SOFT COMPUTING APPROACHES TO UNCERTAINTY PROPAGATION IN ENVIRONMENTAL RISK MANAGEMENT

Thesis submitted in accordance with the requirements of the **Department of Chemical Engineering · University of Rovira I Virgili** for the degree of

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by

Vikas Kumar

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SOFT COMPUTING APPROACES TO UNCERTAINTY PROPAGATION IN ENVIRONMENTAL RISK MANGEMENT
Vikas Kumar
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Marta Schuhmacher, professora Titular del Departament d'Enginyeria Química de la Universitat Rovira i Virgili

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Tarragona, 2 de Juny de 2008-06-02

Dra. Marta Schuhmacher

Professora Titular d'Universitat

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SUPERVISOR

Dr. Marta Schuhmacher Ansuategui

Environmental Engineering Laboratory

Chemical Engineering School

Universitat Rovira i Virgili (URV)

Tarragona (Catalonia, Spain)

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Sheffield, S3 7HQ, UK

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School of Medicine
Universitat Rovira i Virgili (URV)
Reus (Catalonia, Spain)

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To aspiring youths of rural Bihar

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SUMMARY

Real-world problems, especially those that involve natural systems, are complex and composed of many non-deterministic components having non-linear coupling. The conventional approaches based on analytical techniques for understanding and predicting the behaviour of such systems can prove to be very difficult and inflexible in order to cope with the intricacy and the complexity of the real-world system. It turns out that in dealing with such systems, one has to face a high degree of uncertainty and tolerate imprecision. Classical system models based on numerical analysis, crisp logic or binary logic have characteristics of precision and categoricity and classified as hard computing approach. In contrast soft computing approaches like probabilistic reasoning, fuzzy logic, artificial neural nets etc have characteristics of approximation and dispositionality. Although in hard computing, imprecision and uncertainty are undesirable properties, in soft computing the tolerance for imprecision and uncertainty is exploited to achieve tractability, lower cost of computation, effective communication and high Machine Intelligence Quotient (MIQ). Until recently, uncertainty, regardless of its nature or source has been treated using probability theory concepts. However, uncertainties associated with real-world systems are not limited to randomness. Uncertainties in the natural system models may originate from randomness or from imprecision due to lack of information. Imprecise, vague, or incomplete information may better be represented by other soft computing approaches, such as fuzzy set theory, possibility theory, belief functions, etc. New approaches which allow utilization of probability theory in combination with other approaches should be investigated. It can provide more holistic framework to treat different kind of uncertainties and insight into the level of confidence in model estimates.

Proposed thesis has tried to explore use of different soft computing approaches to handle uncertainty in environmental risk management. The work has been divided into three parts consisting five papers.

In the first part of this thesis two uncertainty propagation methods have been investigated. The first methodology is generalized fuzzy α-cut based on the concept of transformation method. A case study of uncertainty analysis of pollutant transport in in the

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subsurface using 2-D transport model has been used to show the utility of this approach. Results are compared with commonly used probabilistic method and normal Fuzzy alpha-cut technique. This approach shows superiority over conventional methods of uncertainty modelling. A Second method is proposed to manage uncertainty and variability together in risk models. The new hybrid approach combining probabilistic and fuzzy set theory is called Fuzzy Latin Hypercube Sampling (FLHS). The noncognitive uncertainty such as physical randomness, statistical uncertainty due to limited information, etc can be described by its own probability density function (PDF); whereas the cognitive uncertainty such as estimation error etc can be described by the membership function for its fuzziness and confidence interval by α-cuts. An important property of this theory is its ability to merge inexact generated data of LHS approach to increase the quality of information. The FLHS technique ensures that the entire range of each variable is sampled with proper incorporation of uncertainty and variability. A fuzzified statistical summary of the model results will produce indices of sensitivity and uncertainty that relate the effects of heterogeneity and uncertainty of input variables to model predictions. The feasibility of the method is validated to analyze total variance in the calculation of incremental lifetime risks due to polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/F) for the residents living in the surroundings of a municipal solid waste incinerator (MSWI) in Basque Country, Spain.

The second part of this thesis deals with the use of artificial intelligence technique for generating environmental indices. Two papers have been published in this area. The first paper focused on the development of a Hazzard Index (HI) using persistence, bioaccumulation and toxicity properties of a large number of organic and inorganic pollutants. For deriving this index, Self-Organizing Maps (SOM) has been used which provided a hazard ranking for each compound. Subsequently, an Integral Risk Index was developed taking into account the HI and the concentrations of all pollutants in soil samples collected in the target area. Finally, a risk map was elaborated by representing the spatial distribution of the Integral Risk Index with a Geographic Information System (GIS). The results were used to generate an integrated risk map in the industrial chemical / petrochemical area of Tarragona. The results of this study show that the usefulness of soft computing approaches to support the environmental decision making processes concerning

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environmental pollutants. The second paper is an improvement of the first work. The first work used SOM weight to rank contaminants using their characteristics of persistence, bioaccumulation, and toxicity in order to obtain the HI. It doesn't consider uncertainty associated with contaminants characteristic values. So in this study a hybrid method of probabilistic SOM is used to calculate Integrated Risk Index. New approach called Neuro-Probabilistic HI was developed by combining SOM and Monte-Carlo analysis. This new index seems to be an adequate tool to be taken into account in risk assessment processes. In both papers, feasibility of the methods has been validated by applying it to the chemical/petrochemical industrial area of Tarragona (Catalonia, Spain).

The third part of this thesis deals with decision-making framework for environmental risk management. A new integrated decision-making framework is proposed. Multi-component environmental risk management in uncertain environment has been addressed. The fuzzy risk-analysis model is proposed to comprehensively evaluate all risks associated with contaminated systems resulting from more than one toxic chemical. In this study, an integrated fuzzy relation analysis (IFRA) model is proposed for risk assessment involving multiple criteria. The model is an integrated view on uncertainty techniques based on multi-valued mappings, fuzzy relations and fuzzy analytical hierarchical process. Integration of system simulation and risk analysis using fuzzy approach allowed to incorporate system modelling uncertainty and subjective risk criteria. This model is demonstrated for a multi-components groundwater contamination problem. Results reflect uncertainties presented as fuzzy number for different modelling inputs obtained from fuzzy system simulation. Integrated risk can be calculated at different membership level which is useful for comprehensively evaluating risks within an uncertain system containing many factors with complicated relationships. It has been shown that a broad integration of fuzzy system simulation and fuzzy risk analysis is possible.

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RESUMEN

Los problemas del mundo real, especialmente aquellos que implican sistemas naturales, son complejos y se componen de muchos componentes indeterminados, que muestran en muchos casos una relación no lineal. Los modelos convencionales basados en técnicas analíticas que se utilizan actualmente para conocer y predecir el comportamiento de dichos sistemas pueden ser muy complicados e inflexibles cuando se quiere hacer frente a la imprecisión y la complejidad del sistema en un mundo real. El tratamiento de dichos sistemas, supone el enfrentarse a un elevado nivel de incertidumbre así como considerar la imprecisión. Los modelos clásicos basados en análisis numéricos, lógica de valores exactos o binarios, se caracterizan por su precisión y categorización y son clasificados como una aproximación al hard computing. Por el contrario, el soft computing tal como la lógica de razonamiento probabilístico, las redes neuronales artificiales, etc., tienen la característica de aproximación y disponibilidad. Aunque en la hard computing, la imprecisión y la incertidumbre son propiedades no deseadas, en el soft computing la tolerancia en la imprecisión y la incerteza se aprovechan para alcanzar tratabilidad, bajos costes de computación, una comunicación efectiva y un elevado Machine Intelligence Quotient (MIQ). Hasta hace poco, la incertidumbre, a pesar de su naturaleza o fuente, ha sido tratada usando conceptos teóricos de probabilidad. Sin embargo, las incertidumbres asociadas con los sistemas del mundo real no se deben tan sólo al azar. Las incertidumbres en los modelos de sistemas naturales pueden deberse a la aleatoriedad o bien a la imprecisión debida a una falta de información. La información imprecisa, vaga o incompleta puede ser mejor presentarla a través de otros enfoques de Soft-computing, tal como un conjunto de teorías difusas, teoría de posibilidad, belief functions etc. Es preciso investigar nuevos acercamientos que permitan la utilización de la teoría de probabilidad en combinación con otras aproximaciones. Ello podría aportar un nuevo marco más integral para tratar diferentes tipos de incertidumbres y poder conocer los niveles de confidencia en los modelos estimados.

La tesis propuesta intenta explorar el uso de las diferentes aproximaciones en la informática blanda para manipular la incertidumbre en la gestión del riesgo

medioambiental. El trabajo se ha dividido en tres secciones que forman parte de cinco artículos.

En la primera parte de esta tesis, se han investigado dos métodos de propagación de la incertidumbre. El primer método es el generalizado α-cut fuzzy o difusa, el cual está basada en el método de transformación. Para demostrar la utilidad de esta aproximación, se ha utilizado un caso de estudio de análisis de incertidumbre en el transporte de la contaminación en suelo, para el cual se utilizó el modelo de transporte 2-D. Los resultados obtenidos mediante la utilización de la técnica fuzzy alpha-cut fueron comparados con los obtenidos por métodos clásicos probabilísticos. Esta aproximación muestra una superioridad frente a los métodos convencionales de modelación de la incertidumbre. La segunda metodología propuesta trabaja conjuntamente la variabilidad y la incertidumbre en los modelos de evaluación de riesgo. Para ello, se ha elaborado una nueva aproximación híbrida denominada Fuzzy Latin Hypercube Sampling (FLHS), que combina los conjuntos de la teoría de probabilidad con la teoría de los conjuntos difusos. La incertidumbre no cognitiva como la aletoriedad física y la incertidumbre estadística debida a la información limitada, etc., pueden describirse mediante su función de densidad de probabilidad (PDF); mientras que la incertidumbre cognitiva tal como es el caso de la estimación del error, etc., puede ser descrita mediante la función de pertenencia para los conjuntos difuso, y los intervalos de confianza de los α-cuts. Una propiedad importante de esta teoría es su capacidad para fusionarse entre si los diferentes datos inexactos generados de la aproximación LHS, lo que supone la obtención de una mayor calidad de la información. La técnica FLHS nos asegura una apropiada incorporación de la variabilidad y la incertidumbre en el registro de cada variable. El resumen estadístico fuzzificado de los resultados del modelo generan índices de sensitividad e incertidumbre que relacionan los efectos de la heterogeneidad e incertidumbre de las variables de entrada con las predicciones de los modelos. La viabilidad del método se llevó a cabo mediante la aplicación de un caso a estudio donde se analizó la varianza total en la cálculo del incremento del riesgo sobre el tiempo de vida de los habitantes que habitan en los alrededores de una incineradora de residuos sólidos urbanos en Tarragona, España, debido a las emisiones de dioxinas y furanos (PCDD/Fs).

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La segunda parte de la tesis consistió en la utilización de las técnicas de la inteligencia artificial para la generación de índices medioambientales. Se realizaron dos artículos en esta área. En el primer artículo se desarrolló un Índice de Peligrosidad a partir de los valores de persistencia, bioacumulación y toxicidad de un elevado número de contaminantes orgánicos e inorgánicos. Para su elaboración, se utilizaron los Mapas de Auto-Organizativos (SOM), que proporcionaron un ranking de peligrosidad para cada compuesto. A continuación, se elaboró un Índice de Riesgo Integral teniendo en cuenta el Índice de peligrosidad y las concentraciones de cada uno de los contaminantes en las muestras de suelo recogidas en la zona de estudio. Finalmente, se elaboró un mapa de la distribución espacial del Índice de Riesgo Integral mediante la representación en un Sistema de Información Geográfico (SIG). Los resultados obtenidos fueron aplicados para la generación de un mapa de peligrosidad integral en el área industrial químico/petroquímico de Tarragona. Los resultados de este estudio muestran la utilidad de la aplicación del soft computing en el proceso de la toma de decisiones medioambientales relacionadas con la contaminación ambiental. El segundo artículo es una implementación del primer trabajo. En el primer artículo el ranking de peligrosidad (o Índice de peligrosidad, HI)) de los diferentes contaminantes se obtenía a partir del valor del índice que generaba el SOM en función de sus características de persistencia, bioacumulación y toxicidad. Dicho Índice no consideraba la incertidumbre asociada con los valores de las variables de los contaminantes. Por ello, en este estudio, se creó un método híbrido de los Mapas Auto-organizativos con los métodos probabilísticos, obteniéndose de esta forma un Índice de Riesgo Integrado. Mediante la combinación de SOM y el análisis de Monte-Carlo se desarrolló una nueva aproximación llamada Índice de Peligrosidad Neuro-Probabilística. Este nuevo índice es una herramienta adecuada para ser utilizada en los procesos de análisis. En ambos artículos, la viabilidad de los métodos han sido validados a través de su aplicación en el área de la industria química y petroquímica de Tarragona (Cataluña, España).

El tercer apartado de esta tesis está enfocado en la elaboración de una estructura metodológica de un sistema de ayuda en la toma de decisiones para la gestión del riesgo medioambiental. Se propone un nuevo marco de integración para la toma de decisiones. El modelo propuesto se ha elaborado para gestión de riesgos medioambientales y propone la

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integración del riesgo producido por múltiples-contaminantes, considerando a su vez un medioambiente incierto. El modelo de análisis de riesgo fuzzy elaborado tiene como objetivo la evaluación de todos los riesgos asociados a los sistemas contaminados por más de un contaminante tóxico. En este estudio, se presenta un modelo integrado de análisis de fuzzy (IFRA) para la evaluación del riesgo cuyo resultado depende de múltiples criterios. El modelo es una visión integrada de las técnicas de incertidumbre basadas en diseños de valoraciones múltiples, relaciones fuzzy y procesos analíticos jerárquicos inciertos. La integración de la simulación del sistema y el análisis del riesgo utilizando aproximaciones inciertas permitieron incorporar la incertidumbre procedente del modelo junto con la incertidumbre procedente de la subjetividad de los criterios. El modelo se ha aplicado a un problema de contaminación de las aguas subterráneas por varios compuestos químicos. Los resultados del modelo muestran la incertidumbre en forma de números fuzzy o difusos de los diferentes parámetros de entrada al modelo obtenido tras la simulación del sistema incierto. El riesgo integrado puede calcularse a diferentes niveles de pertenencia lo cual es útil para la evaluación compreniva de los riesgos dentro de un sistema incierto que contiene muchos factores de riesgo con relaciones complicadas entre ellos. Se ha demostrado que es posible crear una amplia integración entre la simulación de un sistema incierto y de un análisis de riesgo incierto.

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CHAPTER 1

INTRODUCTION AND SCOPE OF THE THESIS

1.1 Introduction

Recent emphasis on the preventative and precautionary approaches to environment risk management denotes a shift towards attempts to manage risks to the environment. Preventative approaches concentrate on eliminating waste and pollution at the source. Approaches based on the Precautionary Principle are more demanding and require the adoption of control measures before harm is proven. The latter has been adopted by the European Union as a guiding principle(EU, 2000). It is used when information suggests cause and effect but cannot prove it, or when possible consequences are so undesirable that "business as usual" cannot be chanced. Justification is on grounds of complexity (inability to unambiguously identify all cause-effect pathways) or uncertainty.

Managing risk means finding ways to reduce, mitigate, or simply learning to live with risks. How this is done depends often on acceptability of the risk. The acceptability can be decided by regulators or public. Regulator criteria of acceptability are driven by scientific evidences or public perceptions. The public considers some risks unacceptable and society is prepared to pay a high cost to avoid such risks. Some of the main factors affecting social perception towards risk are credibility of risk assessment process and communication of risk. However at the end of regulators, it’s all about a well informed decision making process. Basic criteria for "good" decision making are efficiency, effectiveness and equity. A further criterion specific to environmental decision making is flexibility. In the context of environmental risk management, efficiency can be interpreted as good process (rather than economic efficiency), and effectiveness as good outcomes. Ideally, if outcomes can be predicted with reasonable certainty, then good process should lead to good outcomes. In practice, the concept of a "good" decision depends on a combination of good process and good outcomes, and, according to the circumstances, different weights may be given to different aspects. In environmental situations, long lead

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time between action and outcome means that deducing effect from cause is not always possible; a decision maker must rely on judgment. Improving decision making therefore requires looking for ways of improving the quality of the judgment of the decision maker.

Environment Risk Assessment (ERA) models very often rely on the evaluation of risks for human and the environment. This evaluation is carried out with the help of models, which simulate the transfer of pollutants from a source to a vulnerable target, for different scenarios of exposure. Currently, there is a trend in risk analysis away from single summary estimates of risk in favour of more comprehensive risk characterisation based on a probabilistic or possibilistic estimate of risk. The range of risks spanned by these estimates encompasses both uncertainty in the factors affecting risk, as well as variability in exposure or susceptibility within the population of interest. For example body weight, which is pertinent to a number of health risks, varies considerably among individuals even of the same age and sex, but is subject to little uncertainty. On the other hand, levels of exposure to dietary risk factors such as food contaminants can be both highly variable and highly uncertain. Most risk factors will be subject to varying degrees of both variability and uncertainty and the assessment of risk requires consideration of all of the possible factors that may influence risk.

1.2 Problem definition

A key issue in the ERA is uncertainty due to various reasons. First of all ERA models are confronted with inherent uncertainty and lack of knowledge that the disciplinary sciences face. Secondly, ERA models have to deal with a variety of types and sources of uncertainty that have to be structured and combined in one-way or another. The data needs for characterizing parametric uncertainties are often substantial, and not necessarily available. And finally, ERA models are prone to accumulation of uncertainties, because of their ambition to cover the whole cause-effect chain of environment problem.

A typology of uncertainties would help to differentiate between different types and sources of uncertainty and to communicate uncertainties in a more constructive manner. For example, uncertainty regarding model parameters may have essentially two origins. It may arise from randomness due to natural variability resulting from heterogeneity of population or the fluctuations of a quantity in time. Or it may be caused by imprecision due

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to a lack of information resulting. In risk assessment, uncertainty issue is struggling with typological problems; no distinction is traditionally made between these two types of uncertainty, both being represented by means of a single probability distribution. So, uncertainty in risk assessment models is generally addressed within a purely probabilistic framework. This approach comes down to assuming that knowledge regarding model parameters is always of random nature (variability). Such knowledge is represented by single probability distributions typically propagated through the risk model using the Monte-Carlo technique. Even if this approach is well-known, the difficulty is to avoid an arbitrary choice of the shape of probability distributions assigned to model parameters. Indeed in the context of risk assessment related to pollutant exposure, knowledge of some parameters is often imprecise or incomplete. The selection of parameter values of environmental models is based as much as possible on the data collected at the time of on-site investigations (phase of diagnosis). However, due to time and financial constraints, information regarding model parameters is often incomplete and imprecise. The use of single probability distribution to represent this type of knowledge becomes subjective and partly arbitrary, and it is more natural to use intervals.

However, the available information is often richer than an interval but less rich than a probability distribution. In practice, while information regarding variability is best conveyed using probability distributions, information regarding imprecision is more faithfully conveyed using probability families encoded either by p-boxes (lower & upper cumulative distribution functions) or by possibility distributions (also called fuzzy intervals) or yet by random intervals using the belief functions of Dempster-Shafer.

Despite the usefulness of these methods in uncertainty analysis, it has not been adopted by environmental risk modellers. One of the reasons is lack of integrated framework to use simulation results from these methods in risk management model. For example, it is often a problem to use fuzzy results (which are in form of membership function) in crisp-set based risk management model. Problem becomes more complicated when it is multi-contaminants multiple risk criteria problem. This complication has discouraged the risk assessment communality to use fuzzy approach in environmental risk management.

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Finally computational cost is also a major problem in many methods. The number of model runs can sometimes be very large, i.e., of the order of many thousands, resulting in substantial computational demands. Thus, the costs associated with uncertainty analysis may sometimes be prohibitively high, necessitating a simplification of model simulations (inadequate sample size) and/or the use of simpler models.

1.3 Scope and Objectives

This thesis deals with uncertainty in environmental risk models with an aim to improve the practice of characterising uncertainty in environmental risk assessment. The assumptions for this work are (i) possibility of making a well-found decision improves if, apart from decision-relevant knowledge, also uncertainty that may be relevant to the decision is carefully addressed in the information on which this is based, (ii) the risk assessment information often suffers from incompleteness and lack of clarity with regard to uncertainty about health risk and (iii) lack of general framework integrating uncertainty assessment and comprehensive risk assessment.

The aim of this thesis is:

``the development of computationally efficient alternative methods for uncertainty propagation that are applicable to different environmental risk models, and the development of auxiliary tools that facilitate easy use of these methods."

The primary objective of this thesis is to investigate uncertainty representability and the development of computationally efficient methods for uncertainty propagation. This is addressed from the perspective of (a) computational requirements of the methods, (b) applicability of the methods to a wide range of models, and (c) ease of use of the methods.

The specific objectives of desertation are:

- Propose practical representation methods according to available information regarding model parameters by using possibility, probability and random sets.
- To develop a general framework for environmental risk management propagating uncertainty and variability through risk model.

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- These alternative methods are tested on simplified real cases, with a view to provide useful inputs for the decision-making process.

These objectives are accomplished via the development of the Fuzzy Hypercube Sampling Method (FHSM) to address issue of parametric variability and uncertainty in models and its evaluation for a range of multi-media risk assessment models. Development of new ranking methods using artificial intelligence methods has been studied to facilitate better decision processes. Self-Organizing Maps (SOM) is used to create ranking system (Hazard Index) for a number of different inorganic and organic pollutants. Further an improvement over previous method has been done by incorporating uncertainty in the ranking process and a new ranking method is developed called neuroprobabilistic Hazard Index. Integrated Fuzzy Relation Analysis (IFRA) has been developed as a generic multicriteria decision model incorporating the fuzzy inputs and propagating the uncertainty in risk assessment model. Furthermore, the IFRA is coupled with fuzzy simulation model to develop a general framework for Integrated Environmental Risk Assessment (IERA), in order to further improve the uncertainty management in environmental risk management practice.

1.4 Outline of the Thesis

This thesis has been divided into four sections.

First section of this thesis gives an introduction to to the subject and cover introduction and background knowledge on the subject mater. This section includes two chapters. Chapter 1, which is current chapter provides a general introduction to the problem, objectives of this thesis and it's outline.

Chapter 2 reviews previous studies on uncertainty propagation in environmental models and different methods used for uncertainty modeling. It also gives background information on fuzzy set and related theories. Review of these efforts provides bases for proposing practical modeling tools for uncertainty modeling in environmental models. Particularly, the existing techniques tackling uncertainties in simulation and risk assessment, such as fuzzy-set and stochastic methods, are examined with their advantages and disadvantages being analysed.

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Second section of this thesis deals with uncertainty propagation methods and includes two chapters on it. Chapter 3 provides comparison of stochastic and fuzzy approaches of uncertainty propagation. A new methodology based on generalized fuzzy α-cut principal and concept of transformation method shows superiority over conventional methods of uncertainty modelling. A case study of uncertainty analysis of pollutant transport in ground using 2-D transport model has been used to show the utility of this approach. Results are compared with commonly used probabilistic method and normal Fuzzy alpha-cut technique. The second method proposed to address the issue of combined uncertainty and variability in risk models. A hybrid approach called Fuzzy Latin Hypercube Sampling (FLHS) has been proposed which incorporates cognitive and noncognitive uncertainties present in risk models. The feasibility of the method is validated with a real case study of municipal solid waste incinerator (MSWI), to analyze total variance in the calculation of incremental lifetime risks due to polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/F) for the residents living in the surroundings of MSWI.

Third Section of this thesis consists two chapters dealing with uncertainty management in environmental indices. The fourth chapter is focused on the development of an integral risk map of the chemical/petrochemical industrial area using Self-Organizing Maps (SOM). The first step was the creation of a ranking system (Hazard Index) for a number of different inorganic and organic pollutants applying Self-Organizing Maps (SOM) to persistence, bioaccumulation and toxicity properties of the chemicals. Subsequently, an Integral Risk Index was developed taking into account the Hazard Index and the concentrations of all pollutants in soil samples collected in the target area. Finally, a risk map was elaborated by representing the spatial distribution of the Integral Risk Index with a Geographic Information System (GIS). The results of this study show that the usefulness of soft computing approaches to help in the environmental decision making processes concerning environmental pollutants. The chapter 5 deals with an improvement over previous work described in chapter four. In the previous work SOM weight is used to rank contaminants using their characteristics of persistence, bioaccumulation, and toxicity in order to obtain the Hazard Index (HI). It doesn’t consider uncertainty associated with contaminants characteristic values. So in this study a hybrid method of probabilistic SOM is used to calculate Integrated Risk Index. New approach called Neuro-Probabilistic HI was

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developed by combining SOM and Monte-Carlo analysis. This new index seems to be an adequate tool to be taken into account in risk assessment processes. In both papers, feasibility of the methods has been validated by applying it to the chemical/petrochemical industrial area of Tarragona (Catalonia, Spain).

Finally section four of this thesis deals with decision-making framework for environmental risk management. In chapter 6, a new integrated decision-making framework is proposed. Multi-component environmental risk management in uncertain environment has been addressed. The fuzzy risk-analysis model is proposed to comprehensively evaluate all risks associated with contaminated systems resulting from more than one toxic chemical. In this study, an integrated fuzzy relation analysis (IFRA) model is proposed for risk assessment involving multiple criteria. The model is an integrated view on uncertainty techniques based on multi-valued mappings, fuzzy relations and fuzzy analytical hierarchical process. Integration of system simulation and risk analysis using fuzzy approach allowed incorporating system modelling uncertainty and subjective risk criteria. The model is demonstrated for a multi-components groundwater contamination problem. Results reflect uncertainties presented as fuzzy number for different modelling inputs obtained from fuzzy system simulation. Integrated risk can be calculated at different membership level which is useful for comprehensively evaluating risks within an uncertain system containing many factors with complicated relationship. It has been shown that a broad integration of fuzzy system simulation and fuzzy risk analysis is possible.

Finally, chapter 7 presents conclusions of this research dissertation. Future directions of uncertainty analysis and integrated risk assessment studies and their applications within a general European context are put forward.

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UNIVERSITAT ROVIRA I VIRGILI
SOFT COMPUTING APPROACES TO UNCERTAINTY PROPAGATION IN ENVIRONMENTAL RISK MANGEMENT
Vikas Kumar
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Chapter 2

BACKGROUND

"The very heart of risk assessment is the responsibility to use whatever information is at hand or can be generated to produce an estimate, a range, a probability distribution-whatever best expresses the present state of knowledge about the effects of some hazard in some specific setting. To ignore the uncertainty in any process is almost sure to leave critical parts of the process incompletely examined and hence to increase the probability of generating a risk estimate that is incorrect, incomplete, or misleading" (Council., 1994).

2.1 Environmental Risk Analysis

There are many situations today in which we may need to assess possible risk to human health or damage to the environment. This is an issue for government, industry, those involved in environment protection or management, and others. The concept of risk can be clarified by exploring its essential components. For many risks, including those affecting people, plants, animals, materials and the environment, three conditions must be met before a risk can occur. First, there must be a source of risk (i.e., a hazard). Second, there must be an exposure process in which people, animals, plants or materials may be brought into contact with the hazard. Third, there must be a process in which the exposure produces adverse effects. These effects may result from exposure to contaminated source. It essentially seeks to determine the risk of a contaminant source causing harm or pollution via a given pathway at an identified receptor and whether or not the risk is acceptable (EA, 2001). Lerner et al. (2000) states that a full risk assessment combines the probabilities of (a) possible source term, i.e. types, quantities and frequencies of pollutant inputs, (b) attenuation along the groundwater pathway, with (c) the effects on a receptor. A link between the source→pathway→receptor is known as a "pollutant linkage" but each of these elements can exist independently(El-Ghonemy et al., 2005). However, all three elements of the linkage must be present for a risk to exist. Fig. 2.1 shows a simple source→pathway→receptor where arrows depict different pathways.

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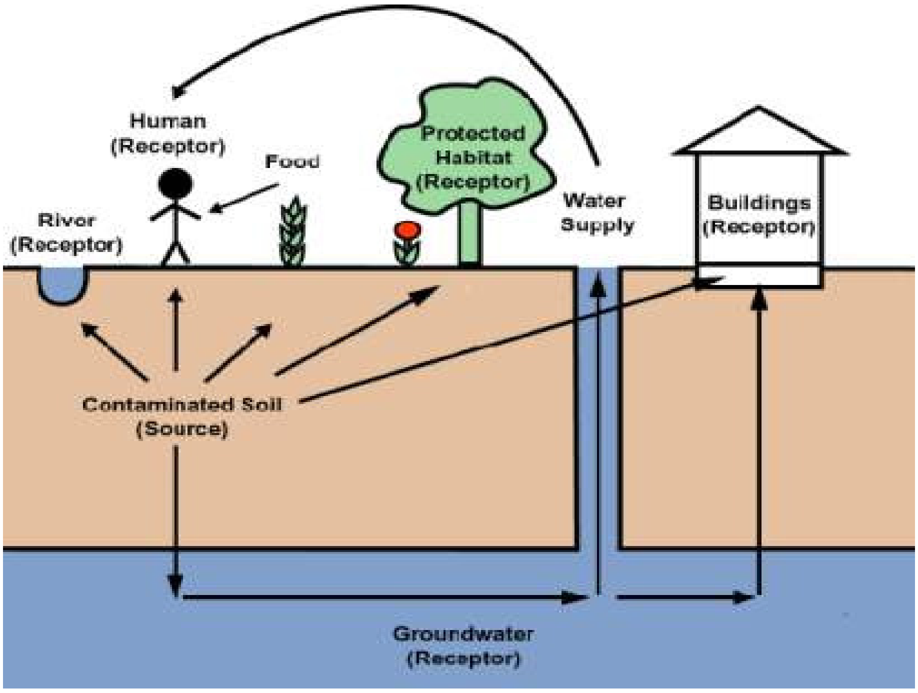

Figure 2.1: Environment Risk Analysis Scenario.

These processes, hazard, exposure, and effect define a risk in the sense that they determine the level and possibility of consequences. Human's perception of risks involves an additional process to evaluate whether the severity, importance, or inequity of the effects is sufficient to be of concern. Therefore, the risk assessment involves considering the likelihood and consequence of an adverse effect. The term 'risk analysis' is employed in its broadest sense to include risk assessment, risk management and risk communication. Risk assessment involves identifying sources of potential harm, assessing the likelihood that harm will occur and the consequences if harm does occur. Risk management evaluates which risks identified in the risk assessment process require management and selects and implements the plans or actions that are required to ensure that those risks are controlled. In other words, risk management is defined as 'the overall process of risk evaluation, risk treatment and decision making to manage potential adverse impacts'. Risk communication involves an interactive dialogue between stakeholders and risk assessors and risk managers which actively informs the other processes. Prerequisite of effective environment risk management is efficient and comprehensive risk analysis and effective communication to stakeholders.

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Essential in risk assessment is the development and use of models for predicting the fate and effect of various environmental pollutants (Nilsen & Aven, 2003). However, various risk assessment models has been developed. Risk Assessment models are frameworks to organize and structure various strands of environment issues. Most frameworks are computer simulation models that describe a specific problem and the cross-linkages and interaction with other problems in specifying cause-effect relationships. This causal description can be done in qualitative sense, through conceptual models, and in a quantitative sense, through different environmental risk models. The latter group is by far the most widely used, and is to reduce the complicated systems into mathematical models. It can be distinguished according to the dominating modelling paradigm in optimization models and system-based simulation models, both deterministic and stochastic.

Risk management involves identifying suitable and practicable measures to ensure that risks remain acceptable. When developing measures against chemical pollution, it is necessary to perform a targeted assessment of the environmental risks that the chemicals may produce on human health or the ecosystem. Environmental risk assessment is performed according to four methods. First, researchers assess whether the chemical compound being assessed causes any damage to humans or living organisms, and if so what kind of harmful effect it has. Second, researchers investigate what degree of effect is caused following exposure to specific amounts of the chemical compound, in order to quantify the strength of the harmful effect. As a chemical compound causes different harmful effects in different species, it is necessary to assess the effect in various organisms. While the most targeted method of assessing the impact on humans would be to analyze actual cases where human health has been damaged, the key objective is to prevent damage to human health before it occurs, so the impact on humans is only assessed after animal experiments. Third, researchers calculate the degree of exposure to the chemical in humans and organisms. The most common method involves estimates based on measurements of environmental concentrations. If the research is to look at preventing damage to human health before any pollution has occurred, researchers assess the degree of exposure using forecasts from mathematical models. Finally, the results of the strength of the harmful effect and the degree of exposure are combined and an environmental risk assessment is made.

