.4. Qualitative Data Processing

Aiming the conversion of the qualitative information (collected through the questionnaire) into a quantitative one, the method proposed by Fernandes et al. (2016b) was followed. According to this method a set of *n* issues regarding a particular subject is itemized into a unitary area circle split into *n* slices, where the marks in the axis correspond to each one of the possible answers, as described in the section IV.4.4.3.

IV.4.3.5. Artificial Neural Networks

The software used to implement ANNs was the Waikato Environment for Knowledge Analysis (WEKA), while maintaining the standard software parameters (Hall et al., 2009; Frank et al., 2016). Aiming to guarantee statistical significance of the results, 20 experiments were applied in all tests. In each simulation, the database was randomly split into two mutually exclusive partitions, i.e., the training set (with two thirds of the cases) and the test set (made up of the remaining examples).

IV.4.3.6. Ethical Aspects of the Study

The respondents took notice of the goals of the questionnaire and participated voluntarily, without any pressure or coercion. The study was conducted in compliance with the relevant laws and institutional guidelines and was approved by the quality manager of the Water Laboratory of Santiago do Cacém Municipality. Furthermore, the participants gave an informed consent to participate in the study.

IV.4.4. Results and Discussion

IV.4.4.1. Sample Characterization

Respondents' age was split into age groups as shown in Figure 46A (i.e., less than 20 years old, 20-30, 31-50, 51-70 and higher than 70 years old). 71% of participants are lesser than 50 years old while 29% are higher than 51 years old (Figure 46A). On the way to an academic qualification, 34% of the cohort stated to have basic education, 39% declared to finish secondary education, 20% affirmed to have a degree and 7% declared to have post graduate education (Figure 46B). Regarding the way customers became familiar with the laboratory, 49% declared that got acquainted through the internet (i.e. web or social networks), 16% said they discovered the laboratory on site, 15% declared to be regular customers and 13% affirmed that knew the lab through close people (Figure 46C).

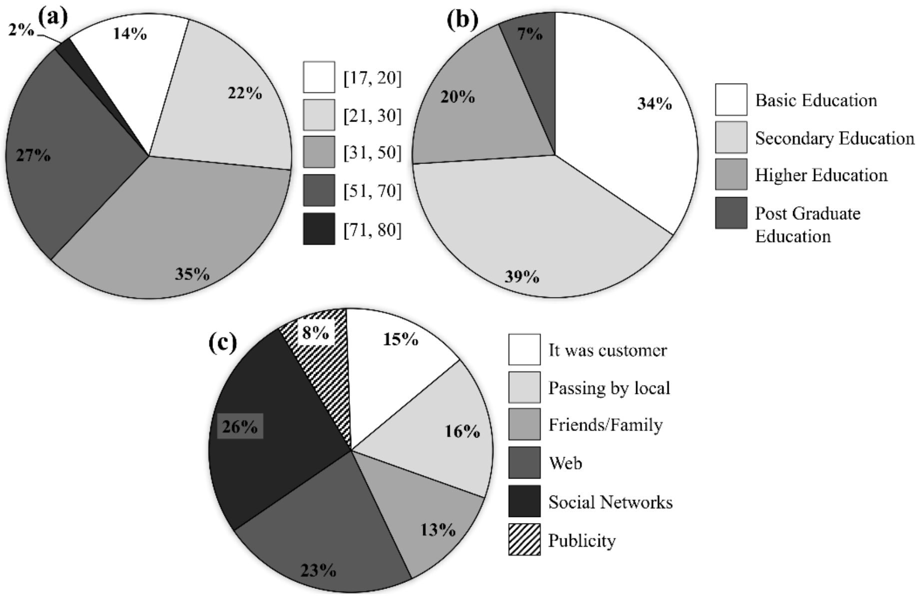

Figure 46 – Sample characterization in terms of age groups (a), academic qualifications (b) and how the customers get acquainted with the laboratory (c).

