DEVELOPMENT OF A HIERARCHICAL FUZZY MODEL FOR THE EVALUATION OF INHERENT SAFETY

A Dissertation

by

MICHELA GENTILE

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

August 2004

Major Subject: Chemical Engineering

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Major Subject: Chemical Engineering

ABSTRACT

Development of a Hierarchical Fuzzy Model for the Evaluation of Inherent Safety.
(August 2004)
Michela Gentile, B.S., Universidad de las Americas, Puebla, Mexico
Chair of Advisory Committee: Dr. M. Sam Mannan

Inherent safety has been recognized as a design approach useful to remove or reduce hazards at the source instead of controlling them with add-on protective barriers. However, inherent safety is based on qualitative principles that cannot easily be evaluated and analyzed, and this is one of the major difficulties for the systematic application and quantification of inherent safety in plant design.

The present research introduces the use of fuzzy logic for the measurement of inherent safety by proposing a hierarchical fuzzy model. This dissertation establishes a novel conceptual framework for the analysis of inherent safety and proposes a methodology that addresses several of the limitations of the methodologies available for current inherent safety analysis. This research proposes a methodology based on a hierarchical fuzzy model that analyzes the interaction of variables relevant for inherent safety and process safety in general.

The use of fuzzy logic is helpful for modeling uncertainty and subjectivities implied in evaluation of certain variables and it is helpful for combining quantitative data with qualitative information. Fuzzy logic offers the advantage of being able to model numerical and heuristic expert knowledge by using fuzzy IF-THEN rules. Safety is traditionally considered a subjective issue because of the high uncertainty associated with its significant descriptors and parameters; however, this research recognizes that rather than subjective, “safety” is a vague problem. Vagueness derives from the fact that it is not possible to define sharp boundaries between safe and unsafe states; therefore the problem is a “matter of degree”.

The proposed method is computer-based and process simulator-oriented in order to reduce the time and expertise required for the analysis. It is expected that in the future, by linking the present approach to a process simulator, process engineers can develop safety analysis during the early stages of the design in a rapid and systematic way.

Another important aspect of inherent safety, rarely addressed, is transportation of chemical substances; this dissertation includes the analysis of transportation hazard by truck using a fuzzy logic-based approach.

To my parents

Mr. Gianpaolo Gentile and Mrs. Eleonora Cuttini

and my brother

Mr. Fabio Gentile

And to all the people
who lost their lives
in a chemical industry-related incident.

ACKNOWLEDGEMENTS

During my years as volunteer paramedic in Mexico I learned one of the most important laws of emergency response: “Heroes do not exist, because they are all dead”.

One of the meanings of this principle is that emergency response is not the result of the efforts of one single person; it is a matter of teamwork. This is also true for process safety, where efforts must be joined in order to reach a safer chemical industry.

But it is also true for this dissertation. Many people, directly or indirectly, knowing or without knowing the importance of their contribution, helped for the realization of this research.

The Chemical Engineering Department at Texas A&M University gave me the opportunity to expand my knowledge on process safety by funding my studies during the last four years. Without this economic support I would not have had such a life-changing opportunity. I would like to acknowledge all the staff for their unconditional dedication to students, especially internationals.

I’m deeply grateful to Dr. Mannan, not only for accepting me into the program (and convincing me to work towards a Ph.D.) but also for allowing me to work on this project. His vision and trust on the potential of his students is unique.

I also appreciate the assistance and help of Dr. Hall, Dr. El-Halwagi, and Dr. Langari, who not only accepted to serve on my committee but also provided fundamental advice for the realization of the research.

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However, the opportunity to work for the MKOPSC would not have existed without Mr. O’Connor, a quiet and visionary man who violated the inviolable second law of

thermodynamics by converting personal tragedy into a legacy for the present and the future of the chemical industry.

Dr. Rogers has also been a fundamental column of this research by providing advice and assistance during my time with the group.

I would like to thank Mr. David Clark, from DuPont, and Dr. Angela Summers, from SIS-Tech, because they were the first "outsiders" to believe that this "fuzzy" project looked interesting, and their interest provided a much needed motivation during the initial "dark ages" of this research. Their comments allowed me to decide to deliberately take the risk of exploring the application of fuzzy logic (which is not very well accepted in the United Sates) for inherent safety analysis rather than following some other more conventional, but less promising, directions.

I'm especially thankful to Mrs. Karen Tancredi, Mr. Clark, and all the Process Safety and Fire Protection Group at Dupont because of the opportunity they gave me to spend summer 2002 with them for an interesting and eye-opening internship.

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CHAPTER I

INTRODUCTION AND SCOPE OF THE PROJECT

Prevention is always better than control; however, process safety for the chemical industry has been traditionally applied as hazard control measures. The process safety approach based on control is known as “extrinsic safety” while the process safety approach based on prevention is known as “inherent safety”.

Inherent safety is based on principles formalized by Trevor Kletz thirty years ago, and although the approach is recognized as the most effective to reduce the overall hazard level of a chemical process, it is still difficult to systematically apply the principles and analyze their effectiveness for hazard reduction.

This dissertation establishes a novel conceptual framework for the analysis of inherent safety and proposes a methodology that addresses several of the limitations of the methodologies available so far for inherent safety analysis. This research proposes a methodology based on a hierarchical fuzzy model that analyzes the interaction of variables relevant for inherent safety and process safety in general.

Fuzzy logic offers the advantage of being able to model numerical and heuristic expert knowledge by using fuzzy IF-THEN rules. Safety is traditionally considered a subjective issue because of the high uncertainty associated with its significant descriptors and parameters; however, this project recognizes that rather than subjective, “safety” is a vague problem. Vagueness derives from the fact that it is not possible to define sharp boundaries between safe and unsafe states; therefore the problem is a “matter of degree”. While traditional mathematics can deal with vagueness only by using arbitrary “categories” that generate discrete indices, fuzzy logic is a natural approach to describe vagueness as a continuous function between the two extremes, safe and unsafe.

This dissertation follows the style and format of *Trans IChemE, Part B, Process Safety and Environmental Protection.*

The proposed method is computer-based and process simulator-oriented in order to reduce the time and expertise required for the analysis. It is expected that in the future, by linking the present approach to a process simulator, process engineers can develop safety analysis during the early stages of the design in a rapid and systematic way.

Chapter II introduces the basic principles of inherent safety and summarizes the limitations and expected benefits from the applications of this safety approach. The second part of the chapter explores the approaches suggested so far by other researchers and presents an analysis of strengths and limitations of the methodologies.

A more ambitious goal of this project is to break the traditional boundaries of safety ideology associated with the idea that safety is subjective and hence non-quantifiable. One of the ideas of the present research is that safety is not subjective because safety is not a matter of opinion. The laws of physics, chemistry, and thermodynamics govern safety and these laws do not care about what a design engineer thinks is or is not safe. The only aspect of safety that is subjective is associated with human factors.

As explained in Chapter II, several methodologies have been proposed for inherent safety analysis, but in general they tend to be simplistic and not computer-based. These methods therefore cannot describe the complexity of a chemical plant and the interrelations between chemical properties and design parameters. Complexity implies uncertainty however, as explained in Chapter III, not all uncertainty has a statistical nature. These type of problems can be described by fuzzy models, which are introduced in Chapter III along with the basic elements of fuzzy set theory.

The present project evolved from the interest and the industrial need to develop a methodology to analyze inherent safety. Several methods have been proposed for inherent safety and many others have been developed to analyze extrinsic safety, it seems that industry does not need another “traditional” methodology that follows the same pattern of thinking established by the historical approaches of risk assessment and the Dow Fire and Explosion Index.

As discussed in Chapters III and IV, the way process safety is understood today is a legacy of the requirements and design philosophy of the past (i.e., safety as an end-of-the-pipe solution) which are derived form the technical limitations existing thirty years ago (i.e., no computers and all their implications) during the time of fastest growth rate of the chemical industry. However, the technological development available today and the new demands of the industry justify the effort to explore different approaches to process safety and to challenge the field to look beyond the usual solutions.

This dissertation explores the state-of-the art of inherent safety and, by taking a look at the history of process safety and history of mathematics, Chapter IV discusses why we use the methodologies we use today. Chapter IV introduces a conceptual background on which the proposed fuzzy logic-based methodology for inherent safety analysis is built. The attempt to fuzzify the problem of inherent safety quantification by applying fuzzy logic and fuzzy modeling opens up the opportunity to explore challenging and unusual questions such as what is safety and what are the limitations associated with its analysis and measurement. By analyzing the problem form its roots it is evident that the usual approaches to safety analysis are inadequate to describe inherent safety while the lack of knowledge and deep, holistic understanding of the problem sets boundaries that can only be broken by thinking out of the box and attempting new approaches, sometimes borrowed by improbable sources (i.e., non-engineering fields) such as social sciences.

Chapters V and VI introduce the fundamental concepts and definitions of fuzzy logic and fuzzy models, which are applied for the development of the hierarchical model proposed in this dissertation. The basic structure of the hierarchical model for inherent safety analysis is described in Chapter VII, while Chapter VIII describes the technical background used for the design of the model. A simple case study is presented in Chapter IX to show how the model is used and its potential for the analysis of the interactions of parameters relevant for process safety.

An important aspect of inherent safety, rarely addressed, is transportation of chemical substances. Because minimization of stored volumes of chemicals is the most applied principle in order to reduce the hazard level of a chemical plant, larger amounts of substances are “stored on wheels” outside chemical facilities. Therefore, the chemical hazard is moved from the plant to the community. In order to evaluate the overall impact of volume minimization it is necessary to include transportation. The topic is briefly addressed in Chapter X.

Except for Chapter V and part of Chapter VI, the language is kept simple in order to demonstrate the transparency and interpretability of the fuzzy model proposed and also to be congruent with one of the principles of inherent safety that demands to "keep things simple". As indicated by Gupta (2003) a methodology developed for the evaluation of inherent safety must be simple in principle. The model proposed by this research achieves both goals; it is simple in nature but because of the hierarchical structure, it can capture the complexity of a chemical process by modeling the interactions of the variables.

CHAPTER II

INTRODUCTION TO INHERENT SAFETY*

Inherently Safer Design is a concept known since 1870, but it was not until a hundred years later when engineers considered it significantly. Despite the encouraging results obtained from past applications, there is a general resistance to adopt and systematically apply inherent safer design principles. The main purpose of Inherently Safer Design is quite different in comparison with the aim of the traditional concepts of Safety. While the former aims to eliminate or to reduce the hazards present in a process facility, the latter aims to control hazards and to reduce the consequences of a possible accident by using add-on barriers. Thus the hazard may still be present and “safety” depends upon the reliability of the protective barriers, which present other disadvantages such as high installation and maintenance costs [Lutz, 1997].

Inherent safety has been recognized as a design approach useful to remove or reduce hazards at the source instead of controlling them with add-on protective barriers. However, inherent safety is based on qualitative principles that cannot be easily evaluated and analyzed, and this is one of the major difficulties for the systematic application and quantification of inherent safety in plant design. The present chapter summarizes the history of inherent safety and reviews its strengths and limitations. The most important methodologies currently available for quantification and analysis of inherently safer design are briefly introduced and discussed.

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2.1 “WHAT YOU DON’T HAVE CAN’T LEAK”

“What you don’t have can’t leak” is a very simple and straightforward idea that proved to be the tip of the iceberg enclosing a very complex and multifaceted problem.

This concept is just not-so-common “common sense” that represents a new and powerful paradigm in process safety. It is also a concept that lies between art and science, and it challenges engineering with its uncertainty and intriguing complexity. This idea is a legacy of the tough lessons of the past and a reminder that they will happen again if we don’t learn from them.

This was also the main concept of a lecture presented by Dr. Trevor Kletz, on December 14, 1977 in England. Dr. Kletz further expanded this concept during another lecture in 1985 in the US during the 19th Loss Prevention Symposium, of the American Institute of Chemical Engineers (AIChE). Since then it has become the lemma of an approach to process safety known as “inherent safety” or “intrinsic safety”, and it has been the central topic of an increasing number of papers, regulatory attempts, and several research projects.

2.1.1 The growth of the idea and its principles

As Kletz recognizes [Kletz, 1996] “every idea has a pedigree” and the roots of inherent safety can be found in early attempts to improve chemical processes. The first known application is attributed to Ludwig Mond during the 1870s when the Solvay process for the production of sodium carbonate was modified to reduce ammonia leaks from a manhole at the top of a column when it had to be opened to feed powder lime. The problem of ammonia releases was eliminated by pumping milk of lime into the column. Another classical example of early application of inherent safety is the redesign of the nitroglycerine reactor. The batch vessel, with a residence time of two hours and containing a mass of 1 ton, was substituted by a small well-mixed continuous reactor with a residence time of two minutes and containing a mass of 1 kg. This improvement represented a dramatic reduction of explosion hazard but happened only during the 1950s [Kletz, 1998].

Kletz was exposed to the nitroglycerine example in 1970 and his attention was captured by the different approach used to increase safety as summarized by Kantyka "...it is far better to avoid the need for complex safety or control systems rather than to install them" (as cited by Kletz, 1996). As in the case of the Solvay process, the hazard reduction was achieved by modification of the design and removal of hazards rather than by addition of complex control systems or protective barriers. In both cases, the hazards were significantly reduced but not totally eliminated, hence demonstrating the essence of the inherently safer design [Kletz, 1996].

An inherently safer design is achieved by reduction and/or elimination of hazard sources by means that are integral parts of the processes and plants and thus cannot be separated as different entities or protective systems. However inherently safer design is different from inherently safe design. Since it is not possible to completely eliminate all the hazard sources, inherently safe designs cannot be achieved because a residual hazard will always be present. However, through inherently safer design the magnitude of the residual hazard can be sufficiently reduced in order to pose small or insignificant threat in case of an incident that can be controlled by simpler extrinsic protective systems.

In 1974 the Flixborough explosion, UK, was a significant and revealing event to Kletz, who observed that one of the reasons why the incident was so devastating was the large quantities of hazardous chemicals stored or in-process. During the next ten years Kletz collected information on other incidents, presented lectures, and slowly convinced the chemical engineering community about the "logic" of inherent safety [Kletz, 1996]. Few weeks later in 1984 the next legacy in the chemical industry history was delivered by the most deadly industrial incident: Bhopal, India. The leak of methyl isocyanate (MIC) killed more than 2000 people. The event produced a profound impact on the chemical industry and new demands for higher safety.

In the United States the inherently safer approach was introduced by Kletz in 1985 at the 19th Loss prevention Symposium of the AIChE and was recognized as the most significant paper of the meeting [Bollinger et al, 1996]. Since then, an increasing number of papers have been published, analytical methodologies have been proposed, and the interest has grown to a point where regulatory attempts have been proposed [Kletz, 1996; Johnson, 2003] and attempted [Corzine bill, 2001].

2.1.2 The principles of inherent safety and friendly plants

Kletz first formalized the inherent safety principles in 1984 as strategies to reduce hazard sources and achieve inherently safer designs. The principles upon which the inherently safer design is based are:

- INTENSIFICATION: Reduction of the inventories of hazardous materials.
- SUBSTITUTION: Replacement of the chemical substances by less hazardous chemicals.
- ATTENUATION: Reduction of the quantity of hazardous materials required in the process. Design processes working at less dangerous processing conditions by reducing temperature, pressure, flow, or other relevant variables.
- LIMITATION of EFFECTS: The facilities must be designed in order to minimize the effects of the release of hazardous chemicals or energies.

The list of principles has been extended by Kletz to include other aspects that make plants friendlier by reducing error opportunities or reducing the plant sensitivity to errors and abnormal situations. The principles for inherently friendlier plants include the following [Kletz, 1998]:

- SIMPLIFICATION: Design simpler plants that provide fewer opportunities for error or wrong operation.
- AVOIDING KNOCK-ON EFFECTS: Design plants in such a way that when incidents occur the domino effect doesn’t happen.
- MAKING INCORRECT ASSEMBLY IMPOSSIBLE: When it is not possible to assemble something in more than the correct way, errors and incidents are prevented.

- MAKING STATUS CLEAR: Friendlier plants or equipment allow clear understanding of their status.
- TOLERANCE: Safer plants forgive operator errors, poor installation, and equipment failures.
- EASE OF CONTROL: By simplification of a plant, less instrumentation is required. Processes with slower response are more tolerant with respect to operation upsets.
- SOFTWARE: Software must be simple to use and understand. It should be homogeneous for all the plant control systems.

2.1.3 The benefits of inherently safer design (ISD)

Several authors analyze the benefits and problems associated with both ISD and the traditional approach [Lutz, W.K., 1997; Gupta and Edwards, 2002b], and Zwetsloot et al. (1999) present cases where ISD has proven to be not only technologically feasible but also economically attractive for productive chemical facilities. Inherent safety is a concept that is naturally related to environmental protection. When a plant is designed to reduce or eliminate the hazards, not only does it become safer but possible emissions to the environment are also reduced or eliminated. The possible application of the inherent safety concepts to environmental protection has been recognized by Kletz (1996) and it has been referred to by many others. The relation between the principles of inherent safety and pollution prevention has been described, along with some successful applications, by Askounes-Ashford and Zwetsloot (2000). Therefore the environmental damage resulting from the release of chemicals during an incident can be significantly reduced. Moreover, contamination resulting from releases or leaks occurring during normal operations is also reduced because the quantities of chemicals or their hazards are limited. Thereby, both process and environmental safety of processing plants are increased.

Inherent safety is sometimes referred to as “primary prevention” and it is also an approach to chemical incident and pollution prevention that is different compared to “secondary accident prevention” and mitigation. Inherent safety is based on the use of technologies and chemicals that reduce or eliminate the possibility of incidents. This approach is in direct contrast to the traditional safety concept that relies on the reduction and mitigation of the consequences of an incident by controlling the hazard sources rather than eliminating them. This last approach alone is unable to avoid or reduce the risk of serious chemical incidents [Askounes-Ashford and Zwetsloot , 2000] as it is based on add-on protective barriers that are supposed to mitigate the consequences of an accident or release. This approach is parallel to pollution control and remediation measures.

In contrast, inherent safety is parallel to pollution prevention given that its purpose is to avoid the occurrence of incidents that can produce environmental and human harm by removing the possibility of occurrence at the source. When these two concepts, inherent safety and pollution control, are brought together under one unique mathematical methodology, the resultant analysis tool becomes a powerful instrument to achieve not only safer processes but also a clean and sustainable chemical industry [Askounes-Ashford and Zwetsloot , 2000].

2.1.4 Problems and limitations

Although the inherent safety approach is thought to be convenient not only from the safety viewpoint but also from the economic and operative viewpoint, it represents the technical and administrative challenges as reported by Kletz (1996) and Gupta and Edwards (2002a).

Inherent safety and pollution prevention are similar but they pursue apparently two different objectives that sometimes seem to be at odds with each other. One of the most notorious examples concerns the refrigerant gases chlorofluorocarbons (CFC) thought to be inherently safer due to their low toxicity and flammability compared to ammonia and propane [Hendershot, 1995]. However the use of CFC has resulted in ozone layer depletion, bringing the hazard to another time scale and risk level. The CFC example exhibits three major problems associated with safety evaluation (inherent or traditional) and the integration of environmental factors:

a) Process safety focuses mainly on acute environmental effects and long-term human health consequences. Environmental protection focuses mainly on avoiding both long term and acute consequences to the biota and society. Safety applied to process design is mainly focused on the reduction of likelihood of a chemical incident, fire and, explosion. The long-term effects of small releases that do not pose fire or explosion hazards are rarely taken into consideration unless there are specific environmental regulations imposing limits on the type, flow, or concentration of released contaminant streams.

b) The limited knowledge available on the long-term effects of chemicals on the environment due to accumulation and slow degradation kinetics can drive the decision process into hazardous directions. As discussed previously, a classic example is the substitution of ammonia and propane with CFC. However, the recognition of the lack of information or data related to a specific chemical can be used as an additional piece of information for the assessment. For instance, if there is inadequate information about the life-cycle of a chemical (i.e., transportation across different environmental systems) its evaluation, from the environmental safety perspective, should be less favorable than the evaluation of another chemical whose properties are well known and supported by scientific data.

c) In the chemical industry it is a common misconception that a chemical with low toxicity is environmentally safe. However, the evaluation of environmental hazard requires the analysis of specific chemical properties such as photo and biodegradation rates, water solubility, and bioaccumulation.

When an industry is forced to undertake measures to move towards an inherently safer approach it is possible to interpret the principles in such a way that will impact other related aspects of safety. For instance, one of the easier ways to improve the inherent safety level is by reducing the inventory of hazardous chemical substances. However, if this step requires an associated increase in the frequency of shipments of chemicals, the net effect could be an increased transportation hazard. This example shows why transportation consideration must be part of the inherent safety analysis of the plant and cannot be studied as a separate risk entity. Transportation of chemical raw materials and chemical products plays a very important role in the analysis of the inherent safety level of a chemical plant. Transportation, as well as an inherent safety and environmental hazard evaluation, share the problems of data uncertainty, complexity due to the many factors [Bonvicini et al, 1998] that should be analyzed, subjectivity, and lack of a quantification methodology.

During the earlier stages of plant design, it is sometimes possible to choose the safer chemicals in order to obtain an inherently safer plant. However, the idea of "safer chemical" should be based not only on toxicity, reactivity, or flammability aspects, but also in terms of volumes, transportation, and environmental aspects. For instance, if two chemicals could be used, one required in small quantities and supplied from a nearby site but with hazardous toxicity and reactive properties, the other one with more benign properties but required in large quantities and supplied from a plant located far away, the question would be: "Which is the safer chemical?"

It is therefore essential that the hazards posed by chemical plants and their chemicals be understood and analyzed jointly by an analytical methodology capable of integrating both aspects. Lack of knowledge and willingness to change along with the lack of reliable and simple methodologies are cited as causes of the slow acceptance and implementation ISD. Similar results were presented by Kletz (1996) and Moore (1999) while Gowland (1996) summarized the problems into two fundamental questions:

- How can the effects of the changes (to inherently safer process or equipment in the plant) be measured?
- How to know if the plant follows the inherent safety principles or not?

Several techniques and tools have been developed to overcome this problem. However these techniques analyze specific aspects of the factors that affect the inherent safety level, and it is difficult to integrate all the results under one unique evaluation. Among other limitations for the application of inherent safety, organizational and managerial barriers, as well as lack of economic incentives and regulatory barriers have been identified by [Askounes-Ashford and Zwetsloot, 2000; Zwetsloot and Askounes-Ashford, 2002]. The regulatory controversy is discussed in the following section.

2.1.5 Regulatory efforts

In October 2001 inherent safety became a political topic when the so-called Corzine Bill (2001) was introduced. Because goals of inherent safety address hazard reduction and elimination, it seemed an effective antiterrorism strategy given the fact that traditional layers of protection are designed under specific assumptions that do not include intentional events such as criminal attack. Under such extreme conditions any traditional layer of protection is likely to fail, and the only plausible strategy is inherent safety through the reduction or elimination of the possibility of releases of chemical substances able to threaten the public and the environment. The Bill (2001) refers to "inherently safer technology" as the "...input substitution, catalyst or carrier substitution, process redesign (including reuse or recycling of a substance of concern), product reformulation, procedure simplification, and technology modification..." according to the inherently safer design principles.

The Contra Costa County, CA, was the first in the nation to try to regulate inherent safety through the passage and implementation of a county ordinance similar to the Corzine Bill. The attempt highlighted a fundamental misunderstanding of the inherently safer design approach and a lack of consistency in the interpretation of the principles within the same company and even among safety experts [Johnson, 2003]. The response to the Bill and the Contra Costa ordinance has been varied from different stakeholder groups and a number of papers have been published in order to increase awareness about the technical limitations and the difficulties associated with the implementation of the Bill's requirements [Mannan et all, 2003]. One of the main impediments for government regulation of inherent safety is the complex nature of chemical plants and processes that goes beyond the capability of regulatory authorities due to the lack of an objective decision-making tool to analyze compliance with the regulatory requirements.

As recognized by Mansfield et al. (1997) two of the most important process safety regulations, OSHA PSM (29 CFR 1910.119) in the US and the Seveso II Directive in Europe, use inventory thresholds as a trigger for compliance requirements. However, this type of regulation that does not address inherently safer approaches can encourage chemical companies to reduce their volumes of stored chemicals to quantities just below the thresholds in order to avoid compliance requirements. When inventory reduction becomes the goal without analysis of the impact from a plant-wide perspective, the resulting overall hazard reduction may not be very significant. In fact, the overall risk may increase if, as discussed earlier, transportation and other associated effects are not considerate.

A similar problem occurs with technical engineering standards and codes because of their prescriptive nature that can hinder the application of the inherently safer principles. An example of this are the codes requiring overpressure relief valves even when it would be possible to design the vessel strong enough to withstand the maximum expected pressure [Mansfield et al, 1997]. Another limitation of the standards is that they are generic and focus on minimum acceptable design conditions [Snyder, 1996].

While regulation could be a stimulus for the application of inherently safer design, as has happened with some environmental regulations that forced industry toward emission reduction and pollution control measures, the regulation itself turned out to be a major obstacle towards real progress. While in the US the principles of inherent safety have not been widely accepted and fully understood, the phantom of a regulation has moved the general attitude from a positive and inquiring attitude to a cautious and defensive one.

2.2 INHERENT SAFETY MEASUREMENT: METHODS, ADVANTAGES, AND LIMITATIONS

Since the introduction of the inherent safety principles, many people have embraced the concepts and the number of specialized publications has increased, but integration of the ideas into a systematic methodology has been slow. The published literature can be classified into four general categories:

- Ideology and analysis of problems/benefits
- Application of the inherent safety approach to real cases
- Quantification methodologies
- Application of the inherent safety approach to design methodologies

Each one of these categories has its own importance with respect to the diffusion and acceptance of the inherent safety approach. The explanation of the concepts, principles, problems, and benefits opens the forum not only for discussion of the approach but also challenges the readers to look for solutions and applications. Information about real cases of successful applications provides examples about how the approach can be implemented during early stages of the life cycle of a plant and also during the productive stage when changes are more difficult and expensive to implement. Literature about the ideology and application cases has been published by Kletz (1996), Englund (1995), Mansfield (1996), Snyder (1996), Zwetsloot and Askounes-Ashford (1999), Askounes-Ashford and Zwetsloot (2000), Lutz (1997), Hendershot (1995, 1997a, and 1997b), and Bollinger et al. (1996). As indicated by Kletz (1996), inherent safety principles can be applied also to environmental protection. The similarities between inherent safety and pollution prevention have been explained (Zwetsloot and Askounes-Ashford (1999); Askounes-Ashford and Zwetsloot (2000), and application in European companies has been successful. The integration of inherent safety ideas for a systematic approach to plant design is an aspect that is being explored; for instance Palanippan et al.

(2002) proposed a design methodology to reduce waste and at the same time perform a safety evaluation by using an intelligent decision support system.

2.2.1 Overview of the analytical methodologies

The lack of a measurement methodology has been recognized as one of the reasons for the slow implementation of the inherently safer design approach. Several published papers deal with quantification issues, and associated problems and limitations. In general, the quantification methodologies can be classified into three groups:

- Collection of several well-known indices used to evaluate various safety aspects. The results cannot be aggregated under an overall index.
- Single overall index that evaluates aspects relevant to inherent safety and the results aggregated under an overall number.
- Other methods such as risk-based approach and material-centric approach.

The first category, collection of indices, includes indices based on a compilation of other well know indices such a the Dow Fire and Explosion Index (F&EI), but they do not attempt the integration of individual indices under one overall number because they are based on different scales that cannot be directly compared. A methodology proposed by Hendershot (1995, 1997a, and 1997b) is based on a weighted scoring method and a decision analysis process similar to the Kepner-Tregoe method. This method uses well-known indices such as the Dow Fire and Explosion Index (F&EI), the ICI Mond Index, and others. The use of the F&EI index also has been proposed by Gowland (1996) and Etowa, et al. (2002), while Gupta (1997) reviewed the application of the F&EI index in the developing countries. The INSET Tool kit developed by the INSIDE Project (INherent SHE In DEsign) includes thirty-one tools for four stages of the entire life-cycle of a plant [Mansfield, 1997]. The tools are helpful to evaluate several safety aspects in an easy, simple, and flexible form. The tools can be used separately as required depending on the actual stage of the plant under analysis, and the indices should be interpreted individually because they are not meant to be aggregated under a unique index. A graphical approach has been proposed by Gupta and Edwards (2002a). In this method the individual hazard indices rather than being added together are plotted individually and then analyzed. This approach is based on some of the recommendations and the expert advice collected by Lawrence (1996) in his thesis.

The first overall index for the inherent safety assessment of a chemical synthesis route was proposed by Lawrence (1996), and Cave and Edwards (1997). The index for chemical route selection was extended and applied by Heikkila et al. (1996 and 1999) to the earlier stages of the life cycle of a plant (conceptual design and process synthesis).

A risk-based approach was used by Khan and Abbasi (1998a) where the inherent safety evaluation is based on a "rapid risk analysis" that requires the definition of a specific scenario and acceptance criteria, selection of a design solution that is evaluated with deterministic calculations, and the evaluation of the results with acceptance criteria. An intelligent decision support system useful for inherently safer design and environmentally benign processes was proposed by Palaniappan et al. (2002).

2.2.2 Overview of three relevant methodologies

In this section the following three methodologies are reviewed in detail due to its relevance to the present project:

1) Inherent safety index for chemical process route selection [Lawrence, 1996].
2) Inherent safety index for process synthesis [Heikkila, 1999].
3) INSIDE Project and INSET Toolkit [Mansfield, 1997].

The Dow Fire and Explosion Index and Mond Index are briefly described in the next chapter because they were originally developed for hazard identification. However, as mentioned above, they served as basis for the development of the inherent safety index for chemical process route selection and the inherent safety index for process synthesis.

2.2.2.1 Inherent safety index for chemical process route selection

The methodology developed by Lawrence (1996), is conceived on the idea that the greatest benefit of the inherent safety approach is obtained when hazards are identified and eliminated during the early stages of the life-cycle of a chemical plant. Hence the method assesses the inherent safeness of a chemical route by targeting the first stage of process development and by focusing on raw materials and chemical reactions required for the chemical synthesis of a specific substance. This stage represents the earliest point at which inherent safety can be applied and it is also the stage that will set the future technical needs and constraints on the final design of the plant. After the chemical route for a product is decided, a preliminary flow-sheet is generated and the engineering design phase begins.

As reported by Lawrence (1996) "...This index is designed to indicate a quantitative assessment of inherent safety of a chemical route. It is not designed to be extremely accurate, hence it is defined as an index, giving an indication of the level of inherent safety. It is quantitative in order to remove the subjectivity from the comparison of the routes." Furthermore, "... The index is intended to act as a guide and it does not lead to hard and fast recommendations on which route should be chosen." The index serves three main purposes:

- Assigns a score to each chemical route, which serves as a tool to compare several possible synthetic pathways for the production of a specific substance in terms of inherent safety.
- Permits the evaluation and ranking of chemical routes for common products in terms of safety rather than from the economic viewpoint only.
- Allows identification of the impact of changes that are made to each chemical route.

The aspects analyzed by this index are:

a) Chemical substances
    - Raw materials

  - Intermediates
- b) Products of waste
- c) Reaction conditions
- d) Number of reaction steps

The list of potential indicators of the inherent safety level of a chemical route included nineteen parameters, however, in order to simplify the application only seven parameters were chosen. The logic behind the selection was based on two points:

- Information on the parameters should be available at the early stage of route selection
- The parameters should have a strong influence on the inherent safety level of the route

The parameters that were not selected are: conversion, reaction rate, side reactions, catalytic action, heat of reaction, number of steps and uniformity of reaction steps (as a measure of chemical synthesis complexity), phase of the reaction, phase change, viscosity, corrosiveness, waste and co-products generation. The seven selected parameters are:

1) Temperature: represents a measure of energy content but also affects the phase and properties of the materials. The range selected goes from -25 to 900 °C and is divided into fourteen subintervals with assigned scores between 0 ($10\ °C \leq T < 30\ °C$) and 10 ($T < -25\ °C$ and $900\ °C < T$).
2) Pressure: represents another measure of the energy content of the reactor and also affects the possibility of leaks and explosion. This variable ranges from 0 to 8000 psi and is divided into ten subintervals with assigned scores between 0 ($0\ psi \leq P < 90\ psi$) and 10 ($6001\ psi \leq P < 8000\ psi$).
3) Yield: represents a measure of the overall reaction efficiency and is a function of conversion and selectivity. Low selectivity implies that reactants follow other reaction routes that can lead to undesired and potentially hazardous chemicals or

conditions. The range of this parameter goes from 0 to 100% and is divided into eleven subintervals with assigned scores between 0 (yield = 100%) and 10 (0% ≤ yield < 9%).

4) Inventory of the reactor: related to residence time and reaction rate. The range of this parameter goes from 0.1 to 100,000 tons and is divided into ten subintervals with assigned scores between 0 (0.1 ton ≤ inventory < 250 tons) and 10 (80,001 ton ≤ inventory < 100,000 tons).
5) Toxicity: measures the potential to produce harmful physiological effects. The range of toxicity varies between 0.001% and 1.0%, and is divided into nine subintervals with assigned scores between 0 (TLV < 0.001%) and 8 (1.0% ≤ TLV).
6) Flammability: measures the potential to generate fire and explosions and depends on flash point and flammability limits. The evaluation of this parameter is based on NFPA scores (i.e., 0 to 4, NFPA 704 (2001)).
7) Explosiveness: represents the potential to generate deflagrations and detonations and depends on the explosive limits of the chemical. This variable is based on the difference between the upper and lower flammability limits (i.e., S = UFL-LFL), therefore the range of the variable varies between 0% and 100%. This interval is divided into eleven subintervals with assigned scores between 0 (i.e., for 0% = S < 10%) and 10 (i.e., 90% = S < 100%).

Several of the parameters are selected and analyzed according to the guidelines provided by the Dow Fire and Explosion Index (F&EI) and the Mond Index. The initial structure of the index was selected in order to keep the analysis simple and was formed by two sub-indices, (i.e., a chemical sub-index and a process sub-index) that were added to obtain the final overall evaluation. The chemical sub-index was obtained by adding the scores for inventory, flammability, explosiveness, and toxicity; the process sub-index was the summation of the scores for pressure, temperature, and yield. The procedure was applied to each step in the chemical route, and then the indices were added to evaluate the overall synthesis route.

The index was applied to six chemical routes for the production of industrial chemicals, and the results were submitted to experts with surveys focused on the evaluation of the whole methodology. The observations returned by the experts included the following observations:

- The scale and subdivision used for describing the inventory is based on the Mond index however, it was suggested that a vessel larger than 250 tons is likely to be a storage tank and hence should not be taken into account by this index.
- The Mond and F&EI treat inventory as a separate variable, however it would be better to combine it with other parameters rather than evaluating it as one single variable.
- The division and scoring of several parameters was too simplistic, and it was suggested to assign relatively higher score to the sub-ranges that implied larger hazards (i.e., higher temperature).
- The parameters have the same importance with regard to the final results. However, weighting factors should be introduced to capture the larger impact of certain parameters on inherent safety. It was also suggested to identify equivalent levels of inherent safety for each parameter.
- The calculation of the overall score based on simple addition of all the sub-scores was not considered appropriate, since values with different measurement units (e.g., pressure, temperature, volume) should not be combined by addition.
- The combination of the indices for several steps of a chemical route was also questioned since it was assumed that all the steps had the same importance.

The resultant index combines the selected parameters by using weighting factors derived from expert comments on the parameter ranking according to its relevance. Based on the expert comments, the structure of the index was modified to a structure based on three components:

a) Inventory and hazard assessment: includes storage volumes, reaction volumes, and separation equipment volumes. These volumes are estimated based on preliminary equipment design. The hazard assessment is based on unit-inventory and includes fire, explosion, and toxic effects. The estimation of the number of fatalities is based on the work of Marshall (1977) as reported by Lawrence (1996).
b) Probability of release: based on the propensity of runaway reactions, release due to corrosion or extreme temperature or pressure. The parameters evaluated are: high/low temperature, corrosion and corrosion behavior in contact with air or water, heat of reaction, chemical stability, autoignition temperature, and pressure.
c) Effect of modified factors: describe how much the hazard could be attenuated or increased due to factors such as flashing liquids, and environmental chemical persistency. The effect of the modifiers is given by the evaluation of flammable limits, vapor density, waste and by-products, odor and color, and viscosity. The scores calculated for each modifier are added to obtain the overall effect of the multipliers.

The final procedure includes sixteen steps. The first two steps require the division of the route into individual steps (i.e., single reactions) and calculate the flowrates for each chemical. Then inventory volumes are calculated for storage steps, reaction steps, and purification steps. For each type of inventory, the consequences are assessed by estimating the potential number of fatalities due to fire, explosion, and toxicity. Finally the results are multiplied by the value of release probabilities, and are modified by multiplying by the factors calculated for the effect of the modifiers.

2.2.2.2 Inherent safety index for process synthesis

An inherent safety index for process synthesis was developed by Heikkila et al, (1996) and then published by the Technical Research Center of Finland [Heikkila, 1999]. The index aims at the conceptual design stage and process synthesis, which are the earliest engineering stages in the life-cycle of a chemical plant after the selection of the chemical route. While the inherent safety index for chemical route selection [Lawrence, 1996] proposes a methodology to select the inherently safest reaction pathway, Heikkila et al. (1996) extended it towards chemical plant design by including other parameters to describe the effect of processing characteristics.

The inherent safety index for process synthesis is divided into two parts, chemical inherent safety and process inherent safety. Both sub-indices are also divided into two subparts, which are described by several parameters as follows:

1) Chemical inherent safety: describes how the raw materials, products, sub-products, and intermediates affect the overall safety level:
    a) Reaction hazards: the following parameters are included:
        - Heat of main reaction
        - Heat of side reactions
        - Incompatibility of chemicals (chemical interactions)
    b) Hazardous substances: the following parameters are included:
        - Flammability
        - Explosivity
        - Toxicity
        - Corrosivity
1) Process inherent safety: describes how the type of unit operations, type of equipment, and operation conditions affect the overall safety level.
    a) Process conditions: the following parameters are included:
        - Inventory of chemicals
        - Process temperature
        - Process pressure
    b) Process conditions: the following parameters are included:
        - Equipment safety: inside battery limits
        - Equipment safety: outside the battery limits
        - Process structure

The range of interest of each parameter is divided into sub-ranges that receive a score, which represents the positive or negative contribution on the inherent safety level. The minimum score for each parameter is set to zero, while the maximum scores are set in order to represent a weighting effect according to the work done and expert judgment collected by Lawrence (1996). It is assumed that a wider range (i.e., 0 to 6) implies a greater impact for the overall safety evaluation. Inventory and toxicity are identified as the aspects with the most important impact on inherent safety, hence their maximum score is set, respectively, to 5 and 6. Process structure is also assigned with a maximum score of 5. Corrosivity is assumed to be the least important of the parameters and receives a maximum score of 2, while the parameter for equipment safety outside the battery limits is assigned a maximum score of 3. The rest of the parameters are assumed to have the same importance and receive a maximum score of 4.

The parameters for heat of main and side reactions describe the hazards associated with fast exothermic reactions able to release large amounts of heat that can start violent chemical reactions or can release gases and vapors. The parameter has been selected because the reaction rate and the presence of specific unstable chemical groups cannot be easy related to the hazard of a reaction. The range of the parameter goes from thermally neutral reactions with heat of reaction ≤ 200 J/g up to extremely exothermic reactions with heat generation ≥ 3,000 J/g.

The parameter for chemical interaction evaluates the hazards associated with the consequences of chemical incompatibility among chemical substances and is based on the EPA matrix [Hatayama et al, 1980 as cited by Heikkila, 1999]. Fire and explosions are assumed to be the worst possible outcomes of an unintended interaction and receive the highest score (i.e., four) while the formation of nontoxic nonflammable gasses are classified as the least hazardous consequences and receive a low score (i.e., one).

Flammability is described by the value of the flash point and the range goes from combustible substances (i.e., flash point > 55 °C) up to very flammable (i.e., flash point

< 0 °C and boiling point ≤ 35 °C). The classification is based on the European Union directives as indicated by Heikkila (1999). The explosiveness parameter is based on the difference between the upper and lower flammability limits expressed as % by volume. The basic idea is that a substance flammable over a wide range of concentrations represents a higher hazard.

Toxicity is described by the threshold limit value (TLV) expressed in ppm and the range goes from TLV > 10,000 for low toxicity up to TLV ≤ 0.1 for highly toxic chemicals. The hazard associated with corrosivity is evaluated indirectly by assigning a score to the construction material required to manage the chemical. It is assumed that carbon steel is suitable for low-hazard chemicals hence receives a score of 0, while stainless steel receives a score of 1. Any other material receives a score of 2.

The score for the evaluation of the impact of inventory on the hazard level is divided into two parts: inside the battery limits (e.g., process vessels) and outside the battery limits (e.g., storage tanks). The sub-ranges for process vessels go from volumes between 0-1 ton up to volumes larger than 1,000 ton; the sub-ranges for storage vessels go from volumes between 0-1 ton up to volumes larger than 10,000 ton. In both cases information from Lawrence (1996) and the Mond Index [AIChE, 1994a] is used.

The range for process temperature goes from temperature < 0 °C up to 600 °C. The sub-range with the lowest score is between 0-70 °C which is harmless to people, while temperatures below zero receive a score of 1 indicating the mechanical hazards associated to this condition. For pressure, the range between 0.5 to 5 bars receive a score of 0 while pressures between 200-1,000 bars receive a score of 4. These ranges are based on the Dow Fire and Explosion Index [AIChE, 1994b].

The overall score for process hazard is calculated by adding the sub-indices for flammability, explosiveness, and toxicity. The chemical with the highest score is selected as the most hazardous chemical of the process. This score is then added to the four sub-indices for reaction hazard (i.e., heat of main reaction, heat of side reactions, incompatibility, and corrosivity).

The evaluation of the index for process inherent safety is developed in a similar way; each parameter receives a score, which is added to the other scores to calculate the index for the process evaluation. For the evaluation of equipment safety inside the battery limits, the suggested distances required between equipment are taken into account and several sources were analyzed by Hekikila (1999). Equipment that handle nontoxic and nonflammable chemicals receive the lowest score (i.e., zero), while furnaces and fired heaters receive the highest penalty (i.e., four). In a similar fashion, the scores for equipment outside the battery limits go from zero, for equipment handling non-hazardous chemicals, to three for flares, boilers, and furnaces.

The evaluation of the process configuration is based on several sources of information and expert knowledge as well as incident reports, sound engineering practice and accepted engineering standards. The parameter is formed by six groups of equipment and systems characterized by the type of information available for their safe operation. The first group receives a score of zero and is for equipment recommended by safety standards; the second group is for equipment selected with basis in sound engineering practice, and known reliable systems. Equipment that lacks information regarding hazardous operation receives a score of two, while the fourth group includes equipment of which safe operation is questionable. For equipment for which minor incidents have occurred are included in the fifth group, while the sixth group receives the highest score (i.e., five) and is for equipment with documented major incidents.

The final overall inherent safety index is then obtained by addition of the chemical and process inherent safety indices.

2.2.2.3 INSIDE Project and the INSET Toolkit

The INherent Safety health and environment Evaluation Tool (INSET) was developed in Europe between 1994 and 1997 by the INSIDE Project Team; an integral version of the report and the Toolkit were released in 2001 [Mansfield, 2001]. The toolkit presents the results of a three-year research effort co-founded by the European Union and industrial and research partners. The main goal of the project was to develop a systematic tool to increase awareness toward inherent safety principles among engineers and chemists and to encourage the application of inherent safety to process and plant design.

During the first stage of the project a survey was performed across the European chemical industry to assess awareness, acceptance, and application of the inherent safety approach. The results indicated a general lack of recognition of the concept and application of the principles driven by economic pressure or incidents and near-miss experience. The need for a methodology to analyze the application of inherent safety through the life-cycle of a processing plant was recognized as well as the need for case studies to demonstrate the benefits of the approach. The INSET Toolkit was developed to address the lack of analytical methods and focused on raising the awareness toward inherent safety during the early stages of the selection of a chemical route and during the following engineering stages for the design of the chemical process and plant.

The INSET Toolkit is a collection of thirty-one tools and methods divided into four stages that cover the early stages of the plant life-cycle, assuming that most of the decisions that affect the safety, health, and environmental hazards (SHE) of a plant are taken during these stages:

Stage I: chemistry route selection: a simple screening methodology proposed is useful to identify the few routes that should be further analyzed.

Stage II: Chemistry route detailed evaluation: evaluation of detailed relevant chemical information about the selected potential chemical routes. One or two routes are selected for optimization during the next stage.

Stage III: Process design optimization: The operation conditions are optimized and the implications of a large-scale industrial operation are analyzed.

Stage IV: Process plant design: The preliminary process design is developed and optimized in order to identify potential flowsheet, conditions, and equipment to maximize the plant performance.

The tools allow the systematic identification and evaluation of potential hazards, and the whole approach is designed to be flexible enough to be applied to plant optimization based on SHE constraints or other aspects such as process feasibility and economics. The tools are the following:

- Tool A: Detailed constraints and objective analysis:
    - A.1: Detailed constraint analysis
    - A.2: Detailed objective analysis
- Tool B: Process option generation (including process waste minimization)
- Tool C: Preliminary chemistry route option records
- Tool D: Preliminary chemistry route rapid ISHE evaluation method
- Tool E: Preliminary chemistry route detailed ISHE evaluation method
- Tool F: Chemistry route block diagram record
- Tool G: Chemical hazard classification method
- Tool H: Record of foreseeable hazards
- Tool I: ISHE performance indices
    - I.1: Fire and explosion hazard index
    - I.2: Acute toxic hazard index
    - I.3: Health hazard index
    - I.4: Acute environmental incident index
    - I.5: Transport hazard index
    - I.6: Gaseous emission index
    - I.7: Aqueous emission index
    - I.8: Solid waste index

  - I.9: Energy consumption index
  - I.10: Reaction hazard index
  - I.11: Process complexity index
- Tool J: Multiple-attribute ISHE comparative index
- Tool K: Rapid ISHE screening method
- Tool L: Chemical reaction reactivity: stability evaluation
- Tool M: Process SHE analysis/process hazard analysis and ranking
- Tool N: Equipment inventory functional analysis method
- Tool O: Equipment simplification guide
- Tool P: Hazard range assessment for gaseous releases
- Tool Q: Siting and plant layout assessment
- Tool R: Designing for operation

The Toolkit is a paper-based method and has been designed to address safety, health, and environmental aspects (i.e., SHE) during the decision-making process at the early design and engineering stages. However, it does not focus on the overall framework of safety, health, and environmental hazards. Stage I requires the evaluation of Tools A.1, A.2, B, C, D, and E. Stage II requires Tools B, F, G, H, I.1 to I.11, J, and K. Stage III requires Tools B, L, M, I.1 to I.11, and J. Stage IV requires Tools B, I.1 to I.11, J, N, O, P, Q, and R.

The flexibility of the INSET Toolkit is given by the independence of the tools and by the fact that the applied methods depend on the type of plant and the stage of process design. While for completely new processes without a selected chemical route, the analysis can start from the tools developed for Stage I, but if a potential route is already available, then the analysis can start with the Stage II tools. When the chemistry of the process has been selected but it is still possible to make changes to increase the process inherent safety level and its performance, the analysis starts with tools for Stage III. When the flowsheet has been developed but decisions must be made on equipment and configuration as well as pipework-sizing, tools for Stage IV can be used.

For each stage the report presents extensive information regarding suggested tool application flowsheet as well as a detailed description of each tool, information required, and outputs. For each tool, background information is presented with detailed instructions to apply the method and templates for the forms that must be completed.

Zwetsloot and Askounes-Ashford (1999) published a report on the application of the INSET Toolkit by several European chemical companies. The results were encouraging and the general problems associated with the implementation of inherent safety were highlighted.

2.2.3 Limitations of the current methodologies for inherent safety analysis

The low level of industrial application of the inherent safety principles shows that more development is required in terms of analytical approaches. The methodologies proposed so far constitute good starting points and present a diverse spectrum of techniques and approaches upon which new analytical tools can be built.

The limitations of these methodologies are based on their own nature. For instance, it is well known that inherent safety principles can be more efficiently and easily applied during the earlier stages of the design, when changes are easier and cheaper. However, during these initial phases the technical information available is incomplete, which forces the quantification methodologies to be simplistic. The resultant oversimplification cannot capture the complexity and complications involved in the inherent safety evaluation of a chemical plant and might hinder detection of hazards created by combinations of hazard factors and hazards generated in other processing areas due to changes toward an inherently safer process.

Sometimes the limitations are implicit in the mathematical procedure. The division of a range into sub-intervals with certain assigned scores is a common approach for index development. However this division presents problems of low sensitivity along the sub-interval (i.e., if a temperature sub-interval is defined between 100 ^oC and 200 ^oC degrees, the variable will receive the same score for a temperature of 101 ^oC or 199 ^oC degrees).

Oversensitivity is however present near the limits of the sub-ranges (e.g., if the next range is defined between 201 ^oC and 300 ^oC, a temperature of 200 ^oC will receive a lower score than a temperature of 201 ^oC). These over/low sensitivity effects could balance each other, but there is no guarantee that it will not affect the analysis. This effect can be interpreted as lack of continuity in the evaluation caused by a discrete function (e.g., intervals with assigned scores) rather than a continuous one.

In some cases, the tools are based on the identification and evaluation of the worst sources of hazard without taking into consideration the magnitude and frequency of other less hazardous conditions. In other cases, the tools require subjective judgment and do not propose a methodology to assess the effect of those personal evaluations. Industrial skepticism with respect to inherent safety is also based on the fact that inherent safety is a good approach for hazard reduction; however it is not proven that inherently safer plants are cheaper and easier to operate [Lawrence, 1996]. Additionally, when the approach is applied to existing plants there are few opportunities to improve the design without incurring significant expenses, and the application of Inherent Safety may require tradeoffs with other environmental and economic aspects. An additional restriction of the methodologies presented so far is that they require tedious and time-consuming manual work not welcomed by design engineers who usually work under project time and cost constraints.

All these indices are based on classical analytical statistics and mathematics and uses rigorous methodologies to analyze data that in some cases are little more than guesses, since some events are too rare to allow the collection of statistically meaningful information. Combining data with a high degree of uncertainty will increase the overall uncertainty of the analysis [Bowles and Pelaez, 1995]. Other authors have recognized limitations such as conflicts and tradeoffs between inherently safer design and environmental, technological, and economic considerations [Palaniappan et al, 2002; Snyder, 1996; Hendershot, 1997].

Koller et al. (2001) developed a comparison of fourteen methods proposed for the evaluation of inherent safety. Process aspects as well as release, safety, and human health aspects were compared for each method. Other characteristics of the methods such as type of scale used for input data and results, aggregation procedure of different hazards, were analyzed. The analysis required the application of the methods to a selected case study. The comparison of the results showed the tendency of most of the methods to classify very hazardous or very low hazard processes in a similar way. In general, it was found that a rather low degree of agreement exists among the methods, and this is attributed to the different approaches to treat variables such as toxicity. In other cases it was found that a single variable dominates over the others (e.g., volume, temperature).

Based on the requirements of the industry and environmental protection, it is important for the methodologies to be able to capture and measure different type of hazards. Due to the complexity and variety of industrial plant operations, these hazards can be classified into process hazards, environmental hazards, and transportation hazards. Transportation hazards must be taken intoaccount in order to analyze the chemical plant from an overall view point.

This research proposes the application of fuzzy logic to deal with the uncertainty and subjectivity of factors that must be analyzed to assess the process hazard and environmental hazards. The analysis of inherent safety for transportation hazard is introduced in Chapter X.

Fuzzy modeling also allows the analysis of the interaction of the factors relevant for process safety because it works with simple IF-THEN rules that are easy to understand and apply. The rules can model numerical data as well linguistic and heuristic knowledge. Because the approach proposed by this research is computer-oriented it is expected that its application is less time consuming then other methods.

CHAPTER III

INTRODUCTION TO EXTRINSIC SAFETY

As explained in Chapter II, the topic of the present dissertation is “inherent safety” that aims to reduce the hazards rather than control them. However, in order to understand the limitations associated with the application and evaluation of inherent safety, it is important to gain an overview of what process safety is today and how we reached the current state-of-the-art. In the present chapter the word “safety” refers to “extrinsic safety” or traditional safety, understood as “low risk” achieved through the application of protective layers that reduce the likelihood and the magnitude of the expected consequences.

In this chapter, the history of loss prevention is briefly summarized in order to understand how and why chemical engineers became concerned about process safety, and why the present safety state-of-the-art can be improved by looking at the problem from a different perspective.

3.1 HISTORY OF PROCESS SAFETY AND LOSS PREVENTION

Process safety is a relatively new concept that grew and developed with the chemical industry and its tragedies. It is also a thankless issue whose importance is minimized when nothing wrong happens and is blamed when incidents do occur. One of the classic fallacies is that if an incident has not occurred before, it is not likely to happen. These events are not recognized as “incidents waiting to happen” and a false sense of safety is taken for granted.

3.1.1 Process safety and loss prevention

The modern conceptual and methodological framework for process safety was developed during the last fifty years in response to the driving force created from incidents and cross-learning from the nuclear industry. The three major development stages of process safety are [Brown, 1999; Kletz, 1999a]:

1) Technical non-systematic approach (bottom-up): During the 1950s process safety was not a technical and systematic issue and a simplistic view was pursued: if each element of the plant was designed according to technical standards then it was inferred that the whole plant should be safe enough. The older and more experienced maintenance personnel were responsible for taking care of process safety issues. During the 1950s and 1960s, new larger and more complex plants were developed and built and it became clear that the previous bottom-up practice was not enough. The Flixborough disaster, which occurred in UK in 1974, was the precursor of a series of European and American regulations, and an increasing interest was developed to model and understand the consequences of incidents.
2) Quantitative risk analysis development: During the 1970s and early 1980s, methods for consequence analysis, and calculation of incident likelihood and probability were adopted by the chemical industry after the nuclear industry recognized the potential magnitude of incidents. Methods such as reliability analysis and fault tree analysis were developed and applied to the chemical and nuclear industry. This stage of development required scientific research in order to develop fundamental understanding of the physical systems, to model and understand their behavior and the hazard implications. Until the late 1980s between 60 and 90% of the papers published on safety were related to technical and scientific issues [Gibson, 1999].
3) Regulation and process safety management: According to Gibson (1999) during the 1990s the percentage of safety-related papers declined by 75% while regulatory and management issues became popular. Due to the increasing availability of computer power the interest switched toward information technology, control systems, and management, however as reported by Gibson (1999) Kletz said "...There is an

> epidemic of papers and books on safety management but they are no substitute for knowledge and experience. All they can do is ensure that knowledge and experience are applied in a systematic way."

The needs of each stage of development of process safety were different, and several analytical methods for the evaluation of risk were proposed. Some of these procedures have been accepted and improved, and today they form the "toolbox" of loss prevention.

3.2 ANALYTICAL TOOLS FOR PROCESS SAFETY AND LOSS PREVENTION

Regardless of the complexity and uncertainty associated with chemical processes, decisions must be taken in order to identify and reduce the risks. The methodologies developed during the first two stages of the history of process safety reflect the mathematical and computational tools available in the past. In general, they can be divided into qualitative and quantitative methods; while qualitative approaches are simple to use, quantitative methods such as quantitative risk assessment are extremely complex and demanding, which reduces their applicability. However, in both cases, these approaches have set the standards for the modern way of thinking and approaching the problem of safety analysis.

The general concept of safety is related to low risk, where risk is understood as the multiplication of event likelihood and magnitude of the potential consequences. The questions that are sought to be answered are:

- How frequent is the scenario?
- How bad are the consequences?

Therefore, after hazard identification methods have been applied, the types of incidents that can be caused by each specific hazard are identified and risk evaluation (through qualitative or quantitative methods) is developed.

3.2.1 Well-known and accepted methods for process safety analysis and loss prevention

Kletz (1999a) has compiled a review of the most important papers published during the last forty years of the history of loss prevention. The paper also includes original references on safety and risk quantification analysis. Among the methodologies reported as the most important for loss prevention are Hazard and Operability Analysis (HAZOP), Quantitative Risk Analysis (QRA), Checklists and Safety Audits, Fault Tree Analysis (FTA), Failure Mode and Effects Analysis (FMEA), What If Analysis, the Dow Fire and Explosion Index (F&EI), and the Mond Index.

3.2.1.1 Hazard and Operability Analysis (HAZOP)

The HAZOP methodology was developed by ICI in 1963 [Kletz, 1999a] and published in 1974 by Lawley (as cited by Kletz, 1999a). It is the most commonly used methodology to identify potential hazards and it is comprehensively described elsewhere [Lees, 1996a; Kletz, 1999b]. It is based on guide words (i.e., MORE, LESS, NO, REVERSE) that are associated with variables (e.g., MORE flow, LESS flow, NO flow, REVERSE flow) and the resultant condition is assessed in terms of potential negative safety consequences. The method is applied to each individual equipment or system for the unit or plant being analyzed. The methodology is simple and powerful but it is time and resource-intensive since a multidisciplinary team is required to develop a meaningful analysis. Since its introduction, the method has not changed, however its application is nowadays abused by users who claim to perform Hazard and Operability Analysis but only do simple line diagram revisions [Kletz, 1999].

3.2.1.2 Quantitative Risk Assessment (QRA)

The method of Quantitative Risk Assessment (QRA) has been accepted by the chemical industry as a method useful for the systematic identification of priorities based on numerical estimation of incident frequency and consequences. Hazard sources that involve probable large risk must be addressed before other less frequent sources or with less severe consequences. When a high risk is identified, it can be reduced by either reducing the probability of the event by using layers of protection, or by controlling the consequences. The methodology, is described elsewhere [AIChE, 1996; Hendershot, 1996] and it is usually applied in three formats depending on the scope of the study. The qualitative QRA is the simplest, while the quantitative version of the QRA requires failure frequency data and consequence quantification as well as calculation of probabilities of each event.

3.2.1.3 Fault Tree Analysis (FTA)

Fault Tree Analysis (FTA) was developed for the chemical industry in the late 1970s by Lapp and Powers (as reported by Khan and Abbasi, 1998b). It is a powerful methodology able to identify hazardous combination of events, by using AND and OR gates, as well as chains of events that can cause an established scenario (e.g., release of a toxic substance). Starting from the frequency of the initiating events it is possible to calculate the frequency of the top event or scenario. The methodology is comprehensive but very demanding and it is rarely applied to large plants or units unless computerized systems are used. However, the generation of the tree by automated means is still subject of research [Wang et al., 2001] and fault tree generation is one of the main disadvantages of the method. The generation of the tree is the most important and time-consuming step and must be performed by experts who know the methodology but also are familiar with the process under analysis. Furthermore, the method requires the use of incident probabilities and failure frequency data under specific conditions. This type of data is not always available and often must be estimated, increasing the uncertainty of the analysis [Khan and Abbasi, 1998b; AIChE, 1993].

3.2.1.4 Failure Mode and Effects Analysis (FMEA)

Failure Mode and Effects Analysis (FMEA) is used to analyze possible equipment failure modes and event sequences. This is a qualitative method, which does not work well for systems where complex logic is need to explain the failure. Furthermore FMEA cannot describe the interaction of several components [AIChE, 1993].

3.2.1.5 What If analysis

The What If analysis is one of the oldest methods and is based on simple questions such as “What if the pump fails?” The method is straightforward and does not require a safety expert; however it is not systematic, requires a multidisciplinary team and relies mainly on their expertise and experience [AIChE, 1993].

3.2.1.6 Dow Fire and Explosion Index (DF&EI)

The Dow Fire and Explosion Index (DF&EI) was published by Dow Chemical in 1964 and is probably the most frequently used hazard evaluation index [AIChE, 1994b; Scheffler, 1994; Brasie, 1976]. This method requires dividing the plant into units and then calculating the hazards due to chemical substances (i.e., material factor which is then modified by established penalty factors for specific process hazards. Credit factors are also applied for loss control measures and devices, and the cost of safety features is analyzed. This method summarizes expert knowledge and empirical experience into simple steps and penalty/credit factors, however when applied mechanically without taking into consideration the specific situation of the plant, it can lead to oversimplification and misjudgment [King, 1999]. A special case of adjustments needed for to the specific characteristics of the plant or the location is reported by Gupta (1997) who proposed to increase some penalty factors for plants located in developing countries. The adjustments have the objective to take into account situations such as possible lack of appropriate control systems and lack of maintenance capability, inadequate training and equipment availability for emergency response, limitations associated with corrosion control, leak prevention, and inadequate operation procedures (i.e., instructions not properly translated to the local language). The hazard ranking has also been modified.

While the F&EI is easy to understand and apply, the limitations include controversy about the value of the weighting factors required to combine the sub-indices. As Kletz recommends (1980, Loss prevention) the methodology should be used keeping in mind that some of the numbers are arbitrary.

3.2.1.7 Mond Fire and Explosion and Toxicity Index

The Mond Fire and Explosion and Toxicity Index was developed by ICI [AIChE, 1994a], in 1979 and it is based on the Dow F&EI. For the Mond Index, toxicity is included as an additional factor and the overall index is calculated by combining indices for general and special process hazards, quantity hazards, layout hazards, and acute health hazards. This index requires also information on cost for equipment and pipework [King, 1999; Khan and Abbasi, 1998b; Lewis, 1980].

3.2.1.8 Checklists and safety audits

Other methodologies such as checklists and safety audits were the first methodologies applied for hazard identification and management. These methods are simple; however the inherent danger is the tendency to apply them in a mechanical manner and thus over time losing their capacity for detection of potential problems [Kletz, 1999a].

During the last decade the limitations and problems of the previous methods have been addressed and new tools have been developed. In several cases they represent improved or modified version of the Dow F&EI and the Mond Index. In other cases some of the risk assessment concepts have been applied to hazard identification techniques is an attempt to include both tools under a single method. There is a general trend towards automation by using computer interfaces, however in general the methods have not been well received.

3.2.2 Not well-known and accepted methods for process safety analysis and loss prevention

The technical literature includes a large number of other methodologies that have been proposed but have not been fully recognized or used by the industry. Some examples are the following:

- Quantitative multi-attribute approach for risk analysis [Christen, et al, 1994]
- Focused What If analysis [Goodman, 1996]
- Generalized model of hazard systems [Marshall and Ruhemann, 1997]
- Hazard Identification and Ranking (HIRA) proposed by Khan and Abbasi (1998c)
- Computer-based Hazard Identification (HAZID) developed by McCoy et al. (2000)
- Optimum risk analysis [Khan and Abbasi, 2001]
- Safety Weighted Hazard Index (SWeHI) proposed by Khan et al. (2002)
- Hybrid hazard identification [Viswanathan t al., 2002].

Due to the large number of new methodologies proposed, other papers have been published comparing the new safety and risk analysis methodologies. Tixier et al. (2002) reviewed 62 methods and classified them based on the type of input, type of output, data required, type of method (i.e., deterministic, probabilistic, qualitative, quantitative), relation between input and output data, and risk hierarchy. The conclusion reached by the authors indicates that it is required to apply several methods to get a better understanding of the risk, but in order to get meaningful results the user needs experience and expert knowledge.

Another study developed by Rouvroye and Van den Bliek (2002) focused on the comparison of risk analysis techniques that could be used for standards related to Safety Instrumented Systems (SIS) and Emergency Shutdown Systems (ESD). The authors analyzed eight techniques including Hybrid methods, Markov analysis, Reliability block diagrams (RBD), and fault trees (FTA). Kirchsteiger (1999) presented a review on the current practice and use of deterministic and probabilistic risk assessment methods in Europe, United Sates, and Korea.

3.3 APPLICATION OF PROCESS SAFETY AND LOSS PREVENTION

The large number of methodologies proposed to analyze traditional safety, risk, and inherent safety implies that there are safety problems that cannot be analyzed with the methodologies available so far, therefore there is a driving force to propose other approaches. However, in general the methods for safety assessment can be broadly classified into three main categories:

1. Risk-based methodologies that identify hazards and then combine them in different ways with the likelihood of the event and the potential consequences. Another classification of risk analysis is given by Kirchsteiger (1999) and is based on probabilistic and deterministic approaches. The deterministic risk analysis takes into account only “worst case scenarios” and it includes an element of subjectivity because the analyst selects the reasonable scenarios. In the probabilistic approach, all possible sources of hazard are analyzed by using probability distributions and uncertainty ranges.
2. Methods based on indices and the Dow F&EI that represent extension, modification, or improvements of the well-accepted index. These methods are based on arbitrary scales representing different variables, and usually are based on scoring systems assigned to specific discrete intervals. The results are then aggregated by multiplication or addition and then corrected by weighting factors.
3. Other methods based on a variety of approaches such as ranking matrices [Moore, 1997], qualitative approaches, checklists, and other safety measures.

The models in the first category require statistical information about incident frequency and probability, and often the information is not available or has to be inferred through approximations to adapt the data to the analyzed case. In general the data are characterized by high uncertainty degree but it is rarely taken into account due to the complexity of such problems. These models tend to be detailed and able to calculate societal and individual risk, however they are complex and time-intensive requiring the participation of specialized technical expertise.

The second category includes a qualitative and a quantitative index and presents a compromise between simplicity and descriptive capability. In general, the application of this type of models does not require the participation of highly technically skilled personnel and can be applied quickly. The numerical results are calculated by applying a well-defined procedure that allows fast identification of potential hazards. Usually the results are in the form of numerical scores that can be interpreted as the representation of certain level of risk [Khan et al., 2001]. In general, these methods are based on assumptions usually not well explained or justified that can lead to oversimplification of the problem.

All the available methodologies offer different innovative concepts, capabilities, and advantages, however some seem to be better accepted and used than others. Kletz (1999a) suggests that the acceptance is a function of the organization level targeted by the method. Methods that demand time and economic resources (i.e., by requiring large teams of experts) require the commitment from higher management level and this may represent an obstacle for the implementation of the methodology. When safety analytical approaches target the lower levels of the organization and can be implemented by designer and project managers the possibility of acceptance increases.

CHAPTER IV

DEVELOPMENT OF A NOVEL CONCEPTUAL FRAMEWORK FOR INHERENT SAFETY ANALYSIS*

This chapter introduces the problem of safety and explains the philosophy upon which the present project is built. Because the approach proposed here does not follow the conventional thinking path for safety analysis and applies an unusual mathematical framework, it is fundamental to keep in mind the ultimate goal of the project. This goal is the development of a tool useful to process and design engineers for identifying potential hazardous characteristics of materials, operating conditions, and process equipment without the intervention of safety experts.

As explained latter, safety is by itself a complicated issue affected by a large number of aspects and parameters, hence the natural complexity of the problem should not be overlooked or ignored. On the contrary, it is assumed here that complexity is derived from the interaction of several simpler systems and the model developed attempts to capture this fundamental assumption. Because of the intrinsic complex nature of "safety", considerable of time has been dedicated to the development of a conceptual framework to bridge the academic theory and potential "real world" needs.

The history of loss prevention was briefly summarized in Chapter III in order to understand the limitations and problems associated with the conventional "extrinsic" safety approach while the limitations of the methodologies so far developed for inherent safety analysis were explained in Chapter II. The present chapter questions and challenges conventional approaches for process safety and analyzes the reasons why

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safety in general, and specifically inherent safety, is so difficult to quantify. The analysis is based on ideas borrowed from non-engineering disciplines. The last part of the chapter introduces the technical ideology of the project, main objectives, and the mathematical methodology (explained in detail in Chapters V and VI).

4.1 QUESTIONING THE PRESENT SITUATION WITH REGARD TO EXTRINSIC AND INHERENT SAFETY

From the information presented in Chapter II and III some intriguing questions arise and their answer establish the theoretical basis for the present dissertation.

4.1.1 Why so many methods?

From the previous Chapters II and III it is clear that nowadays a large number of methods are available to analyze intrinsic and extrinsic "safety", and each one of them presents advantages and disadvantages. Most of the new methodologies proposed are based on usual and traditional safety and risk concepts, which are bounded by the historic development of the chemical and nuclear industry. The mathematical methodologies used are also bounded by the historical background and the tools developed in the past such as statistical and probabilistic theory.