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2.2 Uncertainty in Environment Risk Models

Uncertainty is a key issue in Environmental Risk Modelling because of two reasons. First Environment models cover a wide variety of uncertainties that originates from a range of different types and sources. And secondly, because ERA models intend to capture and entire set of cause-effect relations involved in a specific problem, they are prone to accumulate uncertainties. For example health risk assessment studies often consider aggregate exposure and cumulative risk calculation. Accumulated uncertainty in the final result can produce a misleading assessment. Studies in risk analysis have shown that consideration of different source of uncertainty may be crucial for reliable results. Uncertainty and ignorance associated with assessments and predictions on which to base policies make the communication even more difficult (van der Sluijs, 2007). Frey & Zhao, (2004) suggested that the characterization and quantification of uncertainty and variability in health risk assessment are important to prevent erroneous inferences in multimedia modelling and exposure assessment, which may lead to major environmental policy implications. Risk modelling techniques for environmental risk assessment are fairly well established, however, data to support risk assessment is still a major problem often leading to questionable risk assessment results. Selecting appropriate data sources and modelling uncertainty helps to improve risk assessment results and can help to make more informed decisions. Risk assessments need to be able to capture existing data with varying uncertainties for risk analysis(Wilcox, 2001).

Several different classifications of uncertainty have been suggested depending on type and origins of uncertainties(Alefeld, 1983; Haimes, 1998; van Asselt & Rotmans, 2002; Walker et al., 2003). In the next section we will provide a brief discussion on uncertainty classification.

2.2.1 Types and Origins of Uncertainty

A typology of uncertainties would help to differentiate between different types and origins of uncertainty and to communicate uncertainties in a more constructive manner. However there is not one overall typology that satisfactorily covers all sorts of uncertainties, but that there are many typologies that have been proposed in the literature. Van Asselt (2000) after extensive screening of the scholarly literature has proposed a typology based on the highest level of aggregation. This typology distinguishes between

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the following two sources of uncertainty: Variability and Lack of knowledge. Variability is an attribute of reality. Due to variability, reality inhibits inherent uncertainty and unpredictability. Different sources of variability can be distinguished, i.e.: *inherent randomness of nature, value diversity, human behaviour, societal randomness, and technological surprises.* Variability as defined by the above sources goes beyond established seasonality. As such, it contributes to lack of knowledge, because due to variability perfect, certain knowledge is anyhow unattainable. Variability can thus be considered as a source of uncertainty due to lack of knowledge(van Asselt, 2000; van Asselt & Rotmans, 2002).

Lack of knowledge partly results out of variability, but knowledge with regard to deterministic processes can also be incomplete and uncertain. There are different degrees of lack of knowledge. A continuum can be described that ranges from: inexactness, lack of observations/measurements, practically immeasurable, conflicting evidence, ignorance, to indeterminacy. The first three degrees of lack of knowledge (i.e., inexactness, lack of measurements and practically immeasurable) are also referred to as unreliability (Funtowicz & Ravetz, 1990). The latter three degrees of uncertainty are also referred to as structural or systematic uncertainty (Morgan & Henrion, 1990). Anderson & Hattis (1999) have also identified two typologies. They called "lack of knowledge" as "uncertainty" and they defined it as Uncertainty represents partial ignorance or the lack of perfect knowledge on the part of the analyst where as Variability represents diversity or heterogeneity in a population (people or events) that is irreducible by additional measurements. Variability is the heterogeneity between individual members of a population of some type, and is typically characterized through a frequency distribution. It is possible to interpret variability as uncertainty under certain conditions, since both can be addressed in terms of "frequency" distributions(Raul & Pedro, 2005).

However, the implications of the differences in uncertainty and variability are relevant in decision making. For example, the knowledge of the frequency distribution for variability can guide the identification of significant subpopulations which merit more focused study. In contrast, the knowledge of uncertainty can aid in determining areas where additional research or alternative measurement techniques are needed to reduce uncertainty.

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Funtowicz & Ravetz (1990) distinguish three types of uncertainty in system modelling: technical, methodological and epistemological uncertainties. Technical uncertainties arise from the quality of appropriateness of the data used to describe the system, from aggregation (temporal and spatial) and simplification as well as from lack of data and approximation. Methodological uncertainties arise from lack of knowledge and refer to questions as: what analytical tools and methods are appropriate? How to model causal relationships in view of incomplete understanding of the processes? What is and adequate frame to structure what we know and what is uncertain? How to interpret the uncertainties? And finally epistemological uncertainties concern the conception of a phenomenon. This type of uncertainty arises from structural uncertainty and variability.

One useful taxonomy for uncertainty based on (Clark & Brinkley, 2001) distinguishes at least five types of uncertainty that can be applied to environmental risk analysis. These include: epistemic, descriptive, cognitive, entropic and Intrinsic. Epistemic uncertainty originates from limited knowledge, its acquisition and validation. Examples of epistemic uncertainty include limited sample size, measurement error (systematic or random), sampling error, ambiguous or contested data, unreliable data, use of surrogate data (e.g. extrapolation from animal models to humans), ignorance of ignorance that gives rise to unexpected findings or surprise. Environmental Risk assessment is evidence-based assessment, primarily using information that is derived from scientific research. Consequently, epistemic uncertainty is a major component of uncertainty in risk assessments (Clark & Brinkley, 2001). The principal forms of descriptive uncertainty include vagueness, ambiguity, under specificity, contextual and undecidability. Qualitative risk assessments can be particularly susceptible to linguistic uncertainty. For example the word 'low' may be ambiguously applied to likelihood of harm, magnitude of a harmful outcome and to the overall estimate of risk. Furthermore, the word 'low' may be poorly defined both in meaning (vagueness) and coverage (underspecificity). Cognitive uncertainty can take several forms, including bias, variability in risk perception, uncertainty due to limitations of our senses (contributing to measurement error) and as unreliability. Cognitive unreliability can be viewed as guesswork, speculation, wishful thinking, arbitrariness, debate, or changeability (Kahneman, 2003).

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Entropic uncertainty is associated with the complex nature of dynamic systems that exist far from thermodynamic equilibrium (Nicolis & Prigogine, 1989), such as a cell, an organism, the ecosystem, an organisation or physical systems (e.g. the weather). Complexity is typically coupled to incomplete knowledge (epistemic uncertainty) where there is an inability to establish the complete causal pathway. Therefore, additional knowledge of the system can reduce the degree of uncertainty. However, complex systems are characterised by non-linear dynamics that may display sensitive dependence on initial conditions. Consequently, a deterministic system can have unpredictable outcomes because the initial conditions cannot be perfectly specified. Complexity is listed as one of the four central challenges in formulating the European Union (EU) approach to precautionary risk regulation (Renn et al., 2003).

Intrinsic uncertainty is due to the inherent randomness, variability or indeterminacy of a thing, quality or process. Randomness can arise from spatial variation, temporal fluctuations, manufacturing variation, genetic difference. Variability arises from the observed or predicted variation of responses to an identical stimulus among the individual targets within a relevant population such as humans, animals, plants, micro-organisms, landscapes, etc. Indeterminacy results "from a genuine stochastic relationship between cause and effect(s), apparently noncausal or noncyclical random events, or badly understood nonlinear, chaotic relationships" (Klinke & Renn, 2002). A critical feature of intrinsic uncertainty is that it cannot be reduced by more effort such as more data or more accurate data. In risk management, safety factors and other protective measures are used to cover this type of uncertainty.

All five types of uncertainty may be encountered in a risk analysis context. To encompass this broader application, uncertainty can be defined as ‘imperfect ability to assign a character state to a thing or process; a form or source of doubt’.

Where: ‘imperfect’ refers to qualities such as incomplete, inaccurate, imprecise, inexact, insufficient, error, vague, ambiguous, under-specified, changeable, contradictory or inconsistent; ‘ability’ refers to capacities such as knowledge, description or understanding; ‘assign’ refers to attributes such as truthfulness or correctness; ‘character state’ may include properties such as time, number, occurrences, dimensions, scale, location, magnitude,

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quality, nature, or causality; ‘thing’ may include a person, object, property or system; and ‘process’ may include operations such as assessment, calculation, estimation, evaluation, judgement, or decision.

For practical point of view, in this thesis, uncertainty have been categorised into two broad classes: parametric uncertainty and model uncertainty. Parametric uncertainty covers all kind of uncertainties associated with model input parameters where as uncertainty associated with model choice comes under model uncertainty. Mathematical models are necessarily simplified representations of the phenomena being studied and a key aspect of the modelling process is the judicious choice of model assumptions. The optimal mechanistic model will provide the greatest simplifications while providing an adequately accurate representation of the processes affecting the phenomena of interest. Hence, the structure of mathematical models employed to represent natural systems is often a key source of uncertainty. In addition to the significant approximations often inherent in modelling, sometimes competing models may be available. Furthermore, the limited spatial or temporal resolution (e.g., numerical grid cell size) of many models is also a type of approximation that introduces uncertainty into model results. Sources of model uncertainties in environmental models can be from model structure, model details, spatial and temporal resolution and boundaries conditions (Isukapalli, 1999).

The parametric uncertainty has been classified on the basis of its source and nature. Sources of parameter uncertainty are measurement errors, sampling errors, variability, and the use of surrogate data (Moschandreas & Karuchit, 2005). Measurement errors refer to random (imprecision) or systematic errors (bias), while sampling errors are errors from small sample size and/or misrepresentative samples. Heterogeneity in environmental and exposure-related data includes seasonal variation, spatial variation, and variation of human activity patterns by age, gender, and geographic location, leading to variability errors. Surrogate data refer to errors from the use of substitute data. Van Asselt and Rotmans (2002) and Walker et al. (2003) classified uncertainty based on its nature. They called it *Epistemic uncertainty/imprecision*, and *Stochastic uncertainty/natural variability*. Epistemic uncertainty which results from incomplete knowledge about the system under study, is reducible by additional studies (e.g. further research and data collection). Stochastic uncertainty which stems from variability of the underlying stochastic process is

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non-reducible for a given system and under specific management scenario. Natural variability has also been termed (basic) variability, randomly uncertainty, objective uncertainty, inherent variability, (basic) randomness, and type-I uncertainty. Terms for epistemic uncertainty are systematic uncertainty, subjective uncertainty, lack-of-knowledge or limited-knowledge uncertainty, ignorance, specification error, prediction error, and type-II uncertainty (Haimes, 1998; Merz & Thieken, 2005; Moschandreas & Karuchit, 2005; Refsgaard et al., 2007; Rotmans & van Asselt, 2001; van Asselt & Rotmans, 2002). In this paper, the term uncertainty is used to denote epistemic, variability to denote stochastic uncertainty, and total variance or simply variance to denote total uncertainty and variability in the outcome.

2.3 Approaches for Representation of Uncertainty

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 including environmental modelling.

Analytical models can be used for problems that have been described by noted mathematician Warren Weaver as “organized simplicity”; statistical models are useful for problems of disorganized complexity(Shannon & Weaver, 1949). 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 & Yuan, 1995). Later various approaches for representing uncertainty have been developed (Isukapalli, 1999; Schulz & Huwe, 1999). Klir (1994) has presented a nice overview of uncertainty representation in the context of different domains of applicability. Among them, probabilistic approaches (e.g. Monte Carlo Simulation) are quite common and have been commonly used in the treatment and processing of uncertainty for solution of system modeling (Schuhmacher et al., 2001). When it was recognized that probability theory is capable of representing only one of the several distinct types of uncertainty, new theories for treating uncertainty emerged. One of the milestones in the evolution of these new

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uncertainty theories is the seminal paper by Lofti A. Zadeh (1965). He proposed a new mathematical tool in his paper and called this new mathematical tool "fuzzy sets." He proposed the concept of fuzzy algorithms in 1968 (Zadeh, 1968), and together with Bellman, proposed a new approach for decision-making in fuzzy environments in 1970 (Bellman & Zadeh, 1970). Fuzzy set theory has been recently applied in various fields including environmental modelling for uncertainty quantification (Cho et al., 2002; Hanss, 2002; Isukapalli, 1999; Kentel & Aral, 2004; Kumar, 2005; Mauris et al., 2001).

Some of the widely used uncertainty representation approaches used in environmental modelling includes probabilistic analysis, interval mathematics, fuzzy set theory. These approaches are presented in the following sections.

2.3.1 Probabilistic Analysis

Probabilistic analysis is the most widely used method for characterizing uncertainty in physical systems, especially when estimates of the probability distributions of uncertain parameters are available. This approach can describe uncertainty arising from stochastic disturbances, variability conditions, and risk considerations. Uncertainty is characterised by the probability associated with events. The probability of an event can be interpreted in terms of frequency of occurrence which can be defined as the ratio of the number of favourable events to the total number of events. In this approach, the uncertainties associated with model inputs are described by probability distributions, and the objective is to estimate the output probability distributions.

There are a number of text books that describe the concepts and application of probabilistic analysis in detail. Feller (1950) presents excellent introductory material for probabilistic analysis, and Papoulis (1991) presents an excellent description on probability and random variables from a mathematical view point. Additionally Gardiner (1983) presents the applications of probabilistic analysis in modelling. This section attempts to merely summarize some basic information on probability and its use in environmental modelling.

Hamed (1999) analyzed the probabilistic sensitivity of public health risk assessment from contaminated soil. Moore et al. (1999) conducted a probabilistic risk assessment of the effects of methylmercury and Polychlorinated Biphenyls (PCBs) on mink and

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kingfishers along East Fork Popular Creek, Oak Ridge, Tennessee, USA. Lahkim & Garcia (1999) conducted stochastic modelling of exposure and risk in a contaminated heterogeneous aquifer based on Monte Carlo uncertainty analysis. Loll & Moldrup (2000) carried out stochastic analyses for field-scale pesticide leaching risk due to the influence by spatial variability in physical and biochemical parameters. Hope (2000) undertook an ecological risk assessment through the generation of probabilistic spatially-explicit individual and population exposure estimates. Bonomo et al. (2000) estimated the target cleanup levels for the site of a former gas plant in northern Italy and compared the results from deterministic and probabilistic methods. In their study, probabilistic methods were used to provide fundamental information to define the cleanup strategies. Schuhmacher et al. (2001) used Monte-Carlo simulation techniques in the risk assessment study of municipal waste incinerator. Ma (2002) has used stochastic modelling for multimedia risk assessment for a site with contaminated groundwater. Lester et al. (2007) and Ma (2002) have a good review on site-specific applications of Probabilistic Health Risk Assessment.

Classically all sort of uncertainty have been modelled through simple probabilistic approaches (e.g. Monte Carlo analysis). However recently second order Monte Carlo or 2D Monte Carlo has been used to separate variability and epistemic uncertainty (Simon, 1999). This technique requires knowledge of parameter values and their statistical distribution from which a formal mathematical description of uncertainty must be developed. However, site investigation is generally not detailed enough to determine values for some of the parameters and their distribution pattern, and sufficient data may not be collected for calibrating a model (Kentel & Aral, 2005). These approaches suffer from an obvious lack of precision and specific site-characterization, making difficult to determine how much error is introduced into the result due to assumptions and prediction.

2.3.2 Interval Analysis

Representing possible value in interval is empirical way of representing uncertainty in measured values(Moore, 1979). Interval mathematics is used to address data uncertainty that arises (a) due to imprecise measurements, and (b) due to the existence of several alternative methods, techniques, or theories to estimate model parameters. Interval analysis can be used to propagate these uncertain values through calculations. The rules of interval arithmetic permit us to compute rigorous bounds on all the elementary mathematical

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operations(Moore, 1979). For example interval analysis may be used to represent interval estimates of likelihood and impact resulting in an overall interval estimate if risk using the product rule for interval numbers. The basics of interval mathematics are fairly obvious, although still it is an active area of research in computer science because of its profound implications for handling round-off error (Alefeld, 1983). Even in uncertainty analysis, in many cases, it may not be possible to obtain the probabilities of different values of imprecision in data; in some cases only error bounds can be obtained. This is especially true in case of conflicting theories for the estimation of model parameters, in the sense that "probabilities" cannot be assigned to the validity of one theory over another. In such cases, interval mathematics can be used for uncertainty estimation, as this method does not require information about the type of uncertainty in the parameters (Alefeld, 1983; Broadwater, 1994). Although it's vastly simpler than probabilistic analysis, it can be a little trickier to use in complex modelling scenarios(Moore, 1979).

2.3.3 Fuzzy Set Theory

Fuzzy set theory replaces the two-valued set-membership function with a real-valued function; that is to say, membership is treated as a possibility or as a degree of truthfulness. Likewise, one assigns a real value to assertions as an indication of their degree of truthfulness. Membership functions define the degree of participation of an observable element in the set. Fuzzy numbers are the fuzzy set defined on the set of real numbers and have special significance. They represent the intuitive concept of *approximate numbers,* such as *"around, close to, approximately etc"*. The fuzzy set that contains all fuzzy numbers with a membership of $\alpha \in [0,1]$ and above is called the *a-cut* of the membership function (Abebe et al., 2000) (Figure. 2.2). So the *α-cut* represents the degree of sensitivity of the system to the behavior under observation. Fuzzy α-cut technique is based on the extension principle (Zadeh, 1965), which implies that functional relationships can be extended to involve fuzzy arguments. It can be used to map the dependent variable as a fuzzy set. In simple arithmetic operations, this principle can be analytically used. However, in most practical modeling applications involving complex structural relationships (e.g. partial differential equations), analytical applications of the extension principle is difficult. Therefore, interval arithmetic can be used to carry out the analysis (Abebe et al., 2000).

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Arithmetic on fuzzy numbers can be defined in terms of arithmetic operations on their α-cuts (on closed intervals).

This principle is generalized as: a membership level $\mu_{P_i}(x) = [0,1]$ is assigned to all elements x (i.e. the elements belong to the set to a certain degree) (Hanss, 2002; Klir & Yuan, 1995). A Gausian fuzzy number, subdivided into intervals is depicted in Figure 2.2. The core of the set is defined as the subset for which $\mu_{\tilde{p}} = 1$. The support is the subset for which $\mu_{\tilde{p}} > 0$ (also known as the input vertex). The α-cut is a generalized support: the subset for which $\mu_{\tilde{p}} \geq \alpha$, with $0 < \alpha \leq 1$. The α-sublevel technique (Hanss, 2002) consists of subdividing the membership range of a fuzzy number into α-sublevels at membership levels $\mu_j = j/m$, for $j = 0, 1, \ldots m$ (Figure 2.2). This allows numerically representing the fuzzy number by a set of $m + 1$ interval $[a_j, b_j]$.

In fuzzy simulation, for each α-level of the parameter, the model is run to determine the minimum and maximum possible values of the output. This information is then directly used to construct the corresponding membership function of the output which is used as a measure of uncertainty.

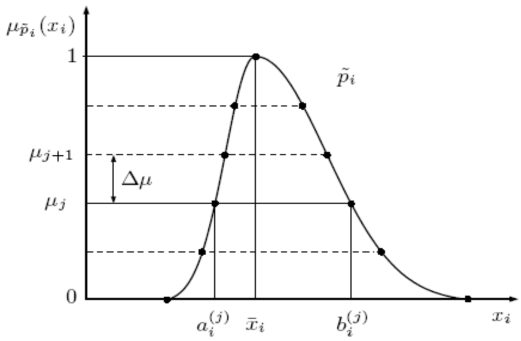

Figure 2.2: Implementation of the i^{th} uncertain parameter as a fuzzy number $\tilde{p}_i$ decomposed into intervals (α-cuts).

There have been considerably less studies using fuzzy theory approach in environmental applications in past. However lately various applications of fuzzy theory have been reported. (Dahab et al., 1994) proposed a rule-based fuzzy-set approach to risk analysis of nitrate-contaminated groundwater by introducing fuzzy sets into a rule-based system for nitrate risk-regulation enforcement. Lee et al. (1995) developed a fuzzy-set

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approach to assess nitrate risk for groundwater contamination. This method can be used when a frequency-based estimation is not available; then fuzzy-set analysis is used to reflect the uncertainty associated risk model processes. Ganoulis et al. (1995) proposed a fuzzy arithmetic for ecological risk management. The methodology consists of fuzzy logic-based calculus combined with ecological modeling. The output variables of the model, such as pollutant concentrations, dissolved oxygen, and biomass were calculated directly as fuzzy numbers. Krause et al. (1997) integrated fuzzy logic into the Zwich Hazard analysis method, which is a logic tool to catalogue hazards and to represent corresponding risks by classifications of frequency and consequence of an undesired event in a risk matrix format. Donald & Ross (1996) presented a similarity measure approach based on fuzzy sets and fuzzy logic for the risk management of hazardous waste sites. In this approach, the so-called similarity measure was given between two fuzzy sets and their corresponding membership functions. Ghomshei & Meech (2000) introduced some thoughts on fuzzy sets and demonstrated the application of fuzzy logic in environmental risk assessment. Abebe et al. (2000) have presented a nice comparison of fuzzy and Monte Carlo analysis in groundwater modelling. More recently Li et al. (2006) presented an integrated fuzzy-set approach for evaluating environmental risks associated with hydrocarbon-contaminated sites through incorporation of a multiphase multi-component modeling system within a general risk assessment framework.

2.3.4 Hybrid Approaches

From a practical viewpoint, it is rare to encounter only one type of uncertainty. Pure variability would mean that all relations and their parameters which describe the random process are exactly known. Pure epistemic uncertainty would mean that a deterministic process is considered, but the relevant information cannot be obtained (e.g. due to the inability to measure the relevant parameters) (Merz & Thieken, 2005). For example, given a parameter X with total variance V_x, it would be straightforward to partition the variance into uncertainty and variability components, where α is the uncertainty component and (1-α) attributable to variability (Figure2.3). Notwithstanding, there also can be an intermediate vague region in which uncertainty and variability commingle. So sometime it is difficult to separate and in that case it needs special handling to measure both uncertainty and variability together.

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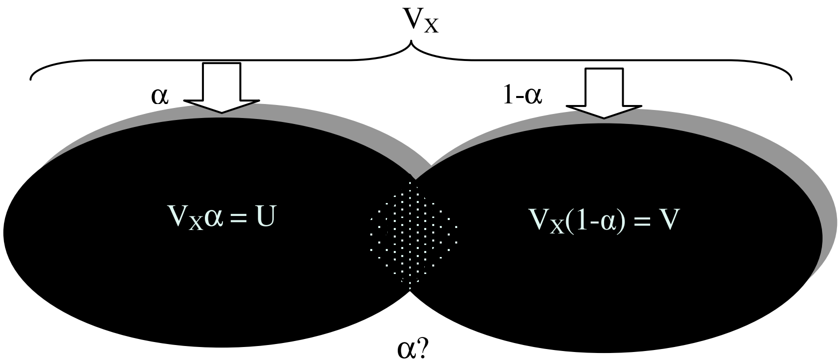

Figure 2.3: Separating uncertainty and variability

Several approaches to uncertainty analysis in environmental risk analysis have been developed. However, all these methods have been developed to handle either variability or uncertainty of the process parameters or they club them together without valid distinction in analysis. Today's challenge is utilization of different approaches in combination to exploit their respective features. Despite the obvious distinction among different type of uncertainty and need of different treatment, it has not been commonly practices(Spencer et al., 2001). Mathematicians in statistics and probability claimed that probability is sufficient to characterize uncertainty and any problem that fuzzy theory can solve can be solved equally well or better by probability theory. Numerous studies on the discussion of probability versus possibility (fuzziness) are provided in the special issue of the IEEE Transactions on Fuzzy Systems (Vol. 2, No. 2, 1994) and in some other publication. Comparisons of probability theory with fuzzy theory, what kind of uncertainties they treat, general definitions of probability theory, and fuzzy set theory concepts in the context of uncertainty modelling are provided in many references(Dubois & Prade, 1993; Klir, 1995; Zadeh, 1995). Lately scientists have started accepting that fuzzy set theory and probability theory are complementary, and they deal with different types of uncertainties" (Spencer et al., 2001). Fundamental procedures to allow combined utilization of fuzzy set theory and probability theory to treat uncertainties have been proposed and developed since the emergence of fuzzy set theory. The concept Fuzzy Probability was introduced by Zadeh (Zadeh, 1984). Recently, a number of authors have suggested adopting other approaches in the data limited situation. Refsgaard et al. (2007) reported: 'The test theory of classical statistics permits the testing of a sample for randomness. If the sample does not exhibit the property of randomness, other uncertainty models such as, e.g. fuzzy randomness must be adopted'. Previously, Möller et al. (2002) presented the idea of Fuzzy Randomness and formalized the concept of random variable and uncertain variable. According to Möller et al. (2002), Objective uncertainty in the form of observed/measured data is modeled as randomness, whereas subjective uncertainty (e.g., due to a lack of trustworthiness or imprecision of measurement results, of distribution parameters, of environmental conditions, or of the data sources), is described as fuzziness. Fuzzy randomness or fuzzy probability simultaneously describes objective and subjective information as a fuzzy set of possible probabilistic models over some range of imprecision (Möller et al., 2002). This hybrid model combines, but not mixes objectivity and subjectivity, which are separately visible at any time. It may be understood as an imprecise probabilistic model, which allows for simultaneously considering all possible probability models that are relevant to describing the problem (Möller et al., 2002). Few recent efforts have been made to use "hybrid models" in environmental applications. Kentel & Aral (2005) introduced 2D Fuzzy Monte Carlo and applied it in the area of health risk assessment. 2D Fuzzy Monte Carlo and Fuzzy Randomness have been classified as hybrid approach mixing the concept of probability and fuzzy set theory. Li et al. (2007) have presented an integrated fuzzy-stochastic modelling approach for risk assessment of groundwater.

There are other approaches for uncertainty representation has also been mentioned in literature like classical set theory, rough set theory, many version of fuzzy set theory (e.g. possibility theory, type 2 fuzzy set etc). Uncertainty is expressed by sets of mutually exclusive alternatives in situations where one alternative is desired. This includes *diagnostic, predictive* and *retrodictive* uncertainties (Kitts, 1978). Here, the uncertainty arises from the nonspecificity inherent in each set. Large sets result in less specific predictions, retrodictions, etc., than smaller sets. Full specificity is obtained only when one alternative is possible. *Rough set theory is* proposed by Pawlak (1991). A rough set is an imprecise representation of a *crisp* set in terms of two subsets, a *lower approximation* and *upper approximation*. Further, the approximations could themselves be imprecise or fuzzy. However these approaches are not very common in environmental application.

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2.4 Uncertainty in Risk Assessment: Trends and Future Hopes

There is an increasing demand in society for knowledge of risks and risk issues, including reactions to risks and how to communicate risk. Concerns within the field include theoretical and empirical research and practical applications across a wide range of areas. A rather fascinating feature of the heterogeneous field of risk communication is that is excludes no one. Today it is commonly accepted that risk management should be more holistic activity involving a better uncertainty propagation approach (Oxley and others 2004; Kumar and Schuhmacher, 2005; Refsgaard, Van der Sluijs et al. 2007). The uncertainty assessment is not just something to be added after the completion of the modelling work. Instead uncertainty should be seen as a red thread throughout the modelling study starting from the very beginning, where the identification and characterisation of all uncertainty sources should be performed (Refsgaard, Van der Sluijs et al. 2007).

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Chapter 3

FUZZY SIMULATION MODELING AND UNCERTAINTY ANALYSIS FOR ENVIRONMENTAL RISK ASSESSMENT USING TRANSFORMATION METHOD

Abstract

With the changing world, there is a great change in risk perception. The present trend from heavy point-source pollution to reduced and scattered contaminant release makes environmental risk analysis a difficult task. With the current environmental legislation, concentration of pollutant has been reduced, pollutant specific signals are difficult to extract but tentacles of dragon has spread many fold which multiplying the overall contamination risk. Old simulation techniques and approaches are no more/less useful and its becoming difficult to impossible to predict environmental risk with old assumption. In this paper, the transformation method has been used for simulation and analysis of environmental system. Transformation method is a special implementation of fuzzy arithmetic based on α-cut principle that avoids the well-known effect of overestimation which usually arise from use of interval computation for fuzzy arithmetic. It has been extended to do sensitivity analysis of uncertain model parameters. This method has been applied to two unsaturated flow problems, one-dimensional solute transport equation for horizontal water and contaminant flow; and two-dimensional equation for unsaturated flow over a complex geometry. Where possible, the results from the transformation method have been compared against other popular methods to determine the accuracy of the method.

Keywords: *Environmental risk, transformation method, transport model, uncertainty analysis, fuzzy α-cut.*

3.1 Introduction

Mechanistic modelling of physical systems is often complicated due to the presence of uncertainties. Commonly environmental models are calibrated to field data to

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demonstrate their ability to reproduce contaminant behaviour at site. However, solute transport modelling presents a big uncertainty due to the lack of reliable field data. On the other hand, specific field situations cannot be extrapolated over larger distances, even in the same site (Sauty, 1980).

Fuzzy set is a mathematical theory for the representation of uncertainty (Zadeh, 1968, 1988). Given a degree of uncertainty in the parameters, fuzzy set theory makes possible to evaluate the uncertainty in the results thereby avoiding the difficulties associated with stochastic analysis, since this method does not require knowledge of probability distribution functions.

Fuzzy set approach has been applied recently in various fields, including decision making, control and modelling (Abebe et al., 2000). However, the application of standard fuzzy arithmetic turns out to be very problematic. Normally, the calculated results of the problem do not only reflect the natural uncertainties, which are directly induced by the uncertainties in the model parameters, they also show some additional, artificial uncertainties generated by the solution procedure itself (Hanss, 2002).

The fuzzy α-cut analysis is based on fuzzy logic and fuzzy set theory which is widely used in representing uncertain knowledge. Uncertain model parameters can be treated as fuzzy numbers that can be manipulated by specially designed operators. But this approach has also been treating independent and strictly dependent variable together. It results in overestimation effect arises from evaluating the arithmetical expression for unreal combination of elements of support of the fuzzy numbers (Hanss & Willner, 1999).

In this paper, fuzzy transformation method has been studied for the practical use in environmental risk analysis. Transformation method is special implementation of fuzzy arithmetic based on α-cut principle that avoids the well-known effect of overestimation which usually arises from use of interval computation for fuzzy arithmetic. The methodology has been applied to two unsaturated flow problems, one-dimensional Richards' equation and solute transport equation for horizontal water and contaminant flow; and two-dimensional Richard's equation for unsaturated flow over a complex geometry. The results will be compared with the results obtained with analytical method of

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Fuzzy α-cut and Monte-Carlo simulation. In the end, some conclusions are drawn and recommendations are made for future research.

3.2 Fuzzy Set Theory

3.2.1 Fuzzy Sets and Numbers

Fuzzy set theory replaces the two-valued set-membership function with a real-valued function, that is, membership is treated as a probability, or as a degree of truthfulness. Likewise one assigns a real value to assertions as an indication of their degree of truthfulness. This principle is generalised as(Hanss & Willner, 1999; Koivo, 2001): a membership level $\mu_A(x) \in [0, 1]$ is assigned to all elements x, i.e. the elements belong to the set to a certain degree. The core of the set is defined as the subset for which $\mu_A = 1$. The support is the subset for which $\mu_A > 0$ (also known as the input vertex). The α-cut is a generalised support: the subset for which $\mu_A \geq \alpha$, with $0 < \alpha \leq 1$. A fuzzy number is a fuzzy set with some specific properties(Koivo, 2001): the set is convex and normal, the membership function is piecewise continuous and the core consists of a single element. A fuzzy number's membership function can be of arbitrary shape, either derived from (limited) experimental data or expert knowledge of the model parameters. Figure 3.1 shows two well-established types: a membership function with a Gaussian and a triangular shape. The triangular shape is widely used for reasons of simplicity: when the exact parameter distribution is not known, it doesn't make sense to assign a more complex-shaped function. The membership functions are possibilistic distribution functions that denote if an input is possible ($\mu_A = 1$), impossible ($\mu_A = 0$) or something in between. The α-sublevel technique (Hanss & Willner, 1999) consists of subdividing the membership range of a fuzzy number into α-sublevels at membership levels $\mu_j = j/m$, for $j = 0, 1, ...m$. This allows to numerically represent the fuzzy number by a set of $m + 1$ intervals $[a^{(j)}, b^{(j)}]$. Figure 3.2 shows a triangular fuzzy number, subdivided into intervals using m = 5.