IV.4.4.2. Answer Frequency Analysis

Figure 47 shows the results of the second part of the questionnaire, in which the respondents expressed their opinion on the statements on two factors, i.e., customer service and quality of service provided. The graphics show the frequency of reactions to the individual factors. Statements S1 to S5 relate to the customer service factor, while statements S6 to S10 relate to the quality of the service provided. Regarding the customer service factor, the analysis of the results shows that the vast majority of respondents (between 83% and 93%) say they are *satisfied* or *very satisfied*. However, more than 20% of the respondents were *very satisfied* with the availability of services (S3), the effectiveness of answering questions (S4) and the clarity of the answers to questions (S5). Conversely, 7.5% of those surveyed stated that they were *very dissatisfied* with the clarity of the answers to questions (S5). In relation to the other statements, only a small percentage, less than 4% of the participants, stated that they were *very dissatisfied*. Regarding the quality of the services provided, the analysis of the results shows that the vast majority of respondents, who are between 83.5% and 96%, think they are *satisfied* or *very satisfied*. The statements on the number and type of available tests (S7), samples (S6) and appropriateness of delivery times (S9) gave more than 90% of the positive answers (96%, 94.5% and 90%). In contrast, the statement with the highest percentage of the most negative answer (7%) relates to the reliability of the results (S8).

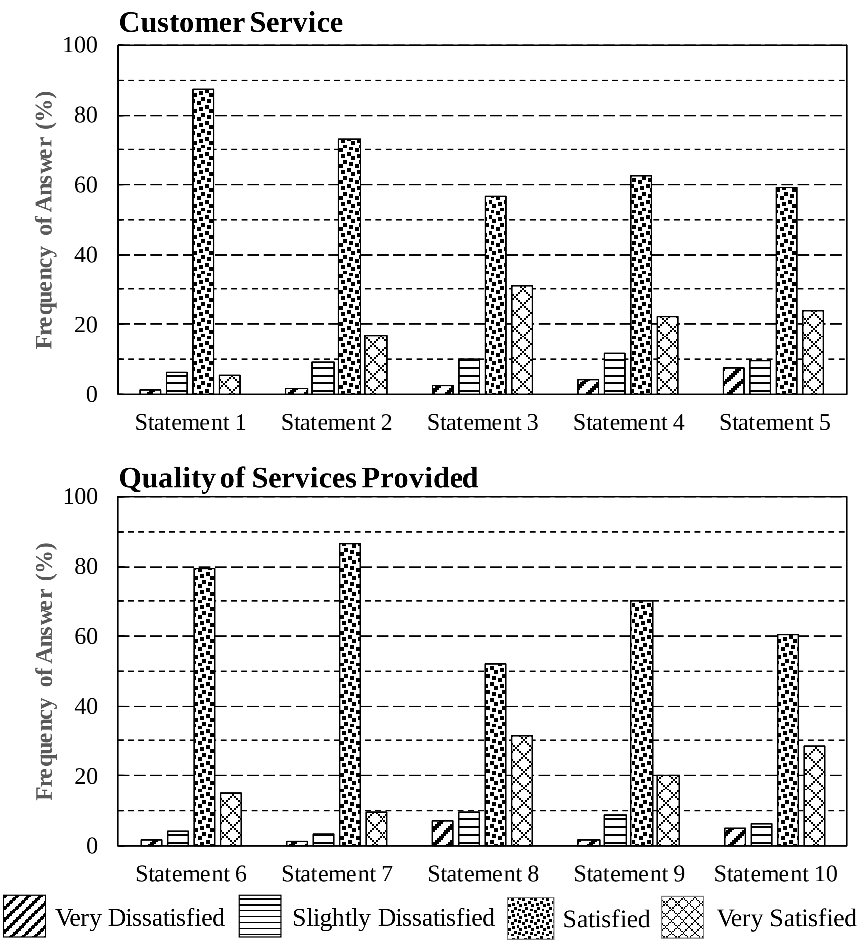

Figure 47 – Frequency of answer to the statements regarding customer service and quality of services provided.

Figure 48 shows the results of the *support documentation*. The diagram shows the frequency of answering the individual instructions. A review of Figure 48 shows that the vast majority of respondents (between 84% and 97.5%) have a positive opinion. However, 16% of the respondents indicated that the analysis reports were negative (S12). This dissatisfaction can be related to both the age of the respondents and their academic qualifications. In fact, 29% of respondents are older than 50 and 34% say they only have basic training (Figure 46).