Nevertheless, the continuous proposal of new tools for process safety highlights the fact that we are still not able to understand what safety is. The answer to the question "How safe is a chemical plant?" has become a circular problem. The more recent methodologies have been shaped around the early and now well-accepted ideas and techniques for safety and risk assessment, hence innovation is itself bounded by the limitations of the original now well-accepted methods. This problem is defined by Walker (1998) as "conceptual inertia".

A different type of innovation requires to "reinvent the details" of the solution by looking at the problem from a different viewpoint. It also requires breaking the usual thinking patterns to explore other approaches. Human history is full of examples on both types of innovation, from the development of the written language to the controversy about how Russia built its atomic bomb [Diamond, 1997].

4.1.2 Why the general safety approach is based on extrinsic safety?

Before the introduction of the inherent safety principles by Kletz, a safe plant could only be achieved through protective layers added after the hazards were detected. This solution to improve the safety level of a plant has historical roots in the limitations and difficulties faced by design engineers such as limited computing power, limited technical information, slow communication with equipment suppliers and very slow drawing capability.

Methodologies for hazard identification and risk analysis require detailed information on chemicals, equipment, and operating procedures (Figure 4.1). This large amount of data was only available at advanced design stages when opportunities for changes were limited, forcing engineers to rely on protective add-on barriers rather than hazard elimination [Mansfield and Cassidy, 1991]. These technical limitations established the modern thinking pattern and plant design systems that rely on protective barriers. Therefore, inherent safety implies not only a paradigm change but also a systematic modification of the design framework.

4.1.3 Risk assessment and data uncertainty

Besides the model complexity associated with quantitative risk assessment, the data requirements regarding failure rates and scenario likelihood constitute a systematic limitation of methodologies based on risk quantification. These indices are based on classical analytical statistics and mathematics and use rigorous methodologies to analyze data that in some cases are little more than guesses, since some events are too rare to allow the collection of statistically meaningful information. Combining data with a high degree of uncertainty will increase the overall uncertainty of the analysis [Bowles and Pelaez, 1995].

Failure data for equipment is reported in databases and specialized literature but are rarely available for the required specific operating condition. Hence, the data must be subjectively adjusted based on expert and technical judgment. While for the nuclear industry the number of equipment, operating conditions and potential scenarios is relatively well defined and limited, the complexity and variety of processes, chemicals, and unit operations make impossible the collection of enough data to describe each situation with a low degree of uncertainty. The problem is further accentuated when the methodology for risk assessment for fixed sites is applied to transportation of chemical substances. In this case the environment around the vehicle (e.g., truck, railcar, and barge) or pipeline is dynamic, non-controllable, and in general non-predictable.

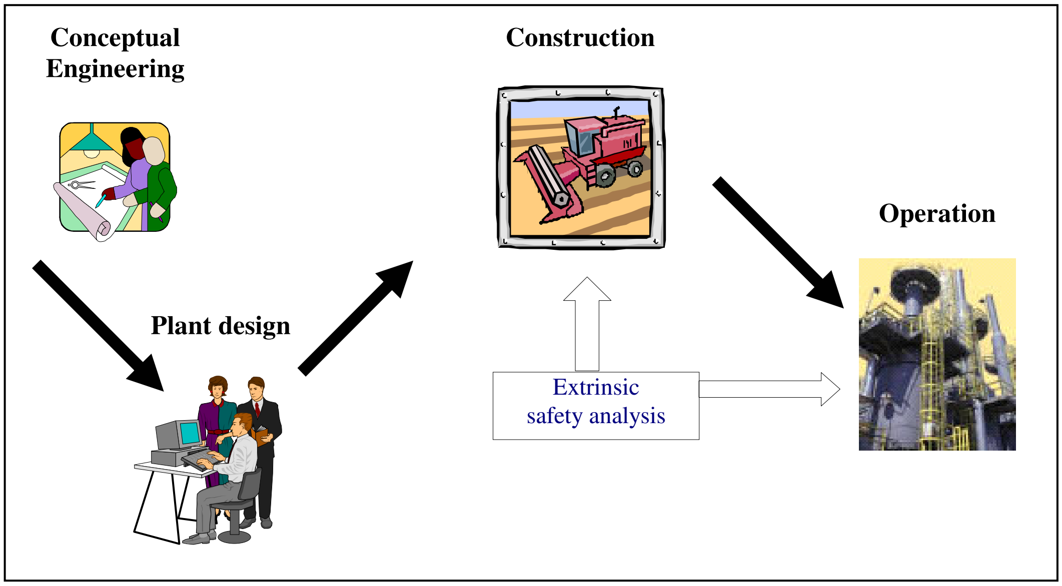


Figure 4.1: Current application of extrinsic safety methodologies during plant design

Risk evaluation requires the calculation of the physical consequences for each selected scenario and this process increases the uncertainty of the analysis since basic assumptions must be made. For instance, weather conditions and wind velocity, population type and density, affect the results of the analysis. Depending on the expected magnitude of the risk, the scope of the study can be selected as a simple qualitative risk analysis or a fully quantitative one. For simple QRA only, few scenarios are analyzed while for more complex problems the complexity of the models and number of analyzed scenarios increases significantly.

The uncertainty associated with the data used as well as the procedure for selection of scenarios and analytical assumptions is not taken into account by the mathematical procedure therefore the results of the risk analysis should then be interpreted on the basis of the quality of information and assumption used.

4.1.4 Is safety a subjective issue?

One of the most important aspects with regard to safety is the subjectivity present in risk evaluation. Risk perception can be biased by economic factors, experience, and knowledge (or lack of them), environmental factors, public perception of the risk, generic technical standards, and lack of specific regulations. Because of the complexity of issues covered under the concept of safety the generally accepted idea is that safety is subject to interpretation, hence it is a subjective matter that can be understood in different ways depending on the situation and the experience of the analyst. Situations that can appear to be safe to somebody may appear to be unsafe to another more experienced person; therefore safety becomes a matter of opinion where event experts can interpret a scenario as safe or unsafe according to their own personal knowledge. For instance, an arbitrarily hazardous chemical can be perceived as less hazardous by somebody used to deal with it; the nuclear industry is perceived as relatively not hazardous by nuclear engineers trained on the matter; however the general public perceives a nuclear plant as great source of hazard even though risk analysis indicates low likelihood of an incident.

Depending on the focus of the problem the definition of safety can acquire different meanings. While risk-based analysis understands safety as low risk to humans and equipment, due to reduced consequences or low likelihood, other methods for extrinsic safety focus on thresholds assuming that if a certain parameter is below a certain value (which can be arbitrary or can have physical meaning) then the hazard is not present, hence a safe state is established. Index-based methods extend the interpretation of safety based on thresholds by establishing arbitrary scales for each source of hazard (e.g., temperature, pressure, toxicity) and assigning scores representative of the implicit danger.

4.1.5 Safety as a simplified problem?

Safety is a complex problem formed by various aspects, and this is one of the reasons why several methodologies looking at different aspects of the same problem are usually required. However, except for Fault Tree Analysis, the rest of the methods tend to oversimplify the analysis by assuming that each variable is an independent source of hazard. For example, a medium reactor working at low pressure and temperature may represent higher hazard than a smaller reactor working at higher pressure and temperature if the volume is sufficiently small. Hence, the amount of material is not enough to generate a serious fire or explosion [Kletz, 1998].

This type of interaction among the significant parameters is difficult to capture when the analytical methods have not been designed with the purpose in mind. Score-based approaches are less likely to identify the interaction because the scores are not proportional to the physical consequences.

4.1.6 On score aggregation and scaling theory

The use of scales and score is common in the field of process safety. One of the more frequently used scales is the National Fire Protection Association standard NFPA 704 (2001) for the evaluation of flammability, toxicity, and reactivity hazards of chemical substances. Depending on certain properties each chemical receives a set of three scores (one per each hazard) on a discrete scale from zero, for no hazard, up to four for maximum danger. This is an ordinal scale able to give an indication of relative hazards but does not provide any information about the proportional threat posed by different chemicals. For instance, if a chemical A has a toxicity score of one and chemical B has a toxicity score of three, then it is possible to conclude that B is more toxic than A, but it is not possible to know how much more toxic.

The type of scale used affects the mathematical operations allowed, however this aspect is in general overlooked and results from different type of scales are combined and aggregated by using addition and weighted multiplication violating the mathematical theory. Koller et al. (2001) noticed the problem for methodologies such as the INSET Toolbox, Dow F&EI, and several other methods. The issue is discussed in more detail in Chapter VII.

4.2 THE PROBLEM OF INHERENT SAFETY

4.2.1 Inherent safety: the issue nobody wants to talk about

Inherent safety is nowadays a controversial topic, and the initial enthusiasm went from efforts to understand and measure it to an unpleasant topic for the industry. In the US the threat of possible regulation due to the proposed Corzine Bill (2001) forced the industry to take a defensive position and focus efforts to highlight the limitations of inherent safety. This position can be misunderstood and can be interpreted as a demonstration that inherent safety is not a reasonable approach to safety. Because of the governmental pressure on inherent safety regulation without a deep understanding of the real technical challenges and limitations for existing plants, inherent safety is becoming the issue many know about but do not want to talk about. The truth is that the present status of inherent safety is not mature enough to be regulated, and a stronger theoretical background as well an analytical framework and new and better processing technologies must be developed. The only plausible regulatory action that can be undertaken at present is the encouragement to consider the application of inherent safety principles whenever it is possible, as done in Europe by the Seveso II Directive.

An example of the effort to show the apparent limitations of inherent safety is the case presented by Hendershot (2002), about the detrimental effects on the stability of a distillation column due to the reduction of bottom liquid inventory. This intensification approach was proposed by Kletz (1998) as an option to reduce the quantity of hazardous materials in a plant. Although the problem presented by Hendershot is a real one it is not a surprise since it is known that large inventories offer increased stability to the process by adding inertia able to buffer control limitations and process upsets. While the target message was "be careful when you apply the inherent safety principles without understanding the behavior of the system because you may get something different from what you expect" it could also be interpreted in a more negative way.

4.2.2 Inherent safety: an approach that can be misunderstood due to hazard migration

The application of inherently safer design requires a holistic approach and a complete understanding of the implications of the changes within the whole plant. When the design of equipment is modified towards an inherently safer option, the achieved local hazard reduction may cause more hazardous conditions in other parts of the plant. When inherent safety is applied only to one single element (e.g., distillation column by reducing liquid space volume) while the other aspects are not improved accordingly (e.g., control system strategy) the expected results probably will not increase the overall safety level (e.g., increased control instability).

This example highlights the fact that not only is it required to analyze variable interactions within the same equipment but also among interrelated units. Furthermore, the normal approach followed by the proposed methodologies for inherent safety analysis usually focuses on "worst hazards" (e.g., largest tank, or most toxic chemical) that cannot capture the complexity associated with hazard migration and hazard interaction.

It is often said that the inherently safest plant is the one that has not being built or is not in operation. However, this is not a correct interpretation of inherent safety because it must be evaluated according to the goal of the plant. The purpose of a chemical plant is to produce certain chemicals with the restriction that the plant must operate in a competitive (i.e., economic) and safe way. The whole plant must be analyzed not only from the processing viewpoint but also from the capital and operating cost, to understand where and how the hazards have been removed (or created) and the economic impact of the proposed changes. Process hazard migration, capital cost, and operation cost change due to plant modification toward inherent safety.

4.2.3 Inherent safety: a paradigm change

While the lack of proven analytical tools for inherent safety analysis represents a strong limitation in practical terms and allows subjectivity to control the design efforts, the true problem of inherent safety is the paradigm change that is required. This change requires the identification of alternative processing options (including chemicals and equipment) with low intrinsic hazard, and the integration of these ideas into design activities during early stages of development. This requires the availability of analytical tools that can be integrated into process simulators in order to reduce the time and effort required for hazard identification and quantification.

Another important paradigm change imposed by inherent safety is the difference between “safety” and “inherent safety”. As explained above, two aspects define the present understanding of safety:

- Reduced consequences
- Low risk

It is possible to see that these two aspects have their roots in the second phases of the historic development of safety and the technical limitations of the past when safety analysis had to be developed at the end of the detailed engineering phase, when only hazard control was possible. However, recent approaches such as Layers of Protection Analysis (LOPA) [AIChE, 2001] follow a similar basic ideology, but mention inherent safety and hazard reduction as the first line of defense and incident prevention. By adding protective barriers the likelihood and consequences of an incident is reduced by ensuring that there are sufficient elements (e.g., relief valves, control systems, alarms, safety instrumented systems) able to stop the sequence of events before they can produce an incident. This concept is illustrated in Figure 4.2a. The width of the arrows at the top indicates the risk without layers of protection while the last arrow is a schematic representation of the amount of risk after the layers of protection. This indicates that without protective barriers the process risk is high however a low risk level can be reached by installing sufficient add-on layers.

Inherent safety, proposes to reduce or eliminate the sources of hazard eliminating or reducing the need for protective barriers, as illustrated in Figure 4.2b. Because the hazards have been eliminated or reduced, the initial arrow is thinner and low risk can be reached with fewer layers of protection. It is important to recognize that absolute inherent safety cannot be reached hence the term “inherently safer” must be used.

From the previous discussion the following conclusions are reached:

- Low risk does not imply low hazard level, but “low risk” is a necessary condition for “low hazard” and hence inherent safety.
- Inherent safety implies low hazard therefore implies low risk, then “low hazard” is a necessary and sufficient condition to ensure “low risk”.

Quantifying inherent safety through risk assessment is conceptually inappropriate, since low risk is achieved by using protective layers, unless the barriers are not taken into consideration. However, this option violates the fundamental goal of risk assessment. On the other hand, in order for the second conclusion to be true, it is important to:

- Identify issues related to hazard migration (e.g., distillation column control instability) as explained above.
- Analyze the process against a goal in order to avoid misleading issues as presented in Chapter II (e.g., car transportation vs. air travel).

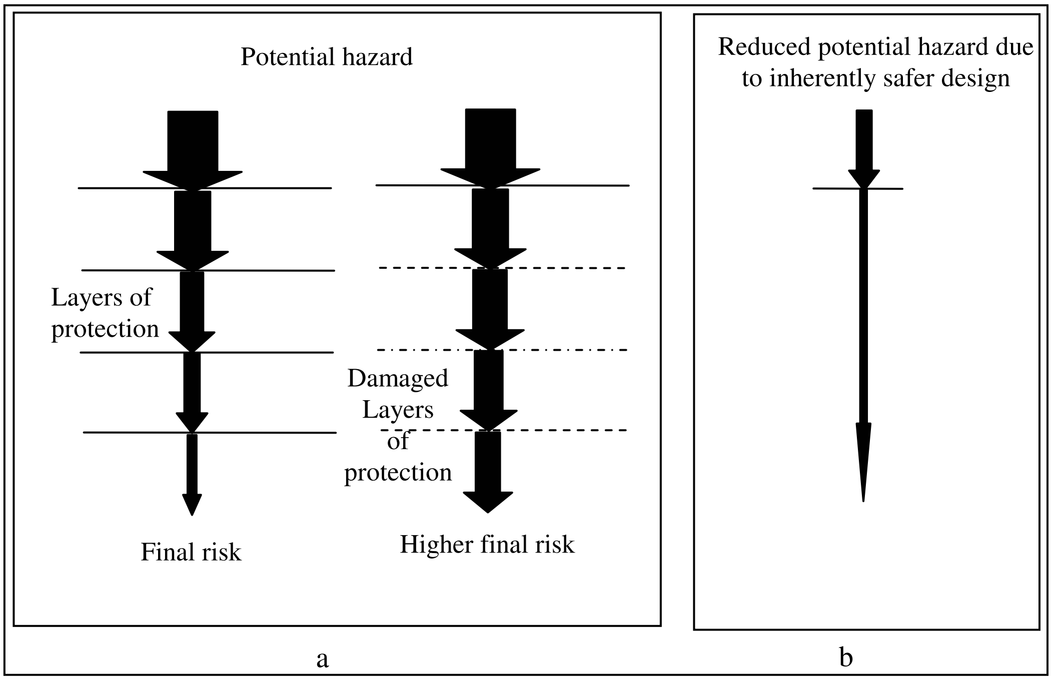


Figure 4.2: Difference between safety achieved through layers of protection (a) and inherent safety (b) [Hendershot, 1998]

4.2.4 Inherently safer design is not inherently safe design

Inherent safety is not the absolute panacea for achieving hazard and risk elimination. A characteristic of inherent safety is that “absolute” elimination of hazards is not possible hence a plant cannot be “inherently safe” but only “inherently safer”. From the modeling viewpoint this aspect is similar to the mathematical concept of limit:

$$\lim_{x \to a} f(x) = b$$

where the limit value of the function f(x) as x approaches a is b. Mathematically the limit cannot be reached, and in the case of an asymptotic function the limit may tend to infinity. If we assume that inherent safety is a function of hazard and is defined in Figure 4.3. Then by applying the concept of mathematical limit:

$$\lim_{HAZARD \to 0} Safety\,(hazard) = +\infty$$
$$\lim_{HAZARD \to \infty} Safety\,(hazard) = 0$$

This concept is in agreement with the idea that only "inherently safer" design can be reached while "inherently safest" design is the practically unachievable limit when hazard tends to zero. As shown in Figure 4.3, and as indicated here, because hazards cannot be totally eliminated, in some cases after applying inherent safety principles, extrinsic safety must be applied by adding protective barriers in order to further reduce the overall risk. Because of this requirement, inherent safety and extrinsic safety are not contradictory but they are complementary and are indicated for different type of situations and processing objectives. For example, a gasoline tank farm has the objective to store large volumes of highly flammable substances, hence inherent safety can be applied only in a limited form (i.e., by simplifying the design to avoid human errors, and to reduce the possible domino effects). In this case, extrinsic safety is indicated instead of inherent safety.

4.2.5 Inherent safety as a tangible activity

Mansfield (1991) suggests that another reason for the preference towards methodologies such as QRA and HAZOP is that these methods require a specific set of activities that can be planned, scheduled, and evaluated. On the other hand, inherent safety as it is used today is understood as a conceptual effort rather than an analytical activity hence cannot be systematically applied and used as a technical decision tool.

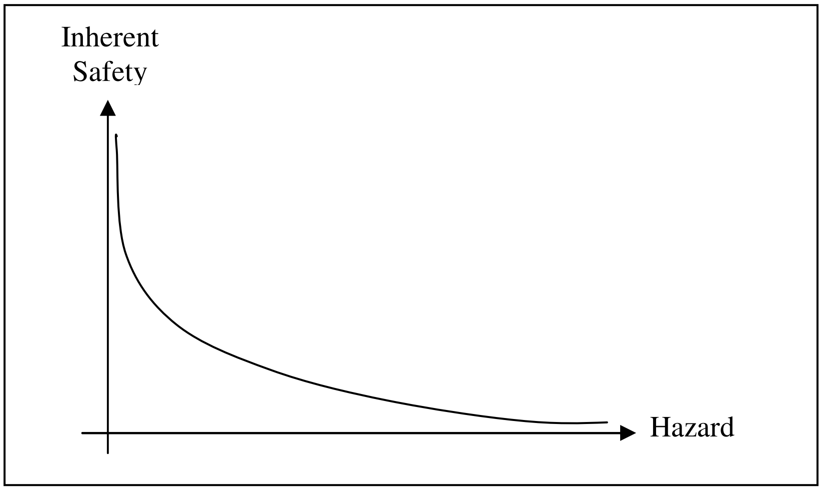


Figure 4.3: As hazard tends to zero, inherent safety increases

4.3 TOWARDS A THEORY FOR SAFETY AND INHERENT SAFETY

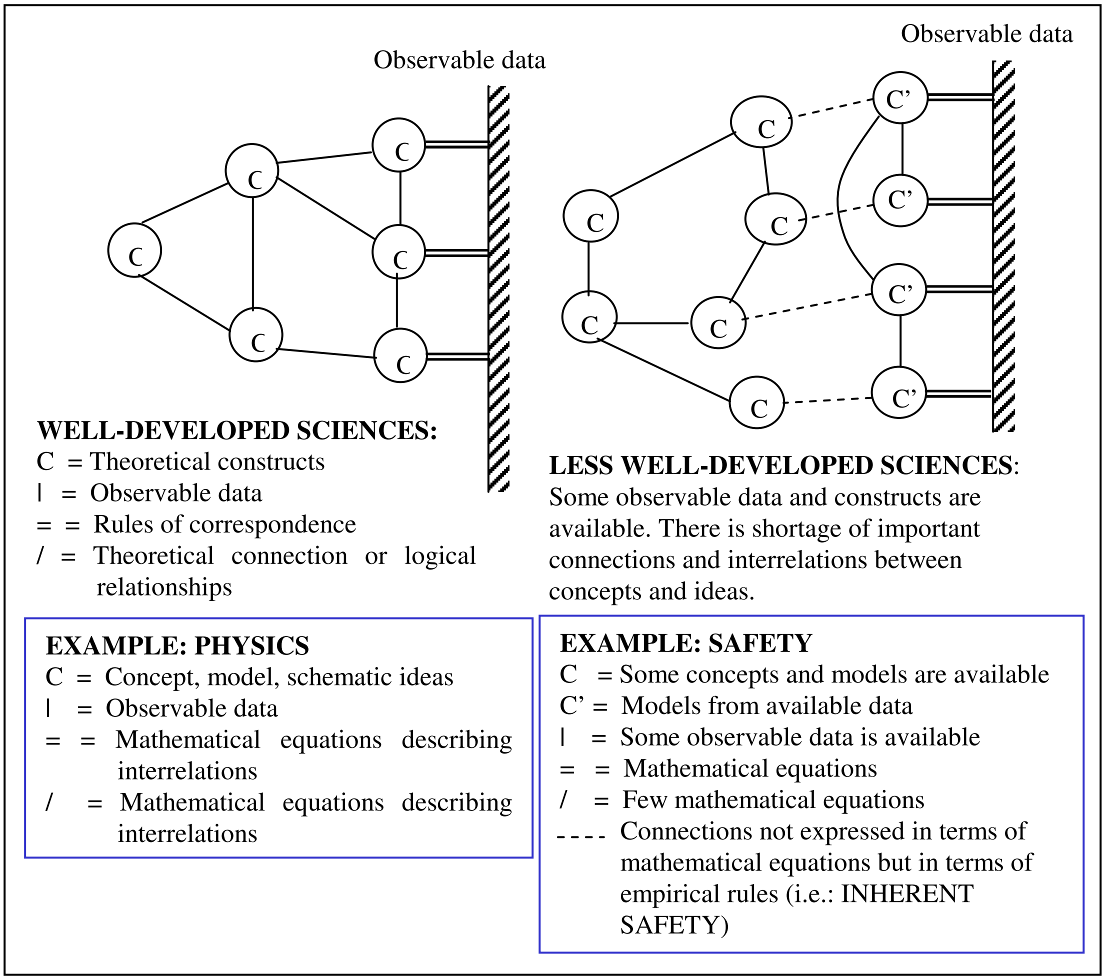
A chemical process plant is a facility composed of a large number of different elements and aspects whose relations are complex and include technical, economic, human, and environmental factors. Several authors have recognized limitations such as conflicts and tradeoffs between inherently safer design and environmental, technological, and economic requirements. Therefore the attempt to develop a rigorous and systematic quantitative measurement of the inherent safety is a challenging problem.

From the previous discussion, it is evident that a measure of safety and inherent safety is required and one of the questions that must be answered is “why is it so difficult to understand, model, and measure safety?

4.3.1 Safety as a non-well-defined science

According to Torgerson (1958) a well-defined science consists of theory and empirical evidence that are connected by rules, logical relationships, and interpretations.

For instance, physics has many constructs (i.e., theory, hypothesis, theorems, ideas, concepts, paradigms), which are connected by quantitative relations such as mathematical equations. The multiple connections of the constructs allow progress from observable data to the theoretical space by means of mathematical equations (Figure 4.4).



WELL-DEVELOPED SCIENCES:
C = Theoretical constructs
| = Observable data
= = Rules of correspondence
/ = Theoretical connection or logical relationships

LESS WELL-DEVELOPED SCIENCES:
Some observable data and constructs are available. There is shortage of important connections and interrelations between concepts and ideas.

EXAMPLE: PHYSICS
C = Concept, model, schematic ideas
| = Observable data
= = Mathematical equations describing interrelations
/ = Mathematical equations describing interrelations

EXAMPLE: SAFETY
C = Some concepts and models are available
C' = Models from available data
| = Some observable data is available
= = Mathematical equations
/ = Few mathematical equations
- - - - Connections not expressed in terms of mathematical equations but in terms of empirical rules (i.e.: INHERENT SAFETY)

Figure 4.4: Difference between a well-developed science and a less developed science [Margenau, (1950) as cited by Torgerson 1958]

However, for a not-well-developed science, such as social and behavioral sciences, the situation is less developed, and there are plenty of observable data but a severe lack of connections such as quantitative models. In some cases there is no universally accepted definition for some concepts or in other cases the concepts are well defined but a measurement method is lacking. Some terms are vague and usually complex [Torgerson, 1958]. Safety is in a very similar situation. Some concepts cannot be defined, others cannot be measured, and in some cases there are enough constructs but no established quantitative connection among them.

From these ideas of not-well-developed science we can take some useful concepts such as property, system, and their interrelation. Properties are the observable aspects and characteristics of the real world and they occur as characteristics of a system, which is formed by elements [Torgerson, 1958]. In the case of safety a system can be a chemical plant composed of equipment, chemicals, instruments, the environment, and people. These elements have observable properties and in our case they must be relevant to inherent safety. For instance, properties of a chemical can be toxicity, volume, and explosiveness. Properties for a vessel can be volume, operating conditions such a pressure and temperature, location, contained chemicals and its own properties. For a pipeline the volume can be substituted by diameter and length, and other factors such as number and type of instruments can be used.

Properties have to be measurable but for not-well-developed sciences the concepts are classificatory (e.g., X is warm, Y is safe) and they use fuzzy terms. When a science is well developed the classificatory terms tend to be replaced by quantitative parameters [Torgerson, 1958]. Classificatory terms are commonly used in process safety, for instance the NFPA scoring system and other score-based methodologies. Type of scales and theory of scaling will be discussed in Chapter VII.

4.3.2 An example of non-developed science to developed science

Thermodynamics allows understanding the transition between the two science development states and can be useful for our case because inherent safety shares several aspects with temperature and enthalpy. Inherent Safety is based on rules (e.g., principles) and fuzzy linguistic terms (e.g., safe, unsafe). In general we can sense situations that are extremely safe or extremely unsafe; similarly we can say if an object is very hot or very cold. However, a temperature scale is needed in order to quantify temperature and to decide how hot or cold an object is. In the case of safety we do not have such a standardized scale yet, but several methodologies, approaches, and concepts have been proposed as measurement means. This situation is very similar to the early history of temperature, when there was a general lack of understanding about the nature of "temperature" and several diverse measurement methodologies were used.

By definition inherent safety involves the reduction or elimination of hazards. And hazards are generated from intrinsic properties of the chemicals, factors related to the plant and also from the interaction of these properties and factors. For instance, a high toxicity may be meaningless by itself in terms of incident possibility (except in very special cases such as toxins or infectious substances), but when combined with large volume the hazardous potential of the scenario becomes evident. If a plant presents a high concentration of hazardous properties and factors, then intuitively the possibility of incident occurrence should be higher compared to plants with fewer hazards.

Intuitively, if temperature is a mathematical variable that provides a measure of hotness or coldness, inherent safety could be understood as a mathematical variable that provides a measure of "safetiness" or "unsafetiness." And, if energy (heat) can be transferred from a body to another changing their temperature, then hazards (represented by the possibility of expressing themselves into an incident) can be removed or added to a process to change the "safetiness" degree of a plant. Heat flows, but hazards also flow because when a modification is made to a part of the plant to increase its inherent safety level, other units could be affected and become inherently unsafer. As the enthalpy function depends on pressure and volume, safety should have some kind of functionality with some parameters (i.e., chemical and physical properties of substances and equipment). The possibility of an incident depends on the type and magnitude of the involved hazards but also on their interaction. Hence a possibility model could be a measure of safety as enthalpy is a measure related to temperature.

4.3.3 Safety as a complex system

When a system is so complex that it cannot be understood it is reduced to more manageable systems that can be modeled with standard mathematical approaches. Complexity, when analyzed from a broad viewpoint, is usually understood as randomness and modeled through a statistical approach. An example of this is flow dynamics where turbulence produces swirls that can appear to behave in an unpredictable form. However, we now know that turbulence swirls result from the fluid and flow properties and can be predicted by fluid flow equations and models. However, the new understanding of turbulence requires approaching the problem from a detailed viewpoint and analyzing the physical phenomena not only at the macroscopic level but also at the microscopic level [Auyang, 2003].

A complex system is formed by a set of subsystems that individually can be simpler but when functioning together establish multiple interrelations and complicate networks of properties and behaviors. Each subsystem may be described by a theory while the whole system may be described by another theory. The connection between the two levels of theory is by itself a complicate issue and may require new ideas. For instance, thermodynamics is connected to mechanics through the theory of statistical mechanics [Auyang, 2003].

When these ideas are applied to safety it can be assumed that safety is by itself a complex system resulting from the interaction of subsystems such as the chemical plant, chemical substances, the natural environment and human beings, and the society. While each one of the subsystems may be more or less understood (i.e., availability of descriptive and predictive models) and can present different hazard sources or be sensitive to hazards in different ways, the overall system lacks a general theory able to describe and analyze “safety”. If we look at safety as a non-well defined science (as described in Section 3.1) with availability of local models, theories and constructs, but with a lack of theories to interconnect the local systems, it appears that safety may be a complex system.

The synthetic analysis required to establish the connections among the subsystems first analyze the overall complex systems in order to identify its main parts and models that independently describe each subsystem. Then interactions among the subsystems are evaluated and the final solution to the original complex problem is finally synthesized. The synthetic analysis is focused on the overall system but it is based on the single parts. On the other hand, a reductionism approach looks only at the single parts [Auyang, 2003].

Looking at the problem of safety it seems that the present state-of-the-art resembles the first stage of a synthetic analysis with a tendency towards a reductionism approach. While some individual systems have been thoroughly analyzed (e.g., gas dispersion for hazard assessment) others have not reached such a predictive power due to lack of driving force or lack of understanding because of high complexity (e.g., environmental modeling). However, the general approach sought so far for safety and loss prevention tends to focus on single elements of the system (e.g., the plant). Due to analytical difficulties and the historical bounds, variable interaction is analyzed only by fault tree analysis while the general approach is to analyze variables independently and then aggregate them in some way.

Several complex systems cannot be grouped into classes; however there are at least two types that can be recognized. Nonlinear dynamic systems are governed by simple rules that can induce chaos when a very small difference of the initial condition produces a large difference in the response. The work of Wolfram (2000) is an example of this behavior. In safety, chaos could be understood as the occurrence of an incident due to the interaction of several factors that form the “right” chain of events. When this type of systems is related to physical quantities that are continuous, a real number cannot represent an exact input condition, since each real number represents an infinite cluster of inputs within a certain error [Auyang, 2003]. This same idea reappears in Section 4.1 regarding the discussion on vagueness as a type of uncertainty present when there is a lack of well-defined boundaries for a variable (i.e., it cannot be divided into crisp subintervals).

Another type of complex systems is given by many-body systems. In this case the complex system is formed by a large number of interacting elements that belong to a reduced number of subsystems. An example of this type is a solid formed by atoms of one or two elements, such as gold [Auyang, 2003]. As explained by Auyang (2003) "…the central aim of many body problems is the micro explanation that relates typical macroscopic properties of the systems to the typical properties of the constituents. As it turns out, this is a very difficult problem, and often demands total reformulation of the problem, i.e., cast the typical properties of the constituents in different forms". This is probably the best description of the ultimate goal of the present project which is directed at the reformulation of the approach to measure inherent safety by analyzing the interaction of the single hazards by starting from the properties of the subsystems (e.g., chemical and physical properties of the substances; physical properties of the plant).

If a complex system is formed by only one type of constituent with property P interconnected by a single type of binary relation R, then each constituent P_i is related to another element P_j by a relation R_{ij}. When all the possible relations are established a complicated network is formed. If one of the constituents P suffers a change, then the network transmits the effect of the change to the other constituents through the specific binary relations [Auyang, 2003]. In the case of safety, this phenomena was mentioned previously as "hazard migration" and constitutes an important property of the system, because it is important to ensure that a design change towards inherent safety does not increase the hazard in other units.

As described by Wolfram (2000) the history of complexity has philosophical roots and can be followed through the development of mathematics and science. In the late 1800s statistics arose as a scientific approach for the treatment of uncertainty in social science; then statistics was applied to explain microscopic physical phenomena in the new field of statistical mechanics. However, until early 1900s the advances of physics focused on simple systems that could be described by mathematical formulas, thus avoiding complexity. Other scientific fields followed the same approach focusing on the development of mathematical formulas for simpler systems. During the last sixty years, computational advances as well as the development of new fields such as artificial intelligence, chaos and fractals, and game theory, and new problems in biology, economics, and mathematics have allowed us to look at problems in a different way even though the tendency to try to develop descriptive mathematical equations remains. In the early 1980s the work on cellular automata [Wolfram, 2000] suggested that complex behavior of a system could be described by general rules that can be very simple.

4.4 APPROACH AND IDEOLOGICAL FOUNDATIONS FOR INHERENT SAFETY MEASUREMENT

The development of a new approach to measure and analyze inherent safety must address the issues identified in the previous discussion. Another methodology that follows the same guidelines already explored by the approaches described in Chapters II and III would not give process engineers an efficient tool to evaluate new designs (assumed to be inherently safer). This practicality describes the objective of the project and establishes the basis upon which the mathematical methodology and technical approach were selected in order to address the problem discussed in Sections 1, 2 and 3 of this chapter.

4.4.1 Question to be answered and definitions

Before starting any project it is important to define which questions should be answered. As noted by Mansfield (1991) in order to measure inherent safety it is necessary to develop an index capable of measuring a “degree” of “inherent safetiness.” In other words, the question that should be asked is “How inherently safer is the plant?” rather than “Is the plant inherently safer?” The difference implicit in these two questions is more evident when the concept “inherent safety” is recognized as an uncertain idea without defined boundaries.

For this project safety is understood as “inherent safety” which is defined as “lack of hazards” therefore as the quantity of hazards of a chemical plant tends to zero the level of safety increases:

$$\text{Inherent safety level} = f(\text{hazards})$$

Hazard is defined as the potential to produce an incident and is function of physical properties of the equipment and chemical/physical properties of the substances:

$$\text{Hazard} = f\,(\text{physical properties of equipment, physicochemical properties of substances})$$

$$\text{Physical properties of equipment} = f(\text{design, operating conditions, task})$$

Physicochemical properties of substances such as toxicity, reactivity, and phase at environmental conditions are inherent only to the nature of the substance; however these properties are affected by other factors such as operating conditions and concentration. The modeling of hazards is therefore based only on measurable (non subjective) parameters, that are however subject to uncertainty (i.e., vagueness) due to their continuous nature (i.e., not describable by discrete intervals) or the experimental variability of their measurement.

The “magnitude of the hazard” is defined in relation to certain values identified as “inherently safer” in terms of the low consequences that could derive from such values.

Because the consequences are physical measurable factors, they are not subjective but remain uncertain and vague since no strict thresholds can be established.

4.4.2 On safety's uncertainty

Safety evaluation is characterized by the presence of uncertainty implicit in the variables and due to subjective evaluations. In order to choose an appropriate mathematical model to work with uncertain variables, it is important to understand the source and type of uncertainty.

In general, uncertainty can be classified into randomness, vagueness, and ambiguity (Lootsma, 1997). The uncertainty for an experiment with several possible outcomes (e.g., casting dice) that can be properly observed is called randomness and can be reduced by performing additional trials and developing a probability density function. This type of uncertainty is associated with the likelihood of stochastic events (ie., non-deterministic events) and can be described by a probabilistic approach. In this case the events are crisp (i.e., well defined) and it is possible to establish sharp and well-defined limits (e.g., "yes/no", numerical values such as x = a).

When the events cannot be properly observed vagueness occurs, and additional experimentation will not reduce this type of uncertainty. An example is casting dice that instead of a specified number of marks have colored faces. If the light is not good enough to allow a clear distinction between colors, uncertainty due to vagueness arises and will not be reduced by performing additional experiments under similar conditions (no better light available) (Lootsma, 1997). The same type of uncertainty arises when either the events are not sharply defined (e.g., "more or less" rather than "yes/no", "x has a value around a" rather than x = a) or the classification intervals are not well defined (i.e., continuous scale rather than discrete scale). The imprecise meaning of words such as "good", "safe", and "reddish" are examples of uncertainty based on linguistic vagueness.

Ambiguity arises when a word has a meaning that depends on the context of the statement. For instance, the expression "the bridge is open" presents uncertainty because it is not possible to understand if the draw-bridge is open to road traffic or to ships (Lootsma, 1997). In this sense, safety is also an ambiguous concept because it is context dependent. For instance, chlorofluorocarbons are inherently safer with respect to ammonia as refrigerant gases because they are not explosive or flammable, however in terms of environmental impact are inherently unsafer due to effects on the Earth's ozone layer.

Fuzziness originates from the imprecise nature of abstract concepts and thoughts rather than from the random properties of an event. Fuzzy logic does not deal with the likelihood that a specific outcome will be observed but deals with the degree of how much the outcome is similar to a particular category. As indicated by Almond (1995), fuzzy logic allows working with imprecision and real-world, vague engineering problems that would otherwise be rejected by the traditional statistical methodologies.

Safety is a fuzzy concept because it defies exact definition. Furthermore, "safety" cannot strictly be classified into the dichotomy safe/unsafe (e.g., Is the plant safe?). A chemical plant is not safe or unsafe on an absolute basis; hazards cannot be totally eliminated, hence a plant will always have a certain quantity of hazards or a certain degree of "unsafeness" that cannot be described by a Boolean (i.e., yes/no, safe/unsafe) approach. A methodology with gradual non-discrete transitions is required (e.g., How safe is the plant?). Safety hazards should not be modeled by a statistical approach, because their uncertainty is not caused by randomness but by fuzziness, vagueness, and ambiguity. Additionally, some events are rare and it is not possible to calculate reliable incident probabilities.

Fuzzy Set Theory and fuzzy logic offer an alternative mathematical framework where vague and imprecise concepts and phenomena can be rigorously modeled and analyzed by allowing an element to belong simultaneously to more than one category or set. A chemical plant that is "more or less" safe belongs to the "safe plants" set and to the "unsafe plants" set with different degrees of membership, which is in contrast with the common Boolean approach where partial membership in a set is not allowed.

4.4.3 Possibility rather than probability

Fuzzy logic is often confused with the traditional probability theory. This controversy is exemplified by a series of seven papers; three are against fuzzy logic (Laviolette et al, 1995a and 1995b; Cheeseman, 1995) while the others (Almond, 1995; Bonissone, 1995; Kandel et al, 1995; Almond, 1995; Zadeh, 1995) recognize that the two approaches, fuzzy logic and probability, are complementary rather than mutually exclusive. Other authors suggest that a possibility distribution can be interpreted as a family of probabilities (Natvig, 1983). However, it is important to recognize that probability theory and possibility theory aim to solve different problems whose fundamental distinction is the type of uncertainty involved.

Regardless of the mathematical controversy between statistics and fuzzy logic, the application of fuzzy set theory to inherent safety quantification, offers the opportunity to solve problems and limitation of the indices based on traditional Boolean logic, and at the same time it offers a systematic methodology to take into account the uncertainty typical of inherent safety evaluation. As noted by Mansfield and Cassidy (1991), in order to measure inherent safety, we must develop an index capable of measuring a "degree" of "inherent safeness." Fuzzy logic offers the opportunity to rank plants according to their degree of inherent safeness through the concept of membership degree (explained in Chapters V and VI). This ranking ability is congruent with the idea that that the concept of inherent safety is a relative state and a plant can only be evaluated with respect to another plant.

Inherent safety aims to eliminate the hazards rather than to control them. This approach is based on the fact that if a hazard is present, the incident could still occur if the protective layers fail during an abnormal situation. In other words, the presence and magnitude of the hazard makes the incident possible; obviously if the hazard is eliminated, the incident cannot occur. This idea is parallel to the relation between probability and possibility: in order for an event to be probable, it has to be possible. Although linguistically the two words can be synonyms, mathematically they have different meanings. While probability is associated with statistics and stochastic uncertainty, possibility is modeled by fuzzy logic (i.e., possibility theory) and deals with vagueness. Human decisions and evaluations are based mainly on possibilistic information rather than probabilistic knowledge and this fact shows the importance of possibilistic theory (Zadeh, 1999). It is interesting to observe that, except when specifically discussing risk assessment or fault tree analysis, the word "possible" is much more common than "probable" in "safety discussions." Ashford and Zwetsloot (2000) also recognize the relation between inherent safety and the reduction of incident possibility while traditional safety can only prevent incidents hence reducing the probability.

If an event is impossible it is also bounded to be improbable. This heuristic rule is known as the possibility/probability consistency principle according to which a possibility distribution acts as an upper limit for the probability distribution. While low possibility implies low probability, high possibility does not imply high probability nor does low probability imply low possibility (Zadeh, 1999). Catastrophic incidents (i.e., high consequences but low probability events) are well described by this characteristic of the possibility theory. It is often assumed that these incidents are almost impossible because they have low probability. However, a measure of the possibility degree can only be developed based on the properties of the systems. For instance, an "incident waiting to happen" (due to a specific combination of factors) is perceived as a very possible event even though it may have low probability.

Possibility theory and fuzzy logic open a new, and apparently natural, approach to inherent safety quantification due to the following properties:

- Inherent safety is a fuzzy concept that can be modeled with fuzzy logic.
- The membership function offers the opportunity to rank plants according to their degree of safetiness, as shown in Figure 4.5.
- High hazard implies high incident possibility, but low risk does not necessarily imply low possibility, as commonly assumed.

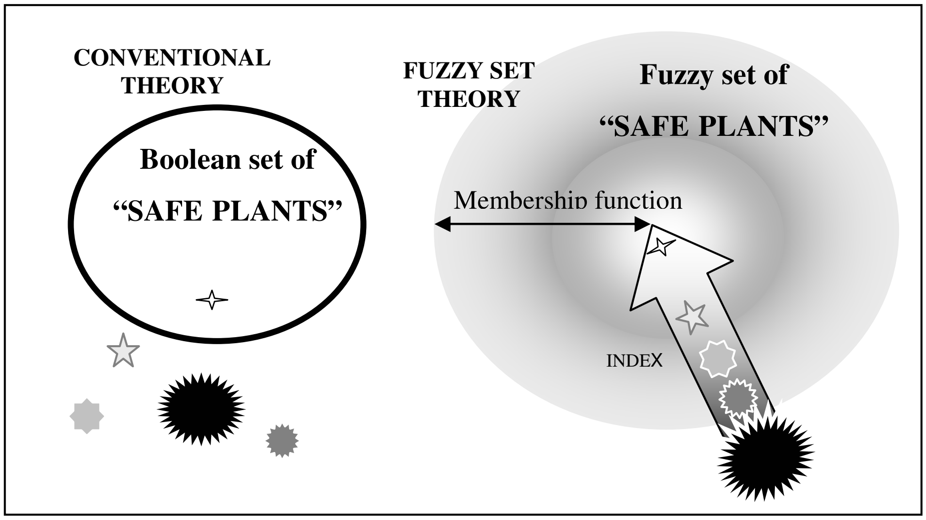


Figure 4.5: Unsafe plant cannot belong to the Boolean set of "safe plants", however according to the fuzzy logic approach plants are ranked in the set according to their degree of inherent safety measured through the membership function in the fuzzy set

4.4 Applicability of the methodology

From the history of process safety and from the limitations of inherent safety it follows that what is needed is a methodology that could be applied during the early stages of plant design by process engineers rather than safety experts (Figure 4.6) as well as for existing plants.

The approach proposed here is derived from knowledge, problems, and limitations reported by other researchers. The main ideas upon which the proposed index is built are:

- The inherent safety index proposed here is based on the quantification of the magnitude of hazards present in a plant due to the chemicals, operating conditions, and type of unit operations. This approach is preferred over a risk minimization approach, because, while low risk can be achieved by protective add-on barriers, low hazards imply low risk as well. To simplify the procedure, the inherent safety principles are not evaluated individually.

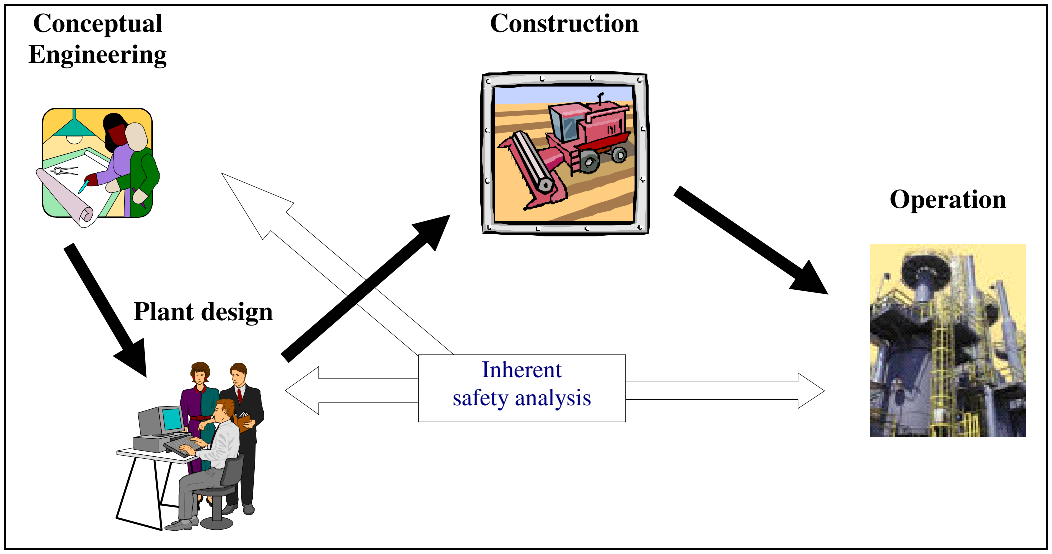


Figure 4.6: Targeted application of the proposed inherent safety index based on fuzzy logic

- The inherent safety index should include enough variables and parameters to describe the possible hazardous situations and interactions that cannot be detected by more simplistic approaches. This index should be useful for the inherent safety analysis of plants in advanced design stages or plants in operation. For designs during early design stages when the information is incomplete, the index uses default values for the required input, which will show high hazard scores to indicate the presence of missing information.
- It is assumed that each piece of equipment contributes an inherent degree of hazard due to the interaction and combination of factors (e.g., chemical hazard, operating

conditions, and mechanical characteristics). The combination of all these contributions should be used, instead of only the worst hazards, to identify phenomena such as hazard migration. Chemicals, equipment, and operating conditions can be hazardous by themselves; however the hazards inherent in a chemical plant are derived from the interaction of hazardous factors. This approach is helpful for solving common controversies. For example, process A requires flammable but low toxicity chemicals, process B requires noncombustible but volatile and moderately toxic chemicals, and process C requires noncombustible nontoxic materials at high pressure. By considering single hazards it is evident that none of the three processes are hazard-free [Englund, 1995], but by analyzing combinations of conditions, process C could be the inherently safer if the vessels are designed to withstand the pressure and the vessels are small. This idea is analogous to the fact that any chemical is toxic if the dose is high enough.

- The inherent safety assessment of existing plants requires the understanding of hazard migration due to changes performed on productive units. The whole plant must be analyzed not only from the processing viewpoint but also from the capital and operating cost viewpoint to understand where and how hazards have been removed (or created) and the economic impact of the changes. Hazard migration, capital cost and operation cost changes due to change toward inherent safety can be analyzed when the index is used with process simulation.

4.4.5 Process simulation

In order to facilitate the application of the proposed methodology during engineering design it is necessary to link the procedure to a process simulator. However, this is usually not pursued [Koller et al, 2001]. The development of an overall inherent safety index based on continuous functions will facilitate the application of inherent safety to process simulation and process synthesis. Process simulation is useful for evaluating the processing alternatives from the processing requirements. When process simulation is linked to cost estimation software, the capital and operating costs can be evaluated, and the results of the analysis can be used by process synthesis to generate better processing alternatives based on the technical, environmental, and economic constraints, as shown in Figure 4.7. The inherent safety index evaluated during process simulation can be used as an additional constraint for the synthesis process, as shown by the dashed line in Figure 4.7. The expected advantages of this procedure are the following:

1) Automated inherent safety evaluation and cost estimation that allow a rapid analysis and generation of processing alternatives when process synthesis is carried out with a systematic generation of design that follows the economic and safety constraints.
2) Possible application to operative plants allowing the identification of processing alternatives according to the cost and environmental constraints. The optimization of a process with respect to environmental restrictions is more efficient when applied during earlier stages of the life-cycle of a plant. However, as demonstrated by El-Halwagi (1997) and Sikdar and El-Halwagi (2001) it is possible to apply the same optimization principles to existing plants to obtain more environmentally friendly processes. A similar application is expected for the inherent safety principles when an inherent safety quantification methodology is available.
3) The application of process simulation presents the additional advantage of permitting analysis of the hazard level of processing areas interconnected to units or equipment modified toward an inherently safer design.

4.4.6 Advantages and disadvantages

The approach presented in this dissertation is expected to solve some of the problems and limitations described previously for more traditional inherent safety evaluation methods. These advantages can be summarized as:

- Understanding of different type of uncertainties involved in inherent safety evaluation, which are then treated with an appropriate mathematical approach based on fuzzy logic and possibility theory. Fuzzy logic allows modeling of uncertainty and subjectivity in a simpler and rigorous way, compared to claimed similar (but more complex) models based on traditional statistics.

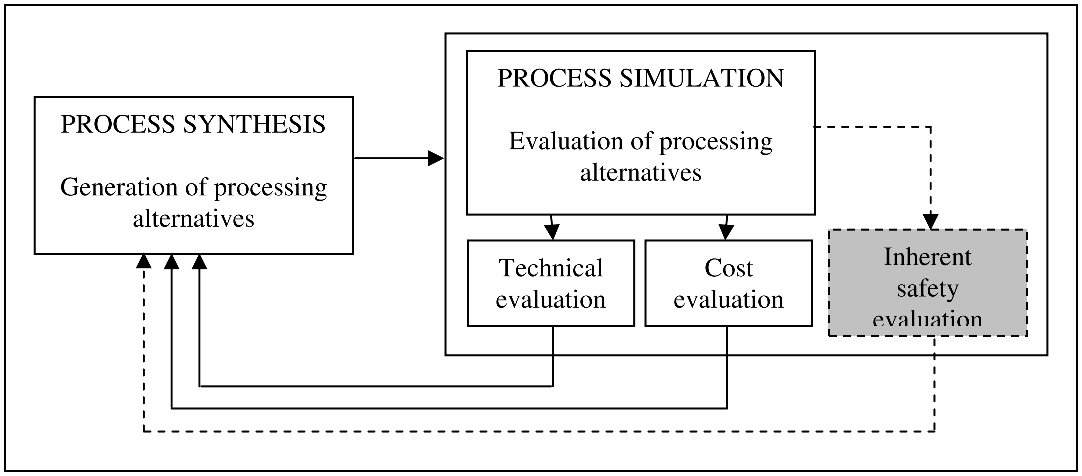


Figure 4.7: Application of the proposed inherent safety index for process simulation and process synthesis

- Solution of the problem relative to lack and excess of sensitivity within and around the limits of subranges are eliminated by smooth and gradual transitions provided by the fuzzy sets. This approach also eliminates the subjective problem of deciding which score should be assigned (or into which adjacent subranges should an element be classified) in uncertain situations (e.g., element around the limits of subranges).
- Combination of numerical information as well as subjective evaluations and heuristic knowledge into a single rigorous mathematical approach, which allows taking into account information that usually is too vague to be translated into accurate numerical indices, such as human factors and linguistic knowledge.

- Modeling of the factors interaction (described either by numerical data or subjective information) by means of IF-THEN rules able to describe general knowledge with respect to the relation between two or more variables, which is especially useful in process safety analysis because of the lack of numerical data. However by means of engineering and expert knowledge, it is possible to develop heuristic rules that can be used in a fuzzy inference system.
- Development of a safety measure based on possibility theory, which is beyond the scope of this work.

However, the present methodology also presents some disadvantages:

- Introduction of uncommon mathematical concepts with which most safety practitioners are not familiar. Nevertheless, the application of abstract concepts is translated into a simple and transparent methodology described in the next sections.
- Limitations due to lack of numerical data to design the membership functions that defines the fuzzy sets. These functions represent the strength of fuzzy logic but at the same time they also are the Achilles' heel when numerical data are not available to apply design methodologies that reduce the uncertainty of the functions. However, the introduction of technical information and expert knowledge is expected to reduce the limitation due to lack of data. Additionally, the modular structure of the approach will allow incorporation of updated data and knowledge when they become available.

4.5 SPECIFIC RESEARCH OBJECTIVES

The hypothesis investigated in this project is work to the evaluation of inherent safety based on a novel theoretical background based on concepts borrowed from complex systems and inspired by the analysis of the limitations and problems of the current process safety and loss prevention state-of-the-art. Inherent safety is explained in the context of a system formed by several subsystems characterized by certain properties capable of posing hazard to the plant, human beings, and the environment. The modeling of hazards and their interactions is based on IF-THEN rules modeled by a hierarchical net of fuzzy inference systems.

The methodology proposed here is based on fuzzy logic and has the objective of establishing a bridge between the theory and the "real industrial world" that demands a tool easy to use and useful for evaluating processing alternatives to select the alternative that poses the lowest overall hazard at a competitive cost. The long-term vision for the methodology is the connection to a process simulator and the application to process synthesis in order to facilitate not only the design stage but also optimization of the plant in terms of safety.

The methodology is based on a hierarchical structure that allows the combination of several factors and at the same time the calculation of sub-indices. For example, sub-indices for process hazard, environmental hazard, and health hazard are combined to form an overall chemical hazard index. The hierarchical structure and the availability of sub-indices allow identification of the type of factors with highest impact on the overall safety (e.g., operation conditions, mechanical design, chemistry) increasing the flexibility of the methodology. Process/equipment changes can target the factors with highest hazard contribution and different technologies or different designs can be analyzed in terms of their specific and overall safety impact.

The main goal of this work is the development of a systematic approach for inherent safety evaluation by measuring the quantity, type, and interaction of hazards inherent to the chemical plant. The specific objectives are:

1) Inherent safety modeling: Identification of the main areas that should be considered by the analysis of inherent safety design and development of the structure of the index.
2) Fuzzy logic modeling: Development of the mathematical methodology based on fuzzy logic for inherent safety evaluation and focused on the integration with a process simulator. The expected future applications to process optimization also require establishing the basis upon which future research can be done.
3) Application and testing of the inherent safety index using a case study.

CHAPTER V

INTRODUCTION TO FUZZY LOGIC

This section provides a brief introduction to the most important concepts of fuzzy logic necessary for understanding the methodology proposed in the next chapters. The following references should be consulted for additional information and examples on fuzzy logic, fuzzy measure, and possibility theory: Berkan and Trubatch (1997); Klir and Folger (1988); Klir and Yuan (1995); Lootsma (1997); Jang et al. (1997); Yen and Langari (1999); Tanaka (1996); Zimmermann (1996).

In the past, the needs of science and classical mechanics forced the development of analytical models, to describe the relation of a small number of variables without taking into account the uncertainty. The development of statistical mechanics and the lack of computational power forced the development of statistical and probabilistic approaches which became useful for a wide variety of disciplines.

Analytical models can be used for problems that have been described by Warren Weaver as “organized simplicity”; statistical models are useful for problems of disorganized complexity. However, these two types of problems represent only the extremes of all the possible situations, but nonlinear problems with a large number of correlated variables lie between the extremes and are described by Weaver as organized complexity as cited by Klir and Yuan (1995).

The driving force behind the development and application of fuzzy logic and fuzzy models is the recognition that traditional bivalued logic along with crisp (Boolean) sets and probability theory are not sufficient to solve real-world problems characterized by high uncertainty, complexity, and ambiguity. Several scientific fields are exploring fuzzification of otherwise unsolvable problems and by doing so they are gaining the flexibility of dealing with non-random uncertainty and imprecision originated from the complexity of the system (i.e., stress distribution in a body with complex geometry) as cited by Klir and Yuan (1995).

Inherent safety presents the characteristics of an organized complexity system where a large number of variables interact with each other in a non-linear fashion. Uncertainty is non-statistical in principle and is caused by a large number of factors and variables that characterize a specific design. One of the objectives of the present project is the fuzzification of the problem of inherent safety quantification through the application of the narrow sense of "fuzzy logic" or fuzzy modeling.

5.1 INTRODUCTION TO CRISP SETS AND CRISP RELATIONS

The theory of fuzzy logic is parallel to the theory of Boolean sets, which is more commonly used and known by the general public. Because of this familiarity, important concepts of set theory are introduced in this section for crisp sets, while in the next section they are expanded to fuzzy set theory.

5.1.1 Introduction to crisp sets

Boolean logic is based on the idea of classical sets that are characterized by a crisp (nonfuzzy) boundary and are represented as a collection of elements a_i:

$$A=\{a_1, a_2, ...,a_n\}$$

where all the elements $a_1, a_2, ...,a_n$ within the set A are listed. Alternatively, a classical set is represented as:

$$A = \{x| P(x)\}$$

where the element x belongs to the set A only and only if the proposition P(x) is true. For crisp sets the proposition P(x) can only be true or false establishing the dichotomy associated with classical logic. This same dichotomy is expressed by the characteristic function χ_A that indicates whether the element x belongs to the set or not:

$$\chi_A(x) = \begin{cases} 1 \text{ for } x \in A \\ 0 \text{ for } x \notin A \end{cases}$$

and takes a value $\chi_A(x)= 1$ when P(x) is true and a value $\chi_A(x)= 0$ when the proposition P(x) is not satisfied. Hence the characteristic function maps elements x of the Universal set X to a two-element set {0, 1}:

$$\chi_A : X \rightarrow \{0, 1\} \qquad \text{where} \quad x \in X$$

Some general sets commonly used are:

- Set of all integers: $Z = \{...,-2,-1,0,1,2,...\}$
- Set of natural numbers: $N = \{1,2,3,...\}$
- Set of nonnegative integers: $N_0 = \{0,1,2,3,...\}$
- Set of n nonnegative integers: $N_n = \{0,1,2,3,...n\}$
- Set of all real numbers: R
- Universal set: X
- Empty set: ϕ
- Ordered n-tuple of elements: $(x_1, x_2, x_3, ..., x_n\}$
- Power set (family of all subsets of A): $P(A)$

For a set A with a finite number of elements, the cardinality is denoted by |A| and indicates the number of elements within A. For any two classical sets A and B the following definitions are established:

- $A \subseteq B$ when all elements of A belong to B, hence A is a subset of B (A is included in B)
- $A = B$ when both sets contain the same elements, hence A and B are equal sets
- $A \neq B$ when at least one element is contained in only one set
- $A \subset B$ when B contains at least one element that does not belong to A ($A \neq B$), hence A is a proper subset of B.

The operations possible on two classical sets A and B, and the Universal set X are defined as:

- Relative complement of A with respect to B : $B - A = \{x|\ x \in B \text{ and } x \notin A\}$
- Absolute complement of A with respect to X: $A = \{x|\ x \in X \text{ and } x \notin A\}$
- Union of two sets A and B: $B \cup A = \{x|\ x \in B \text{ or } x \in A\}$
- Intersection of two sets A and B: $B \cap A = \{x|\ x \in B \text{ and } x \in A\}$

For a family of sets $\{A_i | i \in I\}$ the Union operation can be generalized as:

$$\bigcup_{i \in I} A_i = \{x | x \in A_i \text{ for some } A_i \in I\}$$

and the intersection operation is generalized by:

$$\bigcap_{i \in I} A_i = \{x | x \in A_i \text{ for some } A_i \in I\}$$

The properties of crisp sets are the following:

- Involution: $\overline{\overline{A}} = A$
- Commutativity: $A \cup B = B \cup A$ $A \cap B = B \cap A$
- Associativity: $(A \cup B) \cup C = A \cup (B \cup C)$ $(A \cap B) \cap C = A \cap (B \cap C)$
- Distributivity: $A \cap (B \cup C) = (A \cap B) \cup (A \cap C)$ $A \cup (B \cap C) = (A \cup B) \cap (A \cup C)$
- Idempotence: $A \cup A = A$ $A \cap A = A$
- Absorption: $A \cup (A \cap B) = A$ $A\ n\ (A \cup B) = A$
- Absorption of complement: $A \cup (\bar{A} \cap B) = A \cup B$ $A\ n\ (\bar{A} \cup B) = A \cap B$
- Absorption by X and ϕ: $A \cup X = X$ $A \cap \phi = \phi$
- Identity: $A \cap X = A$ $A \cup \phi = A$
- Law of contradiction: $A \cap \bar{A} = \phi$
- Law of the excluded middle: $A \cup \bar{A} = X$
- DeMorgan's laws: $A \cap B = A \cup B$ $A \cup B = B \cap A$

5.1.2 Introduction to crisp relations

The presence or absence of interaction between elements of two or more crisp sets is known as a crisp relation, which is a subset of a Cartesian product. If X and Y are two crisp sets, their Cartesian product X x Y is given by:

$$X \text{ x } Y = \{(x, y) | \, x \in X \text{ and } y \in Y\}$$

The crisp set X x Y is formed by all possible ordered pairs of elements x and y where the first element belongs to X and the second to Y. Additionally, if $X \neq Y$ then the Cartesian products X x Y and Y x Y will be different. In general, for a family of crisp sets $\{X_1, X_2, ..., X_n\}$ the Cartesian product among the sets is defined as:

$$\underset{i \in N_n}{\mathsf{X}} X_i = X_1 \text{ x } X_2 \text{ x } ... \text{x } X_n = \{(x_1, x_2, ..., x_n) | \, x_i \in X_i \text{ for all } I \in N_n\}$$

When a crisp relation exists among certain elements of the Cartesian product, $\mathsf{X} \, X_{i \in N_n}$ is indicated as $R(X_i | \, I \in N_n)$ or:

$$R(X_1, X_2, ..., X_n) \subset X_1 \text{ x } X_2 \text{ x } ... \text{x } X_n$$

As any other crisp set, the crisp relation R is defined by a characteristic function that describes whether an element (i.e., n-tuple) belongs to R or not:

$$\mu_R (x_1, x_2, ..., x_n) = \begin{cases} \text{if and only if } (x_1, x_2, ..., x_n) \in R \\ 0 \quad \text{otherwise} \end{cases}$$

When the membership of a tuple is one (e.g., $\mu_R (x_1, x_2, ..., x_n) = 1$) the elements $x_1, x_2, ..., x_n$ are mutually related. An example of a binary relation is given by the set of women (X) and men (Y). If the relation $R(X \text{ x } Y) = \{(x,y) | \, x \text{ and } y \text{ are married}\}$ is defined by the set of married persons, then among all the possible pairings xy only married couples belong to R where x is married to y and vice versa. If Mary is married to Bob and Cindy is married to Greg, then R(Mary, Bob)=1 and R(Cindy, Greg)=1, but R(Mary, Greg)=0 and R(Cindy, Bob)=0. When three, four, five or n sets are related, then the respective relations are called ternary, quaternary, quinary, or n-ary. The relations between n crisp sets are conveniently represented by n-dimensional arrays of zeros and ones. For example:

X x R		Y	
		Bob	Greg
X	Mary	1	0
	Cindy	0	1

When the value of the membership function μ_R can receive values smaller than one, a fuzzy relation is established allowing partial membership [Klir and Juan, 1995].

5.2 INTRODUCTION TO FUZZY SETS

This section introduces the basic concepts of fuzzy logic by extending and modifying the principles explained for crisp sets.

5.2.1 Introduction to fuzzy sets

As described above, a crisp set is defined by the characteristic function χ_A that takes values of one or zero when an element x respectively belongs or does not belong to the set A. The characteristic function can be generalized (i.e., $\mu_{\hat{A}}$) by assigning real values within the closed interval [0,1]. In this case when the function has a value of zero or one it is reduced to the specific limiting case where it is the characteristic function for crisp set, indicating respectively full non-membership into the set or complete membership. When the function takes any real value between zero and one, it indicates partial degrees of membership of the element x into the set Â. This generalized characteristic function is known as membership function, $\mu_{\hat{A}}$ defined a:

$$\mu_{\hat{A}} : X \rightarrow [0, 1] \qquad \text{where} \qquad x \in X$$

The membership is defined over the closed interval [0,1] and because it can be partial the set is known as Fuzzy set and is denoted by Â. It is important to note that while $\mu(x)_{\hat{A}}$ indicates the membership of the element x into the fuzzy set Â, $\mu(x_i)_R = \mu(x_1, x_2,...,x_n)_R$ represents the crisp membership of an n-tuple into the crisp relation R. Alternatively, a fuzzy set Â is a set of ordered pairs represented as:

$$\hat{A} = \{(x, \mu_{\hat{A}}(x)) | x \in X\}$$

As discussed in the introduction to this chapter, fuzzy sets are helpful to describe vague concepts. However the representation of the concepts in terms of a membership function depends not only on the definition of the concept by itself, but also on the context of the idea. An example of this is given by the idea of "high temperature" which can be interpreted in several contexts. High temperature for a human body is given by $T > 40\ ^{\circ}C$, while high temperature for a chemical process plant could be as high as $900^{\circ}C$. Thus the concept "high temperature" is defined by different membership functions specific for each context.

The difference between a crisp and a fuzzy set is shown in Figure 5.1 where the characteristic functions are plotted. Set A, defined by its characteristic function χ_A, presents well defined boundaries while the fuzzy set Â, defined by its membership function $\mu_{\hat{A}}$, presents a gradual transition between regions of high membership (i.e., $\mu_{\hat{A}}(x) \approx 1$) and regions of low membership (i.e., $\mu_{\hat{A}}(x) \approx 0$) or no membership (i.e., $\mu_{\hat{A}}(x) = 0$).

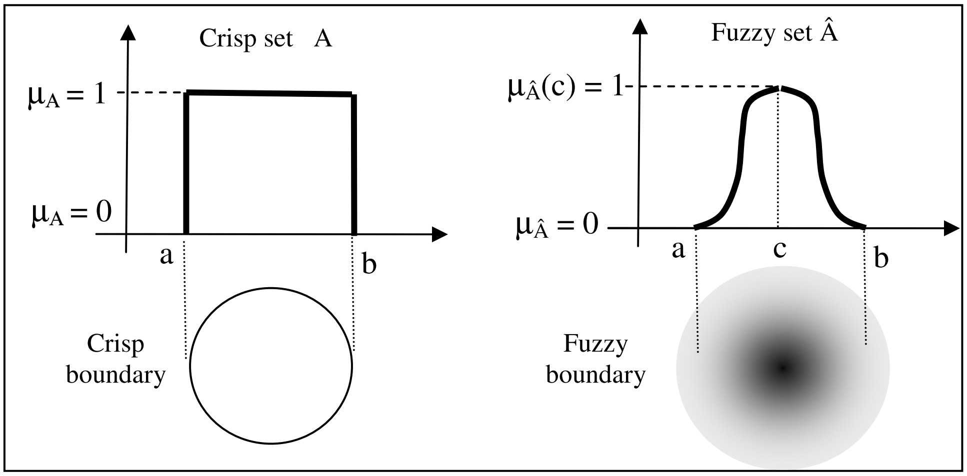


Figure 5.1: Difference between a crisp set and a fuzzy set

Fuzzy sets can be classified in several types, the most common being the ordinary fuzzy sets (also known as Type 1), interval-valued fuzzy sets, and Type 2 fuzzy sets. For ordinary fuzzy sets, the definition is given by the function A: $X \rightarrow [0, 1]$ which assigns a precise membership value to each point on the universe of discourse. As shown in Figure 5.2, for the input x=c the value of the membership function for a fuzzy set Type 1 is exactly $\mu_{\hat{A}}(c)$.