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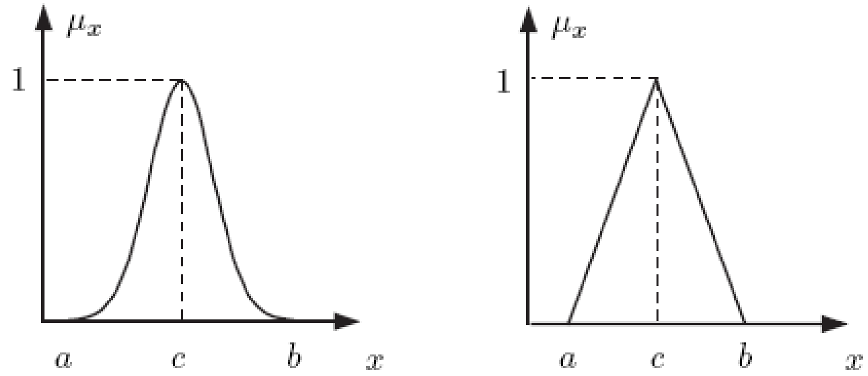

Figure 3.1: Fuzzy numbers with Gaussian (left) and triangular (right) membership function

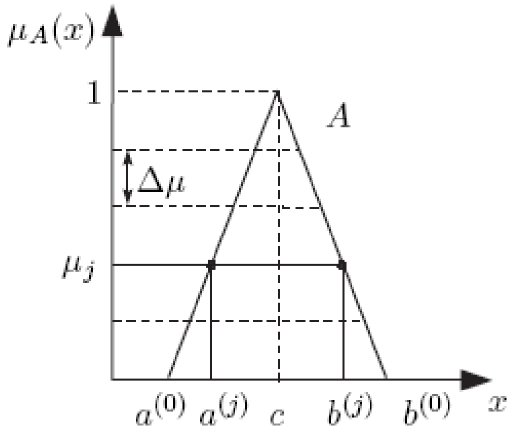

Figure 3.2: The α-cut technique to numerically represent a fuzzy number

3.2.2 **Fuzzy Alpha-Cut (FAC) technique**

An alpha cut is the degree of sensitivity of the system to the behaviour under observation. At some point, as the information value diminishes, one no longer want to be "bothered" by the data. In many systems, due to the inherent limitations of the mechanisms of observation, the information becomes suspect below a certain level of reliability.

Fuzzy alpha-cut technique is based on the extension principle, which implies that functional relationships can be extended to involve fuzzy arguments and can be used to map the dependent variable as a fuzzy set. In simple arithmetic operations, this principle can be used analytically. However, in most practical modeling applications, relationships involve complex structures (e.g. partial differential equations) that make analytical

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application of the principle difficult. Therefore, interval arithmetic can be used to carry out the analysis (Abebe et al., 2000).

Membership functions define the degree of participation of an observable element in the set, not the desirability or the value of the information. The membership function is cut horizontally at a finite number of α-levels between 0 and 1. For each α-level of the parameter, the model is run to determine the minimum and maximum possible values of the output. This information is then directly used to construct the corresponding membership function of the output which is used as a measure of uncertainty. If the output is monotonic with respect to the dependent fuzzy variable/s, the process is rather simple since only two simulations will be enough for each α-level (one for each boundary). Otherwise, optimization routines have to be carried out to determine the minimum and maximum values of the output for each α-level.

3.2.3 **Transformation Method (TM)**

The TM presented by Hanss, (2002) uses a fuzzy alpha-cut approach based on interval arithmetic. The uncertain response reconstructed from a set of deterministic responses, combining the extrema of each interval in every possible way unlike the FAC technique where only a particular level of membership (α-level) values for uncertain parameters are used for simulation. The reduced TM used in the present study will be next explained.

Given an arithmetic function f that depends on n uncertain parameters *x1, x2, ..., xn*, represented as fuzzy numbers, the function output $q = f(x1, x2, ..., xn)$ is also a fuzzy number. Using the α-level technique, each input parameter is decomposed into a set P_i of $m + 1$ intervals $X_i^{(j)}$, $j = 0, 1, ..., m$ where

$$P_i = \{X_i^{(0)}, X_i^{(1)}, ..., X_i^{(m)}\} \tag{1}$$

with $X_i^{(j)} = \left[a_i^{(j)}, b_i^{(j)}\right]$, $a_i^{(j)} \le b_i^{(j)}$, $i = 1,2,...,n,$ $j = 0,1,2,...,m.$ (2)

where $a_i^{(j)}$ and $b_i^{(j)}$ denote the lower and upper bound of the interval at the membership level μ_j .

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Instead of applying interval arithmetic like FAC method, intervals are now transformed into arrays $\hat{X}_i^{(j)}$ of the following form:

$$\hat{X}_i^{(j)} = \left(\overbrace{\alpha_i^{(j)}, \beta_i^{(j)}, \alpha_i^{(j)}, \beta_i^{(j)}, ..., \alpha_i^{(j)}, \beta_i^{(j)}}^{2^{i-1}\, pairs} \right) \tag{4}$$

with $\alpha_i^{(j)} = \left(\overbrace{a_i^{(j)}, ..., a_i^{(j)}}^{2^{i-1}\, pairs} \right), \qquad \beta_i^{(j)} = \left(\overbrace{b_i^{(j)}, ..., b_i^{(j)}}^{2^{i-1}\, pairs} \right) \qquad (5)$

The evaluation of function f is now carried out by evaluating the expression separately at each of the positions of the arrays using the conventional arithmetic. The result obtained is deterministic in decomposed and transformed form which can be retransformed to get fuzzy valued result using recursive approximation.

3.3 Fuzzy Modeling of environmental problems

3.3.1 **Fuzzy Modeling**

Basic principal of fuzzy modeling is based on Zadeh's extension principle (Zadeh, 1968). If all input parameters in a mathematical model are known, also the dependent variables are defined with crisp values and if we assume that the input parameters are imprecise and represented by fuzzy numbers, the resulting outputs of the model will also be fuzzy numbers characterised by their membership functions.

3.3.1.1 Simulation using Transformation method

Consider fuzzy numbers $\tilde{A}_1, \tilde{A}_2, ..., \tilde{A}n$ are the set of n input parameters defined on the real line *R* and suppose x_i, where $i = 1,2,\ldots,n$ denotes the element of $\tilde{A}_i$. Now if y is the output of the system which depends on n inputs $x_1, x_2, ..., x_n$ by the mapping $y = f(x_1, x_2, ..., x_n)$, the n input parameters are modelled as fuzzy numbers with a membership function $\mu_A(x)$ of arbitrary shape. Then the solution to the fuzzy number $\tilde{B}$ in y can be obtained by the following steps using transformation method.

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1. Using the α-sublevel technique, discretise the range of membership [0,1] into a finite number of values. So an input parameter $\tilde{A}_i$ can be decomposed into a set of m+1 intervals $X_i^{(j)}$, $j = 0,1,...m$. The value of discretisation term, m depends on the degree of accuracy needed in approximation.
2. For each membership level *j*, find the corresponding intervals for $\tilde{A}$ in $x_i, i = 1, 2, \ldots, n$. These are the supports of the α_j-cuts of $\tilde{A}_1, \tilde{A}_2, ..., \tilde{A}_N$. So if $\left[a_i^{(j)}, b_i^{(j)}\right]$ is the end points interval of i^{th} input parameter and for j^{th} level of membership denoted by $X_i^{(j)}$ then set $\tilde{A}_i = \{X_i^{(0)}, X_i^{(1)}, ..., X_i^{(m)}\}$. When a_i is equal to b_i, the interval reduce to a point i.e. at α-level 1.

Now instead of applying standard interval arithmetic to the interval $X_i^{(j)}$, they are transformed into arrays using a kind of full factorial at each level. That what makes it Transformation method. Hanss (2002) has proposed two form of transformation methods, one general transformation method and other reduced transformation method. These two methods differ in degree of discretization of particular interval. In this study reduced transformation has been used.

Reduced Transformation method

3. The intervals are transformed into arrays $\hat{X}_i^{(j)}$ of the following forms:

$$\hat{X}_i^{(j)} = \underbrace{\left(\alpha_i^{(j)}, \beta_i^{(j)}, \alpha_i^{(j)}, \beta_i^{(j)}, ..., \alpha_i^{(j)}, \beta_i^{(j)}\right)}_{2^{i-1}\, pairs} \tag{6}$$

with

$$\alpha_i^{(j)} = \underbrace{\left(a_i^{(j)}, ... a_i^{(j)}\right)}_{2^{n-1}\, elements} \;,\; \beta_i^{(j)} = \underbrace{\left(b_i^{(j)}, ... b_i^{(j)}\right)}_{2^{n-1}\, elements} \tag{7}$$

where $a_i^{(j)}$ and $b_i^{(j)}$ denote the lower and upper bound of the interval at the membership level μ_j for the i^{th} uncertain parameter. For each interval level, these arrays combine the interval extrema $a_i^{(j)}$ and $b_i^{(j)}$ in every possible way.

4. Simulation is carried out by evaluating the expression separately at each of the positions of the arrays using the conventional arithmetic for crisp numbers. Thus, if the output $\tilde{B}$ of the system can be expressed in its decomposed and transformed

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form by the arrays $\hat{B}_i^{(j)}$, $j = 0,1,\ldots,m$ the kth element ${}^k b_i^{(j)}$ of the array $\hat{B}_i^{(j)}$ is then given by

$$ {}^k b_i^{(j)} = f\left({}^k \hat{x}_1^{(j)}, {}^k \hat{x}_2^{(j)}, \ldots, {}^k \hat{x}_n^{(j)}\right) \tag{8} $$

where ${}^k \hat{x}_1^{(j)}$ denotes the kth element of the array $\hat{X}_i^{(j)}$.

5. Finally, the fuzzy-valued result $\tilde{B}$ of the problem can be achieved in its decomposed form

$$ \tilde{B}^{(j)} = \left[a^{(j)}, b^{(j)}\right], \quad j = 0,1,\ldots,m \tag{9} $$

by retransforming the arrays $\hat{B}_i^{(j)}$ using recursive formulae

$$ a^{(j)} = \min_k\left(b^{(j+1)}, {}^k \hat{b}^{(j)}\right), \quad j = 0,1,\ldots,m-1, \tag{10} $$

$$ b^{(j)} = \min_k\left(b^{(j+1)}, {}^k \hat{b}^{(j)}\right), \quad j = 0,1,\ldots,m-1, \tag{11} $$

$$ a^{(m)} = \min_k\left({}^k \hat{b}^{(j)}\right) = \min_k\left({}^k \hat{b}^{(j)}\right) = b^{(m)}. \tag{12} $$

3.4 Case Study

3.4.1 **Problem Definition**

A hypothetical problem has been developed to illustrate integrated fuzzy modelling and risk analysis *approach*. The study site contains a leaking underground gasoline storage tank and about 600 m away from the tank area, there is a deep bore well used for rural drinking water supply. The recent groundwater monitoring data indicate high concentrations of several chemical stemming from petroleum products. A Schematic diagram of the solute transport has been shown in Figure 3.3.

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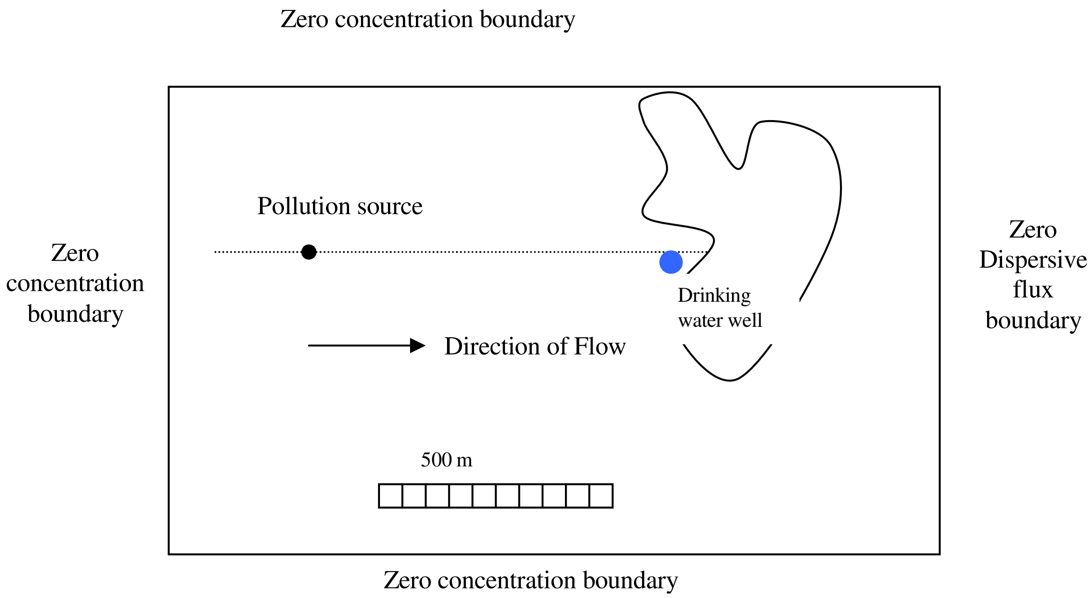

Figure 3.3: Schematic diagram for solute transport

One-Dimension Solute transport

One-dimensional solute movement in a steady uniform flow with a step input concentration C0 at $x = 0$ and a reflection boundary condition at $x = lx$ was used. A numerical model consisting of 40x30 nodal grids with a uniform grid spacing of 50 m in both directions was used to simulate the numerical solution given by

$$C_{i,j}^{n+1} = C_{i,j}^{n} + \Delta t\left(\left(\frac{\alpha_L V}{\Delta x^2} + \frac{V}{\Delta x}\right)C_{i-1,j}^{n} - \left(2\frac{\alpha_L V}{\Delta x^2} + \frac{V}{\Delta x}\right)C_{i,j}^{n} + \frac{\alpha_L V}{\Delta x^2}C_{i+1,j}^{n} \right.$$
$$\left. + \frac{\alpha_L V}{\Delta x^2}C_{i+1,j}^{n} + \frac{M_{i,j}\Delta t}{\Delta x \Delta y \varepsilon b}\right) \quad (13)$$

Two-dimensional Solute Transport

A two-dimensional solute transport, with a continuous point source of pollution in a uniform flow field was studied. For this purpose, numerical solution for contaminant transport model for saturated pores media has been used. Such solution generally requires extreme simplifications, but the results can be used for approximate solutions. They are also very useful to illustrate the sensitivity of different parameters in overall uncertainty. For this case study a finite-difference numerical solution (Dou et al., 1997) has been used for fuzzy simulation.

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$$C_{i,j}^{n+1} = C_{i,j}^{n} + \Delta t\left(\left(\frac{\alpha_L V}{\Delta x^2} + \frac{V}{\Delta x}\right)C_{i-1,j}^{n} - \left(2\frac{\alpha_L V}{\Delta x^2} + 2\frac{\alpha_T V}{\Delta y^2} + \frac{V}{\Delta x}\right)C_{i,j}^{n} + \frac{\alpha_L V}{\Delta x^2}C_{i+1,j}^{n} + \frac{\alpha_T V}{\Delta y^2}C_{i,j-1}^{n} + \frac{\alpha_T V}{\Delta y^2}C_{i,j+1}^{n}\right) + \frac{M_{i,j}\Delta t}{\Delta x \Delta y \varepsilon b} \tag{14}$$

where $C_{i,j}^{n}$ is the concentration of dissolved chemical (mg/L), V is seepage velocity in the x direction (m/day), α_L and α_T are the longitudinal and transverse dispersion coefficients (m), respectively, b is thickness of aquifer (m), ε is effective porosity, Δt is time increment (day), Δx and Δy are grid spacing in x and y direction respectively (m).

A numerical model consisting of 40x30 nodal grid with a uniform grid spacing of 50 m in both direction was used to simulate the two-dimension solute transport using the equation (14). Zero concentration boundaries were placed at the left, upper and lower model boundaries with a constant source placed at 750 m the top boundary.

Characteristics of the uncertain parameters and other data used in the simulation are shown in Table 1 and Table 2 respectively.

Table 3.1: Triangular fuzzy numbers for uncertain parameters

	Low	Medium	High
V(m/day)	0.3	0.6	1.0
α_L (m)	100	200	300
α_T (m)	20	40	60

Table 3.2: Other crisp input data use in simulation

Parameters	Value
Thickness of flow, b	50 m
Source strength, M	120 kg/day
Effective porosity, p	0.17
Grid distance (Δx)	50 m
Grid distance (Δy)	50 m
Time increment	1 day

The membership functions for input parameters that were used for the fuzzy techniques are shown on Figure 3.4.

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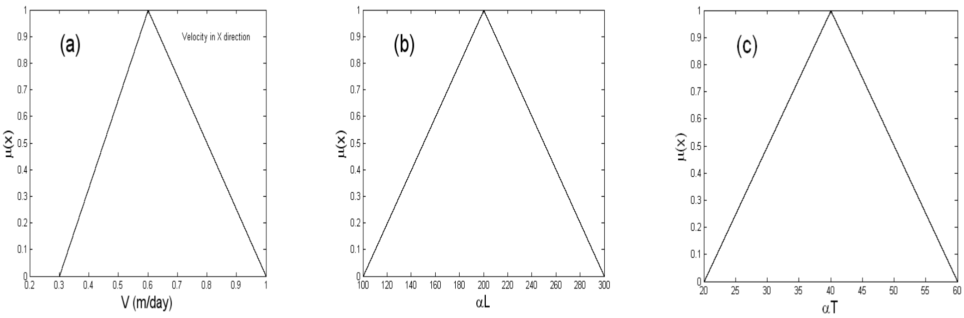

Figure 3. 4: Membership functions of input parameters for 2D solute transport (a) seepage velocity (V), (b) logitudinal dispersivity(α_L), (c) transverse dispersivity(α_T)

3.5 Results and Discussion

Generally in a deterministic model, the model parameters have lot of associated uncertainty. The input data cannot be determined precisely because the state of knowledge is not perfect or near perfect. Assessment of the parameters can be based on expert judgement and sometime expressed as linguistic terms. The crisp set is unable to express this sort of uncertain data which can be best expressed by fuzzy numbers.

In this study, fuzzy transformation method has been used to show usability of fuzzy simulation technique. One-dimensional and two-dimensional transport equation has been used for the example case study.

The results of the simulations are shown in Figures 5 and 6 for 1-D and 2-D solute transport respectively. In these figures, the lower and upper bound of different membership levels of fuzzy number, i.e. 0.0, 0.3, 0.5 and 0.8 of α-cuts respectively has been mapped. For both 1-D and 2-D transport equations, concentration graphs are showing clear narrowing of width of the concentration membership function (upper bound minus lower bound) which converge to one line at 1 α-cut. Our results have been compared with other fuzzy methods reported by (Dou et al., 1997). The width of the concentration membership function obtained from *Transformation method* is narrower than other comparable fuzzy methods like vertex method in the same case study. The difference in the concentration output is mainly due to interaction of the concentration variable in space and time dimensions in Equations (13) and (14). Neglecting this dependency of input variables

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resulted in overestimation of the imprecision of solute concentration. A detailed discussion of the effect of fuzzy number dependence can be found in (Dou et al., 1995).

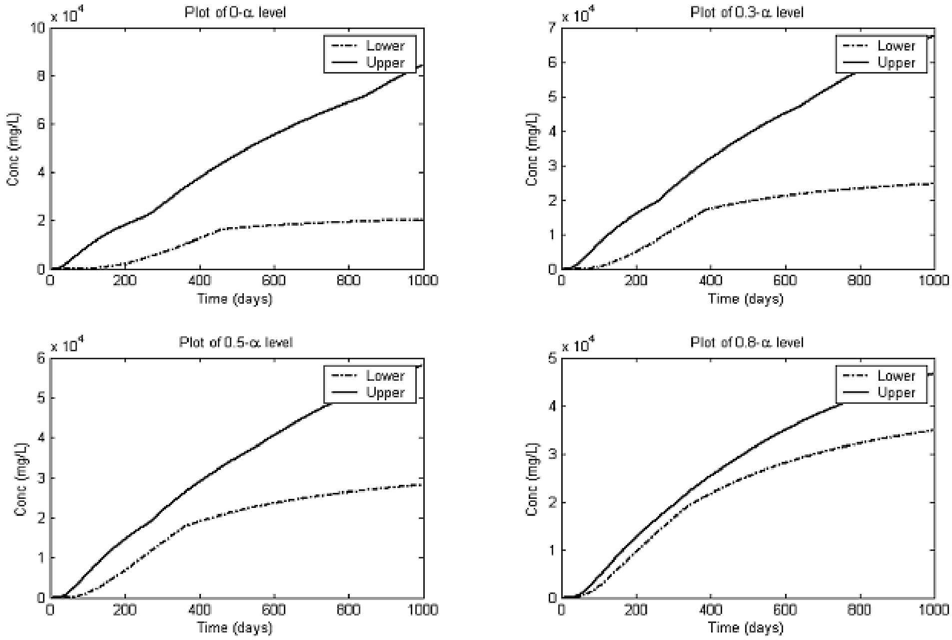

Figure 3. 5: Comparison of solute concentration outputs of 1-D solute transport at different α-levels obtained from Fuzzy Transformation method

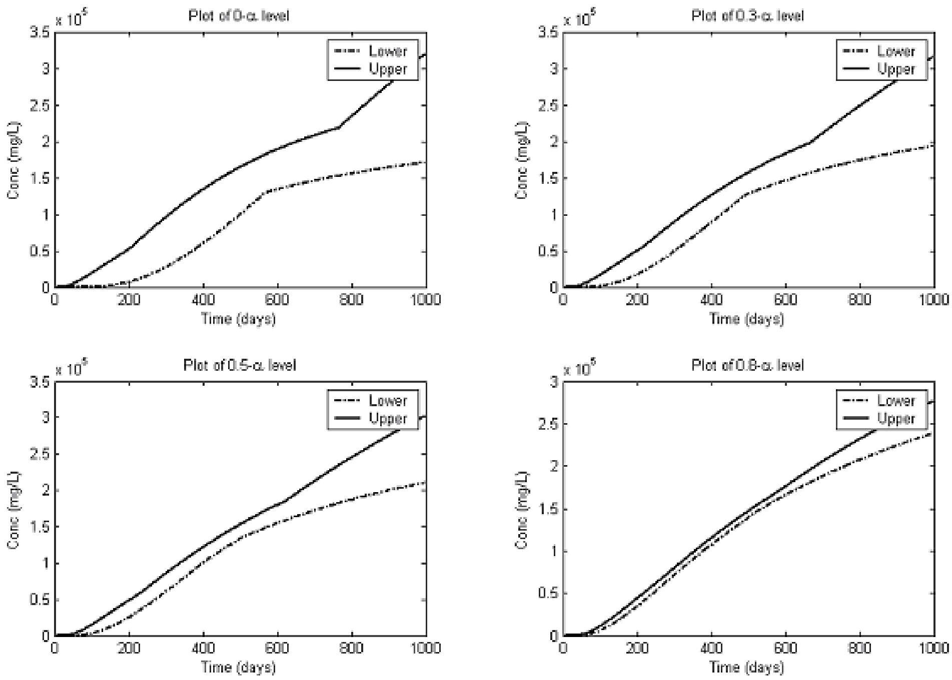

Figure 3.6: Comparison of solute concentration outputs of 2-D solute transport at different α-levels obtained from Fuzzy Transformation method

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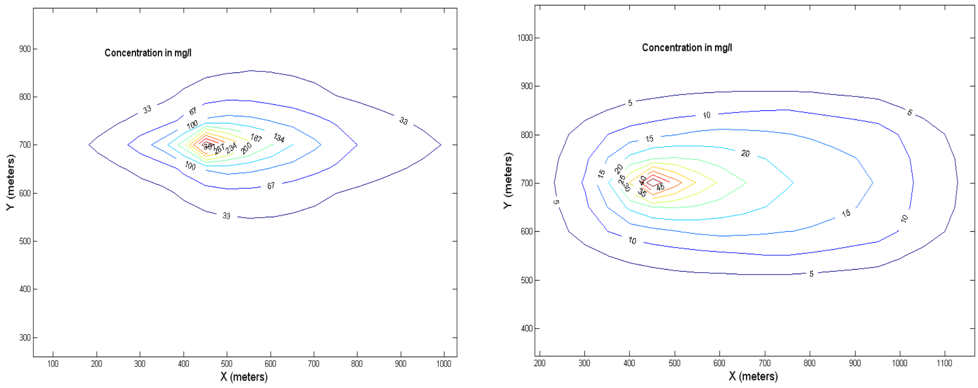

Figure 3.7: Upper(a) and lower(b) bound (0-level cut) solute plum(mg/ l) obtained from *2-D solute transport simulation using* TM method

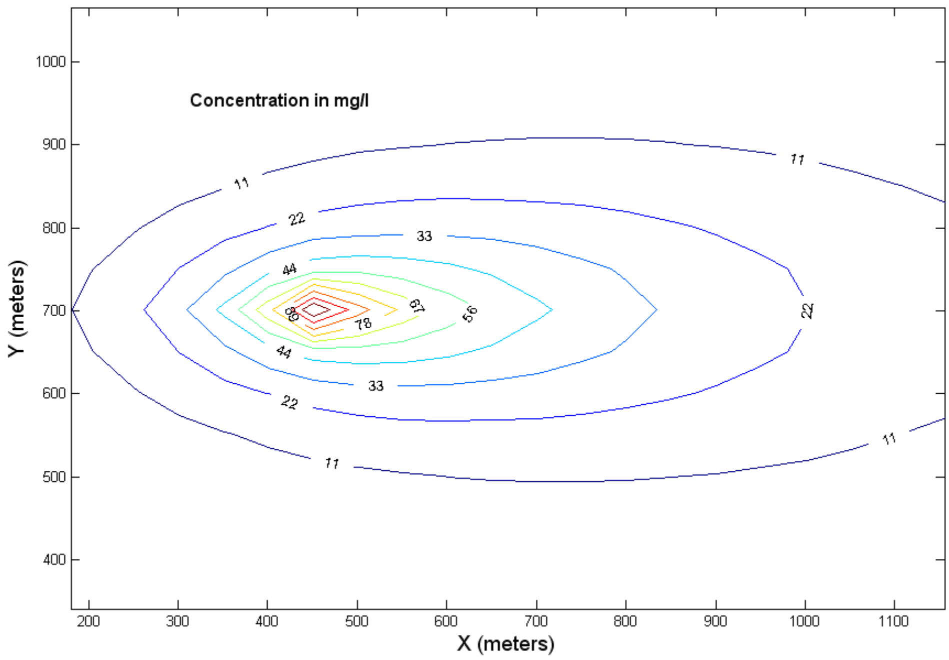

Figure 3.8: 1-level cut solute plum(mg/ l) obtained from 2-D solute transport simulation using TM method

Figure 3.7 and 3.8 present the lower and upper bounds at zero-level cut and one-level cut respectively of the plume concentration after 1000 days calculated using Transformation method. A detailed study of contour maps show that extent of plumes are quite imprecise which is because of imprecise input parameters. Shape of plumes for upper is narrower than lower bounds which has more ellipsoidal shape.

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For comparative study the classical Monte-Carlo Simulation (MCS) was carried out. Comparative measures of uncertainty were devised for comparison of these methods. For point wise analysis, the probability density function (for the MCS technique) and the membership function (for the Fuzzy techniques) of the output (concentration) were analysed at a given point (600 m from the pollution point source). Similarly to evaluate the spatial distribution of uncertainty, the ratio of the standard deviation to the mean concentration of the solute at each grid cell in case of MCS has been compared with the ratio of the 0.1-level support to the value of the concentration for which the membership function is equal to 1 in case of FAC technique and overall influence in case of TM. The results of different methods and effect of different parameters on overall uncertainty using TM are shown in Table 3 and Table 4 respectively.

Table 3.3: Over all uncertainty Of different methods

Methods	Uncertainty
MCS	0.1073
FAC	0.0917
TM	0.0907

Table 3.4: Effect of uncertainty of different parameters on overall uncertainty(TM)

Parameters	% Uncertainty
V	0.4526
α_L	0.1425
α_T	0.4049

Figure 3.9 shows the normalized probability distribution function (PDF) of the concentration obtained from the MCS and the fuzzy number representing the concentration obtained from the TM in the same set of axes. The width of the output membership function is the indication of the sensitivity of the model to uncertain parameters.

In Figure 3.10, the cumulative distribution function (CDF) and the normalized-integrated fuzzy number are plotted. All three methods has shown comparable results, however there is clear indication of more consistency in case of TM and FAC.

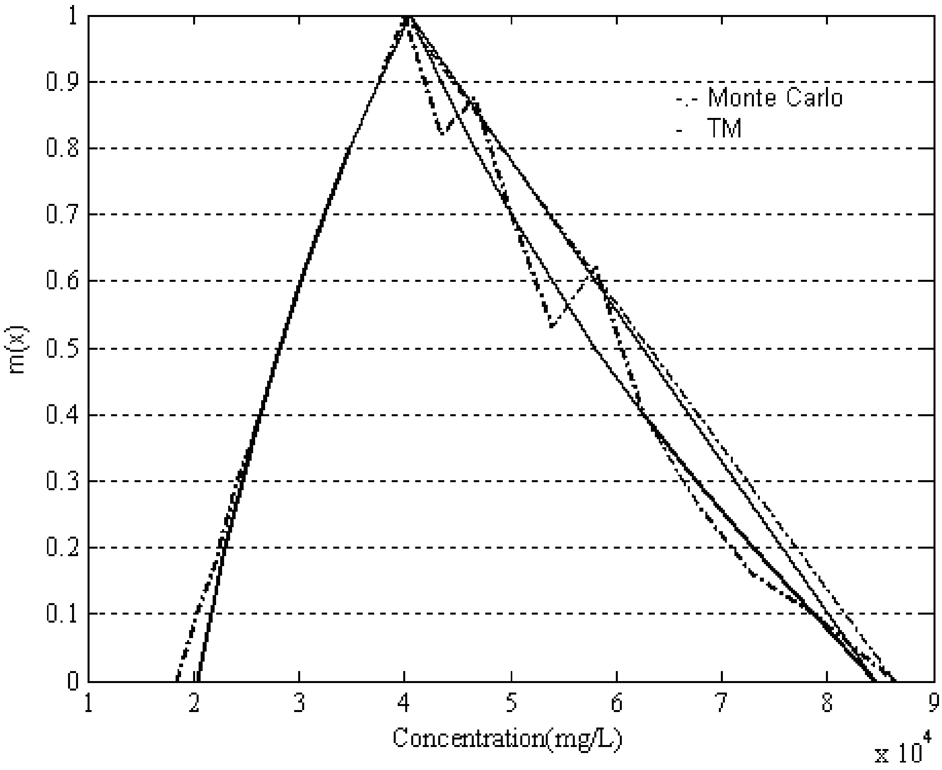

Figure 3.9: Normalized PDF and Fuzzy membership function of the output at the selected point of analysis

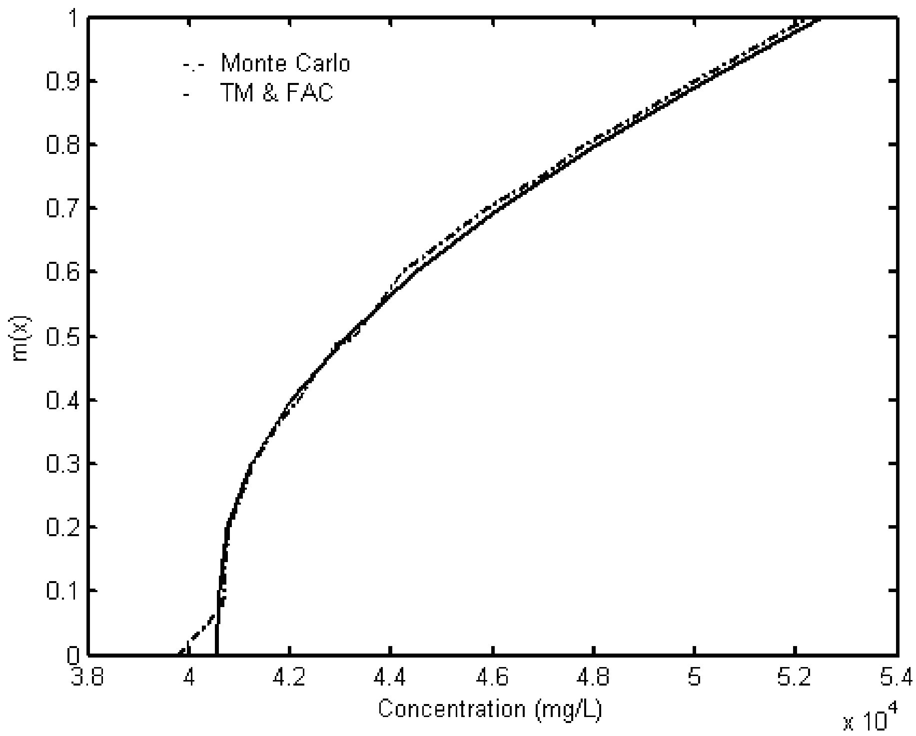

Figure 3. 10: CDF and normalized-integrated membership function

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The output from fuzzy methods agreed well with that from the Monte Carlo method (Figure 3.9 & 3.10), however there is obvious lack of consistency in case of MCS. The other drawback of the Monte-Carlo approach for the present application is its time-consuming character. For the field application, generally a large size of grid simulation has been used. In the present case, decent or rather small grid of 40x30 size has been used. For satisfactory smoothness and accuracy of the results, 500 model runs has been chosen. Simulation has been done for 1000 days of time, which further give a loop of 1000 steps. So the total run of the model is 40x30x500x1000 (60 millions). Mathematical equation for this model is finite-difference equation for 2-D solute transport, which is rather simple among other numerical methods (Dou et al., 1997). A desktop computer with P4 3.0 GHz processor and 1 GB RAM with MATLAB compiler use to take approximately 24-30 hrs of time to complete this simulation. That too is possible after optimization of program. Otherwise a basic computer programme (a common way used by scientists not genius in programming) can easily crash due to lack of memory. Fuzzy arithmetic approach using transformation method for three fuzzy input variables and 10 α-levels of membership need 88 model runs only. Beside that, it is quite difficult in case of Monte-Carlo simulation to select concentration limits for each node of grid and for 1000 days of time, which invariably differ over time. Other approach could be to use a common limit for all grid nodes but it will introduce more uncertainty in the model.