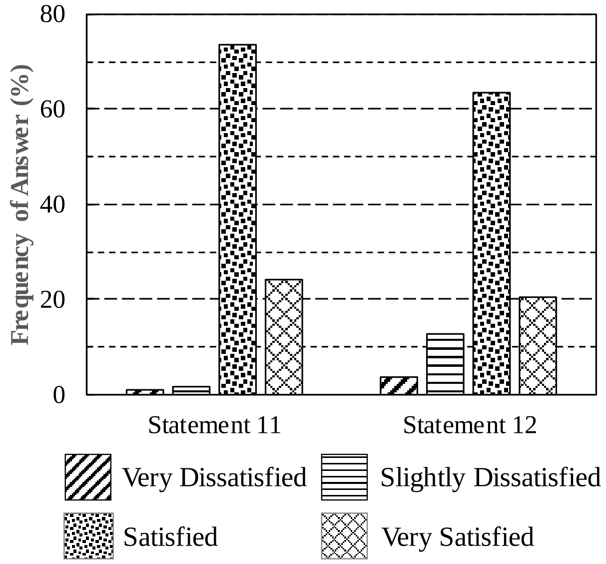

Figure 48 – Frequency of answer to the statements regarding support documentation.

Only 10.7% of respondents replied to the group's explanations on how to deal with complaints. Although this percentage can be considered low in terms of the cohort, the graph shown in Figure 49 indicates that more than 75% of respondents who responded to this group said they were not satisfied with treating their complaints, i.e., solution (S13), response time (S14) and effectiveness (S15). The high percentage of negative opinions on complaints handling suggests that the organization should take these points into account and promote the necessary improvements to address these shortcomings.

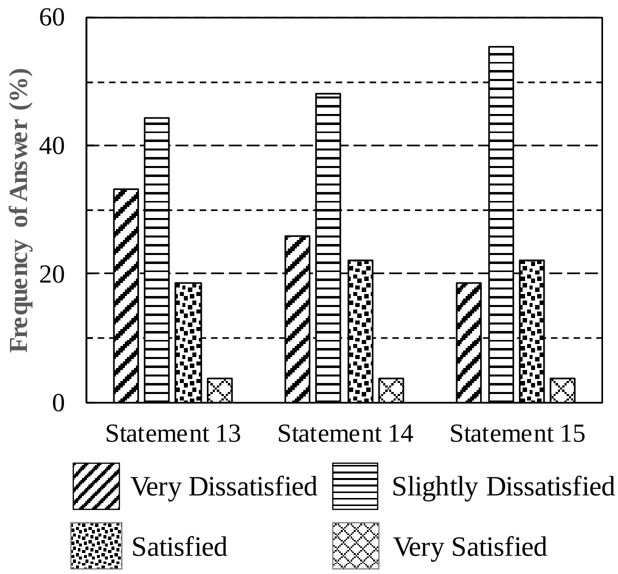

Figure 49 – Frequency of answer to the statements regarding complaint handling.

Figure 50 shows the results of the third part of the questionnaire, in which the respondents expressed their opinion on the overall assessment of the services. A review of Figure 50 shows that the vast majority of respondents have a positive opinion (56% are satisfied and 32% are very satisfied), while 12% of those questioned expressed a negative opinion.

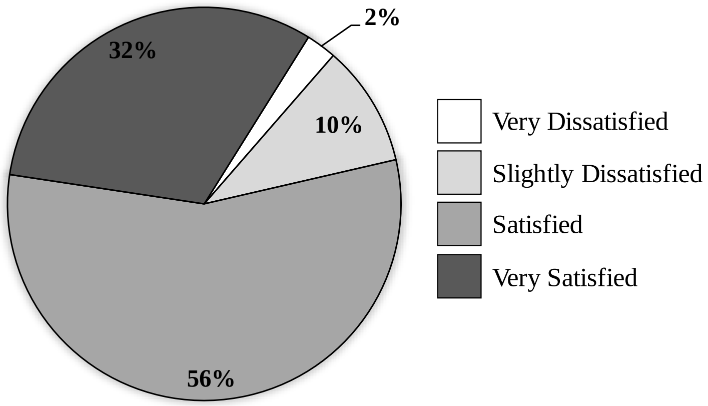

Figure 50 – Frequency of answer to the statements regarding overall assessment of service.

IV.4.4.3. Customer Satisfaction Assessment

In order to gather information about customers' satisfaction, the second section of the questionnaire comprises questions related with the customers' opinions about *Customer Service*, *Quality of Services Provided* and *Support Documentation*.