However, when rather than a precise value, the membership of the point varies between an upper and lower value, the membership function can be defined by a family of intervals over the universe of discourse described as A: $X \rightarrow \xi\ [0, 1]$. In Figure 5.2, for a fuzzy set Type 2, for each value x=a, the value of the membership function varies in the closed interval $[\mu_U(a), \mu_L(a)]$. The expressive potential offered by interval-valued and Type 2 fuzzy sets is higher with respect to Type 1 fuzzy sets, nevertheless the computational complexity increases, being highest for Type 2 sets; however the theoretical background for Type 2 fuzzy set is still limited. Type 1 fuzzy sets offer descriptive power and the low degree of computational complexity, therefore are used for this project.

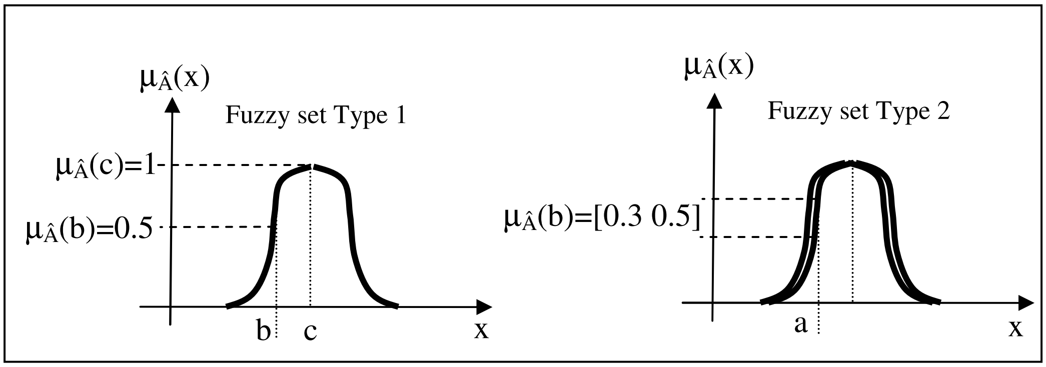


Figure 5.2: Difference between a fuzzy set Type 1 and Type 2

5.2.2 Terminology and basic definitions for fuzzy sets

As defined above, a fuzzy set Â is a set of ordered pairs represented as:

$$Â =\{(x, \mu_{Â}\ (x))| \ x \in X\}$$

where $\mu_{Â}$ (x) are the membership degrees of the elements x within the fuzzy set Â. *X* is the universe of discourse of the set or the numerical range that contains all the possible values taken by the elements x that belong to *X*. The universe of discourse can be classified into three types depending on the type of variable that describes:

- Discrete non-ordered: this universe of discourse is used to model variables formed by unrelated objects or classes. For example, let $X=\{x_1,x_2,x_3\}$={water, steam, heat transfer fluid} and Ŝ=”safe coolant for a specific application” hence, the set of ordered pairs is Ŝ $=\{(x, \mu_{Ŝ}\ (x))| \ x \in X\}$={(water, 0.8), (steam, 0.7), (heat transfer fluid, 0.9)}, where the membership degrees $\mu_{Ŝ}$ (x_i) are assigned according to some subjective expert evaluation.
- Discrete ordered: the modeled variable For example, let $X=\{x_1,x_2,x_3,x_4,x_5,x_6\}=\{0,1,2,3,4,5,6\}$be the number of hazardous chemicals in a plant

and $\hat{S}$ =”number of hazardous chemicals in a low hazard process.” The set of ordered pairs is $\hat{S}=\{(x, \mu_{\hat{S}}(x))| x \in X\}=\{(0, 0.1),(1,0.4),(2,0.7),(3,1.0),(4,0.5),(5,0.2),(6,0.1)\}$, and the membership degrees $\mu_{\hat{S}}(x_i)$ are assigned according to some subjective expert evaluation. An alternative notation for this type of fuzzy set is

$$\hat{S} = \sum_{xi\in X} \mu_A(x_i)/x_i = \mu_A(x_1)/x_1 + \mu_A(x_2)/x_2 + \mu_A(x_3)/x_3 + \ldots + \mu_A(x_n)/x_n$$

It must be noted that the summation symbol symbolizes the union of the discrete membership values, while the division symbol (i.e., /) separates the value of the variable from the value of its membership degree.

- Continuous: For example, let X ={Set of possible ages of human beings} and $\hat{S}$ = “average age of petrochemical operators is about 56 years” The fuzzy set $\hat{S}$ is expressed as $\hat{S} = (x, \mu_{\hat{S}}(x))| x \in X\} = 1/(1+((x-56)/10)^4)$. An alternative notation for this type of fuzzy set is:

$$\hat{S} = \int_X \mu_A(x)/x = \int_X f(x)/x$$

Once again it should be noted that the integral sign symbolizes the union of the membership values and does not indicate a mathematical integration procedure. Similarly, the division symbol (i.e., /) separates the value of the variable from the value of its membership degree and does not indicate mathematical division [Jang et al, 1997].

For this research only continuous universe of discourse are used. The range covered by the universe of discourse X is partitioned into overlapping subranges delimited by the membership function $\mu_{\hat{A}}$, as shown in Figure 5.1. Each membership function defines a fuzzy set and receives a linguistic label (name) that assigns the linguistic value to the set. Therefore, the variable described by fuzzy sets and defined over a specific context-dependent universe of discourse is known as “linguistic variable”. For instance, a continuous variable such as temperature, defined in the context of a living human being, has a universe of discourse between 25 °C (lower survival limit) and 44 °C (upper survival limit). The universe of discourse of the linguistic variable “human body temperature” can be divided into seven fuzzy sets as shown in Figure 5.3, whose linguistic labels (or linguistic values) are “extreme hypothermia”, “severe hypothermia”, “light hypothermia”, ”normal”, “fever”, “hyperthermia”, and “severe hyperthermia”. Each range of abnormal temperature has medical significance and requires different treatment.

Fuzzy sets must present some degree of overlap in order to establish a smooth transition between the partitions of the universe of discourse. Each linguistic variable is characterized by a quintuple (*v, T, X, g, m*) where *v* is the linguistic name of the variable; *T* represents the set of linguistic labels $t \in T$ of the fuzzy sets defined over the range of the universe of discourse *X*; *g* represents syntactic or grammar rules able to generate linguistic terms; and *m* represents semantic rules that assign a meaning (fuzzy set) to each linguistic label *t* [Klir and Yuan, 1995]. From the example shown in Figure 5.3, *v* = “human body temperature”, *T* = {“extreme hypothermia”, “severe hypothermia”, “light hypothermia”, ”normal”, “fever”, “hyperthermia”, “severe hyperthermia”}, *X* = [25 44], *g* generates other linguistic labels such as “high fever” or “very high fever”, and *m* assigns a fuzzy set with a specific shape to each linguistic term $t \in T$.

Each fuzzy set Â is defined over a specific subrange of the universe of discourse and the set of points where the membership function $\mu_{\hat{A}}$ (x) has a value larger than zero is known as support of the fuzzy set:

$$\text{support}(\hat{A}) = \{x \mid \mu_{\hat{A}}(x) > 0\} \quad \text{where } x \in X$$

For example, the support for the fuzzy set “fever” is [38 42] over the centigrade temperature scale. Similarly, the core of a fuzzy set Â occurs where the value of $\mu_{\hat{A}}$ (x) has a value of 1:

$$\text{core}(\hat{A}) = \{x \mid \mu_{\hat{A}}(x) = 1\} \quad \text{where } x \in X$$

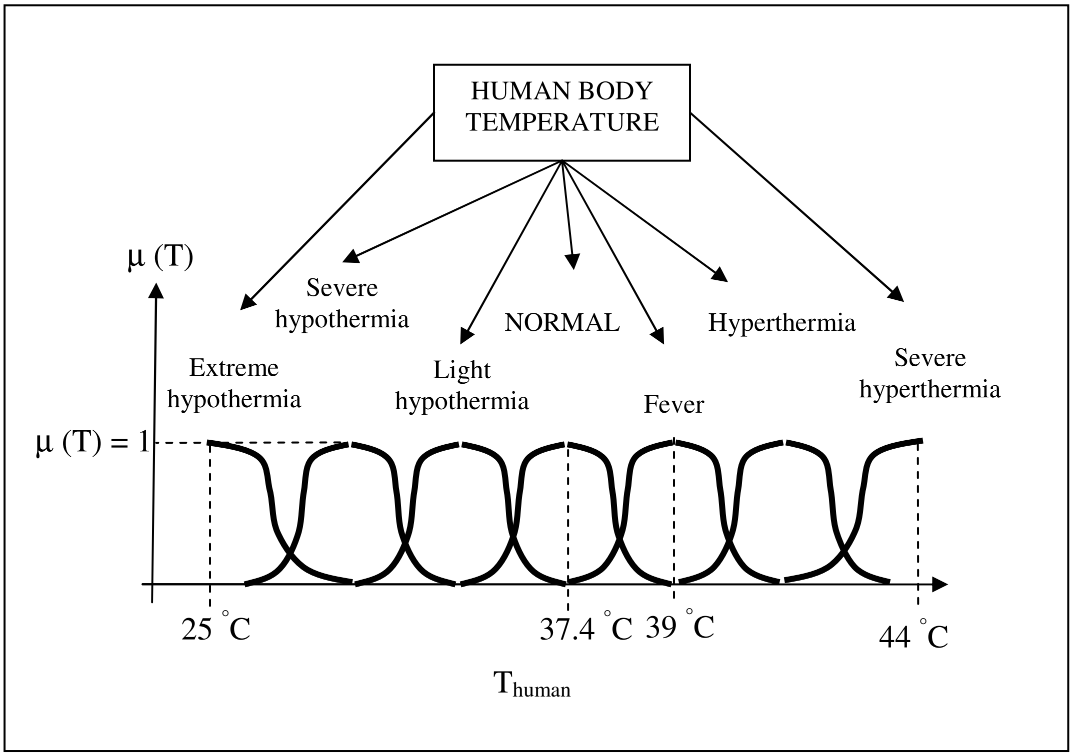


Figure 5.3: Example of linguistic variable (human body temperature) and linguistic values (e.g., extreme hypothermia)

For example, the core for the fuzzy set "fever" is [39] over the centigrade temperature scale while the core for the set "normal" is 37 °C. Depending on the shape of the fuzzy set, the core can be a range (e.g., for a trapezoidal set), a single point (hence the fuzzy set becomes a singleton or a triangular function), or nonexistent (e.g., for a subnormal set).

A singleton is a fuzzy set with a support X containing a single element x (i.e., $X = \{x\}$) with a full membership $\mu_{\hat{A}}(x) = 1$. The height of a fuzzy set is given by the value of the largest membership degree within the set:

$$\text{Height}(\hat{A}) = h(\hat{A}) = \sup \hat{A}\,(x) \quad \text{where} \quad x \in X$$

When a fuzzy set $\hat{A}$ has a Height($\hat{A}$) = 1 or, in other words has a non-empty core (i.e., there is at least one point x where $\mu_{\hat{A}}(x) = 1$), it is known as normal set. When Height($\hat{A}$) < 1 then Core($\hat{A}$) = 0 and the set is known as subnormal. Although a fuzzy set can be defined with maximum membership occurring at any value (e.g., Height($\hat{A}$) = 8), by convention normalized sets are defined based on height values of one. The values x where Height(x) = 0.5 are known as crossover points or equilibrium points and are defined as:

$$\text{crossover}\ (\hat{A}) = \{x|\ \mu_{\hat{A}}\ (x) = 0.5\} \quad \text{where}\ \ x \in X$$

Another property of the crossover point is that the membership value of the set $\hat{A}$ is the same as the membership value of the complement $\overline{\hat{A}}$ (i.e., $\overline{\hat{A}}\ (x) = 1 - \hat{A}(x)$).

When a fuzzy set $\hat{A}$ defined on X is intersected by a horizontal line at Height(x) = α, where $\alpha \in [0,1]$, the part of the set above the line is a crisp set known as strong α-cut, $\hat{A}'_{\alpha}$,and is defined as:

$$\hat{A}'_{\alpha} = \{x|\ \mu_{\hat{A}}\ (x) > \alpha\} \quad \text{where}\ \ x \in X$$

A variant of the strong α-cut occurs when the line $\mu_{\hat{A}}\ (x) = \alpha$ is included into the crisp set, and the α-cut $\hat{A}_{\alpha}$ is defined as:

$$\hat{A}_{\alpha} = \{x|\ \mu_{\hat{A}}\ (x) \geq \alpha\} \quad \text{where}\ \ x \in X$$

By applying the previous definition, the support of a fuzzy set $\hat{A}$ is the same as the strong α-cut set when α=0 (i.e support ($\hat{A}$) = $\hat{A}_{\alpha=0} = \{x|\ \mu_{\hat{A}}\ (x) \geq \alpha = 0\}$ where $x \in X$) while the core of $\hat{A}$ is given by the α-cut when $\alpha = 1$. Both types of α-set follow the inclusion property:

$$\hat{A}_{\alpha=1} \supseteq \hat{A}_{\alpha=2} \supseteq \hat{A}_{\alpha=3} \quad \text{where}\ \ \alpha_1<\alpha_2<\alpha_3$$
$$\hat{A}'_{\alpha=1} \supseteq \hat{A}'_{\alpha=2} \supseteq \hat{A}'_{\alpha=3} \quad \text{where}\ \ \alpha_1<\alpha_2<\alpha_3$$

Another form of this property is given by the following equations:

$$\hat{A}_{\alpha=1} \cap \hat{A}_{\alpha=2} = \hat{A}_{\alpha=2} \text{ and } \hat{A}_{\alpha=1} \cup \hat{A}_{\alpha=2} = \hat{A}_{\alpha=1}$$
$$\hat{A}'_{\alpha=1} \cap \hat{A}'_{\alpha=2} = \hat{A}'_{\alpha=2} \text{ and } \hat{A}'_{\alpha=1} \cup \hat{A}'_{\alpha=2} = \hat{A}'_{\alpha=1}$$

An important requirement of fuzzy set is convexity defined by [Klir and Yuan, 1995]:

$$\mu_{\hat{A}}(\lambda x_1+(1-\lambda)x_2) \geq \min\{\mu_A(x_1), \mu_A(x_2)\}$$

where x_1 and $x_2 \in X$ and $\lambda \in [0,1]$. According to the previous definition, the convex combination (i.e., $(\lambda x_1+(1-\lambda)x_2)$) of any two points x_1 and x_2 that belong to a set Â, should be part of the set. In other words, it is required that each crisp α-set $\hat{A}_\alpha$ is formed by a single line, implying that zones of low membership cannot be located between two zones of high membership. The definition of set convexity is less strict than the definition of convexity for a mathematical function f(x)

$$f(\lambda x_1+(1-\lambda)x_2) \geq \lambda f(x_1)+(1-\lambda)f(x_2)$$

hence a fuzzy set Â can be convex while its membership function $\mu_{\hat{A}}$ could be non convex according to the conventional definition of function convexity.

5.2.3 Relation between fuzzy sets and crisp sets

The concepts of α-cuts ($\hat{A}_\alpha$) and strong α-cuts ($\hat{A}'_\alpha$) introduced above creates a connecting bridge between fuzzy and crisp sets [Klir and Yuan, 1995]. Any fuzzy set Â can be generated either form the family of all α-cuts or strong α-cuts (which are crisp sets) hence the properties of crisp sets are extended to fuzzy sets. When the properties generalized from crisp to fuzzy sets are preserved in all α-cuts $\hat{A}_\alpha$ for $\alpha \in (0,1]$ they are called cutworthy while if they are preserved only in the strong α-cuts $\hat{A}'_\alpha$ for $\alpha \in [0,1]$ they are called strong cutworthy property.

5.2.4 Extension principle

In order to generalize the concept of mathematical function to the fuzzy set domain, the extension principle is applied with the objective of extending the crisp one-to-one mapping to fuzzy sets. According to this principle, when a mathematical function is applied to fuzzy sets, it operates over each element of the set [Klir and Yuan, 1995]. If f is a function mapping the domain of X to Y, and if Â is a fuzzy set defined on X as $\hat{A} = \mu_{\hat{A}}(x_1)/x_1 + \mu_{\hat{A}}(x_2)/x_2 + ... + \mu_{\hat{A}}(x_n)/x_n$ then a fuzzy set Ê defined on Y is the image of Â on Y and is obtained by $\hat{E} = \mu_{\hat{E}}(x_1)/y_1 + \mu_{\hat{E}}(x_2)/y_2 + ... + \mu_{\hat{E}}(x_n)/y_n$ where $v_i = f(x_i)$ for $i = 1...n$. N

When f is a function mapping many-to-one then it is possible that there exist several elements x_i with same image $y_i = f(x_i)$. If for $x_1, x_2 \in X$, $f(x_1) = f(x_2) = y^* \in Y$, then the degree of membership of Ê(y) defined on Y at $y = y^*$ is the same as the highest degree of membership of Â evaluated at $x = x_1$ or $x = x_1$. This is generally indicated as: $\mu_{\hat{E}}(y) = \max \mu_{\hat{E}}(x)$ where $x = f^{-1}(y)$. As an example, if $\hat{A} = 0.1/\text{-}2 + 0.4/\text{-}1 + 0.8/0 + 0.9/1 + 0.3/2$ and $f(x) = x^2 - 3$, then $\hat{E}(y) = 0.1/f(-2) + 0.4/f(-1) + 0.8/f(0) + 0.9/f(1) + 0.3/f(2)$ or $\tilde{N}(y) = 0.1/1 + 0.4/\text{-}2 + 0.8/\text{-}3 + 0.9/\text{-}2 + 0.3/1$. However, after applying the function to the membership degrees of the fuzzy set Â there are two different membership values for values of $y = 1$ and for $y = -2$. In this case the extension principle requires the choice of the highest membership value: $\hat{E}(y) = (0.1 \vee 0.3)/1 + (0.4 \vee 0.9)/\text{-}2 + 0.8/\text{-}3 = 0.8/\text{-}3 + 0.9/\text{-}2 + 0.3/1$.

The extension principle can be applied also to continuous universes and membership functions, however when there is a many-to-one mapping the max operator (i.e., selecting the highest membership value) can cause discontinuities in the resultant membership function over Y. In general, if f is a crisp function $f(x_1, x_2, x_3, ... x_n) = y$ mapping from an n-dimensional Cartesian product $X = X_1 \times X_2 \times ... \times X_n$ to a one-dimensional universe Y, and if $\hat{A}_1 ... \hat{A}_n$ are fuzzy sets defined respectively on $X_1 ... X_n$ then the resultant fuzzy set Ê(y) induced over Y is given by:

$$\mu_{\hat{E}}(y) = \begin{cases} \max\limits_{(x1,\, x2,\ldots,xn)= f^{-1}(y)}[\min(\mu_{\hat{A}}(x_1),\ldots, \mu_{\hat{A}}(x_n)] & \text{if } f^{-1}(y) \neq 0 \text{ otherwise} \\ 0 & \text{if } f^{-1}(y) = 0 \end{cases}$$

In the previous definition the min operator is used because each element of the input vector $(x_1, x_2,\ldots,x_n)$ occurs simultaneously implying an AND operation.

5.3 INTRODUCTION TO BASIC AND STANDARD OPERATIONS FOR FUZZY SETS

The generalization of the classical set operations (i.e., complement, intersection, and union) result in the respective standard fuzzy operations, which behave as their crisp counterpart when the membership functions are restricted to the normalized set of two elements {0,1}. The generalization is possible because the characteristic functions for fuzzy and crisp sets are equivalent. The following definitions apply for fuzzy sets operations:

- Standard fuzzy complement : $\overline{\hat{A}}(x)=1-\hat{A}(x)$ for all $x \in X$
- Standard fuzzy union of two sets Â and Ê: $(\hat{A} \cup \hat{E})(x) = \max[\hat{A}(x), \hat{E}(x)]$ for all $x \in X$
- Standard fuzzy intersection of two sets Â and Ê: $(\hat{A} \cap \hat{E})(x) = \min[\hat{A}(x), \hat{E}(x)]$ for all $x \in X$

The standard fuzzy intersection is represented by the logical AND and modeled by the min operator; the standard fuzzy union is represented by the logic OR and modeled by the max operator. However, contrary to the classical set operations, in the case of fuzzy sets the definitions of the operations are context-dependent and several functions for each fuzzy operation can qualify as a generalization of the related classical operation. The definition of the operations depends on its empirical justification based on intuitive arguments or axiomatic concepts. The family of definitions for fuzzy intersection is known as t-norms (triangular norms) while the family of functions for a fuzzy union is known as t-conorms or s-norms. In spite of the variety of functions, the standard definitions offer attractive properties being the only operations that follow the cutworthy and strong cutworthy properties [Klir and Yuan, 1995].

5.3.1 Fuzzy complement

If $\hat{A}$ is a fuzzy set for all $x \in X$, then $\mu_{\hat{A}}(x)$ indicates the degree to which each element x belongs to the set $\hat{A}$. If c is a complement function and is applied to $\hat{A}$, then $c\hat{A}$ is the type c complement of $\hat{A}$, and $\mu_{c\hat{A}}(x)$ indicates the membership degree of x into the complement set $c\hat{A}$. Alternatively, $\mu_{c\hat{A}}(x)$ indicates how much x does not belong to $\hat{A}$, while $\mu_{\hat{A}}(x)$ indicates how much x does not belong to the set $c\hat{A}$. The complement operator c is a continuous function $c: [0,1] \rightarrow [0,1]$ that for each element x in $\hat{A}$ with membership degree $\mu_{\hat{A}}(x)$ assigns a new membership degree $\mu_{c\,\hat{A}}(x)$ on the set $c\hat{A}$ (i.e., $c(\mu_{\hat{A}}(x)) = \mu_{c\hat{A}}(x)$).

5.3.2 Introduction to the triangular norms

The concept of triangular norms was developed from the theory of probabilistic metric spaces by Menger in 1942 as cited by Pedrycz and Gomide (1998) and then developed by several mathematicians during the decade of the ‘80s and early ‘90s. When applied to fuzzy logic, triangular norms form the basis for the general classes of fuzzy sets operations for intersection and union. A triangular norm, known as t-norm, is a binary operation defined by $t: [0,1]^2 \rightarrow [0,1]$ and that satisfies the following requirements:

i. Monotonicity: for $x \leq y$ and $w \leq z$ then $x\,t\,w \leq y\,t\,z$

ii. Commutativity: $x\,t\,y = y\,t\,x$

iii. Associativity: $x\,t\,(y\,t\,z) = (x\,t\,y)\,t\,z$

iv. Boundary conditions: $(0\,t\,1) = 0$ and $(1\,t\,x) = x$

Another construct associated with the triangular norm, is the triangular co-norm, known as s-norm, which is a binary operation defined by $s: [0,1]^2 \rightarrow [0,1]$ and that satisfies the following requirements:

i. Monotonicity: for $x \leq y$ and $w \leq z$ then $x\, s\, w \leq y\, s\, z$

ii. Commutativity: $x\, s\, y = y\, s\, x$

iii. Associativity: $x\, s\, (y\, s\, z) = (x\, s\, y)\, s\, z$

iv. Boundary conditions: $(0\, s 1) = 1$ and $(1\, s\, x) = 1$

From the properties of t-norms and s-norms it is clear that the standard fuzzy intersection operator, defined by the min operator, is a t-norm while the standard fuzzy union operation, defined by the max operator, is a s-norm. t-norms and s-norms are related by the fact that:

$$x\, s\, y = 1-(1-x)\, t\, (1-y) \quad \text{and} \quad x\, t\, y = 1-(1-x)\, s\, (1-y)$$

and when rewritten as:

$$1-(x\, s\, y) = (1-x)\, t\, (1-y) \quad \text{and} \quad 1-(x\, t\, y) = (1-x)\, s\, (1-y)$$

the relations are recognized as the De Morgan's laws which are followed by fuzzy sets in the form of the standard fuzzy complement (i.e $\overline{\hat{A}}(x) = 1-\hat{A}(x)$) which is involutive, because the complement of the complement of a fuzzy set Â is the original set Pedrycz and Gomide (1998).

5.3.3 Fuzzy intersections: t-norms

If Â is a fuzzy set for all $x \in X$, then $\mu_{\hat{A}}(x)$ indicates the degree to which each element x belongs to the set Â. If Ê is a fuzzy set for all $x \in X$, then $\mu_{\hat{E}}(x)$ indicates the degree to which each element x belongs to the set Ê. The intersection of the two fuzzy sets Â and Ê is defined by a function $i: [0,1]x[0,1] \rightarrow [0,1]$ that for each element $x \in X$

takes the degrees of membership $\mu_{\hat{A}}$ (x) and $\mu_{\hat{E}}$ (x) and assigns a new degree of membership $\mu_{\hat{A} \cap \hat{E}}$ (x) into the set ($\hat{A} \cap \hat{E}$), or in other words:

$$(\hat{A} \cap \hat{E})(x) = i[(\mu_{\hat{A}}(x) \cap \mu_{\hat{E}}(x)] = \mu_{\hat{A} \cap \hat{E}}(x)$$

As in the case of the fuzzy complement, the functions for the fuzzy intersection must follow specific intuitive axioms in order to produce meaningful results. One of the most studied functions for fuzzy intersection is known as t-norm and has been accepted as equivalent to the class of fuzzy intersection. As mentioned previously only the membership values simplified as $\mu_{\hat{A}}(x) = a$ and $\mu_{\hat{E}}(x) = n$ where $a,b,n \in [0,1]$ will be used. The axioms for fuzzy intersection are the following:

i. Boundary conditions: $i(a,1) = a$
ii. Monotonicity: for all $a,b,d \in [0,1]$, if $b \leq d$ then $i(a,b) \leq i(a,d)$
iii. Commutativity: $i(a,b) = i(b,a)$
iv. Associativity: $i(a,i(b,d)) = i(i(a,b),d)$
v. Continuity: i is a continuous function
vi. Subidempotency: $i(a,a) < a$
vii. Strict monotonicity: $a_1 < a_2$ and $b_1 < b_2$ then $i(a_1,b_1) < i(a_2,b_2)$

The first four axioms (i.e., (i) to (iv)) are known as the "axiomatic skeleton for fuzzy intersections/t-norms". These axioms require that when the sets are crisp their intersection follows the classical definitions: $i(0,1) = 0$ and $i(1,1) = 1$ are implied by axiom (i). When the degree of membership of either fuzzy set $\hat{A}$ or $\hat{E}$ increase, the result of the intersection of both sets cannot increase as indicated by axiom (ii) requires that $i(0,0) = 0$ and axiom (iii) that requires that $i(1,0) = 0$. Additionally, the commutativity axiom ensures that intersection is a symmetric operation hence independent on the combination order of the sets. Intuitively the intersection, when one of the elements shows full membership, should be equal to the other membership value. When the intersection operation occurs over more than two sets, axiom (iv) ensures that the operation can be performed by pairwise grouping in any order. This axiom allows performing the intersection of several fuzzy sets in a recursive form.

Axioms (v), (vi), and (vii) reduce the class of fuzzy intersection (t-norms) by setting additional requirements. Axiom (v) avoids discontinuities by ensuring that the result of the fuzzy intersection is not strongly affected by small variations in the membership degree of either one of the pair of fuzzy sets being intersected. Axiom (vi) is a weaker requirement compared to idempotency (i.e., i(a,a) = a) hence it is called subidempotency and implies that the intersection of two sets with the same membership degree cannot exceed that value. A stronger requirement for monotonicity is expressed by axiom (vii).

The standard fuzzy intersection is the only idempotent t-norm (i.e., i(a,a) = a). Other commonly used t-norms for fuzzy intersections are [Klir and Yuan, 1995]:

- Standard intersection: $i(a,b) = \min(a,b)$
- Algebraic product: $i(a,b) = ab$
- Bounded difference: $i(a,b) = \max(0,a+b-1)$
- Drastic product: $i(a,b) = \begin{cases} a & \text{if } b = 1 \\ b & \text{if } a = 1 \\ 0 & \text{otherwise} \end{cases}$

Triangular norms cannot be linearly ordered, however fuzzy intersection t-norms are bounded between the drastic product and the min operator which is the standard definition for fuzzy intersection [Klir and Yuan, 1995]:

$$i_{\min}(a,b) \le \max(0,a+b-1) \le ab \le \min(a,b) \text{ for all } a,b \in [0,1].$$

In order to give the flexibility to adapt to different contexts, authors have developed parameterized families of t-norms. An example of this is the intersection operator proposed by Yager and defined by Klir and Yuan (1995). Other classes of parameterized functions for the fuzzy intersection have been reported in the literature and for additional information the reader is referred to Zimmerman (1996) and Klir and Yuan (1995). The latter reference includes a discussion on increasing and decreasing generators for the construction of t-norms. It is important to recognize that although there exist several classes of operators for the fuzzy intersection, when the membership degrees are restricted to the range [0,1] they perform exactly in the same or similar form as for instance the algebraic product and the min-operator.

5.3.4 Fuzzy unions: t-conorms or s-norms

If $\hat{A}$ is a fuzzy set for all $x \in X$, then $\mu_{\hat{A}}(x)$ indicates the degree to which each element x belongs to the set $\hat{A}$, while for all $x \in X$, $\mu_{\hat{E}}(x)$ indicates the degree to which each element x belongs to the fuzzy set $\hat{E}$. The union of the two fuzzy sets $\hat{A}$ and $\hat{E}$ is defined by a function u: $[0,1]x[0,1] \rightarrow [0,1]$ that for each element $x \in X$ takes the degrees of membership $\mu_{\hat{A}}(x)$ and $\mu_{\hat{E}}(x)$ and assigns a new degree of membership $\mu_{\hat{A} \cup \tilde{N}}(x)$ into the set $(\hat{A} \cup \hat{E})$, or in other words:

$$(\hat{A} \cup \hat{E})(x) = u[(\mu_{\hat{A}}(x) \cup \mu_{\tilde{N}}(x)] = \mu_{\hat{A} \cup \tilde{N}}(x)$$

As in the previous case axioms for the fuzzy union must be satisfied in order to guarantee meaningful results and t-conorms or s-norms u are used to model fuzzy union. The fuzzy union is a binary operation on the unit interval [0,1] that satisfies the following axioms for the membership values $\mu_{\hat{A}}(x) = a$ and $\mu_{\hat{E}}(x) = n$ where $a, b, n \in [0,1]$:

i. Boundary conditions: $u(a,0) = a$
ii. Monotonicity: for all $a,b,d \in [0,1]$, if $b \leq d$ then $u(a,b) \leq u(a,d)$
iii. Commutativity: $u(a,b) = u(b,a)$
iv. Associativity: $u(a,u(b,d)) = u(u(a,b),d)$
v. Continuity: u is a continuos function
vi. Superidempotency: $u(a,a) > a$
vii. Strict monotonicity: $a_1 < a_2$ and $b_1 < b_2$ then $u(a_1,b_1) < u(a_2,b_2)$

Axioms (i) to (iv) are known as the axiomatic skeleton for fuzzy unions/t-conorms, and when compared with the axiomatic skeleton for fuzzy intersection it is clear that the only difference is in the boundary condition (i.e., for fuzzy intersection i(a,1) = 1). Axioms (i) to (iii) require that the fuzzy union is reduced to the classical set union when the sets A and N are crisp (i.e., u(0,0) = 0, u(0,1) = u(1,0) = 0, and u(1,1) = 1). Axioms (v) to (vi) are analogous to the axioms for fuzzy intersection except by the requirement of superidempotency rather than subidempotency as in the case for intersection [Klir and Yuan, 1995]. Examples of t-conorms commonly used for fuzzy intersection are the following; however, the only idempotent t-conorm is the standard fuzzy union (i.e., u(a,a) = a):

- Standard intersection: $u(a,b) = \max(a,b)$
- Algebraic sum: $u(a,b) = a + b - ab$
- Bounded sum: $u(a,b) = \min(1, a + b)$
- Drastic union: $u(a,b) = \begin{cases} a & \text{if } b = 0 \\ b & \text{if } a = 0 \\ 1 & \text{otherwise} \end{cases}$

5.3.5 Aggregations operations

When several fuzzy sets must be combined into one single set, aggregation operators are used. An example of the problem is the calculation of the overall performance of a student expressed in terms of percentages by aggregating the grades obtained in three courses, expressed in terms of linguistic labels such as very high, high, average, low, and very low.

The aggregation of n fuzzy sets $\hat{A}_1$, $\hat{A}_2$... $\hat{A}_i$... $\hat{A}_n$, where $n \geq 2$ and each fuzzy set $\hat{A}_i$ is defined over *X*, is expressed by the function $h;[0,1]^n \rightarrow [0,1]$ that operates over the membership degrees of each set for each $x \in X$. In other words the aggregated set $\hat{A}$ is obtained by:

$$\hat{A} = h(\hat{A}_1(x), \hat{A}_2(x),\ldots \hat{A}_i(x)\ldots \hat{A}_n(x)) \quad \text{for } x \in X$$

As for the fuzzy intersection and fuzzy union, the aggregation operations must satisfy specific axioms that guarantee meaningful results [Klir and Yuan, 1995]:

i. Boundary conditions: $h(0,0,...,0) = 0$ and $h(1,1,...,1) = 1$

ii. Monotonicity: For any pair $(a_1, a_2,..., a_n)$ and $(b_1, b_2,..., b_n)$ of n-tuples such that $a_i,b_i \in [0,1]$ for all $I \in N_n$ if $a_i \leq b_i$ for all $i \in N_n$ then $h(a_1, a_2,..., a_n) \leq h(b_1, b_2,..., b_n)$

iii. Continuity: h is a continuous function

iv. Symmetricity: $h(a_1, a_2,..., a_n) = h(a_{p(1)}, a_{p(1)},..., a_{p(n)})$ where p(i) indicates any permutation p on N_n.

v. Idempotency: $h(a,a,...a) = a$ for all $a \in [0,1]$

Axiom (ii) indicates that the aggregation function h is monotonically increasing in all the arguments; axiom (iv) indicates that h is symmetric in all its arguments or, in other words, that all the arguments are equally important. When equal fuzzy sets are aggregated the result should be the same set, as indicated by axiom (v) as well as by axiom (i).

Fuzzy intersection and fuzzy union functions are aggregation operations, and despite they fact they have been defined only for two arguments, their associativity property allows the expansion to any number of arguments, hence qualifying the t-norms and t-conorms as aggregation operators. However, only the standard min and max operations follow the idempotency axioms for aggregations. It is important to note that any aggregation function h that follows axioms (ii) and (v) satisfies the following inequality for all n-tuples $\langle a_1, a_2,...,a_n \rangle$, $a_i \in [0,1]^n$:

$$\min(a_1, a_2,...,a_n) \leq h(a_1, a_2,...,a_n) \leq \max(a_1, a_2,...,a_n)$$

If the previous inequality is not violated, by axiom (v) the following is also satisfied:

$$a = \min(a,a,...,a) \leq h(a,a,...,a) \leq \max(a,a,...,a) = a$$

implying that aggregation operators h constrained between the standard fuzzy intersection (i.e., min) and the standard fuzzy union (i.e., max) are idempotent and they are known as Averaging Operators. Two classes of Averaging Operators are the Generalized Means and the Ordered Weighted Averaging Operations [Klir and Yuan, 1995]. The Generalized means operators are defined by:

$$h_\alpha(a_1, a_2,...,a_n) = [(a_1^\alpha + a_2^\alpha +,...,+ a_n^\alpha)/n]^{1/\alpha}$$

When α= -1 the aggregation function is known as Harmonic Mean while when $\alpha = 1$ the function becomes the arithmetic mean:

$$\alpha = -1 \qquad h_{-1}(a_1, a_2,...,a_n) = [n/(1/a_1 + 1/a_2 +,...,+ 1/a_n)]$$

$$\alpha = 1 \qquad h_1(a_1, a_2,...,a_n) = (a_1 + a_2 +...+ a_n)/n$$

When $\alpha \to 0$ the aggregation function becomes the Geometric Mean, and if $\alpha \to -\infty$ or $\alpha \to +\infty$ the aggregation function respectively becomes the Minimum or Maximum aggregator:

$$\alpha \to -\infty \qquad h_{-\infty} (a_1, a_2,...,a_n) = \min(a_1, a_2,...,a_n)$$

$$\alpha \to 0 \qquad h_0(a_1, a_2,...,a_n) = (a_1 + a_2+...+a_n)^{1/n}$$

$$\alpha \to +\infty \qquad h_{+\infty} (a_1, a_2,...,a_n)= \max(a_1, a_2,...,a_n)$$

The Ordered Weighted Averaging operators (known as OWA) are defined by the following function:

$$h_w(a_1, a_2,...,a_n) = w_1b_1 + w_2b_2 +,...,+ w_nb_n = \sum_{i=1}^{n} w_ib_i$$

$$\mathbf{w} = \langle\ w_1, w_2,...,w_n\ \rangle \text{ where } w_i \in [0,1]^n \text{ for all } i \in N_n \quad \text{and} \quad \sum_{i=1}^{n} w_i = 1$$

where **w** is the weighting vector. This function requires the sorting of the element a_i in a decreasing order. After the sorting is performed, $\langle b_1, b_2,...,b_n \rangle$ is a permutation vector of $\langle a_1, a_2,...,a_n \rangle$ where $b_i \in [0,1]^n$ for all $i \in N_n$ represents the i^{th} largest element in such a way that $b_i \geq b_j$ when $i < j$. This operator satisfies axioms (i) through (v) and the upper (h_w^*) and lower (h_{w*}) bounds are given by the max and min operators:

$$h_{w*}(a_1, a_2,...,a_n) = \min(a_1, a_2,...,a_n) \quad \text{where} \quad \mathbf{w}_* = \langle w_1, w_2,...,w_n \rangle = \langle 0,0,...,1 \rangle$$

$$h_w^*(a_1, a_2,...,a_n) = \max(a_1, a_2,...,a_n) \quad \text{where} \quad \mathbf{w}^* = \langle w_1, w_2,...,w_n \rangle = \langle 1,0,...,0 \rangle$$

If the weight vector $\mathbf{w} = \langle 1/n, 1/n,...,1/n \rangle$ the operator h_w becomes the arithmetic mean. It is clear that by varying the values of the weights in the vector **w** between $\mathbf{w}_*$ and $\mathbf{w}^*$, it is possible to cover the range of aggregation bounded by the max and min aggregation operators [Klir and Yuan, 1995].

Other aggregation functions have been proposed; however, the selection of a specific aggregation function must be based on the characteristics of the problem and the requirements of the model. Hence, the selection of aggregation operation is context dependent and it is helpful to follow the following criteria [Klir and Yuan, 1995]:

1) Axiomatic strength: when two operators show similar performance, the one that should be selected is the one that is less limited by the axioms and properties that must satisfy.
2) Empirical fit: besides the mathematical requirements, the chosen operator must be able to model the behavior of the system that is being analyzed. Empirical testing is required in order to check the criterion.
3) Adaptability: since every context and application is different a large number of operators should be used. Another possible approach is the utilization of adaptable parameterized operators able to model different situations by modifying the value of the parameter. For example, the max and min operators

are not adaptable but they are attractive in specific problems due to their mathematical simplicity.

4) Numerical efficiency: operator's mathematical complexity becomes important for large problems and the least mathematically complex operator able to model the problem should be used. While fuzzy max and min are numerically efficient, they are not adaptable and can only be applied in specific contexts.

5) Compensation: if an aggregation operation is defined as: $\mu_{agg}(x_k) = f(\mu_{\hat{A}}(x_k), \mu_{\hat{E}}(x_k)) = k$ then the operator defined by the function f is compensatory when the result k can be obtained by modifying the value of $\mu_{\hat{E}}(x_k)$ when the value $\mu_{\hat{A}}(x_k)$. In other words low membership in one set is compensated by higher membership in the other set. The min-operator does not follow this criterion while the product does.

6) Range of condensation: when the range of compensation is large the operator should be preferred. For instance, the range of compensation for the product operator spans the complete interval (0, 1).

7) Aggregating behavior: when normal or subnormal fuzzy set are aggregated the result is a function of the number of aggregated sets. For example, when several sets are aggregated by using the product-operator, the resultant aggregate membership degree tends to be reduced.

8) Required scale level of membership functions: the scale type (i.e., nominal, interval, and ratio) selected for the design of the fuzzy sets to be aggregated restricts the type of operator that can be used. For example, while the min-operator can be used with ordinal scales, the product-operator cannot. When an operator can be applied to low-level scales (i.e., nominal) it is preferable over operators that require higher scale level (i.e., absolute, ratio).

5.4 INTRODUCTION TO FUZZY RELATIONS

As explained previously for conventional set theory, a crisp relation expresses the existence or lack of a specific relation between the elements of two crisp sets. Since the definition of a fuzzy set is the generalization of a crisp set, the definition of a fuzzy relation can be seen as the generalization of the definition of a crisp relation. The total/null association of elements in a crisp relation is generalized by a degree of association, which indicates the strength of the relation. When there is full or null association the fuzzy relation is reduced to the crisp case [Klir and Yuan, 1997].

While for the crisp relation the boundaries are well defined, in the case of a fuzzy relation the boundaries are vague due to the smooth transitions between regions of full membership (i.e., full relations among X and Y) and areas of null membership. When fuzzy relations occur among fuzzy sets, the result is a fuzzy set on a multidimensional space. The fuzzy relation among two fuzzy sets (i.e., age and height) is given by a 2-dimension fuzzy set on a Cartesian product space.

5.4.1 Definitions

The membership function for fuzzy sets is similar to the characteristic function for crisp sets in the sense that it allows degrees of membership. Similarly, in the case of fuzzy relations, the characteristic function of a crisp relation is expanded to allow degrees of association among the element of the fuzzy sets. The crisp relation R, between all the possible combination of elements $x_1 \in X_1$, $x_2 \in X_2,...,x_n \in X_n$ that belong to the relation defined on the Cartesian product $R = X_1 \text{ x } X_2 \text{ x...x } X_n$ is defined by a characteristic function that describes whether an element $(x_1, x_2,...,x_n)$ (i.e., n-tuple) belongs to R or not:

$$\mu_R(x_1, x_2,...,x_n) = \begin{cases} 1 & \text{if and only if } (x_1, x_2,...,x_n) \in R \\ 0 & \text{otherwise} \end{cases}$$

When the membership of a tuple is one (i.e., $\mu_R(x_1, x_2,...,x_n) = 1$) the elements $x_1, x_2,...,x_n$ are mutually related. When instead of a total/null relationship, degrees of relation are allowed between the elements of the n-tuple, the characteristic function for a crisp relation becomes a membership function for a fuzzy relation:

$$\mu_{\hat{R}}(x_1, x_2,...,x_n) = [0, 1] \text{ if } (x_1, x_2,...,x_n) \in \hat{R}$$

A binary fuzzy relation, is a subset of a Cartesian product X x Y. If X and Y are two crisp sets, the fuzzy relation $\hat{R}$ among all possible ordered pairs of elements $(x, y) \in X \times Y$, where $x \in X$ and $y \in Y$, is given by:

$$\hat{R} = \{(x, y), \mu_{\hat{R}}(x, y) | (x, y) \in X \times Y\} \quad \text{and} \quad \mu_{\hat{R}}\, x, y)=[0,1]$$

When for all possible ordered pairs of elements $(x, y) \in X \times Y$, the relation values are {0,1}, then the fuzzy relations becomes a crisp relation where no partial membership is allowed [Zimmerman 1996; Klir and Yuan,1995]. A fuzzy relation established among elements of crisp sets can be expressed as a matrix, called fuzzy matrix.

If $X = \{x_1, x_2,...,x_n\}$ and $Y = \{y_1, y_2,...,y_m\}$, the binary fuzzy relation $\hat{R} = \{(x, y), \mu_{\hat{R}}(x, y) | (x, y) \in X \times Y\}$ can be expressed as:

$$\hat{R} = \begin{array}{c|ccccc|} & y_1 & y_2 & & y_{m-1} & y_m \\ x_1 & \mu_{\hat{R}}(x_1, y_1) & \mu_{\hat{R}}(x_1, y_2) & \cdots & \mu_{\hat{R}}(x_1, y_{n-1}) & \mu_{\hat{R}}(x_1, y_m) \\ x_2 & \mu_{\hat{R}}(x_2, y_1) & \mu_{\hat{R}}(x_1, y_2) & \cdots & \mu_{\hat{R}}(x_2, y_{n-1}) & \mu_{\hat{R}}(x_2, y_m) \\ & \cdots & \cdots & & \cdots & \cdots \\ x_n & \mu_{\hat{R}}(x_1, y_1) & \mu_{\hat{R}}(x_1, y_2) & \cdots & \mu_{\hat{R}}(x_{n-1}, y_{n-1}) & \mu_{\hat{R}}(x_n, y_m) \end{array}$$

where the value of $\mu_{\hat{R}}(x_n, y_m) = [0,1]$. An example of this type of fuzzy relations can be established about the distances existing between two sets of cities in two states. If $X = \{x_1, x_2, x_3\}$ = "cities in New York State" and $Y = \{ y_1, y_2, y_3\}$ = "cities in New Jersey"; the fuzzy relation $\hat{R}$ represents the distance between each pair of cities describing the concept of "closeness". If the distance between x_1 and y_2 is very short then it is implied that the two cities are "very close" hence the pair has full membership in the fuzzy set represented by the relation $\hat{R}$, or in other words $\mu_{\hat{R}}(x_1, y_1) = 1$. If x_x is very far away from y_3 then the membership into the relation $\hat{R}$ is low and $\mu_{\hat{R}}(x_2, y_3) = 0.1$. When the membership degrees are representing the degree of "closeness", they are assigned to all the n x m pairs, the resulting fuzzy relation, expressed as a fuzzy matrix is:

$$\hat{R} = \begin{pmatrix} 1 & 0.6 & 0.3 \\ 0.4 & 0.9 & 0.1 \\ 0.5 & 0.2 & 0.7 \end{pmatrix}$$

The fuzzy relation can be reduced to a crisp relation R if the concept "close" is related to a physical measure such as 100 km. In this case when the distance among a pair of cities (x_n, y_m) is larger than the threshold the membership value into the relation becomes zero (i.e., $\mu_{\hat{R}}(x_n, y_m) = 0$) since they are assumed to be farther away than the distance that can be assumed to be short enough to be classified as "close". When the distance is shorter than 100 km, then $\mu_R(x_n, y_m) = 1$ indicating a full membership in the crisp set 'close". In this case the relation is expressed in terms of a binary matrix as follows [Tanaka, 1996]:

$$R = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Fuzzy relations can also be established between fuzzy sets. If $X,Y \in \hat{R}$ and two fuzzy numbers are defined as:

$$\hat{A} = \{(x, \mu_{\hat{A}}(x)) \mid x \in X\} \quad \text{and} \quad \hat{E} = \{(x, \mu_{\hat{E}}(y)) \mid y \in Y\}$$

Then the fuzzy relation $\hat{R}$ is defined as:

$$\hat{R} =\{[(x, y), \mu_{\hat{R}}(x, y)] \mid (x, y) \in X \text{ x } Y\} \quad \text{and} \quad \mu_{\hat{R}}(x, y)=[0,1]$$

When $\mu_{\hat{R}}(x, y) \leq \mu_{\hat{A}}(x) \quad \forall(x,y) \in X \text{ x } Y$

$\mu_{\hat{R}}(x, y) \leq \mu_{\hat{E}}(y) \quad \forall (x,y) \in X \text{ x } Y$

and an additional requirement is: $\mu_{\hat{R}}(x, y) \leq \min\{\mu_{\hat{A}}(x), \mu_{\hat{E}}(y)\} \quad \forall (x,y) \in X \text{ x } Y$

The conditions required for fuzzy relations ensure that the degree of membership of the relation $\mu_{\hat{R}}(x,y)$ is not larger that the membership in each single set $\mu_{\hat{A}}(x)$ and $\mu_{\hat{E}}(y)$ [Zimmerman, 1996]. Because fuzzy relations are multidimensional fuzzy sets on a product space, the set and algebraic operations can be applied in a similar form. If $\hat{R}$ and $\hat{O}$ are two fuzzy relations on the same product space, then the fuzzy union (i.e., $\hat{R} \cup \hat{O}$) and fuzzy intersection (i.e., $\hat{R} \cap \hat{O}$) operation are defined as [Zimmerman, 1996]:

$$\mu_{\hat{R} \cup \hat{O}}(x, y) = \max\{\mu_{\hat{R}}(x, y), \mu_{\hat{O}}(x, y)\} \quad \text{where } (x, y) \in X \text{ x } Y$$

$$\mu_{\hat{R} \cap \hat{O}}(x, y) = \min\{\mu_{\hat{R}}(x, y), \mu_{\hat{O}}(x, y)\} \quad \text{where } (x, y) \in X \text{ x } Y$$

CHAPTER VI

INTRODUCTION TO FUZZY SYSTEMS DESIGN

Fuzzy logic and fuzzy systems have been applied to a variety of scientific areas. The first practical applications are attributed to process control and civil engineering during the late ‘70s and early ‘80s. E.H. Mamdani developed the first application for process control and the model he created was named after him and was the first fuzzy logic controller used during the 1980s. The Takagi-Sugeno-Kang (TSK) model was developed by T. Takagi, M. Sugeno, around 1985 and K.T. Kang later, and since the 1990s has been used particularly for control applications [Tanaka, 1997]. Since then, other disciplines became aware of the fuzzy logic approach. In safety management, fuzzy logic has been applied to reliability engineering [Bowles, 1995], environmental impact evaluation and ecotoxicology [Stoms et al, 2002; Friederichs et al, 1996], and transportation risk analysis [Bonvicini et al, 1998; Gentile et al, 2002].

The application of fuzzy modeling is relatively new, but the foundations are already well established. This chapter introduces the basic ideas and concepts of fuzzy modeling required for the development of the hierarchical model for the evaluation of inherent safety, described in Chapters VII and VIII.

6.1 OVERVIEW OF FUZZY MODELING

In order to understand the purpose of this work it is helpful to establish an analogy between traditional mathematical and statistical modeling procedures with similar methodology for fuzzy systems.

A traditional model is constituted of a set of mathematical equations that describe the behavior and interaction of its independent variables. When the equation is solved, the dependent variables are assigned numbers, which are the solution of the equation. If the model is built from physical principles, a mathematical equation or set of equations is obtained, which are then tested against real experimental data. In traditional mathematics, when enough data is available a regression model can be fitted by using a statistical approach to fit a correlation.

In fuzzy logic, the equivalent of the traditional independent variables, are fuzzy sets defined for specific linguistic variables. Each fuzzy set is combined to the fuzzy sets of the other variables by IF-THEN rules that describe the relation existing between the sets. Procedures for fuzzy modeling can be classified in a similar way as for traditional models.

When enough data is available, it is possible to use fuzzy neural networks such as ANFIS (Adaptive Neural Fuzzy Inference System) [Yen and Langari, 1999] to generate membership functions and fuzzy IF-THEN rules, which constitute the fuzzy model. This procedure is analogous to statistical regression. When ANFIS is used, the interpretability of the model can be lost because rules and fuzzy sets are designed for a specific set of data. In order to generate general models it is then required to obtain a data set representative of a large number of situations. In the case of process safety, this type of generalization may not be possible.

If data that are available is insufficient, ANFIS cannot be used and the membership functions and IF-THEN rules must be designed from the underlying physical principles of the system. This is analogous to traditional mathematical modeling, but instead of obtaining an equation, the fuzzy model is formed by fuzzy sets and IF-THEN rules.

A third type of fuzzy modeling does not require fuzzy IF-THEN rules and works in a more abstract mathematical level using the theory of fuzzy relational equations. While for linguistic models the fuzzy relation is given by rules and fuzzy sets, for relational models the fuzzy relation is expressed in terms of a fuzzy matrix. However, the linguistic meaning of fuzzy matrices is not explicit; therefore relational models are more abstract and less interpretable than linguistic models. A methodology to extract fuzzy IF-THEN rules from relational models has been proposed by Campello and Amaral (2001).

The fuzzy modeling methodology used for this research is based on linguistic modeling; therefore fuzzy sets and rules are built by identifying physical principles of the selected linguistic variables. The choice is based on the fact that for inherent safety modeling there is a general lack of data, but a large amount of information and empirical knowledge can be used to build the system.

6.1.1 Computing with words

As indicated by Zadeh (1996) fuzzy logic is a methodology that allows computing with words and no other modeling method offers such flexibility. The basic concept upon which "computing with words" is based is the "granule" that groups points that have similar features; in other words a granule is a fuzzy set. A granule can be atomic (e.g., safe) or composite (e.g., very safe) and is represented by a word which is a fuzzy constraint on the variable. For example, for the proposition "Mary is young" the word "young" represents a granule that groups certain ranges of ages and act as a fuzzy constraint (i.e., fuzzy set) on the linguistic variable "age".

When there are several propositions expressed in terms of IF-THEN rules, as for example:

IF X is small THEN Y is small
IF X is medium THEN Y is large
IF X is large THEN Y is small

the rules describe a function f: $U \rightarrow\in V$, $X \in U$, $Y\in V$. The function f is approximated by the fuzzy graph f^*:

$$f^* = \text{small x small + medium x large + large x small}$$

where the symbols x and + indicate disjunction and Cartesian product (introduced in Chapter V). For example, if A and B are two words, then the expression AxB represents a Cartesian granule (shown as gray rectangles in Figure 6.1), therefore the fuzzy graph f

*can be understood as a disjunction of Cartesian granules. In other words, a fuzzy graph f^* is an approximation of a function or relation f as shown in Figure 6.1.

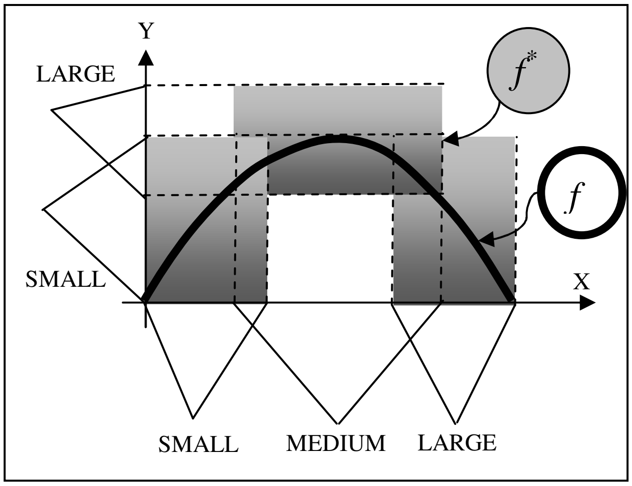


Figure 6.1: Unknown function f approximated by a fuzzy graph f^* built from the linguistic granules of the linguistic variables X and Y.

Computing with words is defined by Zadeh (1996) as "…a necessity when the available information is too imprecise to justify the use of numbers, and when there is a tolerance for imprecision which can be exploited to achieve tractability, robustness, low solution cost, and better rapport with reality..."

When the concepts of "computing with words" are applied to the problem of inherent safety quantification, several advantages become evident. In inherent safety quantification function f is unknown, but heuristic and empirical knowledge is available. The inherent safety principles are an example of the type of knowledge that can be modeled through the “computing with words” methodology in order to approximate the unknown “safety function” f_s through a fuzzy graph f_s^*. The procedure for the selection of the variables, definition of the granules, and definition of the rules is described in the following section. The application to the specific problem of inherent safety is described in Chapters VII and VIII.

Computing with words requires working with language and knowledge. Klir (1994) indicates that language is associated with vagueness and, in order to model vague concepts, the used logic does not need to follow the law of excluded middle and the law of contradiction, introduced in Chapter V.

6.1.2 Theory of possibility

Zadeh (1999, reprinted from 1978) indicated that in several cases the information used for decision making and information analysis is possibilistic rather than probabilistic because of the issue of vagueness. Fuzzy logic is often confused with traditional probability theory, however when uncertainty is associated with vagueness a possibility approach should be used; only when uncertainty is derived from stochastic variability a probabilistic method can be used.

An event must be possible in order to be probable; however a high possibility degree does not imply a high likelihood. The concept of possibility is related to the concept of fuzzy set that acts as an elastic (i.e., not crisp) boundary on the values that the linguistic variable can accept. Therefore, partial membership (allowed by fuzzy sets but not by Boolean sets) does not represent frequency, but it describes how much that element satisfies the properties that characterize the fuzzy set [Laviolette et al, 1995a; Lootsma, 1997].

6.2 INTRODUCTION TO FUZZY REASONING: MAMDANI MODEL

Fuzzy reasoning requires inference rules expressed in IF-THEN format. There are three model based on fuzzy rules [Yen and Langari, 1999]:

- Mamdani's method
- Takagi and Sugeno's method (TSK)
- Kosco's additive model (SAM)

The models TSK and SAM are based on similar inference algorithms for the aggregation of the conclusions of the fired rules. This inference uses weighted sum, therefore TSK and SAM are classified as "additive rule models". The Mamdami model combines the rule outputs by using superimposition, therefore is a "nonadditive rule model" [Yen and Langari, 1999].

One of the most common reasoning methods is the Mamdani procedure, which is based on a simple structure of max and min operations. Mamdami's method uses rules such as:

$$\text{IF } x \text{ is } \hat{A}_i \text{ AND } y \text{ is } \hat{E}_j \text{ THEN } z \text{ is } \hat{C}_k$$

where $\hat{A}$, $\hat{E}$, and $\hat{C}$ are fuzzy sets and x, y, and z are linguistic variables divided respectively into i, j, and k fuzzy sets, whose relation is described by the rule.

The Takagi and Sugeno method (TSK) uses rules such as

$$\text{IF } x \text{ is } \hat{A}_i \text{ AND } y \text{ is } \hat{E}_j \text{ THEN } z \text{ is } c_k$$

where $\hat{A}$ and $\hat{E}$ are fuzzy sets but c is either a constant value or a traditional mathematical expression.

The Mamdami method presents advantages with respect to the TSK models because it is easier to understand and allows defining the output of the system in terms of fuzzy sets. Therefore the Mamdami model is also convenient for the present work because it is more transparent and offers better interpretability of fuzzy sets and fuzzy rules.

6.2.1 The Mamdami fuzzy inference algorithm

Many other fuzzy reasoning methods have been proposed, however the methodology presented here is based on a Mamdani model that uses groups of r rules such as:

Rule 1: IF x is $\hat{A}_{i1}$ AND y is $\hat{C}_{j1}$ THEN z is $\hat{E}_{k1}$
Rule 2: IF x is $\hat{A}_{i2}$ AND y is $\hat{C}_{j2}$ THEN z is $\hat{E}_{k2}$
. . .
Rule r: IF x is $\hat{A}_{ir}$ AND y is $\hat{C}_{jr}$ THEN z is $\hat{E}_{kr}$

where $\hat{A}$, $\hat{C}$, and $\hat{E}$ are fuzzy sets; x, y, and z are linguistic variables, and r is the number of rules (r = 1… r). This type of rule is defined by the generalized modus ponens (i.e., based on the modus ponens of the traditional two-valued logic) [Yen and Langari, 1999]:

Premise 1 (fact)	x is $\hat{A}_i$ and y is $\hat{C}_j$
Premise 2 (rule)	IF x is $\hat{A}$ AND y is $\hat{C}$ THEN z is $\hat{E}$
Consequence (conclusion)	z is $\hat{E}_k$

In the rules the connector AND can be replaced by OR depending on the requirements of the physical model. The connectors AND and OR are evaluated respectively by the standard operations of intersection ($\mu_{\hat{A}\text{ and }\hat{E}}(x) = \mu_{\hat{A}\cup\hat{E}}(x) = \mu_{\hat{C}}$) and union ($\mu_{\hat{A}\text{ or }\hat{E}}(x) = \mu_{\hat{A}\cap\hat{E}}(x) = \mu_{\hat{C}}$) described in Chapter V. The linguistic variables x, and y are the input variables, while the linguistic variable z is the output. The linguistic variables x is divided into i fuzzy sets while the variables y and z are divided into j and k fuzzy sets, respectively.

Fuzzy rules with two antecedents (e.g., $\hat{A}$ and $\hat{C}$) are represented by $\hat{A} \times \hat{C} \rightarrow \hat{E}$, which is known as a fuzzy relation between x, y, and z. The first step of fuzzy reasoning requires the conversion of the fuzzy IF-THEN rules into fuzzy relations $R_{\hat{A} \times \hat{C} \rightarrow \hat{E}}$; in the second step the conclusion Ê is inferred from the input $\hat{A}_i$ and $\hat{C}_j$ by applying the compositional rule of inference:

$$\hat{E}_k = (\hat{A}_i \text{ and } \hat{C}_j) \circ (R_{\hat{A} \times \hat{C} \rightarrow \hat{E}}) = (\hat{A}_i \circ \hat{C}_j) \circ (R_{\hat{A} \times \hat{C} \rightarrow \hat{E}})$$

Expressed as:

$$\hat{E}_k = \hat{A}_i \circ (\hat{C}_j \circ R_{\hat{A} \times \hat{C} \rightarrow \hat{E}}) = \hat{C}_j \circ (\hat{A}_i \circ R_{\hat{A} \times \hat{C} \rightarrow \hat{E}})$$

The resultant fuzzy set has a membership function expressed as:

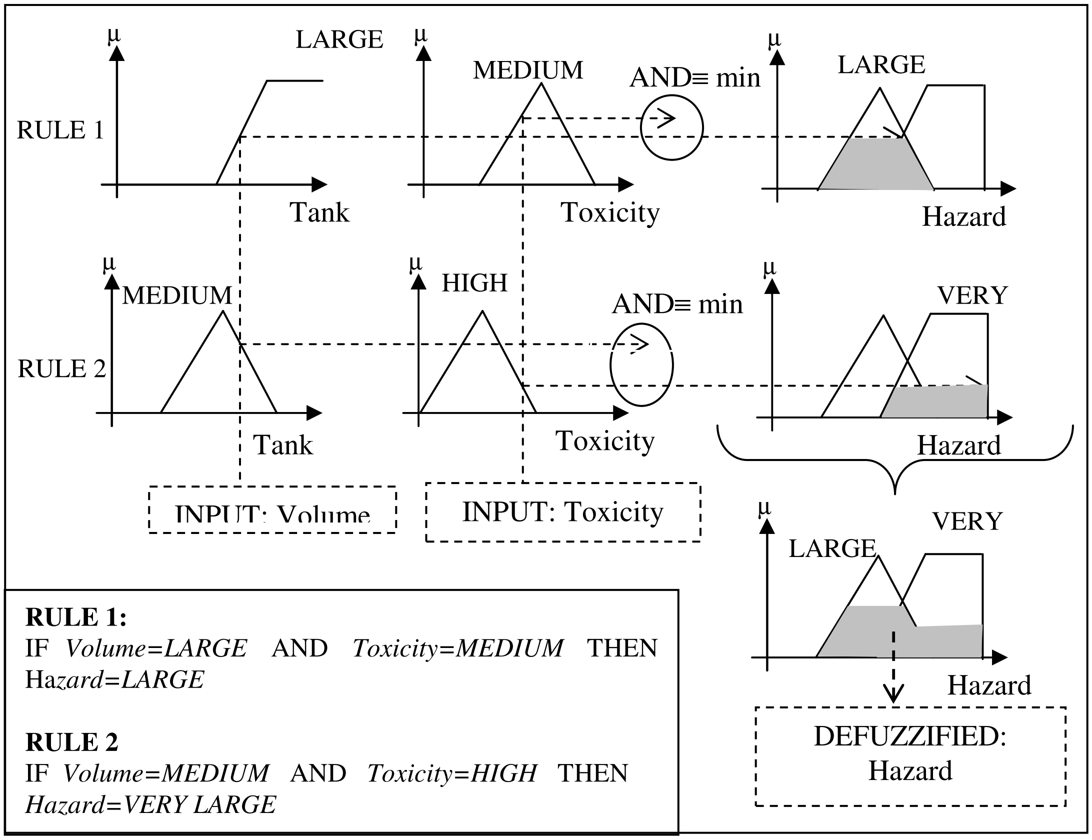
$$\mu_{\hat{E}} = \mu_{(\hat{A} \circ \hat{C}) \circ R}(x) = \max\{\min[\mu_{\hat{C}}(x), \max[\min(\mu_{\hat{A}}(y), \mu_R(x, y, z))]]\}$$

which is a combination of max-min composition.

After the rules have been evaluated, the output fuzzy sets $\hat{E}_r$ for each rule must be aggregated by using $\hat{E} = \bigcup_{r=1}^{n} \hat{E}_r$ where r is the number of rules. The obtained fuzzy set Ê is the fuzzy output of the inference system and must be defuzzified to obtain a crisp result.

The defuzzification methodology used is the center of mass (although there are several possible methods) of the resultant fuzzy set Ê, because it takes into account the strength of the fuzzy set $\mu_{\hat{E}}(x)$ and its support, where $\mu_{\hat{E}}(x)>0$.

A simplified version of the fuzzy inference process based on the Mamdami model is shown in Figure 6.2 for a system formed by two linguistic variables, “Tank Volume” and “Toxicity’, each described by two fuzzy sets, “Large” and “Medium”, and “Medium” and “High”, respectively. The output is represented by the variable “hazard” described by two sets, “large” and “very large”.



RULE 1:
IF *Volume=LARGE* AND *Toxicity=MEDIUM* THEN Ha*zard=LARGE*

RULE 2
IF *Volume=MEDIUM* AND *Toxicity=HIGH* THEN *Hazard=VERY LARGE*

Figure 6.2: Mamdami fuzzy inference algorithm

6.3 ELEMENTS OF A FUZZY MODEL

The concepts of membership function and fuzzy set represent the weakest aspect of fuzzy logic, which are at the same time the most powerful aspects of the methodology because they allow the modeling of uncertainty and allow the conversion of information and data into linguistic terms. Membership functions are the mathematical representation of fuzzy sets, and in order to design them, it is required to define the following aspects [Oliveira, 1995]:

- Number of fuzzy sets assigned to each linguistic variable: as indicated by Lootsma (1997) human beings can only process seven categories at most, therefore, the granularity of a linguistic variable should not exceed that number.
- Position of the natural zero: when the physical system has a point that can be assumed to be the natural zero, a fuzzy set should represent it. As indicated in Chapter IV, inherent safety can be assumed to have a natural limit when no hazard is present. While in some cases the natural zero exists (e.g., volume), in others (i.e., temperature) the physical zero exists under specific conditions only (e.g., absolute temperature scale).
- Universe of discourse: fuzzy sets should be assigned in such a way that they cover the whole range of the universe of discourse.
- Normalization of the membership functions: because each membership function should fully represent at least one point of the universe of discourse, it must be a normal function (i.e., with a height of one).
- Distinct semantic meaning: each fuzzy set must have a specific meaning, therefore it should be possible to distinguish it from any other set for the same linguistic variable.

The following sections summarize techniques used for membership function design.

6.3.1 Fuzzy set and membership functions design

The design of fuzzy sets involves the design of membership functions that assign linguistic values to the linguistic variables. A fuzzy variable is known as linguistic variable and its universe of discourse (i.e., range) is divided into fuzzy sets defined by the membership function, which indicates the degree of membership of each point into that set. Fuzzy sets represent the linguistic value of the linguistic variable for a specific input value x. For example, in Figure 6.3, the variable "environmental temperature" is divided into three fuzzy sets, "Low", "Moderate", and "High". The universe of discourse of the fuzzy set "Moderate" is [0 30] $^{\circ}$C and the set is normal because there is at least one point, x=15, with $\mu_{moderate}=1$. The input temperature of x=10 °C belongs partially to the fuzzy set "moderate" with $\mu_{moderate}(x=10)=0.4$ and belongs partially to the fuzzy set "low" with $\mu_{low}(x=10)=0.1$.

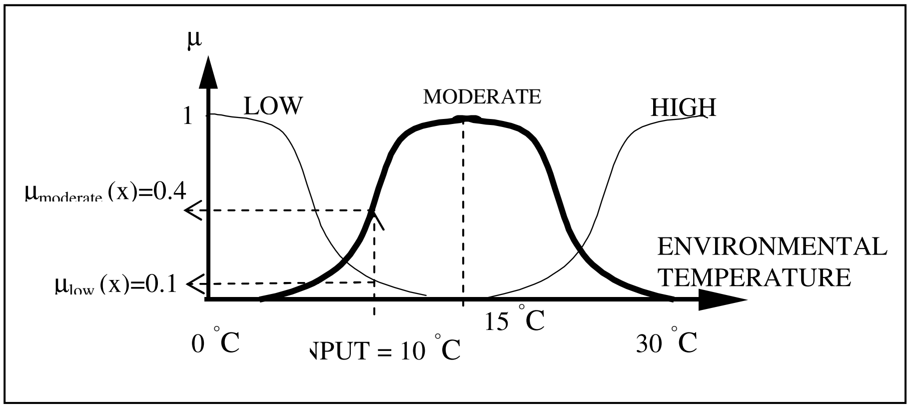


Figure 6.3: Example of linguistic variable "ENVIRONMENTAL TEMPERATURE", in terms of fuzzy sets "HIGH", "MEDIUM", "LOW".