With regard to standard fuzzy methods, the serious drawback is the uncertainty of result for the same problem. Results of standard fuzzy arithmetic method depends on the form of solution procedure applied (Hanss, 2002). Also there is widening of the fuzzy value set which is due to multi-occurrence of variables in function expression. TM is not dependent on solution procedure and can also prevent widening of the fuzzy value set. This method was first shown in vertex method (Dong & Shah, 1987) which also used the interval analysis but that was only suitable for uniform solution space. However TM can be applied for both uniform and non-uniform solution space. In case of FAC technique, it requires less model runs compare to TM but it has been reported to overestimate uncertainty value due to dependencies among uncertain variables. FAC seriously lack the detail analysis of uncertainty, like sensitivity of different uncertain parameters, uncertainty

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at different membership levels. Also for non-monotonic problems, it lacks a clear procedure.

3.6 Conclusion

Fuzzy Transformation method has been analysed and its ability to predict system with uncertain parameters has been shown. Test cases from environmental domain have been considered in order to show its applicability in environmental engineering in general and environmental risk analysis in particular. One and tow-dimensional solute transport processes has been modelled using Fuzzy Transformation method which have some uncertain parameters. Based on the structure of the explicit finite-difference equation for solute transport, the transformation method has been applied to solve the fuzzy equation at each node and each time step. Compare to the vertex method which has been reported to overestimate the uncertainty, TM has given comparable or better results and has sorted out the problem of overestimation due to dependencies among uncertain variables at different nodes.

We can safely conclude that fuzzy transformation method presents a strong alternative to the probabilistic and general fuzzy approach. A faster and accurate result in case of monotonic function and near proper result in case of non-monotonic can be achieved. The transformation method holds the potential to be an effective tool for modelling and analysis of Environmental Risk.

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Chapter 4

PARTITIONING TOTAL VARIANCE IN RISK ASSESSMENT: APPLICATION TO A MUNICIPAL SOLID WASTE INCINERATOR

Abstract

Comprehensive health risk assessment based on aggregate exposure and cumulative risk calculations requires a better understanding of exposure variables and uncertainty associated with them. Although there are many sources of uncertainty in system models, two basic kinds of parametric uncertainty are fundamentally different from each other: natural/stochastic and epistemic uncertainty. However, conventional methods such as standard Monte Carlo sampling (MCS), which assumes vagueness as random property, may not be suitable for this type of uncertainty analysis. An improved systematic uncertainty and variability analysis can provide insight into the level of confidence in model estimates, and it can aid in assessing how various possible model estimates should be weighed. The main goal of the present study was to introduce, Fuzzy Latin Hypercube Sampling (FLHS), a hybrid approach for incorporating epistemic and stochastic uncertainties separately. An important property of this technique is its ability to merge inexact generated data of the LHS approach to increase the quality of information. The FLHS technique ensures that the entire range of each variable is sampled with proper incorporation of uncertainty and variability. A fuzzified statistical summary of the model results produces a detailed sensitivity analysis, which relates the effects of variability and uncertainty of input variables to model predictions. The feasibility of the method has been tested with a case study, analyzing total variance in the calculation of incremental lifetime risks due to polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs) for the residents living in the surroundings of a municipal solid waste incinerator (MSWI) in the Basque Country, Spain.

***Keywords**: Uncertainty; Variability; Fuzzy set; Latin Hypercube sampling; Municipal solid waste incinerator; Health risks*

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4.1 Introduction

Recent health risk assessment studies often consider aggregate exposure and cumulative risk calculation. Accumulated uncertainty in the final result can produce a misleading assessment if it is not incorporated adequately. Studies in risk analysis have shown that consideration of different sources of uncertainty may be crucial for reliable results. Uncertainty and ignorance associated with assessments and predictions on which to base policies make the communication even more difficult (van der Sluijs, 2007). The characterization and quantification of uncertainty and variability in health risk assessment are important to prevent erroneous inferences in multimedia modeling and exposure assessment, which may lead to major environmental policy implications (Frey & Zhao, 2004).

Several different classifications of uncertainty have been suggested (Alefeld, 1983; Haimes, 1998; van Asselt & Rotmans, 2002; Walker et al., 2003). However, for the objectives of the current study, only parametric uncertainty has been considered. The parametric uncertainty has been classified on the basis of its source and nature. Sources of parameter uncertainty are measurement errors, sampling errors, variability, and the use of surrogate data (Moschandreas & Karuchit, 2005). Measurement errors refer to random (imprecision) or systematic errors (bias), while sampling errors are errors from small sample size and/or misrepresentative samples. Heterogeneity in environmental and exposure-related data includes seasonal variation, spatial variation, and variation of human activity patterns by age, gender, and geographic location, leading to variability errors. Surrogate data refer to errors from the use of substitute data. Van Asselt and Rotmans, (2002) and (Walker et al., 2003) classified uncertainty based on its nature. They called it *Epistemic uncertainty/imprecision*, and *Stochastic uncertainty/natural variability*. Epistemic uncertainty which results from incomplete knowledge about the system under study, is reducible by additional studies (e.g. further research and data collection). Stochastic uncertainty which stems from variability of the underlying stochastic process is non-reducible for a given system and under specific management scenario. Natural variability has also been termed (basic) variability, randomly uncertainty, objective uncertainty, inherent variability, (basic) randomness, and type-I uncertainty. Terms for epistemic uncertainty are systematic uncertainty, subjective uncertainty, lack-of-knowledge

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or limited-knowledge uncertainty, ignorance, specification error, prediction error, and type-II uncertainty (Haimes, 1998; Merz & Thieken, 2005; Moschandreas & Karuchit, 2005; Refsgaard et al., 2007; Rotmans & van Asselt, 2001; van Asselt & Rotmans, 2002). In this paper, the term uncertainty is used to denote epistemic, variability to denote stochastic uncertainty, and total variance or simply variance to denote total uncertainty and variability in the outcome.

In spite of this obvious distinction, uncertainty and variability have been used as synonym. Some of the reasons are the blurred knowledge about uncertainty and variability and the lack of commonly agreed guidelines on uncertainty characterization and appropriate methodology. Consequently, in uncertainty estimation both type of uncertainty are clubbed together and treated as random event, though epistemic uncertainty is not random in nature. The purpose of uncertainty analysis is to provide decision makers with a complete spectrum of information concerning the assessment and its quality. It also gives some scope to improve predictive results (Rotmans & Asselt, 2005). When the uncertainty in the risk estimate is unacceptable for decision-making, additional data are acquired for the major uncertainty contributing model components. This process is repeated until the level of residual uncertainty is acceptable. For this we need to identify uncertainty components which are reducible. Further, separate measurements can provide us relevant information to the risk management decision (Spencer et al., 2001).

From a practical viewpoint, it is rare to encounter only one type of uncertainty. Pure variability would mean that all relations and their parameters which describe the random process are exactly known. Pure epistemic uncertainty would mean that a deterministic process is considered, but the relevant information cannot be obtained (e.g. due to the inability to measure the relevant parameters) (Merz & Thieken, 2005). For example, given a parameter X with total variance V_x, it would be straightforward to partition the variance into uncertainty and variability components, where α is the uncertainty component and (1-α) attributable to variability (Figure 4.1). There also can be an intermediate vague region in which uncertainty and variability commingle. So sometime it is difficult to separate and in that case it needs special handling to measure both uncertainty and variability together.

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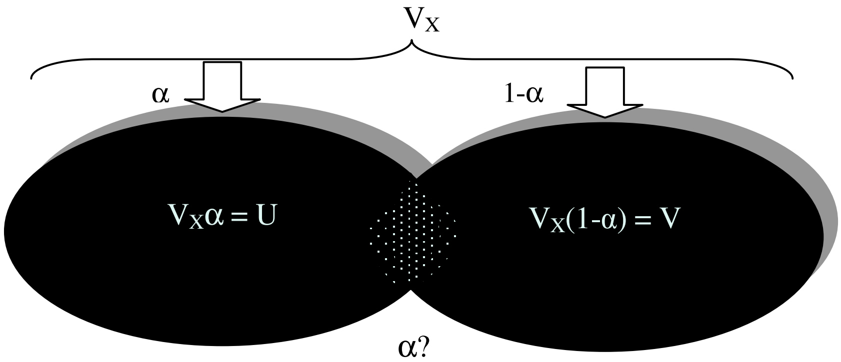

Figure 4.1: Separating uncertainty and variability

Several approaches to uncertainty analysis in environmental risk analysis have been developed (Isukapalli, 1999; Schulz & Huwe, 1999). Among them, probabilistic approaches (e.g. Monte Carlo Simulation) are quite common and have been commonly used in the treatment and processing of uncertainty for solution of system modelling (Schuhmacher et al., 2001). Another prominent approach based on fuzzy set theory (e.g. fuzzy alpha-cut analysis) has been recently applied in various fields including environmental modelling for uncertainty quantification (Cho et al., 2002; Hanss, 2002; Isukapalli, 1999; Kentel & Aral, 2004; Kumar, 2005; Mauris et al., 2001). However this model has been branded as too conservative and basically applied in pure epistemic condition (Mauris et al., 2001). However, all these methods have been developed to handle either variability or uncertainty of the process parameters or they club them together without valid distinction in analysis. Few recent efforts have been made to treat them separately. One common approach used in this field is 2D Monte Carlo Analysis, which classifies epistemic uncertainty as second order uncertainty (Simon, 1999). This technique requires knowledge of parameter values and their statistical distribution from which a formal mathematical description of uncertainty must be developed. However, site investigation is generally not detailed enough to determine values for some of the parameters and their distribution pattern, and sufficient data may not be collected for calibrating a model (Kentel and Aral, 2005). These approaches suffer from an obvious lack of precision and specific site-characterization, making difficult to determine how much error is introduced into the result due to assumptions and prediction. Recently, a number of authors have suggested adopting other approaches in the data limited situation. (Refsgaard

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et al., 2007) reported: 'The test theory of classical statistics permits the testing of a sample for randomness. If the sample does not exhibit the property of randomness, other uncertainty models such as, e.g. fuzzy randomness must be adopted'. Previously, (Möller et al., 2002) presented the idea of Fuzzy Randomness and formalized the concept of random variable and uncertain variable. (Kentel & Aral, 2005) introduced 2D Fuzzy Monte Carlo and applied it in the area of health risk assessment. 2D Fuzzy Monte Carlo and Fuzzy Randomness have been classified as hybrid approach mixing the concept of probability and fuzzy set theory. The present study aims to continue this area of research and introduces a new hybrid approach, Fuzzy Latin Hypercube Sampling (FLHS), for uncertainty and variability analysis. It need less computational effort and allows incorporating parameters correlation. Further we present a way to apply sensitivity analysis in fuzzy-stochastic modeling paradigm. The feasibility of the method has been validated analyzing total variance in the calculation of incremental lifetime risks due to polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs) for the residents living in the surroundings of a municipal solid waste incinerator (MSWI) in the Basque Country, Spain.

4.2 Background

4.2.1 Fuzzy sets and numbers

Fuzzy set theory replaces the two-valued set-membership function with a real-valued function; that is to say, membership is treated as a possibility or as a degree of truthfulness. Likewise, one assigns a real value to assertions as an indication of their degree of truthfulness. Membership functions define the degree of participation of an observable element in the set. Fuzzy numbers are the fuzzy set defined on the set of real numbers and have special significance. They represent the intuitive concept of *approximate numbers,* such as *"around, close to, approximately etc"*. The fuzzy set that contains all fuzzy numbers with a membership of $\alpha \in [0,1]$ and above is called the *a-cut* of the membership function (Abebe et al., 2000) (Figure 4.2). So the *α-cut* represents the degree of sensitivity of the system to the behavior under observation. Fuzzy α-cut technique is based on the extension principle (Zadeh, 1965), which implies that functional relationships can be extended to involve fuzzy arguments. It can be used to map the dependent variable as a fuzzy set. In simple arithmetic operations, this principle can be analytically used. However,

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in most practical modeling applications involving complex structural relationships (e.g. partial differential equations), analytical applications of the extension principle is difficult. Therefore, interval arithmetic can be used to carry out the analysis (Abebe et al., 2000). Arithmetic on fuzzy numbers can be defined in terms of arithmetic operations on their α-cuts (on closed intervals).

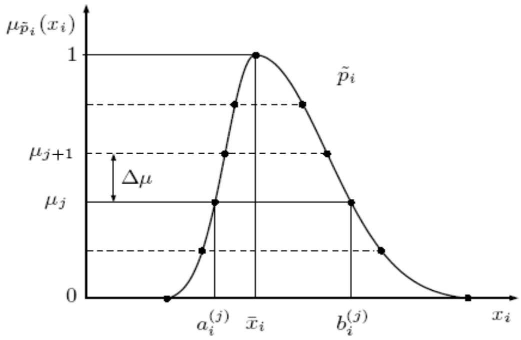

Figure 4.2: Implementation of the i^{th} uncertain parameter as a fuzzy number $\tilde{p}_i$ decomposed into intervals (α-cuts)

This principle is generalized as: a membership level $\mu_A(x) \in [0, 1]$ is assigned to all elements x (i.e. the elements belong to the set to a certain degree) (Hanss, 2002; Klir & Yuan, 1995). The core of the set is defined as the subset for which $\mu_A = 1$. The support is the subset for which $\mu_A > 0$ (also known as the input vertex). The α-cut is a generalized support: the subset for which $\mu_A \geq \alpha$, with $0 < \alpha \leq 1$. The α-sublevel technique (Hanss, 2002) consists of subdividing the membership range of a fuzzy number into α-sublevels at membership levels $\mu_j = j/m$, for $j = 0, 1, ...m$ (Fig. 2). This allows numerically representing the fuzzy number by a set of $m + 1$ interval $[a_j, b_j]$. A triangular fuzzy number, subdivided into intervals using $m = 5$, is depicted in Figure 4.2.

In fuzzy simulation, for each α-level of the parameter, the model is run to determine the minimum and maximum possible values of the output. This information is then directly used to construct the corresponding membership function of the output which is used as a measure of uncertainty.

4.2.2 Latin Hypercube Sampling (LHS)

The LHS technique proposed by (McKay et al., 1979) is a type of stratified Monte Carlo sampling, where the range of each of the K variables included in the uncertainty analysis $X_1, X_2, ...X_k$ is divided into N intervals in such a way that the probability of the

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variable falling in any of the intervals is $1/N$. One value is selected at random from each interval. The N values obtained for the first variable X_1 are randomly paired with the N values of the second variable X_2. These pairs are furthermore randomly combined with the sampled values of the third variable, and so on. It finally results in N combinations of k variables. This set of k-tuples is the Latin hypercube sample that is used for successive execution of model runs. When using LHS, the variable space is sampled with relatively few samples and the number of samples recommended in the literature span from 4*K/3 ((Iman & Helton, 1985), to 2*K ((McKay, 1992), to much larger ((Pebesma & Heuvelink, 1999).

4.3 Method

4.3.1 Concept: Fuzzy Latin Hypercube Sampling technique

In this study, the Fuzzy Latin Hypercube Sampling (FLHS) technique is proposed. This technique uses a combination of probability and possibility theory to include imprecise probabilistic information in risk analysis model. It allows the characterization of both uncertainty and variability in one or more input variables. Parameters can be uncertain, variable, or uncertain-variable. The variability in the random variables of the model is treated using probability density functions (PDFs), while the uncertainty associated with them is treated using fuzzy membership functions for the parameters of these random variables. Thus, means and standard deviations of these PDFs are modeled as fuzzy numbers. This modeling structure gives a generalized framework for uncertainty analysis. All three uncertainty cases can be represented by a single definition. In the case of only uncertain parameters, standard deviation can be zero, whereas in the case of only variable parameters membership function (MF) can represent the highest degree of certainty (i.e. $\mu(x)=1$). Generally, membership functions used are triangular and trapezoidal. One important difference between triangular membership function and triangular PDF is that the area below the PDF is equal to the unity. The support of the membership function provides all possible values for the variable, and any number outside the support is not possible according to fuzzy set definition. The base of the probability density function covers all the values, which have positive probabilities. Our purpose was not to provide an alternative approach to 2D MCA, which treated imprecise probability or second order uncertainty, but to use FLHS for the same purpose although with a different concept. FLHS is treating uncertainty and variability in the parameters separately using hybrid fuzzy probability set theory. For a detailed discussion on Fuzzy probability, the readers can refer to the seminal paper of (Zadeh, 1984). This framework of uncertainty analysis encourages the modelers for detailed uncertainty characterization, and at the same time gives enough space to carry out modeling task in case of insufficient information on parameters distribution. If the available information is sufficient for detailed characterization of uncertainty and variability, the method can provide a detailed analysis of uncertainty and variability contribution in the final result. However, in all cases the method can give insight into uncertainty and variability contribution of different parameters in the final result, which would help modeler/decision maker to collect more data or to improve observation of major parameters in order to improve results. The readers may also refer to (Guyonnet et al., 2003) for a brief discussion of the same topic.

Since our main goal was neither to convert probability density functions into membership functions, nor to utilize one in place of another, no direct numerical comparisons for the calculated risk estimates are provided. Some researchers have attempted to compare fuzzy and stochastic simulation results but they have adopted different measures for their comparison. Guyonnet et al. (2003) have proposed possibility and necessity measures at different α-cut levels to be compared with percentile value at corresponding probability level. However (Abebe et al., 2000) have used the ratio of the 0.1-level support to the value of for which the membership function is equal to 1 from fuzzy α-cut simulation to be compared with a measure of derived from ratio of the standard deviation to the mean value from Monte Carlo simulation. Kentel and Aral, (2004) have used overlapped membership function and the bar chart of the normalized frequency distribution to compare the results. Clearly these differences are due to inherent differences in the definition, meaning and treatment of the uncertainty as utilized in each method. Further research is needed to define the comparison criteria and then one should attempt to provide such a comparison We here provide computational framework for the FLHS and the interpretation of the information generated from the proposed method.

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4.3.2 **Modeling procedure**

There is no clearly agreed upon definition of Fuzzy probabilistic modeling. However, three components are nearly always at the heart of all risk modeling: 1) variability/uncertainty characterization (use of probability distributions or fuzzy distribution/membership function to describe and represent uncertainty), 2) propagation of uncertainty through sampling (statistical, fuzzy etc) of the input parameter distributions and multiple model runs, and 3) presentation of model outputs (again as probability distributions or fuzzy distribution) (Crowe, 2002). The FLHS implementation has been also restricted to this basic framework of risk modeling except the two tiered propagation of variability and uncertainty in the model simulation. Nevertheless, a comparison should not be drawn with other classical methods.

4.3.2.1 Characterization of uncertain variables

Given an arithmetic function f that depends on n uncertain parameters $X_1, X_2, ..., X_n$, represented as fuzzy numbers, the function output $q = f(X_1, X_2, ..., X_n)$ is also a fuzzy number. Using the α-level technique, each input parameter is decomposed into a set P_i of $k+1$ intervals $X_i^{(j)}$, $j = 0, 1,..., k$ where

$$P_i = \{ X_i^{(0)}, X_i^{(1)}, ..., X_i^{(k)} \} \tag{1}$$

$$\text{with } X_i^{(j)} = [a_i^{(j)}, b_i^{(j)}] \;,\; a_i^{(j)} \le b_i^{(j)},\;\; i = 1,2,...,n,\, j = 1,2,...,k \tag{2}$$

where $a_i^{(j)}$ and $b_i^{(j)}$ denote the lower and upper bound of the interval at the membership level μ_j for the i^{th} uncertain parameter. Instead of applying interval arithmetic like fuzzy α -cut (FAC) method (Abebe et al., 2000), now all parameters are transformed into an array using combinatorial combination taking each end of the interval one at a time for each parameters and at each membership level separately. A similar transformation has been used by Hanss, (2002). Purpose of this transformation is to evaluate the target function for each possible combinations arising from discretisation of uncertain parameters. These transformed arrays $\hat{X}_i^{(j)}$ take the following form:

$$\hat{X}_i^{(j)} = \underbrace{\left(\alpha_i^{(j)}, \beta_i^{(j)}, \alpha_i^{(j)}, \beta_i^{(j)}, ..., \alpha_i^{(j)}, \beta_i^{(j)}\right)}_{2^{i-1}\, pairs} \tag{3}$$

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with

$$\alpha_i^{(j)} = \underbrace{\left(a_i^{(j)},...a_i^{(j)}\right)}_{2^{n-1} elements}, \quad \beta_i^{(j)} = \underbrace{\left(b_i^{(j)},...b_i^{(j)}\right)}_{2^{n-1} elements} \tag{4}$$

The evaluation of function f is now carried out by evaluating the expression separately at each of the positions of the arrays using the conventional arithmetic. The obtained result is a deterministic multi-valued decomposed interval, which can be retransformed to get a fuzzy valued result using recursive approximation (Zimmermann 1991).

4.3.2.2 Characterization of random variables

Characterization of random variables has been done using Latin hypercube sampling (LHS). LHS selects *N* different values from each of *n* variables $X_1, X_2, \ldots, Xn$ in the following manner. The range of each variable is divided into *N* non-overlapping intervals on the basis of equal probability. One value from each interval is randomly selected with respect to the probability density in the interval. The *N* values thus obtained for X_1 are paired in a random manner (equally likely combinations) with the *N* values of X_2. These *N* pairs are combined in a random manner with the *N* values of X_3 to form *N* triplets, and so on until *N n*-tuplets are formed. These *N n*-tuplets are the same as the *N n* - dimensional input vectors described in the previous paragraph. It is convenient to think on this sample (or any random sample of size*N*) as forming an (*N n*) matrix of input where the i^{th} row contains specific values of each of the *n input* variables to be used on the i^{th} run of the computer model.

4.3.2.3 Fuzzy-stochastic measures

Taking the clue from fuzzy probability function proposed by Kato et al. (1999) when the mean and standard deviation are fuzzy number, we here propose a fuzzy version of stochastic measures. Using the heuristic of this method together with interval analysis and vertex method, the fuzzy cumulative distribution function (FCDF) and fuzzy linear correlation coefficient (FLCC) for fuzzy random variables can be calculated. This procedure, for a fuzzy-stochastic variable $\tilde{X}$ that has a normal distribution with fuzzy mean $\tilde{m}$, and fuzzy standard deviation $\tilde{\sigma}$, is next summarized:

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4.3.2.3.1 Fuzzy CDF

For standardized normal variables, the Cumulative Distribution Function (CDF) $F(x;m,\sigma^2)$ can be defined as:

$$F(x;m,\sigma^2) = \Phi(\frac{x-m}{\sigma}) \tag{5}$$

Here F is an arithmetic function with three uncertain parameters. Suppose $\tilde{x}_i$ is the realization of fuzzy-stochastic variable $\tilde{X}$ *(*which in this case are derived from output of FLHS simulation run of target model*) and* $\tilde{m}$, $\tilde{\sigma}$ are the fuzzy mean and fuzzy standard deviation of fuzzy-stochastic variable $\tilde{X}$. *So* all three parameters are fuzzy-random variables which can be decomposed (as in equation 2) using the α-level technique, into a set of $k+1$ intervals $\tilde{m}^{(j)}$, $\tilde{\sigma}^{(j)}$, $\tilde{x}_i^{(j)}$ $j = 0,1,..., k$

$$\tilde{m} = \{\tilde{m}^{(0)}, \tilde{m}^{(1)},...,\tilde{m}^{(k)}\} \tag{6}$$

$$\tilde{\sigma} = \{\tilde{\sigma}^{(0)}, \tilde{\sigma}^{(1)},...\tilde{\sigma}^{(k)}\} \tag{7}$$

$$\tilde{x}_i = \{\tilde{x}_i^{(0)}, \tilde{x}_i^{(1)},...\tilde{x}_i^{(k)}\} \tag{8}$$

where

$$\tilde{m}^{(j)} = \left[\tilde{m}_l^{(j)}, \tilde{m}_u^{(j)}\right], \ \tilde{\sigma}^{(j)} = \left[\tilde{\sigma}_l^{(j)}, \tilde{\sigma}_u^{(j)}\right] \text{ and } \tilde{x}_i^{(j)} = \left[\tilde{x}_l^{(j)}, \tilde{x}_u^{(j)}\right] \tag{9}$$

where l and u denote the lower and upper bound of the interval at the membership level μ_j.

Now all three parameters are transformed into an array using similar combinatorial combination as used in equation 3. The resultant array will have 8 combinations at each membership level. So for α-cut level j, the vertex of $\Phi(x)$ can be calculated as:

$$\begin{gathered}
F_1 = \Phi\left(\frac{\tilde{x}_l - \tilde{m}_l^{(j)}}{\tilde{s}_l^{(j)}}\right), F_2 = \Phi\left(\frac{\tilde{x}_l - \tilde{m}_l^{(j)}}{\tilde{s}_u^{(j)}}\right), F_3 = \Phi\left(\frac{\tilde{x}_l - \tilde{m}_u^{(j)}}{\tilde{s}_l^{(j)}}\right), \\
F_4 = \Phi\left(\frac{\tilde{x}_l - \tilde{m}_u^{(j)}}{\tilde{s}_u^{(j)}}\right), F_5 = \Phi\left(\frac{\tilde{x}_u - \tilde{m}_l^{(j)}}{\tilde{s}_l^{(j)}}\right), F_6 = \Phi\left(\frac{\tilde{x}_u - \tilde{m}_l^{(j)}}{\tilde{s}_u^{(j)}}\right), \\
F_7 = \Phi\left(\frac{\tilde{x}_u - \tilde{m}_u^{(j)}}{\tilde{s}_l^{(j)}}\right), F_8 = \Phi\left(\frac{\tilde{x}_u - \tilde{m}_u^{(j)}}{\tilde{s}_u^{(j)}}\right) j = 0,1,...m
\end{gathered} \tag{10}$$

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The fuzzy-valued result $\tilde{F}(\tilde{x})$ of the CDF can be achieved in its decomposed form:

$$\tilde{F}(\tilde{x}_i) = \left[\tilde{F}(\tilde{x}_i)_l^{(j)}, \tilde{F}(\tilde{x}_i)_u^{(j)}\right], \; j = 0,1,\ldots,m \tag{11}$$

by retransforming the arrays $\tilde{F}(\tilde{x})$ using recursive formulae (Zimmermann 1991)

$$\tilde{F}(\tilde{x}_i)_l^{(j)} = min\left(F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8\right), \; j = 0,1,\ldots,m-1, \tag{12}$$

$$\tilde{F}(\tilde{x}_i)_u^{(j)} = max\left(F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8\right), \; j = 0,1,\ldots,m-1, \tag{13}$$

4.3.2.3.2 Sensitivity analysis measures

The sensitivity contribution of the model parameters to the model output can be quantified by various measures (Janssen et al., 1992). Many of these measures are based on regression and correlation analyses and commonly used for stochastic model analysis. They are applied to the original parameter and output values or to their rank-transformed values in case of a monotonic nonlinear relation. Given that some of these measures lead to similar results in identifying the sensitive parameters (Manache, 2001), only the linear correlation coefficient (LCC) are considered in this study. However other similar measures like the standardized regression coefficient (SRC), the semipartial correlation coefficient (SPC) can be derived in similar fashion.

Fuzzy Linear Correlation Coefficient (FLHS)

Given a sample of n-independent pairs of observations (x_1, y_1); (x_2, y_2);… ;(x_n; y_n), the sample correlation coefficient r_{xy} between x and y is calculated as

$$r_{xy} = {cov(x,y)} \Big/ {\sigma_x \times \sigma_y} \tag{14}$$

Clearly r_{xy} is an arithmetic function with three parameters. Here all three parameters may not be fuzzy-random variables. Let us assume that X_i represents input parameters which may be fuzzy, fuzzy-stochastic or stochastic variable and y denotes the out of target model, so in this case it will be output of FLHS simulation which will be fuzzy-stochastic variable provided any of input parameter is fuzzy combined with other stochastic variable or fuzzy-stochastic variable. Similar to Fuzzy CDF derivation, parameters are decomposed using the α-level technique, into a set of $k+1$ intervals and

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then transformed as in equation 3. Depending on type of X_i it can have 4 to 8 functional combination of r_{xy} from which $\tilde{r}_{xy}$ can be derived using recursive formulae.

Similarly the fuzzy standardized regression coefficient (FSRC), the fuzzy semipartial correlation coefficient (FSPC), and other sensitivity measure for fuzzy-stochastic variables can also be calculated. Selection of estimators depends on the problem and objective of the study. For example Regression based estimator can yield results that may be statistically insignificant or counter intuitive (Neter *et al.*, 1996).

4.4 Case Study

Recently, a new MSWI which treats around 250,000 tones per year of domestic wastes started its regular operations in the Basque Country (North of Spain). The facility is placed at 3 km from a metropolitan area with a population around a million of inhabitants. In order to estimate the impact of the new MSWI on the environment and the population living in the neighborhood, fate and transport models were applied to estimate PCDD/F concentrations in different compartments. In turn, these concentrations were used to estimate the exposure of the local population and to assess human health risks. The methodology is summarized in four main steps:

1) Definition of the area of study. Receptor sites were the nearest villages, in some of which agricultural activities are important.

2) Fate and transport model. PCDD/F concentrations were estimated in different compartments (soil, plants, meat and milk) using a multi-compartmental model.

3) Human exposure model. Inhalation of air and resuspended dust, dermal absorption, and ingestion of soil and local foods (vegetables, meat and milk) were the exposure pathways considered.

4) Risk characterization. Together with exposure results, safety PCDD/F benchmarks were used to evaluate the carcinogenic and non-carcinogenic risks (Katsumata and Kastenberg, 1997; Van Leeuwen et al., 2000).

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Information about the equations used in the multi-compartmental model, the exposure model, and the characterization of the health risk model for this case study can be found in the Annex I.

4.4.1 Estimation of parameters uncertainty

The first step of uncertainty and variability analysis is the uncertainty characterization. Once all available information has been collected and evaluated, appropriate probability density functions and membership functions can be specified for variable and uncertain parameters, respectively. Estimations are based on site specific data, previously reported values, as well as some basic assumptions (Schuhmacher et al., 2001). Parameters are characterized as crisp, random/variable, uncertain/fuzzy, and uncertain-variable/fuzzy-random. Crisp variables do not contain any uncertainty. Thus, they are represented by a single value. Variability associated with random variables is represented by probability density functions. Uncertainty associated with fuzzy variables is represented by membership functions, whereas uncertainty-variability of fuzzy-random variables is represented by fuzzy-probability density functions. As an example, sample data set is provided in Table 1. A detailed list of characterized input parameters used in the multi-compartmental model is given in Annex II.