Figure 51 shows the answers of respondent #1 to the mentioned part of the questionnaire. In order to quantify the qualitative information presented in Figure 51, the method proposed by Fernandes et al. (2016b) was followed. For each dimension (i.e., *Customer Service*, *Quality of Services Provided* and *Support Documentation*) the correspondent answers were itemized into a unitary area circle. The marks in the axis correspond to the possible answer, i.e., *very dissatisfied*, *slightly dissatisfied*, *satisfied* and *very satisfied*. Taking as an example the dimension customer service, the answer of respondent #1 to statements 1 and 5 (S1 and S5) was *satisfied* and the correspondent areas is computed as $\frac{1}{5} \times \pi \times \left(\frac{3}{4} \times \frac{1}{\sqrt{\pi}}\right)^2 = 0.11$, in the statements 2 and 4 (S2 and S4) was chosen the alternative *very satisfied* and the corresponding areas are $\frac{1}{5} \times \pi \times \left(\frac{4}{4} \times \frac{1}{\sqrt{\pi}}\right)^2 = 0.2$. Finally, for statement 3 (S3) the answer was *slightly dissatisfied* and the areas are $\frac{1}{5}\times\pi\times\left(\frac{2}{4}\times\frac{1}{\sqrt{\pi}}\right)^{2} = 0.05$. The total area (i.e., 0.67) is the sum of the partial ones, being the quantitative value regarding the dimension customer service for respondent #1 (Figure 52). For the remaining dimensions the procedure is similar and the results are shown in Table 21.

CUSTOMER SATISFACTION QUESTIONNAIRE

PART II

For each statement tick the option that best reflects your opinion.

CUSTOMER SERVICE	Very Dissatisfied	Slightly Dissatisfied	Satisfied	Very Satisfied
S1. Easiness of contact.	☐	☐	☒	☐
S2. Response time to requests.	☐	☐	☐	☒
S3. Service availability.	☐	☒	☐	☐
S4. Effectiveness in the clarification of questions.	☐	☐	☐	☒
S5. Clarity in answers to questions.	☐	☐	☒	☐

QUALITY OF SERVICES PROVIDED	Very ~ Dissatisfied	Slightly Dissatisfied	Satisfied	Very Satisfied
S6. Sampling.	☐	☐	☒	☐
S7. Number and type of tests available.	☐	☐	☒	☐
S8. Reliability of results.	☐	☒	☐	☐
S9. Appropriateness of delivery times.	☐	☐	☐	☒
S10. Delivery deadlines.	☐	☐	☐	☒

SUPPORT DOCUMENTATION	Very Dissatisfied	Slightly Dissatisfied	Satisfied	Very Satisfied
S11. Presentation of the commercial proposals.	☐	☐	☒	☐
S12. Presentation of analysis reports.	☐	☒	☐	☐

COMPLAINT HANDLING (IF APPLICABLE)	Very Dissatisfied	Slightly Dissatisfied	Satisfied	Very Satisfied
S13. Resolution of complaints.	☐	☐	☐	☐
S14. Timely response to complaints.	☐	☐	☐	☐
S15. Effectiveness in handling of complaints.	☐	☐	☐	☐

Figure 51 – The answers of respondent #1 to the second part of the questionnaire.

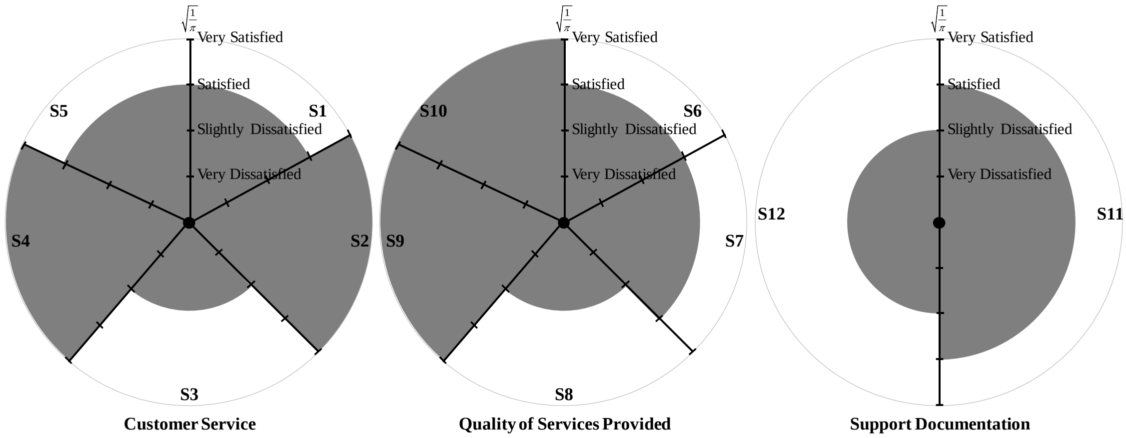

Figure 52 – A view of the qualitative data processing.