The methods available for the construction of membership functions can be classified into direct and indirect methods [Despic and Simonovic, 2000]; direct methods imply a direct relation between the values x and the interval [0 1], while indirect methods rely on relations existing between the elements of the inputs. A brief description of six classes of experimental methods is presented by Pedrycz (1998). Methods such as fuzzy clustering can be used when a data set is available. In this case the set of data is partitioned into overlapping clusters that are then used to design the membership functions. Another methodology is based on pairwise-comparison which is based on the methodology proposed by Saaty for analytical hierarchy processing (AHP) as cited by McCauley-Bell and Badiru (1996 a and 1996b).

Another classification of methodologies for the design of membership functions is based on two types of information used: data-driven (bottom-up approach) and linguistic design (top to bottom approach). The data-driven approach requires a set of numerical data from which the rules are inferred by looking at the data, or by using algorithmic approaches such as clustering and ANFIS. The linguistic design is used when no numerical data is available or when the data is insufficient and, in this case, heuristic knowledge is required. Both methods are explained by Berkan and Trubatch (1997).

Because of the lack of data, this research is based on linguistic design. Under this approach, several steps are required [Berkan and Trubatch, 1997] to define the following parameters of the membership functions:

- Granularity (number of membership functions)
- Shape
- Location on the universe of discourse
- Fuzzy rules

These aspects have an important impact on the performance of the fuzzy system, and the following procedure is used in order to ensure the accuracy of the inference results [Berkan and Trubatch, 1997]:

- The first step requires the determination of the IF-THEN rules from the information available on the physical behavior of the system. This step also defines the granularity, which should not exceed seven fuzzy sets per linguistic variable.
- The following step requires the identification of shape and location of each membership function on the universe of discourse of the variable. In order to locate the membership functions it is necessary to identify the decision boundaries of the sets; the decision boundaries indicate which output set corresponds to which input set. In other words local models are created as shown

in Figure 6.1 where each rectangular gray area reflects the decision boundaries of two sets.

- The shape of the functions must be selected according to the physical meaning of the variable. This step requires following some design principles for the analysis of the shape.

An additional step is required for the selection of hedges (e.g., very, more or less, almost) that modify the shape of the function. However, for the present project, hedges are not used.

As described by Berkan and Trubatch (1997), the analysis of the shape of the membership function defines the following parameters of each membership function:

- Shape
- Height
- Overlap degree

The shape of the functions affects the performance of the inference system but in a limited form compared to the effect of number and location of the functions. The membership functions can have several shapes such as piece-wise-linear (e.g., triangular and trapezoidal), curve, S-shaped, π-shaped and other functions. Commonly used shapes are presented in Figure 6.4.

In general, triangular and trapezoidal functions offer a good compromise between descriptive power and computational simplicity, therefore these are the functions used for the hierarchical model developed for inherent safety quantification.

The height of the function indicates the maximum possibility value that can be produced by the inference rule related to the specific set. If the height of the set is lower than one (i.e., subnormal fuzzy set), then the rule will always produce an output set with less importance compared to the output generated from a normal set. Output fuzzy sets designed with a height less than one will produce paralysis (insensitivity) for a certain range of input values [Berkan and Trubatch, 1997]. For the proposed model, only normal input and output sets are used.

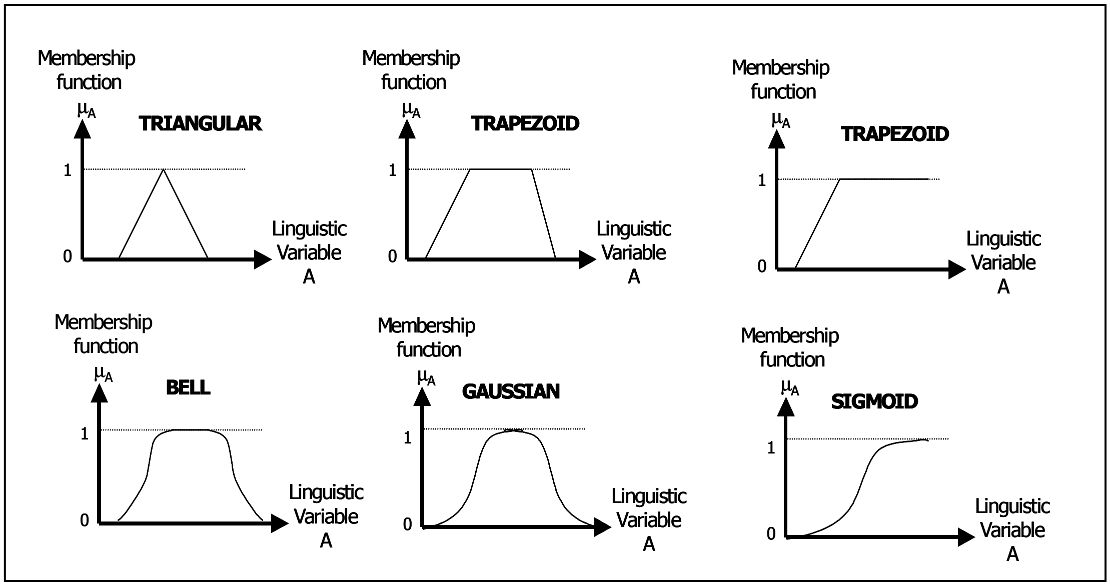


Figure 6.4: Common shapes for membership functions

An aspect of the paralysis phenomena is given by the geometric scaling of the output functions. When the output is defined over a large scale (compared with the range of μ which is the close interval [0 1]) and the method used for defuzzification is the centroid (explained in the next section), the functions are stretched [Berkan and Trubatch, 1997] as shown in Figure 6.5. Because the centroid defuzzification method is based on the calculation of the clipped output set (e.g., gray areas in Figure 6.5), when the sets are stretched (because of a wide scale of the universe of discourse of the output) the method becomes insensitive to changes in the inputs. To avoid this problem the range of the output is normalized on a scale [0 1], [Berkan and Trubatch, 1997].

A similar phenomenon occurs with the scale of the inputs, because when it is too wide and the sets are not equally spaced (e.g., toxicity intervals) then the narrower sets are lost compared to the wider sets. To solve this problem, a logarithm transformation is applied to the scale of the linguistic variable.

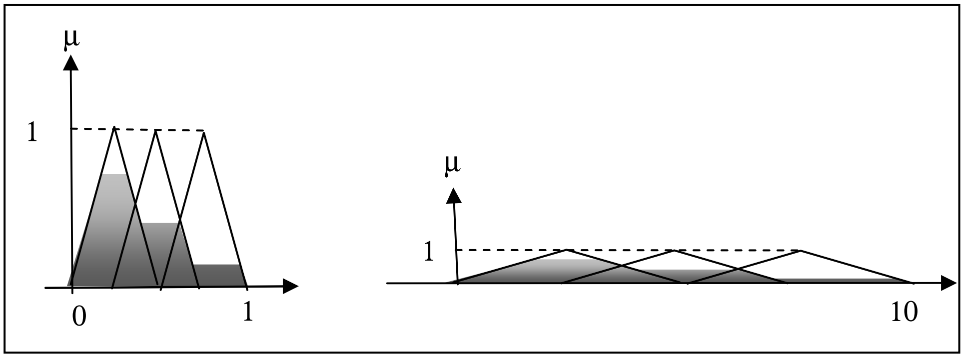


Figure 6.5: Effect of the output scale

The election of the shape of the membership function requires understanding the inherent uncertainty of the linguistic term. In the case of triangular functions it is assumed that only one value of the support of the set has full membership (i.e., μ=1.0) while the rest of the support represents the uncertainty or possible range of variability of the linguistic term. For example, the normal temperature of operation of a reactor can betaken to be the point with full membership, while the normal range of variability of the operation temperature can be represented by the two extremes of the triangular membership function. A triangular membership function implies strict standards for the antecedent variable since only one point is assigned with full membership [Berkan and Trubatch, 1997].

The trapezoidal shape indicates that several input points have full membership in the set; therefore the use of this shape implies that the requirements for full membership are less strict compared to the triangular function. The trapezoidal shape also indicates the degree of tolerance of the set; shapes with narrow regions of high membership (i.e., triangular function) are conservative (since they represent stricter requirements in order to assign high membership) while a trapezoidal function is assumed to be more tolerant because a wider region is assigned with high membership values [Berkan and Trubatch, 1997].

As shown in Figures 5.2 and 5.3 the membership functions for an input linguistic variable must present some degree of overlap. The overlap permits a smooth transition from one set to the other, which is an important characteristic of fuzzy systems. As indicated by Berkan and Trubatch (1997), the degree of overlap also increases the speed of the response of the rule and the degree of cooperation among rules. When the overlap increases, the cooperation of the rules also increases making the response smoother. A common practice for fuzzy systems design is to define membership functions with crossover points at $\mu = 0.5$ in order to establish a balance between sensitivity and smoothness of the response. A lower overlap may indicate the presence of undefined regions, while a larger overlap may indicate lack of knowledge about the linguistic variable or lack of sufficient partitioning.

For the model proposed in the next chapter, the membership functions have been designed using the principles summarized above and other principles discussed by Berkan and Trubatch, (1997). The selected shapes are triangular and trapezoidal, and in general they are defined in such a way that the indications on overlap are obeyed.

According to the Mamdami algorithm, each fuzzy IF-THEN rule can receive a weight factor that assigns more or less importance to the rule in comparison to the other rules of the rule-basis. The effect of the weights is analyzed by Ishibuchi and Nakashima (2001), and by Nauck and Kruse (1998). By changing the weights, the rectangular decision area of each rule is modified accordingly allowing the fuzzy graph to be changed as required. When the rule base is not complete (i.e., some rules are missing) the decision areas are no longer rectangular, however the same approach of modifying the relative membership functions can be used [Ishibuchi and Nakashima, 2001]. In both cased it is indicated that the use of weights can be replaced by modifying the shape of the antecedent and consequent membership functions.

For the hierarchical model proposed for inherent safety evaluation, while rule weights are not used, the functions are tuned manually by trial and error in order to obtain smooth fuzzy graphs whose behavior resembles the expected behavior of the physical system.

6.3.2 Defuzzification methods

The step of defuzzification is the last step of the fuzzy inference algorithm where the aggregated fuzzy output is converted into a crisp number. Defuzzification is defined as a function F^{-1} mapping a fuzzy set Â to a certain element (x) of the support of the output (as shown in Figure 6.6) and defined as:

$$F^{-1} : F(x) \rightarrow x$$

Several methods have been proposed for this purpose, however the method chosen should be based on the properties of the defuzzification method and the requirements of the system. The properties of the defuzzification methodology can be classified into static and dynamic properties [Runkler, 1997].

Static properties are consistency, monotonicity, scale invariance, and compatibility. The property of consistency is related to the fact that the defuzzification method should map convex crisp sets to their centroid (e.g., center of a crisp subinterval). Monotonicity requires that the result of the defuzzification moves towards the areas of higher membership when the opposite part is changed to a lower degree of membership. Scale invariance is related to the type of scale (i.e., ordinal, interval, ratio) used to define the linguistic variables (as discussed in Chapter VII). The property of scale invariance is not required when the degree of membership are defined on interval, ordinal, and ratio scales.

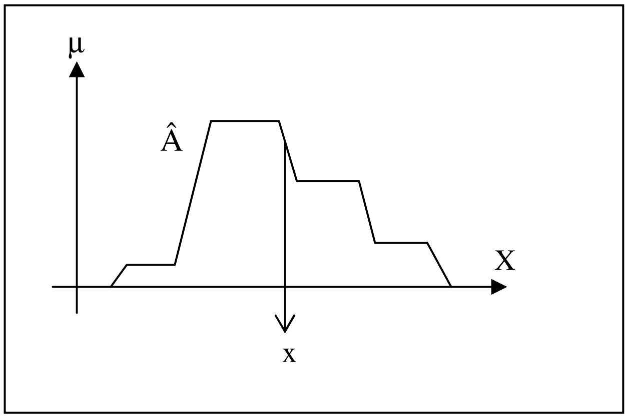


Figure 6.6: Defuzzification of the output fuzzy set Â

Compatibility is important for rule-based inference systems because the selected defuzzification method must be compatible with the used operators and implication methods. The dynamic properties of the defuzzification methods are related to the change in response caused by a small change in the input. Other important properties have been reported by Leekwijck and Kerre (1999).

The most important defuzzification methodologies are [Runkler, 1997]:

- Centroid: it is one of the standard methods and calculates the center of gravity (COG) of the area delimited by the membership function of the output set:

$$F^{-1}(\hat{A}) = \int \mu_{\hat{A}}(x)\, x\, dx \,/ \int \mu_{\hat{A}}(x)\, dx$$

This method follows the properties of consistency, monotonicity, but does not follow the property of scale invariance.

- Center of area: calculates the point x where the areas under the membership function to its right and left are equal and it follows the properties of consistency, monotonicity, and scale invariance.
- Maxima methods: these methods focus on the maximum values of the fuzzy set rather than on the area under the membership function (as in the case of centroid and center of area). Several methods are classified under this category such as: first of maxima, last of maxima, mean (average of maxima), and center of maxima (median of maxima).

Other methods have been reported by Runkler(1997), Ali and Zhang (2001), and Leekwijck and Kerre (1999). Other criteria for the selection of defuzzification methods are related to the specific application such as computational efficiency, transparency, and continuity as indicated by Leekwijck and Kerre (1999). While efficiency is related to the number of mathematical operations required by each specific method, transparency is related to the degree of complexity of the approach. Efficient and transparent operators are preferred.

For the model proposed in this work for the evaluation of inherent safety, the selected defuzzification method is the standard center of mass or centroid because of its characteristics and the fact that it is the most widely used method for the Mamdami model. As explained below, the linguistic variables used are based on continuous ordinal scales, which do not required the defuzzification method to follow the scale-invariance property. The test performed also showed that the continuity of the response is ensured.

6.4 HIERARCHICAL FUZZY SYSTEMS

The application of fuzzy logic to complicated process control problems with a large number of inputs highlights the problem of rule-explosion. If a system requires n input variables each partitioned into m membership functions, the total number of rules required to model the system by using one single fuzzy inference system is m^n. As the complexity of the problem increases, the number of required inputs increases too, requiring an exponentially larger number of rules. In order to deal with the problem rule-explosion, the development of hierarchical fuzzy systems has been proposed. In hierarchical systems, the number of rules increases linearly with the number of inputs rather than exponentially [Lee et al., 2003]. The structure of a normal fuzzy system is shown in Figure 6.7 and the classical structures of hierarchical fuzzy systems are shown in Figure 6.8:

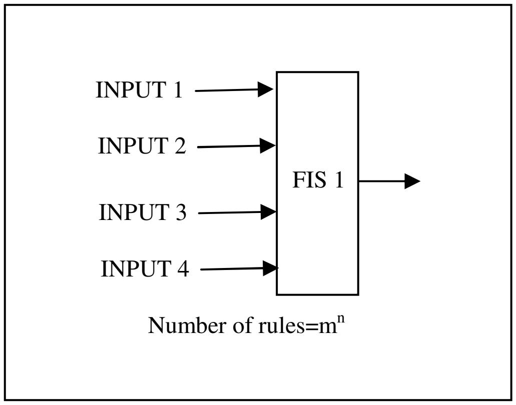


Figure 6.7: Structure for conventional single-layer fuzzy systems

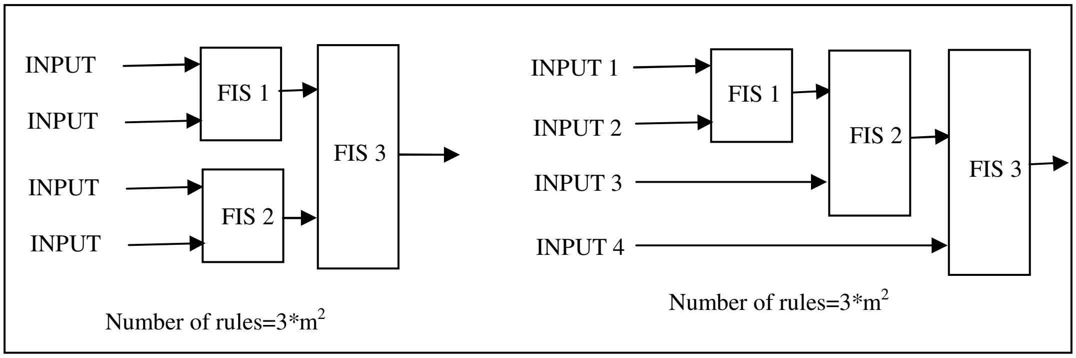


Figure 6.8: Structure for hierarchical fuzzy systems

For hierarchical fuzzy systems, the outputs from certain FIS are used as inputs for the following FIS, which are difficult to design because the intermediate outputs do not have physical meaning. As the number of layers of FIS increases, the difficulty associated with their design increases due to the loss of physical meaning [Lee et al, 2003]. A new model that further reduces the number of rules for hierarchical systems, and reduces the limitations associated with the loss of the physical meaning of intermediate outputs/inputs has been proposed by Lee et al., (2003). Examples of hierarchical fuzzy systems for applications other than control have been published by Stoms (2002) for assessment of land stability, Sasikala and Petrou (2001) for the estimation of the risk of desertification, and Despic and Simonovic (2000) for decision making in water resources management.

The problem of inherent safety quantification is a complex problem that requires the use of several inputs. For example, as indicated in Chapter VII, the proposed prototype requires 25 inputs that correspond to linguistic variables partitioned into 2 to 5 fuzzy sets. Assuming an average of 3 fuzzy sets per input a total number of 3^{25}=8.47*10^{11} rules would be required. By using the hierarchical structure described in Chapter VII and formed by 35 FIS, less than 900 rules are required. Because the variables are combined in such a way that the physical significance of intermediate outputs is not lost, the classical structures for hierarchical systems are used.

The aggregation of intermediate outputs from the lower layers of the hierarchical fuzzy model is generally achieved by using aggregation operators; a brief introduction to these methodologies is provided in Chapter V. Additional information on aggregation is given by Yager (2004) who presents a review of aggregation operations and type of problems where information fusion is required; the selection of aggregators for multi-attribute decision making in engineering is revised by Scott and Antonsson (1998). A review of aggregation methods and a case study comparing benefit and limitations of each method is provided by Smolikova and Wachowiak (2002); the example demonstrates some guidelines about how to select weights for the ordered weighting operators (OWA) from the characteristics of the system. Another approach for the selection of weight for OWA functions has been proposed by O'Hagan (as cited by Yager and Kelman, 1996) and is based on the selection of a single coefficient of optimism from which all the weights are estimated.

Depending on the requirements of the problems and the criteria for the selection of the aggregation operators, several methods may be used for describing different parts of the problem. The problem of selection for an aggregation methodology is not trivial and must be carefully analyzed. In the case of ordered weighted operators (OWA) a vector of weights representing the importance of each element must be selected; if data is not available to calculate the weights, expert judgment must be used. However, subjectivity associated with the expert's previous knowledge (or lack of it) affect the aggregation methodology and inconsistent results may be obtained [Despic and Simonovic, 2000]. When parameterized operators (e.g., Zimmermann's γ-family of operators) are used, the values of the parameters must be selected but their meaning is not intuitive. An alternative aggregation methodology proposed by Zadeh et al. (1987) as citeted by Despic and Simonovic (2000) suggests the use of a fuzzy-algorithmic approach based on fuzzy IF-THEN rules.

In the case of the proposed hierarchical model for inherent safety evaluation, sources of hazard represented by physical factors are combined by fuzzy rules and their aggregated outputs represent a measure of the inherent hazard. These measures of hazards are then used by the next layers of the hierarchical model; however, since the measure of hazard is related to the potential physical consequences, they keep a physical significance. Therefore, the aggregation methodology chosen is based on the use of fuzzy IF-THEN rule bases.

In hierarchical systems, when the outputs from previous FIS are used as inputs for the next FIS, problems associated with rule chaining can arise due to the fuzziness of the used outputs, as shown in Figure 6.2. The output obtained from the evaluation of a set of rules is a fuzzy set whose support (i.e., width of its base) is a measure of the uncertainty of the result. When the output is defuzzified a single real number is obtained as result, however the information about uncertainty is lost. When rule chaining is used, as in the case of hierarchical systems, the output is fed to the next set of rules as a fuzzy set or as a crisp real number. Each option presents advantages and disadvantages:

- The option of using fuzzy output from previous layers as fuzzy input for the next fuzzy inference system presents the advantage of preserving the information about uncertainty. However, when the fuzzy set is too wide it fires several rules of the new FIS generating therefore a very uncertain result (i.e., very wide set). As indicated by Driankov and Hellendoorn (1995) even areas of the fuzzy output (used as fuzzy input) with very low membership degree will fire rules and the resulting new output will be composed by sets that should not have been used.
- When the output is used as a crisp number with no uncertainty, only few rules will be fired reducing the uncertainty of the new result, but information is lost. As indicated by Driankov and Hellendoorn (1995) when the crisp output is obtained from the defuzzification of a non-convex set, the obtained crisp result is associated with a lower membership degree.

An additional problem of these two approaches is that the final result may not be the expected. For instance, if one rule is “IF X is A THEN Y is B”, and the following rule is “IF Y is B THEN Z is C”, because of the problems described above, probably the rule “IF X is A THEN Z is C” will not be obeyed [Driankov and Hellendoorn, 1995].

A compromise between the two options is presented by Driankov and Hellendoorn (1995) by decomposing the defuzzification of the output used as input for the next FIS into two or more crisp singletons corresponding to the points of highest membership. In this case the limitation associated with non-convex sets is solved, and the problem related to the chaining of rules is reduced.

For the hierarchical model proposed for inherent safety evaluation, a compromise among the three methods described above is applied by using only the part of the fuzzy output with membership degree $\mu_{output} \geq 0.4$. The resultant fuzzy set is then converted to a triangular fuzzy set by taking the lowest and highest values of the support of the output where $\mu_{output} = 0.4$. This approach is shown in Figure 6.9. The original fuzzy output is shown in white and its relative defuzzificated value is indicated. The modified fuzzy output (i.e., $\mu_{output} \geq 0.4$) is shown in light gray and the resultant triangular fuzzy set is indicated in dark gray.

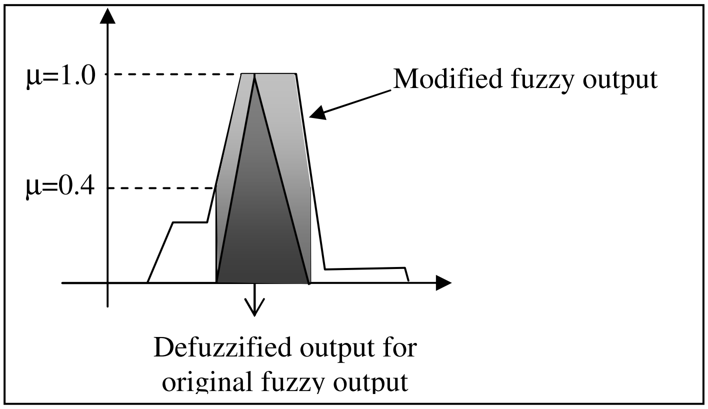


Figure 6.9: Approach used to modify fuzzy outputs used as inputs by other inference systems.

The value of 0.4 was chosen in order to reduce the effect of parts of low membership degree on the FIS that takes the fuzzy set as input (e.g white parts of the set in Figure 6.9). However, the parts of the function with $\mu_{output} < 0.4$ is taken into account by the crisp defuzzified value that is used as the second parameter of the triangular function. By the test performed on the systems, in general the defuzzified value is found within the support limited by $\mu_{output} \geq 0.4$. When the defuzzified result falls outside the range of the support limited by $\mu_{output} \geq 0.4$ the inputs are located in areas of high uncertainty and the defuzzified output is adjusted to coincide with either the lowest or highest value of the support where $\mu_{output} = 0.4$.

6.5 INTRODUCTION TO FUZZY MODELING

Fuzzy logic captures and models expert knowledge by using linguistic rules, which simplify the modeling process. The main steps for designing fuzzy logic system are:

1) Expert knowledge collection about the most important factors that affect the systems and the behavior of the variables.
2) Modeling of the knowledge by selecting the inputs to the system. The membership functions, fuzzy set and the fuzzy IF-THEN rules are developed at this stage.
3) The fuzzy system is integrated by fuzzy logic software, and after test and validation the system must be optimized to ensure its reliability and accuracy.

The development of the overall model for the evaluation of inherent safety is based on several steps. The first stage is the knowledge acquisition from technical information and literature, general models, expert knowledge, and data. The main objective of this stage is the identification of the most important parameters (i.e., linguistic variables) for the description of the each relevant aspect of the system, and the identification of the relations among the selected factors (i.e., fuzzy IF-THEN rules). This is a critical step that requires the deep understanding of the physical behavior of each subsystem in order to identify the most significant factors. For instance, the hazard due to chemical releases is usually assessed by calculating the area covered by a potential chemical plume under specific release conditions and other factors such as atmospheric stability and ground characteristics. These factors, along with the characteristics of the population present around the release source, affect the overall risk. However, from the inherent safety viewpoint, the hazard magnitude is a function of the system only (e.g., chemical and vessel) and the comparison of factors such as type of phase released and general behavior of the substance at environmental conditions control the possibility of a cloud generation and dispersion. Following the basic idea of inherent safety, if the cloud cannot be formed then the hazard is eliminated.

The knowledge acquisition for the present project is based on specialized literature review, simulation (e.g., dispersion modeling), engineering models, and expert assessment. Expert knowledge compilation through survey was not used because other researches have collected similar information [Lawrence, 1996] which has been used to identify weaknesses of other methodologies that have been addressed by the fuzzy-logic approach. This type of information collection was deliberately avoided in order to focus on the "reformulation of the problem" as indicated in Chapter IV and avoid the temptation to use traditional risk-based approaches.

The second step of the fuzzy model development is the design of fuzzy sets and membership functions. The objective of this step is the identification of physical characteristics of each selected variables that can have a potential impact on the magnitude of the resultant hazard. To ensure the modeling capability the membership functions must describe the general physical meaning of each point on the range of the variable. For instance, in the case of operation temperature, points such as the boiling temperature and the flash point of the substance affect the potential formation of explosive clouds (in case of a flammable chemical) and their dispersion. These two points were used to design the granularity of the variable "temperature". The granularity (i.e., number) and shape of functions for each variable was selected following the design criteria proposed by Berkan and Trubatch (1997) and by applying the technical information collected during the previous stage. In some cases (e.g., corrosion evaluation) the granularity and shape of the membership functions depends on the chemical, hence they are variable and adaptive. In this case the user of the software is required to feed some parameters that are used to design the specific functions for the case analyzed. For certain linguistic variables (e.g., toxicity) with a wide universe of discourse (i.e., domain of a linguistic variable) a logarithm transformation was applied in order to preserve the narrower fuzzy sets (e.g., very low concentrations of highly toxic chemicals).

The sensitivity of the model to the shape of the functions has been qualitatively analyzed comparing the response with the expected physical behavior (based on the knowledge of the system) and performing tests for the local systems. The potential utility of Adaptive Neural Fuzzy Inference Systems (ANFIS) algorithms for the design of membership functions was explored; however, the lack of data prevented the application of automated means for the design of membership functions and rules.

The next step consists of the development of rule-base for each fuzzy inference system. The model selected for this application is the Mamdami model and it is based on IF-THEN rules. The rules must be able to describe the relation between the inputs for the local model and the output (e.g., hazard degree). As described in Chapter VI, this is equivalent to establishing a functionality between input variables and outputs but rather than being based on a traditional function such as $z = f(x,y)$ here the obtained fuzzy graph is an approximation of the unknown relation. In other words, fuzzy logic modeling allows transforming the general knowledge expressed in terms of IF-THEN rules into a continuous non-linear mapping.

The next step requires the design of the inference engine and the definition of the connectors AND and OR (as explained in Chapter V), the selection of the implication and aggregation operators, as well as a defuzzification methodology.

CHAPTER VII

FUZZY HIERARCHICAL MODEL FOR INHERENT SAFETY ANALYSIS

This chapter introduces the general model developed for the evaluation of inherent safety including the assumptions and general features of the selected fuzzy inference systems.

7.1 FUZZY MODELING

The steps for the development of a fuzzy model were explained in Chapter VI. This section describes the characteristics of the hierarchical model for the evaluation of inherent safety.

7.1.1 Fuzzy model specifications

The used fuzzy model is the Mamdami algorithm because it works with IF-THEN rules whose antecedents and consequents are based on linguistic variables defined in terms of fuzzy sets. The Mamdami model is used rather than the TSK because the consequent part of the rules is expressed by fuzzy sets, instead of linear functions. Fuzzy sets are more convenient for the present application because they can express linguistic concepts and are easier to interpret. Because of this the obtained model is more transparent to the user and highly interpretable since the rules are easy to understand and visualize.

The overall system is formed by 35 fuzzy inference systems (FIS) arranged in a hierarchical tree where the output from the lower levels are used as inputs for the lower levels. The user is required to provide 25 input values for the chemical substance, operating conditions, and vessel design. Other 11 parameters are required for the design of adaptive membership functions for the evaluation of dispersion hazard, corrosion potential, and vessel operating conditions. The list of required inputs is reported in Tables 7.1 and 7.2.

Table 7.1: List of required input parameters (linguistic variables)

HUMAN TOXICITY	**UNITS**	**FIS WHERE INPUT IS USED**
Acute oral toxicity	mg/kg	CHH1a
Acute dermal toxicity	mg/kg	CHH1a
Acute respiratory toxicity (vapor)	ppm	CHH2a
Acute respiratory toxicity (gas)	mg/l	CHH2a
Acute respiratory toxicity (dust/mist)	mg/l	CHH3a
Human cancer evidence	%	CHHc
Animal cancer evidence	%	CHHc
ENVIRONMENTAL IMPACT	**UNITS**	**FIS WHERE INPUT IS USED**
Chemical water toxicity	LD_{50}	CHEdt, CHEat
Half-time chemical life	days	CHEdt
Bioaccumulation factor	-	CHEat
Troposphere half-time chemical life	days	CHEp
Data quality: troposphere half-time	%	CHEp
FIRE AND EXPLOSION	**UNITS**	**FIS WHERE INPUT IS USED**
Normal boiling temperature	°C	CHPFa, DISP, DISPTX
Flash temperature	°C	CHPFa, DISP
Maximum potential density	W/ml	CHPR
Water heat of mixing	cal/gr.	CHPRh2o
Unit average obstruction fraction	%	COOB
Unit average congestion fraction	%	COOB
Flame burning velocity	cm/s	COOB
DISPERSION	**UNITS**	**FIS WHERE INPUT IS USED**
Vessel operation temperature	°C	DISP, DISPTX, CORRH
Vessel operation pressure	°C	DISP, DISPTX
Boiling temp. at vessel conditions	°C	DISP, DISPTX
DESIGN	**UNITS**	**FIS WHERE INPUT IS USED**
Volume of vessel	gal	ISIMECH
Nozzle diameter	in	NLD
Nozzle level	%	NLD

Table 7.2: List of required input parameters for adaptive membership design

DISPERSION	UNITS	FIS WHERE INPUT IS USED
Normal boiling temperature	°C	DISP, DISPTX *
Flash temperature	°C	DISP *
Atmospheric temperature	°C	DISP, DISPTX
CORROSION	**UNITS**	**FIS WHERE INPUT IS USED**
Temp. for excellent resistance (metal)	°C	CORRH
Temp. for good resistance (metal)	°C	CORRH
Temp. for satisfactory res. (metal)	°C	CORRH
Temp. for unsatisfactory res. (metal)	°C	CORRH
Temp. for unsatisfactory res. (plastic)	°C	CORRH
NOZZLE	**UNITS**	**FIS WHERE INPUT IS USED**
Maximum operation level	%	NLD
Normal operation level	%	NLD
Low normal operation level	%	NLD
Minimum operation level	%	NLD
Drain level	%	NLD

* also used for evaluation (Table 7.1)

Binary fuzzy relations evaluate the effect of the interaction of the linguistic variables or inputs (e.g., “overall mechanical hazard” is combined with “volume”). By combining only two (or three at most) variables per fuzzy inference system it is possible to obtain defuzzified surfaces that can be examined to ensure that the system behavior is as expected. Except for the fuzzy inference systems DISP and DISPTX that require three inputs (i.e., three antecedents are combined by the IF-THEN rules) the rest of the FIS require only one or two inputs. The system is designed in this way in order to facilitate the comprehension of the rules and allowing the analysis of the FIS by plotting the output, or fuzzy graph.

The linguistic variables are combined by IF-THEN rules that are not modified by weights; therefore it is implicitly assumed that all the linguistic variables (i.e., inputs) have the same importance. In some cases, synergetic effects among input variables have been assumed, and the rule set takes care of it.

The logic operators (i.e., AND, OR) are based on the standard max and min operators. The choice of the operators for intersection and union (minimum (min) for intersection and maximum (max) for union) is not unique. Several operators have been proposed in the literature and each one targets specific characteristics of different problems. The operators selected here (min and max) are the classical operators in fuzzy logic and they are analogous to the logical operators AND (Boolean conjunction) and OR (Boolean disjunction). In the case of the classical fuzzy intersection or min operator, the lowest degree of membership involved in the intersection dictates the result of the operation. This situation is similar to the common metaphor that a chain is as strong as its weakest link.

On the other hand, for fuzzy union, the max operator chooses the highest degree of membership among the involved values. These standard fuzzy operators are the only ones that satisfy all six required mathematical axioms, explained in Chapter V. Two of the most important axioms require the operators to be continuous and idempotent. In other words, the continuity axiom ensures that a small change in the membership function of one set (e.g., either $\hat{A}$ or $\hat{C}$) will not produce a large change in the membership function of the set $\hat{E}$ given by union or intersection. The independency axiom ensures that the union or intersection of one fuzzy set with itself will result in the same fuzzy set [Klir and Folger , 1988].

The implication operators are based on a Mamdani type, while the defuzzification methodology chosen is the center of mass (COM) approach. These options for implication methodology and defuzzification are commonly used for the Mamdani algorithm.

7.1.2 Variable type and fuzzy set design

The variables selected for the proposed model are identified among the most relevant for the evaluation of inherent safety. The main idea on which they have been selected is their physical significance in terms of objective interpretation based on physical consequences (e.g., explosion overpressure) and physically meaningful thresholds. This characteristic is required in order to eliminate the uncertainty derived from subjective interpretation.

One of the problems associated with variable selection is the fact that while some hazards depend only on chemical characteristics, others depend on the combination of chemical and design factors. A finer classification is shown in Table 7.3, where the variable type is classified by type of threshold and type of property.

Table 7.3: Variable types

VARIABLE TYPES	
BASED ON THRESHOLDS	BASED ON PROPERTIES
On inputs	Physicochemical properties
On outputs	Design properties
Mixed	Interaction

An example of a variable type based on input thresholds is flammability, which is defined based on boiling and flash temperature; once the system has reached specific conditions based on these parameters it is considered to be in the flammable range. Toxicity is an example of a variable based on output thresholds; a chemical is classified as more or less hazardous depending on the effects on living organisms such as mice and rabbits. Even though, other toxicological parameters affect the outcome (i.e., dosage, time, body mass, stress level during intoxication) they are not taken into account for the toxicological classification. An example of variables that could be classified under a combination of output and input thresholds is chemical reactivity. Although this is subject of intensive investigation around the world, there is not yet a consensus on a methodology for reactivity classification. While the NFPA has developed a scoring system based on output threshold (i.e., instantaneous power density or IPD) the use of onset temperature could be classified as an input-based threshold. However, design and operating parameters may also have an effect on the classification of reactivity.

For the classification of variables based on properties, while some of the variables common in process safety depend only on physicochemical properties of the substances, others depend on design factors, and some others require a combination of physicochemical properties and design characteristics. Burning velocity of a chemical is a physicochemical property only but the flame speed velocity for the same substance depends on the combination of the burning velocity and design factors (e.g., degree of confinement) that affects the turbulence. For example, hydrogen and propane are both classified as highly flammable gases (NFPA flammability score of 4) but, while hydrogen has one of the highest burning velocities (320 cm/sin air and 1175 cm/s in oxygen, [Lees, 1996]), propane has a low burning velocity (45 cm/s in air and 390 cm/s in oxygen [Less, 1996)]. However, depending on the confinement degree of the unit where the release happens, the effects of the flame velocity will change generating more or less destruction. An example of a variable that depends only on design parameters is volume of the vessel or equipment.

The variable type based on thresholds is important because it affects the methodology followed for the design of the membership functions and fuzzy inference systems. In the case of variables that depend on output thresholds (e.g., toxicity), the physical effects (i.e., rules outputs) are already defined in terms of comparable values, while the rules antecedents are also defined as a function of the outputs. Toxicity is an example of this type of variables. When the variable is based on input thresholds (e.g., flammability), then in order to design the rule consequent (i.e., output) it is required to use simulation in order to identify the consequences and translate them into a scale of physical effects. Explosion is an example of this type of variables, and the rules output is designed based on source models for releases, dispersion modeling, and overpressure evaluation.

Variable type based on design is important for the structure of the proposed hierarchical tree, because the design properties must be combined with physicochemical inputs in order to evaluate their interaction and obtain a better idea of the resultant hazard. The evaluation of fire and explosion hazards requires the combination of flammability (i.e., chemical property) with the unit obstruction and congestion measures (i.e., design parameters). The evaluation of design hazard due to nozzle location and diameter is based only on equipment characteristics.

After the selection of the variables presented in Table 7.1, the granularity (i.e., number of fuzzy sets and location) for each one of them was decided based on physical principles, as explained in Chapter VIII. The maximum number of membership function for each variable is seven as indicated in Chapter VI, because of the limited human capacity to manage a larger number of categories. The shapes used for the membership functions are triangular and trapezoidal because they represent a tradeoff between modeling flexibility and simplicity. The details of the selection of each shape for each particular variable are explained in Chapter VIII.

The universe of discourse (i.e., range of interest of the variables) is defined by their physical units, however in order to follow the design principles suggested by Berkan and Trubatch (1997), when the range is too wide (e.g., more than 150 units) a logarithm transformation is used (e.g., toxicity range goes from 0.001 ppm to 1,000 ppm) in order to preserve the effect of the narrower sets (e.g., high toxicity sets) with respect to the wider ones (e.g., low toxicity). The transformation does not affect the rest of the algorithm; however it has an impact on the value of membership of the input. Because the range of membership degree μ is [0,1], if the universe of discourse is very wide the membership function would be stretched (as explained in Chapter VI) reducing their sensitivity to the inputs.

Fuzzy logic allows working with uncertain information. This is achieved through the use of membership functions and the use of inputs based on fuzzy numbers rather than crisp values. This characteristic of fuzzy systems is particularly important for the present model where most of the required inputs present high degrees of vagueness and uncertainty. Because of this problem, the proposed system allows the user to feed inputs either as crisp or fuzzy numbers. In the case of fuzzy inputs, the available information regarding a input variable is converted to a fuzzy number by defining the lowest possible value, most likely value, and most likely maximum value. In the case of operating conditions, the range could represent the normal variability of the process (e.g., normal operating temperature fluctuates between 40 and 50 °C).

Hierarchical trees combine several fuzzy inference systems and the inputs to the upper branches are the outputs from the lower branches of the tree (as shown in Figures 7.1 to 7.9). The output of a fuzzy inference system can be a fuzzy set or the defuzzified crisp value. The system developed here uses both outputs to define the input to the next branch. However, in order to reduce the uncertainty given by low-membership values (i.e., $\mu < 0.4$) the fuzzy output is clipped at $\mu = 0.4$, defining then the fuzzy number by three parameters:

- Minimum value for the input fuzzy set: minimum value of the output fuzzy set where $\mu = 0.4$
- Most likely value: defuzzified result of the output set
- Maximum value for the input fuzzy set: maximum value of the output fuzzy set where $\mu = 0.4$

Other proposed approaches have been explained in Chapter VI but the selected one offers a good compromise between accuracy and simplicity. The sensitivity of the model to the shape of the functions has been qualitatively analyzed comparing the response with the expected physical behavior (based on the knowledge on the system) and performing tests as proposed by Boston (1995). The potential utility of Adaptive Neural Fuzzy Inference Systems (ANFIS) algorithms for the design of membership functions was explored; however, the lack of data avoided the application of automated means for the design of membership functions and rules.

7.1.3 Output design

The design of the output requires special consideration because it is common to all the fuzzy inference systems and must give an indication of the physical hazard. The interval [0,1] is the range chosen for the output; 0 indicates total lack of hazard and 1 indicates a very hazardous situation. The lack of hazard is only achievable when equipment and chemicals have specific safe conditions, which are expressed through strict IF-THEN rules. In general, as shown by the figures in Chapter VII, the absolutely non-hazardous states are single points at the origin of the defuzzified surface plots, therefore they are difficult to achieve.

An additional reference point on the output scale is set at 0.5; this fuzzy threshold establishes a separation between conditions of low hazard, assumed to be inherently safer, and conditions that tend to be hazardous and therefore cannot be classified as inherently safer. If the value of the output is smaller than 0.5, then the degree of inherent safety increases until becoming “absolute” when it reaches the limit (i.e., 0). When the value of the output is larger than 0.5 it is assumed that the principles of inherent safety must be applied in order to reduce the inherent hazard.

The relative importance between the real values on the output scale is not ensured; for example output = 0.3 cannot be understood as being twice as safe as an output = 0.6. However, special care has been taken in order to provide correspondence for the output of the different FIS. For example, 0.5 represents the threshold between the inherently safer region and the non-inherently safer region for all the inference systems. The equivalence is based on the potential physical impacts on the combinations of input parameters. When there is possibility of irreversible effects on population, environment, or equipment, then the output must always be above 0.5; as the magnitude of the consequences increases, the index must also then increase to 1. When the consequences are reversible then the index should be below 0.5 with a tendency to zero when the magnitude of the consequences is negligible. The selected approach simplifies the aggregation process by mapping the inputs and their interaction to a common “hazard possibility index”.

7.1.4 Rule design

For each one of the 35 FIS, a different set of IF-THEN rules was designed according to the general knowledge and information regarding the physical behavior of each system. The purpose of the rules is to map each combination of fuzzy sets for the input variables to a fuzzy set for the output variable. The rules must be able to describe and capture the expected behavior of the physical system when the values of the input factors correspond to the specific range defined for the input fuzzy sets.

When a specific rule requires two inputs each one with i and j fuzzy sets respectively, the completely specified rule-bases requires (i x j) rules. However, in order to simplify and optimize the system it is possible to eliminate certain rules. For this work, most of the fuzzy inference systems are based on completely specified rule-bases; however, in certain cases simplification were made. In other cases some of the rules do not have physical significance but are part of the rule-matrix to ensure the behavior of the system along the borders of the region of physical significance. An example of this case is the combination of “high congestion” with “low obstruction” for the evaluation of the degree of congestion of a unit.

The Mamdani algorithm allows the specification of weighting factors to assign different degrees of importance to each rule, but for the present model it is assumed that all the rules have the same significance, hence all the weights are set to 1. As indicated by Berkan and Trubatch (1997), when hierarchical systems are used, the individual rule design is not affected; however, care must be taken in order to ensure that the overall behavior of the system is as required. The test of individual rules and rules sets is described in Chapter VII and is mainly related to the evaluation of specific cases.

7.1.5 Software

The software used for the design and evaluation of the fuzzy inference systems is MATLAB® and the basic software for the functions for the Mamdami algorithm and fuzzy operations are from Hines (1997). The basic algorithm has been adapted to the needs of this research.

7.2 ON SCALE THEORY AND VARIABLE TYPE

As explained in Chapter IV several of the indices used in process safety have a classificatory nature, due to the lack of understanding of the physical phenomena to convert them into quantitative measures. According to Torgerson (1958) the classificatory concepts about properties are substituted by quantitative measures as science progresses. The transition from classificatory indices to quantitative measures offers several advantages [Torgerson, 1958]:

- Ordering of lumped elements: a quantitative measure allows establishing a logic relative sequence of elements classified under the same category. For instance, while the vague concept "warm" can group several objects whose temperature is neither high nor low, the use of the quantitative construct "temperature" allows classifying the object within the same category of warm. A similar problem exists in safety and as indicated in Chapter II, score-based indices exhibit lack of sensitivity within the limits of the subintervals and excess of sensitivity at the sub-range thresholds. For example, if the temperature range between $0 \leq T < 70$ °C receives a score of 0, the range between $70 \leq T < 150$ °C receives a score of 1 and the range between $150 \leq T < 300$ °C receives a score of 2 [Heikkila, 1999], then a temperature of 70 °C has the same significance as a temperature of 140 °C. However, since the physical implications of a temperature of 69.9 °C are practically the same as the implication at

70 °C (but they receive different scores), and 150.1 °C can be assumed to be the same as 150 °C, then 69.9 °C and 150.1 °C should also be the same (and with them the rest of the intervals between 70-150 °C and 150-300 °C). This is the same paradox introduced in Chapter VI by the discussion about the vagueness associated with weather classification.

- Increased descriptive capability: quantitative measures allow the formulation of general physical models. For instance, the relation between temperature change and the variation of height of a mercury column cannot be established by using classificatory concepts.
- Application of theories of higher mathematics: when a quantitative measure is used the general laws can be expressed in terms of equations (e.g., the calibration curve for a mercury thermometer expresses the relation between temperature and mercury height) and can be linked to other theories (i.e., the concept and measurement of temperature played a fundamental role in the development of thermodynamics).

A fundamental distinction between two important types of constructs, systems and properties, must be established here. While systems are formed by objects and properties, only the latter can be measured while the former can only be classified. Properties of a system can be observed, hence measured, however the system by itself cannot be measured [Torgerson, 1958].

A type of construct that is important in safety is the consequences of an incident. The consequences can be assumed to be another system formed by objects and properties. For instance, the consequences of a fire can be explosion, damage due to overpressure, fatalities and injuries. Some of them are objects (e.g., fire and damage) while others are properties. The distinction becomes important when measuring safety because fire cannot be measured hence flammability is assessed by using intrinsic properties of the chemicals representative of the degree of easiness with which the chemical is ignited. The effect of the explosion can however be measured in terms of the magnitude of the overpressure generated from the explosion (i.e., TNO multi-energy model). On the other hand, the consequence of exposure to a toxic chemical could be different type of systemic injuries, and fatalities. In this case the potential toxic effects of a chemical are assessed by using the effects of the chemicals (i.e., LD $_{50}$) rather than its intrinsic properties. These are examples of "proxies" [Bradley and Schaefer, 1998] which are characteristics used to describe entities that cannot be measured.

7.2.1 Measurement scale types

After the properties that need to be measured are selected an isomorphism must be established by developing a one-to-one relationship between a certain quantity of the property and a specific number that is assigned to the measured quantity. The numbers assigned are located on the real axis (or real number series) and have the following characteristics:

- Order: the numbers are ordered
- Distance: the difference between a pair of numbers is ordered with respect to difference between any other pair (e.g., larger, equal, or smaller)
- Origin: the real number series has a unique origin (i.e., zero).

Depending on how many characteristics are obeyed by the isomorphism, the obtained measurement scale is different. Order is the only property held by all scales then, depending on the presence of the other two properties, four different unidimensional scales can be obtained:

1. Ordinal scale: in this case there is no natural origin and the property of distance is not obeyed. Data on this scale is ordered but not in a quantitative way. The numbers assigned to the magnitude of the property follow the same relative order as the relative order of magnitude.
2. Ordinal scale with natural origin: this ordinal scale has the additional restriction that the lack of the property receives a score of zero. An example of this is the NFPA scoring system; a score of 3 for flammability means that the chemical is more "flammable" than another chemical with a score of 2 or 1. When the score is 0, the

chemical is classified as nonflammable. However, in the case of flammability the score indicates the relative distance between flash temperature and boiling point with the atmospheric temperature, as described in Chapter VII. Ordinal scales are described by monotonic increasing functions such as $f(x) > f(y)$ if $a > b$.

3. Interval scale: in this case there is no origin but the order of the number assigned to a specific magnitude of the property follows the same relative order of the magnitude, and additionally the difference between two scores is representative of the difference in magnitude between two states of the property. An example of this type of scale is time. Other examples are the Celsius and Fahrenheit temperature scales. Here a positive linear transformation such as $f(x) = ax + b$ where $x > 0$ is used. However, the position of the zero is not fixed and varies with the value of b.
4. Ratio scale: when the interval scale has a meaningful zero indicating a natural origin (i.e., lack of the specific property), hence here the distance is related to the origin. In this case the ratio between two numbers is meaningful. Examples of this type of scale are the Kelvin and Ranking, temperature scales, length, and weight. A similarity transformation of the type $f(x) = ax$ with $x > 0$ is used and implies that no matter the value of a, the zero does not change.

An additional scale, the nominal scale, is the simplest and only requires categorization without following a logical order. Each category receives a name, which cannot be logically ordered with respect to other classes. For instance, type of processing equipment classified according to unit operation. The objects must be classified according to a specific property or set of properties, however for this scale only the presence or absence of the specific property is important, while for the other scale the “amount” or magnitude of property present is required.

This type of scale is similar to the classification of a chemical processing plant as safe/unsafe based on the presence/absence of a specific set of properties (i.e., low risk from the traditional safety viewpoint). However, in Chapter IV it was noted that safety cannot be classified in such a dichotomy because of the complexities involved in the problem, and it would be better to use “degree of safetiness” as also indicated by Mansfield and Cassidy (1991). Torgerson (1958) presents further analysis about scale types and conceptual interpretations from various authors.

Assuming that our system is a specific type of equipment (e.g., vessel) and we are interested in measuring the degree of hazard inherent in the vessel due to its mechanical design, its operating conditions or the chemical, we need to identify measurable properties that can be related to the “degree of hazard”. Since inherent safety deals with the elimination or reduction of hazards, it is possible to infer that the “degree of inherent safety” is directly related to the “degree of hazard” of the vessel. As explained in Chapter IV, the absolute state of inherent safety occurs when all sources of hazard have been removed; therefore the degree of hazard is zero. This limit establishes a natural origin for the measurement of inherent safety, hence the only scales that can be used are ordinal with origin or ratio (which is the interval scale with origin).

7.2.2 Application to safety evaluation

While the information presented in Chapter IV suggests that it should be possible to develop an interval or ratio scale for inherent safety evaluation, the lack of information as well as the lack of a “theory of safety” able to connect the available constructs, limits the progress toward the development of such “safety scale”. A scale for inherent safety could be developed by comparing the magnitude of the physical consequences associated with certain combination of parameters to the consequences of a standard set of conditions whose known consequences can be assumed to be “inherently safer” because they do not pose a substantial hazard. For example, the release of a flammable chemical in vapor form at low pressure implies a lower hazard degree than the release of the same chemical in a liquid form at high pressure and temperature. The reference states should be chosen for each set of rules and requires not only consensus among safety practitioners (in order to make sure that the selected “inherently safer” reference state is widely accepted) but requires also the development of data through modeling and simulation, and in some cases a better scientific understanding of the phenomena involved, as in the case of reactive chemicals. Because of the previous limitations and research challenges, for this prototype model, the scale of “inherent safety” is based on a continuous ordinal scale between 0 and 1 with two fixed points: 0 for no hazard and 0.5 for the reference threshold as explained in section 1.4 of this chapter.

7.3 MODEL OVERVIEW FOR INHERENT SAFETY

This section introduces the general inherent safety model proposed by this research however, the hierarchical fuzzy model described in next section, only focuses on the first part of the overall model.

7.3.1 Description of the overall inherent safety model

In Chapter II and IV it was indicated that inherent safety is complementary to the traditional safety model, and it is suggested as the first option in order to reduce process hazards and the consequent risk. It was also stated that inherent safety must be applied by looking at the whole chemical plant as a system in order to identify hazard migration problems. Another aspect that must be taken into account is the fact that hazard will “migrate” outside the boundary of the plant if hazard reduction is sought through reduction of storage capacity and transportation of chemical substances is not taken into consideration.

Therefore, following the format of fuzzy IF-THEN rules to capture all the relevant aspects related to inherent safety, the next two overall rules can be developed. The first rule is:

IF “chemical hazard” is “LOW” AND “dispersion potential” is “LOW”
AND “design hazard” is “LOW” THEN “inherent safety level” is “HIGH”

The evaluation of “chemical hazard” is based on chemical properties that describe the potential toxicological, environmental, and explosion hazard. The “dispersion potential” depends on chemical properties but also operating conditions, while “design hazard” depends mainly on characteristics of the plant but also on some chemical properties. This is the part of the overall model addressed by this research and the proposed hierarchical model is explained in the next section.

It is assumed that each equipment, pipe, and element of a plant contributes in some degree to the overall hazard; therefore the previous rule must be applied to each equipment and pipe. The summation of all the indices will represent the overall hazard score for the plant. This idea is similar to the concept of cost, where the total cost of the plant is the summation of the individual costs of each equipment and pipe.

However, inherent safety cannot always be achieved because of technical or economic limitations in the application of the principles. As a result, options to reduce risk (but not hazard) such as the application of passive and active layers of protection, and administrative controls, are used to increase the extrinsic safety level.

Looking at another aspect of the problem, true inherent safety can only be achieved without minimizing the transportation hazards, although this could decrease the chances for eliminating plant hazards by inventory reduction. The rule here should be:

IF “inherent safety level” is “LOW” AND “transportation hazard” is “LOW”
THEN “overall inherent safety level” is “HIGH”

Transportation is addressed in this research by evaluating chemical transportation by train and the proposed preliminary model is briefly described in Chapter X.

An additional fuzzy inference system can be developed in the future in order to evaluate the relation between the size of a plant and its overall inherent safety index (calculated as the contributions for each piece of equipment). A large plant with a low inherent safety index can have a lower hazard density than a small plant with a low index. Plants with high hazard density could have more opportunities for design improvement than plants with low hazard density. A small plant with high inherent safety index (hence very high hazard density) could be very inherently unsafe. Several tests must be performed before the set of rules for the consistency rules can be designed because it is necessary to analyze several case studies on real plants, which is outside the reach of this project.

7.4 DESCRIPTION OF THE INHERENT SAFETY HIERARCHICAL MODEL

The basic assumption upon which the methodology is based is that every piece of equipment and pipeline acts as a vessel with a double objective:

- accomplish a specific processing task (i.e., unit operation)
- keep the chemical substances confined avoiding releases to the environment

For example, the task of a storage tank is to accumulate a certain volume of chemicals, while the task of a pump is to increase the pressure of a specific stream. For a process vessel, the task could be mixing to obtain a homogeneous chemical mixture or to ensure homogenous heat transfer. The loss of the mixing action (due to malfunction or other upsets) may imply the appearance of hazards due to heterogeneous properties such as hot spots or points with concentrations different from specifications. In the case of reactive chemicals, the heterogeneity can result in a runaway reaction. Hence there are hazards inherent to the specific task of the equipment.

Regardless of the specific task, every equipment and pipeline has a common purpose related to avoidance of releases of chemicals. Based on this assumption a general model for the evaluation of hazards and their interactions can be developed. The general hazards analyzed by the proposed model are:

- explosion due to continuous release of flammable chemicals
- toxic dispersion and environmental impact due to continuous release of toxic substances

The model can analyze these hazards for pure chemicals, released from vessels such as storage tanks and process drums. The application to towers, heat exchangers, and pipelines is possible by modifying the basic model. For instance, heat exchangers can be modeled as two vessels; however, the hazard derived from mixing the two streams is not accounted for. Distillation towers can be modeled by assuming that the normal liquid level is the one present for the reboiler. The following aspects are not considered:

- Internal explosions
- Sudden release of chemicals (i.e., puff dispersion model)
- Domino effect
- Stability of process control related to volume intensification
- Mixtures of chemicals (unless the required mixture properties are calculated by using accepted methodologies)
- Reactivity with air or incompatible chemical contaminants
- Toxicity of combustion products
- Toxicity of reaction products due to environmental degradation
- Reaction due to mixture of incompatible chemicals
- External corrosion due to specific environments
- Corrosion under insulation

However, in the future, specific models for each type of hazard and each type of equipment can be developed by adding the required design parameters and developing the fuzzy IF-THEN rules.

7.4.1 Description of the basic hierarchical model for vessel i in unit j

The basic event taken into account by the model is the release of chemical substances and the possible consequences in terms of fire and explosion, toxic effects on humans and the environment as well as long-term effects on the atmosphere. Problems associated to the loss of production due to process upsets that reduce the quality of the final product are not considered.

The model takes into account the interaction of several parameters, by using 35 sets of IF-THEN rules arranged in a hierarchical tree-like structure that describes the potential hazard due to combinations of specific conditions such as chemical properties, operating conditions, and equipment design parameters. Figure 7.1 presents the explanation of the symbols used for the diagrams in Figures 7.2 through 7.9.

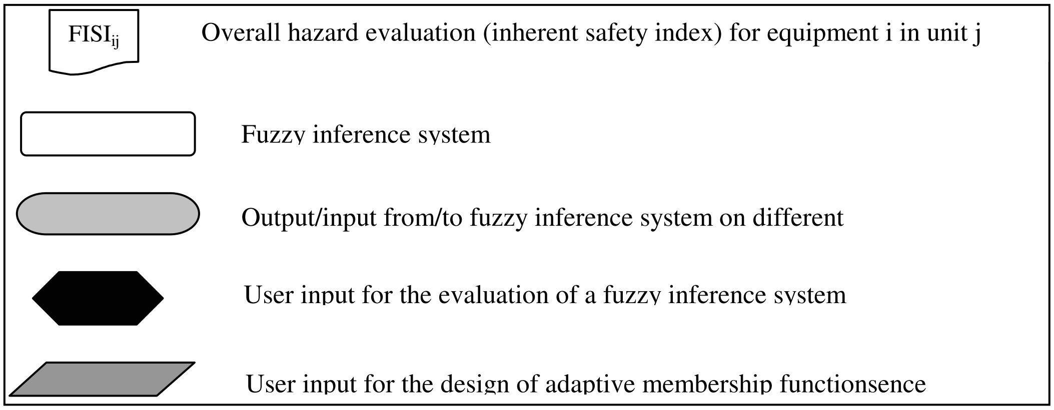


Figure 7.1: Explanation of symbols used in Figures 7.2 through 7.9

The first layer of the tree (i.e., Layer 1 in Figure 7.2) describes the inherent safety level (ISL) as a fuzzy index (FISI$_{ij}$) of the equipment i located in unit j as a function inversely proportional to the amount of hazard inherent to the chemical properties of the substances (which are also affected by specific operating conditions) and the characteristics of the design of the equipment including volume. The description of the interaction between the two main sources of hazards is obtained by the first set of IF-THEN rules of the form:

IF (“chemical hazard” is ____) AND (“mechanical hazard” is ____) THEN (ISL is ____)

This rule expresses the principles of “intensification”, “moderation”, and “substitution”, by indicating that “chemical hazard” can be reduced either by selecting a less hazardous chemical and/or less hazardous processing conditions (evaluated in Layer 2.1) while the potential consequences of “mechanical hazard” can be reduced by using smaller volumes and/or more benign operating conditions (evaluated in Layer 2.2) as shown in Figure 7.2. However, in order to assign each a high degree of inherent safety (i.e., low inherent hazard, $FISI_{ij} < 0.5$) both conditions, “chemical hazard” and “mechanical hazard”, must be low. The outputs from Layer 2.1 and Layer 2.2 are used as the inputs for Layer 1, and they are calculated by evaluating respectively the fuzzy inference systems for “chemical and design hazards” (ISICHEM), and “mechanical and design hazards” (ISIMECH) as indicated in Figure 7.2.

The combination of hazards posed by the chemical substances present in the equipment i being analyzed is evaluated by the FIS called “Hazard due to chemical and design factors” (ISICHEM) whose IF-THEN rules combine the results of the inference systems that evaluate toxic chemical hazard (for humans and environmental) and hazards due to flammability and reactivity behavior. The IF-THEN rules evaluated for ISICHEM have the following general structure:

IF (“fire/explosion/reactivity hazard” is ____) AND (“toxicity/environmental
impact” is ____) THEN (ISL is ____)

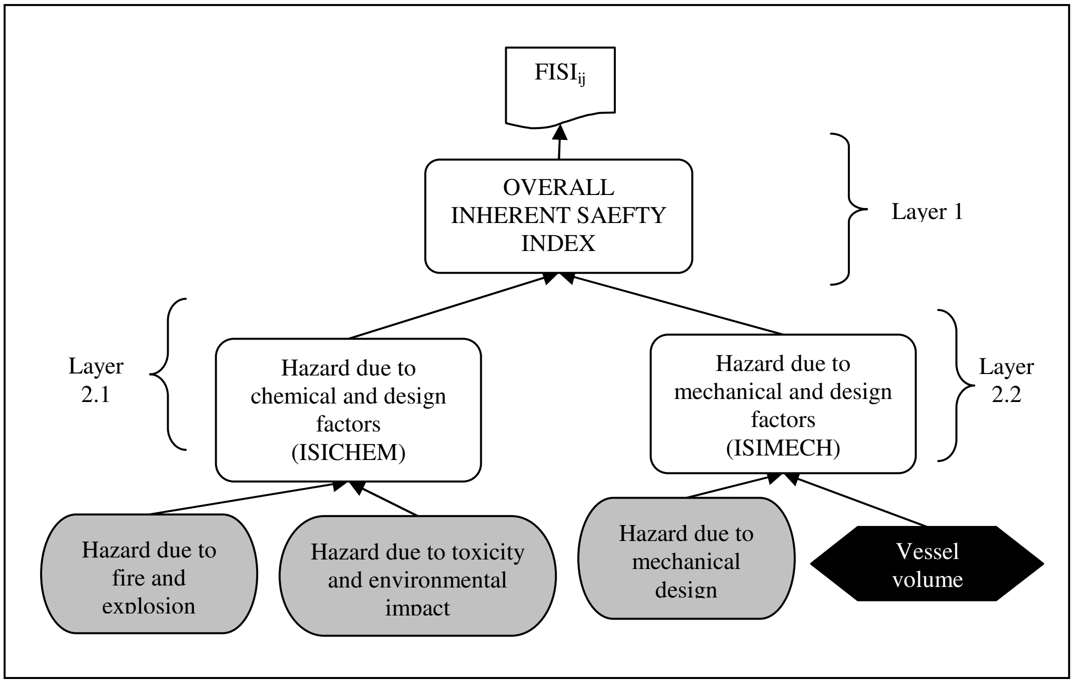


Figure 7.2: Hierarchical tree for Layer 1 and Layers 2.1 and 2.2

The objective of this set of rules is the identification of conflicts between process safety requirements and environmental requirements. In order to be considered inherently safer a chemical must show low toxicity, be environmental friendly, and have low flammability and reactivity. If any of these properties is high then the inherent hazard posed by the substance in equipment i will increase. It is important to clarify that design factors, such as operating conditions, are able to modify the inherent hazard due to chemical properties of the substances; however, this is taken into account by the next layer as explained below. The inherent safety principle evaluated is “substitution”.

As shown in Figure 7.2, the hazards due to the interaction of mechanical and design factors is evaluated by the FIS called ISIMECH which describes principles such as “minimization”, “moderation” and “simplification”. The general objective of this set of rules is to capture the possibility of release occurrence due to vessel failure caused by internal corrosion, or chemical release due to failure of vessel connections such as nozzles and other penetrations of the wall of the tank. The set of IF-THEN rules evaluated for ISIMECH has the following general form:

IF (“hazard due to mechanical design” is ____) AND (“volume” is ____)
THEN (ISL is ____)

An important factor used as input for this FIS is the volume of the vessel. For this FIS the effect of the volume plays a double role since it affects the amount of chemical substance contained, but also is an indication of the area of plastic or metal surface exposed to the chemical and subject to corrosion or other forms of mechanical failure. If the potential for failure is high but volume is small, then the overall hazard obtained by the interaction of the two factors is reduced.

By including the variable “volume” at this point it is possible to capture the importance of this variable for inherent safety, as recognized by several authors and also often misunderstood, as explained in Chapter IV, when volume reduction is seen as the sole approach for reaching an inherently safer design. The value of volume has the power to minimize or magnify the hazard posed by chemical properties, operating conditions, or mechanical design. If the potential for mechanical failure is low but the volume is large then the overall hazard due to the interaction is high but must be combined with the chemical hazard; if chemical hazard is low then the overall hazard will be low to giving then a high degree of inherent safety, but if the chemical substance presents a high degree of hazard (which is obtained by combining chemical properties and operating conditions) then the overall hazard level will be higher yielding a lower inherent safety level.

7.4.2 Description of the hierarchical model for chemical hazard: toxicity

The inherent chemical hazard due to toxicity combines two factors, hazards due to human toxicity and due to environmental impact, with the dispersion potential in case of release. The hierarchical tree is shown in Figure 7.3.

The fuzzy inference system called "Hazard due to toxicity, environmental impact, and potential dispersion" (AGCHM) is formed by a set of IF-THEN rules of the type:

IF ("human/environmental chemical hazard" is ____) AND
("hazard due to toxic dispersion" is ____) THEN (ISL is ____)

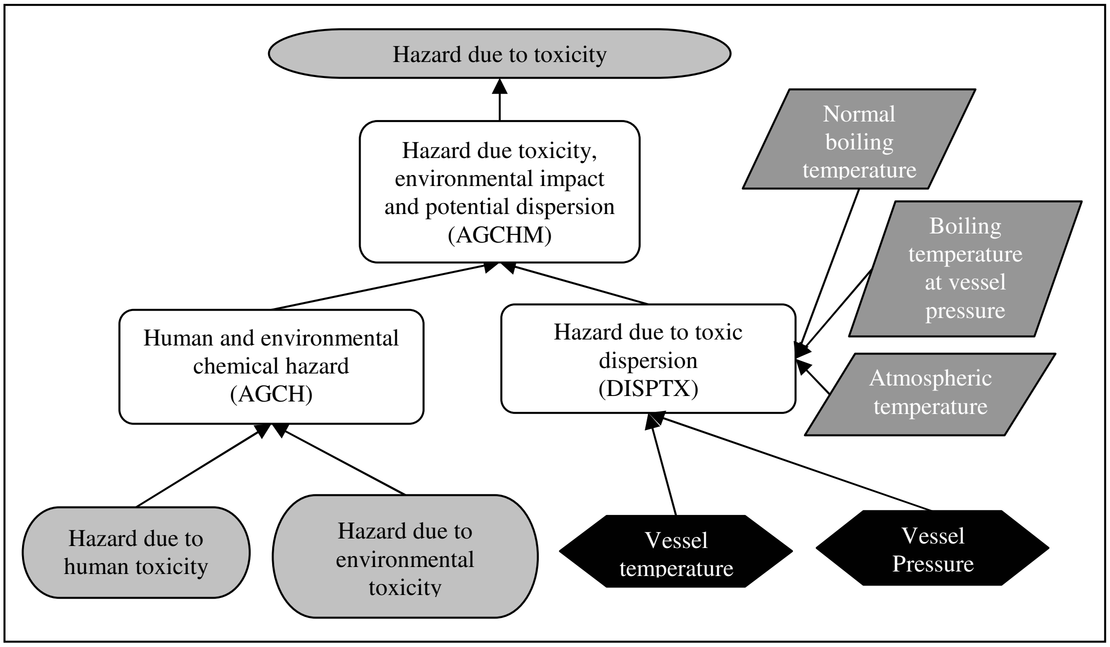


Figure 7.3: Hierarchical tree for the evaluation of hazards due to chemical properties

The rules evaluate the interaction between the toxicity potential with the possibility of releasing the substance in a physical form capable of dispersing into the environment. The analyzed inherent safety principles are “substitution” and “moderation”. If the chemical is not toxic or the operating conditions are able to reduce the dispersion potential, then the hazard posed by the vessel is reduced. However, if the chemical is toxic for humans and/or the environment and is managed at conditions such as high pressure and/or high temperature, then the potential for releasing large quantities able to vaporize and disperse increases, reducing the inherent safety level of the equipment (expressed as high hazard level).