4.4.2 Simulation and propagation of uncertainty

After characterizing the uncertainty and/or variability associated with each input parameters, the FLHS technique is used to propagate these uncertainty. The total variance in the result can then be estimated. This propagation results in a fuzzy probability distribution functions for the estimated risk. Even though the Latin Hypercube Sampling needs lesser sample size compared to normal Monte-Carlo, a higher sample size (1000) has been used to validate the results from previous work of(Schuhmacher et al., 2001). Further 11 levels (0-0.1-1 α-cuts) of fuzzy discretisation have been used which have further been discretised into lower and upper bounds. Under consideration of the fuzzy randomness of the uncertain input values, the obtained result values were also fuzzy random variables.

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Table 4. 1:Sample data sets uncertainty characterization

Parameters	Definition	Units	Uncertainty Type	Distribution /Value*	Note
TD	Total time period of deposition	year	Uncertain	Tri(30, 40, 60)	1
May	Average annual moisture (rainfall, snowfall)	cm/yr	variable	Min: 100.04; Mean: 111.74; Max: 128.93 Std: 11.06	2
Vd	Dry deposition velocitya	cm/sec	Uncertain &Variable	UniTri([4.98E-03 2.73E-02 7.41E-02], [6.22E-03 7.18E-02 1.235E-01])	3
BD	Bulk density	g/cm3	Variable	Uni(0.93-1.84)	4

[1.] Expected life time of MSWI could be 30-60 years. [2]Extracted from 10 years data of the area (1994-2004). [3]Depends on the size of the air particles. [4]From Hoffman and Baes (1979)
[*] Tri = Triangular, Uni = Uniform, UniTri = Uniform Triangular (represent variability and uncertainty respectively).
[a] Detailed calculation is provided in Annex II (Table 2).

FLHS simulation produces two PDFs/CDFs (i.e., one for upper and one for lower bound) for each α-cut level. For the triangular membership function used in this case study, the lower and the upper bound at α-cut 1.0 are the same. Thus, a total of 21 risk PDFs/CDFs were generated with 11 levels of fuzzy discretisation**.** These discrete distributions were used to generate fuzzy risks values corresponding to each percentile. To represent the results, box plots were used. The simplicity of the box plot makes it ideal as a means of comparing many samples simultaneously. It was used to compare distributions at different possibilities level. Box plots of the individual α-cut levels were lined up side by side on a common scale, and the various attributes of the results compared at a glance. Obvious differences were immediately apparent. Data which will not lend itself to standard analysis can be identified. In the current case study, the box plots have been used to show the 5th, 25th, 50th, 75th, and 95th, percentiles of model outcome, in this case PCDD/F concentrations or risk due to exposure to PCDD/Fs. It has been drawn separately for lower and upper membership functions.

The box length gives an indication of the sample variability, while the line across the box shows where the sample is centered. The length of the notch (along the box, not its depth into the box) is a "robust estimate of uncertainty about the median". The notches should be interpreted as a rough indication of the magnitude of a significant difference. The position of the box in its whiskers and the position of the line in the box also indicate whether the sample is symmetric or skewed, either to the right or left. For a symmetric distribution, long whiskers, relative to the box length, can betray a heavy tailed population and short whiskers, a short tailed population. The commonly accepted method among

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statisticians for drawing the whiskers is 1.5 times the interquartile range (IQR). Any data value larger than that should be marked as an outlier.

The membership function of mean and standard deviation of different results has also been plotted to represent uncertainty associated with the result. Further sensitivity analysis to calculate relative contribution of different uncertain parameters to the total uncertainty has been also done. This is useful to handle reducible source of uncertainty in parameters.

4.5 Results and discussion

The output of FLHS simulation is fuzzy probabilistic distributions, which can be represented in various forms (multi-plot of PDF/CDFs over different α-cuts). Several forms of information can be extracted from the results. In the present case study, results have been shown according to the conventional way used by risk modeler community. The frequency distribution has been plotted at three levels of uncertainty, lower α-0, α-1 and upper α-0, which basically represent min-mode-max pattern in triangular membership function (MF). The box plots have been plotted for all 11 α-cut levels at lower and upper uncertainty levels. Further minimum, mode and maximum values for respective triangular MFs have been shown for mean and standard deviation to represent possibilistic uncertainty distribution of fuzzy variability. Sensitivity analysis is presented in Tables and pie-charts. Analysis has been broken down at each step of modeling exercise involving compartmental sub-models from air deposition models and exposure models.

4.5.1 **Results from multi-compartmental model**

A fuzzified statistical summary of PCDD/F concentrations in different media obtained from the multi-compartmental model is shown in Table 2. Large uncertainty in the output has been observed on the current characterization of input parameters. The distribution of PCDD/F concentrations in soil due to air deposition of the MSWI emission is depicted in Figure 4.3. The distributions at different α-cut levels show a different behavior. The most possible value (α-cut 1) shows a normal distribution, whereas the minimum value (lower α-cut 0) is displaying a negative skewness, and the maximum value (upper α-cut 0) is displaying a positive skewness. In turn, the box plots at 11 α-cut levels (Figure 4.4) show a high variability across different possibility levels (α-cut levels). Since

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the notches in the box plot do not overlap, it can be concluded with 95% confidence that the true medians differ. Sensitivity analysis shows how much each uncertain parameter contributes to the overall uncertainty of the prediction. Major contributors to uncertainty in soil deposition are soil loss constant (ks) (55%), dry deposition velocity (Vd) (30%), and volumetric washout ratio for particulates (Wp) (14%) (Figure 4.5). Surprisingly, the concentration of PCDD/Fs in air (Cair) is not a major source of uncertainty, which emphasizes the need to collect more site specific data. The approximated membership function of the fuzzy expected value of PCDD/F in soil concentrations is also depicted in Figure 4.5.

Similar analysis of PCDD/F concentrating in milk exhibits distributions at different α-levels (Figure 4.6). In this case, all three uncertainty levels exhibited a positive skweness. However, the most possible value (α- cut 1) has shown a similar distribution pattern to lower α-cut 0 (minimum value), which can further be confirmed from box plots (Figure 4.7). It can be interpreted as the PCDD/F concentrations in milk would likely be at a lower side of estimation than to the max-value. There are a large number of outliers across all the possibility levels. However, those are mostly mild outliers as they hardly go beyond 3rd Interquartile ranges (3IQRs). At the upper lowest possibility level (upper α-cut 0) of the PCDD/F concentrations in milk, there are some extreme outliers which explain the high uncertainty toward max-value side of the α result. Sensitivity analysis shows fraction of wet deposition (Fw) (33%), plant surface loss coefficient (kp) (23%), particle deposition velocity (Vd) (22%), and volumetric washout ratio for particulates (Wp) (11%) as major contributors towards uncertainty (Table 3). However PCDD/F concentrations in air (Cair), the total time period of deposition (TD) are not a major source of uncertainty (Table 3). The approximated membership function of the fuzzy expected value of PCDD/F concentrations in milk is shown in Figure 4.8. The most expected value of PCDD/F concentrations in milk denotes closeness to minimum possibility level, which can be interpreted as ‘expected value of PCDD/F concentrations in milk would be low to moderate, or it has low possibility of getting maximum value’.

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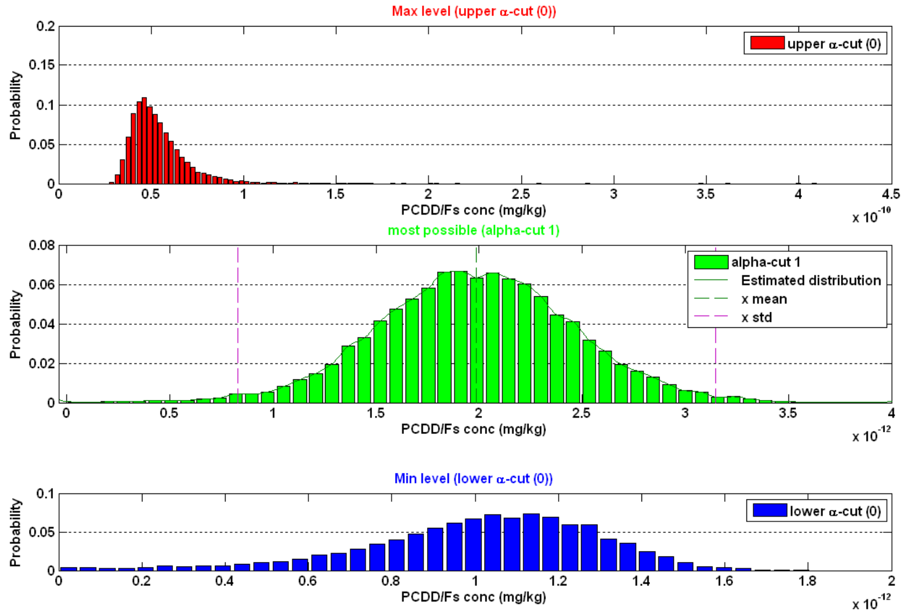

Figure 4. 3: Distribution of PCDD/F concentrations in soil at three uncertainty levels (upper α-cut 0, α-cut 1; and lower α-cut 0)

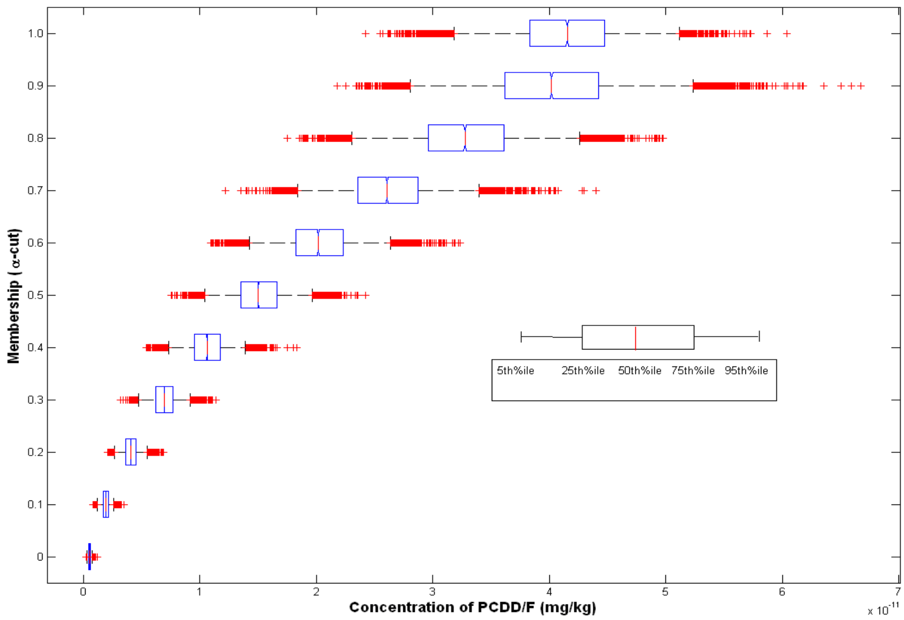

Figure 4. 4: Box plot of PCDD/F concentrations in soil at lower level of membership (lower α-cut levels)

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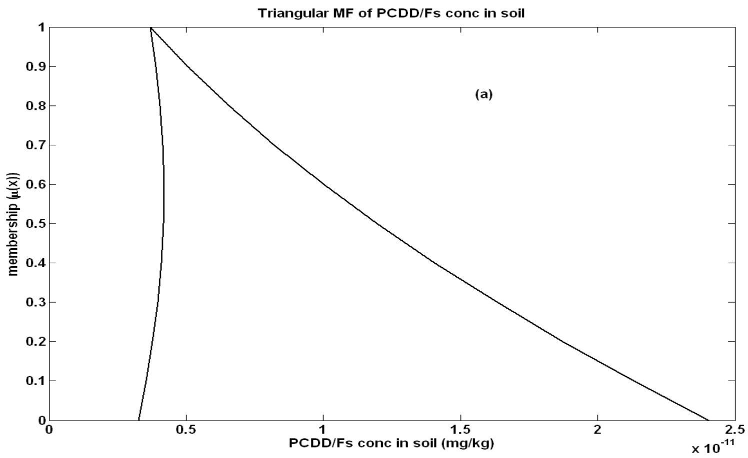

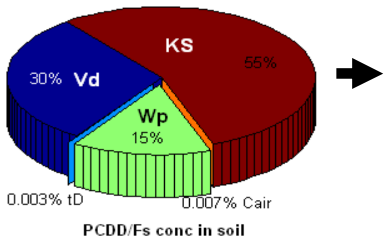

(b)

Parameters	Fraction contribution of total uncertainty
Vd	0.3035
Cair	0.00007
Wp	0.1464
TD	0.00003
ks	0.55

Figure 4. 5 (a) Membership Function of PCDD/F concentrations in soil and (b) sensitivity chart of uncertain parameters used in calculating PCDD/Fs concentration in soils

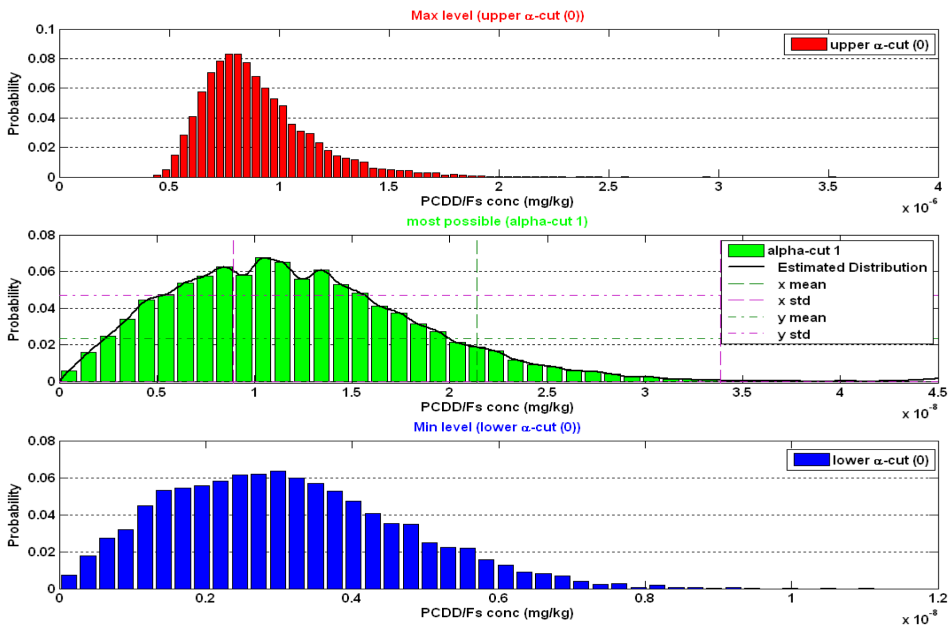

Figure 4. 6: Distribution of PCDD/F concentrations in milk with at three uncertainty levels (Upper α-cut 0, α-cut 1, and Lower α-cut 0)

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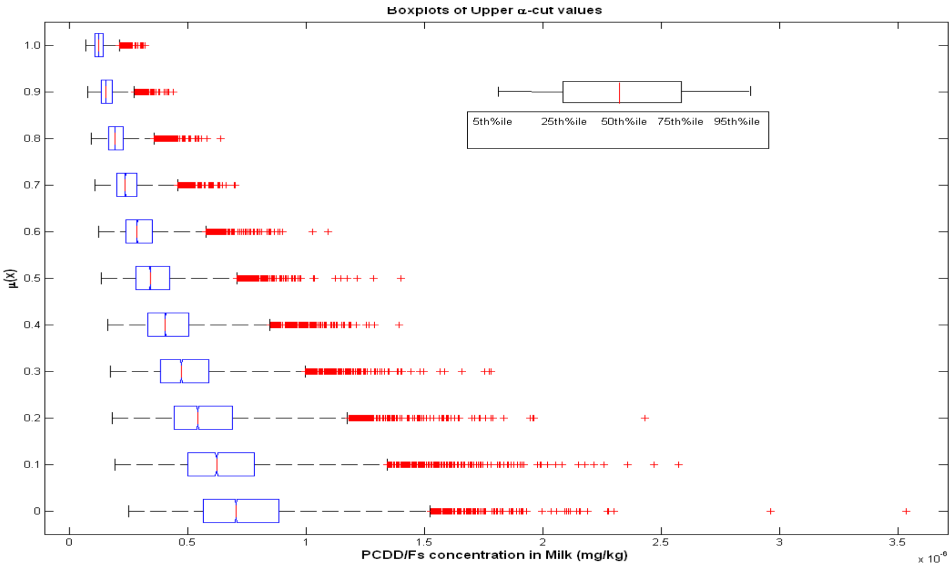

Figure 4.7: Box plot of PCDD/F concentrations in milk at upper level of membership (upper α-cut level)

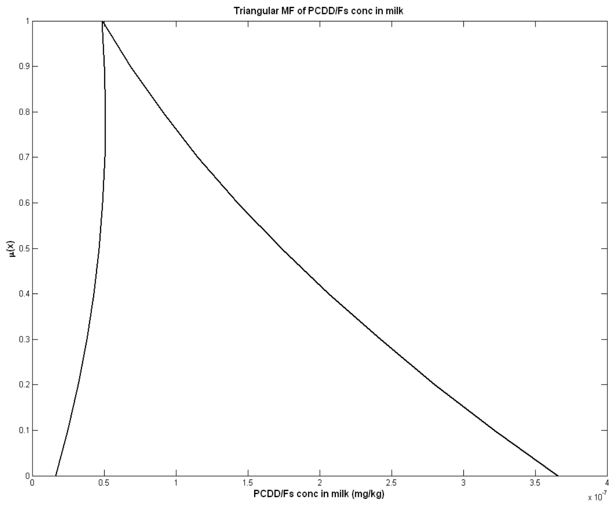

Figure 4.8: Membership Function of PCDD/F concentrations in milk

Table 4.2: Mean and standard deviation of PCDD/Fs concentration in different media obtained from air deposition model with three levels of uncertainty (lower α-cut 0, α-cut 1, and upper α-cut 0)

Media	Mean concentration [min mode max]	Uncertainty (Triangular Std) [min mode max]
Soil	[1.01, 1.98, 54.7]* E-12	[0.28, 0.48, 23.6] * E-12
Meat	[0.2, 0.9, 109.2] * E-8	[0.12, 0.53, 33.72] * E-8
Milk	[0.3, 1.2, 90.85] * E-8	[0.2, 0.6, 25.9] * E-8
Fruits	[0.3, 0.9, 20.1] * E-10	[0.12, 0.23, 37.18] * E-10
Vegetables	[0.2, 0.4, 10.0] * E-10	[0.01, 0.12, 1.86] * E-10

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Table 4.3: Sensitivity analysis for diet intake

Parameters	Fraction contribution of total uncertainty
Vd	0.224
Cair	1.6E-11
Wp,	0.1078
TD	2.8E-13
ks	0.0627
Fw	0.3311
kp	0.2364
SIR	0.0379

4.5.2 Results from exposure models

A fuzzified statistical summary of exposure to PCDD/Fs by the population living in the vicinity of the MSWI is presented in Table 4.4. The distribution of exposure due to air inhalation with three level of uncertainty band is depicted in Figure 4.9. It is a positively skewed extreme value normal distribution with higher variability toward max-value. The distribution of total exposure to PCDD/Fs to the population through different media is shown in Figure 4.10, which are positively skewed at all three levels of uncertainty. Estimated mean and standard deviation has been also shown for most possible distribution (i.e. for α-cut 1). Detailed possibilistic-probabilistic analysis can be done from box plots of lower and upper α-cut levels. Since most of the notches in the boxes do not overlap, we can conclude with 95% confidence that the true medians differ across different possibility levels. Further analysis of whiskers show how distribution has been skewed at different possibility levels. It also shows the mild and extreme outliers present across the possibility levels. For example, outliers present at lower α-cut 0.8 or upper α-cut 0 are quite notable. From these data, it can be interpreted that there is less likelihood of getting these maximum risk value and result decision should not be based on these values. Outliers can be the result of conceptualization or modelling error so at least a detail validity analysis should be performed before considering it for risk decision. This information is particularly important comparing with classical worst case risk analysis method which doesn't give information on likelihood of decision variable.

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Table 4.4: Mean and standard deviation of PCDD/Fs intake through different exposure media with three levels of uncertainty (lower α-cut 0, α-cut 1, and upper α-cut 0)

Exposure Media	Mean exposure [min, mode , max]	Uncertainty (Triangular Std) [min mode max]
Food ingestion	[0.3, 0.8, 130.5] *E-12	[0.3, 0.9, 129.2] *E-12
Air inhalation	[0.22, 0.29, 0.34] *E-13	[0.07, 0.09, 0.1]* E-13
Dermal absorption	[0.0, 0.2, 10.77]* E-16	[0.0, 0.07, 4.79]* E-16
Soil ingestion	[2.0, 3.6, 205.2]* E-20	[0.9, 1.6, 111.7] * E-20
Resuspended particles inhalation	[0.4, 0.66, 24.17] *E-32	[0.17, 0.25, 12.46] *E-32

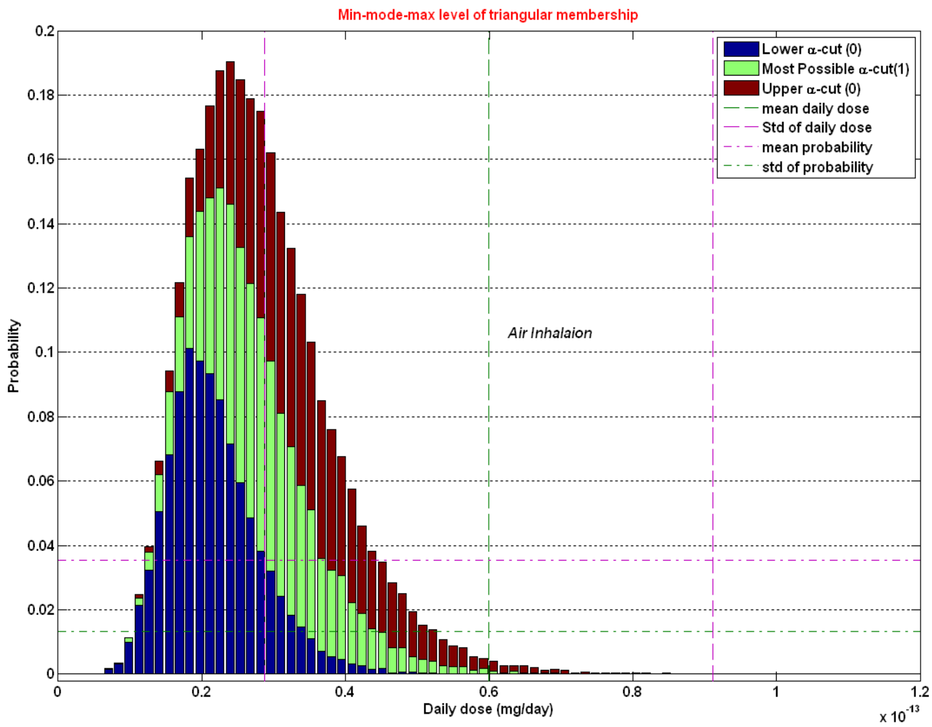

Figure 4.9:Distribution of air inhalation with uncertainty band

Table 4.5: Non-carcinogenic risk: Mean, standard deviation, and 10th, 50th, 90th percentiles with three levels of uncertainty (lower α-cut 0, α-cut 1, and upper α-cut 0)

		Direct Risk [min, mode , max]	Diet Risk [min, mode , max]	Total Risk [min, mode , max]
Mean		[1.1 1.5 1.8]*E-5	[0.2 3.4 69]*E-3	[0.21 3.41 69.02]*E-3
SDa		[4.1 5.5 6.4]*E-6	[1.2 1.7 31]*E-4	[1.2 1.72 31.2]*E-4
Percentiles	10th	[0.5 0.6 0.8]*E-5	[0.0 0.3 6.5]*E-3	[0.01 0.36 6.58]*E-3
	50th	[0.8 1.1 1.3]*E-5	[0.1 1.9 3.9]*E-3	[0.11 1.91 3.91]*E-3
	90th	[1.7 2.2 2.6]*E-5	[0.4 6.6 13.8]*E-3	[0.42 6.62 13.83]*E-3

[a] *SD = standard deviation*

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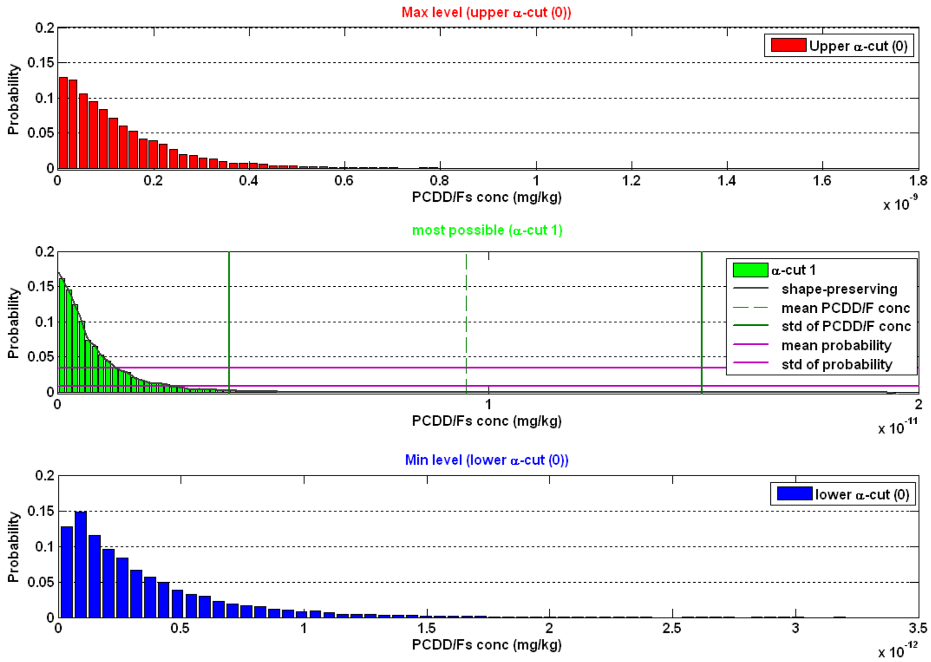

Figure 4.10: Distribution of total doses at three uncertainty levels (upper α-cut 0, α-cut 1; and lower α-cut 0)

Sensitivity analysis (Figure 4.11 b) shows that 99% risk is from exposure to PCDD/F contaminated diets source. Less that 1% of the total PCDD/F exposure is due to the direct MSWI emissions, which can also be validated from previous results in this area (Schuhmacher et al., 2001). The tolerable average intake levels of PCDD/Fs established by the WHO are between 1 and 4 pg WHO-TEQ/kg/day for lifetime exposure (Schuhmacher et al., 2001). Closer examination of box plots (Figure 4.12) reveals that excluding the extreme outliers, most values lie within 1 pg WHO-TEQ/kg/day limit. Also, the total exposure value at 50th percentile (below 0.1 pg WHO-TEQ/kg//day) and 90th percentile (below 0.2 pg WHO-TEQ/kg//day) are far below to the tolerable limit. Consequently, it can be concluded that in the current case study the MSWI would not mean a substantial risk to the population living in the area under potential influence of the emissions of the facility.

4.5.3 Risk evaluation

The non-carcinogenic and carcinogenic risks from direct, indirect (food source), and total exposure are shown in Tables 5 and 6, respectively. The results show the mean, standard deviation, 10^{th} percentile, the central tendency of risk (50^{th} percentile), and the reasonable maximum exposure (RME) (90^{th} percentiles). All this statistical measures have been calculated at three levels of uncertainty: minimum value (lower α-cut 0), most possible value (α-cut 1), and maximum value (upper α-cut 0). It can be seen that the median

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(50th percentile) of non-carcinogenic risk due to PCDD/Fs for the population living in the surroundings of the MSWI is in the range of 0.0001 – 0.004 and most likely risk would be 0.002 (Table 4.5). The results also reveal that the uncertainty of the risk estimated, as defined by the ratio of the 90th to 10th percentile (Schuhmacher et al., 2001) is in the range of 0.06 – 1383, and the most likely value would be 18.4 (Table 4.5).

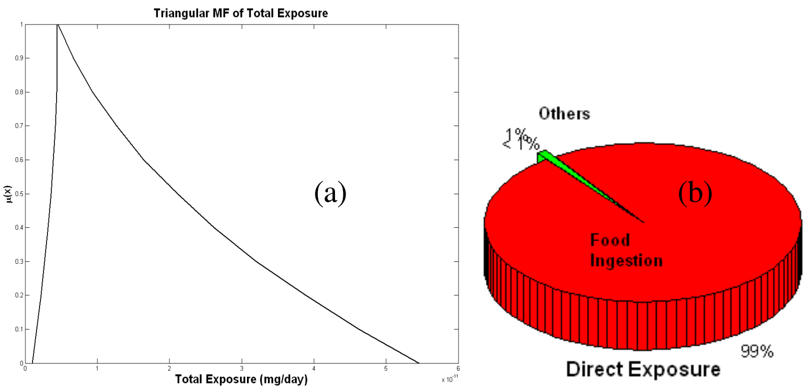

Figure 4.11: (a) Membership Function of total exposure to PCDD/Fs and (b) sensitivity analysis for total exposure

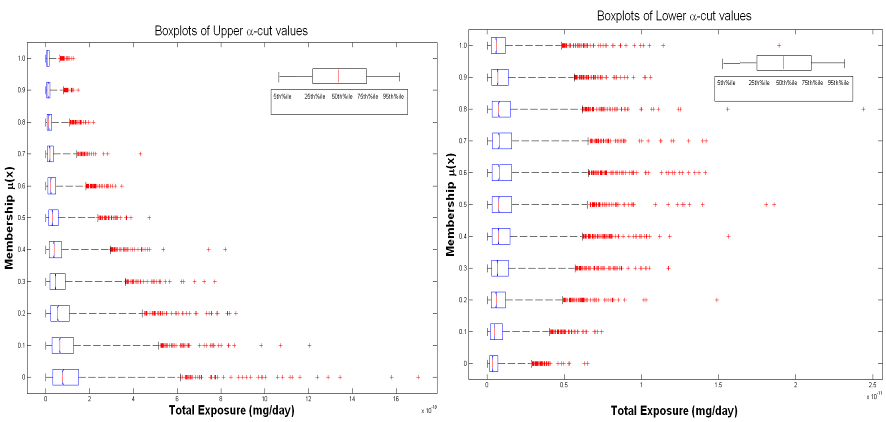

Figure 4.12: Box plot of total exposure for lower and upper level of membership (lower and upper α-cut levels)

With respect to the total carcinogenic risk, the median increment in individual lifetime is in the range of $(3.2 – 1148)\times10^{-7}$, and the most likely value would be 5.53×10^{-7} (Table 4.6). Similarly, the uncertainty of the risk estimated is in the range of 0.16 – 9642, being the most probable value 44.84 (Table 4.6). From the obtained results, it can be concluded that according to the WHO recommendations neither the emissions from the

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MSWI (direct exposure), nor the indirect exposure (diet) to PCDD/Fs would mean any additional risk for the health of the general population living in the vicinity of the MSWI during its life time.

Table 4.6: Carcinogenic risk: Mean, standard deviation, and 10th, 50th, 90th percentiles with three levels of uncertainty (lower α-cut 0, α-cut 1, and upper α-cut 0)

		Direct Risk [min, mode , max]	Diet Risk [min, mode , max]	Total Risk [min, mode , max]
Mean		[1.9 2.5 3.0]*E-10	[0.3 5.5 114.8]*E-8	[0.32 5.53 114.81]*E-8
SDa		[1.5 2.1 2.4]*E-10	[0.4 7.8 16.9]*E-9	[0.50 7.82 17.01]*E-9
Percentiles	10th	[0.3 0.4 0.4]*E-10	[0.03 0.3 5.1]*E-8	[0.03 0.31 5.11]*E-8
	50th	[1.5 2.1 2.4]*E-10	[0.1 2.7 56.5]*E-8	[0.12 2.82 56.52]8E-8
	90th	[4.0 5.3 6.2]*E-10	[0.7 13.8 289.1]*E-8	[0.80 13.90 289.26]*E-8

4.6 Conclusions

In the current case study, only parametric uncertainty consisting of natural variability and epistemic uncertainty has been analyzed. However, the proposed methodology (FLHS) can be used to evaluate other uncertainty components (e.g. model uncertainty and scenario uncertainty). FLHS technique can encompass uncertainty in the inventory, in fate and transport processes, and in exposure pathways to potential receptors. The outputs of these models are also fuzzy probability distributions that, if correctly constructed, represent an expected or "all possible estimates" of the risk and the uncertainty associated with that estimate, conditioned on the model assumptions. As other probabilistic models which generally include probabilistically based sensitivity and uncertainty analyses, FLHS can also give sensitivity measures that can be used in uncertainty reduction and measurement of the value of uncertainty reduction. However, in contrast to classical probabilistic sensitivity measures which failed to separate uncertainty and variability, FLHS can do it effectively. In summary, FLHS clearly separates controllable and uncontrollable uncertainty associated with models, which helps the models /and decision makers to identify the priority area in order to improve the results.