The data presented in Table 21 were used as input variables in the training of an *ANN* in order to obtain the output variable, i.e., the *costumers' satisfaction assessment* (Figure 53). The *ANN* approach to data processing enables not only that data are processed in a system context but also to capture complex/unknown relationships between inputs and outputs (Vicente et al., 2012b; Vilhena et al., 2017). *ANNs* simulate the structure of the human brain, being populated by multiple layers of neurons, with a valuable set of activation functions (Haykin, 2009).

Table 21 – A fragment of the knowledge base for costumers' satisfaction assessment.

#	Customer Service	Quality of Services Provided	Support Documentation
1	0.67	0.67	0.41
2	0.29	0.54	0.31
…	…	…	…
253	0.64	0.60	0.82

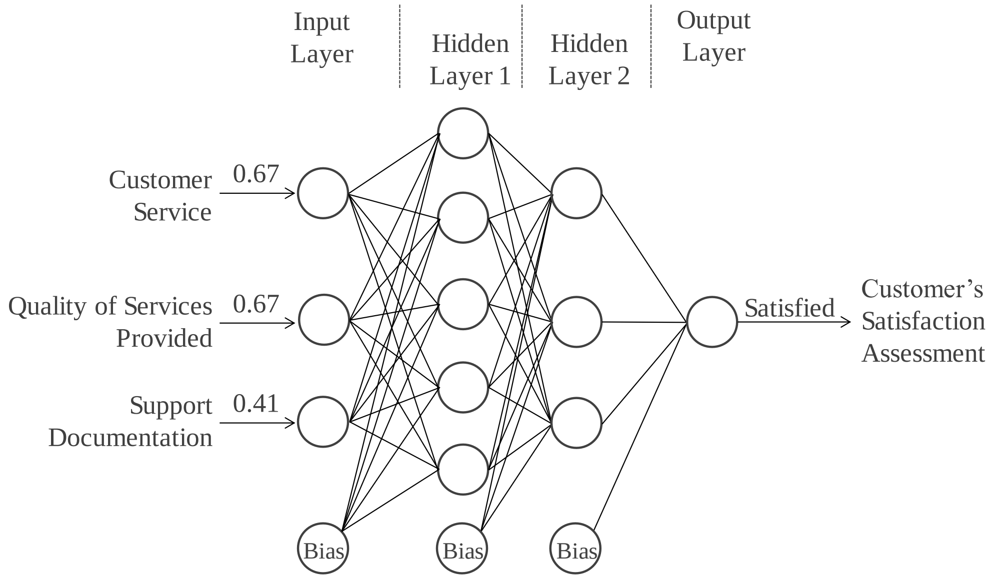

Figure 53 – ANN model for customers' satisfaction assessment.

The assessment of *ANN* model performance can be done using the confusion matrix (Vilhena et al., 2017). Table 22 presents the confusion matrix for the *ANN* model shown in Figure 53 (the values refer to an average concerning 20 experiments). The values shown in Table 22 allow computing the model accuracy for training set (94.7%, i.e., 160 well classified in 169) and for test set (91.7%, i.e., 77 well classified in 84). Therefore, the predictions of customers' satisfaction using the *ANN* model are satisfactory, achieving accuracies higher than 90%. The coincidence matrix also allows to compute the *Sensitivity*, *Specificity*, *Positive Predictive Value* (*PPV*) and the *Negative Predictive Value* (*NPV*) of the model (Vilhena et al., 2017). The sensitivity and specificity for training and test sets were 94.2%, 93.1%, 95.4%, and 88.5%, respectively. Thus, the proportion of positive opinions correctly identified ranges between 93.1% and 94.2%, while the proportion of negative ones well classified varied between 88.5%, and 95.4%. Regarding the confidence that can be put when the model classifies a case as positive (i.e., the *PPV*) 97.0% and 94.7% were obtained for training and test sets. Concerning negative cases, the values obtained were 94.4% and 85.2% respectively. These results seem to reveal a good overall ability of the model to discriminate between the output classes, i.e., the *ANN* model exhibits a good performance in the assessment of customers' satisfaction.