The “hazard due to toxic dispersion” (DISPTX) requires inputs from the user in order to evaluate the rules but also to define the parameters of the membership functions, which for this fuzzy inference system are adaptive. The information required for the design of the membership functions is;

- Normal boiling temperature
- Boiling temperature at vessel pressure
- Atmospheric temperature

The input parameters for the FIS are:

- Operation temperature of the vessel
- Operating pressure of the vessel

The values for these inputs can be provided as crisp numbers (e.g., operation temperature = 45 °C and pressure = 4 atm) or they can be given as fuzzy numbers representing the expected variation in the vessel temperature and pressure (e.g., maximum operation temperature = 55 °C, normal operation temperature = 45 °C, minimum operation temperature = 35 °C). The use of a range of temperature and pressure increases the uncertainty of the analysis, (i.e., more rules are fired) but increases the flexibility of the methodology because rather than exploring one single operation point, the whole region where the equipment is likely to operate is analyzed. The objective of the IF-THEN rules for this FIS is the detection of operating points near the saturation curves. In this region, when the chemicals are released in the liquid phase (e.g., operating temperature lower than saturation temperature at the vessel pressure) the released mass flow is higher compared to a vapor release (e.g., operating temperature higher than saturation temperature at the vessel pressure). However, if the released chemical is in the liquid phase and the vessel operates at a temperature higher than the normal boiling point, then the liquid will totally or partially vaporize producing a vapor cloud that will be dispersed. If the pressure of the vessel is higher than the atmospheric pressure, then the released flow rate increases but also increases the possibility of aerosol formation that increases the evaporation rate. The fuzzy IF-THEN rules used for DIPTX have the following general form:

IF (“vessel temperature” is ____) AND (“vessel temperature” is ____) AND
(“vessel pressure” is ____)
THEN (ISL is ____)

The input “vessel temperature” is used by two linguistic variables and the logic behind this requirement is explained in Chapter VII. The traditional approach for dispersion modeling requires weather and wind parameters (e.g., atmospheric stability, wind velocity) however in this case it is assumed that in order to be dispersed a chemical has to be released. If the mass of the released chemical is small then the hazard is reduced regardless of weather conditions. However, if the released mass is large and has the potential to quickly evaporate and form a toxic cloud, then the toxic hazard will be large. A similar approach is followed by Hendershot (2003) to demonstrate the effect of phase type on the total mass of released chlorine from a pipeline of liquid chlorine and another of gas chlorine. The weather and wind parameters change the shape (e.g., length, width, height) of the cloud in predictable ways and, and unless the wind is strong enough to quickly dilute the cloud, the dispersion hazard remains.

The fuzzy inference system “Human and environmental hazard” (AGCH) shown in Figure 7.3 has the objective to combine the effect of the chemicals on human as well on water organisms, animal, and the troposphere. The IF-THEN rules have the general form:

IF (“human toxicity” is ____) AND (“environmental impact” is ____)
THEN (ISL is ____)

and evaluate the inherent safety principle “substitution”. In order to be considered inherently safer a chemical must show low or no human toxicity but also low or no environmental impact. If either two effects are capable of producing adverse consequences, then the hazard level increases reducing the degree on inherent safety.

The hierarchical tree for the evaluation of the environmental hazard due to toxicity is shown in Figure 7.4.

The evaluation of environmental impacts is divided in two main parts, water/soil and air impacts, combined by the FIS called “Hazard due to water/soil and troposphere toxicity” (AGET). This set of rules evaluates the environmental part of the inherent safety principle “substitution” in the sense that, in order to be inherently safer from the environmental view point, a chemical must show certain characteristics given by the outputs from two other FIS: “Hazard due to atmospheric stability” (CHEp), and “Hazard due to bioaccumulation potential and degradability” (CHPF). The IF-THEN rules for AGET have the form:

IF (“bioaccumulation/degradability” is ____) AND (“atmospheric stability” is ____)
THEN (ISL is ____)

The ISL index will be high only when both antecedents of the rules reflect low inherent hazard; if both or either antecedent imply high hazard, the ISL index will be low.

As shown in Figure 7.4, “atmospheric stability” is evaluated by a FIS whose inputs have to be fed by the user for the chemical used by the equipment being evaluated. The required information is:

- Troposphere half-life time
- Quality of used data

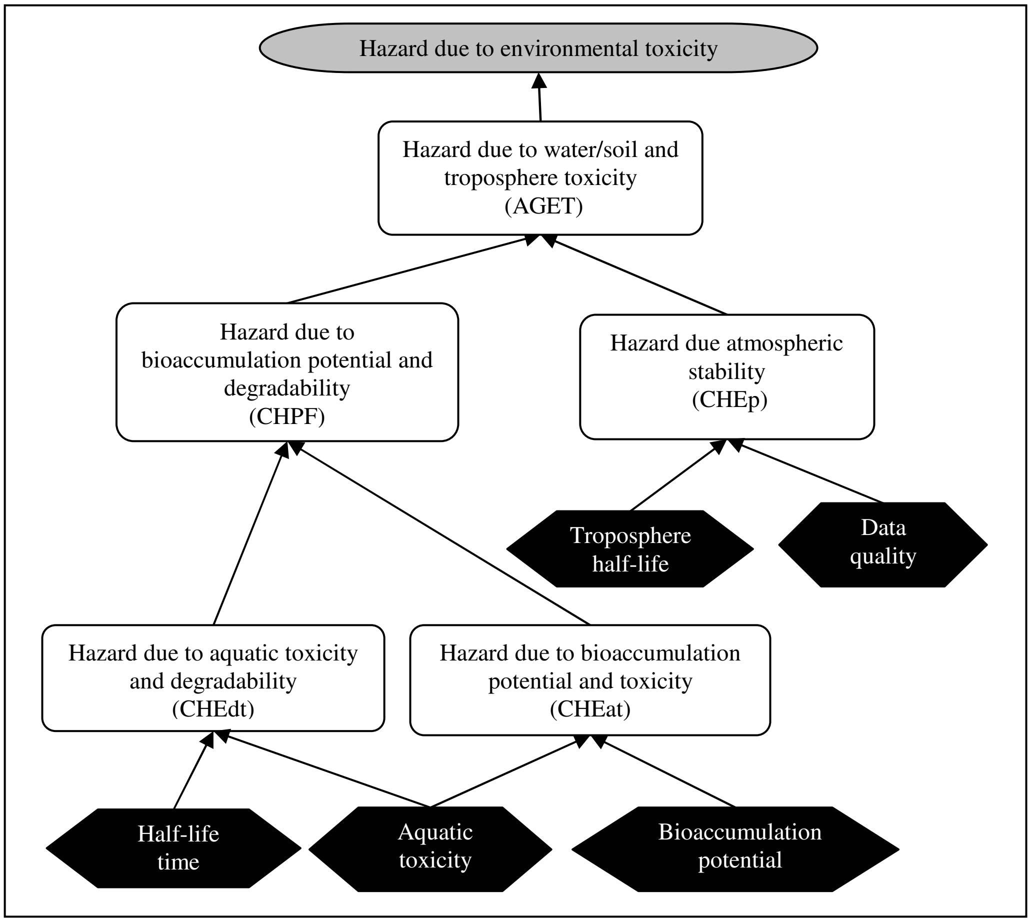


Figure 7.4: Hierarchical tree for the evaluation of environmental hazard due to chemical properties

As implied by the second input, the information required for the evaluation of the chemical impact on the atmosphere is highly uncertain. The troposphere half-life time can be fed as a fuzzy number indicating the possible range of values that can be assigned to the parameter. This option reduces the uncertainty associated with the decision about which number to choose from a possible set of values given by different references.

On the other hand, each source of information can have a different level of accuracy and credibility and this type of uncertainty is also taken into account by the second input. The details of the FIS are explained in Chapter VII. The set of IF-THEN rules for CHEp has the following general form:

IF (“troposphere half-life time” is ____) AND (“quality of information” is ____)
THEN (ISL is ____)

If the half-life time in the troposphere is large then the chemical tends to be less degradable therefore will accumulate. An example of this type of behavior is given by the chlorofluorocarbons that not only accumulate but also interact with the ozone layer. In this case the possibility of atmospheric reaction is not included because of the lack of information easily accessible to non-experts in the field.

The evaluation of the chemical hazard to the biota is estimated by the fuzzy inference system called “hazard due to bioaccumulation potential and degradability” (CHPF), as shown in Figure 7.4. This FIS combines the effects due to bioaccumulation, water and animal toxicity, and degradability; when either of these characteristics, or its combination, implies threat to the biota the overall hazard level increases reducing the degree of inherent safety. Therefore, this FIS evaluates another aspect of the principle of “substitution”. The general format of the IF-THEN rules fro CHPF is:

IF (“hazard due to toxicity/bioaccumulation” is ____) AND (“hazard due to
toxicity/degradability” is ____) THEN (ISL is ____)

The principal concept behind the rules are explained in Chapter VII, but in general when the chemical substance presents high bioaccumulation potential (i.e., due to liposolubility) and toxic effects, the inherent hazard to animals increases which increases the possibility of chemical accumulation in the higher links of the food chain. If the chemical substance presents low degradability then the possibility of accumulation in soil increases and if this effect is combined with toxic potential, the overall hazard level become high. Chemical products generated by degradation reactions, which can be more toxic than the original chemicals, are not taken into consideration. Additional rule sets can include this hazard.

As shown in Figure 7.4, the inputs for the fuzzy inference system CHPF are calculated by two FIS; the first one is called "Hazard due to aquatic toxicity and degradability" (CHEdt), while the second is called "Hazard due to bioaccumulation potential and toxicity" (CHEat). The inputs for these two FIS are given by the user for the specific substance. For the inference system CHEdt the required inputs are the following:

- Half-life time
- Aquatic toxicity

For the inference system CHEat the required inputs are the following:

- Bioaccumulation potential
- Aquatic toxicity

In both cases, the inputs can be provided as single numbers, with a low degree of uncertainty, or as fuzzy numbers able to describe the possible range of values. The information required for the evaluation of these two FIS must be obtained from several references and data sources, therefore it is assumed that in most of the cases the inputs are uncertain and, in order to avoid losing the information regarding their uncertainty, the option of using fuzzy number reduces the problem of deciding which crisp value would be the best. This approach is useful when the user is not an expert in environmental chemistry but requires getting a general idea about the potential effects of a specific chemical.

As shown in Figure 7.3, the next branch of the hierarchical tree for the evaluation of chemical toxicity is related to humans, as shown in Figure 7.5. The fuzzy inference system called "Hazard due to human acute and chronic toxicity" (AGHEA) combines the potential short and long term effects due to exposure to the specific chemical present in the analyzed equipment i in unit j. The general format of the IF-THEN rules for this FIS is the following:

IF ("hazard due acute human toxicity" is ____) AND
("hazard due to chronic human toxicity" is ____)
THEN (ISL is ____)

The objective of this set of rules is the evaluation of the inherent safety principle "substitution" in terms of human toxicity, by implying that if the chemical is capable of producing acute effects or long-term consequences such as cancer, then the potential hazard associated with a release and human exposure due to dispersion increases, reducing therefore the overall level of inherent safety. The input for the antecedent related to chronic effects is the output of the fuzzy inference system called "hazard due to chronic human toxicity" (CHHc) which combines the information regarding the potential hazard of human cancer. This type of information is highly uncertain and must rely not only on human data but also on animal test. Because of this the required inputs are the following:

- Human cancer evidence
- Animal cancer evidence

Due to the uncertainty of this information because of lack of data, extrapolation of information across species, and the complexity of living organisms the inputs are characterized by high uncertainty, which is addressed by the model by allowing the use of a range of data through fuzzy numbers. The general structure of the IF-THEN rules is the following:

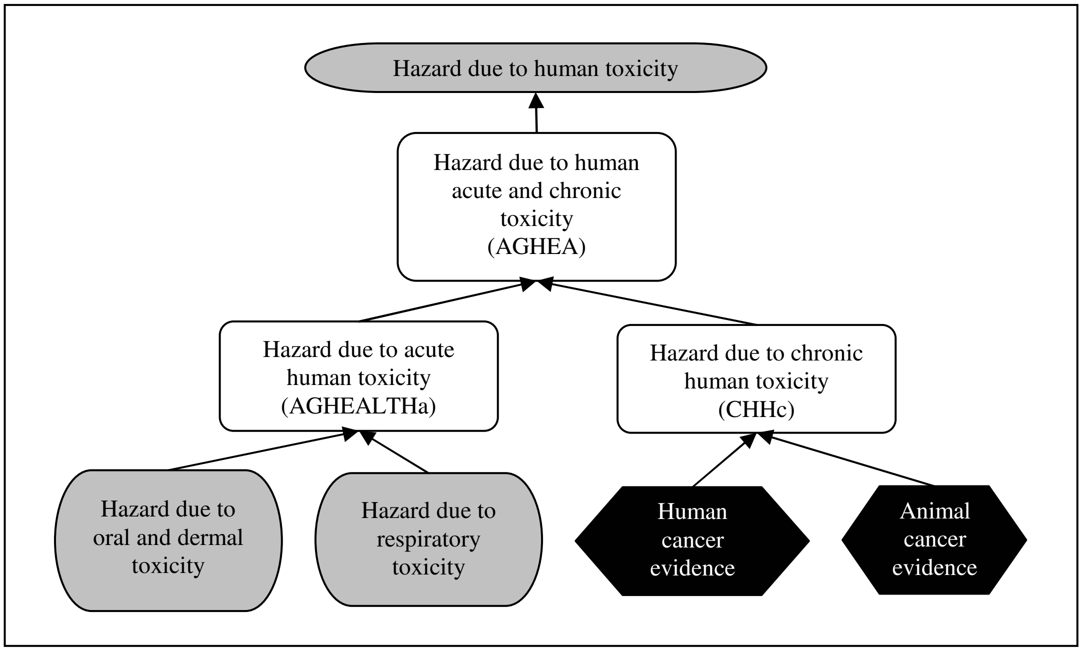


Figure 7.5: Hierarchical tree for the evaluation of human toxicity

IF (“human cancer evidence” is ____) AND (“animal cancer evidence” is ____)
THEN (ISL is ____)

If there is enough information about the human response to a certain chemical in relation to cancer occurrence, regardless of the lack of animal evidence, the resultant inherent hazard will be high. On the other hand, if human information is not available but there is enough animal evidence about the potential occurrence of human cancer, then the inherent hazard is also assumed to be high. The only situation when the inherent cancer hazard is low occurs when the evidence for both, animals and humans, suggest so.

The evaluation of acute toxic effects for humans is evaluated by the FIS called “hazard due to acute human toxicity” (ACHEALTHa), as shown in Figure 7.5. This set of rules evaluates the inherent safety principle “substitution” in terms of the potential short-term effects on human health caused by the chemical substance used in the equipment being evaluated. The structure of the general rules for this FIS is the following:

IF (“hazard due to respiratory toxicity” is ____)
AND (“hazard due to oral/dermal toxicity” is ____) THEN (ISL is ____)

The structure of the rule is based on the assumption that dermal and oral exposure to the chemical requires direct contact with the substance as in the case of an operator. Hence, this part of the rules is mainly focused on industrial hygiene practice and people not supposed to work with the specific chemical should have less possibility of being exposed through these routes. Exceptions to this assumption are emergency response personnel who might respond to emergency events. Respiratory toxicity is assumed to present a broader impact due to the possibility of cloud generation and dispersion exposing larger number of people and general public.

The inputs for this fuzzy inference system are the outputs obtained from the evaluation of other two sets of rules, “hazards due to respiratory toxicity” and “hazards due to oral and dermal toxicity” (CHH1a), shown in Figure 7.6.

The evaluation of the set of rules for CHH1a combines the evidence of toxicity due to ingestion of the chemical and due to acute dermal contact. The general structure of the IF-THEN rules is the following:

IF (“acute oral toxicity” is ____) AND (“acute dermal toxicity” is ____)
THEN (ISL is ____)

The objective of the rule is to identify the potential occurrence of adverse health effects due to either characteristic or due to a combination of both. The chemical is evaluated with a low degree of inherent hazard only when both types of toxicity are low; therefore the chemical is assumed to be inherently safer with respect to these specific aspects of the acute human toxicity. The evaluation of the FIS requires the input of:

- Human acute oral toxicity

- Human acute dermal toxicity

As in the previous cases, the information regarding toxicity is highly uncertain, and the system takes it into consideration by allowing the input of both crisp and fuzzy numbers. When only a range of toxicity values is available and it is not possible to decide which number to use, the fuzzy number can be formed by the lowest most likely value, the average value, and the highest possible value.

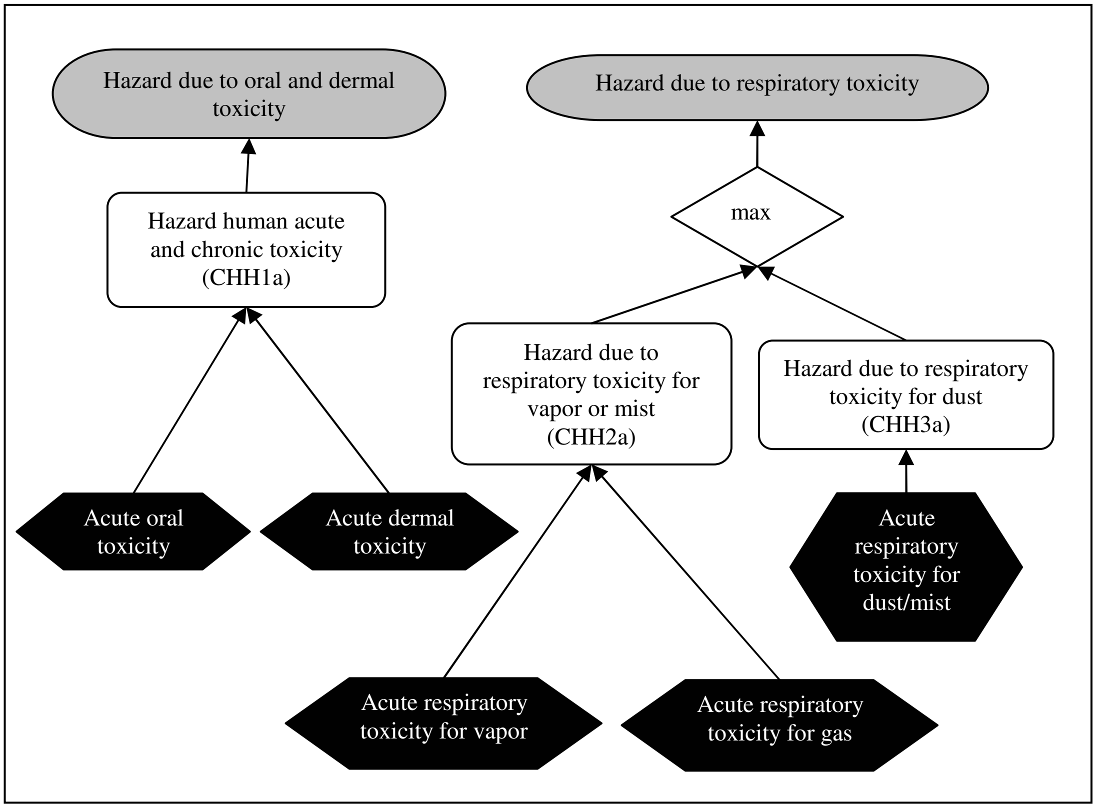


Figure 7.6: Hierarchical trees for the evaluation of hazards due to human oral/dermal toxicity and respiratory toxicity

The evaluation of respiratory toxicity requires the distinction of the physical phase of the chemical. When the substance is in a powder or dust form, the inhalation hazard is evaluated by the FIS called "hazard due to respiratory toxicity for dust" (CHH3a) while when the physical form is liquid, vapor, gas, or mist, the hazard is evaluated by the FIS called "hazard due to respiratory toxicity for vapor or mist"(CHH2a). The general IF-THEN rule format for CHH3a is the following:

IF ("acute dust toxicity" is ____) THEN (ISL is ____)

In this case the rules map a range of toxicity from concentration units to a common scale of potential hazard. This step is required in order to facilitate the aggregation of results in the upper layers of the hierarchical tree. The input required from the user is the value of dust toxicity. The general IF-THEN rule format for CHH2a is the following:

IF ("acute vapor toxicity" is ____) AND ("acute gas/mist toxicity" is ____)
THEN (ISL is ____)

In order for the chemical to receive a low degree of inherent hazard, it must present low vapor and gas/mist toxicity. The structure of the rule is also based on the availability of the data, as explained in Chapter VII. The inputs required from the user are:

- Human acute toxicity for vapors
- Human acute toxicity for mist and/or gases

As explained earlier, the higher uncertainty associated with toxicity information justifies the use of fuzzy numbers as inputs.

7.4.3 Description of the hierarchical model for chemical hazard: fire and explosion

As shown in Figure 7.2, the second part for the evaluation of "hazards due to chemical and design factors" (ISICHEM) requires the evaluation of the fire and explosion potential. The hierarchical tree for the estimation of this hazard is shown in Figure 7.7. The overall evaluation of fire and explosion hazards is accomplished by the fuzzy inference system called "hazard due to fire and explosion" (AGEXPL), whose general IF-THEN rules are of the form:

IF ("hazard due to fire/explosion and congestion/obstruction" is ____)
AND ("hazard due to dispersion" is ____)
THEN (ISL is ____)

The structure of these rules combines the chemical potential for adverse consequences such as explosions with the potential of forming a cloud that could reach an ignition source. As in the case of toxic chemicals the possibility of formation of a cloud depends on the physicochemical properties of the substance but also on the operating conditions, hence the set of rules evaluates the principles of "substitution" and "moderation" by combining chemical properties, design factors, and operating conditions.

The evaluation of the interaction is fundamental for this FIS because regardless of the chemical potential for fires and explosions (i.e., due to intrinsic flammability, reactivity, and explosiveness of the substance) if the operating conditions reduce the potential for cloud formation (e.g., low temperature and pressure) the overall hazard is reduced. However, if the chemical is flammable, and is managed at hazardous conditions (e.g., high pressure, temperature above normal boiling temperature) then the hazard can still be reduced by designing the unit providing sufficient ventilation (e.g., low obstruction and low congestion) to avoid the formation of clouds and/or pockets of gas within the explosive range (e.g., concentration between lower and upper flammability limits). The structure of the rules offers the opportunity to take into account factor interactions and to develop and evaluate different design strategies in order to reduce the hazard due to fire and explosion.

As shown in Figure 7.7, the fuzzy inferences system AGEXPL requires the input from other two sets of rules. The first one is called "hazard due to dispersion" (DISP) which calculates the potential of cloud formation based on operating conditions and some properties of the chemical; the second one is called "hazard due to fire/explosion and congestion/obstruction" (ACOFRV) that estimates the inherent chemical hazard due to the substance properties and other design factors.

The fuzzy inference system for dispersion, DISP, is the most complex set of rules used by the whole hierarchical tree. It is formed by three set of similar rules with the following general structure:

IF ("vessel temperature" is ____) AND ("vessel temperature" is ____)
AND ("vessel pressure" is ____) THEN (ISL is ____)

The input "vessel temperature" is used by two linguistic variables in order to detect the type of phases inside and outside the vessel. The set of rules detects the phase of the chemical inside the vessel and the potential phase of the chemical outside the vessel. For toxic dispersion, it is assumed that if the released flow rate is liquid (e.g., vessel temperature below boiling temperature at vessel pressure) then the total mass available for vaporization and dispersion is much larger compared to the case of the release of a vapor phase. The leak flowrate is also proportional to the operating pressure; if the pressure is higher than the atmospheric then the flowrate is increased as well as the possibility of aerosol formation. Additional explanation of the physical phenomena and the assumptions is given in Chapter VII.

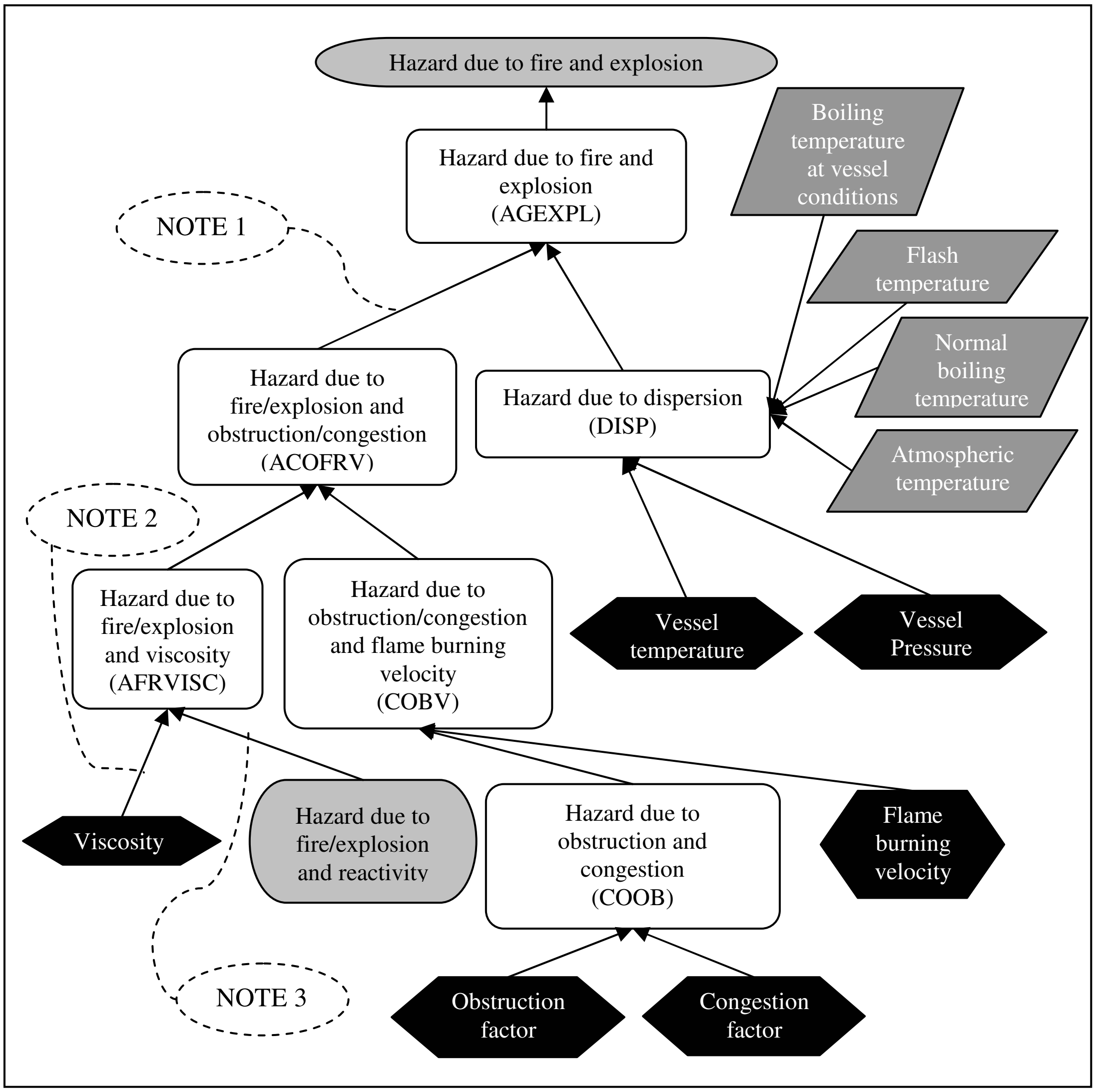


Figure 7.7: Hierarchical tree for the evaluation of fire and explosion hazards

The FIS for dispersion is based on adaptive membership functions whose parameters depend on physical properties of the evaluated chemical substance. Depending on the values of those properties, one of the three sets of rules is chosen to distinguish between chemical released as very cold liquids (e.g., vessel temperature below flash temperature of the chemical), liquids around environmental temperature, and vapor or gas phase

The inputs that the user must provide for the design of the membership functions are:

- Flash temperature for the chemical substance
- Normal boiling temperature
- Atmospheric temperature

The flash temperature is understood according to the NFPA definition as being the temperature at which the chemical can generate enough vapors to reach the lower flammability limit. For the evaluation of the dispersion potential the user must provide the following input values:

- Vessel operating temperature
- Vessel operating pressure

The user can choose to provide a crisp value or a fuzzy number for each required input. In the case of operating conditions, the fuzzy number describes the range within which temperature and pressure vary during normal operation. A second approach can include the expected maximum, normal, and minimum values expected during abnormal situations, start-up, and shutdown.

As shown in Figure 7.7, the second input required for the overall fire and explosion hazard (AGEXPL) is the output from the fuzzy inference system called “hazard due to fire/explosion and obstruction/congestion” (ACOFRV). This set of IF-THEN rules has the following general structure:

IF (“fire/explosion potential” is ____) AND
(“obstruction/congestion/burning velocity” is ____)
THEN (ISL is ____)

The rules evaluate the interaction of chemical factors with design parameters. The inherent safety principles evaluated are “moderation”, “simplification” and “substitution”. In order to generate a hazardous situation the chemical must be reactive or flammable but also the equipment must be located in an area with low ventilation (e.g., high obstruction) or high ventilation but high congestion where turbulence effects can enhance the flame front burning velocity (which depends on design factors and chemical properties). Regardless of the degree of congestion and obstruction, the flame burning velocity characteristic of the chemical (which is an inherent characteristic of the substance) can increase or decrease the hazard degree by modifying the resultant explosive overpressure.

The output from the fuzzy inference system ACOFRV, as shown in Figure 7.7, can be combined with another set of rules, indicated as NOTE 1, which can be added in future revisions of the model. Fire and explosions are likely to produce domino effects when the release of the flammable substance occurs in congested units where other equipment are likely to suffer damage and release more flammable chemicals. Another consequence of explosions is the possibility of damage to adjacent equipment due to missiles projected from the exploding equipment towards other areas of the plant. For the evaluation of possibility of the domino effect, design factors should be taken into account; for instance, equipment layout, spatial arrangement, distance between hazardous processing equipment, and hazard degree of other units. A special case of domino effect is described by Lees (1996) as pressure piling, and depends on the possibility of pressure waves generated from exploding internals to vessels towards other interconnected equipment. Khan and Abbasi (1998d) have proposed a model called DOMIFFECT that can serve as starting point for the development of the fuzzy inference systems that could be integrated into this prototype model.

The inputs for the fuzzy inference system ACOFRV are the outputs from other systems, as shown in Figure 7.7. The first one is the “hazard due to obstruction/congestion/flame burning velocity” (COBV), while the second is the “hazard due to fire/explosion and viscosity” (AFRVISC).

The objective of the fuzzy inference system ACOFRV is the combination of the hazards due to congestion and obstruction, and flame burning velocity. The general structure of the IF-THEN rules is:

IF (“obstruction/congestion” is ____) AND (“flame burning velocity” is ____)
THEN (ISL is ____)

The inherent safety principles evaluated by this set of rules are “substitution” because flame burning velocity is a chemical property and “simplification” because the physical arrangement of the unit affects the overall hazard resulting from the interaction of these parameters. The evaluation of this set of rules requires two inputs. One is the output from the FIS called ”hazard due to obstruction and congestion” (COOB) and the other is provided by the user and is the characteristic flame burning velocity. This parameter, as in the case of the other user inputs can be fed as a crisp number or as a fuzzy number.

The FIS called ”hazard due to obstruction and congestion” (COOB) evaluates the combination of two design parameters, hence it is related to the inherent safety principle of ”simplification”. The general structure of the IF-THEN rules for COOB is:

IF (“obstruction fraction” is ____) AND (“congestion fraction” is ____)
THEN (ISL is ____)

In general, when obstruction is high, it is expected that congestion will also be high, and vice versa, unless the unit equipment is arranged in such a way that corridors and tunnels are left open between two rows of equipment. The inputs required from the user are:

- Processing unit congestion fraction
- Processing unit obstruction fraction

These two values are highly uncertain due to the approximation required for its calculation (as explained in Chapter VII) and because they should reflect the average for the whole unit. When the degree of congestion and/or obstruction is variable within the processing unit, it is possible to estimate a range (i.e., maximum and minimum value) for each one of the two inputs and feed them as fuzzy numbers that reflect the physical variability.

As shown in Figure 7.7, the evaluation of the overall hazard due to fire/explosion and congestion/obstruction (ACOFRV) requires the input from the fuzzy inference system called “hazard due to fire/explosion and viscosity” (AFRVISC). This set of rules combines chemical and design properties evaluating the principles ”substitution”, “moderation” and ”simplification”. The principle of substitution is related to the chemical properties of flammability and reactivity. The principle of moderation is related to less hazardous form of the chemical substance and here viscosity is implicitly related to mixing and possibility of generating heterogeneous properties within the vessel. When viscosity of the chemical is high, it is assumed that more mixing power is required in order to reach homogeneous properties. In case of mixing failure the occurrence of hot spots or zones of higher/lower than specification concentration can occur. In the case of reactive chemicals, this abnormal lack of homogeneity can cause runaway reactions while in the case of flammable chemicals (i.e., low flash temperatures, low boiling points, and/or low autoignition temperature) the reduced heat transfer rate can generate a temperature rise sufficient to reach hazardous conditions.

The general structure of the IF-THEN rules for AGOFR is:

IF (“viscosity” is ____) AND (“flammability/explosivity/reactivity” is ____)
THEN (ISL is ____)

While the input for the second part of the rule is given by the output from the FIS called “hazard due to fire/explosion and reactivity” (AGOFR), shown in Figure 8, the input for viscosity is given by the user. Since viscosity is a function of temperature it can be fed as a fuzzy number whose maximum value is given by the maximum viscosity in relation of the minimum (or maximum) vessel temperature; the minimum value of the fuzzy number is given by the minimum expected value of viscosity obtained at the maximum (or minimum) expected temperature of the vessel. The option of using fuzzy numbers for entering the value of viscosity is especially important for chemicals such as sulfur whose viscosity presents an inversed strong dependence with temperature.

Other factors that could be added in the future to the fuzzy logic-based model prototype are the estimated requirement of mixing power in order to keep the vessel contents in a homogeneous phase. While viscosity describes part of the problem of fluid homogeneity, other aspects such as mixing of multiphase, as in the case of immiscible liquids or solid suspensions, cannot be modeled by using only viscosity as an input factor. An example of this type of hazard is the rollover (or boilover) of oil tanks when heated due to external fires if water is accumulated at the bottom [King, 1990; AIChE, 1993]. Similar hazardous situations can occur when mixing is lost and two or more phases can be formed due to miscibility and density gradients.

The overall objective of the set of rules for AFRVISC is the combination of flammability and reactivity hazards with the possibility of generating heterogeneous properties due to high viscosity of the mixture and, in an implicit form, due to lack of appropriate mixing. When high flammability and/or reactivity are combined with highly viscosity, the implicit degree of hazard of the equipment is high; if viscosity is low for high flammable chemicals the hazard degree is slightly reduced due to the possibility of maintaining homogeneous properties even with lack of mechanical mixing because of convective forces. When the chemicals are not flammable and/or reactive regardless of the value of the viscosity, the hazard will be low.

The second input for AFRVISC is the output from the FIS called “hazard due to fire/explosion and reactivity” (AGOFR) that aggregates the three types of hazards (Figure 7.8). The format of the IF-THEN rules for AGOFR is the following:

IF (“flammability” is ____) AND (“reactivity” is ____) THEN (ISL is ____)

In terms of inherent safety principles, the set of rules evaluates "substitution" by identifying hazardous chemical characteristics. If either of two properties implies high hazard, the resultant degree of inherent safety is reduced. It is assumed that reactivity can trigger fire and explosions hence a certain degree of synergy between the two hazards is taken into account by the rules.

As indicated by note 3 in Figures 7.7 and 7.8, additional IF-THEN rules set can be added in order to take into consideration hazards due to static electricity generated by fluids of low conductivity in vessels and equipment whose design does not provide grounding means or minimization of energy-generating operations such as splashing during filling [Crowl and Louver, 2002].

As shown in Figure 7.8, the evaluation of flammability and reactivity is based on the FIS called "hazard due to fire ad explosion" (CHPF) whose IF-THEN rules have the following format:

IF ("boiling temperature" is __) AND ("flash temperature" is __) THEN (ISL is __)

The rules describe the relation between normal boiling and flash temperature established by specialized flammability standards such as NFPA and the UN ratings. The general knowledge expressed by the rules is that if the flash temperature is low and boiling temperature is lower or around the environmental temperature, then the possibility of fire, and hence explosion, is high. A detailed description of the systems is presented in Chapter VII. The user is required to feed the following inputs:

- Normal boiling point of the chemical
- Flash temperature

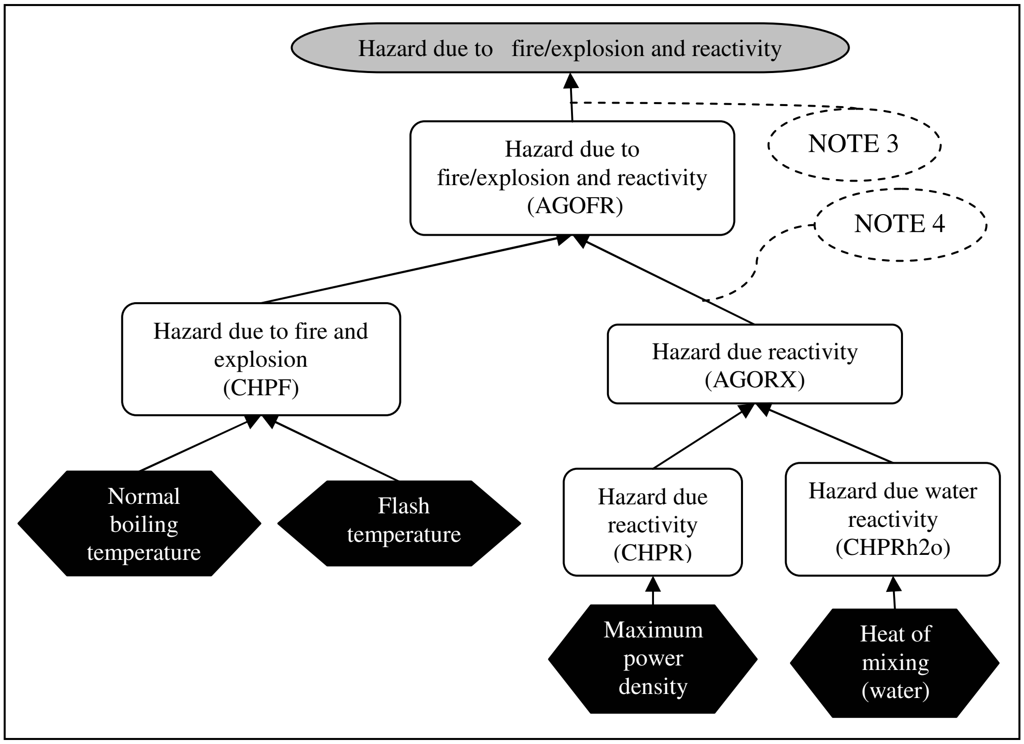


Figure 7.8: Hierarchical tree for the evaluation of hazards due to flammability and reactivity

The systems takes such input uncertainty into account by allowing the user to use fuzzy numbers defined by lower, average, and maximum values for the two temperatures.

As shown in Figure 7.8, the evaluation of reactivity is based on the FIS called "hazard due to reactivity" (AGORx) whose IF-THEN rules have the following format:

IF ("chemical reactivity" is ____) AND ("water reactivity" is ____) THEN (ISL is ____)

The rules describe the relation between reactivity behaviors inherent to the molecular structure due to incompatibility with water. In order to present low reactivity hazard, both inputs to the rule must imply low hazard. The effect of side reactions, reactions due to air reactivity, or reactions due to incompatibility with impurity and/or contamination are not taken into account.

The inputs to the rule set AGORx is given by the outputs from two other simple set of rules; the possibility of chemical reactivity intrinsic to the kinetics of the reaction is given by the FIS called "hazard due to reactivity" (CHPR), while the water reactivity hazard is given by the FIS "hazard due to water reactivity" (CHPRh2o).

The general format of the IF-THEN rules for CHPR is:

IF ("maximum power density" is ____) THEN (ISL is ____)

The user is expected to provide the maximum power density (MPD) for the reaction, however it can be substituted by the "initial power density" (IPD) as explained in Chapter VII, if the MPD is not available. When the value of the MPD is high, the overall hazard increases due to the possibility of runaway reaction. If IPD is used, the uncertainty is much greater due to the fact that while a low MPD implies a low IPD, a low IPD may be followed by a higher MPD. The input can be fed either as crisp number or as a fuzzy number. The general format of the IF-THEN rules for CHPRh2o is:

IF ("heat of mixing with water" is ____) THEN (ISL is ____)

The user is expected to provide the estimated value for heat generated due to mixing of the evaluated chemical with water. When the heat of mixing, is high the hazard increases. As in the previous case the parameter can be fed a as crisp number or as a fuzzy number.

The purpose of both set of rules set is to convert a physical scale into the hazard possibility scale used for the rest of the fuzzy inference systems.

The efforts to understand and model chemical reactivity are an ongoing area of research [Saraf, 2003; Aldeeb, 2003] around the world. The parameters selected for the model proposed by this research are based on the NFPA 704 (2001) approach, however only cover a limited type of chemicals (e.g., flammable as classified by the NFPA scoring system) and phenomena (e.g., water reactivity and simple reaction kinetics). In the future, when more information and understanding of the reactivity phenomena is available, the model can be expanded by including additional IF-THEN rule sets and hierarchical trees able to describe the new knowledge. This current lack of information is highlighted in Figure 7.8 by the label Note 4.

7.4.4 Description of the hierarchical model for design hazard

The design aspects that are not already taken into account during the evaluation of chemical hazards, are evaluated under the branch indicated in Figure 7.2 as “hazard due to mechanical and design factors” (ISIMECH). One of the inputs for ISIMECH is given by the FIS known as “hazard due to nozzle failure and corrosion” (CORNZ) that has the objective of combining the potential hazards from mechanical failure of the shell of the vessel, connection points to the rest of the process such as nozzles, or other penetration of the wall for instrumentation and other devices. The inherent safety principle evaluated are “simplification”, ”moderation”, and “substitution” because chemical properties of the substances interacting with the mechanical design and vessel construction material are involved.

The general structure of the IF-THEN rules for CORNZ, shown in Figure 7.9, is the following:

IF (“corrosion potential” is ____) AND (“nozzle failure hazard is” is ____)
THEN (ISL is ____)

It is assumed that if either the failure of the vessel wall is possible or failure of any nozzle or wall penetration is possible, the hazards due to leak of chemicals increase, hence the level of inherent safety is reduced.

The branch of the tree that evaluates the corrosion potential is formed by the fuzzy inference system called "hazard due to corrosion potential" (CORRH), shown in Figure 7.9.

The general structure of the IF-THEN rules for CORRH is:

IF ("operation temperature" is ____) THEN (ISL is ____)

The rule structure is based on the fact that temperature is one of the most important factors for the occurrence of corrosion for a specific pair chemical-construction material.

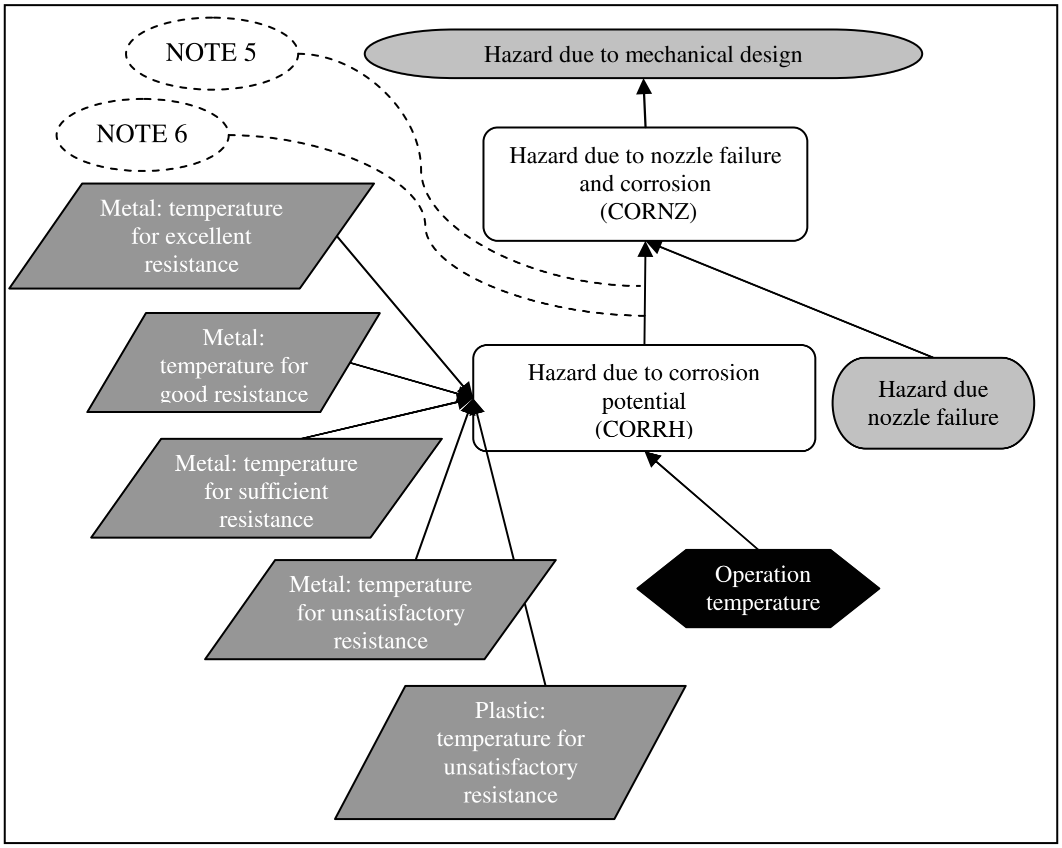


Figure 7.9: Hierarchical tree for the evaluation of mechanical failure

Other factors such as impurities and abrasives, galvanic effects, pH, fluid velocity, metallurgy, mechanical stress and detailed equipment design are important, however in order to capture their effects additional sets of rules are required. As indicated by Note 5 in Figure 7.9, additional IF-THEN rule sets can be added to model the effect of specific type of corrosion, and to include the effect of the environment characteristics that can affect external corrosion, such as the presence of contaminant such as sulfur dioxide, chlorides, and salts.

In order to model the specific interaction between the chemical and the construction material of the vessel, the fuzzy inference system is based on adaptive membership functions whose parameters must be provided by the user and are the following:

- For metals:
    - Temperature at which the corrosion rate is excellent
    - Temperature at which the corrosion rate is good
    - Temperature at which the corrosion rate is satisfactory
    - Temperature at which the corrosion rate is unsatisfactory

- For plastics:
    - Temperature at which the corrosion rate is unsatisfactory

In general, only one or two values are available for each material, therefore the user is not required to submit all the inputs and the FIS will work with a limited number of functions (i.e., minimum two if only the unsatisfactory value is provided or up to five if all the values for metals are available).

In order to model other factors that can produce the mechanical failure of the vessel, such as sudden pressure increase due to relief valve failure or due to runaway reaction, more IF-THEN rule sets can be added. These factors can be inserted as indicated by note 6 in Figure 7.9.

Another scenario for the release of chemicals to the environment is the failure of nozzles such as indicated in Figure 7.10. It is assumed that the vessel has up to four nozzles (however the number can be increased) and each one presents a different degree of hazard depending on its position (e.g., height from bottom) and diameter. In the case of a vessel with liquid contents, a nozzle located at the bottom of the tank, in case of failure will release a liquid phase, increasing therefore the hazard of large mass flowrate releases; when a nozzle is located above the maximum liquid level of the vessel the hazard is reduced since the released chemical will be in a vapor phase. The released flowrate is also a function of the diameter of the nozzle; however this parameter also affects the possibility of failure, since small bore pipes (e.g., diameter smaller than 2 in) are more likely to fail. The general structure of the IF-THEN rules for the fuzzy inference system called "hazard due to nozzle failure" (NLD) is the following:

IF ("nozzle location is" is ____) AND ("nozzle diameter is" is ____)
THEN (ISL is ____)

The FIS is based on adaptive rules whose parameters must be provided by the user and are related to the liquid levels of the vessel:

- Overflow level
- Normal high level
- Normal operation level
- Normal low level
- Minimum level (or drain)

The inputs required for each of the nozzles for the evaluation of the hazard are:

- Level at which the nozzle is located
- Diameter of the nozzle

The hazard levels calculated for each nozzle are then aggregated and the result is used as input for the fuzzy inference system CORNZ.

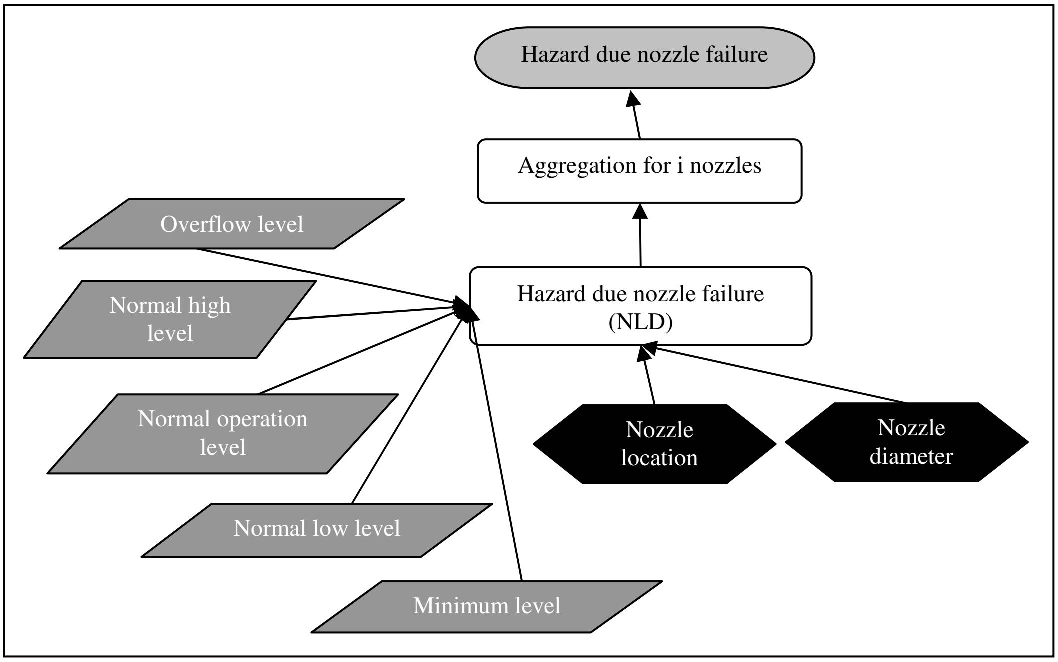


Figure 7.10: Hierarchical tree for the evaluation of nozzle failure

CHAPTER VIII

DESIGN OF MEMBERSHIP FUNCTIONS AND IF-THEN RULES

This chapter introduces the general physical theory upon which the fuzzy inference systems are designed. The most important IF-THEN rule sets, with its linguistic variables and membership functions are described in order to show the rationale behind the design procedure. The parameters reported for the membership functions correspond to the vertices of the triangular or trapezoidal functions.

As mentioned in previous chapters, the evaluation of hazards is based on a scale defined on the real interval [0 1], where 0 indicates absolute absence of hazard (i.e., inherently safest option) and 1 indicates extreme hazard. A reference state for the outputs (i.e., hazards) is set at 0.5 and indicates the threshold between different degrees of inherent safety and different degrees of hazards. The hazard inherent to the reference value of 0.5 is assumed to be low enough to be considered as acceptable or manageable by simple layers of protection such as procedural controls or simple control systems. The significance of the output values is related to the identification of the combination of conditions that raise the hazard level beyond the reference state of 0.5 and that must be analyzed in order to identify design options to reduce the source of hazard.

The chapter is divided in four main topics covering fire and explosion models, human and environmental toxicity, design hazards, and aggregation rules.

8.1 REACTIVITY, FIRE AND EXPLOSION FUZZY MODELS

As indicated in Chapter VII, fire and explosion hazards for this research are related to the continuous release and dispersion of flammable chemicals. Internal explosions capable of destroying the vessel and sending projectiles towards other equipment inducing a domino effect are not covered, but can be added in the future.

For the evaluation of fire and explosion hazards, six fundamental fuzzy inference systems (FIS) are used; this FIS require the input of physical and chemical parameters for the specific substance and equipment being evaluated. Other 5 FIS integrate the information generated from the fundamental FIS. Tables 8.1 and 8.2 shows the names of the 11 FIS and the list of inputs they require. As indicated in Tables 7.1 and 7.2, some of the inputs are used for the design of adaptive membership functions, as in the case of the evaluation of the dispersion potential (DISP).

As mentioned previously, in order to eliminate the subjectivity derived from interpretation of the phenomena, the model must be based on sound technical principles. In the next section the fundamental physical principles used to design the fuzzy inference systems for the evaluation of fire and explosion hazard, including dispersion of flammable chemicals, are summarized. Section 1.2 reports the parameters of the membership functions for some representative FIS, as well as the sets of IF-THEN rules.

Table 8.1: List of fundamental FIS and required input parameters

FIS NAME	INPUT	UNITS
CHPF “Hazard due to fire and explosion “	Normal boiling temp. Flash point	°C °C
CHPR “Hazard due to reactivity “	Power density	W/ml
CHPRh2o “Hazard due to water reactivity “	Heat of mixing	cal/gr
DISP “Hazard due dispersion “	Normal boiling temp. Flash point Atmospheric temperature Vessel boiling temperature Vessel temperature Vessel pressure	°C °C °C °C °C atm
COOB “Hazard due congestion/obstruction “	Congestion factor Obstruction factor	% %
COBV “Hazard due COOB and burning velocity“	Flame burning velocity	cm/s

Table 8.2: List of aggregation FIS and input parameters

FIS NAME		INPUT	UNITS
AGORX	"Hazard due to reactivity "	CHPR CHPRh2o	HP* HP*
AGOFR	"Hazard due to fire/explosion and reactivity "	CHPF AGORX	HP* HP*
AGOFRVISC	"Hazard due to fire/expl./react. and viscosity "	AGOFR Viscosity	HP* cp
ACOFRV	"Hazard due to fire/expl./react. and viscosity and cong./obstr."	AGOFRVISC COBV	HP* HP*
AGEXPL	"Overall explosion hazard"	ACOFRV DISP	HP* HP*

* HP = hazard potential index

8.1.1 Theoretical foundation for the design of IF-THEN rules and membership functions

As reported by Lees (1996) several types of fire and explosion have occurred in the chemical industry. The type of fires addressed here are vapor cloud fires, jet fires, and pool fires with explosion. Fireballs and solid fires are not addressed. It is assumed that explosions will occur due to releases of flammable gases that are then ignited. Davletshina (1998) indicates that "…flammability can only be subjectively defined…" because several parameters affect the hazard evaluation, some substances are assumed to be flammable because of their heat content (e.g., fuel oils) but they have high flashpoint; others have low flash point and low heat content too. King (1999) reports several physicochemical, design, and firefighting factors that should be used in order to evaluate the overall fire hazard. Kondo et al. (2001 and 2002) propose a flammability measure based on flammability limits and heat of combustion. Glassman and Dryer (1980) present a general discussion of flammability and the experimental uncertainty of parameters relevant to flammability and flame spreading.

Looking at flammability as a type of variable defined with basis on input thresholds (as explained in Chapter VII) only chemical properties can be used. This approach simplifies the problem for the prototype fuzzy logic-based model proposed in this research, however in the future it will be possible to include additional design factors. Physicochemical factors that describe flammability are:

- Boiling temperature
- Flash temperature
- Flammability and explosivity limits
- Flame burning velocity
- Autoignition temperature
- Vapor density

8.1.1.1 Flammability hazard

The boiling point and flash temperature are the base variables used by NFPA 704 (2001) and other systems, such as the US Department of Transportation (DOT) and the EU Risk Phrases to classify substances based on to their potential to get ignited. The relation between the thresholds used by each system is shown in Figure 8.1.

The Risk Phrases assign the label R12 to “extremely flammable chemicals”, R11 to “highly flammable substances”, and R10 to chemicals that are flammable (INSET, 2001). The DOT classes of flammables (i.e., IA, IB, IC, II, and III) are assigned to chemicals with different degrees of flammability, Class IA being the most hazardous. According to the NFPA system, a score of 4 is assigned to substances that vaporize at ambient conditions and burn fast [NFPA 704, 2001]. A score of 2 is assigned to materials that must be exposed to a relatively high temperature before releasing enough vapors to be ignited. NFPA 2 and DOT Class IIIA are the states taken as a reference threshold for inherent safety, as explained in Chapter VII. Chemicals with NFPA scores of 1 and 0 are assumed to be inherently safer than chemicals with scores 3 ad 4; from Figure 8.1 the conclusions can be extrapolated to the DOT classes and the Risk Phrases.

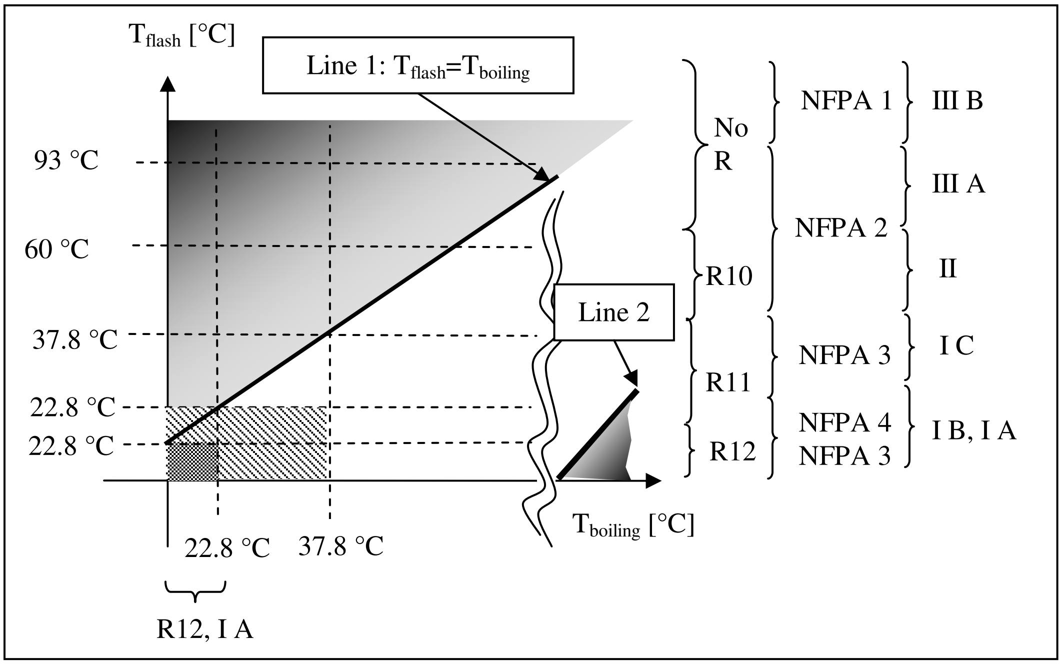


Figure 8.1: Relation between the flammability thresholds used by NFPA, DOT, and Risk Phrases

The information summarized in Figure 8.1 is used to design the fuzzy IF-THEN rules for the evaluation of flammability as shown in section 1.2; however it must be noted that certain regions do not have physical meaning. For example, by definition $T_{flash} < T_{boiling}$, therefore the region above line 1 in Figure 8.1 is physically not possible. Similarly, the region below line 2 requires a very low flash temperature with a high boiling point. By testing chemicals listed in NFPA 325 (1994) with a score of 3 and with high boiling temperature none was found to have high boiling temperatures (i.e., located under line 2).

8.1.1.2 Dispersion hazard

The potential for the formation of an explosive cloud is based on the location of the operation point of the vessel (i.e., temperature or pressure) with respect to the vapor pressure curve for the specific chemical. When a flammable liquid is released it forms a vapor-liquid equilibrium in air, hence the system is binary (i.e., air-flammable chemical) and should be described by a binary VLE diagram (Figure 8.2). The approach explains why the flash temperature is lower than the boiling temperature of the pure substance. Flash temperature corresponds to the temperature at which the equilibrium composition is the lower flammability limit (i.e., $x = x_{LFL}$). Similarly, the composition of the upper flammability limit (i.e., $x = x_{UFL}$) corresponds to a temperature higher than the T_{flash} but lower than $T_{boiling}$, however this temperature is rarely reported, as indicated by King (1999). A closed vessel working at $T > T_{UFL}$ generates a vapor too rich in terms of the flammable vapor, therefore outside the flammable composition. This is not true for open systems, where ventilation can modify the concentration of the cloud.

When the three-dimensional envelope for the binary VLE at different pressures is projected on the PT plane, a diagram similar to Figure 8.3 is obtained; this figure exemplifies the reasoning for the modeling of inherent hazard when a liquid chemical with a flash temperature lower than the atmospheric temperature (i.e., $T_{flash} < T_{atm}$) is released.

Due to the low boiling point of air, the two saturation curves for pure components (e.g., air and flammable chemicals) are separated quite a bit. At constant pressure (i.e., $P = P_{atm}$), the distance between the two pure boiling temperatures represents also the range of composition between pure air (i.e., $x_A = 0$) and pure flammable chemical (i.e., $x_A = 1$). Therefore, when the location of temperatures at upper and lower flammability limits are transported on the composition axis, the flammable range for a flammable chemical in a closed system is obtained (i.e., T_{LFL} and T_{UFL}).

When a chemical is released to the environment the system is no longer closed and dilution effects can take place due to transport phenomena and turbulence generated by wind flow. Therefore, for an open system it is assumed that when the chemical is released at a temperature higher than T_{flash} , the formation of a flammable cloud is possible if the plume is not diluted. The assumed flammability range for an open system is shown in Figure 8.3 by the larger arrow.

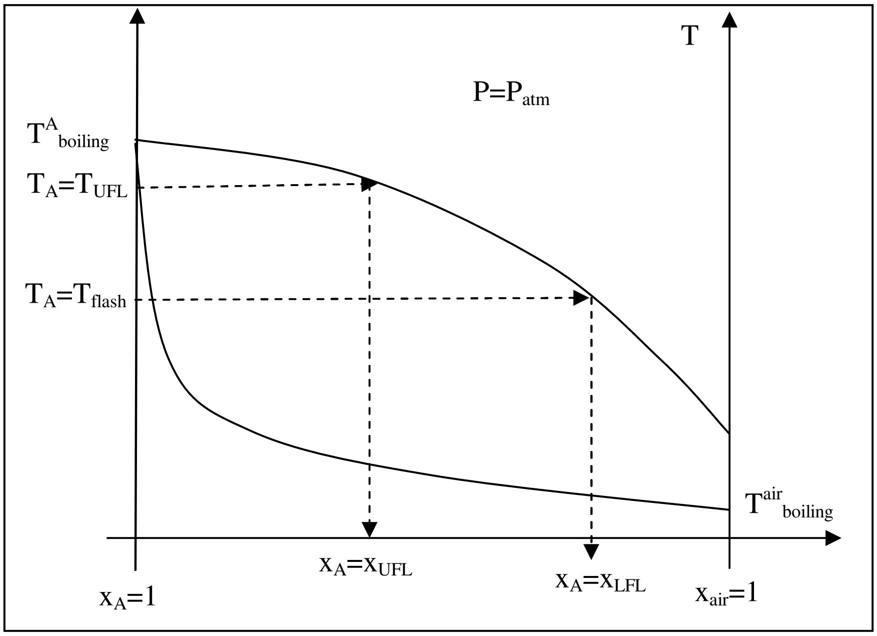


Figure 8.2: Relation between the flash temperature and composition at the lower flammability limit for a closed vessel

Flammability limits are often used as a parameter to classify the possibility of ignition of a chemical (e.g., Heikkila index as described in Chapter II). For the model proposed in this research the flammability limits are taken into consideration in an indirect form by DISP, which is the FIS that evaluates the potential of formation and dispersion of flammable clouds after the chemical has been released.

Flammability limits are taken as crisp thresholds for the analysis of flammability hazards; however, they present high uncertainty due to their dependence on several system characteristics such as size of the experimental vessel, experimental procedure, and pressure [Lees, 1996; Takahashi et al., 2003]. Therefore due to their inherent uncertainty flammability limits should be used as fuzzy thresholds. For the hierarchical model proposed in this research, the flammability limits are modeled by using the flash temperature only.

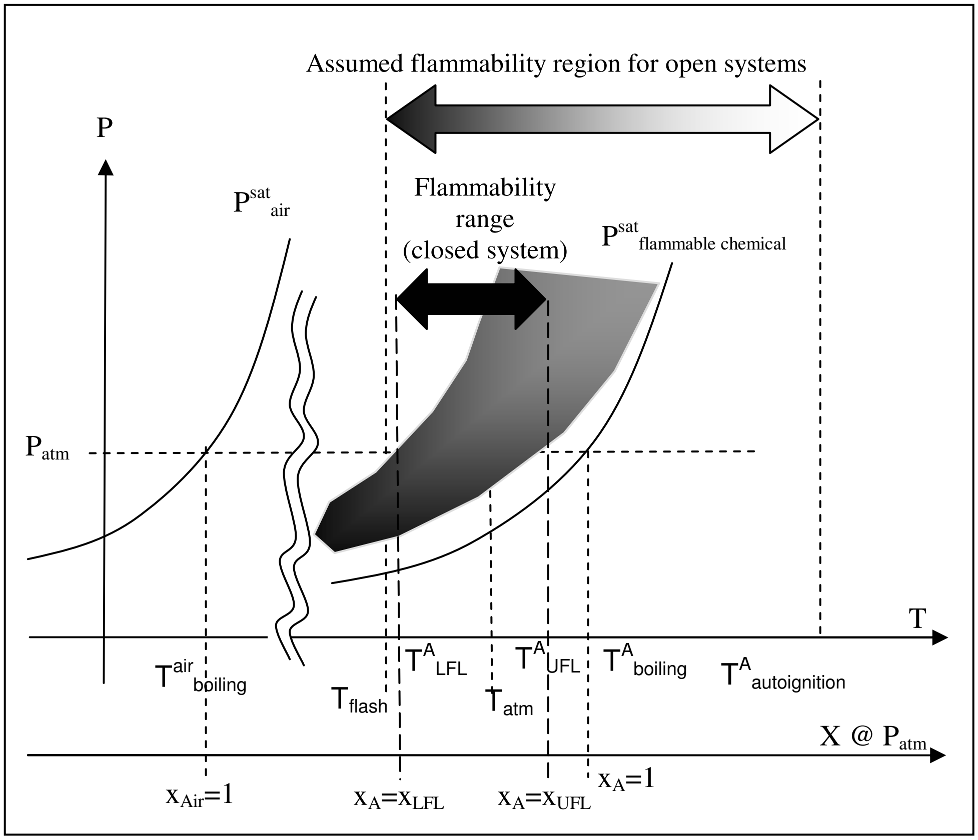


Figure 8.3: Projection of the binary (Air-Flammable liquid) vapor-liquid equilibrium PTx envelop on the plane PT, and effect of pressure on flammability region for closed and open systems

The upper flammability limit is unknown for open systems due to ventilation effects that modify the concentration. However, when the temperature of the system is higher than the flash temperature the potential for formation of an explosive cloud increases. The dependence of the flammability limits with respect to pressure is indicated in Figure 8.3 by the gray region.

The design of the membership functions for the analysis of the hazard inherent to the formation of flammable clouds is based on the idea that the flash point can be assumed to be the lowest temperature at which the chemical generates enough vapor to be ignited. Although in order to sustain the flame the temperature must be higher (i.e., fire temperature) as indicated by NFPA 704 (2001), the two values are only few degrees apart, therefore the flash temperature is one of the parameters, with boiling and atmospheric temperature, used to design the membership functions.