Further validation is needed to test the degree of satisfaction of compliance guideline. For example different risk compliance guidelines have been developed to compare results from stochastic simulation; similar guidelines should be developed to give general uncertainty estimates in accordance with U-V classification. Guyonnet et al. (2003)

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has proposed possibility and necessity measures to test the degree of satisfaction of the compliance guideline. However it still needs to be tested and adopted by different regulatory bodies before used by modeler community.

It also offers new research direction to modeler community to further improve the uncertainty analysis approach. In environment risk analysis, an immediate need is to develop more uniform guidelines to characterize uncertainty and variability associated with different environmental models. In this study, no attempt has been made to compare FLHS with other evolving techniques in this area considering fundamental differences in assumption of defining uncertainty and variability. Comparison of the FLHS results is not straight forward. However, FLHS results can be compared with other similar modeling paradigm like 2D Monte-Carlo, or even second order fuzzy simulation. Notwithstanding, as all these emerging modeling techniques, it needs further research, and then an adequate comparison can be performed. Also further research performed in order to develop decision analysis models, which directly use U-V outcomes in decision making process and improve risk estimation, will enhance the framework.

Software Availability

A toolbox for Matlab has been developed for use in health risk assessment. It is still in beta version and very specialized for health risk assessment. However, in due time a generalized version will be released. It can be made available upon specific request.

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ANNEX I: RISK CHARACTERIZATION MODEL

Table 4.7: Compartmental concentrations

COMPARTMENTAL CONCENTRATIONS	
Environmental concentrations *Soil* $Cs = \frac{100(Dp + Dv + L_{DIF})}{ks \cdot BD \cdot Zs}\left(1 - \exp(-ks \cdot TD)\right)$ where: $Dp = 0.31536 \cdot Vd \cdot Cpa$ $Dv = C_{air} \cdot May \cdot Wp \cdot 10^{-8}$ $L_{DIF} = 0.31536 \cdot Kt \cdot Cva$ $Kt = \left(\frac{Da}{Zs}\right) \cdot \left(1 - \left(\frac{BD}{\rho_S}\right) - \theta_{SW}\right)$	Cs: concentration of contaminant in soil (µg/g); Dp: yearly dry deposition rate (g/m^2 year); Dv: yearly wet deposition rate (g/m^2 year); L_{DIF}: atmospheric diffusion flux (g/m^2 year); ks: soil loss constant (yr^{-1}); TD: time period over which deposition occurs (yr); Zs: soil mixing depth (cm); BD: bulk density (g/cm^3); Vd: dry deposition velocity (cm/sec); Cpa: particle bound concentration of contaminant (µg /m^3); Cair: concentration of contaminant in air (µg /m^3); May: average annual moisture (cm/yr); Kt: gas phase mass transfer coefficient (cm/s); Cva: vapor phase air concentration of contaminant (µg/m^3); Da: diffusion coefficient of contaminant in air (cm^2/s); ρs: solids particle density (g/cm^3); θsw: volumetric soil water content (ml/cm^3); Cpd: concentration in plant due to particle deposition (µg/g); Fw: fraction of wet deposition that adheres to plant surfaces (unitless); Kp: plant surface loss coefficient (yr $^{-1}$); Tp: time of plant's exposure to deposition (yr); Yp: yield or standing crop biomass (kg/m^2); Cpr: concentration plant due to root uptake (µg/g); Br: soil to plant bioconcentration factor (g soil/g plant); C_{beef}: concentration in beef (mg/kg); Fi: fraction of plant grown on contaminated soil and eaten by the animal (unitless); Qp: quantity of plant eaten by the animal (kg plant/d); Cp= Cpd + Cpr (µg/g); Qs: quantity of soil eaten by the animal (kg soil/d); Ba_{beef}: biotransfer factor for beef (d/kg); C_{milk}: concentration in milk (mg/kg); Ba_{milk}: biotransfer factor for milk (d/kg). s: quantity of soil eaten by the animal (kg soil/d); Ba_{beef}: biotransfer factor for beef (d/kg); C_{milk}: concentration in milk (mg/kg); Ba_{milk}: concentration in milk (mg/kg); Ba_{milk}: biotransfer factor for milk (d/kg)
Plants Deposition $Cpd = \frac{1000 \cdot (Dp + Fw \cdot Dv)}{kp \cdot Yp} \cdot \left(1 - \exp(-kp \cdot Tp)\right)$ Root uptake $Cpr = Cs \cdot Br$	
Food chain concentrations *Beef* $C_{beef} = (\Sigma\, FiQp \cdot Cp + Qs \cdot Cs) \cdot Ba_{beef}$ Milk $C_{milk} = (\Sigma\, FiQp \cdot Cp + Qs \cdot Cs) \cdot Ba_{milk}$	

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Table 4.8: Exposure model

EXPOSURE MODEL	
Air inhalation $ADD_{inh} = \frac{C_{air} \cdot IR \cdot AFI_i \cdot EF}{1000 \cdot BW \cdot 365}$ Inhalation of resuspended dust $ADD_{res} = \frac{Cres \cdot IR \cdot RET \cdot AFI_i \cdot EF}{1000 \cdot BW \cdot 365}$ where: $C_{res} = 10^{-6} \cdot Cs \cdot Cpa \cdot Fres$	ADD_{inh}: inhalation of air average daily dose (mg/kg day); Cair: PCDD/F air concentrations g I-TEQ/m^3; IR: inhalation rate (m^3/day); AFI_i: adsorption factor for inhalation; EF: exposure frequency (day/year); BW: body weight (kg); ADD_{res}: inhalation of resuspended dust average daily dose (mg/kg day); Cres: concentration in resuspended dust (µg/m^3); RET: fraction retained in the lung (unitless); Cpa: particle concentration in air (µg/m^3); Fres: fraction of resuspended soil in particle concentration (unitless); Cs: soil concentration (µg/g); ADD_d: dermal absorption daily dose (mg/kg day); AF: adherence factor (mg/cm^2); SA: exposed skin surface (m^2/day); ABS_d: dermal absorption factor (unitless); ADDs ingestion average daily dose (mg/kg day); CRs: soil consumption rate (mg/day); AFI_g: gastrointestinasl absorption factor (unitless); ADD_f: food ingestion average daily dose (mg/kg day); CF_i: concentration in "i" food (µg/g): CRF: consumption rate of each "i" food type (g/day); Fi; fraction of food each "i" food type produced in the contaminated area (unitless).
Dermal absorption $ADD_d = \frac{Cs \cdot AF \cdot SA \cdot ABS_d \cdot EF}{10^2 \cdot BW \cdot 365}$	
Ingestion of soil $ADD_s = \frac{Cs \cdot CRs \cdot AFI_g \cdot EF_s}{10^6 \cdot BW \cdot 365}$	
Ingestion of contaminated food $ADD_f = \frac{CFi \cdot CRF_i \cdot Fi \cdot AFI_g \cdot EF_f}{1000 \cdot BW \cdot 365}$	

Table 4.9: Health risk characterization model

HEALTH RISK CHARACTERIZATION	
No carcinogenic risk	ADD: average daily dose (mg/kg day); HQ: Hazard quotient (unitless); RfD: reference dose (mg/kg day); ER: excess cancer risk (unitless); ED: exposure duration (yr); SF: slope factor $(mg/kg\ day)^{-1}$; AT: average lifetime (yr).
$HQ = ADD / RfD$	
Carcinogenic risk	
$ER = ADD \cdot ED \cdot SF / AT$	

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ANNEX II

Table 4.10:General parameters of multi-compartmental model

Parameter	Symbol	Units	Uncertainty Type	Distribution /Value	Comments/References
Total time of deposition	TD	yr	Uncertain	Tri(30, 40, 60)	Expected life time of MSWI was assumed to be 30-60 years
Soil mixing depth	Zs	cm	Variable	Uni(10-20)	(US EPA, 1998)
Average annual moisture (rainfall, snowfall)	May	cm/yr	Variable	Min: 100.04; Mean: 111.74; Max: 128.93 Std: 11.06	Extracted from 10 years data of the area (1994-2004) (Ministerio de Medio Ambiente)
Bulk density	BD	g/cm^3	Variable	Uni(0.93-1.84)	(Hoffman and Baes, 1979)
Volumetric soil water content	θsw	ml/cm^3	Variable	Uni(0.03-0.40)	(Hoffman and Baes, 1979)
Solids particle density	ρs	g/cm^3	Variable	Uniform(2.6-2.7)	(Hillel, 1980; Blake and Hartge, 1996)
Yield crop biomass of plant group (vegetables/fruits)	Yp	kg/m^2	Variable	Uni(0.24-0.31)	(Belcher and Travis, 1989; Shor et al., 1982)
Quantity of plant eaten by the animal	Qpi	kg/day	Variable	Dairy Cattle: Uni(2.6-11); Beef cattle: Uni(0.47-8.8)	Derived from data of seven types of grains, two types of forage and two types of silage for beef and dairy cattle (US EPA , 1997)
Soil consumption rate (animal)	Qs	kg/day	Variable	Dairy Cattle: Uni(0.1367-2.64); Beef cattle: Uni(0.13-1.17)	(US EPA, 1997) (1-18% of dry matter intake)
Time of plant's exposure to deposition per harvest	Tp	yr	Variable	Uni(0.0822- 0.1644)	(Belcher and Travis, 1989)
Dry deposition velocity*	Vd	cm/sec	Uncertain &Variable	UniTri([4.98E-03 2.73E-02 7.41E-02], [6.22E-03 7.18E-02 1.235E-01])	Depends on the size of the air particles. Estimation is shown in Table 2

* Separate calculation has been provided in next table

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Calculation of deposition velocity

The emissions were modeled in three size classes of particles.

Table 4.11:Particle size distribution and velocity estimation

Particles Size	AbsoluteVelocity (cm/sec)	Particle Percentage (%)	Estimated Velocity (cm/sec)
< 2 μm	7.11E-03	70.0- 87.5	4.98E-03-6.22E-03
< 2-1000 μm	2.87E-01	9.5- 25.0	2.73E-02-7.18E-02
>1000 μm	2.47	3.0-5.0	7.41E-02-1.235E-01
[2 500 1000]	[7.11E-03 2.87E-01 2.47]		Tri_Uni([4.98E-03 2.73E-02 7.41E-02], [6.22E-03 7.18E-02 1.235E-01])

Table 4.12:Contaminant Specific parameters (in this case PCDD/Fs)

Parameters	Symbol	Units	Uncertainty Type	Value/Distribution	Comments
Contaminant air concentration	Cair	mg/m^3	Uncertain & Variable	Tri([2.10E-10, 9.27E-11, 3.50E-10], [1.05e-13, 1.05e-12, 1.05e-10])	Derived from routine sampling in the area (10 samples)
Water partition coefficient	Kow		Variable	(4.62E+06, 0.73)	Caltox database
Fraction of food produced in the contaminated area	Fi	unitless	Variable	Uni(0.01 0.1)	The consumption of food produced in contaminated area was assumed to be 1-10%.
Diffusion coefficient of contaminant in air	Da	cm^2/s	Variable	Normal(4.2E-1, 0.08)	Caltox database
Fraction of wet deposition that adheres to plant surfaces	Fw	unitless	Uncertain	[0.5 0.6 0.7]	(US (EPA, 1998))
Soil loss constant	Ks	yr^{-1}	Uncertain &Variable	Uni([0.76 0.81 0.90], [0.03 0.07 0.11])	Calculated using formula in (EPA, 1998)
Volumetric washout ratio for particulates	Wp	unitless	Uncertain	[1.00E+2 1.05E+2 1.1E+2]	(US (EPA, 1998))
Plant surface loss coefficient	Kp	unitless	Uncertain	[14.0 18.0 21.0]	(US (EPA, 1998))

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Table 4.13: Input Parameters for exposure model

Parameters	Symbol	Units	Uncertainty Type	Value/Distribution	Observation
Body weight	BW	Kg	Uncertain &Variable	Lognormal(67.52 ± 12.22)	(Arija et al., 1996)
				Lognormal(77.1 ± 13.5)	(Smith, 1994)
Inhalation Rate	IR	m^3/day	Uncertain &Variable	Lognormal(20 ± 2)	(Shin et al., 1998)
				Uniform(5.05-17.76)	(Finley, 1994a)
Fraction retained in the lung	RET	unitless	Uncertain	Tri(45 60 70)	(Nessel et al., 1991)
Absorption factor for inhalation	AFIi	unitless	Uncertain	100	(Nessel et al., 1991)
Soil ingestion rate (human)	CRs	mg/day	Uncertain &Variable	Lognormal(3.44 ± 0.8)	(LaGrega et al., 1994)
				Tri 25 (0.1- 50)	(Lagoy, 1987)
Consumption rate of vegetables	CRF_{veg}	g/day	Variable	Lognormal (99 ± 80)	(Arija et al., 1996)
Consumption rate of fruit	CRF_{fruit}	g/day	Variable	Lognormal (236 ± 174)	(Arija et al., 1996)
Consumption rate of milk	CRF_{milf}	g/day	Variable	Lognormal (226 ± 177)	(Arija et al., 1996)
Consumption rate of beef	CRF_{beef}	g/day	Variable	Lognormal (180 ± 84)	(Arija et al., 1996)
Gastrointestinal absorption factor	AFI_g	unitless	Uncertain	Tri(40 60 100)	(Nessel et al., 1991)
Exposed skin surface area (Adult surface area: head, hands, forearms, lower legs)	SA	m^2/day	Uncertain	Tri(0.20 0.53 0.58)	(US EPA, 1992)
Adherence Factor	AF	mg/cm^2	Uncertain	Tri (0.52 71 0.9)	(Finley, 1994b)
Dermal absorption factor	ABSd	unitless	Uncertain	Tri (0.001 0.003 0.03)	(Katsumata and Kastenberg, 1997)
Exposure Frequency	EF	day/yr	Variable	Tri 345 (180-365)	(Smith, 1994)

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Table 4.14: Specific chemical parameters (PCDD/Fs) for risk evaluation

Parameters	**Symbol**	**Units**	**Uncertainty Type**	**Value/Distribution**	**Observation**
Average Lifetime	AT	yr	Variable	Lognormal (75 ± 5)	(Frey, 1993)
Exposure duration (adult resident)	ED	yr	Variable	Lognormal (11.4 ± 13.7)	(Israeli, 1992)
Tolerable Daily Intake	TDI	mg/kg day	Variable	Uniform (1E-9 - 4E-9)	(van Leeuwen et al., 2000)
Slope Factor	SF	$(mg/kg\ day)^{-1}$	Variable	Uniform (34000-56000)	(Katsumata and Kastenberg, 1997)

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UNIVERSITAT ROVIRA I VIRGILI
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Vikas Kumar
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CHAPTER 5

DEFINITION AND GIS-BASED CHARACTERIZATION OF AN INTEGRAL RISK INDEX APPLIED TO A CHEMICAL/PETROCHEMICAL AREA

Abstract

A risk map of the chemical/petrochemical industrial area of Tarragona (Catalonia, Spain) was designed following a 2-stage procedure. The first step was the creation of a ranking system (Hazard Index) for a number of different inorganic and organic pollutants: heavy metals, polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs), polychlorinated biphenyls (PCBs) and polychlorinated aromatic hydrocarbons (PAHs) by applying Self-Organizing Maps (SOM) to persistence, bioaccumulation and toxicity properties of the chemicals. PCBs seemed to be the most hazardous compounds, while the light PAHs showed the minimum values. Subsequently, an Integral Risk Index was developed taking into account the Hazard Index and the concentrations of all pollutants in soil samples collected in the assessed area of Tarragona. Finally, a risk map was elaborated by representing the spatial distribution of the Integral Risk Index with a Geographic Information System (GIS). The results of the present study show that the development of an integral risk map can be useful to help in making-decision processes concerning environmental pollutants.

Keywords: *Environmental pollutants; Risk map; Hazard Index; Self-organizing maps; Geographic Information System; Tarragona (Catalonia, Spain)*

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5.1 Introduction

The assessment of health risks due to exposure to environmental pollutants has been usually focused on analyzing the impact of a single compound over groups of population. However, people are rarely exposed to individual substances, but to a notable variety of chemicals (Haddad et al., 2001). In recent years, new efforts have been made in order to take into account the possible adverse health effects of an exposure to pollutant mixtures, rather than to single chemicals (Cizmas et al., 2004; Jonker et al., 2004; Monosson, 2005; Pohl et al., 2003; Wilbur et al., 2004). One of the main fields has been the development of ranking and scoring systems to prioritize substances (Lerche et al., 2004; Lerche & Sorensen, 2003; Swanson & Socha, 1997). These new methodologies are aimed to establish an order of importance of different chemicals depending on individual characteristics, such as human and ecological effects. The US Environmental Protection Agency (US EPA) and the European Union have been working in PBT Profiler (US EPA, 2004) and EU Risk Ranking Method (Hansen et al., 1999), respectively, as methods to rank substances. Often, ranking systems have been based on 3 basic characteristics to quantitatively assign a score to each substance: Persistence, Bioaccumulation and Toxicity, commonly known as PBT (Knekta et al., 2004). Thus, the US EPA developed the Waste Minimization Prioritization Tool (WMPT) (US EPA, 1997b), where a single score is calculated in terms of those three categories (Pennington & Bare, 2001). In turn, Snyder et al. (2000) described a Chemical Scoring and Ranking Assessment Model (SCRAM), which was developed according to the same PBT categories. In this latter tool, uncertainty related to lack of knowledge was incorporated as an additional element in order to allow assessment of those chemicals for which data are limited (Mitchell et al., 2002).

The basic aim to create new risk assessment methodologies is to help in the making-decision processes. Therefore, these techniques must be easily understandable and usable by all the stakeholders (scientists, politicians, general public, etc.). Recent advances in the computational field have increased not only the capacity and robustness of data treatment. A notable improvement has been also made to get quickly comprehensible results. Kohonen Self-Organizing Maps (SOM) have become a largely used methodology to classify large amounts of data (Nadal et al., 2004a; Park et al., 2004). Originally

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developed by Kohonen (1982), this is an unsupervised artificial neural network (ANN). It is considered a future step in comparison to the classic statistical tools. SOM, which is based on *data mining*, allow to deal very efficiently with uncorrelated and heterogeneous data (Brosse et al., 2001). SOM, as well as other ANN techniques, have been successfully applied to characterize environmental pollution in particular areas (Dan et al., 2002; Nadal et al., 2004c; Olcese & Toselli, 2004; Shang et al., 2004). Likewise, the Kohonen's map has been successfully applied for ranking in environmental assessment (Tran et al., 2003). On the other hand, Geographic Information Systems (GIS) are very powerful tools not only to design maps of a specific territory, but also to explore data in order to simulate present and future stages. In environmental sciences, GIS have been widely used to analyze a huge variety of land characteristics, and to solve problems related to human activities (Blanco & Cooper, 2004; Carlon et al., 2001; Elbir, 2004; Facchinelli et al., 2001; Nam et al., 2003; Thums & Farago, 2001).

Since approximately 30 years ago, one of the largest chemical/petrochemical complexes in Southern Europe is located in Tarragona County (Catalonia, Spain). A big oil refinery is placed in the zone, together with a number of important chemical and petrochemical industries. In response to the concern of the local population to these facilities, in recent years we initiated a wide survey focused on determining the current levels of various inorganic and organic pollutants in the area (Nadal et al., 2004b, 2004c; Schuhmacher et al., 2004). The purpose of the present study was double. Firstly, to develop a SOM-based Integral Risk Index to assess the global pollution of a potentially polluted area. Secondly, to elaborate a risk map of the chemical/petrochemical area of Tarragona by applying a GIS-characterization of the Index.

5.2 Materials and methods

5.2.1 **Artificial neural networks**

Artificial neural networks (ANN) are systems of elementary computing units that model the information-processing abilities of biological neural networks (Cross et al., 1995; Gagne & Blaise, 1997; Hernandez-Borges et al., 2004). They are capable of learning from examples and are often implemented as a computer program. These biologically-inspired

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methods of computing are thought to be the next major advancement in the computing industry. With the advances in biological research and better understanding of the natural thinking mechanism, many models have been proposed based on different mechanisms of neuron system. One of the major capabilities of the human brain is its self-organizing capacity. According to this, a self-organizing neural network system called SOM was proposed by Kohonen (1982). Since then, SOM has been intensively used as a tool for visualization and classification of data.

5.2.2 **Integral risk index**

The Integral Risk Index was obtained by the following equation:

$$\text{Integral Risk Index} = \frac{\Sigma\,(\text{Hazard Index} \times \text{Pollutant Concentration})}{\text{No. Pollutants}} \qquad (1)$$

5.2.2.1 Hazard Index

The Hazard Index (HI) was a slight modification of the WMPT developed by the US EPA (Pennington & Bare, 2001). The HI shows the relative hazard of a compound respect to the rest. It is based on 3 independent categories:

a) Persistence: given by half-lives in air, water, soil and sediments (Mackay et al., 2000).
b) Bioaccumulation: given by the Bioconcentration Factor logarithm (log BCF). The BCF was obtained from octanol-water constant (Kow) by EPI software BCFWin (Meylan, 1999).
c) Toxicity: given by the non-carcinogenic effects (Reference Dose, RfD), through inhalation, dermal absorption and ingestion, as well as the carcinogenic effects (Slope Factor, SF), through inhalation, dermal absorption and ingestion. Toxicity data were obtained from the Risk Assessment Information System (RAIS, 2005) .

In the present study, the HI was calculated by a set of different organic and inorganic pollutants. The analyzed heavy metals were arsenic (As), cadmium (Cd), chromium (Cr), mercury (Hg), manganese (Mn), lead (Pb), and vanadium (V). In turn, 10 PCDD/F homologues (corresponding to 2,3,7,8-substituted congeners), 7 PCBs (28, 52,

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101, 118, 153, 138, and 180), and 16 PAHs were included as organic contaminants. Therefore, a matrix consisting on 41 pollutants and 11 parameters was elaborated.

To normalize the criteria, a SOM was applied to all data. Kohonen's map becomes really interesting to establish similarities among a huge number of different chemicals by using a single picture. Moreover, SOM was also used as a further normalization system in order to avoid extreme values for each variable. Once the results of the SOM were obtained, they were grouped by PBT categories. Subsequently, the following weighting was applied to each category: a) Persistence received a weight of 3, b) Bioaccumulation was also given a weight of 3, and c) Toxicity weight was 4, divided into 2 for each, non-carcinogenic and carcinogenic toxic effects. The HI was calculated as the single addition of the weighted values. In its totality, unlike WMPT whose score ranged 3-9, the HI could have a value between 0 and 10.

5.2.2.2 Pollutant Concentrations

Soil samples were collected in several locations around the chemical/petrochemical industrial area of Tarragona (Catalonia, Spain) (Figure 5.1). Levels of all pollutants were determined and the results were recently reported. Sampling and analysis methodology were described elsewhere (Nadal et al., 2004b, 2004c; Schuhmacher et al., 2004). In brief, 24 soil samples were collected in 4 different areas (chemical, petrochemical and residential zones, as well as unpolluted areas), and dried at room temperature. Heavy metals were determined through digestion with nitric acid and analyzed by inductively coupled mass spectrometry (ICP-MS) (Nadal et al., 2004c). After extraction and clean-up, the chlorinated compounds (PCDD/Fs and PCBs) were determined by high-resolution gas chromatography/high-resolution mass spectrometry (HRGC/HRMS), following US EPA method 1625 (Schuhmacher et al., 2004). Finally, PAH levels were determined by gas chromatography (GC-FID) (Nadal et al., 2004b).

The concentration of each individual compound/congener was properly normalized, according to the following equation:

$$X_{norm} = \frac{X - X_{\min}}{X_{\max} - X_{\min}} \tag{2}$$

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where X_{norm} is the normalized concentration, X is the individual amount of a compound for each sample, X_{min} is the lowest value of the range, and X_{max} is the maximum. If unpolluted areas are also sampled, X_{min} should ideally correspond to blank samples.

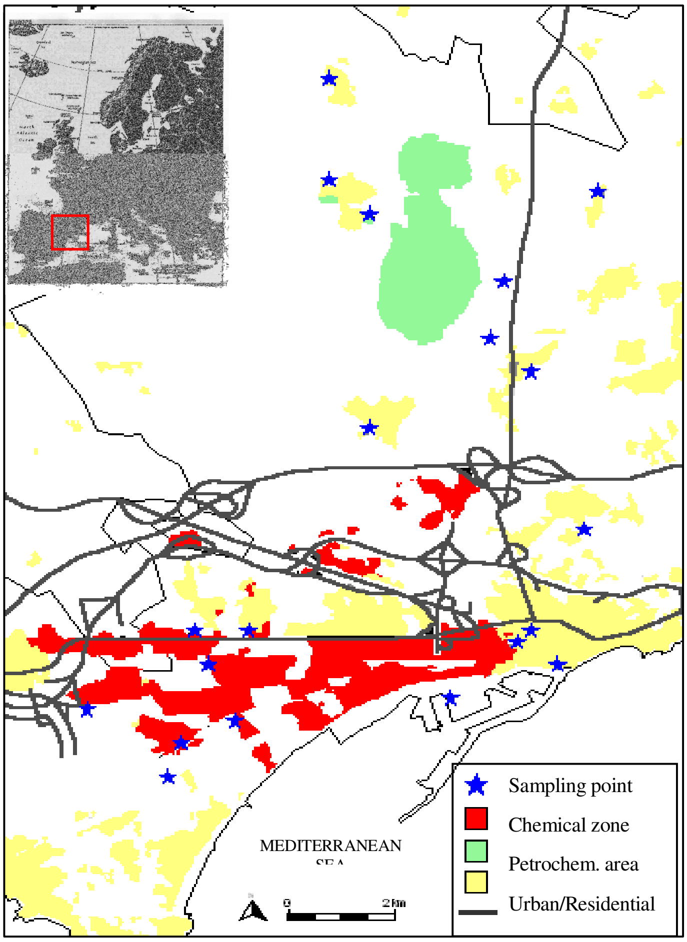

Figure 5.1: Sampling points in the area of study

5.2.3 **GIS mapping**

Spatial distribution of the concentration of all groups of pollutants, as well as the Integral Risk Index, were mapped out with MiraMon© 5.0 GIS software. This tool was developed by the "Centre de Recerca Ecològica i Aplicacions Forestals" (CREAF, Barcelona, Spain). It has been widely used in environmental sciences research (Pons, 2000; Serra et al., 2003). Inverse distance weighted was carried out in order to interpolate geo-referenced data. This method is based on assuming that each input point has a local

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influence that diminishes with the distance (Panagopoulos et al., in press). In the present study, the Risk Map was overlapped with a spatial distribution of soil uses. The main objective was to point out the most impacted areas, not only because of high risk levels, but also due to the closeness to agricultural and/or inhabited areas.

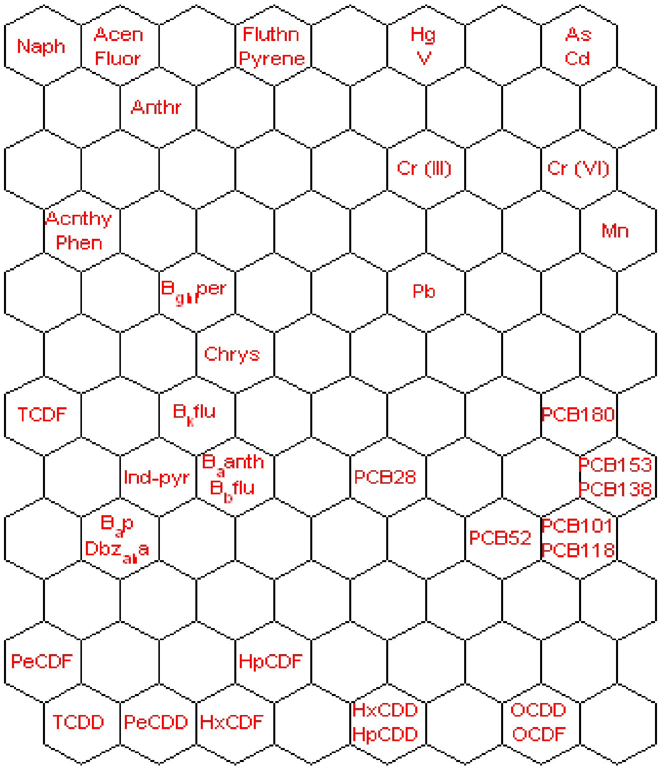

Figure 5.2: Kohonen self-organizing map (SOM) obtained in PBT (Persistence, Bioaccumulation and Toxicity) values of the pollutants under study[1]

5.3 Results and discussion

5.3.1 Hazard Index

The application of self-organizing algorithm to PBT data of all pollutants is depicted in Figure 5.2. The map structure was based on a rectangular grid with 96 hexagons (12 x 8). The learning phase was broken down with 10,000 steps, and the tuning phase consisted on 10,000 additional steps. All chemicals were spread over the 96-units grid,

[1] Abbreviations: Naph: naphthalene; Acen: acenaphthene; Fluor: fluorene; Fluthn: fluoranthene; Anthr: anthracene; Acnthy: acenaphthylene; B_{ghi}per: benzo[g,h,i]perylene; Chrys: chrysene; $B_k$flu: benzo[k]fluoranthene; Ind-pyr: indeno[1,2,3-cd]pyrene; $B_a$anth: benzo[a]anthracene; $B_b$flu: benzo[b]fluoranthene; B_ap: benzo[a]pyrene; Dbz_{ah}a: dibenzo[a,h]anthracene.

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according to similarities of persistence, bioaccumulation and toxicity. Five main clusters were formed: 1) PCDD/F homologues appeared in the lowest part of the grid, 2) PCBs were grouped in the right, 3) heavy PAHs appeared in the middle part of the map, 4) light PAHs were grouped in the left high-corner, and finally, 5) heavy metals were grouped in the right high-corner.

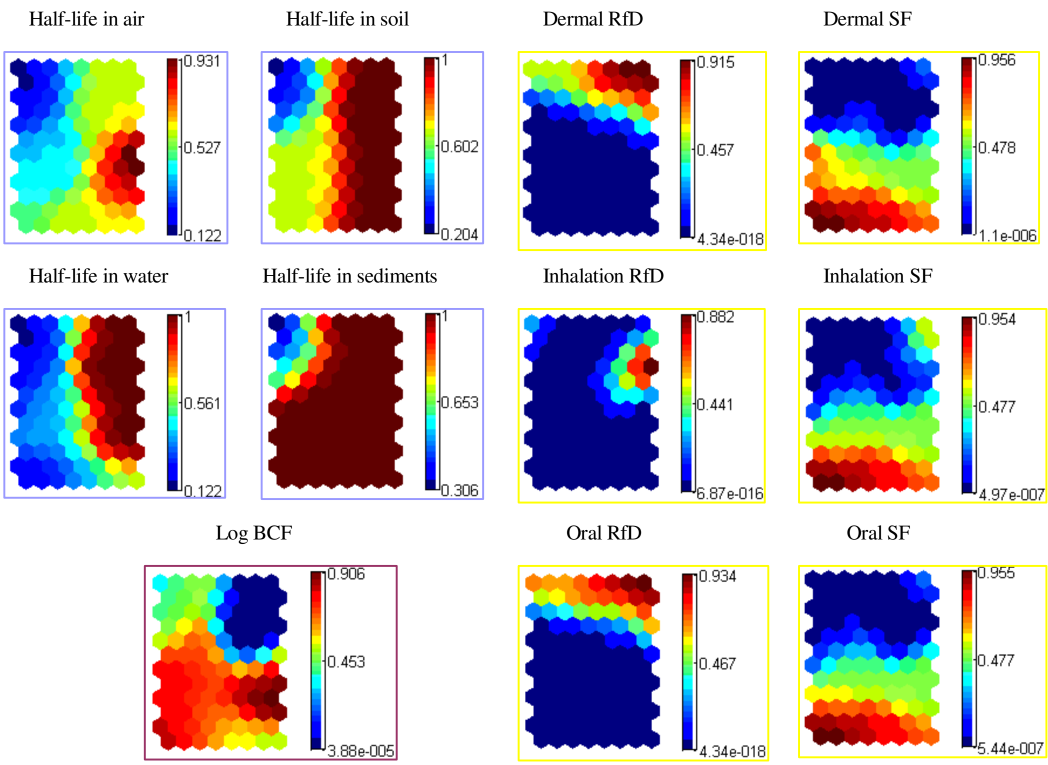

Figure 5.3: Component planes (c-planes) of the SOM results for all pollutants under study

Data treatment with SOM was also used for "correlation hunting". This is to say; to compare the influence of each variable over input data. To illustrate it, component planes (c-planes) are depicted in Figure 5.3. C-planes represent the normalized PBT value of each virtual unit of the map. This value ranged between 0 and 1. The individual score for the PBT variables of all pollutants is summarized in Table 5.1. In turn, the resulting Hazard Indexes are numerically shown in Table 5.2.