Table 22 – Confusion matrix regarding ANN model for customers' satisfaction assessment.

Target	Predictive				
	Training set			Test set	
	Satisfied (+)	Dissatisfied (–)		Satisfied (+)	Dissatisfied (–)
Satisfied (+)	97	6		54	4
Dissatisfied (–)	3	63		3	23

IV.4.5. Conclusions

Water analysis is of enormous importance, especially if it is intended for human consumption. The results of the water analysis also serve to assess the damage to the aquatic environment and to trigger measures to reduce the environmental impact. The water analysis can also be used to estimate the measures required to comply with the applicable laws. In addition, water analysis can ensure that the water is free of chemicals or microorganisms that can harm human health. Indeed, health is central to the well-being of society and people play an increasingly central role in the proper functioning of the health system. This study was carried out in a water laboratory in which a management system according to the ISO/IEC17025 standard is implemented. The results show that the vast majority of respondents rate the performance of the laboratory worldwide as positive. This work also introduces an intelligent decision support system to assess customer satisfaction. The formal basis lies in Logic Programming for Knowledge Representation and Logical Thinking, supplemented by an approach of Artificial Neural Networks for computing, which enables the handling of incomplete, unknown, or even contradictory information. This approach focuses on the processing of information gathered through questionnaire surveys and enables the full integration of factors related to *Customer Service*, *Service Quality* and *Support Documentation*. It can provide reasonable answers with an overall accuracy of more than 90%. This system can not only recognize the weakness of the laboratory organization, but also design and develop future improvement measures to promote customer satisfaction. In fact, customers today are better informed and more critical of the quality of the services provided.

IV.4.6. Customer Satisfaction Questionnaire

CUSTOMER SATISFACTION QUESTIONNAIRE

The continuous improvement of the services provided is the main commitment of the Water Laboratory.

In this sense, knowing the degree of customer satisfaction is fundamental to create new alternatives and leads to an increasingly effective service.

For improvement suggestions use the space for the effect at the end of the questionnaire.

Note: The Laboratory protects your privacy.

The personal data collected will be processed by computer and will not be transferred to any other institution not used for any purpose other than the support to the Internal Quality Management System.

PART I

CUSTOMER DATA

Tick the box that corresponds to your case or fill the blanks.

Gender	Feminine ☐	Masculine ☐

Academic Qualifications	Basic Education	Secondary Education	Higher Education	Post Graduate Education
	☐	☐	☐	☐

Age	______________ **years old**	**Locality**	______________

How did you find the Lab?	It was Customer	Passing by local	Friends or Family	Web	Social Networks	Publicity
	☐	☐	☐	☐	☐	☐

PART II

For each statement tick the option that best reflects your opinion.

CUSTOMER SERVICE				
	Very Dissatisfied	**Slightly Dissatisfied**	**Satisfied**	**Very Satisfied**
S1. Easiness of contact.	☐	☐	☐	☐
S2. Response time to requests.	☐	☐	☐	☐
S3. Service availability.	☐	☐	☐	☐
S4. Effectiveness in the clarification of questions.	☐	☐	☐	☐
S5. Clarity in answers to questions.	☐	☐	☐	☐

CUSTOMER SATISFACTION QUESTIONNAIRE

QUALITY OF SERVICES PROVIDED	Very ~ Dissatisfied	Slightly Dissatisfied	Satisfied	Very Satisfied
S6. Sampling.	☐	☐	☐	☐
S7. Number and type of tests available.	☐	☐	☐	☐
S8. Reliability of results.	☐	☐	☐	☐
S9. Appropriateness of delivery times.	☐	☐	☐	☐
S10. Delivery deadlines.	☐	☐	☐	☐

SUPPORT DOCUMENTATION	Very Dissatisfied	Slightly Dissatisfied	Satisfied	Very Satisfied
S11. Presentation of the commercial proposals.	☐	☐	☐	☐
S12. Presentation of analysis reports.	☐	☐	☐	☐

COMPLAINT HANDLING (IF APPLICABLE)	Very Dissatisfied	Slightly Dissatisfied	Satisfied	Very Satisfied
S13. Resolution of complaints.	☐	☐	☐	☐
S14. Timely response to complaints.	☐	☐	☐	☐
S15. Effectiveness in handling of complaints.	☐	☐	☐	☐

PART III

Tick the option that best reflects your global opinion about the service provided by the lab.