In order to design the consequent part of the rule, which evaluates the potential for the formation of a flammable cloud, the dispersion potential is estimated as a function of the released phase. Three parameters are used:

- Difference between the ambient temperature and the normal boiling point of the chemical
- Difference between the ambient temperature and the vessel temperature
- Vessel pressure

The general heuristic knowledge modeled by these three variables is the following:

- As the boiling point of a substance increases, its volatility decreases reducing the hazards due to vaporization and dispersion. The effect of heavy gases is not taken into account by the model, because as indicated by Lees (1996) the cloud density depends on physicochemical factors of the released chemical (e.g., molecular weight) but also on other dynamic factors such as temperature of the cloud, presence of mist or aerosol, environmental humidity, and temperature.
- As the storage temperature increases the hazard due to dispersion increases, especially around the saturation curve. The hazard reduction due to high temperature

release (e.g., release of very hot gases that produce a chimney effect carrying the cloud away from the site, hence reducing the hazard of rain out) is not taken into account by the used rules.

- As the storage pressure increases the mass flow from a leak increases and the possibility of aerosol formation is higher. Hazard reduction due to jet mixing (e.g., concentration dilution due to entrapped air) is not taken into account.

The general principles summarized above are graphically represented by Figure 8.4 for a volatile liquid and by Figure 8.5 for a gas.

According to King (1999) when the operation region of a vessel with a flammable chemical is located in region a in Figure 8.4, the inherent hazard in case of release is very high because the released phase is liquid but vaporizes immediately (cooling down until it reaches the normal boiling temperature) generating a large explosive cloud. For pressurized vessels (e.g., region b and c, Figure 8.4), the liquid flow rate is increased, and the possibility of aerosol formation is also increased. When the liquid is stored at very low temperatures (e.g., region c, Figure 8.4) the sudden release to the environment initially generates high vaporization that cools the formed pool to an equilibrium temperature at which the vapor release is slower [Lees, 1996]. As indicated by Kletz (1998) refrigerated storage is inherently safer than pressurized storage. Region e in Figure 8.4 is under vacuum; hence the pressure effects are derived only by the hydrostatic liquid height above the leak point. An additional hazard, not taken into account by the model is the reactivity of the substance with atmospheric humidity or air.

Two types of liquids can be identified according to the value of the flash point with respect to the atmospheric temperature; when $T_{flash} < T_{atm}$ the liquid is assumed to be more hazardous due to higher volatility, however, a liquid with $T_{flash} > T_{atm}$ can also become hazardous if heated above its flash point [Lees, 1996]. These effect of pressure is also relevant when the formation of mist and aerosol is possible, since, they can be ignited at temperatures lower than the flash point [Lees, 1996; Zabetakis, 1965].

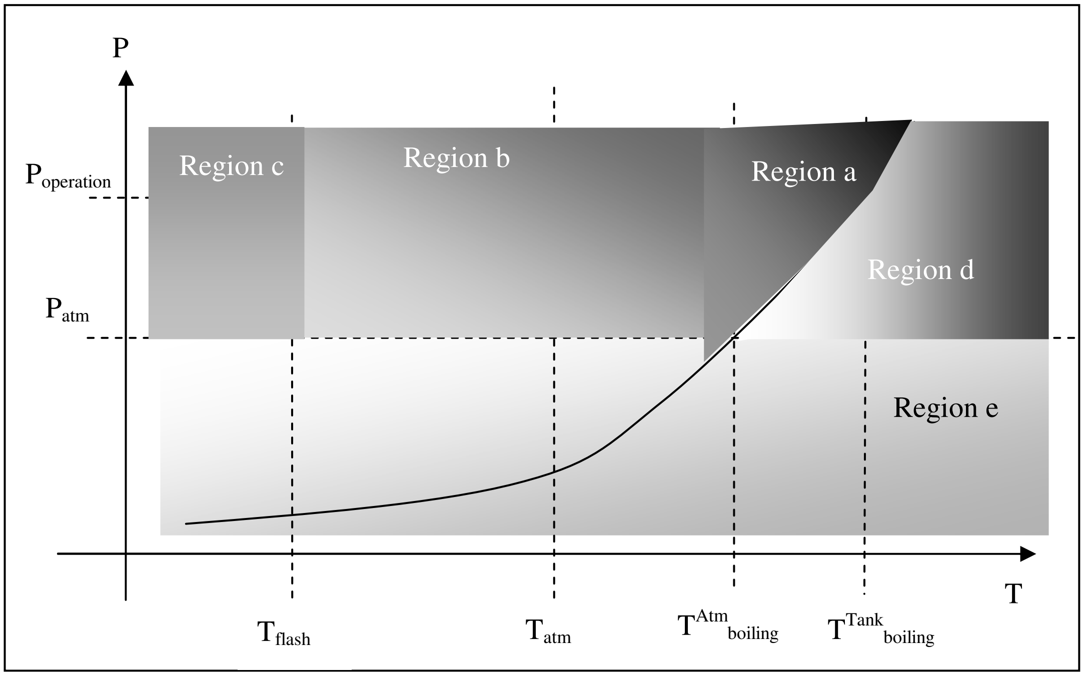


Figure 8.4: Hazard regions for a flammable liquid with T_{flash}<T_{atm}

In the case of flammable gases region b in Figure 8.5, is also hazardous due to the effect of pressure that increases the release rate and the density of the substance. Gases under cryogenic conditions (e.g., region b, c, and d, Figure 8.5) when released from a liquid pool that boils violently [Lees, 1996; Jensen, 1983] releasing large quantities of vapor and mist until the temperature of the pools drops below the substance's normal boiling point.

The normal procedure for dispersion modeling of gases and vapors (both flammable and toxic) is complex and it is developed by specialized models based on different approaches depending on the characteristic behavior of the chemical (e.g., dense gas). Each model is based on different assumptions (e.g., box models assume that dense gases disperse generating a flat pancake-like cloud) and mathematical tools. The uncertainty of the models is also a function of atmospheric conditions, wind speed and direction, height of release, and type of source model. All these factors increase the uncertainty of the final result. In the case of flammable and explosive chemicals, other factors affect the hazard degree of the release event, such as the amount of gas that will contribute to the explosion [Lees, 1996].

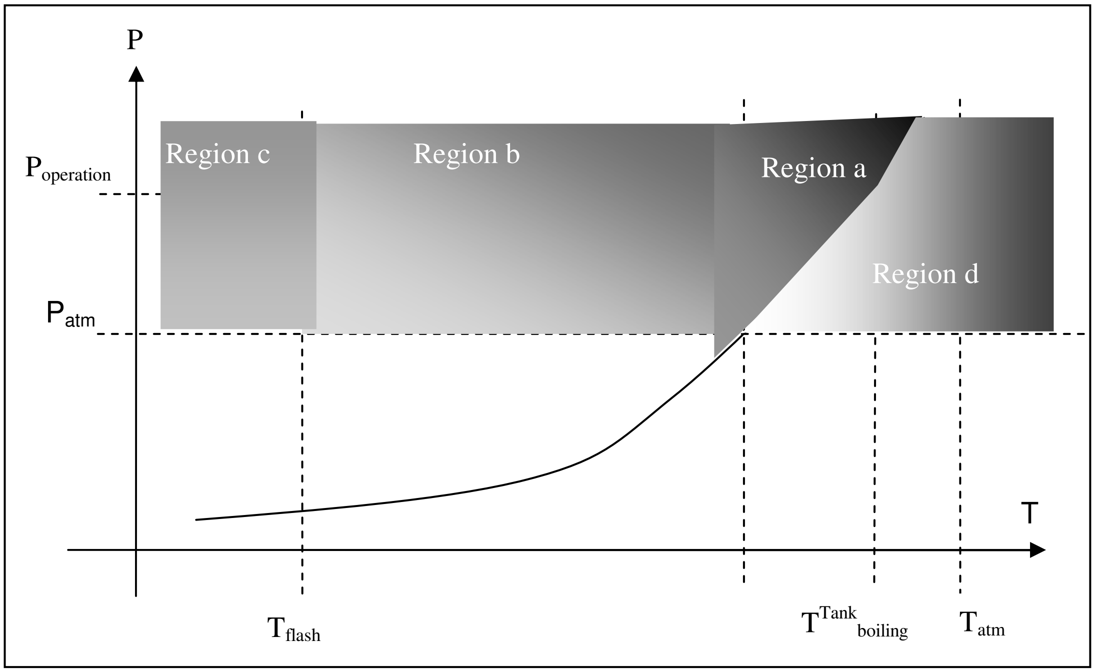


Figure 8.5: Hazard regions for a flammable gas

The hierarchical model proposed in this research evaluates the sources of hazards based on the potential for cloud formation and dispersion, and does not use uncontrollable conditions such as wind velocity and direction. Because of this the uncertainty associated with weather are not taken into account by the fuzzy model.

After the flammable chemical is released, it is assumed that an ignition source is present. As indicated by Davenport (1977 cited by Kletz (1980)), the probability of ignition is proportional to the size of the cloud (hence the quantity of released substance) and in general clouds drift less than 100 m before exploding. Similar information is also reported by Wiekema (cited by Lees (1996)). Kletz (cited by Lees, 1996) indicates that there is no theoretical threshold relating the release quantity of flammable substance to the strength of the explosion but it is possible to infer that as the mass increases the size of the cloud increases too; therefore, as indicated previously the possibility that the flammable cloud finds an ignition source is also higher. A similar conclusion regarding the influence of the spilled amount of chemical is reported by Wiekema (cited by Lees (1996).

Based on this information, the evaluation of the dispersion potential by the FIS DISP does not depend on the size of the inventory (i.e., vessel volume) but on the potential of forming a large vapor cloud, which is inferred by applying the information summarized by Figure 8.3, 7.4 and 7.5, as well as from the fact that at high pressure the possibility of aerosol and mist formation is high.

8.1.1.3 Congestion and confinement of the processing unit

Two factors identified as relevant to the consequence potential of a vapor cloud explosion are chemical reactivity and confinement degree of the processing unit. In general these two aspects are also related to cloud inhomogeneity that increases flame speed and overpressure, because of the formation of pockets of high or low concentration of gas. The cloud geometry has an additional impact on the generation of overpressure; for heavy gases the pancake shaped-cloud allows venting pressure buildup and gases through the top reducing the compression of the gases in front of the flame front, reducing then the flame speed. However, when the chemical is released in congested areas the venting effect is reduced [Wiekema (1984) cited by Lees (1996)].

The degree of obstruction generates turbulence and increases the flame speed, however the reactivity of the chemical is also important. As reported by Lees (1996) for a low reactivity gas exploding in an area of low obstruction, the velocity increase is negligible. However, in presence of confinement, the overall effect of obstruction/confinement is significant even for low reactivity gases. The combination of all these factors leads to generate high flame velocity, increasing therefore the negative impact of the explosion.

In order to take into account the interaction of confinement, obstruction, and flame reactivity, a system of two fuzzy inference systems has been designed. The first FIS (COOB) combines degree of congestion with degree of obstruction, and the result of this first FIS is combined by the second FIS (COBV) with the reactivity of the fuel, expressed in terms of burning velocity.

The degrees of confinement and congestion are calculated following the guidelines provided by Hjertager et al. (1992), Mercx et al. (2000), Clutter (2001), Wingerden and Zeeuwen (1983), and Fothergill et al. (2003) and based on a concept of porosity. Two parameters are required: the "overall volume blockage fraction" and the "degree of confinement".

The "overall volume blockage fraction" is obtained by using the average sizes of pipelines, equipment, and vessel to calculate the volume occupied with respect to the total volume of the unit:

$$\text{Overall volume blockage fraction} = V_{\text{obstruction}}/V_{\text{tot}}$$

$$\text{Where } V_{\text{obstruction}} = \sum V_{\text{equipment}} + \sum V_{\text{vessels}} + \sum V_{\text{pipelines}}$$

Since the blockage fraction can vary within the same unit, it is possible to estimate the range of variation (e.g., maximum and minimum blockage fraction) and use the values as a fuzzy number. The "Degree of confinement" is estimated from the percentages of face obstruction of the unit. It is assumed that the processing unit is a parallelepiped with five possible open faces, each one covering 20% of the possible area, as shown in Figure 8.6a. The calculation of the degree of confinement requires the estimation of the percentage of coverage of each one of the five sides. This is an approximate calculation (unless specialized technical drawing software is used), however, because the fuzzy system accepts a range of inputs rather than a crisp number, a rough estimate is sufficient. After the percentages of coverage of each side are defined the weighted summation of the five values gives the result for the degree of confinement. For example, in Figure 8.6b sides 3 and 4 are totally obstructed, while side 1 has an approximate 50% of obstruction, therefore the overall percentage of face obstruction of the unit is given by 0.2*(0.5)+0.2*(0)+0.2*(1)+0.2*(1)+0.2*(0) = 0.5.

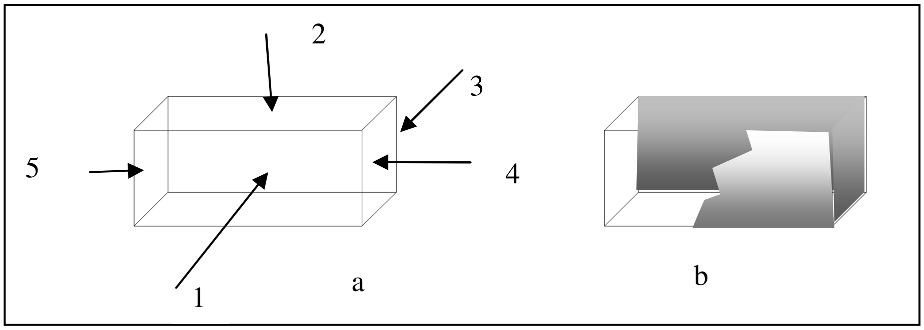


Figure 8.6: Processing unit totally unconfined (a), and unit with 50% of confinement (b)

These concepts and the guidelines of the TNO multy-energy model for the classification of the classes of blast are used to design the membership functions for the FIS COOB. For instance, obstruction is assumed to be high when the overall blockage fraction is larger than 30%. Parallel confinement occurs when walls or other barriers block two or three sides of the unit, therefore when the degree of confinement is at least 40 to 60% [Lees,1996; Van der Berg, 1985].

8.1.1.4 Burning velocity

The burning velocity is the other factor that can modify the overpressure generated by an explosion, and it is a property of the mixture air-flammable chemical. Burning velocities are affected by pressure, temperature, and concentration; for example, the burning velocity for paraffinic hydrocarbons varies between few cm/s the flammability limits up to 45 cm/s at the stoichiometric concentration [Lees, 1996]. Depending on the value of the burning velocity, for the TNT equivalent models for explosion, chemicals are classified as Low, Medium, and High reactivity [Lees, 1996]. A low reactivity material is relatively uncreative as for instance propane and butane whose burning velocity are respectively 45 cm/s and 40.5 cm/s; a moderately reactive material is ethylene that has a burning velocity of 68.8 cm/s; acetylene is classified as a highly reactive material and has a burning velocity of 173 cm/s [Lees, 1996]. These values are used to design the membership functions for burning velocity.

8.1.1.5 Viscosity

Mixing is required in order to ensure homogeneous properties of the contents of process vessels and reactors and it is important for mass and heat transfer. When liquids contained in a vessel can separate in multiple phases due to loss of mixing (e.g., mixer failure) or when viscous mixtures require heat transfer to maintain a specific temperature, the loss of mixing can create hazardous conditions. For instance, hot spots and concentration gradients can initiate runaway reactions. While for low viscosity mixtures the loss of mixing for heat transfer can be partially substituted by convective forces, in the case of viscous chemicals convection cannot take place, creating therefore heterogeneous bulk conditions.

The effect of fluid viscosity on the shape and flow pattern of gas bubbles in viscous liquids was published by Benuzzi et al. (1989) while Oster et al. (1990) and Bell and Morris (1991) considered the hydrodynamic aspects of emergency venting of vessels when the contained fluids are high-viscosity. Because of the hydrodynamic effects of viscous fluids on gas bubbles generated at the bottom of the vessel, high viscosity liquids present two-phase emulsions which indicate that the liquids swell more and for longer times compared with less viscous fluids.

Fluids with viscosity between 13-19 cp are considered low viscosity [Bell and Morris, 1991]. The value of viscosity also affects the type and design of mixer and impeller that can be used to achieve efficient mixing. For low viscosity fluids up to 4000 cp, propellers with three blades can be used, while for up to 100,000 cp turbines with vertical blades can be used [Walas, 1988].

An additional inherent hazard related to viscosity is the complication associated with the design of relief systems for two-phase viscous flows. Melhem et al. (2002) present estimates of flow reduction with respect to water due to viscosity increase; while for fluids with up to 100 cp, the flow is reduced 32%, for viscosity up to 10,000 cp the flow is reduced 59%.

Common procedures for relief design are based on low-viscosity fluids, however in the case of higher viscosity friction effects reduce the mass flowrate that can be vented [Fisher et al., 1992]. When the viscosity is below 50 cp, the fluid is assumed to be low viscosity, while fluids with viscosity values in the hundreds are assumed to be high viscosity [Fisher et al., 1992].

From the revised references, the membership functions for viscosity are designed as follows: viscosity up to 25 cp are assumed to be low, between 25 to 75 the viscosity is classified as low to medium, between 75 and 130 cp the viscosity changes from medium to high. For these three sets, low viscosity is associated with low hazard; while for medium values the hazard is high, and for high viscosity the hazard is very high.

8.1.1.6 Reactivity

Reactivity is another aspect that is taken into account for the evaluation of fire and explosion hazard. A list of physical and chemical properties that affect the reactivity hazard is provided by Lees (1996).

For the model proposed for inherent safety analysis, the evaluation of chemical reactivity is divided into two aspects: chemical reactivity inherent to the property of the substance (evaluated by the FIS CHPR) and chemical reactivity with water (evaluated by the FIS CHPRh2o). The problem of reactivity is complex and is being investigated extensively because of the difficulty in understanding and predicting the possibility of runaway reaction. For the modeling of these two aspects several approaches have been tested such as the use of the onset temperature for runaway reactions, and the approach proposed by Saraf et al. (2001). However, due to the complexity of the problem and the uncertainty associated with the lack of predictive models, the NFPA [NFPA 704, 2001; Hofelich et al., 1997] ratings for reactivity hazards and water reactivity have been used.

The NFPA scoring methodology for reactivity and thermal stability is based on the parameter called “Instantaneous Power Density” (IPD) which indicates the quantity of energy that the material at 250 °C will initially release if it suffers a chemical reaction due to decomposition or incompatibility with other materials. As indicated by Saraf et al. (2001) and by Kossoy (2003) this approach has the disadvantage of being applicable only for a zero-order reaction. When the expected reactive behavior does not follow single stage reaction without self-acceleration, the calculated IPD can be lower than the maximum power density (MPD). Therefore, Kossoy (2003) suggests the use of MPD rather than IPD for the evaluation of the reactivity hazard. The disadvantage of this approach is that the data is not available for a large number of chemicals and its calculation is not a simple task.

Therefore, in order to simplify the application of the proposed methodology for the evaluation of inherent safety, the NFPA methodology based on IPD is used, however it should be kept in mind that when MPD data is available it should be used instead of IPD. Kossoy (2003) also introduces the software Thermal Safety Software (TSS) useful for the calculation of IPD and kinetics values. The evaluation of water reactivity is based on the NFPA 704 approach [NFPA, 2001] that uses heat of mixing as suggested by Hofelich et al. (1997). The hazard associated with water reactivity is evaluated with respect to the violence of the decomposition reaction with water.

8.1.1.7 Aggregation of hazards

The outputs from the fundamental fuzzy inference systems are then combined, in order to obtain the overall evaluation of chemical hazard due to fire, explosion, and reactivity. As mentioned at the beginning of the chapter, the outputs are on a continuous scale [0 1], and the rules for the fuzzy inference systems have been designed in relation to specific “inherently safer” fuzzy thresholds which are assigned to the “medium hazard” output fuzzy set. The “medium hazard” fuzzy set is located at 0.5±0.25. When the index obtained from a FIS is below 0.5 the set of conditions evaluated for that FIS are assumed to have a high degree of inherent safety; when the index is higher than 0.5 then the evaluated conditions imply higher hazard than the selected “inherent safety” threshold.

Each fuzzy inference system for aggregation of outputs is based on rules designed intuitively according to technical information (e.g., high congestion increases the explosion hazard which is a consequence of the chemical properties). These rules could be designed in a systematic form by simulating and modeling releases of several chemicals under different operating conditions and unit congestion. From the results of the simulation it would then be possible to generate rules that can have a quantitative meaning (i.e., ratio scale).

For the present project, the FIS for aggregation are used to rank the results with respect to the threshold 0.5. In the case of dispersion hazard, the dispersion modeling software Canary was used to model the dispersion of hexane under several conditions of pressure, temperature, and unit congestion. The data for maximum overpressure was then used as an indication of hazard due to vapor cloud explosion.

The overpressure threshold is established at 3 psi according to the IRI (1992) which indicates that steel frames are damaged. The distance where the 3 psi overpressure is generated has been used as ranking parameter with respect of the distance obtained from the selected reference case. The reference case used is refrigerated liquid, since it is assumed to be inherently safer due to slow generation of vapors. While the design of the output of the rules (i.e., hazard degree related) for dispersion modeling has quantitative tendency, the other aggregation FIS are more qualitative because modeling and simulation was not used to generate data.

8.1.2 Example of the design of IF-THEN rules and membership functions

The membership functions and set of IF-THEN rules for flammability are designed according to the information summarized in Figure 8.1. The membership functions for the input are shown in Figure 8.7, and their parameters are reported in Table 8.3.

In Figure 8.7 the first two membership functions for the boiling temperature present a degree of overlap higher than that suggested in Chapter VII; however the overlap is required to obtain a faster and smoother response of the fuzzy graph. The last two fuzzy sets for flash temperature have been extended assuming a very high upper limit (i.e., 800 °C) in order to model chemicals that are not flammable. By examination of the list of chemicals included in NFPA 325 (1994), the highest flash temperature reported is 360 °C for tert-Butyl tetralin that has a NFPA flammability score of 1.

Figure 8.8 shows the membership functions for the output and the fuzzy graph obtained after defuzzification of all possible combination of inputs; Table 8.4 shows the parameters of the output functions. The matrix of rules used to estimate the flammability index by the inference system CHPF is reported by Table 8.5.

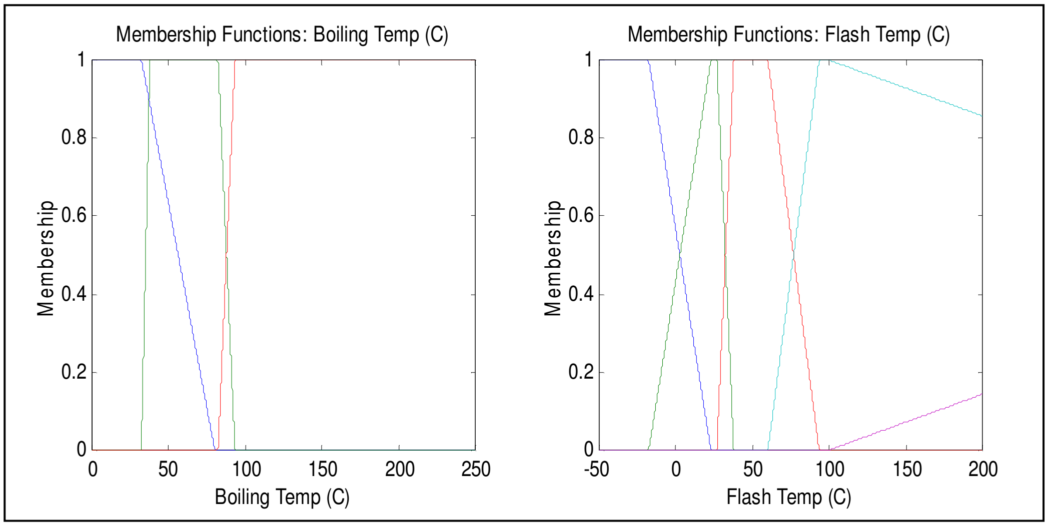


Figure 8.7: Membership functions for FIS CHPF

Table 8.3: Parameter for CHPF inputs

INPUTS	NAME	DESCRIPTION	SHAPE	PARAMETERS [°C]
Boiling Temp. Tb	**VLTb**	Very Low Tb	Trapezoidal	[0 0 32.2 80]
	LTb	Low Tb	Trapezoidal	[32.2 37.8 82.2 93.2]
	HTb	Medium Tb	Trapezoidal	[82.2 93.2 250 250]
Flash Temp Tf	**VLTf**	Very Low Tf	Trapezoidal	[-50 -50 -17.8 22.8]
	LTf	Low Tf	Trapezoidal	[-17.8 22.8 26.7 37.8]
	MTf	Medium Tf	Trapezoidal	[26.7 37.8 60 93.4]
	HTf	High Tf	Trapezoidal	[60 93.4 100 800]
	VHTf	Very High Tf	Trapezoidal	[100 800 800]

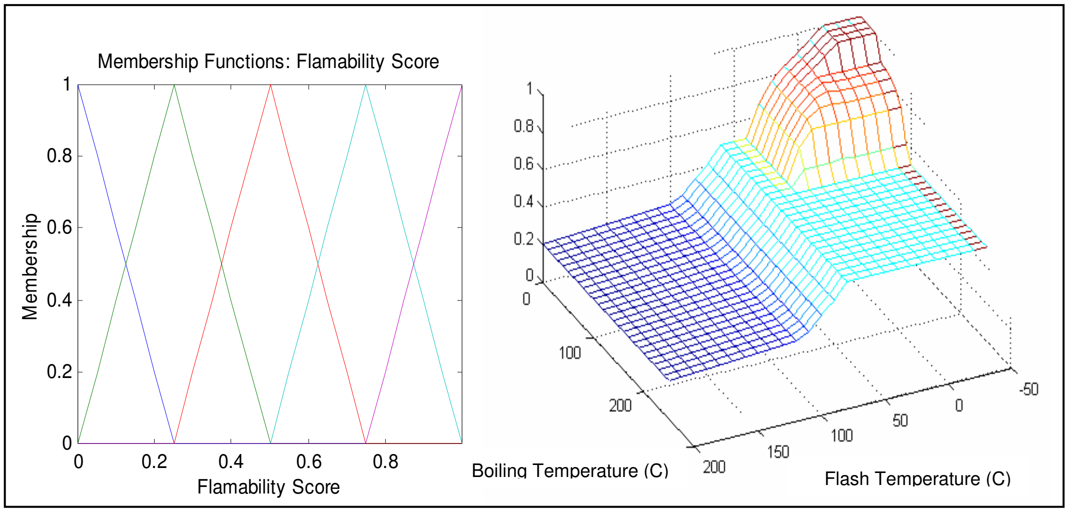


Figure 8.8: Membership functions for output of FIS CHPF and related fuzzy graph

Table 8.4: Parameter for CHPF output

OUTPUT	NAME	DESCRIPTION	SHAPE	PARAMETERS [°C]
Hazard Potential	**VLH**	Very Low Hazard	Triangular	[-0.25 0 0.25]
	LH	Low Hazard	Triangular	[0 0.25 0.5]
	MH	Medium Hazard	Triangular	[0.25 0.5 0.75]
	HH	High Hazard	Triangular	[0.5 0.75 1]
	VHH	Very High Hazard	Triangular	[0.75 1 1.25]

Table 8.5: Fuzzy IF-THEN rules for CHPF. The general rule is: IF (“boiling temperature” is ____) AND (“flash temperature” is ___) THEN (HP is ___)

HP		**Boiling temperature**		
		VLTb	**LTb**	**HTb**
Flash Temp.	**VLTf**	VHH	VH	MH
	LTf	VH	VH	MH
	MTf	MH	MH	MH
	HTf	LH	LH	LH
	VHTf	VLH	VLH	VLH

As mentioned previously some of the rules in Table 8.5 do not have physical meaning (e.g., gray cells) but are included in the rule base in order to ensure the model sensitivity along the limits of region with physical meaning. This is required because of the fact that several rules are fired at the same time.

From the rule matrix, it is clear that only chemicals with very high flash temperature represent low fire and explosion hazard. The fuzzy set MH (medium hazard) is assumed to be the reference state that indicates the threshold between the different degrees of inherent safety and conditions of higher hazard and it corresponds to the NFPA flammability score 2.

The membership functions for reactivity due to water are reported in Figure 8.9 and the parameters for input and output fuzzy sets are shown in Tables 8.6 and 8.7; the IF-THEN rules are reported in Table 8.8. In the case of water reactivity the values of heat of mixing used by NFPA to define the categories (i.e., 30 cal/gr, 100 cal/gr, 600 cal/gr) are transformed to a logarithmic scale for the design of the membership functions and the values are used to define the crossover points of the fuzzy sets.

The membership functions for chemical reactivity based on Instantaneous Power Density (IPD) are similar to the functions for water reactivity; however they have one more set, according to the NFPA scoring system. The NFPA score 2 for reactivity is used as the reference inherently safer state. The reference state for inherent safety is assumed to be the output fuzzy set "Very low heat of mixing" because the other sets imply the potential of vapor and gas generation that can overpressurize the vessel. The discrete scale of NFPA scores is on the range [0 3] and the score of 1 is used by the model proposed by this research as the inherently safer reference value. This score is for materials that react vigorously but not violently with water however, they can still generate gases and toxic vapors.

The membership functions for the potential hazard due to dispersion of flammable and volatile chemicals (i.e., $T_{flash} < T_{atm}$) are shown by Figure 8.10.

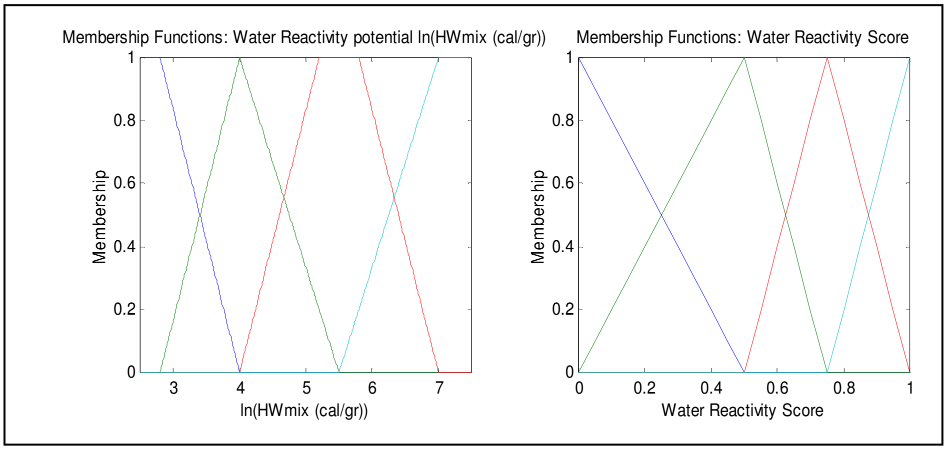


Figure 8.9: Input and output membership functions for hazard due to chemical reactivity CHPRh2o

Table 8.6: Parameter for CHPRh2o inputs

INPUTS	NAME	DESCRIPTION	SHAPE	PARAMETERS ln[cal/gr]
Heat of water mixing	**VLHWmix**	Very Low H mix	Trapezoidal	[0.6 2.2 2.8 4.0]
	LHWmix	Low H mix	Triangular	[2.8 4 5.2]
	MHWmix	Medium H mix	Trapezoidal	[4 5.2 5.8 7]
	VHHWmix	Very high H mix	Trapezoidal	[5.8 7 8 9.2]

Table 8.7: Parameter for CHPRh2o outputs

OUTPUTS	NAME	DESCRIPTION	SHAPE	PARAMETERS [cal/gr]
Hazard	**VLH**	Very low hazard	Triangular	[-1 0 1]
	MH	Medium hazard	Triangular	[0 1 2]
	HH	High hazard	Triangular	[1 2 3]
	VHH	Very high H mix	Triangular	[2 3 4]

Table 8.8: Fuzzy IF-THEN rules for CHPF. The general rule is: IF ("heat of water mixing" is ____) THEN (HP is ____)

		HP
Heat of mixing	**VLHWmix**	VLH
	LHWmix	MH
	MHWmix	HH
	VHHWmix	VHH

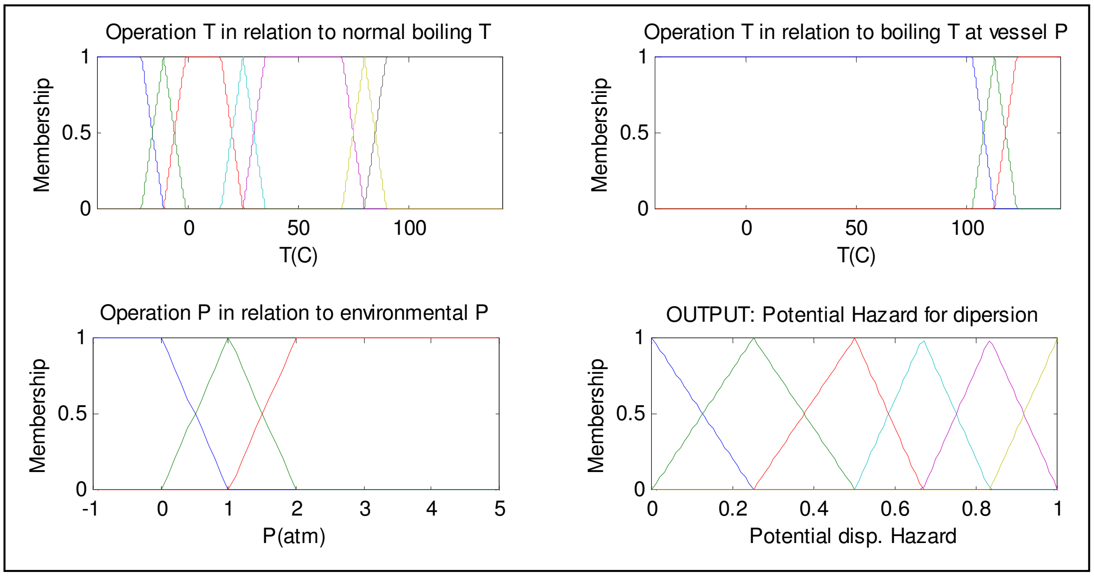


Figure 8.10: Input and output membership functions for the evaluation of the dispersion potential

The design of the membership function for pressure is based on the fact that for gases when the pressure of the vessel is $P > (1.7 - 1.9) \times P_{atm}$ the flow becomes sonic. The principle does not apply to liquids, however here it is taken as an approximate physical indication for the design of the symmetric functions for pressure. The parameters of the membership functions are not reported because they change according to the location of the fuzzy set for the flash temperature and the normal boiling temperature.

The rules reported in Table 8.9 have the following meaning: VLH = very low hazard LH = low hazard, MH = medium hazard (and this is also the reference state), VH = high hazard, HH = very high hazard, VVHH = extremely high hazard.

Table 8.9: Fuzzy IF-THEN rules for DISP. The general rule is: IF (“vessel temperature” is __) AND (“vessel temperature” is __) AND (“vessel pressure” is _) THEN (ISL is __)

	$T^t < T_b^t$			$T^t \cong T_b^t$			$T^t > T_b^t$		
	$P^t < P_{atm}$	$P^t \cong P_{atm}$	$P^t > P_{atm}$	$P^t < P_{atm}$	$P^t \cong P_{atm}$	$P^t > P_{atm}$	$P^t < P_{atm}$	$P^t \cong P_{atm}$	$P^t > P_{atm}$
$T^t < T_f$	LH	MH	MH	LH	-	-	VLH	-	-
$T^t \cong T_f$	VLH	VLH	VLH	VLH	-	-	VLH	-	-
$T^t > T_f$	VLH	VLH	LH	VLH	-	-	VLH	-	-
$T^t \cong T_{atm}$	LH	LH	MH	LH	-	-	VLH	-	-
$T^t < T_b^N$	MH	MH	HH	MH	-	-	LH	-	-
$T^t \cong T_b^N$	-	-	VVHH	-	HH	-	MH	-	-
$\mathbf{T^t > T_b^N}$	-	-	VVHH	-	-	VVHH	VLH	MH	HH

Where:

T^t: vessel temperature

T_b^t: boiling point at the vessel pressure

T_f: Flash temperature

T_{atm}: Atmospheric temperature

T^t: vessel temperature

P_{atm}: Atmospheric pressure

-: combination of input sets without physical meaning

For the case of the evaluation of the hazard derived from the degree of confinement and obstruction and the burning velocity of the chemical, Figure 8.11 shows the input membership functions, and Figure 8.12 shows the output functions and the fuzzy graph. Table 8.10 reports the parameters of the input functions and Table 8.11 reports the parameters for the output sets.

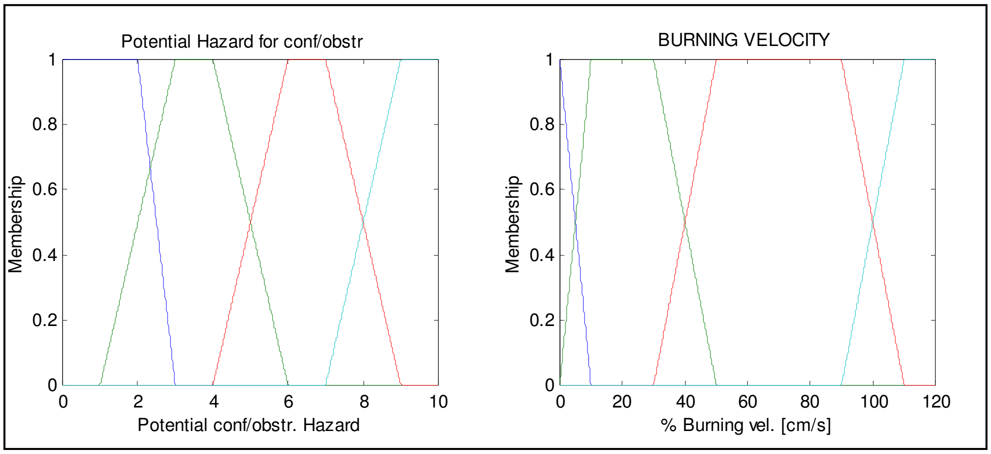
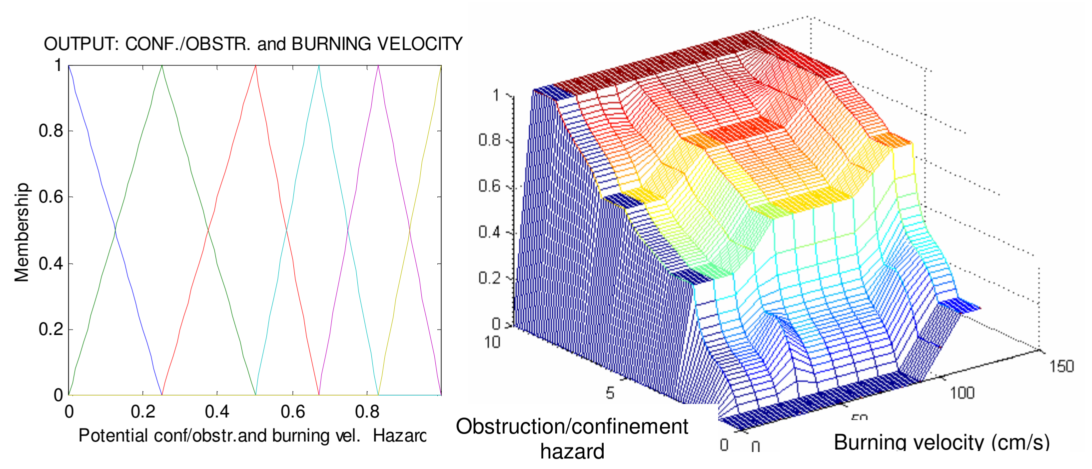


Figure 8.11: Membership functions for the FIS COBV

As shown in Figure 8.12a, the last three output sets are narrower than the first three in order to emphasize the hazard associated with conditions of high obstruction and congestion, when the chemical is flammable and capable of producing a strong overpressure due to an explosion. The fuzzy sets for COOB are the output set for the FIS that combines the degree of obstruction and confinement, and they describe the potential strength of the explosion.



a

b

Figure 8.12: Output membership functions (a) and fuzzy graph for FIS COBV (b)

Table 8.12 reports the rules used for the FIS COBV; the gray cells indicate a region of high uncertainty because of the firing of four rules over the whole range of the output. In this case, the strength of each rule's output determines the location of the defuzzified value (i.e., the hazard degree). The rules are designed in this way in order to generate a rapid increase of the hazard score.

Table 8.10: Parameter for COBV inputs

INPUTS	**NAME**	DESCRIPTION	SHAPE	PARAMETERS [cm/s]
COOB HP	**WEAK**	Low overp.	Trapezoidal	[0 0 2 3]
	MED	Med. overp.	Trapezoidal	[1 3 4 6]
	STRONG	High overp.	Trapezoidal	[4 6 7 9]
	VSTRONG	Very high overp.	Trapezoidal	[7 9 10 10]
Burning velocity [cm/s]	**NOBV**	No reactivity	Trapezoidal	[0 0 10]
	LOWBV	Low reactivity	Trapezoidal	[0 10 30 50]
	MEDHBV	Medium reactivity	Trapezoidal	[30 50 90 110]
	HIGHBV	High reactivity	Trapezoidal	[90 110 120 120]

Table 8.11: Parameter for COBV output

OUTPUT	**NAME**	DESCRIPTION	SHAPE	PARAMETERS [°C]
Hazard Potential HP	**VLH**	Very Low Hazard	Triangular	[-0.25 0 0.25]
	LH	Low Hazard	Triangular	[0 0.25 0.5]
	MH	Medium Hazard	Triangular	[0.25 0.5 0.67]
	HH	High Hazard	Triangular	[0.67 0.83 1]
	VHH	Very High Hazard	Triangular	[0.83 1.0 1.17]

Table 8.12: Fuzzy IF-THEN rules for COBV. The general rule is: IF ("obstruction/congestion" is __) AND ("flame burning velocity" is __) THEN (HP is __)

HP		**Burning velocity**			
		NOBV	**LOWBV**	**MEDBV**	**HIGHBV**
	WEAK	VLH	VLH	VLH	LH
COOB	**MED**	VLH	MH	HH	VHH
	STRONG	VLH	HH	VHH	VVHH
HP	**VSTRONG**	VLH	VVHH	VVHH	VVHH

8.2 FUZZY MODELS FOR TOXICITY AND ENVIRONMENTAL HAZARD

The evaluation of chemical substances from the view point of their toxic effect and the impact on the environment and the troposphere has the objective to identify potential negative consequences other than fire and explosion. Process safety design is mainly focused on the reduction of likelihood of a chemical incident, fire and, explosion. The long-term effects of small releases that do not pose fire or explosion hazards are rarely taken into consideration unless there are specific environmental regulations imposing limits on the type, flow, or concentration of released contaminants streams.

When a chemical is evaluated from the environmental viewpoint, the properties used for evaluating its process safety characteristics are not sufficient compared to properties as photo and biodegradation rates, water solubility, and bioaccumulation. For instance, paper is one of the most common supplies of the modern world, and it is thought to be biodegradable and environmentally friendly. However, even if it does not pose a toxic hazard (it can pose a fire hazard if stored in large quantities) it poses an environmental problem since its biodegradation process is very slow.

The evaluation of environmental effects is restricted to water toxicity and atmospheric persistence. The impact on soil and biota is modeled by assuming that if the chemicals are hard to degrade and bioaccumulable, the potential for persistence in soil and accumulation in the food chain is possible. The purpose of this part of the proposed hierarchical model for inherent safety evaluation is the identification of potential environmental hazards. Chemical fate modeling is not part of the scope of the project; however, the results derived from environmental simulation can be applied to develop general rules (as in the case of dispersion modeling in air) that can then be used to expand the hierarchical model.

The evaluation of acute toxic effects for humans is based on the three potential routes of exposure: dermal, oral, and respiratory. Chronic effects are restricted to the potential for carcinogenicity based on information for animals and humans. The combination of both sources of data is required because of the limited quantity of information for humans; however because carcinogenicity in animals must be extrapolated across species, when human data is available, it is assumed to be more reliable. Other chronic effects such as teratogeneity, cell mutations, respiratory and skin sensitization, are not taken into consideration due to the lack of data easily accessible to non-experts such as process design engineers.

For the evaluation of toxic and environmental hazards, eight fundamental fuzzy inference systems (FIS) are used while six integrate the information generated from the fundamental FIS. Tables 8.13 and 8.14 report the names and required inputs for the 14 FIS. As indicated in Tables 6.1 and 6.2, some of the required inputs are for the design of adaptive membership functions, as in the case of toxic dispersion potential evaluation (DISPTX).

Table 8.13: List of fundamental FIS and required input parameters for toxicity

FIS NAME		INPUT	UNITS
CHEp	"Hazard due atmospheric stability"	Troposphere half-life Data quality	days %
CHEat	"Hazard due to bioaccumulation potential and toxicity"	Bioaccumulation factor Aquatic toxicity (LD_{50})	Log K_{ow} µg/l
CHEdt	"Hazard due to aquatic toxicity and degradability"	Half-life time Aquatic toxicity (LD_{50})	days µg/l
DISPTX	"Hazard due to toxic dispersion"	Normal boiling temperature Atmospheric temperature Vessel boiling temperature Vessel temperature Vessel pressure	°C °C °C °C atm
CHHc	"Hazard due to chronic human toxicity"	Human cancer evidence Human cancer evidence	% %
CHH1a	"Hazard human acute and chronic toxicity"	Acute oral toxicity Acute dermal toxicity	mg/kg mg/kg
CHH2a	"Hazard due to respiratory toxicity for vapor or gas/mist"	Acute respiratory tox.: vapor Acute respiratory tox.: mist	mg/l ppm
CHH3a	"Hazard due to respiratory toxicity for dust"	Acute respiratory tox.: dust	mg/l

Table 8.14: List of aggregation FIS and input parameters for toxicity

FIS NAME		INPUT	UNITS
AGCHM	"Hazard due toxicity, environmental impact and potential dispersion"	AGCH DISPTX	HP* HP*
AGCH	"Human and environmental chemical hazard"	AGHEA AGET	HP* HP*
AGET	"Hazard due to water/soil and troposphere toxicity "	CHPF CHEp	HP* HP*
CHPF	"Hazard due to bioaccumulation potential and degradability"	CHEdt CHEat	HP* HP*
AGHEA	"Hazard due to human acute and chronic toxicity'	CHHc AGHEALTHa	HP* HP*
AGHEALTHa	"Hazard due to acute human toxicity"	CHH1 CHH2a/CHH3a	HP* HP*

* HP = hazard potential index

As for fire and explosion hazard, in order to eliminate the subjectivity derived from interpretation of the phenomena, the model is based on accepted toxicological and ecotoxicological principles. In the next section the fundamental concepts used for the design of the fuzzy inference systems for the evaluation of toxic and environmental hazard, including dispersion of toxic chemicals, are summarized. Section 2.2 reports the parameters of the membership functions for representative FIS, as well as the sets of IF-THEN rules.

8.2.1 Theoretical foundation for the design of IF-THEN rules and membership functions

The limited knowledge available on the long-term effects of chemicals on the environment due to accumulation and slow degradation kinetics can mislead the decision process into hazardous directions. An example is the substitution of ammonia and propane by CFC. However, the recognition of the possible lack of information or data related to a specific chemical can be used as an additional piece of data. For instance, if there is not specific information about the life-cycle of a chemical (i.e., how it is transported across different environmental systems, how it is degraded, and how long does it take to be bio-decomposed) its evaluation, from the environmental view point, should be less favorable than the evaluation of another chemical whose properties are well known and supported by scientific data. This approach is used by the GDCh-Advisory Committee (1989).

To understand the environmental problems it is necessary to introduce the concepts of Environmental Risk Analysis (ERA), and ecotoxicology.

8.2.1.1 Environmental hazard

The environmental impact analysis (EIA) has the objective of identifying and evaluating the importance and duration of the possible impacts and benefits to the natural and social environment due to an activity or project. The impact is defined by a spatial component (i.e., a defined area) and a temporal component (i.e., a specified period of time) produced by the change in an environmental parameter (Wathern, 1988).

The subjectivity along with uncertainty inherent in the environmental factors, the reliability of the information, and the low-probability events that must be addressed, increases the uncertainty of the analysis. However, this aspect is rarely taken into consideration.

The environmental impact assessment (EIA) and the environmental risk assessment (ERA) have many common, and in some case overlapping points. However they have been developed by two professional communities emphasizing different aspects. The community interested in EIA is generally related to biological and environmental sciences, resource management, and sociology. Professionals related to ERA can be grouped into toxicologists, epidemiologist, and biostatisticians as well as engineers. The focus of both studies is different, and while EIA emphasizes the effects on the natural ecosystems, ERA emphasizes human health consequences (Wathern, 1988).

With respect to the environment, the risk is related to hazards imposed on the ecosystems by the properties of the substances, their degradation products, or other chemicals generated during the manufacturing processes. The impact of the substances can occur on any of the compartments of the ecosystems, and some of the most important hazardous properties include low degradability (hence high persistence), bioaccumulation, and mobility.

Environmental risk is characterized by uncertainty and time dependency. The probability of causing environmental damage is given by a set of conditional probabilities defined over a specific period of time. However the risk should be judged in different ways depending on the time length the risk will exist and its severity. In general an ERA should include the evaluation on the type, quantity, and extent of risk, control mechanisms and transport mechanisms able to move the source of hazard to sites where the environmental damage can occur. The general targets for environmental risk are sensitive environments and humans. In both cases assessment factors include surface and ground waters, air routes, fire and explosion, and direct contact.

Environmental risk assessment relies on ecotoxicology knowledge to identify and evaluate chemical hazards due to exposure to specified doses. When ERA is performed as a predictive evaluation, it should include levels of toxicity to the biological systems and the potential environmental distribution and fate of the chemicals. The evaluation should start from physical and chemical properties of toxicants (Bacci, 1994).

Ecotoxicology is a branch of toxicology formed by the union of environmental chemistry and ecology and aims to produce criteria and standards for pollution prevention and minimization. Another goal of ecotoxicology research is the evaluation of acceptable risk levels for the biological systems. The study of contamination is focused on the protection of human health, however it is understood that this could not be achieved unless wildlife and ecosystem would be also preserved.

Ecotoxicology is based on models to predict the behavior of the substances in the environment and to detect possible impacts on the compartments. The models are based on the physicochemical properties of the substances that define the environmental behavior and the hazards intrinsic to the nature of the chemicals (Bacci, 1994). In general, five parameters are required to describe the environmental hazard:

- Rate of entry
- Stability
- Movement
- Bioconcentration
- Toxicity

Each one of the parameters can be measured by using physicochemical properties. Movement can be evaluated by using water solubility and vapor pressure; stability is evaluated by the rates of hydrolysis, photodegradation and biodegradation; bioconcentration is evaluated by using the octanol-water partition coefficient and the bioaccumulation and biomagnification factors; the toxicity can be evaluated by using carcinogenic data and the LD_{50} (Golden et al., 1979).

Other properties describe chemical partitioning and fate. Environmental partitioning is controlled by properties such as boiling and melting points, gas and liquid densities, surface tension, vapor pressure, air-water partition coefficient, and sorption coefficient for soil and sediment. The environmental transport and fate are controlled by the diffusivity in air and water, the phase transfer coefficient for air-water and for soil-air. Only for a few of the required properties, information is available in the literature. However, estimation methods exist but should be used only when the experimental information is difficult to assess (Baum, 1998).

The criteria used to estimate the potential hazard to the environment are the following:

- Degradability: The resistance to degradation by biological or chemical mechanisms, is one of the major sources of hazards when combined with toxic properties of the chemicals or their products of side. The degradation of chemical substances can occur either due to biological effects (biodegradation) or chemical reactions such as reduction, oxidation, photolysis, and hydrolysis (Bacci, 1994).
- Bioconcentration: This is one of the three possible mechanisms according to which the chemicals are partitioned with water. Bioconcentration is related to the intake of chemicals from air or water via respiration that produces higher chemical concentration in the organism than in the water; bioaccumulation is referred to the chemical intake from any possible source for an organism (e.g., contact, respiration, ingestion, etc.) and happens because the intake rate exceeds the organism capacity to degrade it FROM its parts. Both bioconcentration and bioaccumulation are species-specific parameters due to different transport mechanisms inside the organism. However, bioconcentration depends solely on the physicochemical properties of the substances (Bacci, 1994). This parameter is a measure of the amount of chemicals absorbed by an organism and stored into the tissue. These chemicals are not degraded by the metabolism or excreted from the organism (Connell et al., 1999) therefore they have the potential for biomagnifcation (i.e., accumulation in higher levels of the trophic chain).

- Aquatic toxicity: This is the potential of the substance to produce harm and can be divided into acute and chronic toxicity. Paracelsus stated (as cited by Bacci, 1999) "all substances are poisons; there is no one which is not a poison; the right dose makes the difference between poison and remedy" and this represents the dose-effect relationship associated with the toxicity concept. The effect caused by the exposure to a chemical is described by the surface response-concentration-duration from which the curve dose-response is derived. Acute toxicity occurs at high chemical concentrations during short exposure times (i.e., 24-96 hrs or as short as 30 min for highly toxic substances). The physical effects of acute toxicity are associated with breakdown of physiological systems. Acute toxicity is given by the lowest concentration at which effects are evident within few days of continuous exposure; subchronic effects occur when the organism is exposed at the highest concentration in order for the effects to become evident around one-tenth of the lifespan of the animal; this data is useful to understand the mode of action of the chemical. Chronic effects are given by the highest concentration tolerable by the organism without presenting life threatening effects for the whole life-span of the organism [Verschueren, 1996].

For short-term exposure one of the significant parameters is the median lethal dose LD_{50} while for chronic studies other response levels (i.e., LD_{01}) are used. When chemicals are present in a mixture the overall toxicity can be modified; when the chemicals act independently the effect of the mixture can be predicted by adding the individual toxic effects. On the other hand, the toxic effects can be similar but independent, synergetic or antagonistic (Bacci, 1994). These combined effects are not taken into consideration here.

Other important parameters are the vapor pressure, boiling and melting temperatures, water solubility, Henry's Law constants, molecular diameter and surface area, molecular structure, partition coefficients (soil/sediment, vegetation/air, etc.), surface tension, diffusivity, and sorption coefficients. These properties affect the concentration of the chemicals in air, water, soil, biota, and sediments and should be taken into consideration for improved models. Rate of entry into the environment is important and can be estimated from mass balances of the chemical plants, production rates, and dispersion rates due to fugitive emissions, spills, and accidental releases, waste effluents and controlled emissions to the atmosphere.

The design of the membership functions for the evaluation of the environmental hazards due to toxic effects is based on three main documents: the Harmonized Integrated Classification System for Human Health and Environmental Hazards of Chemical Substances and Mixtures [OECD, 2001], published by the Environmental, Health and Safety Division of the Environmental Directorate of the Organisation for Economic Cooperation and Development (OECD); the Toxic Release Inventory (TRI) relative risk-based environmental indicators methodology [Bouwes and Hassur (1996)]; GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance (BUA), [GDC, 1989].

The purpose of the Harmonized system [OECD, 2001], is relevant for this research because it is focused on the development of a system for the classification of hazardous chemical substances based on their inherent physical and chemical properties based on the following general principle: "…harmonization means establishing a common and coherent basis for chemical hazard classification and communication, from which the appropriate elements relevant to means of transport, consumer, worker and environmental protection can be selected…". Based on the previous principle, common cut-offs for each hazard category, are proposed and must be accepted as a fundamental basis for any type of application. The harmonized system developed thresholds for categories of chemical hazard by integrating the threshold specified by other classification systems.

The TRI [Bouwes and Hassur (1996)] is also relevant for the present project because of the effort to develop environmental indicators based on risk using scores assigned according to the relative importance of each class. Therefore, the ordinal scale used includes information on a relative basis.

For the present research the evaluation of environmental effects is focused on the aquatic environment and the air compartment only. Effects on soil are not taken into account. For the aquatic environment the indicators taken into account by the hierarchical system are:

- Aquatic toxicity
- Bioaccumulation potential
- Degradability

The criteria used to estimate the potential hazard to the environment are the following:

- **Degradability**: Environmental degradation occurs due to biotic and abiotic factors. Chemical substances can be classified into readily degradable when 70 to 80% of the initial content is degraded. The uncertainty in the results is derived from the different experimental methodologies that can be used. Particular attention should be paid to mixtures, which are not addressed by this project. The five possible degradation reactions can be analyzed separately to obtain information about the behavior of the chemical in the different compartments (e.g., hydrolysis rate is more important for water environment, while photolysis is not important for areas that do not receive sunlight). However, they can be grouped into a first-order global reaction rate, $k_{R,}$ which is used to define the overall half-life $t_{½\ overall}$ parameter (Bacci, 1994):

$$k_R = k_{hydrolysis} + k_{photolysis} + k_{oxidation} + k_{reduction} + k_{biodegradation}$$

$$t_{½\ overall} = (\ln 2)/k_R$$

Under natural conditions the half-life time for the degradation of a substance can show considerable variability. However it is constant under controlled experimental conditions and this is helpful for comparative ranking of different chemicals (Connell, 1999). The uncertainty associated with the variability in the environment is taken into account by the proposed hierarchical model by allowing the user to work with a range of values (expressed by a triangular fuzzy input) rather than a single crisp value. Mackay (1992) and Bouwes and Hassur (1996) indicated the following classes (Table 8.15) for mean half-life times:

The values reported in Table 8.15 are used for the design of the membership functions for the evaluation of the degradability of the chemicals. The linguistic variable is however, on a logarithmic scale (i.e., $\ln(t_{1/2})$) because of the wide range of the universe of discourse.

Table 8.15: Suggested classes for half-time according to Mackay (1992) and Bouwes and Hassur (1996)

[Mackay, 1992]			[Bouwes and Hassur, 1996]	
CLASS	MEAN HALF-TIME	RANGE [hr]	SCORE	
1	5 hrs	< 10	12	1 day < t
2	17 hrs (~ 1 day)	10 - 30		
3	55 hrs (~ 2 days)	30 - 100	10	1 day < t < 2 weeks
4	170 hrs (~ 1 week)	100 - 300		
5	550 hrs (~ 3 weeks)	300 - 1,000		
6	1700 hrs (~ 2 months)	1,000 - 3,000	5	2 weeks < t < 8 weeks
7	5500 hrs (~ 8 months)	3,000 -10,000	3	8 weeks < t < 52 weeks
8	17,000 hrs (~ 2 years)	10,000 - 30,000	0	t > 1 year
9	~ 5 years	> 30,000		

- **Bioconcentration:** This parameter is chosen because it is independent on the properties of the organism or ecosystem. The bioconcentration potential is evaluated either by the bioconcentration factor (BCF) or by the fish-water partition coefficient (K_{FW}), which is correlated to the n-octanol-water partition coefficient (K_{OW}). Several correlations have been proposed [Verschueren, 1996], but the most frequently used is the one proposed by Mackay, which assumes that fish behave as if it was a mixture of 4.8% octanol in water (the percentage is similar to the fish lipid content) (Bacci, 1994):

$$BCF = K_{FW} = 0.048\ K_{OW}$$

The previous equation also implies that the thermodynamics of the partition coefficient water-octanol is similar to the partition between water-lipid (Baum, 1998). However, the equation should be used only for non-polar substances because polar chemicals can affect the transport properties and can produce complexation reactions modifying the results. When a substance has a $\log(K_{OW})>6.5$ it is defined as superhydrophobic, and the results obtained with $BCF = K_{FW} = 0.048\ K_{OW}$ are overestimated with respect to the experimental values due to longer times required to achieve the equilibrium state and solubility differences (Bacci, 1994). Another possible explanation is that the chemical solubility in lipids reaches the maximum when BCF = 6. As an example BFC for chlorobenzenes reaches a maximum of 5.5 in fish when $\log(K_{OW}) = 6.0$ and then decreases as K_{OW} increases (Baum, 1998).

According to Bouwes and Hassur (1996) and the Harmonized system [OECD, 2001], the preferred measure of bioaccumulation and bioconcentration is the Bioconcentration factor (BCF) obtained experimentally by comparing the chemical concentration in water and in the tissue of the test organism. However, when the information is not available, the BCF can be approximate by the octanol-water partition coefficient (i.e., $\log(K_{OW})$) or by water solubility. For this research the bioconcentration potential of a chemical is evaluated by using the $\log(K_{OW})$ because of the easier accessibility to the information.

The values reported in Table 8.16 are used for the design of the membership functions for modeling bioaccumulation. When $\log(K_{OW}) < 3$ the bioconcentration potential is considered low while when it is larger than 3 it is considered high [GDC, 1989]. According to the Harmonized system [OECD, 2001] when the $\log(K_{OW}) < 4$ the toxic effects of the chemicals on the aquatic ecosystem are considered acute, while when $\log(K_{OW}) > 4$ they are assumed to be chronic.

Chemicals that are highly liposoluble (i.e., high octanol/water partition coefficient) have low water solubility therefore they do not undergo rapid biological transformation. Bioconcentration and biomagnification become important for chemicals with low acute toxicity because they accumulate and they may produce chronic effects [Verschueren, 1996].

Table 8.16: Suggested classes for bioconcentration according to Bouwes and Hassur (1996)

BCF	Log Kow
$BCF < 1$	<0.8
$1 < BCF < 10$	0.8-2.0
$10 < BCF < 100$	2.0-3.2
$100 < BCF < 1000$	3.2-4.5
$1000 < BCF < 10000$	4.5-5.5
$BCF > 10000$	5.5-6.0

- **Aquatic toxicity:** The evaluation of this parameter is mainly based on acute toxicity and is described by the parameter LD_{50} (for solids and liquids) and LC_{50} (for gases). When $LD_{50} < 1$ mg/kg the substance is classified as extremely toxic while a chemical with $LD_{50} < 50$ mg/kg is highly toxic. Another commonly used parameter is the threshold limit value (TLV), but this is not a measure of toxicity (Golden, 1979). Criteria for acute aquatic toxicity and acute fish toxicity are reported in Table 8.17 by the indicated sources.

Table 8.17: Categories proposed for the classification of aquatic acute toxicity

	[VCH, 1989]	[Bouwes and Hassur, 1996]	[OECD, 2001]
Specie Exposure time	Fish or Daphnia		Fish 96 hrs
Very High Toxicity	$LC_{50} < 1$	$LC_{50} < 0.1$	$LC_{50} < 1$
High toxicity		$0.1 < LC_{50} < 1$	
Average toxicity	$1 < LC_{50} < 100$	$1 < LC_{50} < 10$	$1 < LC_{50} < 10$
Low toxicity	$100 < LC_{50} < 1000$	$10 < LC_{50} < 100$	$10 < LC_{50} < 100$
No toxicity	$1000 < LC_{50}$	$100 < LC_{50}$	

* LC_{50} in mg/l

For simplicity, fish or daphnia aquatic toxicity are used as inputs for the hierarchical model proposed here, rather than the acute mammalian toxicity values (based on LD_{50} for oral, dermal, and inhalation absorption). The values proposed by [Bouwes and Hassur, 1996] are used for the design of the membership functions because are similar to the values given by the Harmonized system [OECD, 2001] but they include two additional category that allow finer granulation of the linguistic variable "aquatic toxicity". In case that data for fish are not available, the ranges given by the Harmonized systems can also be applied to crustacean with exposure time of 48 hrs (in this case EC_{50} is used with the same ranges given for LC_{50}) or to algae and aquatic plants with exposure times of 72 to 96 hrs (in this case ErC_{50} must be used with the same ranges given for LC_{50}), [OECD, 2001].

The fuzzy system for the evaluation of the environmental impact due to aquatic acute toxicity, bioaccumulation potential, and degradability is composed by three sets of rules, as explained in Chapter VII. The first set of rules "hazard due to aquatic toxicity and degradability (CHEdt) evaluates the combination of toxicity and degradability. Highly toxic and degradable chemicals have the potential to produce short-term negative effects on the environment; if these chemicals are not degradable the negative impact is higher

[OECD, 2001]. In both cases (i.e., toxic degradable chemicals and toxic non-degradable substances) these chemicals are assumed to represent very high inherent hazard for the environment; however, in the case of high degradability, the effects can be localized therefore the evaluation is conservative.

Chemicals with low toxicity and low degradability can generate chronic consequences therefore they imply high environmental hazard. Chemical with low toxicity and high degradability are assumed to have a low hazard degree. The reference states for inherent safety are represented by chemicals with medium or high toxicity and easy to degrade. Another reference state is given by non-degradable and non-toxic chemicals that do not imply adverse effects on the environment.

The second set of rules "hazard due to bioaccumulation potential and toxicity", (CHEat) combine the hazards due to toxicity and bioaccumulation potential. If chemicals are toxic, regardless their bioaccumulation potential, they receive high hazard scores. The lowest hazard degree is assigned to chemicals with low or no toxicity and with low or null accumulation potential; the reference for inherent safety is assumed to be for chemicals with low toxicity and low accumulation potential and for non-toxic chemicals with high bioaccumulation potential.

The combination of the outputs from the fuzzy systems CHDT and CHEdt is evaluated by the FIS "hazard due to bioaccumulation potential and degradability" (CHPF) which evaluates the aggregated effect of acute aquatic toxicity, degradability, and bioaccumulation potential. It is assumed that if either one of the inputs implies high hazard, the inherent hazard is high while both inputs must imply low hazard in order to obtain an overall low inherent hazard for the aquatic environment.

- **Tropospheric half-time:** An additional parameter that must be considered is the impact of chemicals on the atmosphere and the future global warming potential. As proposed by the Environmental Performance Indicators (EPI) project developed in 1999 under a partnership between several entities lead by the Association of the Dutch Chemical Industry (VNCI), several effects can be taken into account. Examples of relevant aspects are the potential for greenhouse effect, potential for depletion of the ozone layer, potential for atmospheric acidification, and the potential for ozone creation [EPI, 2001]. The EPI approach could be translated into a fuzzy system that could be added to the prototype proposed in this research.

However, for this work only the degradability in air based on photochemical reactions is modeled by using the tropospheric half-time of the chemicals. According to the report “Existing Chemicals of Environmental Relevance” [GDC, 1989], when the tropospheric half-life of a substance is less than one day, it is considered easy to degrade; if the half-life is between 1 and 10 days the chemical is assumed as potentially degradable, but if the half-life is longer than 10 days then it is classified as hardly degradable. In order to reach the troposphere, a chemical must be volatile therefore for a chemical substance with low volatility the impact on the atmosphere is assumed to be negligible.

Another possible approach for the design of the membership functions is based on the six classes proposed by IPUAC [2001] (i.e., 1day, 10 days, 100 days, 365 days); this system allows finer granulation of the linguistic variable and it is used for the design of the fuzzy sets.

The information regarding the air half-life is becoming a common parameter reported by the Material Safety Data Sheets (MSDS) and therefore it was selected. However, due to the high uncertainty associated with the parameter, for the design of the fuzzy IF-THEN rules that evaluate the atmospheric impact an additional parameter is required, “quality of the information”, in order to take into account the reliability of the source of information. When the reference is considered highly reliable and published by experts (e.g., research institutes, governmental and specialized reports) the linguistic variable should be assigned a value, or range of values, above 0.9; if the half-life value is estimated by using analytical models the input for “information quality” should receive a value between 0.25 and 0.75; if the source is not very reliable, then the parameter should receive a value below 0.5. The rule set “hazard due to atmospheric stability“, (CHEp) combines the estimated atmospheric hazard with the quality of information.

The aggregation of the overall aquatic inherent hazard and the hazard due to the atmosphere is evaluated by the fuzzy inference system called “hazard due to water/soil and troposphere toxicity”, (AGET). The inputs are assumed to have equal importance, therefore only when both aspects imply very low hazard the overall aggregated evaluation is set to low hazard; if both imply medium hazard, then a synergistic effect is assumed and the overall hazard is assumed to be high.

The reference states for inherent safety (i.e., overall hazard assumed to be medium) occur when the tropospheric hazard is medium and aquatic hazard is either low or very low; other reference states are assigned when aquatic hazard is medium and tropospheric hazard low or very low.

8.2.2 Human toxicity

Toxic effects in humans can occur due to exposure to a chemical substance through three main routes, inhalation, ingestion, and dermal contact, and the effects can be acute or chronic. While acute effects are produced by exposure to high doses of chemical for a short time, with immediate consequences for human health, chronic effects occur due to exposure to lower doses for a long period of time and the symptoms can be latent or gradual [Lees, 1996]. In terms of toxicity, chemical substances can be classified according to their effects on the human organism. For instance, gases can be simple asphyxiants when they only displace oxygen but are biologically inert (e.g., methane and carbon dioxide); chemical asphyxiants affect the absorption of oxygen by displacing it or destroying its transport mechanics (e.g., carbon monoxide, cyanide, hydrogen sulfide); irritants produce injury of the mucosa and, depending on their water solubility will affect the upper or lower airways (e.g., ammonia affects upper airways, while phosgene, sulfur dioxide, and chlorine affect the lower airways); asphyxiants and irritants affect the airways in both forms, by reducing the oxygenation and by injuring the respiratory tract. Other forms of toxicants may cause sensitization of specific organs such as respiratory system, liver, eyes and skin; in other cases chemicals can produce cancer, or they may have reproductive and teratogenic consequences.