Table 5. 1Individual score[1] of all variables for each pollutant after SOM application

Chemicals	log BCF[2]	Dermal RfD[3]	Inhalation RfD	Oral RfD	Dermal SF[4]	Inhalation SF	Oral SF	Half-life air	Half-life water	Half-life soil	Half-life sediments
Arsenic	1.47E-04	9.10E-01	9.40E-02	9.30E-01	2.20E-01	5.50E-01	2.20E-01	6.00E-01	1.00E+00	1.00E+00	1.00E+00
Cadmium	1.47E-04	9.10E-01	9.40E-02	9.30E-01	2.20E-01	5.50E-01	2.20E-01	6.00E-01	1.00E+00	1.00E+00	1.00E+00
Chromium (III)	1.81E-02	6.00E-01	1.30E-01	5.80E-01	8.60E-03	6.30E-02	8.30E-03	5.90E-01	9.80E-01	9.90E-01	1.00E+00
Chromium (VI)	7.77E-04	7.60E-01	6.90E-01	7.30E-01	5.30E-02	4.00E-01	5.20E-02	6.00E-01	1.00E+00	1.00E+00	1.00E+00
Lead and compounds	4.11E-02	9.30E-02	2.80E-01	7.40E-02	2.30E-02	3.30E-02	2.30E-02	6.00E-01	9.80E-01	9.90E-01	1.00E+00
Manganese	1.24E-02	6.30E-01	8.80E-01	6.00E-01	1.70E-02	2.40E-01	1.70E-02	6.10E-01	1.00E+00	1.00E+00	1.00E+00
Mercury	5.43E-02	8.60E-01	1.10E-02	7.00E-01	2.80E-02	6.80E-02	2.70E-02	5.80E-01	9.40E-01	9.70E-01	1.00E+00
Vanadium	5.43E-02	8.60E-01	1.10E-02	7.00E-01	2.80E-02	6.80E-02	2.70E-02	5.80E-01	9.40E-01	9.70E-01	1.00E+00
Acenaphthene	4.05E-01	5.20E-01	1.10E-01	6.50E-01	3.30E-06	2.60E-06	2.80E-06	1.80E-01	1.80E-01	3.00E-01	4.50E-01
Acenaphthylene	4.70E-01	4.30E-02	7.50E-03	5.50E-02	1.80E-02	6.00E-03	6.50E-03	2.20E-01	2.20E-01	3.70E-01	5.50E-01
Anthracene	4.42E-01	4.60E-01	4.40E-02	5.80E-01	2.00E-04	1.60E-04	1.70E-04	2.20E-01	2.20E-01	3.60E-01	5.40E-01
Benzo[a]anthracene	7.25E-01	6.40E-07	1.50E-05	5.20E-07	5.40E-01	4.80E-01	5.10E-01	4.10E-01	4.10E-01	6.80E-01	1.00E+00
Benzo[a]pyrene	7.72E-01	1.10E-09	2.10E-09	3.80E-04	6.40E-01	5.50E-01	5.80E-01	4.10E-01	3.80E-01	6.70E-01	1.00E+00
Benzo[b]fluoranthene	7.25E-01	6.40E-07	1.50E-05	5.20E-07	5.40E-01	4.80E-01	5.10E-01	4.10E-01	4.10E-01	6.80E-01	1.00E+00
Benzo[g,h,i]perylene	6.93E-01	7.10E-03	2.00E-04	9.00E-03	1.70E-01	1.30E-01	1.50E-01	3.60E-01	3.60E-01	6.00E-01	9.00E-01
Benzo[k]fluoranthene	7.33E-01	1.20E-05	1.50E-05	1.40E-05	4.90E-01	4.10E-01	4.30E-01	4.00E-01	4.00E-01	6.70E-01	1.00E+00
Chrysene	7.18E-01	5.60E-04	4.20E-04	5.60E-04	3.50E-01	3.00E-01	3.20E-01	4.00E-01	4.00E-01	6.70E-01	9.90E-01
Dibenzo[a,h]anthracene	7.72E-01	1.10E-09	2.10E-09	3.80E-04	6.40E-01	5.50E-01	5.80E-01	4.10E-01	3.80E-01	6.70E-01	1.00E+00
Fluoranthene	4.75E-01	6.00E-01	2.50E-03	7.00E-01	7.90E-05	1.80E-04	7.50E-05	3.80E-01	4.30E-01	6.40E-01	9.10E-01
Fluorene	4.05E-01	5.20E-01	1.10E-01	6.50E-01	3.30E-06	2.60E-06	2.80E-06	1.80E-01	1.80E-01	3.00E-01	4.50E-01
Indeno[1,2,3-cd]pyrene	7.54E-01	1.50E-07	2.60E-07	1.90E-07	5.80E-01	4.80E-01	5.00E-01	4.00E-01	3.90E-01	6.70E-01	1.00E+00
Naphthalene	3.62E-01	5.30E-01	2.50E-01	6.70E-01	1.10E-06	5.00E-07	5.40E-07	1.20E-01	1.20E-01	2.00E-01	3.10E-01
Phenanthrene	4.70E-01	4.30E-02	7.50E-03	5.50E-02	1.80E-02	6.00E-03	6.50E-03	2.20E-01	2.20E-01	3.70E-01	5.50E-01

[1] Score is unitless. Range: 0-1;
[2] BCF: Bioconcentration Factor
[3] RfD: Reference Dose
[4] SF: Slope Factor

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Pyrene	4.75E-01	6.00E-01	2.50E-03	7.00E-01	7.90E-05	1.80E-04	7.50E-05	3.80E-01	4.30E-01	6.40E-01	9.10E-01
TCDD	8.24E-01	4.20E-18	6.90E-16	5.40E-18	9.60E-01	9.50E-01	9.50E-01	4.80E-01	2.10E-01	6.70E-01	1.00E+00
PeCDD	7.85E-01	3.20E-17	1.00E-13	2.70E-17	9.40E-01	9.40E-01	9.40E-01	5.20E-01	2.20E-01	6.70E-01	1.00E+00
HxCDD	5.71E-01	1.10E-13	1.10E-09	1.10E-13	8.50E-01	8.50E-01	8.50E-01	6.00E-01	2.60E-01	9.50E-01	1.00E+00
HpCDD	5.71E-01	1.10E-13	1.10E-09	1.10E-13	8.50E-01	8.50E-01	8.50E-01	6.00E-01	2.60E-01	9.50E-01	1.00E+00
OCDD	5.26E-01	6.10E-12	3.30E-09	5.80E-12	7.40E-01	7.40E-01	7.40E-01	6.10E-01	5.90E-01	1.00E+00	1.00E+00
TCDF	7.78E-01	7.10E-06	4.80E-07	9.60E-06	7.30E-01	2.00E-01	2.10E-01	3.90E-01	2.80E-01	6.60E-01	9.80E-01
PeCDF	8.29E-01	3.10E-15	6.30E-15	4.20E-15	9.10E-01	9.00E-01	9.10E-01	4.90E-01	2.20E-01	6.70E-01	1.00E+00
HxCDF	7.16E-01	6.50E-16	6.80E-12	2.70E-17	9.10E-01	9.00E-01	9.00E-01	5.80E-01	2.60E-01	7.00E-01	1.00E+00
HpCDF	6.71E-01	1.40E-12	5.10E-09	1.00E-12	8.60E-01	8.50E-01	8.50E-01	5.80E-01	3.30E-01	7.30E-01	1.00E+00
OCDF	5.26E-01	6.10E-12	3.30E-09	5.80E-12	7.40E-01	7.40E-01	7.40E-01	6.10E-01	5.90E-01	1.00E+00	1.00E+00
PCB-28	7.63E-01	3.80E-05	5.40E-03	3.10E-05	4.90E-01	4.90E-01	4.90E-01	6.00E-01	7.60E-01	9.30E-01	1.00E+00
PCB-52	8.87E-01	5.90E-06	6.80E-04	5.70E-06	5.00E-01	5.10E-01	5.10E-01	8.20E-01	9.70E-01	1.00E+00	1.00E+00
PCB-101	9.06E-01	1.20E-05	3.20E-04	1.10E-05	5.00E-01	5.00E-01	5.00E-01	8.60E-01	9.90E-01	1.00E+00	1.00E+00
PCB-118	9.06E-01	1.20E-05	3.20E-04	1.10E-05	5.00E-01	5.00E-01	5.00E-01	8.60E-01	9.90E-01	1.00E+00	1.00E+00
PCB-153	8.68E-01	4.00E-04	2.90E-03	3.80E-04	4.90E-01	4.90E-01	5.00E-01	9.30E-01	1.00E+00	1.00E+00	1.00E+00
PCB-138	8.68E-01	4.00E-04	2.90E-03	3.80E-04	4.90E-01	4.90E-01	5.00E-01	9.30E-01	1.00E+00	1.00E+00	1.00E+00
PCB-180	7.60E-01	7.10E-03	4.80E-02	6.80E-03	4.60E-01	4.70E-01	4.70E-01	9.30E-01	1.00E+00	1.00E+00	1.00E+00

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Table 5.2: Persistence, Bioaccumulation and Toxicity (PBT) scores and Hazard Index (HI) for all pollutants, ordered according to the HI value

	Persistence (0-3)	Bioaccumulation (0-3)	Toxicity (0-4)	HAZARD INDEX
PCB-101	2.888	2.719	1.000	6.61
PCB-118	2.888	2.719	1.000	6.61
PCB-153	2.948	2.603	0.989	6.54
PCB-138	2.948	2.603	0.989	6.54
PCB-52	2.843	2.660	1.014	6.52
PCB-180	2.948	2.279	0.975	6.20
TCDD	1.770	2.472	1.907	6.15
PeCDF	1.785	2.488	1.813	6.09
PeCDD	1.808	2.354	1.880	6.04
HxCDF	1.905	2.149	1.807	5.86
PCB-28	2.468	2.288	0.984	5.74
HpCDF	1.980	2.014	1.707	5.70
HxCDD	2.108	1.713	1.700	5.52
HpCDD	2.108	1.713	1.700	5.52
OCDD	2.400	1.578	1.480	5.46
OCDF	2.400	1.578	1.480	5.46
Benzo[a]pyrene	1.845	2.317	1.180	5.34
Dibenzo[a,h]anthracene	1.845	2.317	1.180	5.34
Indeno[1,2,3-cd]pyrene	1.845	2.261	1.040	5.15
Benzo[a]anthracene	1.875	2.176	1.020	5.07
Benzo[b]fluoranthene	1.875	2.176	1.020	5.07
Benzo[k]fluoranthene	1.853	2.198	0.887	4.94
TCDF	1.733	2.334	0.760	4.83
Arsenic	2.700	0.000	1.949	4.65
Cadmium	2.700	0.000	1.949	4.65
Chrysene	1.845	2.155	0.648	4.65
Chromium (VI)	2.700	0.002	1.790	4.49
Manganese	2.708	0.037	1.589	4.33
Fluoranthene	1.770	1.426	0.869	4.06
Pyrene	1.770	1.426	0.869	4.06
Benzo[g,h,i]perylene	1.665	2.080	0.311	4.06
Mercury	2.618	0.163	1.129	3.91
Vanadium	2.618	0.163	1.129	3.91
Chromium (III)	2.670	0.054	0.927	3.65
Lead and compounds	2.678	0.123	0.351	3.15
Anthracene	1.005	1.325	0.723	3.05
Acenaphthene	0.833	1.216	0.853	2.90
Fluorene	0.833	1.216	0.853	2.90
Naphthalene	0.563	1.086	0.967	2.62
Acenaphthylene	1.020	1.409	0.091	2.52
Phenanthrene	1.020	1.409	0.091	2.52

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According to the Hazard Index, PCBs were the most hazardous pollutants, with values ranging from 5.74 to 6.61. Although toxicity values were lower than those corresponding to PCDD/Fs, they are more persistent in the environment and bioaccumulate more easily in the body. Only the lightest PCB, PCB-28, presented a relatively lower Hazard Index, appearing in the position 12 of the list. This is basically due to the fact that it has a lower persistence than those more weighted compounds in the aqueous and atmospheric compartments. Sinkkonen and Paasivirta (2000) suggested PCB-28 half-lives of 72 and 1450 hr in air and water, respectively. This fact contrasted with values of persistence above 1500 and 3000 hr, respectively, for PCB-52 and heavier congeners. PCBs were followed by PCDD/F homologues, which appeared inversely ordered according to their chlorination degree. PCDD/Fs showed Hazard Indexes between 5.46 and 6.15, with a level of toxicity ranging 1.5-1.9, over a global of 4. Some authors have noted that non-carcinogenic effects of PCDD/Fs may be more important than cancer hazards (Greene et al., 2003). Although a tolerable daily intake (TDI) for PCDD/Fs has been established in the range 1-4 pg TEQ/kg body weight (Van Leeuwen et al., 2000), no differentiation for the TDI has been carried out according to PCDD/F congeners and/or homologues. Consequently, since the US EPA has not recommended the derivation of a reference dose for these compounds yet (US EPA, 2000), non-carcinogenic toxicity was considered as zero. Since 2,3,7,8-TCDD is considered the most toxic congener, a toxic equivalency factor (TEF) of 1 is associated to it (Van den Berg et al., 2000). Specially high carcinogenic slope factors have been established for 2,3,7,8-TCDD, with values of $3 \cdot 10^5$, $1.16 \cdot 10^5$ and $1.5 \cdot 10^5$ kg·day/mg for dermal, inhalation and oral exposure, respectively (RAIS, 2005). Since a TEF of 1 has been assigned to 1,2,3,7,8-PeCDD by WHO (Van den Berg et al., 2000), this congener may be considered so toxic as 2,3,7,8-TCDD. However**,** the Toxicity Value of PeCDDs in the Hazard Index was slightly lower because slope factors for 1,2,3,7,8-PeCDD have not been modified yet. Therefore, TCDD and PeCDD homologues did not appear in the same cell, but in contiguous units. Slope factors for 1,2,3,7,8-PeCDD and 1,2,3,7,8-PeCDF have been identified to be one-half of that for 2,3,7,8-TCDD (RAIS, 2005). Among PCDD/F homologues, TCDF presented a relatively low value, basically due to their characteristics of relatively low persistence and toxicity.

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With regard to PAHs, the carcinogenic compounds presented the highest value. Benzo(a)pyrene and dibenzo(ah)anthracene are considered the most toxic PAHs, according to toxic equivalency factors associated to them. Nisbet and LaGoy (1992) established a value of 1 and 1.1 benzo(a)pyrene equivalents (B[a]P-eq) for benzo(a)pyrene and dibenzo(ah)anthracene, respectively. In the present study, both pollutants presented a Hazard Index of 5.34. Indeno(123-cd)pyrene, with a toxicity of 0.1 B[a]P-eq, accounted for a hazardous level of 5.15. Some of the remaining 16 PAHs appeared jointly with heavy metals, whereas the lightest hydrocarbons (i.e., naphthalene, acenaphthylene) seemed to be the less hazardous compounds. In spite of their high half-lives in all the environmental compartments, inorganic pollutants showed a low Hazard Index, mainly because of their extremely low bioaccumulation factors. Among these pollutants, As, Cd and Cr^{6+} were the most dangerous. In fact, these elements seemed to be even more toxic and persistent than PCDD/Fs. However, bioaccumulation was negligible. It must be taken into account that EPIWin software cannot derive a bioaccumulation factor for inorganic chemicals. Consequently, an extremely low value of 0.5 is supposed for all heavy metals. Although it is known that elements can bioaccumulate differently, a large uncertainty still remains around the establishment of reliable values of accumulation in the human body, based on a common base.

5.3.2 Case study

In 2002, a large environmental program was started near the petrochemical area of Tarragona. The levels of PCDD/Fs, PCBs, PAHs and 7 heavy metals were determined in several soil samples. The organic pollutants presented a very similar profile: the highest levels were found in soils collected in the chemical and the residential areas. These were followed, by far, by samples corresponding to the petrochemical zone, whose concentrations were only slightly higher than those of the unpolluted sampling sites. Differences between the most concentrated (chemical and residential areas) and the less impacted (petrochemical and unpolluted zone) were significant for PCDD/Fs and PCBs. However, for PAHs, they did not reach the level of statistical significance. With regard to heavy metals, industrial levels were also higher than those found in samples corresponding to urban and unpolluted areas.

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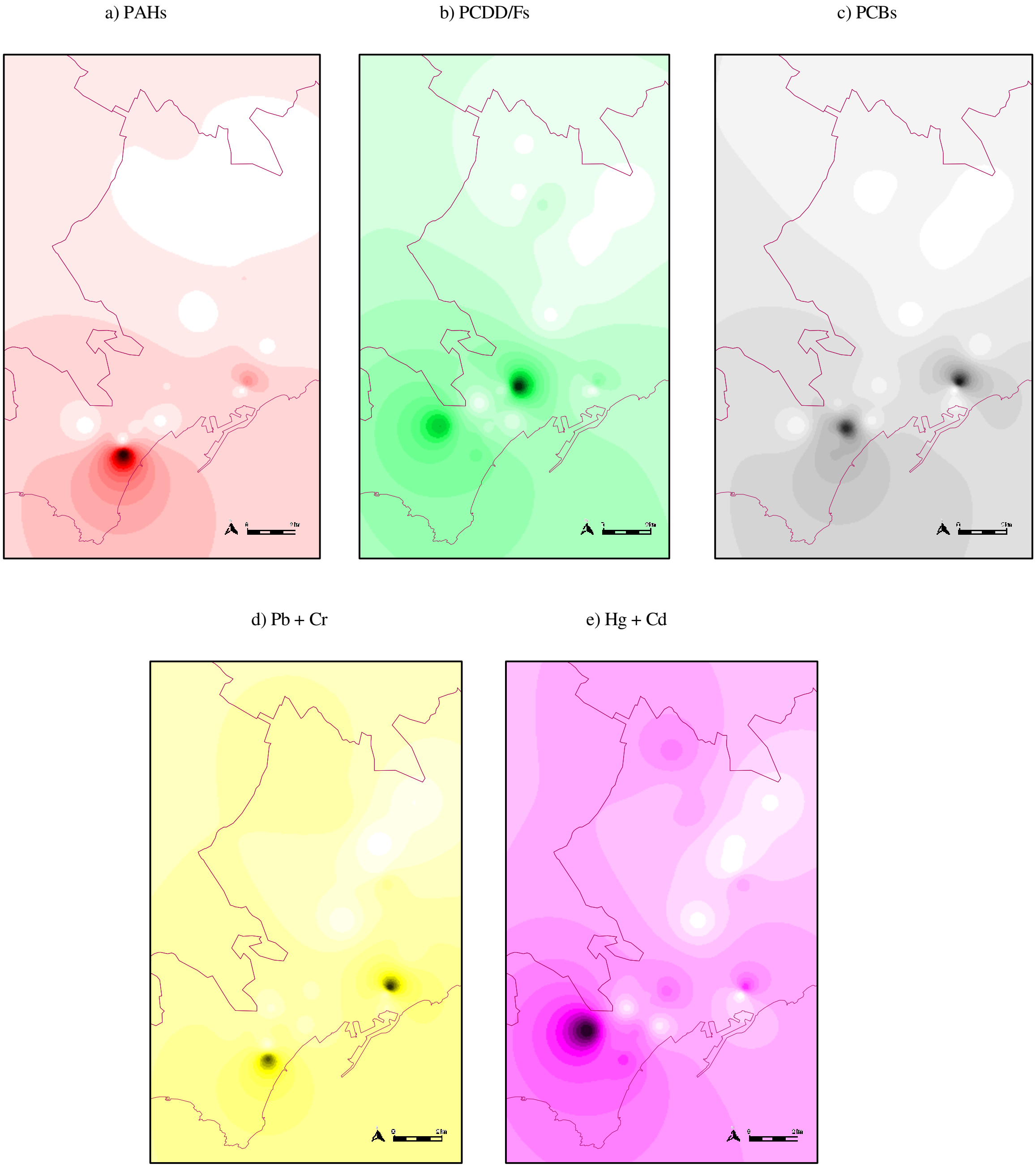

Figure 5. 4: Spatial distribution of the levels of various pollutants in soil samples collected in the industrial area of Tarragona, Spain

Geospatial analysis of data was developed in order to establish a possible common pattern of pollution according to the levels of contaminants. The spatial distribution of the concentrations in soils of PCDD/Fs, PCBs, PAHs, as well as two groups of heavy metals (Pb and Cr, and Hg and Cd) is depicted in Figure 5.4. Resulting maps for PAHs, PCBs and

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Pb were similar. Two different "hot spots" were identified: 1) in the south-western corner of the chemical area, basically due to the fact that predominant wind blows from north, pollutants released to air by industries are deposited here, and 2) in Tarragona downtown, where traffic is known to be a major source of pollution, specially of PAHs and Pb. In turn, although levels of Hg and Cd were relatively high in the urban area, it was observed that the most impacted area by these elements was the western part of the chemical pole. The reason could be due to the presence of an important chlor-alkali plant in this zone. Likewise, the georeferenced map for PCDD/Fs suggested that this source might be a potential source of PCDD/Fs. Notable levels of PCDD/Fs were also found in a sampling point located in the northern area of the chemical pole, which is adjacent to a residential suburb. It has been suggested that uncontrolled waste could have been previously dumped in this specific location (Schuhmacher et al., 2004).

A GIS-characterization based on the Integral Risk Index in the industrial area of Tarragona was carried out. According to equation 1**,** the Integral Risk Index corresponding to each sampling point was calculated. Since concentration profiles were similar for all pollutants, the resulting pattern was expected. The chemical and residential areas showed the highest Risk Index, with values of 1.49 ± 0.62 and 1.01 ± 0.52, respectively. Statistically significant lower levels of risk ($p < 0.01$) were observed in the petrochemical and unpolluted zones (0.44 ± 0.72 and 0.20 ± 0.59, respectively). The risk map of the industrial area of Tarragona, considered as the spatial distribution of the Integral Risk Index, is depicted in Figure 5.5. Three "hot spots" were identified, with pollution levels remarkably higher than the mean of contamination of the region. A large area comprising the SW and W corners of the chemical area were the most impacted zone, with a risk value up to 2.33. This relative high risk area might be due to the concentration of highly hazardous compounds, such as PCBs and PCDD/Fs, together with other chemicals (i.e., PAHs, Pb and V). However, special attention should be paid to the other "hot spots", because they belong to inhabited areas. Northern part of the southern pole presented higher levels of PCDD/Fs, while pollution in Tarragona downtown was due to a mixture of different chemicals (PCBs, Pb and PAHs, mainly). Since this tool is oriented to help

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making-decision stakeholders, and human health is the main aspect to be protected in risk management policies, polluted residential areas should be specially taken into account.

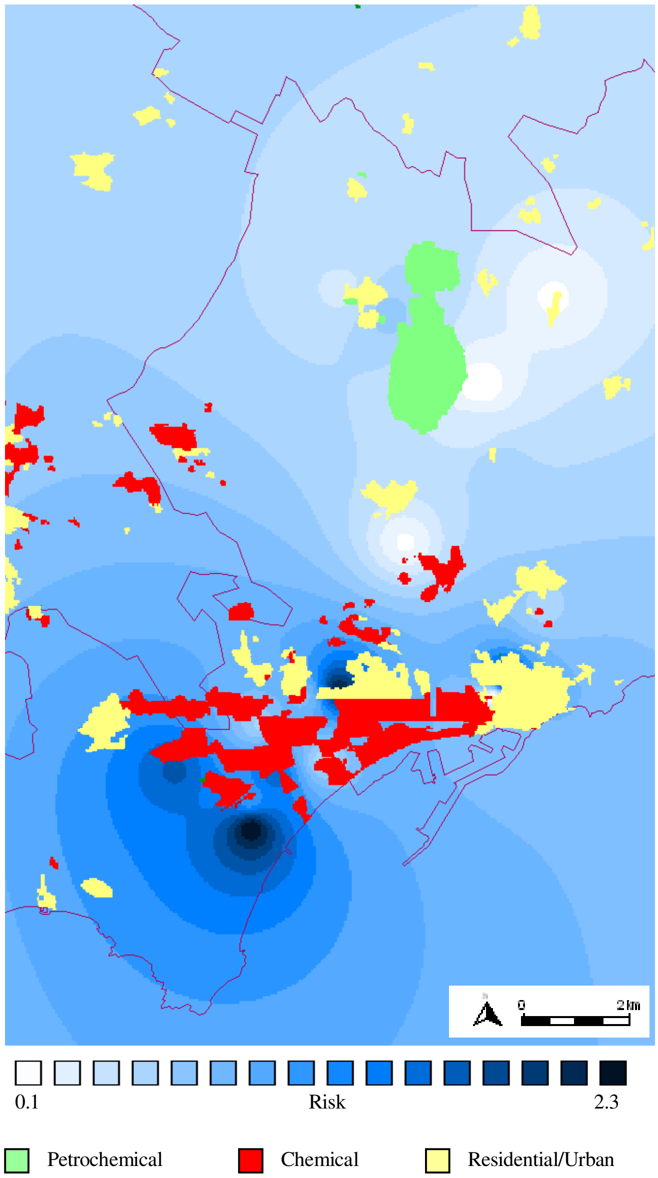

Figure 5.5: Risk map of the chemical/petrochemical area of Tarragona, Spain

In spite of the above, the GIS-based Integral Risk Index is only a relative way to show the risk of a particular area. In these terms, a maximum Risk Index was calculated on the basis of maximum allowed concentrations of different pollutants in soils according to the Catalan and Spanish legislations (BOE, 2005; Busquet, 1997). Thus, considering the

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soil quality guidelines of several heavy metals (As, Cd, Cr, Hg, and Pb), PAHs, and PCBs, the Maximum Integral Risk Index would be around 130 (Table 5.3). It is again corroborated that, although some specific zones of the chemical and residential areas of Tarragona could present a relative higher risk than others, the current environmental pollution does not pose, in principle, a significant risk for the population living in the vicinity of the chemical/petrochemical area.

Table 5.3: Maximum allowed concentrations (mg/kg) of heavy metals[a], PAHs[b] and PCBs[b] according to the Catalan and Spanish legislations

Arsenic	30	Pyrene	6
Cadmium	3.50	Chrysene	20
Chromium	200	Benzo(a)anthracene	0.20
Mercury	10	Benzo(k)fluoranthene	2
Lead	300	Benzo(b)fluoranthene	0.2
Naphthalene	1	Benzo(a)pyrene	0.02
Acenapthene	6	Indeno(123-cd)pyrene	0.3
Fluorene	5	Dibenzo(ah)anthracene	0.03
Anthracene	45	□ PCB	0.01
Fluoranthene	8		
Maximum Integral Risk Index			**130.8**

Risk communication and risk management can be defined as two subsequent stages of the health risk assessment process, consisting on 4 steps: hazard identification, dose-response analysis, exposure assessment, and risk characterization (Goldstein, 2005; NRC, 1993). These two further stages are more related to risk perception of public and political authorities, and they involve not only scientists, but also all other stakeholders (politicians, general public, technicians…). In recent years, different approaches such as Decision Support Systems, have been developed in order to give real alternatives to help the members who take part in the ultimate process of making-decision (Gheorghe & Vamanu, 2004; Pojana et al., 2003). Therefore, the development of friendly-visualize tools to help the making-decision stakeholders has been proved to be important. We think that the role of the scientist must emphasize other aspects of risk analysis, such as risk communication and management. Considering this, in the present study the Integral Risk Index has been defined and presented as a new methodology to carry out integral risk assessments due to chemical mixtures. The GIS-characterization of this Index might be a first approach to present diverse data of environmental pollution, which could make easier the making-decision process. Anyhow, further studies should be focused on applying this technique to other presumably polluted areas and/or enlarge the number of chemicals to be incorporated. Moreover, uncertainty related to data knowledge of the pollutants and the land scenarios should be added as an additional measure to check the validity of the Integral Risk Index.

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CHAPTER 6

APPLICABILITY OF A NEURO-PROBABILISTIC INTEGRAL RISK INDEX FOR THE ENVIRONMENTAL MANAGEMENT OF POLLUTED AREAS: A CASE-STUDY

Abstract

Recently, we developed a GIS-integrated Integral Risk Index (IRI) to assess human health risks in areas with presence of environmental pollutants. Contaminants were previously ranked by applying a Self-Organizing Map (SOM) to their characteristics of persistence, bioaccumulation, and toxicity in order to obtain the Hazard Index (HI). In the present study, the original IRI was substantially improved by allowing the entrance of probabilistic data. A Neuro-Probabilistic HI was developed by combining SOM and Monte-Carlo analysis. In general terms, the deterministic and probabilistic HIs followed a similar pattern: polychlorinated biphenyls (PCBs) and light polycyclic aromatic hydrocarbons (PAHs) were the pollutants showing the highest and lowest values of HI, respectively. However, the bioaccumulation value of heavy metals notably increased after considering a probability density function to explain the bioaccumulation factor. To check its applicability, a case-study was investigated. The probabilistic integral risk was calculated in the chemical/petrochemical industrial area of Tarragona (Catalonia, Spain), where an environmental program is being carried out since 2002. The risk change between 2002 and 2005 was evaluated on the basis of probabilistic data of the levels of various pollutants in soils. The results indicated that the risk of the chemicals under study did not follow an homogeneous tendency. However, the current levels of pollution do not mean a relevant source of health risks for the local population. Moreover, the Neuro-Probabilistic HI seems to be an adequate tool to be taken into account in risk assessment processes.

Key Words: *Probabilistic self-organizing maps; Monte-Carlo; Hazard Index; integral risk; Tarragona (Catalonia, Spain)*

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6.1 Introduction

Chemicals are present in the environment mainly as a result of human activities (industries, traffic, agriculture…) or the release from natural sources. Humans may be potentially exposed to an important amount of hazardous substances. In the last decade, several methodologies of chemicals prioritization have been studied and/or started to be used by national agencies, international organizations, and private companies. For instance, the European Risk Ranking Method (EURAM) and the Chemicals Hazard Evaluation for Management Strategies (CHEMS) have been developed by the European Union and the US EPA, respectively.(Hansen et al., 1999; Swanson et al., 1997) Their ultimate aim is not only to screen or to rank sets of chemicals, but also to help in the decision-making process through human health risk assessment. In addition, because of the need to assess global pollution, instead of considering individual components the importance of developing multicomponent risk indexes has increased in recent years.

A common criterion about the best mathematical approach to be used in the construction of rankings has not been established yet. In recent years, based on the capacity to predict and to classify information, Artificial Neural Networs (ANNs) have become a very useful tool to manage large databases.(Wang et al., 2004) Moreover, when combined to Geographic Information Systems (GIS), ANN can help to identify patterns from remotely sensed data.(Shatkin & Qian, 2004) Among the different kinds of ANNs, Kohonen's Self-Organizing Maps (SOM) are one of the most used. In environmental studies, they have been commonly used to characterize pollution of specific areas and forecast future situations.(Ferré-Huguet et al., 2006; Tran et al., 2003) On the other hand, most methodologies to prioritize chemicals are based on Persistence, Bioaccumulation and Toxicity (PBT) characteristics of the substances.(Bodar et al., 2002; Carlsen & Walker, 2003; Mekenyan et al., 2005; Moss et al., 2001) In 2005, we developed a SOM-based integral risk index on the basis of PBT characteristics of a set of 41 inorganic and organic pollutants. The applicability was examined in a case-study.(Nadal et al., 2006)

Since 1980s, it has been observed that the variability and uncertainty are becoming critical in the 4-steps process of human health risk assessment. The uncertainty stems from

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partial ignorance or lack of perfect knowledge, while variability explains the heterogeneity inherit to the population.(Matthies et al., 2004; US EPA, 2001) Consequently, risk assessment must be performed from a probabilistic point of view, rather than by considering deterministic aspects. Among the probabilistic tools, in order to include the above aspects the use of Monte-Carlo analysis has been increasing in recent years.(Binkowitz & Wartenberg, 2001; Burmaster & Anderson, 1994; Lester et al., 2007; Nadal et al., 2004d; Öberg & Bergbäck, 2005; Price et al., 1996; Sander et al., 2006; Sanga et al., 2001; Sharma et al., 2005; Smith, 1994) This method has the advantage of allowing the analyst to account for relationships between input variables and to provide the flexibility to investigate the effects of different modeling assumptions.(US EPA, 1997a)

Since risk assessment tools must include aspects of probability, the previously developed index risk(Nadal et al., 2006) was implemented by including Monte-Carlo analysis. In the present study, Monte-Carlo and SOM were integrated in order to create a neuro-probabilistic risk index by applying Probabilistic Artificial Neural Networks. Specifically, a Probabilistic SOM (PRSOM) was applied by varying the SOM mathematical algorithm to allow the entrance of probability density functions (PDFs) instead of point values.(Anouar et al., 1998; Saraceno et al., 2006; Wu & Chow, 2005) On the other hand, the applicability of the index was investigated in a case-study: the chemical/petrochemical industrial zone of Tarragona (Catalonia, Spain), where a wide environmental monitoring program is currently being carried out.