OVERALL ASSESSMENT OF SERVICE	Very Dissatisfied	Slightly Dissatisfied	Satisfied	Very Satisfied
S16. Service provided by the laboratory.	☐	☐	☐	☐

SUGGESTIONS FOR IMPROVEMENTS

Thank you very much for your collaboration!

IV.5. Synopsis

The Total Quality methodologies had a strong impact on the operation of the laboratories. The main methodologies adopted in Portugal include accreditation and certification, based on international models, whose final objectives are satisfaction, on one hand, and compliance with legal and regulatory requirements affecting the sector, on the other hand. In this context, the paper **"An Assessment of the Data Guidelines in Cryopreservation Laboratories"** assesses the implementation of GDPR in a cryopreservation laboratory, based on the use of ANNs.

Due to the exceptional situation and the proliferation of registered cases of contagion by the new coronavirus, SARS-COV-2, it is urgent that organizations apply extraordinary measures in terms of training employees, acquiring resources, cleaning procedures and disinfection. In this context, the paper **"A Case-Based Approach to Assess Employees' Satisfaction with Work Guidelines in Times of the Pandemic"** combines the concept of innovation and TQM. In this work, a model is presented, using Case-Based Reasoning, to assess employee satisfaction with the new procedures related to the current pandemic crisis. In this study, through the analysis of responses to a questionnaire, built for this purpose, insights are obtained that can contribute to a better adaptation of organizations to this situation, increasing employee satisfaction and involvement. Knowing employee satisfaction is important but also customer satisfaction, which is an indicator of the quality present in most organizations. In the paper **"Customers' Satisfaction Assessment in Water Laboratories",** customer satisfaction at a water analysis laboratory, accredited according to the ISO/IEC 17025 standard, was analysed. In general, it was found that for all parameters analysed, whether they are related to Management Requirements or Technical Requirements, a high level of satisfaction was obtained. These results show that the existence of a management system according to the ISO/IEC 17025 framework contributes to meeting customers' requirements.

Chapter V. Concluding Remarks and Future Perspectives

V. Concluding Remarks and Future Perspectives

Laboratories have undergone intense changes due to increasing technical and regulatory requirements. On one hand, legal guidelines, new expectations, recommendations from scientific societies, technological innovations and competition put pressure on laboratories to supply a variety of new products and services to the market. On the other hand, laboratory managers and their teams are continually challenged to demonstrate increasing levels of technical excellence in order to guarantee the reliability of results, in line with the necessary cost reduction, reduction of response time, minimization of consumption of reagents and the constant need for updating. The routine of a laboratory is complex, either because of the multiplicity of processes that must be controlled, or because of the variety of equipment used. This framework increasingly requires better preparation of professionals and the adoption of effective Quality Management Systems. However, current methods of quality control and management are time consuming, complex, expensive and involve a large number of technical and financial resources (calibrated equipment, infrastructure, qualified technicians and reagents). All this complexity promotes dispersion and hinders quick access to the information needed to make predictions and make the best decisions in a timely manner.

The present work contributes to the resolution of problems in the technical area and in quality management in laboratories, using Artificial Intelligence tools. It presents different models that can be applied to obtain valid results and strategic business actions. Its application in water and/or health laboratories allows to promote the quality of services and, therefore, the reduction of waste, the minimization of consumption, the guarantee of legal compliance, the improvement of working conditions, the prevention of diseases, the development of new therapies and, finally, the satisfaction of clients/patients. In fact, the introduction of these models in Biochemistry-based laboratories makes it possible to take another step up of innovation and better laboratory performance, privileging health and in line with customers' expectations.

The results obtained allow to sustain new developments and new investigations, with a view to the application of the proposed models to other sectors. As future work, it is proposed, viz.

- The creation of a platform that integrates all the models presented and, in this way, provide organizations with tools to assess their efficiency as a whole; and
- The adaptation of the platform to other activities to promote quality and provide excellent services.

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