The toxic effect of a chemical depends on several factors, such as its physicochemical properties, exposure time, dosage, and toxic mechanism. Therefore the evaluation of a chemical from the toxicology viewpoint is a complex task and relevant information is usually incomplete or nonexistent [Lees, 1996]. Toxicity is assessed in several ways such as microorganism test, animal testing, and epidemiological assessment. In the case of animal testing the common objective is to determine the lowest dosage capable of killing 50% of the specimens; if the substance is administered orally the obtained value is the LD_{50} (i.e., lethal dose that kills 50% of the animals) while if it is administered through the respiratory route the result is LC_{50} (i.e., lethal concentration that kills 50% of the animals). The epidemiological approach is possible when a group of people are exposed to the chemical and a comparison with non-exposed persons is possible. However, besides the implications for the exposed people, this approach also implies technical uncertainty due to the impossibility of determining the degree of exposure in terms of dosage and time [Lees, 1996].

When information on chemical toxicity is obtained from microorganisms and animals, additional uncertainty is added to the estimation because the data must be extrapolated between different species. Because of physiological differences the response of different species to the same chemical can vary. In general, it is assumed that if results are similar for three animal species then they can be extrapolated to humans with caution. Another source of uncertainty is the variability of the human response to chemicals depending on general health of the individual, fitness and stress level, as well age and gender [Lees, 1996].

Another measure of toxicity derived from industrial hygiene standards is the Threshold Limit Values (TLV) which can be time-weighted average (TLV-TWA), TLV for short-term exposure limit (TLV-STEL), or TLV for a ceiling concentration (TLV-C). However, as indicated by Lees (1996) TLV are not sharp lines that divide safe from unsafe concentrations and the best approach is to keep the chemical concentration as low as possible. Other toxicity measures are reported and explained by Lees (1996).

When toxicity values are used for risk assessment it must be kept in mind that the values are based on the assumption that the organism is static; however, in emergency conditions people will be under stress and performing physical activity, increasing therefore the air intake, and the potential for injury may be more severe than expected.

Probit equations are common models for the analysis of toxicity and they are available for several industrial gases; however probit equations are based on animal experimental data, therefore present the limitation of not taking into account the physical activity factor. Another model, known as SLOT (Specified Level Of Toxicity) developed by the HSE (Health and Safety as cited by Lees, 1996) is based on values of LD_{05} or LD_{01} rather than LD_{50} which are values that can exist for humans and can then be used as reference limits. Other models proposed by several entities for the analysis of gas toxicity are presented by Lees (1996).

The hierarchical model proposed for inherent safety analysis, evaluates the potential hazards derived from the chemical toxicity for humans based on the guidelines suggested by the Harmonized system whose criteria are based on the guidelines issued by the United Nations Committee of Experts on the Transport of Dangerous Goods (UNCETDG) [OECD, 2001].

The model is divided into acute and chronic toxicity; acute effects take into account respiratory, oral, and dermal toxicity, while chronic effects evaluate the cancer potential of the substance. Other acute effects such as eye and skin irritation and corrosion are not included due to the lack of data easily accessible to non-experts; similarly, chronic effects such as respiratory sensitization, reproductive toxicity and germ cell mutagenicity are not included. However, these aspects of human toxicity can be included in future improvements of the model.

- **Human acute toxicity:** This aspect is divided into three main categories shown in Table 8.18; the toxicity values are based on approximate values of LD_{50} for the oral and dermal route, and values of LC_{50} for the respiratory route, based on exposure times of 4 hrs.

Table 8.18: Categories proposed for the classification of human acute toxicity [OECD, 2001]

CATEGORY	1	2	3	4	5
Oral toxicity [mg/kg]	5	20	300	2000	5000
Dermal toxicity [mg/kg]	50	200	1000	2000	
Respiratory toxicity					
Gases [ppm]	100	500	2500	5000	
Vapors [mg/l]	0.5	2	10	20	
Dust and mist [mg/l]	0.05	0.5	1	5	

When data are available for exposure times of 1 hour they must be converted to the required time-scale by dividing them by 2 for gases and vapors and by 4 for mists and dusts [OECD, 2001]. The values for inhalation are divided into three categories in order to take into account the physical form of the substance; when the chemical is a saturated vapor or is a mixture of vapor and mist, it presents experimental challenges for the estimation of the toxicity values, therefore the concentrations are expressed as mg/l rather than ppm. Category 5 is for chemicals that present very low toxicity but can pose some toxicological hazard to sensitive people. Values of respiratory toxicity for mist and dust must be related to tests performed on rats, due to the aerodynamic characteristics of particles between 1 and 4 mm the chemical is deposited on the whole respiratory tract of these animals [OECD, 2001].

The values reported in Table 8.17 have been used as crossover points for the design of the membership functions for the linguistic variables for the FIS “Hazard due to respiratory toxicity for vapor or gas”, (CHH2a), “hazard due to respiratory toxicity for dust and mist” (CHH3a), and “hazard due to human acute and chronic toxicity” (CHH1a). In the three cases the variables have to be converted to logarithmic scales in order to preserve the narrower sets for high toxicity (i.e., categories 1 and 2) with respect to the wider sets for low toxicity (i.e., categories 4 and 5).

Because volatile chemicals can exist either as saturated vapor or as gases, only one input is expected for the set of rules CHH2a. The output from these rules is compared with the output from the set of rules CHH3a to select the largest hazard of respiratory toxicity. Oral and dermal toxicity are evaluated together assuming that this type of exposure occurs under specific circumstances such as close contact with the chemical (i.e., operator). Respiratory exposure can occur due to close contact but also because exposure due to dispersion of the released chemical outside the limits of the plant. In this case the general public will also be affected.

- **Human chronic toxicity:** The evaluation of long-term effects on the human health is focused on the potential to cause cancer. Carcinogenicity potential is estimated according to the guidelines given by the Toxic Release Inventory (TRI) relative risk-based environmental indicators methodology [Bouwes and Hassur (1996)]. According to this system, the cancer potential can be classified into six categories depending on experimental and epidemiological evidence available from humans and animals. The carcinogenicity categories are shown in Table 8.19.

Table 8.19: Carcinogenicity classes according to Bouwes and Hassur (1996)

CLASS	EPIDEMIOLOGICAL EVIDENCE	ANIMAL STUDIES
A	Sufficient evidence	
B1	Limited evidence	Sufficient evidence
B2	Inadequate or no data	Sufficient evidence
C	No evidence	Limited evidence
D	Inadequate or no data	Inadequate or no data
E	No evidence of carcinogenicity	

Additional explanation regarding the proposed categories and the type of data are provided by Bouwes and Hassur (1996). The information reported in Table 8.19 is used for the design of the membership functions for inputs and outputs. The inputs required by the fuzzy inference system “hazard due to chronic human toxicity” (CHHc), are the linguistic variables “human cancer evidence” and “animal cancer evidence”; these variables are defined over a range of [0 1], and are divided into four fuzzy sets representing the degree of evidence available (i.e., sufficient, limited, inadequate, nonexistent). When the evidence is sufficient the value of the input should be between 0.65 and 1; however, when the evidence is strong enough to support the relation between chemical exposure and cancer, the input value should be lower than 0.95. When the evidence of potential to cause cancer is limited, the input value should be between 0.35 and 0.95, while when the evidence is inadequate the input value should be between 0.05 and 0.65. When there is no evidence that supports the possibility of the chemical to generate cancer, the input value should be between 0 and 0.35; when the input is below 0.05 the chemical is considered not carcinogenic.

The fuzzy sets for the output are designed with reference to the carcinogenicity categories presented in Table 8.19, and the information reported by [Sabljic and Peijnenburg, 2001] which classify chemicals into five categories (i.e., carcinogenic, probable carcinogenic, possible carcinogenic, not classifiable, and probably not carcinogenic) based on the type of evidence available. The fuzzy IF-THEN rules describe the relation between the type of information available and the input and output fuzzy sets. Because the information regarding carcinogenicity is uncertain and vague, it is possible to define a range of values for the two inputs and feed them as fuzzy numbers.

The fuzzy system “hazard due to human acute and chronic toxicity “ (AGHEA), combines the evaluation of acute human toxicity and chronic human toxicity by using qualitative rules that assign equal importance to both adverse effects. Only when the two types of toxicity imply very low or null hazard for the human health, the chemicals are assigned an overall null hazard degree. The reference state for an inherently safer combination of acute and chronic toxicity is obtained when acute toxicity hazard is medium and the chemical is not carcinogenic, and when the acute toxicity is low or very low and the evidence for cancer effects is not enough to classify is as carcinogenic.

8.2.3 Hazards aggregation and toxic dispersion

The combination of human toxicity and environmental toxicity are aggregated by the qualitative fuzzy IF-THEN rules of the fuzzy inference system “human and environmental chemical hazard” (AGCH). For this inference system, human toxicity and environmental toxicity are assigned the same importance therefore in order for a chemical to represent low overall inherent hazard must also imply low toxicity for humans and low environmental impact.

The dispersion of toxic chemicals after being released is evaluated by “hazard due to toxic dispersion” (DISPTX), following the same guidelines and rules developed for fire and explosion (i.e., DISP). It is assumed that a toxic chemical stored at high pressure and at a temperature above the normal boiling point presents higher hazard due to increased flowrate and vaporization potential. The dispersion of toxic chemicals is more dependent on weather conditions than the dispersion of flammable chemicals [Lees, 1996]. However, for this research it is assumed that, as in the case of flammable substances, if the chemical has the potential to vaporize (either due to its physicochemical properties or because of the operation conditions) then the inherent degree of hazard is high. Another factor important for toxic dispersion is the degree of ventilation of the processing unit as indicated by Lees (1996). Ventilation is low when the degree of congestion and obstruction is high. While the aspects of confinement are taken into account for the evaluation of the explosion hazard, are not used for toxic dispersion, but they can be added in the future.

The potential hazard of cloud formation expressed by DISPTX is then combined with the overall hazard for humans and the environment (i.e., AGCH) by the FIS “hazard due toxicity, environmental impact and potential dispersion” (AGCHM). This inference system is based on qualitative rules that assign a low or very low hazard score only when both hazard aspects represent a low degree of hazard. The reference inherently safer combination of human and environmental hazards require medium or low hazard for either inputs, combined with low or very low hazard for the other input; if human hazard is evaluated as medium and environmental hazard is evaluated as medium, then a synergistic effect is assumed and the overall aggregated hazard is assumed to be hazardous.

The aggregation of toxic hazard for humans and the environment, and the chemical hazard for fire and explosion, is performed by the fuzzy inference system “Hazard due to chemical and design factors” (ISICHEM).The fuzzy IF-THEN rules for this system assign more importance to explosion hazards because of the larger destructive power that can increase the release of toxic chemicals. While the release of a toxic chemical affects human health and the environment, it cannot cause fire and explosion (unless the chemical is also flammable) therefore the destructive power is lower. Low hazard scores are given only for combination of low toxicity and low flammability, while the reference state for inherent safety is assumed to be the combination of medium toxicity (or explosivity) hazards with low explosivity hazards (or toxicity hazards).

8.2.4 Examples of the design of membership functions and fuzzy sets

The input fuzzy sets used as inputs for the evaluation of human toxicity for gases and vapors are given in Figures 8.13 and 8.14 show the output sets.

In Figure 8.14 four additional sets are used in order to smooth the output and the fuzzy graph. Table 8.20 shows the parameters for the input fuzzy sets for vapor and gas toxicity and Table 8.21 shows the rule-base used for the evaluation of overall respiratory human toxicity for a chemical in vapor or gas state.

In Table 8.21 the output fuzzy sets with * indicate a hazard between that set and the next level of hazard; for example, MH* indicates a level of hazard higher than medium hazard (MH) and lower than high hazard (HH). The finer granulation of this output allows increasing or reducing the sensitivity of certain areas of the output fuzzy graph.

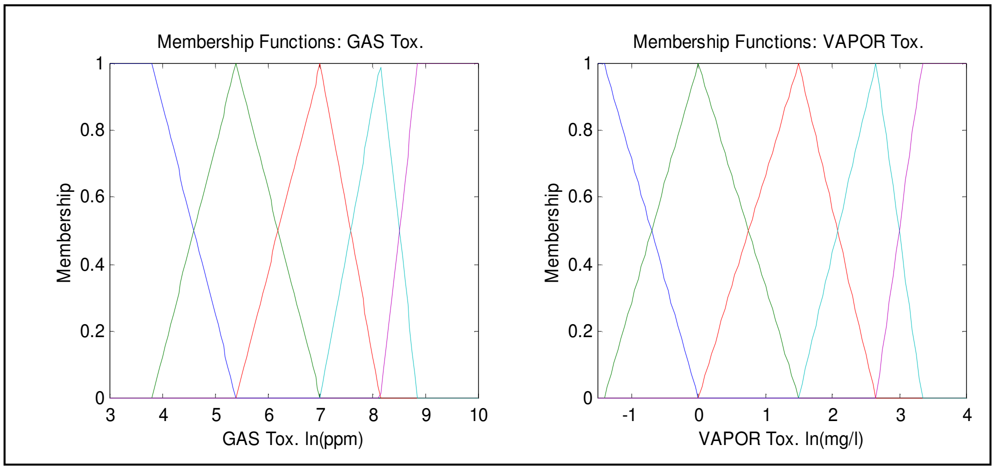


Figure 8.13: Input fuzzy sets for CHH2a (human toxicity for gases and vapors)

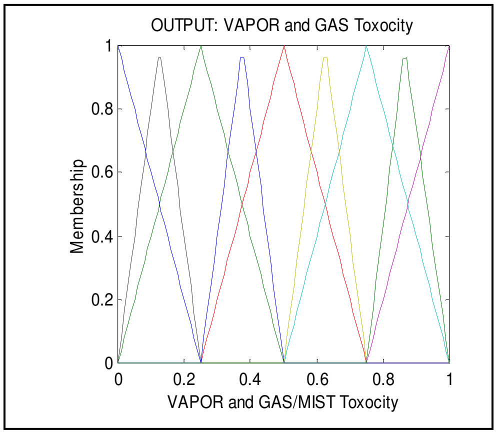


Figure 8.14: Output fuzzy sets for CHH2a (human toxicity for gases and vapors)

Table 8.20: Parameters for CHH2a inputs

INPUTS	NAME	DESCRIPTION	SHAPE	PARAMETERS
Gas toxicity ln[mg/l]	**VHGtox**	Very high toxicity	Trapezoidal	[1.4 2.2 3.8 5.4]
	HGtox	High toxicity	Triangular	[3.8 5.4 7]
	MGtox	Medium toxicity	Triangular	[5.4 7 8.14]
	LGtox	Low toxicity	Triangular	[7 8.14 8.85]
	VLGtox	Very low toxicity	Trapezoidal	[8.14 8.85 10.15 10.49]
Vapor toxicity ln[ppm]	**VHVAPtox**	Very high toxicity	Trapezoidal	[-1.5-1.5 -1.4 0]
	HVAPtox	High toxicity	Triangular	[-1.4 0 1.5]
	MVAPtox	Medium toxicity	Triangular	[0 1.5 2.65]
	LVAPtox	Low toxicity	Triangular	[1.5 2.65 3.34]
	VLVAPtox	Very low toxicity	Trapezoidal	[2.65 3.34 4 4]

Table 8.21: Fuzzy IF-THEN rules for COBV. The general rule is: IF ("acute vapor toxicity" is ____) AND ("acute gas toxicity" is ____) THEN (ISL is ____)

HP		**Gas toxicity**				
		VHGtox	**HGtox**	**MGtox**	**LGtox**	**VLGtox**
Vapor toxicity	**VHVAPtox**	VVHH	VVHH	VVHH	VVHH	VVHH
	HVAPtox	VVHH	VHH	VHH	VH	MH*
	MVAPtox	VVHH	VHH*	MH*	MH	LH*
	LVAPtox	VVHH	HH	MH	LH	VLH*
	VLVAPtox	VVHH	MH*	LH*	VLH*	VLH

The fuzzy sets for the evaluation of the environmental impact due to toxicity and degradability are shown in Figure 8.15. Tables 8.22 reports the parameters of the input functions, and Table 8.23 shows the rules used to evaluate the environmental impact.

In Table 8.23 the shaded rules indicate a region of high uncertainty that increases the sensitivity of the fuzzy inference system. The rules located in the right side of the table are associated with acute effects because of the rapid degradability of the substance, while the rules on the left side of the table are associated with long-term effects because the chemical will accumulate.

Table 8.24 shows the rules used for the aggregation of the evaluation of the toxic effects for humans (AGHA) and the environment (AGET):

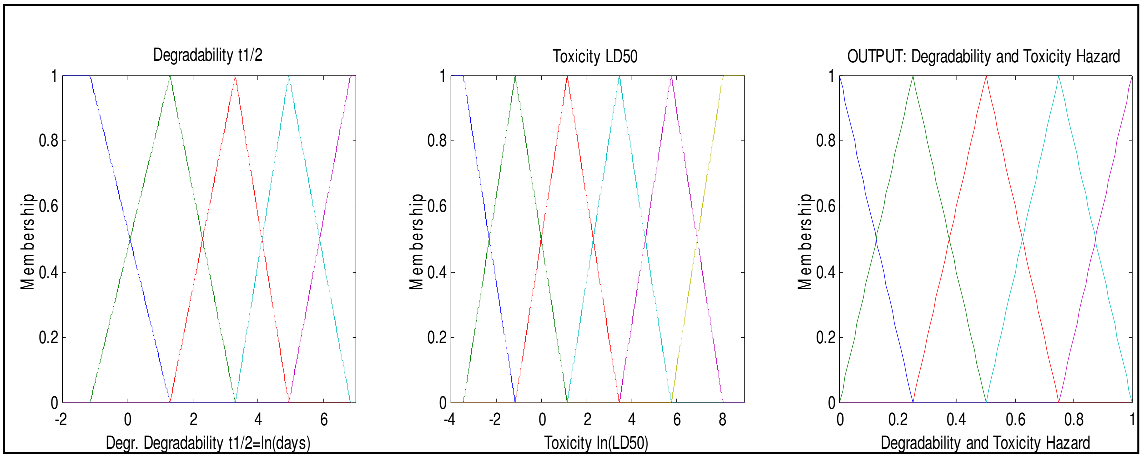


Figure 8.15: Input and output fuzzy sets for CHEdt

Table 8.22: Parameters for CHEdt inputs

INPUTS	NAME	DESCRIPTION	SHAPE	PARAMETERS
Half Life time ln[$t_{1/2}$]	**VHDegr**	Very high degrad.	Trapezoidal	[-2.3 -2.3 -1.15 1.3]
	HDegr	High degradability	Triangular	[-1.15 1.3 3.3]
	MDegr	Medium degrad.	Triangular	[1.3 3.3 4.94]
	LDegr	Low degradability	Triangular	[3.3 4.94 6.83]
	VLDegr	Very low degrad.	Trapezoidal	[4.94 6.83 7 7]
Chemical toxicity ln[LD_{50}]	**VVHtox**	Extreme toxicity	Trapezoidal	[-4 -4 -3.45 -1.15]
	VHtox	Very high toxicity	Triangular	[-3.45 -1.15 1.15]
	HLtox	High toxicity	Triangular	[-1.15 1.15 3.45]
	Mtox	Medium toxicity	Triangular	[1.15 3.45 5.75]
	Ltox	Low toxicity	Triangular	[3.45 5.75 8.05]
	Ntox	Very low toxicity	Trapezoidal	[5.75 8.05 9 9]

Table 8.23: Fuzzy IF-THEN rules for CHEdt. The general rule is: IF ("hazard due to toxicity" is ____) AND ("hazard due degradability" is ____) THEN (HP is ____)

HP		**Half-life time**				
		VHDegr	**HDegr**	**MDegr**	**LDegr**	**VLDegr**
Toxicity	**VVHtox**	VHH	VHH	VHH	VHH	VHH
	VHtox	VHH	VHH	VHH	VHH	VHH
	HLtox	VH	VH	VH	VHH	VHH
	Mtox	LH	MH	VH	VH	VH
	Ltox	VLH	LH	MH	VH	VH
	Ntox	VLH	VLH	LH	MH	MH

Table 8.24: Fuzzy IF-THEN rules for CHEdt. The general rule is: IF ("human toxicity" is ____) AND ("environmental impact" is ____) THEN (HP is ____)

HP		**Environmental impact (AGET)**					
		VLH	**LH**	**MH**	**HH**	**VHH**	**VVHH**
Human impact (ACHEA)	**VLH**	VLH	LH	MH	HH	VHH	VHH
	LH	LH	LH	MH	HH	VHH	VVHH
	MH	MH	MH	MH	HH	VHH	VVHH
	HH	HH	HH	HH	VHH	VVHH	VVHH
	VHH	VHH	VHH	VHH	VVHH	VVHH	VVHH
	VVHH	VVHH	VVHH	VVHH	VVHH	VVHH	VVHH

The rules in Table 8.24 are based on the fact that no interaction is assumed between the two types of hazards.

8.3 FUZZY MODELS FOR DESIGN HAZARD

Inherent safety is the result of the complex interaction of factors related to the chemical substances and the properties of the equipment of the plant. In the previous two sections the chemical aspects have been evaluated and some design factors have been taken into account when required (i.e., operation conditions for dispersion potential assessment). However, there are other design aspects that must be evaluated and concern mainly the integrity of the equipment and the possibility of failure and release of chemicals. The model proposed in this project is mainly related to vessels, and it is based on the concept that each piece of equipment and pipework can be assumed to be a vessel. Each equipment, besides the specific task dictated by the unit operation they are intended for, must avoid releases of chemicals to the environment. The basic model for vessels can then be modified in order to describe other equipment.

The aggregated mechanical hazard is obtained by combining the potential for wall failure (i.e., corrosion potential) and the hazard due to failure of the connection to other units (i.e., nozzle failure). The overall mechanical hazard is then combined to the volume of the vessel, which indicates not only the amount of substance that can be released but also the surface of the vessel exposed to the hazard. It is assumed that larger vessels have larger areas increasing the chances of failure.

The design aspects taken into consideration are related to the corrosion potential and potential of nozzle failure; in both cases, if the potential for loss of integrity due to failure of the vessel wall or failure of the connection to other parts of the process is high, the possibility of chemical release increases decreasing the level of inherent safety.

The two aspects evaluated here are only representative and the model must be expanded in the future to include effects of overpressure due to runaway reactions or other scenarios that can increase the hazard of vessel failure. In this case it must be noted that the source of hazard can be external to the analyzed vessel as in the case of overpressure due to failure of pressure regulation upstream of the vessel or side reaction due to contamination.

For the evaluation of the corrosion potential and hazard due to nozzle failure, 2 fundamental fuzzy inference systems (FIS) are used and other 2 FIS integrate the information generated from the fundamental FIS. Tables 8.25 and 8.26 report the names and required inputs for the 4 FIS. As indicated in Tables 7.1 and 7.2, some of the required inputs are for the design of adaptive membership functions, as in the case of corrosion potential evaluation (CORRH).

8.3.1 Theoretical foundation for the design of IF-THEN rules and membership functions

The following subsections describe the theoretical information upon which the design aspects are analyzed.

8.3.1.1 Corrosion hazard evaluation

The analysis of the potential for corrosion in a very complex problem, which requires detailed mechanical information, as well as chemical and environmental data. Types and modes of corrosion have been described by several authors such as Shreir et al. (1991), ASM (1997), Lees (1996), King (1990), CCPS (1993), and Jones (1996). In general, the most important factors for corrosion are the following [Lees, 1996]:

- Environmental chemistry: this factor is related to the properties of the fluids directly in contact with the metal, such as pH, concentration, and gas content.
- Physical conditions: this factor takes into account the properties of the system such as operating temperature, flow velocity, presence of solids and bubbles that can have erosive effects, and heat transfer. Stress and fatigue can also derive from the design and operation of the equipment.
- Operating cycles: in the case of heating/cooling cycles the corrosion potential is affected by modification of the chemical and system properties. Other aspects of cyclic operations are stagnant periods of operation and cleaning procedures.
- External environmental properties: the presence of corrosive gases within the plant, generated from fugitive emissions or vents, can affect the corrosion rate. Other aspects are humidity, temperature, and salt and pollutant concentration in air.
- Mechanical aspects: the presence of stresses such as tensile and cycling forces can modify the material resistance to other factors that can enhance corrosion.

Table 8.25: List of fundamental FIS and required input parameters for design

FIS NAME		INPUT	UNITS
CORRH	"Hazard due to corrosion potential"	Vessel temperature	°C
		Metal: Temp. excellent res.	°C
		Metal: Temp. good res.	°C
		Metal: Temp. sufficient res.	°C
		Metal: Temp. unsatisf. res.	°C
		Plastic: Temp. unsatisf. res.	°C
NLD	"Hazard due to nozzle failure"	Nozzle location	%
		Nozzle diameter	in
		Overflow level	%
		Normal high level	%
		Normal level	%
		Normal low level	%
		Minimum level	%

Table 8.26: List of aggregation FIS and input parameters for design

FIS NAME		INPUT	UNITS
CORNZ	"Hazard due to nozzle failure and corrosion"	COPRH	HP*
		NLD	HP*
ISIMECH	"Hazard due to mechanical and design factors"	CORNZ	HP*
		Volume	gal

* HP = hazard potential index

Depending on the mechanism, corrosion can be classified as localized and uniform. In the case of localized corrosion, pitting and crevice formation occurs. Other corrosion types are intergranular corrosion, environment induced cracking such as stress corrosion cracking, erosion-corrosion, dealloying, and galvanic corrosion. The type of metal (e.g., carbon steel, austenitic stainless steel, nickel alloys) and the composition (i.e., alloy concentration) affect the susceptibility of the material to a certain type of corrosion. For example, nickel-chromium alloys are susceptible of intergranular corrosion. The concentration of chemical substances affects the behavior of the metal but also the presence of traces of contaminants can trigger corrosive processes. The mechanical design of the equipment also modifies the potential for corrosion; for example, dissimilar metals can generate electrochemical cells that are responsible for galvanic corrosion.

Detailed classifications of corrosion processes, as well as the analysis between relevant chemical and mechanical aspects are presented by authors mentioned above. The development of predictive models able to detect hazardous combinations of conditions is an open research area and due to the complexity of the problem some authors investigated the application of neural networks for the modeling of CO_2 corrosion [Nesic et al., 2001] and atmospheric corrosion due to several contaminants such as SO_2 and Cl^-.

For the hierarchical model proposed in this research, several approaches were explored in order to model the corrosion potential. The approach of generating rules for each metal type interacting with specific classes of chemicals under certain conditions was discarded because of the large number of cases that must be analyzed. The use of isocorrosion graphs which are developed for each chemical in contact with a specific chemical under different temperatures is a possible approach however it presents the same limitations of the previous case. The third approach explored was the evaluation of each type of corrosion depending on the combination of chemical, environmental, mechanical, and design factors; however, in this case detailed information regarding mechanical characteristics was required, and it is assumed that such data may not be available.

Therefore the approach selected for the modeling of the potential hazard due to corrosion is based on the information provided by material resistance tables. The corrosion resistance tables published by Schweitzer (1991) are taken as model because they present the information for a large number of chemicals in contact with plastic and metallic materials, at a range of temperatures. The most common types of metallic corrosion for the chemical process industry, as reported by DuPont and cited by cited by CCPS (1993), are general corrosion, stress corrosion cracking, and pitting. The material tables published by Schweitzer (1991) report general notes when the analyzed material for the specific chemical under the required operating conditions is susceptible to any of them. Therefore the designer can identify design modifications that can control or avoid the specific corrosion type.

The fuzzy inference system for the evaluation of the corrosion potential called "hazard due to corrosion potential" (CORRH), is based on adaptive membership functions that divide the linguistic variable "temperature" into fuzzy sets that describe the ranges of temperature where the specific material for the specific chemical present excellent, good, sufficient, and unsatisfactory corrosion resistance. Schweitzer (1991) indicates that a corrosion rate < 2 mills penetration/year is considered excellent, a corrosion rate < 20 mills penetration/year is considered good, a corrosion rate < 50 mills penetration/year is considered satisfactory, while a corrosion rate > 50 mills penetration/year is considered unsatisfactory. These values are used as crossover points for the membership functions. Usually, only one or two points are available for each material, therefore the FIS is designed to recognize which information has been submitted and designs only the appropriate sets. In the case of plastic materials, only the temperature that divides a region of satisfactory resistance form non-satisfactory resistance is required, and only two fuzzy sets are used.

For example, for acetic acid with a concentration of 80%, stainless steel 316 presents excellent resistance up to 90 °F, good resistance up to 150 °F, satisfactory resistance up to 230 °F, and unsatisfactory resistance above that. Therefore, four fuzzy sets are designed. In the case of the same acid, monel presents excellent resistance up to 110 °F, good resistance up to 219 °F, and unsatisfactory resistance above that; therefore only three sets are designed.

The operation temperature of the equipment is used as input for the specific system being analyzed and the membership into each set is evaluated by the fuzzy algorithm.

Fuzzy IF-THEN rules are then used to evaluate the hazard inherent in the systems due to the combination of material, chemical, and temperature; it is assumed that an operation temperature within the unsatisfactory set represents the highest hazard, while the operation within the excellent region implies the lowest hazard.

By following the described modeling approach it is possible to model internal corrosion by taking into account some degree of detail by including the essential information of the specific system (i.e., chemical substance, material, and operation temperature) and at the same time achieve a general model that can work for a wide range of cases. However, factors such as stress and fatigue, external corrosion due to pollution or other environmental conditions, and other technical details responsible for specific type of corrosion are not taken into account. These effects can be added in future revisions of the hierarchical model proposed in this research.

8.3.1.2 Nozzle hazard evaluation

The presence of nozzles in a vessel is assumed to be a potential source of hazard, whose magnitude depends on the position with respect to the level of the liquid and the size of the wall penetration. As indicated by Lees (1996) in the case of pressure vessels, it is better to have discharge and filling pipes entering the vessel above the level of the liquid in order to reduce the leak flowrate in case of failure. This approach is based on the same ideas presented for the evaluation of dispersion; a liquid release at high pressure is more hazardous than a vapor release because of the quantity of material leaked is much larger and capable of forming larger clouds.

For the evaluation of the potential hazard associated with the failure of nozzles of a storage or process vessel the approach indicated by Lees (1996) about reducing the number of penetrations below the level of the liquid, is used as a general approach to reduce the possibility of liquid releases. In order to evaluate this type of hazards, the fuzzy inference system “hazard due to nozzle failure” (NLD) is based on adaptive membership functions whose design depends on the normal operation levels of the vessel being analyzed. The required operation levels are:

- Overflow level
- Normal high level
- Normal operation level
- Normal low level
- Minimum level (or drain)

For vessels working under stable conditions the range of variation of the normal levels (i.e., high level, operation level, and low level) should be narrow while for vessels working under oscillating and cycling conditions the range is wider. It is assumed that in case of failure, nozzles located at or above the drain will release only vapors, while nozzles located below the normal minimum operation level will release liquids. In the case of vessels containing vapors or gases only, the liquid level is assumed to be located at the bottom of the tank and therefore the release will always imply reduced hazard. In the case of vessels full of vapors that can condense, it is assumed that the resultant liquid phase will occupy a small volume, hence implying low hazard.

Another factor that is important in order to estimate magnitude of the potential chemical release due to nozzle failure is the size of the nozzle which affects also the possibility of failure itself. According to Lees (1996) for pressure systems, small-bore pipes (i.e., diameter smaller than 1 in) are more likely to fail, being damaged, or producing leaks. However, the amount of released material is also relatively low. Larger pipes (i.e., diameter ≥ 6 in) are less likely to fail but the quantity of materials that can be released is much larger. The data presented by Lees (1996) for pressure systems is used as baseline and extended to non-pressure pipes too. The failure frequency for five pipe diameters (i.e., 1 in, 1.5 in, 2 in, 3 in, 4 in, and 6 in) are compared with the failure frequency of small-bore pipes, and the relative factor is then used for the design of the membership functions for the evaluation of the possibility of failure. The flowrate that can be released through each pipe size is calculated at fixed conditions (i.e., liquid level and vessel pressure) and the flows for each nozzle size are compared with the flowrate that can be released by a 12 in pipe. The values are used to design the membership functions for the evaluation of the relative hazard inherent to the magnitude of the flow released due to size of the nozzle.

The fuzzy inference system NLD combines the two factors, possibility of hazard due to liquid release and possibility of nozzle failure due to its diameter (which includes the magnitude of the flow), by using IF-THEN rules. The highest hazard is derived from large nozzles located at low levels below the normal low liquid level; the lowest hazard is assigned to medium size nozzles (i.e., 2, to 3 in) located in the vapor space of the vessel. Three conditions (or rules) are assumed as inherently safer and are given by medium nozzles located around the normal liquid level, and larger nozzles located above the normal liquid level.

The hierarchical model is set up to evaluate up to four nozzles for each vessel and it is assumed that each one contributes independently to the overall hazard of the vessel, therefore the individual contributions taken as fuzzy numbers (by using the procedure explained in Chapter VII) are added by using fuzzy addition. Because the evaluation of each nozzle is based on a scale on the range [0 1] the aggregated hazard score is on the scale [0 4].

The inference system “hazard due to nozzle failure and corrosion” (CORNZ), combines the hazard due to chemical release caused by two factors:

- Mechanical failure of the wall of the vessel because of corrosion,
- Hazard due to release of chemical substances by mechanical failure of the nozzles of the vessel.

The fuzzy IF-THEN rules used to combine the overall hazard given by the interaction of the possibility of wall failure and nozzle failure, are based on qualitative judgment and require that both type of failure present low potential. When the failure due to corrosion potential is high, the overall hazard is high; if the potential for high release rate due to nozzle failure under the liquid level is high, then the overall hazard is high.

8.3.1.3 Hazard due to volume

The output from the inference system CORNZ is used as input for the system "hazard due to mechanical and design factors" (ISIMECH), is combined with the linguistic variable "volume" which is related to the size of the vessel. The fuzzy sets for volumes are designed with reference to the values used by NFPA 30 [NFPA, 1990] for storage of class I, II, IIIA, and unstable liquids; the standard indicates distances to the property line of the plant for different sizes of storage tanks. These values are assumed to represent a measure of potential hazard associated with each vessel size and are therefore useful to define membership functions according to the potential physical implications of a potential release. Kletz (1980) indicates that vessels with less than 5 tons are not likely to generate unconfined vapor cloud explosions; the size of these vessels (assumed to be around 1,300 gallons) is taken as the reference state; volumes smaller than 1,300 gallons are assumed to be safer than the reference state while larger volumes are more hazardous. The scale of volume taken into account is between 0 and 3,000,000 gallons but a logarithmic transformation is applied to preserve the fuzzy sets for the smaller volumes.

The fuzzy IF-THEN rules that combine the potential for mechanical failure and the size of the volume have the capability of reducing high hazard due to mechanical failure to lower hazard levels if the volume is small because even if the release happens, a reduced amount of chemical will be released. On the other hand if the potential for mechanical failure is very small but the volume is very large, the resultant overall hazard is very high. These type of rules is required in order to carry the potential hazard due to large volumes to the fuzzy inference system that combines the potential chemical hazard with the mechanical hazard and volume.

8.3.2 Examples of the design of membership functions and fuzzy sets

The membership functions for the evaluation of corrosion are shown in Figure 8.16, when the temperatures for excellent and good resistance are available. The parameters are not shown because the functions are adaptive therefore they move along the temperature axis according to the characteristics of the chemical-metal interaction. Table 8.27 shows the rules used for the potential hazard due to corrosion.

In Table 8.27, ETcr represents the set that covers the range of temperature where the material presents excellent corrosion resistance for the specific chemical substance; when the operation temperature is within the range covered by the set for good resistance (i.e.,GTcr) the hazard is low but if the operation temperature is within the set of satisfactory resistance the hazard for potential corrosion increases and is maximum when the temperature is within the set of unsatisfactory corrosion resistance (i.e., UTcr).

The membership functions for the evaluation of the overall mechanical hazard (ISIMECH) by combining the hazard due to potential corrosion and nozzle failure with the volume of the vessel are shown in Figure 8.17. Table 8.28 reports the parameters of the fuzzy sets and Table 8.29 report the rules used.

The rules shown in Table 8.29 indicate that a vessel could imply high inherent hazard due to either large volume or high corrosion potential. However, the output from this fuzzy inference system must be combined with the aggregated chemical hazard (ISICHEM) in order to combine the mechanical and chemical hazard.

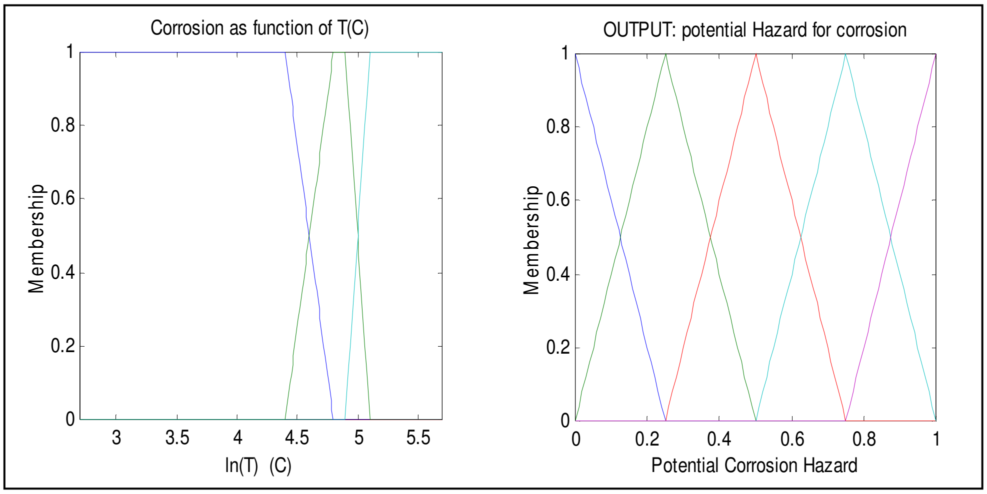


Figure 8.16: Membership functions for corrosion when the temperature for excellent and good resistance is available

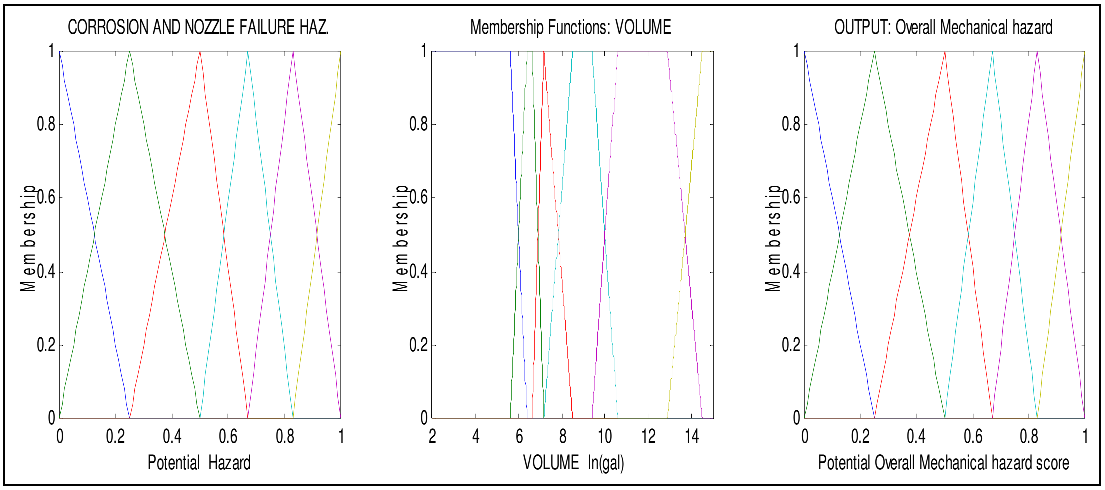


Figure 8.17: Membership functions for ISIMECH

Table 8.27: Fuzzy IF-THEN rules for CORRH. The general rule is: IF ("operation temperature" is ____) THEN (HP is ____)

	Corrosion temperature			
	ETcr	**GTcr**	**STcr**	**UTcr**
Hazard	VLH	LH	MH	VVHH

Table 8.28: Parameters for ISIMECH inputs

INPUTS	NAME	DESCRIPTION	SHAPE	PARAMETERS
HP mechanical Failure	**CVLH**	Very low hazard	Triangular	[0 0 0.25]
	CLH	Low hazard	Triangular	[0 0.25 0.5]
	CMH	Medium hazard	Triangular	[0.25 0.5 0.67]
	CHH	High hazard	Triangular	[0.5 0.67 0.83]
	CVHH	Very high hazard	Triangular	[0.67 0.83 1]
	CVVHH	Extreme hazard	Triangular	[0.83 1 1]
Volume Ln(gal)	**AVLH**	Very small volume	Trapezoidal	[2 2 5.62 6.4]
	ALH	Small volume	Trapezoidal	5.62 6.4 6.62 7.18]
	AMH	Medium volume	Trapezoidal	[6.62 7.18 8.5]
	AHH	Large volume	Trapezoidal	[7.18 8.5 9.39 10.59]
	AVHH	Very large volume	Trapezoidal	[9.39 10.59 12.89 14.59]
	AVVHH	Large storage tank	Trapezoidal	[12.89 14.5 15 15]

Table 8.29: Fuzzy IF-THEN rules for ISIMECH. The general rule is: IF ("hazard due to mechanical design" is ____) AND ("volume" is ____) THEN (HP is ____)

		Volume					
		AVLH	**ALH**	**AMH**	**AHH**	**AVHH**	**AVVH**
Mechanical hazard	**CVLH**	VLH	VLH	LH	MH	VH	VHH
	CLH	VLH	VLH	LH	MH	VH	VVHH
	CMH	VLH	LH	MH	VH	VHH	VVHH
	CHH	LH	MH	VH	VHH	VVHH	VVHH
	CVHH	MH	VH	VHH	VVHH	VVHH	VVHH
	CVVHH	MH	VH	VVHH	VVHH	VVHH	VVHH

8.4 FUZZY MODELS FOR HAZARD AGGREGATION

The last fuzzy inference system has the purpose of aggregating the two main hazards, as shown in Table 8.30, inherent to the chemical properties of the substances and to the design characteristics of the equipment.

The fuzzy IF-THEN rules upon which the overall hazard is based are qualitative rules shown in Table 8.31. The rules require low chemical and mechanical hazard in order to obtain an overall low hazard and therefore a high inherent safety index for the evaluated equipment.

When the methodology is applied to several equipment (i) for the same unit (j), the individual evaluations for each single equipment must be added by using fuzzy addition in order to obtain the overall index for the whole unit.

Table 8.30: List of aggregation FIS and input parameters

FIS NAME	INPUT	UNITS
OVERALL INHERENT SAEFTY INDEX	ISICHEM	HP*
	ISIMECH	HP*

* HP = hazard potential index

Table 8.31: Fuzzy IF-THEN rules for ISI. The general rule is: IF (“chemical hazard” is ____) AND (“mechanical hazard” is ____) THEN (ISL is ____)

ISI		ISIMECH					
		VLH	**LH**	**MH**	**HH**	**VHH**	**VVHH**
ISICHEM	**VLH**	VLH	VLH	VLH	VLH	VLH	LH
	LH	VLH	VLH	VLH	LH	LH	MH
	MH	VLH	LH	MH	VH	VHH	VHH
	HH	LH	MH	VH	VHH	VVHH	VVHH
	VHH	MH	VH	VHH	VHH	VVHH	VVHH
	VVHH	MH	VH	VVH	VVHH	VVHH	VVHH

CHAPTER IX

CASE STUDY

In this chapter a simple case study is presented and analyzed in order to show how the fuzzy hierarchical model is applied. In the first section a description of the processing unit is presented with the data of the two vessels analyzed. Then results obtained by applying the fuzzy model are presented with the explanation of the results. For the first vessel three design modifications are tested in order to show the potential of the model.

9.1 UNIT DESCRIPTION

The case selected as example for this methodology is one unit of the process of hydrodealkylation of toluene for the production of benzene. This information used is reported by Turton et al. (1998). Only two pieces of equipment are modeled; the first is the storage tank TK-101 and the second is the process vessel V-102 which is the reflux drum of the distillation column for the purification of benzene. Figure 9.1 shows the location of the two vessels.

The information regarding the two analyzed vessels is reported in Figures 9.2 and 9.3. Additional information for the vessel TK-101 is the following:

- Operation temperature: 59 °C
- Operation Pressure: 2.0 atm
- Operation levels: normal high = 60%, normal = 50%, normal low = 40%
- Material of construction: carbon steel
- Volume = 4,426 gal
- Unit where it is located is assumed to be obstructed 90% on three sides, while one is 50% obstructed and the other is totally open. Therefore the fraction of

confinement is 84%. It is assumed that the overall volume blockage fraction (i.e., volume of equipment/volume of unit) is around 60%.

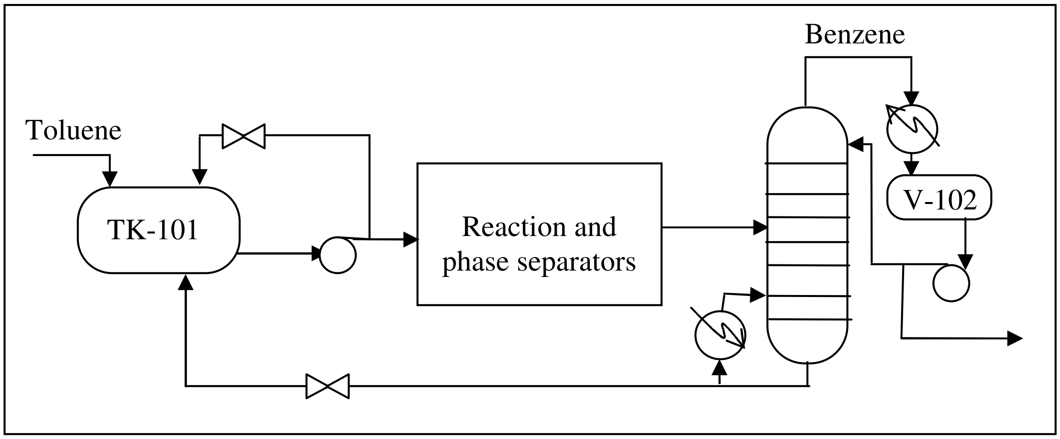


Figure 9.1: Diagram of the hydrodealkylation unit

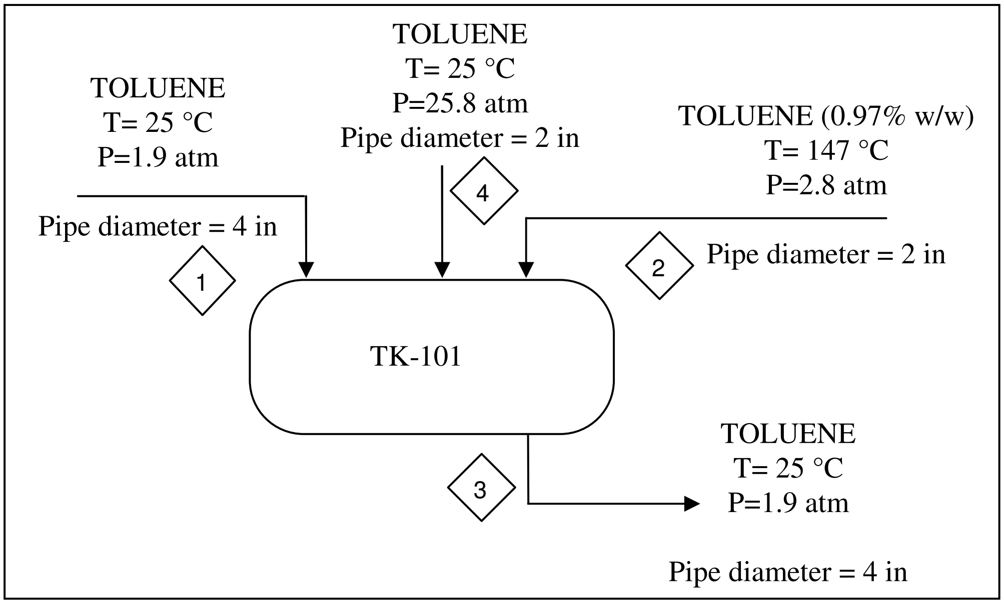


Figure 9.2: Diagram of the storage tank TK-101

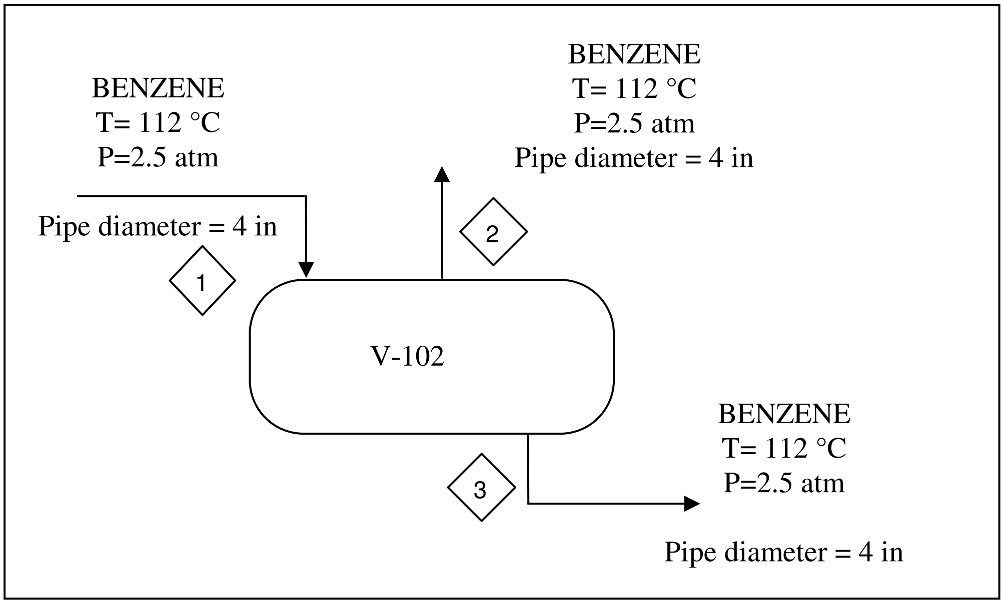


Figure 9.3: Diagram of the vessel V-102

- Carbon steel has an excellent corrosion resistance for toluene up to 350 °F
- The wall penetrations for instrumentation and sampling are not taken into consideration.

Additional information for the vessel V-102 is the following:

- Operation temperature: 112 °C
- Operation Pressure: 2.5 atm
- Operation levels: normal high = 60%, normal = 50%, normal low = 40%
- Material of construction: carbon steel
- Volume = 1,368 gal
- Unit where it is located is assumed to be obstructed 80% on two sides, while other two are 50% obstructed and the other is totally open. Therefore the fraction

of confinement is 72%. It is assumed that the overall volume blockage fraction (i.e., volume of equipment/volume of unit) is around 60%.

- Carbon steel has an excellent corrosion resistance for toluene up to 350 °F
- The wall penetrations for instrumentation and sampling are not taken into consideration.

The information about toxicity and other properties of toluene and benzene are reported in Table 9.1, with all the used inputs. When a variable X appears as X1, X2, and X3, the user can feed the values of the variable as a fuzzy number. If the values given are equal, then they are taken as a crisp number.

Table 9.1: Input values used for the analysis

INPUT	**TOLUENE**	**BENZENE**	**DESCRIPTION**
Tb1	111	80.1	Lower limit for Boiling temperature (°C)
Tb2	111	80.1	Normal Boiling temperature (°C)
Tb3	111	80.1	Upper limit for Boiling temperature (°C)
Tf1	4	-11	Lower limit for Flash Temp. C
Tf2	4	-11	Normal Flash temperature (°C)
Tf3	4	-11	Upper limit for Flash temperature (°C)
Fnfpa	3	3	Decision variable: NFPA flammability score
MPD1	0	0	Lower limit for Max. power density (W/mL at 250 °C)
MPD2	0	0	Average Maximum power density
MPD3	0	0	Upper limit for Maximum power density
HWmix1	0	0	Lower limit for the Water heat of mixing [cal/gr]
HWmix2	0	0	Average Water heat of mixing [cal/gr]
HWmix3	0	0	Upper limit for the Water heat of mixing [cal/gr]
Tt1	25	112	Lower limit for operation temperature (°C)
Tt2	55	112	Operation temperature (°C)
Tt3	70	112	Upper limit for operation temperature (°C)
Pt1	1.9	2.5	Lower limit for operation pressure (atm)
Pt2	2.0	2.5	Operation pressure (atm)
Pt3	2.8	2.5	Upper limit for operation pressure (atm)
Tbt1	115	112	Lower limit for Boiling temperature (C): at lowest vessel conditions
Tbt2	115	112	Boiling temperature (°C): at lowest vessel conditions
Tbt3	115	112	Upper limit for Boiling temperature (°C): at lowest vessel conditions
Tatm1	25	25	Lower limit for atmospheric temperature (°C)

Table 9.1: Continued

INPUT	INPUT	INPUT	INPUT
Tatm2	25	25	Average atmospheric temperature (°C)
Tatm3	25	25	Upper limit for atmospheric temperature (°C)
Ovbf1	0.6	0.6	Lower limit for the overall volume blockage fraction = Vobstr/Vtot=Veq/Vtot
Ovbf2	0.6	0.6	Average overall volume blockage fraction
Ovbf3	0.6	0.6	Upper limit for the overall volume blockage fraction
Ocf1	0.84	0.72	Lower limit for the overall confinement fraction
Ocf2	0.84	0.72	Average overall confinement fraction
Ocf3	0.84	0.72	Upper limit for the overall confinement fraction
Fbv1	10	10	Lower limit for the chemical flame burning velocity (cm/s)
Fbv2	10	10	Average chemical flame burning velocity (cm/s)
Fbv3	10	10	Upper limit for the chemical flame burning velocity (cm/s)
Vis1	0.35	0.6	Lower limit for Viscosity [cp]
Vis2	0.0.4	0.6	Average Viscosity [cp]
Vis3	0.6	0.6	Upper limit for Viscosity [cp]
To1	5,000	4,700	Lower limit for Oral Toxicity (mg/kg)
To2	5,000	4,700	Average oral Toxicity (mg/kg)
To3	5,000	4,700	Upper limit for Oral Toxicity (mg/kg)
Td1	12,124	2,900*	Lower limit for Dermal Toxicity (mg/kg)
Td2	12,124	2,900*	Average dermal Toxicity (mg/kg)
Td3	12,124	2,900*	Upper limit for Dermal Toxicity (mg/kg)
phase	Vm	vm	DECISION VAR: liquid then phase='vm'
GMc1	4,600	7,800	Lower limit for respiratory Toxicity: Gas concentration
GMc2	4	9,000	Average respiratory Toxicity: Gas concentration
GMc3	4	13,700	Upper limit for respiratory Toxicity: Gas concentration
Che1	0.05	0.7	Lower limit of confidence in Human evidence for Cancer (range 0-1)
Che2	0.05	0.7	Average confidence in Human evidence for Cancer
Che3	0.05	0.7	Upper limit for confidence in Human evidence for Cancer
Cae1	0.95	0.6	Lower limit for confidence in Animal evidence for Cancer
Cae2	0.95	0.6	Average confidence in Animal evidence for Cancer
Cae3	0.95	0.6	Upper limit for confidence in Animal evidence for Cancer
Halft1	2	2	Lower limit for degradability: Half time (days)
Halft2	7	9	Average degradability: Half time (days)
Halft3	14	16	Upper limit for degradability: Half time (days)
LD501	6.4	6	Lower limit for Aquatic toxicity LD$_{50}$
LD502	13	11	Average Aquatic toxicity LD$_{50}$
LD503	24	22	Upper limit for Aquatic toxicity LD$_{50}$
LogKow1	2.69	2.13	Lower limit for Bioaccumulation factor LogK$_{ow}$
LogKow2	2.69	2.13	Average Bioaccumulation factor LogK$_{ow}$
LogKow3	2.69	2.13	Upper limit for Bioaccumulation factor LogK$_{ow}$
HalftTr1	0.25	3	Lower limit for Tropospheric Degrad.: Half time (days)
HalftTr2	0.5	4	Average Tropospheric Degradability: Half time (days)
HalftTr3	1	5	Upper limit for Tropospheric Degrad.: Half time (days)

Table 9.1: Continued

INPUT	INPUT	INPUT	INPUT
Info1	0.7	0.7	Lower limit for confidence in Type of information available [0 1]
Info2	0.8	0.8	Average confidence in Type of information available [0 1]
Info3	0.9	0.9	Upper limit for confidence in Type of information available [0 1]
crEm	350	350	T(°F) at which METAL Corrosion resistance is EXCELLENT (cr<2 mills/yr)
crGm	15*	15*	T(°F) at which METAL Corrosion resistance is GOOD (2<cr<20 mills/yr)
crSm	15*	15*	T(°F) at which METAL Corrosion resistance is SATISFACTORY (20<cr<50 mills/yr)
crUm	15*	15*	T(°F) at which METAL Corrosion rate (mills) for UNACCEPTABLE resistance (cr>50 mills/yr)
N1	1	1	Level of nozzle 1: (0-100% vessel height)
N2	1	1	Level of nozzle 2: (0-100% vessel height)
N3	0	0	Level of nozzle 3: (0-100% vessel height)
N4	1	-	Level of nozzle 4: (0-100% vessel height)
D1	4	3	Diameter of nozzle 1: (in)
D2	2	4	Diameter of nozzle 2: (in)
D3	4	4	Diameter of nozzle 3: (in)
D4	4	-	Diameter of nozzle 4: (in)
OFL	1	1	Overflow level
NHL	0.6	0.6	Normal high level
NOL	0.5	0.5	Normal op level
NML	0.4	0.4	Normal low level
DRL	0	0	Min level
VOL	4,426	1,368	Vessel volume [gal]

* These values are set at upper or lower limit of the variable because not used or out of range

9.2 CASES

The vessel V-102 is evaluated according to the parameters reported in Table 8.1 The vessel is working under hazardous conditions because the operating conditions are saturated and the pressure is relatively high compared with the atmospheric pressure. The conditions of confinement and obstruction are also very high. The storage tankTK-101 is evaluated at the same conditions reported in Table 8.1; this vessel works at less hazardous conditions since the operating temperature is not close to the normal boiling temperature. However, the pressure is relatively high and it is assumed that in case of failure of the pressure regulators on line 2, it can be pressurized.

The values reported in Table 9.1 are assumed to be the normal operating conditions, therefore for Case 1, vessel V-102 is assumed to be equipment 1 of unit 1 and its overall hazard index will be $FISI_{11}$; storage tank TK-101 is assumed to be equipment 2 of unit 1 therefore its overall fuzzy hazard index will be $FISI_{12}$. If more equipment and pipelines were evaluated they would be equipment i of unit 1, where i = 0…n. Therefore, in order to obtain the overall index for unit j = 1, all the $FISI_{ij}$ should be added by using fuzzy addition. This step is exemplified below.

For Case 2 only TK-101 is reevaluated by reducing the overall fraction of confinement but the operating pressure is not changed. For Case 3, TK-101 is reevaluated by reducing the operating pressure at atmospheric and using the high degree of confinement; in Case 4, TK-101 is evaluated with low operating pressure and low degree of confinement.

9.3 RESULTS AND ANALYSIS

This section reports the results obtained for each case. The obtained results are plotted indicating the possible range of variability of the hazard degree and the value that is given by defuzzification and therefore is the crisp solution. The plots have been developed according to the advise given by Kletz (2003). The tables of results report at the top the values of $FISI_{ij}$ and the two overall evaluations for the chemical hazard (ISICHEM) and the mechanical hazard (ISIMECH). Below the three main indices, the rest of the indices are reported.

The vertical axis of the plot represents the scale of hazard, which is on the real interval [0 1] and the value of 0.5 indicates the threshold between conditions that represent relevant hazards and therefore cannot be considered inherently safer. Values lower than 0.5 represent conditions associated with low hazard degrees that should not require complex layers of protection to control them and therefore are assumed to be conditions within the “inherently safer” region.

9.3.1 Results and analysis for Case 1

The values for each index for the Vessel TK-101 are reported in Table 9.2, and they are presented graphically in Figures 9.4 to 9.9.

The lower part of the figures presents arrows that show which indices are aggregated to obtain the index indicated by the arrow, which is circled.

From Figure 9.4 it is possible to detect that the major hazard contribution to the overall hazard for the storage tank TK-101 is given by the overall chemical hazard (i.e., ISICHEM) while the mechanical contribution is not important (i.e., ISIMECH). From Figure 9.5 the hazard due to corrosion is negligible while the major contribution for the nozzle (or pipe connection) for nozzle 3 (i.e., NLD 3) is the most important due to its size (i.e., 4 in) at its location at the bottom of the vessel.

From Figure 9.6 it is possible to see that the hazard derived form the degree of obstruction and congestion (i.e., COBV) is very high, and although the explosive hazard due to flammability and reactivity is relatively low (i.e., AGOFR) as shown in Figure 9.7, when combined with high congestion the hazard increases (i.e., AGEXPL). The hazard due to dispersion is relatively high because TK-101 works under pressurized conditions, but the temperature is lower than the normal boiling point of toluene.

The overall hazard due to flammability and reactivity (i.e., AGOFR) is low because toluene is flammable (CHPFa) but is not reactive (AGORX) and therefore cannot undergo a runaway reaction. Because of the low viscosity of toluene, the hazard for the generation of heterogeneous hazardous conditions reduces the aggregated hazard of flammability and reactivity (i.e., AFRVISC).

Table 9.2: Results for the vessel TK-101

INDICES	**Upper limit**	**Lower limit**	**Most possible**
FISI$_{12}$	0.93	0.74	0.75
ISICHEM	1.00	0.74	0.88
ISIMECH	0.60	0.35	0.50
ISIMECH			
CORNZ	0.15	0.00	0.00
CORRH	0.40	0.10	0.25
NLD	2.35	1.60	2.15
1	0.60	0.35	0.53
2	0.15	0.00	0.09
3	1.00	0.90	1.00
4	0.60	0.35	0.53
ISICHEM			
AGEXPL	1.00	0.57	0.77
DISP	0.76	0.57	0.60
ACOFRV	0.91	0.59	0.70
COBV	1.00	0.90	0.89
AFRVISC	0.58	0.38	0.42
AGOFR	0.60	0.35	0.44
CHPFa	0.65	0.35	0.50
AGORX	0.00	0.00	0.00
CHPR	0.00	0.00	0.00
CHPRh2o	0.00	0.00	0.00
AGCHM	1.00	0.57	0.79
DISPTX	0.76	0.57	0.60
AGCH	1.00	0.57	0.83
AGHEA	0.40	0.00	0.23
AGHEALTH	0.40	0.00	0.10
CHHc	0.15	0.00	0.00
AGET	1.00	0.74	0.77
CHEadt	1.00	0.60	0.80
CHEdt	0.90	0.35	0.57
CHEat	1.00	0.60	0.86
CHEp	0.40	0.00	0.20

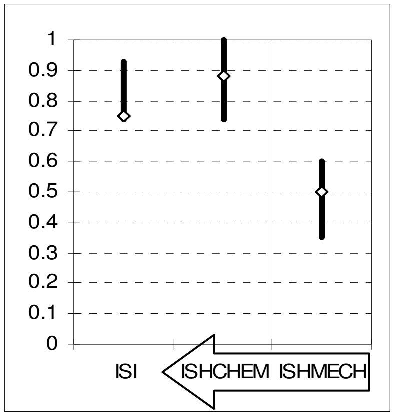


Figure 9.4: Main overall hazard indices for storage tank TK-101

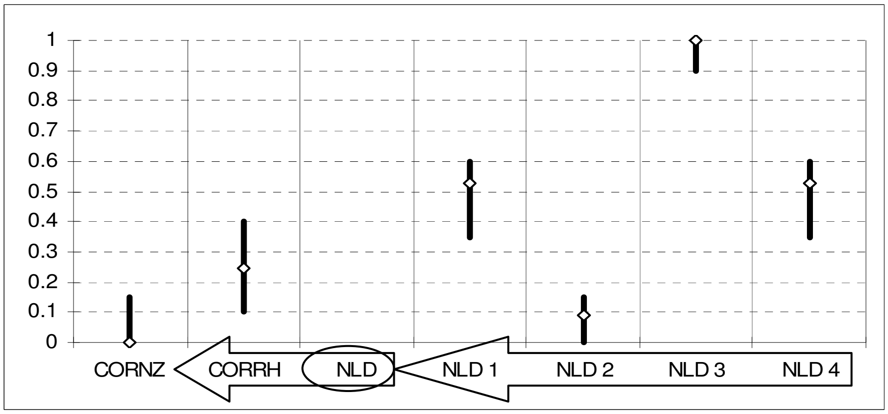


Figure 9.5: Overall mechanical hazard indices for storage tank TK-101

The overall hazard due to environmental impact (i.e., AGET) as shown in Figure 9.8 is relatively high because of the combination of the toluene toxicity, degradability, and bioaccumulation characteristics (i.e., CHEadt, CHEdt,CHEat,ad CHEp) which are relatively high as shown in Figure 9.9.

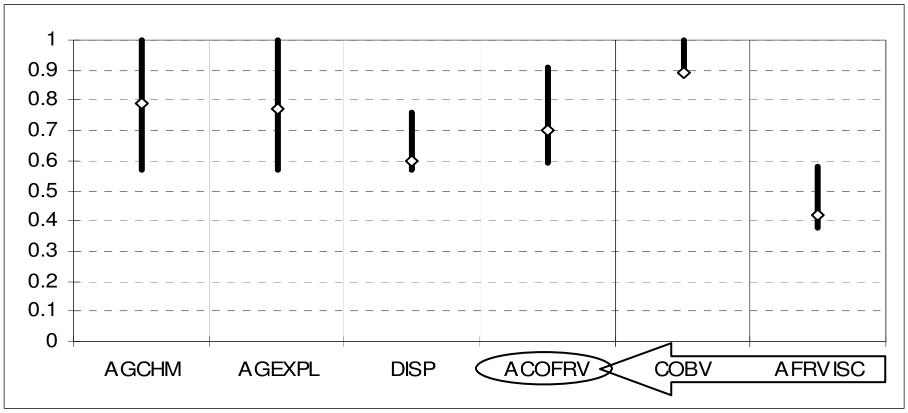


Figure 9.6: Overall mechanical and chemical indices for storage tank TK-101

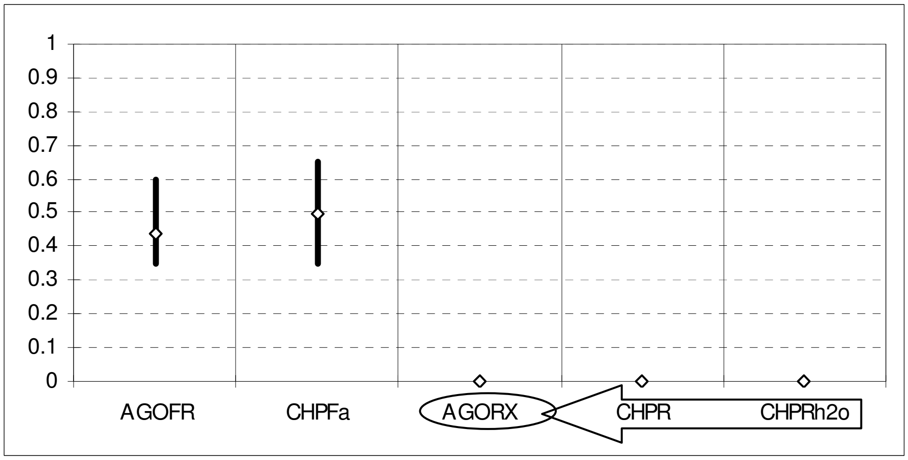


Figure 9.7: Overall chemical hazard indices for storage tank TK-101

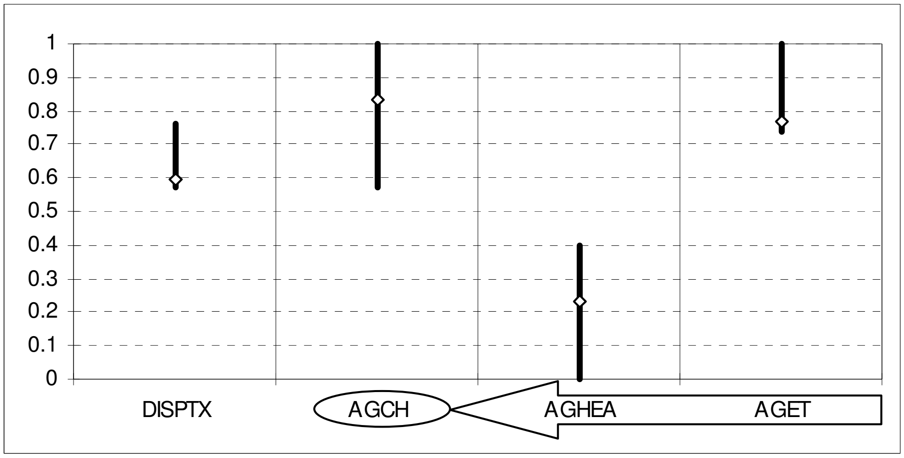


Figure 9.8: Overall aggregated hazard indices for storage tank TK-101

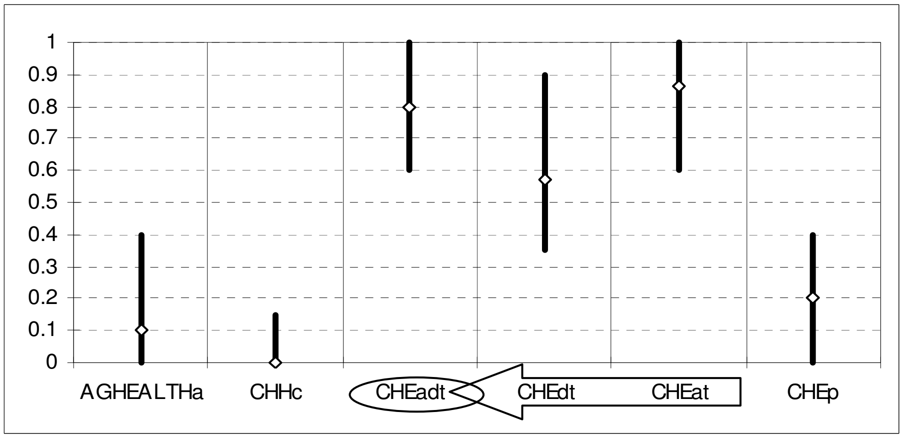


Figure 9.9: Overall aggregated environmental indices for storage tank TK-101

The overall human toxicity and environmental hazard (i.e., AGCH) is high mainly due to the contribution of the environmental hazard. The overall hazard for humans (i.e., AGHEALTHa) as shown in Figure 9.9 is relatively low due to low dermal and respiratory toxicity and the proven absence, and therefore low uncertainty, for the toluene potential to produce cancer in humans and animals (i.e., CHHc).

The length of the lines representing each index indicates the uncertainty associated with each value (represented by white squares). Depending on the number of rules fired for each fuzzy inference system, the uncertainty can increase or be reduced. This effect is caused by the fact that some sets of IF-THEN rules have areas of high uncertainty (i.e., an output of LH next to an output of VH) to increase the speed on hazard increase or decrease. The uncertainty is also derived from the fact that in several cases the inputs are submitted as fuzzy numbers rather than crisp values.

The values for each index for the Vessel V-102 are reported in Table 9.3, and they are plotted in Figures 9.10 to 9.15.

Figure 9.10 shows the overall hazard index for the process vessel TV-102 which is relatively high (but lower than the overall index for the storage tank TK-101) and again the major contribution is given by the overall chemical hazard (i.e., ISICHEM). The chemical hazard is mainly caused by the operating conditions of the vessel that works at saturation conditions and under pressure. The mechanical hazard is low because of the excellent corrosion resistance and the relatively low volume of the vessel that reduces the overall mechanical hazard. As indicated in Figure 9.12, the explosion and dispersion hazards (i.e., AGEXPL and DISP) are high due to the saturation conditions and the high degree of obstruction and congestion (i.e., COBV).

The hazard due to flammability (i.e., CHPFa) is high as shown in Figure 9.13 while the reactivity is low. Therefore the aggregated reactivity and flammability hazard is dominated by the flammability. It is interesting to note that while benzene and toluene have the same NFPA flammability score (i.e., 3) the flammability hazard score assigned to benzene is higher than the score resultant for toluene because the boiling temperature for benzene is thirty degrees lower than the boiling temperature of toluene, and the flash temperature of benzene is fifteen degrees lower than the flash point for toluene.

Table 9.3: Results for the vessel V-102

INDICES	**Upper limit**	**Lower limit**	**Most possible**
FISI$_{11}$	0.93	0.57	0.65
ISICHEM	1.00	0.90	1.00
ISIMECH	0.40	0.10	0.32
ISIMECH			
CORNZ	0.15	0.00	0.00
CORRH	0.40	0.10	0.22
NLD	2.20	1.60	2.05
1	0.60	0.35	0.53
2	0.60	0.35	0.53
3	1.00	0.90	1.00
4	0.00	0.00	0.00
ISICHEM			
AGEXPL	1.00	0.90	1.00
DISP	1.00	0.90	1.00
ACOFRV	1.00	0.75	0.86
COBV	1.00	0.90	0.89
AFRVISC	0.75	0.59	0.65
AGOFR	0.76	0.57	0.70
CHPFa	0.90	0.60	0.75
AGORX	0.00	0.00	0.00
CHPR	0.00	0.00	0.00
CHPRh2o	0.00	0.00	0.00
AGCHM	1.00	0.90	1.00
DISPTX	1.00	0.90	1.00
AGCH	1.00	0.74	0.88
AGHEA	0.93	0.57	0.73
AGHEALTH	0.40	0.00	0.10
CHHc	0.90	0.60	0.75
AGET	1.00	0.74	0.77
CHEadt	1.00	0.60	0.79
CHEdt	0.90	0.35	0.57
CHEat	1.00	0.60	0.78
CHEp	0.40	0.00	0.15

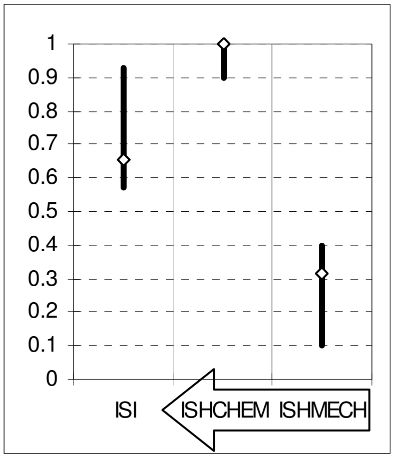


Figure 9.10: Main overall hazard indices for vessel TV-102

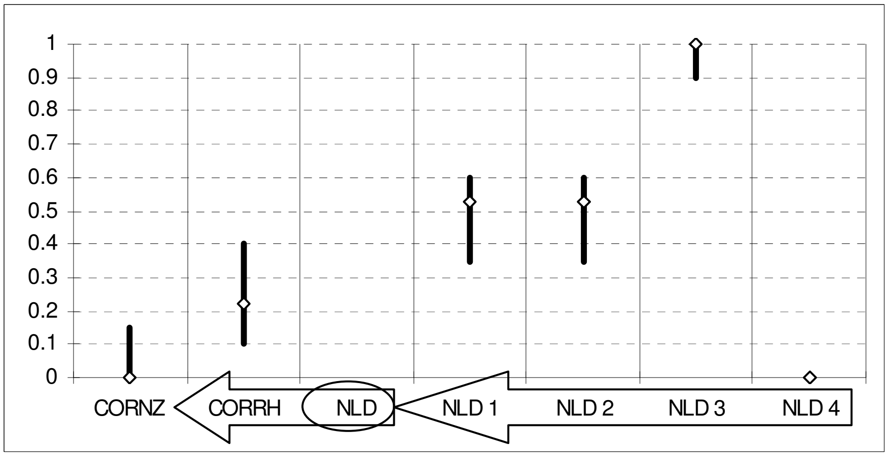


Figure 9.11: Overall mechanical hazard indices for vessel TV-102 (NLD not shown because larger than 1)

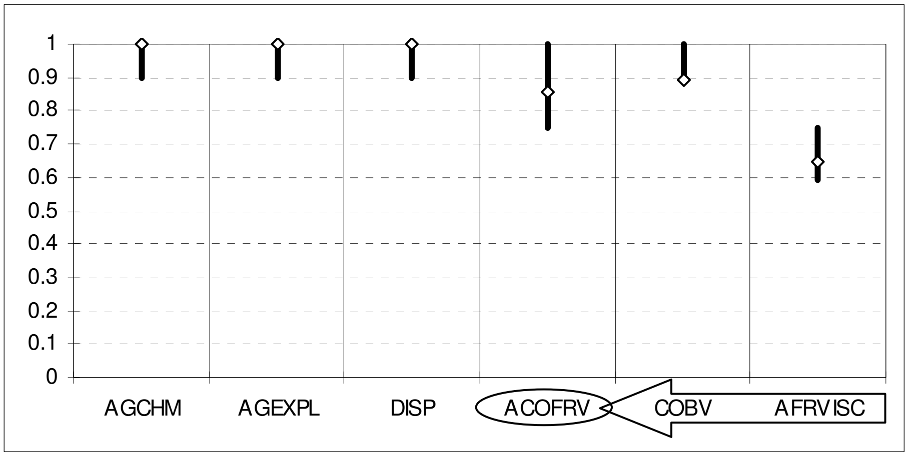


Figure 9.12: Overall mechanical and chemical hazard indices for vessel TV-102

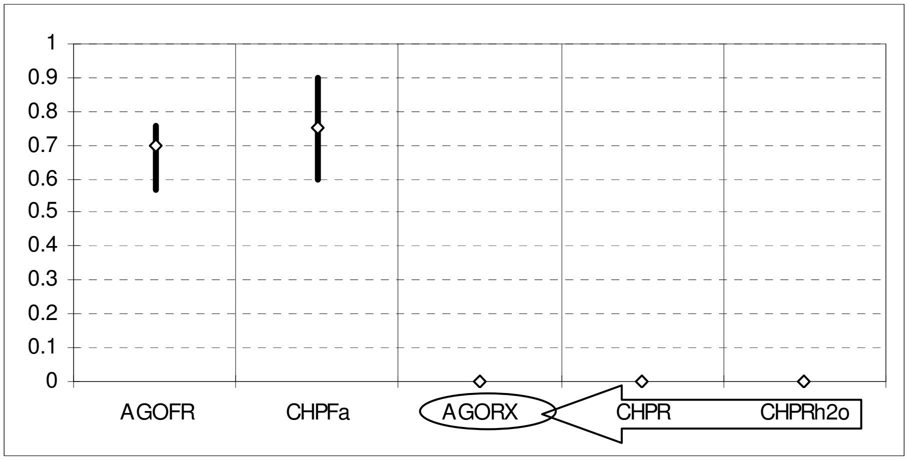


Figure 9.13: Overall chemical hazard indices for vessel TV-102

As shown in Figures 9.12, 9.14 and 9.15 overall hazard for human health and the environment is high (i.e., AGCHM) because of the potential environmental consequences and the high dispersion hazard (i.e., DISPTX) given by the operating conditions of the vessel. The environmental hazard is caused by water toxicity and bioaccumulation (i.e., AGET, CHEadt), and the human toxicity. While the toxicity of benzene for humans is relatively low (i.e., AGHEALTHa) the cancer potential is high (i.e., CHHc).

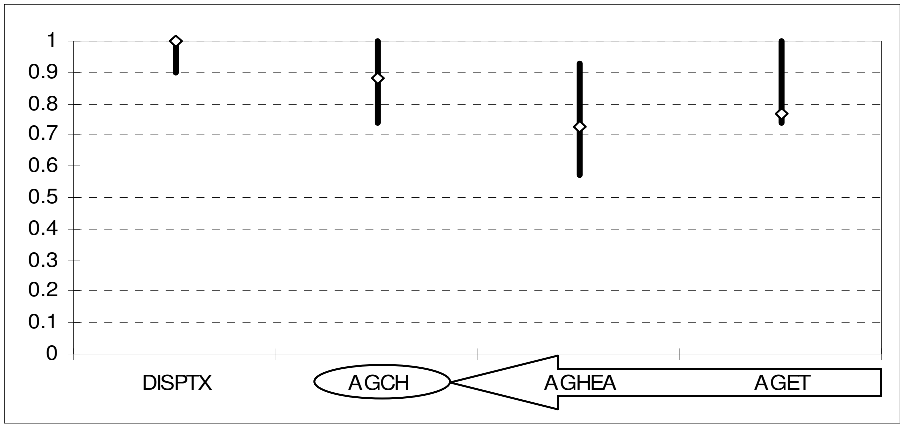


Figure 9.14: Overall aggregated hazard indices for vessel TV-102

Assuming that the processing Unit 1 is formed only by storage vessel TK-101 and process vessel V-102, the overall inherent hazard can be obtained by adding the fuzzy triangular numbers obtained for $FISI_{11}$ and $FISI_{12}$ as shown in Table 9.4. Therefore the fuzzy hazard indices obtained for each equipment are used in a similar way as “cost” assuming that the overall hazard is given by the individual contributions of each piece of equipment.

Because the range of each individual index is [0 1] when two vessels are present, the overall range is [0 2], and the assumed inherent safety threshold would be located around 1. Because the most possible value for $FISI_1$ is 1.4 the overall unit presents a hazard level than what could be considered inherently safer and other extrinsic measures must be taken to reduce the potential consequences of a chemical release.

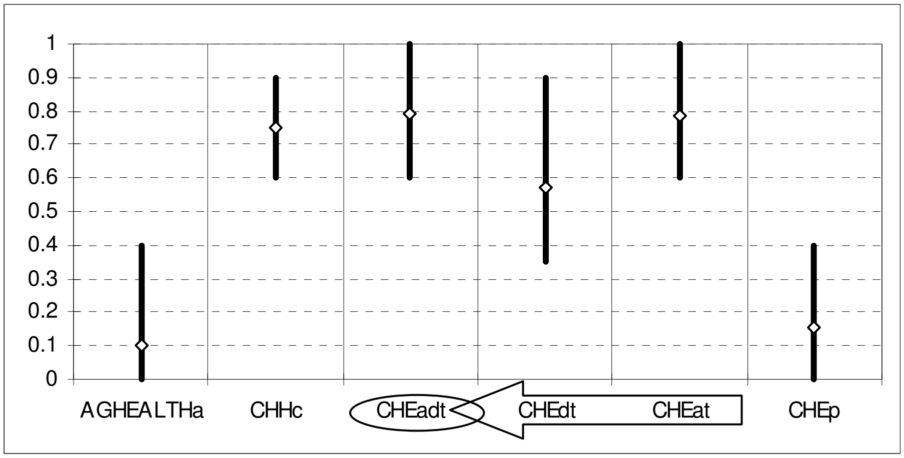


Figure 9.15: Overall aggregated environmental hazard indices for vessel TV-102

Table 9.4: Results for the Unit 1

INDICES	Upper limit	Lower limit	Most possible
Storage tank TK-101			
$FISI_{12}$	0.93	0.74	0.75
Process vessel V-102			
$FISI_{11}$	0.93	0.57	0.65
PROCESSING UNIT			
$FISI_1$	1.86	1.31	1.40

The hazard is mainly produced by the flammability of the chemicals and the operating conditions (i.e., pressurized vessels) however the relatively small volumes help to reduce the mechanical hazards and the overall equipment hazard.

9.3.2 Results and analysis for Case 2

For this case, only the storage vessel TK-101 is analyzed; the input conditions presented in Table 9.1 are used but the degree of obstruction and confinement are reduced to 20% in order to analyze the potential hazard reduction effects due to a less congested unit design. Table 9.5 presents the relevant results.

The overall hazard index $FISI_{12}$ is lowered (e.g., values for Case 1 are: 0.93, 0.74, and 0.75) due to the reduction of the chemical hazard while, as expected, the mechanical hazard does not change. The hazard due to dispersion does not change because it depends only on the operating conditions, but the overall explosion hazard AGEXPL is reduced (e.g., values for Case 1 are: 1.0, 0.57, and 0.77) because of the reduction of the congestion degree. Figure 9.16 and Figure 9.17 show the new indices.

Table 9.5: Results for the vessel TK-101 when congestion is reduced

INDICES	**Upper limit**	**Lower limit**	**Most possible**
$FISI_{12}$	0.93	0.57	0.66
ISICHEM	1.00	0.57	0.79
ISIMECH	0.60	0.35	0.50
ISICHEM			
AGEXPL	0.93	0.35	0.69
DISP	0.76	0.57	0.60
ACOFRV	0.75	0.38	0.50
COBV	0.60	0.35	0.39

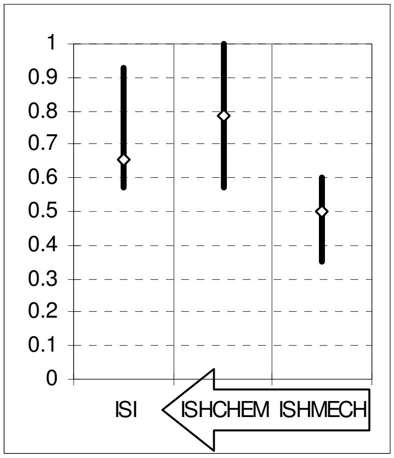


Figure 9.16: Main overall hazard indices for storage tank TK-101 for Case 2

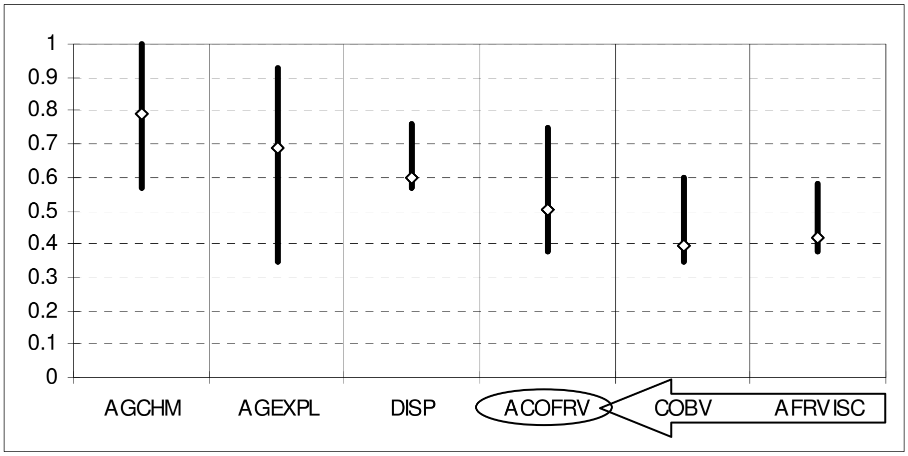


Figure 9.17: Explosion hazard indices for storage tank TK-101 for Case 2

9.3.3 Results and analysis for Case 3

For this case, only the storage vessel TK-101 is analyzed; the input conditions presented in Table 9.1 are used but the operation pressure is reduced to atmospheric and the obstruction and confinement factors are high, as for Case 1. Table 9.6 presents the relevant results. Figures 9.18 and 9.19 show the results.

The overall hazard indices are similar to the values obtained for Case 2, however the hazard reduction is achieved through reducing the dispersion hazard (e.g., values for Case 2 are 0.76, 0.57, and 0.60) but, because of the high degree of congestion, the overall hazard is constant.

Table 9.6: Results for the vessel TK-101 for Case 3

INDICES	Upper limit	Lower limit	Most possible
$FISI_{12}$	0.93	0.57	0.63
ISICHEM	1.00	0.57	0.69
ISIMECH	0.60	0.35	0.50
ISICHEM			
AGEXPL	0.93	0.35	0.62
DISP	0.60	0.35	0.40
ACOFRV	0.91	0.59	0.70
COBV	1.00	0.90	0.89

9.3.4 Results and analysis for Case 4

For this case, only the storage vessel TK-101 is analyzed; the input conditions presented in Table 9.1 are used but for this case the operation pressure is reduced to atmospheric and the degree of congestion is low, as in Case 2. Table 9.7 presents the relevant results.

The overall hazard indices are reduced by the combined effect of operating pressure reduction and lower congestion. While for Case 1 the inherent safety index for $FISI_{12}$

was [0.93, 0.74, 0.75], in Case 4 the index is located around the inherent safety threshold. The hazard due to the chemical properties cannot be removed by design, unless the chemicals are substituted. Figures 9.20 and 9.21 show the indices for Case 4.

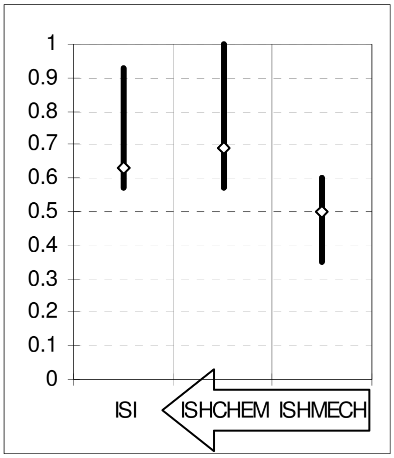


Figure 9.18: Main overall hazard indices for storage tank TK-101 for Case 3

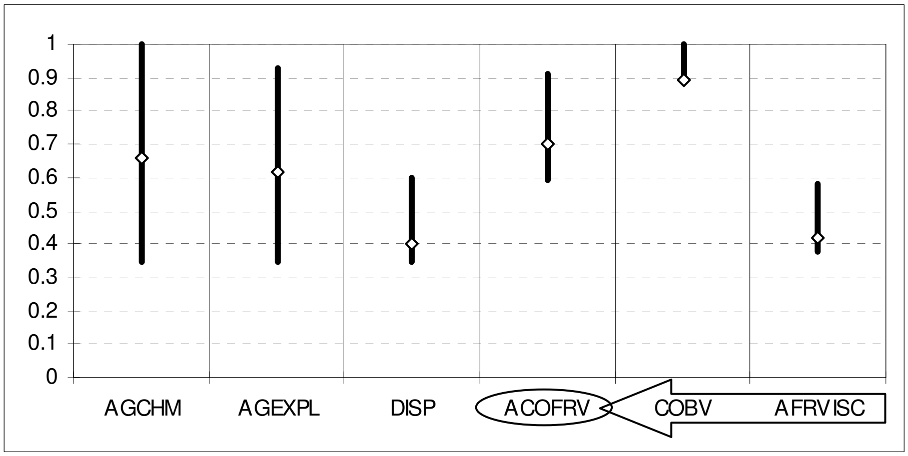


Figure 9.19: Explosion hazard indices for storage tank TK-101 for Case 3

For Case 4, the uncertainty of several indices is increased because the new values are located in regions of the sets of rules that imply fast change, and this is reflected in the values of the obtained results. This is a problem associated with the fact that fuzzy numbers are used for the inputs rather than crisp numbers.

Table 9.7: Results for the vessel TK-101 for Case 4

INDICES	**Upper limit**	**Lower limit**	**Most possible**
$FISI_{12}$	0.93	0.35	0.53
ISICHEM	1.00	0.35	0.66
ISIMECH	0.60	0.35	0.50
ISICHEM			
AGEXPL	0.76	0.10	0.52
DISP	0.60	0.35	0.40
ACOFRV	0.75	0.38	0.50
COBV	0.60	0.35	0.39

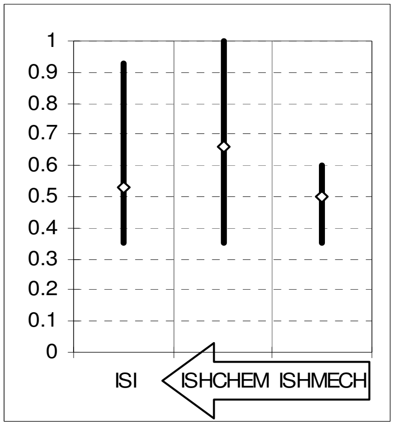


Figure 9.20: Main overall hazard indices for storage tank TK-101 for Case 4

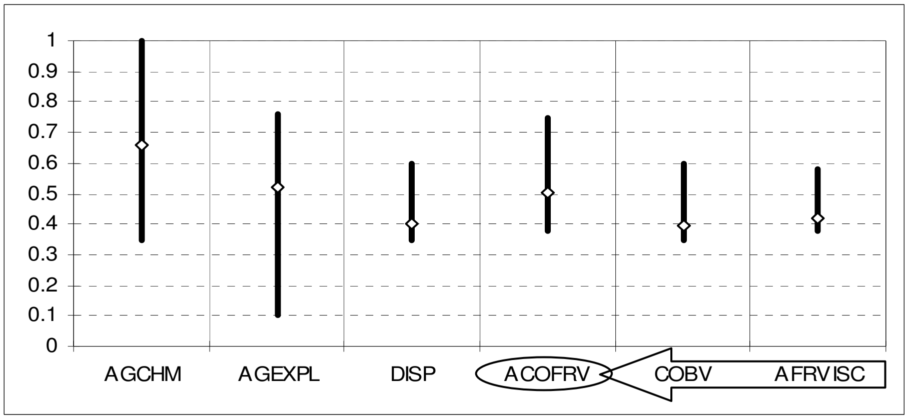


Figure 9.21: Explosion hazard indices for storage tank TK-101 for Case 4

CHAPTER X

INHERENT SAFETY APPLIED TO TRANSPORTATION

Raw materials, chemical products, and subproducts must be transported to/from the chemical facilities that produce or use them, and this activity extends the chemical hazards from the processing plant to the community. Therefore, to obtain a general evaluation of the inherent safety level of a chemical plant, it is necessary to consider the hazards due to transportation of chemicals and treat these as an additional “property” of the substance.

This chapter presents an overview of a prototype of inherent safety index based on fuzzy logic, which is useful to extend the concepts of inherent safety to transportation of chemical substances. An example evaluates the transportation step of chemical substances, shows how the index works, and describes how it can be applied to different stages of the life cycles of a chemical facility.

It must be noted that the principles used for the design of the model for transportation are similar to the approach described in the previous chapters, but this chapter is based on the concept of risk, because the possible impact on the population is taken into account. Therefore the results obtained at the end of this chapter are not comparable with the results presented in Chapter VIII.

10.1 TRANSPORTATION AS AN ELEMENT OF INHERENT SAFETY

Transportation of chemical raw materials and chemical products plays a very important role in the analysis of the inherent safety level of a chemical plant. Transportation and inherent safety share also the common problems of data uncertainty, complexity due to the many factors that should be analyzed, subjectivity, and lack of a quantification methodology. The mathematical approach proposed in this chapter is based on the fuzzy set theory rather than probability and statistics.

Inherent safety is based on the elimination of hazards rather than control of them. When an industry is forced to move towards an inherently safer approach, it is possible to interpret the principles in a way that will impact other related aspects of safety. For instance, one of the easier ways to improve the inherent safety level is to reduce the inventory of hazardous chemical substances. However, if this step causes an increase in the frequency of shipments of chemicals to or from the plant, the overall effect could be an increased transportation hazard. This example shows why transportation must be part of the inherent safety analysis of the plant and cannot be studied as a separate entity.

Transportation of chemical substances is by itself an extremely complex and difficult topic, and when it is joined to the already complex issue of inherent safety quantification, the resultant problem could appear impossible to be solved. However no inherent safety quantification can be complete unless it takes into account the hazards related to transportation. The two questions that naturally appear here are:

- How can transportation be included within inherent safety?
- How to deal with all the complexity, uncertainty, and imprecision common to both inherent safety and transportation?

Traditionally the hazards related to a specific chemical are health hazards (based on properties such as acute and chronic toxicity) and fire and explosion hazards (based on properties such as flammability, explosivity, and reactivity). These hazards are rated by using indices (e.g., NFPA ratings) based on chemical and thermodynamic properties. Following a similar approach, transportation hazards could be analyzed based on specific aspects such as mode of transportation, length of the route, and type of urban/rural areas traveled through. The transportation hazard then can be rated by a “transportation index”, which could be used by the general rules introduced in Chapter VI for the overall model of inherent safety.

Since each transportation mode has a characteristic range of possible volumes (e.g., tank trucks can transport less volume than a rail car) the number of trips per year is a function of the total required volume. The frequency of the shipments depends on the total volume of chemical required by the plant but also by the size of the storage tank. Because of this relation, the hazards posed by transportation are related to the hazards posed by the plant and then can be included within the inherent safety evaluation. This answers the first question.

The answer to the second question requires the understanding of the source and type of uncertainty. The model examined in this chapter is based on fuzzy logic, that as explained in Chapters IV and VI allows one to take into consideration the uncertainty derived from vagueness. In some cases fuzzy logic has been used for risk assessment and fault tree analysis, and an interesting application of fuzzy logic to transportation risk assessment is presented by Bonvicini et al, (1998), where the authors treat the release frequency and rates as fuzzy numbers.

10.1.1 Inherent safety for fixed site facilities

The inherent safety index based on fuzzy logic measures hazards related to the chemical substance, the process, and the equipment present in the plant. The process hazard evaluation takes into account processing conditions such as temperatures and pressures, materials required for the construction of the equipment, protective equipment for workers, and the degree of packing of the evaluated unit or plant. The hazards related to process equipment are related to the type of equipment and the volume and conditions of storage and process tanks. The storage tanks represent a large accumulation of chemical substances and usually they are also a significant source of hazards. Because of this, one of the easier ways to reduce the risk of the plant is by reduction of inventory. When the reduction of stored volumes implies a higher transportation frequency, it is necessary to evaluate the options to identify the safest option. When, during the design stage it is possible to choose between two or more chemicals, the consideration of the transportation factors in the analysis can help one to select the best option.

The evaluation of the chemical substance is based on an approach simpler than the one proposed in Chapters VII and VIII, however the principles are similar.

10.1.2 The transportation problem

Transportation is becoming every day more of a major concern for the chemical industry especially after the events of 9/11 and lately with the controversy associated with the transportation of nuclear waste to Yucca Mountain. Transportation is also assumed to be required, but in some cases it can be avoided or reduced if the chemicals can be substituted, shipped under a different mode, or produced on site.

The typical transportation problem occurs when a plant A requires a certain chemical that can be shipped by different modes (e.g., truck or train) from different plants located at different distances. Each possible route goes through different environments (e.g., populated and rural areas) and consequently has a different risk. The problem is how to choose the best route and the best mode to reduce the hazards. The required storage tank in plant A varies according to the frequency and volume of the shipments, and this dependency links transportation to inherent safety. Additional decisions can improve the inherent safety level of transportation by choosing the type of container and the conditions (e.g., pressure, temperature, and concentration) that reduce the hazards [Bollinger et al., 1996]. Refrigerated storage is usually safer than pressurized storage tanks, but if the total quantity of stored chemicals is small, as in transportation, the observation might not be true [Kletz, 1998]. Because the transportation problem is affected by many external and unpredictable variables, the selection of the conditions that minimize the risk represents also the inherently safer option.

When decisions have to be made, the typical questions asked are related to the associated risk. However, the problem is complex, and the answer is not easy to determine due to the lack of consensus on a systematic methodology (e.g., **Saccomano** (1993)). Traditional risk assessment for transportation is based on the typical risk definition:

RISK = f (Accident rate, Probability of release, Consequences)

The accident rate for transportation is mode specific (e.g., road, railroad, pipeline, barge, ship) but also depends on factors such as the environment (e.g., urban, rural, suburban, remote), contributing factors, and initiating events. The accident rate for trucks depends on the type of truck, the type of road, traffic, and velocity, among others. For railroads, the class of track is important, as well as the location (main track or yard), the number of intersections with roads and highways, among others.

The probability of release describes the likelihood of the tank to suffer a failure following the accident. It depends on the type of tank, the wall thickness, and the pressure of the tank but also on dynamic factors such as the velocity, the type and size of impacted object, the position where the tank of fittings are hit, the material and wall thickness of the tank, and the type of force (e.g., puncture, crush, fire).

The consequences of the accidents depend on several other factors such as the size and position of the hole, the geographical location of the car, the time of the day which affects the number of exposed people, the weather conditions that affect the dispersion modeling, and the direction of the release. The size of the hole in the railcar has been studied by Raj and Turner (1993) and the data are in some case inconclusive. The size of the hole affects directly the release rate of the chemical but the location of the hole is also important. If the hole is in the vapor space the release rate is lower, however the vapor space is not always at the top of the car because the car could be overturned as a result of the accident.

The combination of all the factors produces a large number of possible release scenarios. Additionally, the accident can happen along the selected route in any location, each one characterized by different weather conditions, socioeconomic, and terrain characteristics. Because of all these possible variations, the transportation problem is not so well defined as in the case of a fixed facility. Another factor in the analysis of transportation risk is the presence of accidents characterized by high consequences but low frequency [Brown, 2000].

How to present and analyze the risk is another problem for transportation. The individual risk at any specific location is given by the sum of the contributions of each scenario. While individual risk does not depend on the length of type of the route and is normally very low, societal risk depends on the length of the route and could be potentially unacceptable due to the additive effects along the route [Rhyne, 1994].

10.1.3 The problem about transportation data

Transportation risk assessment is based on the same principles as the fixed site procedure and relies on accident databases for the statistical data required to calculate accident frequencies, release probabilities, and other parameters. However, these databases are not immune to the typical accident data collections such as underreporting (which is difficult to quantify), different reporting criteria, and various reporting parameters and scopes. Because of these problems, database accident data are difficult to compare. However, to develop a transportation analysis, data from several different databases must be used, and this requirement increases the uncertainty and complexity of the analysis. Additionally the required data must span several years during which regulation changes occurred and technical improvement of tank railcars and truck design occurred. The drop in accident rate for railroads during the last 20 years is a good example of this effect. The accident rate dropped from $15.8\text{x}10^{-6}$ accident/train mile in 1977 to 4.6 $8\text{x}10^{-6}$ accident/train mile in 1986. Since then it has been fluctuating around that value with a lowest rate of $4.3\text{x}10^{-6}$ accident/train mile in 1987 [FRA, 2000]. During 1980 the railroad tank cars design was modified with self-couplers and head shields that dramatically reduced risk of head puncture during an accident. In 1990 regulatory changes for transportation of toxic liquids reduced the likelihood of tank failures [Rhyne, 1994]. This and other regulatory changes contributed to the decrease of accident rates and release probabilities, but their effect is not immediate and continues during several subsequent years.

Additional sources of uncertainties are related to the reporting of total number of miles traveled, quantities of transported substances, conditions before and during the accident, and detailed information on the construction of the tanks (such as material and wall thickness). Also the data problem is different for each mode of transportation. For railroad the collected data have a better quality and are more nearly complete with respect to data collected for truck and road transportation.

All these elements together show the complexities associated with the evaluation of the transportation problem. Several methodologies have been proposed, but two of them are the most significant. Saccomano (1993) proposed an exercise where the same specified corridor was analyzed for two transportation modes (truck and railroad) by seven different academic, industrial, or consulting organizations. The goal was to compare the assumptions and results obtained by the seven groups. Each group developed the transportation risk analysis for the given corridor based on very different assumptions and different factors that yielded final results with great variability. For instance the accident rate used for road transportation varied between 0.31 $x10^{-6}$ and 2.6 $x10^{-6}$ accident/train mile.

The AIChE (1995) proposed a transportation risk assessment procedure based on a well-defined and systematic methodology for fixed site facility. However, when most of the expected important factors are taken into account (each one with several possible levels) the complexity of the problem is overwhelming and it becomes difficult to keep track of all the information used. Additionally, the lack of detailed and specific data for the development of the analysis contributes to the difficulty of applying the methodology.

10.2 A FUZZY MODEL FOR TRANSPORTATION

The proposed transportation index is based on nine fuzzy inference systems from the Mamdami [Yen and Langari, 1999] model, and the definition of the AND and OR operation is based on MIN and MAX operations, respectively [Zadeh, 1999] as explained in Chapter V. The software that is used for the calculations is the Fuzzy Logic Toolbox and Simulink from MATLAB.

The model proposed here has the purpose of evaluating the hazards of truck transportation from a macroscopic approach given the fact that during the early stages of process design only fundamental transportation information is available and easy to get. The procedure is based on the general idea that three major components contribute to the transportation risk: accident frequency, release probability, and consequences. Each one of these components must be described by factors that are selected according to knowledge that can be extracted from the statistical information in the databases. Keeping in mind the uncertainty associated with the data, the lack of detailed information, the learning from the corridor exercise, and the problems of complexity for detailed analysis, the development of the transportation index is based on the following steps:

1) Analysis of information and data reported by several studies and literature sources.
2) Selection of the most important macro factors that appeared to be relevant to the specific component (accident rate, release probability or consequences) for which the information can be available during the early design stages.
3) Selection of the data used to extract the knowledge needed to design the membership functions, fuzzy relations, and fuzzy inference systems.
4) Design of fuzzy relations and fuzzy IF-THEN rules to model the behavior of the selected factors and its relations with respect to other factors.

The three major components of the index depend on the following factors, and they are described by three fuzzy inference systems:

1) ACCIDENT RATE:
    a) Environment: rural or urban
    b) Type of road: highway, multilane divided, multilane undivided, two lanes, one-way
2) RELEASE PROBABILITY:

   a) Environment: rural or urban
   b) Type of road: freeway or non-freeway
   c) Type of truck: simple, single trailer, double trailer

3) CONSEQUENCES:
   a) Dispersion hazard: based on boiling point of the substance and transportation temperature
   b) Toxicity: based on the ERPG-2 of the chemical
   c) Flammability and explosivity: based on the NFPA ranking
   d) Volume transported by the truck (which depends on the type and configuration of the truck)

In order to generalize the model and including other important factors that can affect the components, the following correction factors are applied and they are described by three fuzzy inference systems:

1) ACCIDENT RATE: Correction due to the type of the truck
   a) Environment: rural or urban
   b) Type of road: highway, multilane divided, multilane undivided, two lanes, one-way
   c) Type of truck: simple, single trailer, double trailer
2) RELEASE PROBABILITY: Correction for wall thickness
   a) Design pressure of the tank
3) CONSEQUENCES: Correction for population concentration
   a) Number of people/mile^2

The final transportation hazard, TH, is calculated using the following formula:

$$TH_i = \{((\text{ACCIDENT RATE})_i\ (\text{CORR. FACTOR}_1)_i)) * ((\text{RELEASE PROBABILITY})_i\ (\text{CORR. FACTOR}_2)) *$$

* ((VOLUME)(TOXIC INDEX)(EXPLOSIVE/FLAMM. INDEX)(CORR. FACTOR$_3$))} *

* (TOTAL NUMBER OF SHIPMENTS PER YEAR) * (MILES)$_i$

$$TH = \sum TH_i$$

The total number of shipments per year is given by $N = V/ x\ n\ v_{hw}$,where V is the total volume of the chemical required in one year, n is the number of trailers per shipment and v_{hw} is the volume of each trailer. The volume of the tank that must be refilled per shipment is given by $v = x\ n\ v_{hw}$, where x represents the number of trucks required to refill the tank. Adjustment factors are used to calculate N and x when the volumes V, v and v_{hw} yield fractional values for N and x.

The sub-index i represents the different combinations of factors along the route. It is assumed that the route can be divided in segments where the population density, the type of road, and type of environment are constant. The calculations must be performed for each one of the i uniform segments, and the results must be added to obtain the final value. The weather is a major component for assessment of the consequences of a release, but for the purposes of this study, the evaluation of the area covered by the cloud is based on the dispersion index explained below. Additional assumptions are the following:

a) The total hazard index is based on the total length of the route and the number of shipments required per year. The frequency of the shipment is affected by the following variables:
   1. Total amount of chemical required by the plant during one year (V)
   2. Volume of the storage tank (v)
   3. Volume of the tank truck (v_{hw})
   4. Truck type (single truck or single trailer, double trailer)
b) The data used are based on the Harwood and Russell (1990) report and other data reported by Rhyne (1994) and CCPS (1993). The purpose of the present work is the development and testing of an index to evaluate transportation hazards to be used by

the inherent safety index. The limitations and uncertainties associates with the data are recognized, but the analysis of accuracy and goodness of the data is beyond the scope of this work.

The factors selected for the transportation index are described next. For the Accident Rate and the Consequences evaluation, the fuzzy sets and the fuzzy rules used are presented.

10.2.1 Truck accident frequency

Truck accident can happen as a consequence of several factors or combination of factors. Harwood and Russell (1990) and Karlaftis and Golias (2002) reported lists of possible factors. In general they include the truck configuration, including its size and weight, truck operation, including cargo type and human factors associated with the driver, highway or road type, type of environment and geographical location, weather, and temporal factors such as time, day and month. Intuitively any of these factors can have an effect on the accident rate of a truck; however, as pointed out in both studies, the statistical data show that some of them, such as the weather condition, apparently does not affect the accident rate. Other factors, such as environment, road geometry and traffic volumes have been recognized by both studies to have a strong effect on the accident rate. The same conclusion is reached by the two studies although they used different sets of data. Karlaftis and Golias (2002) used the Road Inventory database from the Indiana Department of Transportation (INDOT) and the Accident Information Record from the Indiana State Police for the years 1991 to 1995. These data are for any type of vehicular accidents. Harwood and Russell (1990) used the FHWA Office of Motor Carriers for the Sates of Michigan, Illinois, and California for the years 1984-1985, and these data are for truck accidents.

The common conclusion and the additional analysis presented by Harwood and Russell (1990) indicates that these three parameters are the most important to describe the accident frequency for trucks. For the purpose of this research, the data presented by

Harwood are used here because it reports the accident frequency for the three states based on type of environment and type of roadway.

The type of environment is classified into urban or rural according to the expected population concentration. This is also an indirect measure of the expected traffic (heavier in urban environments) and the possibility of accidents due to vehicular impact. The road type is classified into highway, multilane divided and undivided, and two-lanes. It is expected that the accident rate decrease to the degree that the type of road is similar to a highway.

A scale from 0 to 10 describes the type of environment, while a scale from 1 to 5 describes the type of road. A scale from 0 to 16 describes the accident frequency, and it represents the accident frequencies multiplied by a factor of 10^6. The fuzzy sets are shown in Figure 10.1. The data used and reports the fuzzy set classification used to develop the fuzzy rules, reported in Tables 10.1 and 10.2.

10.2.2 Correction due to type of truck

As reported by Harwood (1990) the type of truck and its configuration can affect the accident rate. The trucks can be classified as: simple, single trailer, and double trailer. Simple trucks are formed by a single unit consisting of the cargo compartment mounted on the same rigid frame as the cab. These trucks are smaller compared to the other two types and are used for short-range routes. Single trailers consist of a tractor and a separate trailer. Double trailers consist of a tractor and two separate trailers.

Because of the different design and dimensions, these three trucks present different driving problems. Large trucks are affected by the geometry of the roads such as curves, horizontal and vertical alignment, interchange ramps, shoulders, and railroad crossing [Harwood and Russell, 1990]. The truck configuration is a parameter that should be taken into account during the design stage to optimize the size of the tank and the transportation hazards.

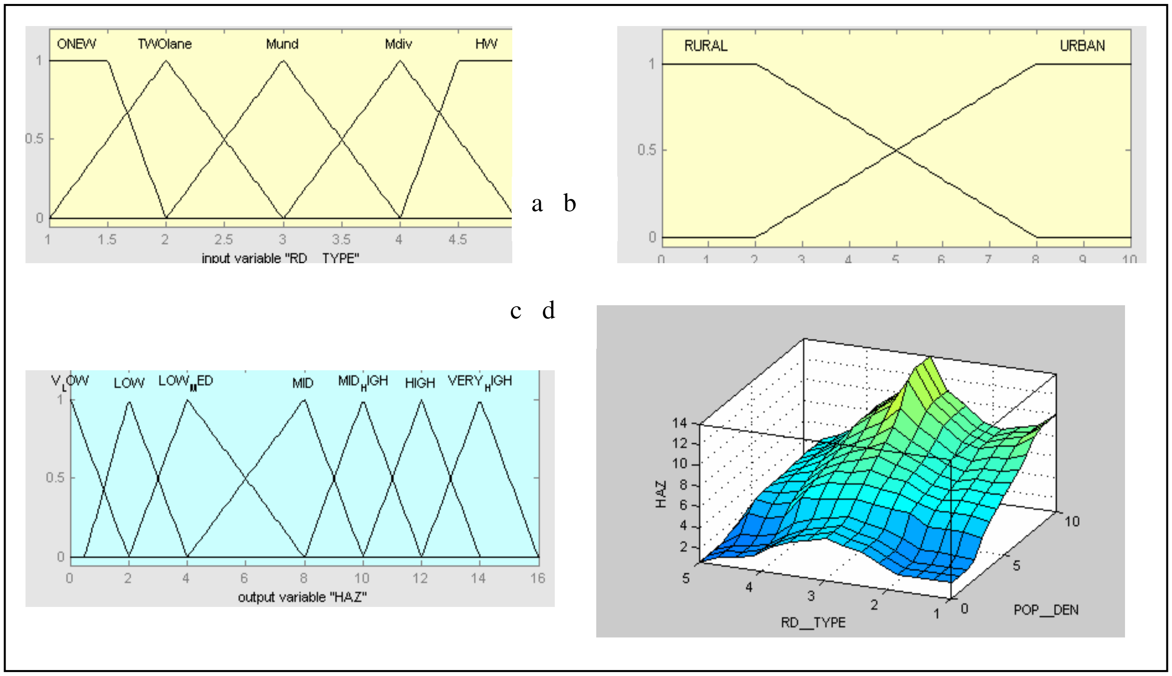


Figure 10.1: Fuzzy sets for the inputs “Type of road” (a), “Type of environment” (b), and for the output “Accident frequency” (c); defuzzified output surface (d)

Table 10.1: Accident frequencies as reported by Rhyne (1994) based on Harwood (1990) data from the averages for California, Illinois, and Michigan

AREA TYPE	ROAD TYPE	ACCIDENT RATE Accident/mi	FUZZY SET
RURAL	TWO-LANE	2.19E-06	Low
RURAL	MULTILANE UNDIVIDED	4.49E-06	Med-low
RURAL	MULTILANE DIVIDED	2.15E-06	Low
RURAL	FREWAY	6.40E-07	V-low
URBAN	TWO-LANE	8.66E-06	Mid
URBAN	MULTILANE UNDIVIDED	1.39E-05	V-high
URBAN	MULTILANE DIVIDED	7.47E-06	Mid
URBAN	FREWAY	2.18E-06	Low
URBAN	ONE-WAY STREET	9.70E-06	Mid-high

Table 10.2: Definition of fuzzy rules that express the knowledge extracted from the data in Table 10.1

	AREA TYPE	
ROAD TYPE	URBAN	RURAL
TWO-LANE	MID	LOW
MULTILANE UNDIVIDED	VERY_HIGH	LOW_MID
MULTILANE DIVIDED	MID	LOW
FREWAY	LOW	V_LOW
ONE-WAY STREET	MID_HIGH	LOW

The data reported by Harwood and based on a study developed by the California Department of Transportation for the years 1979 to 1983 are useful for developing a fuzzy relation between the type of environment (rural or urban), the type of road (freeway or non-freeway), and the type of truck (simple, single trailer, or double trailer). The data indicate that the accident rates are generally higher on non-freeways in urban areas.

This information can be used to modify the accident rate according to the expected type of truck and the route environment. The value for "all trucks" is taken as an average from which deviations occur according to the case. The percentage of deviation is used for designing the fuzzy relation that describes how much the accident rate should be affected. The maximum increase/decrease allowed is 50%.

10.2.3 Release probability

Because of the accident, the tank-truck can suffer different types of damages depending on several factors such as the velocity, dynamics of the accident, type of force and type of terrain that can cause the truck to overturn or not. A detailed analysis of several factors is proposed by Rhyne (1994) based on reports and studies presented by other researchers.

The velocity is the most important factor related to release probability along with the thickness of the wall of the tank. The velocity can be related to the type of road by a fuzzy relation developed using the data presented by Rhyne (1994) and is based on Harwood and Russell (1990). An additional advantage of this set of data is that it is directly related to the set of data used for the accident rate model.

10.2.4 Correction due to thickness of the wall

The analysis of data developed for railroad accidents clearly suggests that the increased thickness of the head of the tanks acting as shields decreases the incidence of tank-car punctures during an accident [Raj and Turner, 1993]. Additionally, the internal pressure of the tank can reduce the tank's resistance to puncture [Phillips and Olson, 1986]. Similar information is not available for tank-trucks, however it can be inferred that as the tank is designed for higher pressures, the wall thickness should increase. Based on this, the classification of tanks presented by AIChE (1995) and based on specific regulations is used here to develop a fuzzy relation based on internal pressure of the tank and the possible effect on the puncture resistance. This fuzzy relation is based only on knowledge, since no data are available to relate these variables and the material tensile strength. The relation is then used to modify (up to 50%) the release probability calculated with the relative fuzzy relation.

10.2.5 Tank volume

The volume of the tank is a direct measure of the amount of chemical transported by the truck (assuming it is full) and it affects the hazard of a release, since larger volumes represent longer leak times and population exposure. This fuzzy variable is designed based on the data presented by AIChE (1995). It is assumed that the volume of the tank can range from 2,000 to 45,000 gal, and this range is transformed by taking the natural logarithm to maintain a good representation of the smaller volumes.

10.2.6 Toxicity, explosivity and flammability indices

As mentioned at the beginning of the section, hazards due to toxicity and flammability are evaluated by using a simpler version of the hierarchical methodology proposed in Chapters VII and VIII, however the general ideas are the same. The fuzzy relation describing the toxicity index is based on the ERPG-2 value of the chemical substances. The chosen scale ranges from a concentration lower than 1 ppm (e.g., phosgene) to concentrations of 500 ppm. The range of the linguistic variable "toxicity" is transformed by taking the natural logarithm of the ERPG-2 range to achieve a good differentiation of the fuzzy sets for the lower (and most toxic) concentrations.

Explosivity and flammability are described by using the NFPA 704 ratings (2002). The fuzzy variable here describes the hazards associated with the flammability and explosivity of the chemical. The linguistic variable here has a range between 0 and 32 and the input is given by the sum of the squares of the two NFPA indices. The square of the index (that varies between 0 and 4) acts as a penalty for the higher scores.

Dispersion of hazardous chemicals after their release is also important for transportation, however the methodology followed here is simpler than the approach proposed in Chapters VII and VIII, but the general principles are the same:

1) The boiling point (Tb) of a substance indicates its phase at normal conditions and its volatility when released at conditions different from the atmospheric temperature and pressure. This behavior is described by $\Delta t1 = 25 - Tb$. When $\Delta t1$ is large the substance will tend to evaporate faster and cover a larger area than a less volatile substance. The range for $\Delta t1$ is (-100, 100) and it is divided into five fuzzy sets, as shown in Table 10.3.
2) The tank temperature (Tt) indicates the condition at which the chemical is shipped (e.g., pressurized or refrigerated). This is described by $\Delta t2 = 25 - Tt$ and it is assumed that when $\Delta t2$ is large the tank is refrigerated and when it is small the tank is pressurized. As noted by Kletz (1998) a refrigerated tank tends to be inherently safer than a pressurized tank because the substance is at low temperature and its vaporization will be slower due to the absorption of heat required to reach the boiling

temperature. Additionally, for a pressurized tank the release rate will be larger than a refrigerated tank due to the higher-pressure difference with respect to the atmospheric pressure, so it is expected that the area covered by the dispersion plume increases as the tank pressures increases. The range for Δt2 is (-100, 100), and it is divided into five fuzzy sets, as shown in Table 10.3. Figure 10.2 shows the resultant defuzzified surface that describes the expected hazard proportional to the size of the dispersion plume.

Table 10.3: Definition of fuzzy rules that express the hazard as a function of the expected area covered by a dispersion plume under steady state conditions

DISPERSION	**Δt2=25-Tt**				
Δt1=25-Tb	VERY LOW	LOW	0	HIGH	VERY HIGH
VERY LOW	MEDIUM	MEDIUM	LOW	VERY LOW	VERY LOW
LOW	HIGH	MEDIUM	LOW	VERY LOW	VERY LOW
0	HIGH	MEDIUM	LOW	VERY LOW	VERY LOW
HIGH	VERY HIGH	HIGH	MEDIUM	LOW	LOW
VERY HIGH	VERY HIGH	VERY HIGH	HIGH	MEDIUM	MEDIUM

10.2.7 Correction for population density

The consequences and hazards of the plume dispersion are related to the density of the population present in the area of the release. Therefore, the dispersion index must be corrected for the expected population density. The location of the population and the variation in density are neglected during the daytime. This correction factor is based on the idea that as the population density increases the hazards of highly negative consequence increases too. The fuzzy sets, shown in Figure 10.3, describing the population density are based on the classification, displayed in Table 10.4, used by the United States Census 2000 [Census, 2000] and are more detailed than the sets used to model the accident rate to provide more sensitivity to the correction factor.

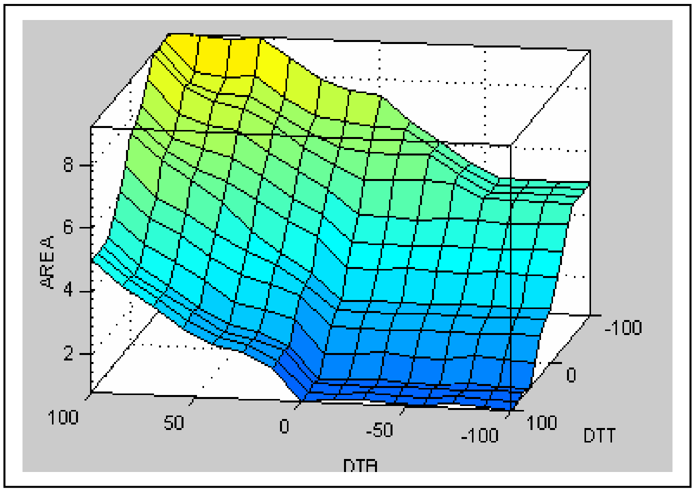


Figure 10.2: Defuzzified output surface for the inputs “Δt2 = 25-Tb” and “Δt2 = 25-Tt”

Table 10.4: Definition of fuzzy set for population density as a correction factor for the dispersion index

CATEGORY	**DENSITY (people/mi^2)**	**SCALED DENSITY Ln(people/mi^2)**
REMOTE	20	3.0
RURAL	100	4.6
SUBURBAN	1,000	6.9
URBAN	3,000	8.0
EXTREMELY HIGH	10,000	9.2

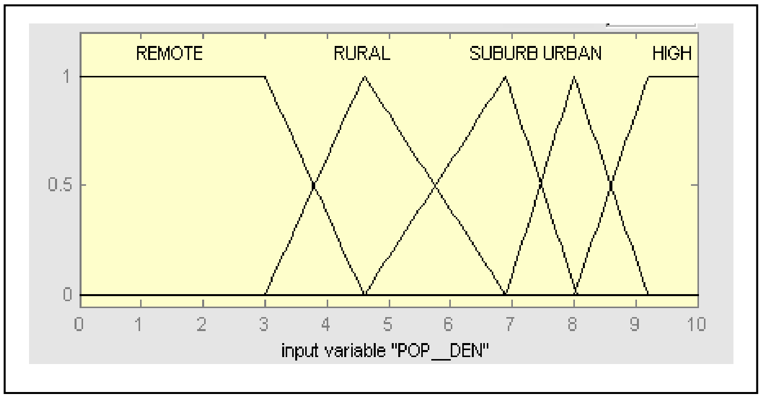


Figure 10.3**:** Fuzzy sets describing the population density from the data in Table 10.4

10.3 CASE STUDY

The fuzzy logic methodology described in this chapter has been applied to three fictitious routes with different lengths and classifications that are reported in Table 10.5. Each route is divided into segments (i) with constant population density, type, and condition of the road. It is expected that this type of information can be easily obtained from the Census data and GIS (Geographic Information System) software.

The index for population density (expressed as ln(people/mi^2)) is used as input in Figure 10.1a, while the index for type of road is used as input in Figure 10.1b. The index for type of road can be increased or decreased according to the expected condition that is evaluated subjectively.

Route 3 is longer than the other two routes but it does not intercept highly populated areas. Four different cases have been used with the three routes. The conditions for each case are presented in Table 10.6.

Table 10.5: Description of the three routes used as example

ROUTE	ENVIRONMENT	POP. DENSITY Ln (people/mi^2)	LENGTH mi	TYPE ROAD	ROAD CONDITION	LENGTH mi
	REMOTE	3	100	TWO LANES	Good condition	2.5
	RURAL	5	50	MUND	Bad condition	2.8
1	SUBURBAN	7	20	MDIV	Many intersections	3.8
	URBAN	9	20	MDIV	Very good	4.3
	VERY HIGH	10	0	MDIV	Bad condition	4
	REMOTE	3	50	TWO LANES	good condition	2.5
	RURAL	5	150	MUND	Bad condition	2.8
2	SUBURBAN	7	20	MDIV	Many intersect.	3.8
	URBAN	9	10	MDIV	Very good	4.3
	VERY HIGH	10	10	MDIV	Bad condition	4
	REMOTE	3	250	TWO LANES	good condition	2.5
	RURAL	5	100	MUND	Bad condition	2.8
3	SUBURBAN	7	10	MDIV	Many intersect.	3.8
	URBAN	9	0	MDIV	Very good	4.3
	VERY HIGH	10	0	MDIV	Bad condition	4

Table 10.6: Description of the four cases used as example

		CASE 1	CASE 2	CASE 3	CASE 4
CHEMICAL	ERPG-2 (ppm)	3	3	3	3
Chlorine	NFPA FIRE	0	0	0	0
	NFPA EXP	0	0	0	0
	Tb (F)	-29	-29	-29	-29
	Type	Single trailer	Single trailer	Double trailer	Single trailer
TRUCK	VOL (gal)	4,000	4,000	4,000	4,000
	T (F)	80	80	80	32
	P rating (psi)	400	400	400	400
STORAGE TANK	VOL (gal/yr)	20,000	20,000	20,000	20,000
	tank VOL (gal)	5,000	8,000	8,000	8,000

The results reported in Table 10.7 are for the first route and the first three cases. It is possible to observe how the accident rate and release probability change depending on the environment and the type of truck. Also, it is possible to observe how the total hazard indices change depending on the route and the conditions of each combination of case and route.

The values of the indices reported in Table 10.7 are based on ideas similar to the ones used in the rest of the research project but because they are not exactly the same. The indices are not comparable. The hazard index for this chapter is based on incident rates modified by the factors listed in the previous section.

In Figure 10.4 the total hazard indices are plotted for Cases 1, 2, 3 and 4 on Route 3. It is possible to observe how Case 3 (double pressurized trailer) seems to present the higher potential hazard while Case 4, single refrigerated trailer, offers the safest option among the four studied.

The fuzzy logic methodology described in this chapter represents a first step in the development of a transportation index that can be included in the overall inherent safety evaluation of a chemical plant. This methodology must be expanded to other transportation modes, such as railroad, pipelines, and barges, and each one of these modes represents a different problem that must be analyzed by taking into account the data available and the knowledge obtained from it. Fuzzy logic provides a flexible approach to model transportation problems because of its ability to work with uncertain data and include subjective evaluations.

Table 10.7: Results for Cases 1, 2, 3 for Route 1

CASE		HAZ INDEX	Rel. Prob.	Acc/mi	Rel. prob.	Rel. rate
1	REMOTE	0.003204	0.000641	5.79E-06	0.0626	3.62E-05
	RURAL	0.003031	0.000606	8.94E-06	0.05747	2.57E-05
	SUBURBAN	0.001582	0.000316	9.94E-06	0.0527	1.05E-05
	URBAN	0.001603	0.000321	8.08E-06	0.05	8.09E-06
	VERY HIGH	0	0	1.06E-05	0.05	0
	Total	**0.00942**				
2	REMOTE	0.001602	0.00032	5.70E-06	0.0626	1.81E-05
	RURAL	0.009093	0.001819	8.94E-06	0.05747	7.71E-05
	SUBURBAN	0.001582	0.000316	9.94E-06	0.0527	1.05E-05
	URBAN	0.0008017	0.00016	8.08E-06	0.005	4.04E-06
	VERY HIGH	0.001104	0.000221	1.06E-05	0.05	5.29E-06
	Total	**0.0141**				
3	REMOTE	0.00801	0.001602	5.78E-06	0.0626	9.06E-05
	RURAL	0.006062	0.001212	9.94E-06	0.05747	5.14E-05
	SUBURBAN	0.000791	0.000158	9.94E-06	0.0527	5.24E-06
	URBAN	0	0	8.08E-06	0.005	0.00E+00
	VERY HIGH	0	0	1.06E-05	0.05	0.00E+00
	Total	**0.0148**				

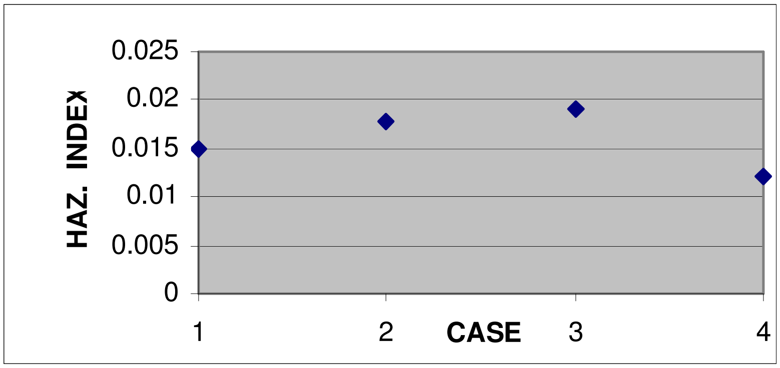


Figure 10.4: Total hazard index for Cases 1, 2, 3, and 4 for Route 3

CHAPTER XI

CONCLUSIONS AND FUTURE WORK

Inherent safety is a concept derived from the learning that no matter how well hazards are controlled by extrinsic measures and protective barriers, there is always a possibility for abnormal events that can degenerate into industrial chemical incidents. Kletz's famous expression "what you don't have cannot leak" became the motto of inherent safety because it summarizes the very essence of the approach: hazard elimination rather than control. Because the idea sounds as a very reasonable approach, regulatory efforts have been undertaken but the application of the inherent safety principle has proven to be complex and difficult to analyze because of the complexity of the chemical industry and the several aspects that must be taken into account.

One of the most important limitations of inherent safety is the lack of a methodology able to measure how well the principles have been applied. As explained in Chapter II several approaches have been proposed and they constitute important starting points from which to develop and explore other approaches. Another limitation associated with the inherent safety analytical methods available so far is the fact that they are based on worst hazards and therefore focus mainly on the most hazardous chemicals and largest vessels. However, because hazards are derived from the interaction of several factors, it is necessary to take into account the contributions of all equipment and pipelines of a plant in order to capture and model the complexity of the chemical plant. Another limitation of the analytical methodologies described in Chapter II is that they are based on interval scales that present limitations associated with sensitivity within and around the limits of the subintervals, giving therefore a discrete overall index.

The present research focuses on understanding how the methodologies and approaches available for safety analysis today were developed and after identifying the fact that they derive from the limitations imposed by the procedure followed for plant design, a conceptual background was proposed. Because safety analysis requires a large amount of information, in the past it was only possible to develop safety analysis after the design stage was completed. However, today, with the availability of computers, mathematical modeling, and process simulators it is possible to move the safety analysis towards earlier stages of the plant design phase. However, this requires the development of analytical methodologies developed for computer use, in order to integrate it into process simulators and facilitate the analysis of safety.

Process safety is similar to a non-well defined science because of the lack of enough constructs to rigorously understand and model "safety". It is therefore necessary to integrate technical information and empirical engineering knowledge. Traditional mathematical methods do not have such capability; hence the model proposed by this research is based on fuzzy modeling that can interpret numerical and linguistic information in a rigorous mathematical approach. Additionally, fuzzy logic can deal with the high uncertainty associated with factors that are relevant for process safety. The proposed fuzzy logic model has the advantage of being transparent and easy to understand, as demanded by the nature of fuzzy logic, without sacrificing the mathematical rigor. Because of the simplicity of the approach it is expected that non-safety-specialized design engineers can apply it to identify potential hazardous combination of conditions during the design stage.

The hierarchical fuzzy model for the analysis of inherent safety proposed in this research is computer-based and relies on information that can be obtained during early design stages by using process simulation, cost estimation, and approximate equipment sizing. Because of the hierarchical nature of the model it is possible to analyze the interaction existing between the hazards inherent to the chemical properties of the substances and to the characteristics and the equipment. The interaction analysis is fundamental for inherent safety analysis because one change toward inherently safer design in one unit can increase the hazard in another part of the process. The model is based on the observation that safety can be understood as a complex system formed by several subsystems that can be modeled by simple sets of local rules; however the interaction of the result of each set of rules can describe the complicated net of interaction among the factors.

The main idea upon which the model is based is that each single equipment and pipeline contributes to the overall hazard of the plant; this concept is parallel to the idea of cost that adds up to the capital cost of the plant. The model is based on a scale of hazard with a lower value of 0 and an upper value of 1. The value of zero implies absolute physical lack of hazard and is therefore the inherently safest option; the value of one implies an extremely high level of hazard whose physical implications are catastrophic. The value of 0.5 is assumed to be the threshold between inherent safety and unsafe design. Because the hazard scale is based on a continuous ordinal scale, it is not possible to establish a relation between two values of hazard, but it is possible to rank the values and identify them as safer or unsafer. However, as the hazard value tends to zero, the level of inherent safety increases while, as it tends to one, the level of inherent safety drops. The problem related to scaling, scale development, and variable type has been discussed in Chapter IV and Chapter VII.

In the case of inherent safety, the contribution of each pipe and piece of equipment adds up to the overall hazard for the plant. It is assumed that when the hazard level is low (i.e., below 0.5) the equipment has a high degree of inherent safety and will therefore require fewer or no protective barriers; if the hazard level is high (i.e., above 0.5) then it is required to reduce it by modifying the design or substituting the chemical or by applying the ideas of extrinsic safety, such as protective barriers.

The model described in Chapter VII and Chapter VIII provides a systematic approach for the evaluation of inherent safety taking into account the subjectivity and uncertainty characteristic of safety evaluations. The application of fuzzy logic provides an ideal approach to model fuzziness and subjectivity. The inherent safety evaluation obtained directly from a process simulation, without requiring extra tedious work for manual safety evaluations, will allow design engineers to apply the inherent safety approach in a more efficient way.

The results presented for the case study show how the model is applied and its sensitivity to design changes. The results are encouraging and show the potential modeling power of the proposed hierarchical fuzzy-based approach. However, this research represents only the first step, and due to underlying complexity can be expanded and improved. As future work, it is suggested to revise the fuzzy inference systems in order to incorporate more linguistic variables and improve the modeling capacity of the system. The designed inference system should be revised by experts and optimized according to their assessments; additionally, the system should be tested on real cases and tuned when discrepancies with reality are found. The model proposed here is mainly for vessels and must be adapted to other equipment such as pumps, pipes, towers, and reactors

Future work is required in order to expand the model including other factors as explained in Chapter VII and to adapt the basic model for vessels to other equipment. Because the software relies on information that is available in equipment datasheets it will be useful to develop a Visual Basic version able to run in Excel and facilitate the application during the plant design stage. On the other hand, by linking the proposed methodology to process simulation and cost estimation, it will be possible to create a powerful engineering tool able to evaluate processing units or plants from often conflicting criteria such as technical requirements, cost limitations, environmental, and safety aspects.

The challenge of designing membership functions based on the magnitude of the potential physical consequences has been addressed by this work for the fuzzy inference systems of dispersion, however additional work is required on the issue. If the approach is used for the other factors, then it would be possible to evaluate inherent safety on a interval or ratio scale that allows direct comparison of the points on the scale.

Transportation is another important aspect that must be included in inherent safety, and while the example presented in Chapter X is a first step, the methodology must be expanded to other transportation modes.

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