6.2 Methods

6.2.1 **Hazard Index**

The construction of the Hazard Index (HI) was previously described.(Nadal et al., 2006) In general terms, it stands on 3 variables: human toxicity (differentiating cancer and non-cancer effects), bioaccumulation potential, and persistence (PBT). Other methodologies, such as the Waste Minimization Prioritization Tool (WMPT) developed by the US EPA(Pennington & Bare, 2001; US EPA, 1998) are based on the same parameters. However, while the same weight is given by the WMPT for the 3 variables, the weighting is slightly different in the HI. Thus, while persistence and bioaccumulation scores can

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account for up to 3 each, toxicity can reach the value of 4. In addition, in the present study HI was constructed using a probabilistic approach. It is acknowledged that risk assessment factors can mostly be described by lognormal distributions.(Haas, 1997; Slob & Pieters, 1998; Swartout et al., 1998) In the current study, the following parameters were used:

a) Persistence: Half-lives in air, water, soil and sediments. The original values were obtained from Mackay et al.(2000) According to Webster et al.(Webster et al., 2005) the persistence of the chemicals can be classified into 10 classes depending on their mean half-life. For each one of these 10 classes, a range of half-lives is also given. The extreme values of this range can be taken as the minimum and maximum half-lives. Thus, a chemical is included in that specific persistence class. Considering the mean, maximum and minimum values, a triangular distribution could be constructed. Finally, the triangular distribution was approximated to a lognormal distribution. The corresponding standard deviation was calculated on the basis of the following expression:

$$\text{St.Dev.} = \sqrt{\frac{a^2 + b^2 + c^2 - ab - ac - bc}{18}}$$

where a, b and c are the minimum, maximum and mean values, respectively.(Fiorito, 2006)

b) Bioaccumulation: Bioconcentration factor logarithm (log BCF). The mean BCF was obtained from the octanol-water constant (K_{ow}) by applying EPI software BCFWin.(Meylan, 1999) The standard deviation of the lognormal distribution corresponding to each chemical was calculated by setting a coefficient of variance (CV) of 0.58.(Lessmann et al., 2005) The CV is the ratio of the standard deviation and the mean of a given property.

c) Toxicity: Non-cancer and cancer properties were separately considered. Non-carcinogenic effects were assessed by means of the Reference Dose (RfD), while carcinogenic effects were evaluated with the Slope Factor (SF). The values corresponding to 3 pathways (ingestion, inhalation and dermal absorption) were used. All these parameters were obtained from the Risk Assessment Information System website.(RAIS, 2006) Because of the difficulty to obtain reliable

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probabilistic data, a conservative value of CV=0.9 was considered.(Lessmann, 2002) This is really arbitrary and reflects a high degree of uncertainty. However, this value has been used for determined environmental parameters in probabilistic exposure assessment in order to cover a range of two orders of magnitude.(Matthies et al., 2004)

In the present study, the HI was calculated for a set of 41 chemicals: arsenic plus various heavy metals (Cd, Cr-VI, Cr-III, Pb, Mn, Hg and V), 10 polychlorinated dibenzo-p-dioxins and furans (PCDD/F) homologues, 7 PCBs (environmental markers; numbers 28, 52, 101, 118, 153, 138 and 180) and, finally, 16 US EPA priority PAHs. The Monte-Carlo distributions of the 11 PBT parameters are summarized in Table I.

A PRSOM was applied to the PBT data. The original SOM algorithm was modified to accept probabilistic instead of deterministic data. In our previous study,(Nadal et al., 2006) the SOM algorithm was modified to get an internal normalized weight vector as an ordered index of pollutant. In the SOM process, the weight initialization is a random process, and the final outcome of weight vector always depends on initial weight, although it is run over many times. To improve the quality of the index, SOM and Monte-Carlo techniques were converted into a Probabilistic SOM.

The SOM criteria were the same as those of our previous study.(Nadal et al., 2006) The map structure was based on a rectangular grid with 96 (12 x 8) hexagons. Likewise, the learning and tuning phases consisted on 10,000 steps. The resulting Kohonen's map indicates the position of the 41 chemicals, which are spread over the grid according to PBT affinities. Complementarily, 2 component planes (or c-planes) are obtained. The first c-plane shows the normalized (0-1) mean values, whereas the second one illustrates the standard deviations. The position of each pollutant in the grid is the same in the map and the c-planes. Consequently, the mean and standard deviation of the HI corresponding to each of the 41 pollutants may be easily obtained. Subsequently, these values were introduced into the Crystall Ball software, where the lognormal PDFs of the 11 PBT parameters were constructed. The following weightings, derived from a slight modification of the US EPA WMPT,(Pennington & Bare, 2001; US EPA, 1998) were then applied to the whole probabilistic parameters: 3 to each persistence and bioaccumulation, and 2 to each

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non-carcinogenic and carcinogenic toxicities. The minimum and maximum values of the HI were 0 and 10, respectively.

In recent years, an important scientific effort has been made to assess the exposure of pollutant mixtures. One of the most important difficulties is the study of potential interactions (synergism or antagonism) when the effects following an exposure to various chemicals are assessed. In fact, the impact of mixtures has been found to be substantially more severe than the linear addition of the impacts of each of these substances only.(Dietz & van der Straaten, 1992) In the present study, a number of inorganic (heavy metals) and organic (PCDD/Fs, PAHs, and PCBs) pollutants were included. PCDD/Fs and PCBs have similar PBT characteristics. Currently, the toxic impact of the different congeners of both pollutants is estimated/given in TEQ (Toxic Equivalents), and the concentrations of PCDD/Fs and PCBs are generally given as a linear sum of the individual TEQ of each group of chemicals. Moreover, since some PAHs show a toxicity mechanism similar to the chlorinated compounds, a PAH TEF-based approach, similar to that of PCDD/Fs, has also been developed. Consequently, a linear aggregation was considered as a good approach for the assessment of a mixtures of the pollutants here analyzed.

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Table 6.1: Original values (mean ± standard deviation) of the 11 PBT parameters for the 41 assessed pollutants (Monte-Carlo distributions)

	BCF		HL-air		HL-water		HL-soil		HL-sedim	
As	3.16E+00	± 1.83E+00	5.50E+02	± 1.45E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
Cd	3.16E+00	± 1.83E+00	5.50E+02	± 1.45E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
Cr-III	3.16E+00	± 1.83E+00	5.50E+02	± 1.45E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
Cr-VI	3.16E+00	± 1.83E+00	5.50E+02	± 1.45E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
Pb	3.16E+00	± 1.83E+00	5.50E+02	± 1.45E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
Mn	3.16E+00	± 1.83E+00	5.50E+02	± 1.45E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
Hg	3.16E+00	± 1.83E+00	5.50E+02	± 1.45E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
V	3.16E+00	± 1.83E+00	5.50E+02	± 1.45E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
Acenaphthene	2.08E+02	± 1.21E+02	5.50E+01	± 1.45E+01	5.50E+02	± 1.45E+02	5.50E+03	± 1.45E+03	1.70E+04	± 4.14E+03
Acenaphthylene	2.16E+02	± 1.25E+02	5.50E+01	± 1.45E+01	5.50E+02	± 1.45E+02	5.50E+03	± 1.45E+03	1.70E+04	± 4.14E+03
Anthracene	5.33E+02	± 3.09E+02	5.50E+01	± 1.45E+01	5.50E+02	± 1.45E+02	5.50E+03	± 1.45E+03	1.70E+04	± 4.14E+03
Benz[a]anthracene	5.44E+03	± 3.15E+03	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Benzo[a]pyrene	1.05E+04	± 6.07E+03	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Benzo[b]fluoranthene	5.63E+03	± 3.27E+03	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Benzo[g,h,i]perylene	2.54E+04	± 1.47E+04	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Benzo[k]fluoranthene	1.01E+04	± 5.86E+03	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Chrysene	5.94E+03	± 3.44E+03	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Dibenz[a,h]anthracene	2.17E+04	± 1.26E+04	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Fluoranthene	1.88E+03	± 1.09E+03	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Fluorene	3.30E+02	± 1.91E+02	5.50E+01	± 1.45E+01	5.50E+02	± 1.45E+02	5.50E+03	± 1.45E+03	1.70E+04	± 4.14E+03
Indeno[1,2,3-cd]pyrene	2.86E+04	± 1.66E+04	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
Naphthalene	6.93E+01	± 4.02E+01	1.70E+01	± 4.00E+00	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	5.50E+03	± 1.45E+03
Phenanthrene	5.42E+02	± 3.15E+02	5.50E+01	± 1.45E+01	5.50E+02	± 1.45E+02	5.50E+03	± 1.45E+03	1.70E+04	± 4.14E+03
Pyrene	1.14E+03	± 6.62E+02	1.70E+02	± 4.14E+01	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
TCDD	4.25E+04	± 2.46E+04	1.70E+02	± 4.14E+01	5.50E+02	± 1.45E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
PeCDD	1.42E+04	± 8.21E+03	5.50E+02	± 1.45E+02	5.50E+02	± 1.45E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
HxCDD	1.43E+03	± 8.27E+02	5.50E+02	± 1.45E+02	1.70E+03	± 4.14E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
HpCDD	1.47E+03	± 8.50E+02	5.50E+02	± 1.45E+02	1.70E+03	± 4.14E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
OCDD	1.47E+03	± 8.50E+02	5.50E+02	± 1.45E+02	5.50E+03	± 1.45E+03	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
TCDF	1.40E+04	± 8.11E+03	1.70E+02	± 4.14E+01	5.50E+02	± 1.45E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
PeCDF	2.37E+04	± 1.37E+04	5.50E+02	± 1.45E+02	5.50E+02	± 1.45E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
HxCDF	1.03E+04	± 5.98E+03	5.50E+02	± 1.45E+02	5.50E+02	± 1.45E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
HpCDF	3.55E+03	± 2.06E+03	5.50E+02	± 1.45E+02	1.70E+03	± 4.14E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04
OCDF	4.15E+02	± 2.41E+02	5.50E+02	± 1.45E+02	5.50E+03	± 1.45E+03	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
PCB-28	1.77E+04	± 1.03E+04	5.50E+02	± 1.45E+02	1.70E+04	± 4.14E+03	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
PCB-52	4.07E+04	± 2.36E+04	1.70E+03	± 4.14E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
PCB-101	1.43E+05	± 8.31E+04	1.70E+03	± 4.14E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
PCB-118	1.84E+05	± 1.07E+05	1.70E+03	± 4.14E+02	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
PCB-153	6.72E+04	± 3.90E+04	5.50E+03	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
PCB-138	2.53E+04	± 1.47E+04	5.50E+03	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04
PCB-180	4.92E+03	± 2.85E+03	5.50E+03	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04	5.50E+04	± 1.45E+04

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Table 6.1 (cont.):Original values (mean ± standard deviation) of the 11 PBT parameters for the 41 assessed pollutants (Monte-Carlo distributions)

Der-RfD	Inh-RfD	Oral-RfD	Der-SF	Inh-SF	Oral-SF
8.13E+03 ± 7.32E+03	1.17E+00 ± 1.05E+00	3.33E+03 ± 3.00E+03	3.66E+00 ± 3.29E+00	1.51E+01 ± 1.36E+01	1.50E+00 ± 1.35E+00
1.00E+05 ± 9.00E+04	1.17E+00 ± 1.05E+00	1.00E+03 ± 9.00E+02	2.35E-05 ± 2.12E-05	6.30E+00 ± 5.67E+00	7.30E-06 ± 6.57E-06
1.33E+02 ± 1.20E+02	1.17E+00 ± 1.05E+00	6.67E-01 ± 6.00E-01	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
1.67E+04 ± 1.50E+04	3.50E+04 ± 3.15E+04	3.33E+02 ± 3.00E+02	2.35E-05 ± 2.12E-05	4.20E+01 ± 3.78E+01	7.30E-06 ± 6.57E-06
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
1.79E+02 ± 1.61E+02	6.99E+04 ± 6.29E+04	7.14E+00 ± 6.43E+00	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.76E+04 ± 4.29E+04	1.17E+00 ± 1.05E+00	3.33E+03 ± 3.00E+03	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
1.43E+04 ± 1.29E+04	1.17E+00 ± 1.05E+00	1.43E+02 ± 1.29E+02	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
5.38E+01 ± 4.84E+01	1.17E+00 ± 1.05E+00	1.67E+01 ± 1.50E+01	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.39E+00 ± 3.95E+00	1.17E+00 ± 1.05E+00	3.33E+00 ± 3.00E+00	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E+00 ± 2.12E+00	3.08E-01 ± 2.77E-01	7.30E-01 ± 6.57E-01
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E+01 ± 2.12E+01	3.08E+00 ± 2.77E+00	7.30E+00 ± 6.57E+00
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E+00 ± 2.12E+00	3.08E-01 ± 2.77E-01	7.30E-01 ± 6.57E-01
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E-01 ± 2.12E-01	3.08E-02 ± 2.77E-02	7.30E-02 ± 6.57E-02
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E-02 ± 2.12E-02	3.08E-03 ± 2.77E-03	7.30E-03 ± 6.57E-03
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E+01 ± 2.12E+01	3.08E+00 ± 2.77E+00	7.30E+00 ± 6.57E+00
8.06E+01 ± 7.26E+01	1.17E+00 ± 1.05E+00	2.50E+01 ± 2.25E+01	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
5.00E+01 ± 4.50E+01	1.17E+00 ± 1.05E+00	2.50E+01 ± 2.25E+01	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E+00 ± 2.12E+00	3.08E-01 ± 2.77E-01	7.30E-01 ± 6.57E-01
6.25E+01 ± 5.63E+01	1.17E+03 ± 1.05E+03	5.00E+01 ± 4.50E+01	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
1.08E+02 ± 9.68E+01	1.17E+00 ± 1.05E+00	3.33E+01 ± 3.00E+01	2.35E-05 ± 2.12E-05	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	3.00E+05 ± 2.70E+05	1.16E+05 ± 1.04E+05	1.50E+05 ± 1.35E+05
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	1.50E+05 ± 1.35E+05	5.78E+04 ± 5.20E+04	7.50E+04 ± 6.75E+04
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	3.00E+04 ± 2.70E+04	1.16E+04 ± 1.04E+04	1.50E+04 ± 1.35E+04
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	3.00E+03 ± 2.70E+03	1.16E+03 ± 1.04E+03	1.50E+03 ± 1.35E+03
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	3.00E+02 ± 2.70E+02	1.16E+02 ± 1.04E+02	1.50E+02 ± 1.35E+02
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	3.00E+04 ± 2.70E+04	3.08E-06 ± 2.77E-06	7.30E-06 ± 6.57E-06
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	1.50E+04 ± 1.35E+04	5.78E+03 ± 5.20E+03	7.50E+03 ± 6.75E+03
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	3.00E+04 ± 2.70E+04	1.16E+04 ± 1.04E+04	1.50E+04 ± 1.35E+04
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	3.00E+03 ± 2.70E+03	1.16E+03 ± 1.04E+03	1.50E+03 ± 1.35E+03
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	3.00E+02 ± 2.70E+02	1.16E+02 ± 1.04E+02	1.50E+02 ± 1.35E+02
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.22E+00 ± 2.00E+00	2.00E+00 ± 1.80E+00	2.00E+00 ± 1.80E+00
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.22E+00 ± 2.00E+00	2.00E+00 ± 1.80E+00	2.00E+00 ± 1.80E+00
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.22E+00 ± 2.00E+00	2.00E+00 ± 1.80E+00	2.00E+00 ± 1.80E+00
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.22E+00 ± 2.00E+00	2.00E+00 ± 1.80E+00	2.00E+00 ± 1.80E+00
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.22E+00 ± 2.00E+00	2.00E+00 ± 1.80E+00	2.00E+00 ± 1.80E+00
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.22E+00 ± 2.00E+00	2.00E+00 ± 1.80E+00	2.00E+00 ± 1.80E+00
4.39E-03 ± 3.95E-03	1.17E+00 ± 1.05E+00	6.67E-04 ± 6.00E-04	2.22E+00 ± 2.00E+00	2.00E+00 ± 1.80E+00	2.00E+00 ± 1.80E+00

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Table 6.2: Concentration of the 41 organic and inorganic pollutants in soils of Tarragona, in the 2002 and 2005 surveys

	2002				2005			
	Chemical	*Petrochemical*	*Urban/Resid.*	*Unpolluted*	*Chemical*	*Petrochemical*	*Urban/Resid.*	*Unpolluted*
As	5.79 ± 0.74	5.17 ± 1.83	4.15 ± 1.66	5.30 ± 1.42	6.24 ± 4.10	6.51 ± 2.64	3.82 ± 2.2	4.23 ± 1.82
Cd	0.25 ± 0.1	0.17 ± 0.08	0.19 ± 0.07	0.15 ± 0.05	0.16 ± 0.08	0.21 ± 0.06	0.14 ± 0.09	0.11 ± 0.03
Cr-III	13.25 ± 2.33	9.42 ± 3.08	8.5 ± 2.7	1.43 ± 0.33	14.58 ± 6.58	13.8 ± 5.75	11.4 ± 3.75	9.9 ± 3.17
Cr-VI	2.65 ± 0.47	1.88 ± 0.62	1.7 ± 0.5	7.17 ± 0.07	2.92 ± 1.32	2.75 ± 5.75	2.28 ± 0.75	1.98 ± 0.63
Pb	46.5 ± 36.5	24.6 ± 17.7	66.1 ± 49.2	14.6 ± 3.1	22.2 ± 13.0	37.8 ± 18.5	42.0 ± 34.9	18.3 ± 7.0
Mn	228.1 ± 77.5	194.7 ± 65.1	191.5 ± 71.8	188.9 ± 13.2	259.3 ± 116.6	268.9 ± 92.0	195.8 ± 67.7	234.8 ± 61.8
Hg	0.12 ± 0.09	0.04 ± 0.02	0.08 ± 0.07	0.04 ± 0.02	0.05 ± 0.07	0.04 ± 0.03	0.06 ± 0.07	0.02 ± 0.02
V	23.2 ± 6.6	14.8 ± 4.0	13.6 ± 3.3	12.2 ± 2.5	25.5 ± 11.4	22.7 ± 7.50	23.5 ± 8.5	18.8 ± 7.1
Acenaphthene	1.3 ± 0.8	1.0 ± 1.0	4.8 ± 3.9	1.0 ± 1.0	1.3 ± 0.9	2.0 ± 1.4	1.9 ± 2.3	1.4 ± 0.9
Acenaphthylene	14 ± 12	12.3 ± 8.7	23 ± 19	4.2 ± 3.7	6.0 ± 10.5	0.5 ± 0.5	3.0 ± 2.3	1.5 ± 1.0
Anthracene	51 ± 90	3.1 ± 4.5	17 ± 27	1.0 ± 1.0	11.4 ± 28.4	7.5 ± 9.4	7.5 ± 9.2	2.4 ± 1.8
Benz[a]anthracene	137 ± 256	11.5 ± 9.4	68 ± 73	1.9 ± 2.4	65.3 ± 180.1	19.3 ± 17.6	27.3 ± 41.8	7.8 ± 13.6
Benzo[a]pyrene	100 ± 130	18 ± 14	56 ± 77	22 ± 24	55.7 ± 144.4	22.5 ± 21.3	35.2 ± 47.7	10.4 ± 18.8
Benzo[b]fluoranthene	9 ± 16	2.9 ± 4.0	2.4 ± 2.6	2.3 ± 1.5	145.9 ± 405.1	27.9 ± 24.1	49.8 ± 67.5	12.2 ± 17.4
Benzo[g,h,i]perylene	41 ± 39	17 ± 12	40 ± 35	50 ± 85	31.3 ± 68.2	15.7 ± 12.8	31.3 ± 37.7	6.3 ± 9.8
Benzo[k]fluoranthene	9.0 ± 9.5	13 ± 17	47 ± 41	1.2 ± 0.4	51.8 ± 143	11.0 ± 10.1	19.2 ± 26.2	5.0 ± 8.0
Chrysene	120 ± 200	14 ± 15	68 ± 73	3.7 ± 5.4	113.3 ± 317.4	21.8 ± 20.5	34 ± 40.9	8.2 ± 12.2
Dibenz[a,h]anthracene	6 ± 13	1.8 ± 1.6	21 ± 25	1.0 ± 1.0	10.7 ± 26.5	4.0 ± 3.0	6.3 ± 8.0	2.2 ± 2.4
Fluoranthene	180 ± 292	21 ± 15	97 ± 115	5.6 ± 3.5	73.7 ± 177.3	44.0 ± 47.1	69.2 ± 87	40.8 ± 39.6
Fluorene	23 ± 49	2.1 ± 1.5	13 ± 21	1.1 ± 0.2	1.1 ± 0.4	0.5 ± 0.5	0.5 ± 0.5	0.5 ± 0.5
Indeno[1,2,3-cd]pyrene	16 ± 20	9 ± 14	60 ± 72	5.3 ± 7.6	33.4 ± 81.6	13.3 ± 10.4	35.2 ± 47	7.1 ± 12.3
Naphthalene	5 ± 10	3.7 ± 3.6	8.3 ± 9.5	1.0 ± 1.0	24.4 ± 19.5	16.6 ± 4.6	21.2 ± 9.4	15.5 ± 11.9
Phenanthrene	131 ± 269	16 ± 16	114 ± 101	7.9 ± 6.3	19.9 ± 21.5	33.9 ± 41.7	37.8 ± 38.4	82.1 ± 138.5
Pyrene	159 ± 268	20 ± 23	96 ± 125	2.5 ± 3.0	140.5 ± 376.2	39.8 ± 43.2	58 ± 74.7	37.6 ± 39.4
TCDD	3.72 ± 1.95	1.48 ± 1.37	3.70 ± 3.83	0.57 ± 0.72	na	na	na	na
PeCDD	4.37 ± 3.78	1.62 ± 1.71	3.60 ± 3.42	0.60 ± 0.61	na	na	na	na
HxCDD	10.05 ± 8.05	2.32 ± 2.21	8.15 ± 5.12	0.89 ± 0.55	na	na	na	na
HpCDD	32.63 ± 28.46	5.32 ± 3.95	34.10 ± 22.95	1.95 ± 1.34	na	na	na	na
OCDD	127.6 ± 134.7	28.5 ± 22.34	155.9 ± 123	6.85 ± 5.25	na	na	na	na
TCDF	21.25 ± 25.35	5.20 ± 5.47	8.98 ± 8.71	1.67 ± 0.87	na	na	na	na
PeCDF	14.15 ± 14.86	3.37 ± 3.93	8.40 ± 6.64	1.24 ± 0.69	na	na	na	na
HxCDF	26.64 ± 29.40	4.62 ± 4.65	14.88 ± 14.13	1.46 ± 0.55	na	na	na	na
HpCDF	25.91 ± 20.68	2.97 ± 2.27	10.59 ± 9.85	0.90 ± 0.34	na	na	na	na
OCDF	93.16 ± 115.8	4.74 ± 3.03	10.87 ± 8.65	1.41 ± 1.00	na	na	na	na
PCB-28	43 ± 9	41 ± 37	28 ± 19	8 ± 6	67 ± 84	59 ± 50	48 ± 41	19 ± 19
PCB-52	463 ± 1102	46 ± 42	231 ± 341	13 ± 8	56 ± 62	204 ± 309	35 ± 39	19 ± 19
PCB-101	1436 ± 2544	167 ± 113	1074 ± 1556	75 ± 58	295 ± 328	752 ± 1334	216 ± 179	47 ± 64
PCB-118	949 ± 1733	164 ± 97	716 ± 1029	54 ± 49	195 ± 237	1081 ± 1933	197 ± 276	44 ± 27
PCB-153	2660 ± 2348	477 ± 340	2266 ± 3659	144 ± 84	1193 ± 1252	922 ± 1285	1148 ± 1057	216 ± 250
PCB-138	3036 ± 3032	564 ± 414	3098 ± 5425	196 ± 114	941 ± 1011	1115 ± 1704	845 ± 713	146 ± 128
PCB-180	3452 ± 3005	505 ± 373	2930 ± 4793	169 ± 83	1886 ± 2125	540 ± 864	1946 ± 2247	275 ± 358

na: not analyzed. Units: heavy metals = μg/g dry weight; PAHs = ng/g dry weight; PCDD/F homologues and PCB congeners = ng/kg dry weight.

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Table 6.3: Values (mean ± standard deviation) of the 11 PTB parameters for the 41 assessed pollutants (SOM distributions)

	BCF	HL-air	HL-water	HL-soil	HL-sedim
As	0.07 ± 0.18	0.26 ± 0.34	0.86 ± 0.34	0.90 ± 0.24	1.00 ± 0.03
Cd	0.07 ± 0.18	0.33 ± 0.29	0.86 ± 0.34	0.90 ± 0.24	1.00 ± 0.03
Cr-III	0.06 ± 0.19	0.36 ± 0.37	0.83 ± 0.34	0.88 ± 0.24	1.00 ± 0.01
Cr-VI	0.07 ± 0.20	0.30 ± 0.36	0.84 ± 0.35	0.95 ± 0.13	1.00 ± 0.01
Pb	0.06 ± 0.19	0.36 ± 0.37	0.83 ± 0.34	0.88 ± 0.24	1.00 ± 0.01
Mn	0.07 ± 0.20	0.29 ± 0.37	0.80 ± 0.37	0.95 ± 0.15	1.00 ± 0.01
Hg	0.07 ± 0.18	0.26 ± 0.34	0.86 ± 0.34	0.90 ± 0.24	1.00 ± 0.03
V	0.06 ± 0.19	0.33 ± 0.34	0.86 ± 0.34	0.90 ± 0.23	1.00 ± 0.02
Acenaphthene	0.08 ± 0.18	0.23 ± 0.33	0.14 ± 0.34	0.20 ± 0.32	0.36 ± 0.27
Acenaphthylene	0.08 ± 0.18	0.23 ± 0.33	0.14 ± 0.34	0.20 ± 0.32	0.36 ± 0.27
Anthracene	0.08 ± 0.18	0.23 ± 0.33	0.14 ± 0.34	0.20 ± 0.32	0.36 ± 0.27
Benz[a]anthracene	0.08 ± 0.19	0.30 ± 0.39	0.08 ± 0.15	0.36 ± 0.18	0.99 ± 0.02
Benzo[a]pyrene	0.09 ± 0.18	0.29 ± 0.36	0.13 ± 0.26	0.37 ± 0.23	0.98 ± 0.04
Benzo[b]fluoranthene	0.08 ± 0.19	0.30 ± 0.39	0.08 ± 0.15	0.36 ± 0.18	0.99 ± 0.02
Benzo[g,h,i]perylene	0.12 ± 0.19	0.31 ± 0.39	0.12 ± 0.24	0.36 ± 0.17	1.00 ± 0.01
Benzo[k]fluoranthene	0.09 ± 0.18	0.29 ± 0.36	0.13 ± 0.26	0.37 ± 0.23	0.98 ± 0.04
Chrysene	0.08 ± 0.19	0.30 ± 0.39	0.08 ± 0.15	0.36 ± 0.18	0.99 ± 0.02
Dibenz[a,h]anthracene	0.12 ± 0.19	0.31 ± 0.39	0.12 ± 0.24	0.36 ± 0.17	1.00 ± 0.01
Fluoranthene	0.07 ± 0.19	0.30 ± 0.39	0.09 ± 0.13	0.37 ± 0.25	0.91 ± 0.14
Fluorene	0.08 ± 0.18	0.23 ± 0.33	0.14 ± 0.34	0.20 ± 0.32	0.36 ± 0.27
Indeno[1,2,3-cd]pyrene	0.12 ± 0.19	0.31 ± 0.39	0.12 ± 0.24	0.36 ± 0.17	1.00 ± 0.01
Naphthalene	0.09 ± 0.23	0.28 ± 0.40	0.14 ± 0.33	0.19 ± 0.33	0.29 ± 0.29
Phenanthrene	0.08 ± 0.18	0.23 ± 0.33	0.14 ± 0.34	0.20 ± 0.32	0.36 ± 0.27
Pyrene	0.07 ± 0.19	0.30 ± 0.39	0.09 ± 0.13	0.37 ± 0.25	0.91 ± 0.14
TCDD	0.20 ± 0.18	0.31 ± 0.39	0.15 ± 0.34	0.39 ± 0.25	1.00 ± 0.02
PeCDD	0.17 ± 0.18	0.32 ± 0.38	0.15 ± 0.34	0.39 ± 0.25	1.00 ± 0.01
HxCDD	0.06 ± 0.19	0.35 ± 0.38	0.16 ± 0.31	0.92 ± 0.13	1.00 ± 0.01
HpCDD	0.06 ± 0.19	0.35 ± 0.38	0.17 ± 0.29	0.95 ± 0.09	1.00 ± 0.01
OCDD	0.06 ± 0.18	0.35 ± 0.38	0.15 ± 0.18	0.94 ± 0.16	0.97 ± 0.11
TCDF	0.12 ± 0.18	0.29 ± 0.35	0.15 ± 0.34	0.39 ± 0.25	1.00 ± 0.02
PeCDF	0.12 ± 0.18	0.29 ± 0.35	0.15 ± 0.34	0.39 ± 0.25	1.00 ± 0.02
HxCDF	0.12 ± 0.18	0.29 ± 0.34	0.15 ± 0.34	0.39 ± 0.25	1.00 ± 0.02
HpCDF	0.07 ± 0.19	0.30 ± 0.39	0.09 ± 0.13	0.37 ± 0.25	0.91 ± 0.14
OCDF	0.06 ± 0.18	0.35 ± 0.38	0.15 ± 0.18	0.94 ± 0.16	0.97 ± 0.11
PCB-28	0.24 ± 0.20	0.38 ± 0.37	0.34 ± 0.18	0.88 ± 0.31	0.91 ± 0.24
PCB-52	0.14 ± 0.18	0.46 ± 0.33	0.74 ± 0.31	0.88 ± 0.24	0.99 ± 0.03
PCB-101	0.73 ± 0.25	0.60 ± 0.33	0.86 ± 0.34	0.86 ± 0.34	0.88 ± 0.31
PCB-118	0.73 ± 0.25	0.60 ± 0.33	0.86 ± 0.34	0.86 ± 0.34	0.88 ± 0.31
PCB-153	0.25 ± 0.16	0.92 ± 0.11	0.86 ± 0.34	0.89 ± 0.27	0.97 ± 0.12
PCB-138	0.14 ± 0.16	0.85 ± 0.15	0.86 ± 0.34	0.90 ± 0.25	0.99 ± 0.08
PCB-180	0.14 ± 0.16	0.85 ± 0.15	0.86 ± 0.34	0.90 ± 0.25	0.99 ± 0.08

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Table 6.3 (cont.): Values (mean ± standard deviation) of the 11 PTB parameters for the 41 assessed pollutants (SOM distributions)

Der-RfD	Inh-RfD	Oral-RfD	Der-SF	Inh-SF	Oral-SF
0.40 ± 0.26	0.14 ± 0.33	0.80 ± 0.29	0.03 ± 0.10	0.03 ± 0.10	0.03 ± 0.10
0.47 ± 0.30	0.32 ± 0.34	0.35 ± 0.27	0.10 ± 0.25	0.10 ± 0.25	0.10 ± 0.25
0.20 ± 0.31	0.33 ± 0.36	0.17 ± 0.33	0.13 ± 0.32	0.13 ± 0.33	0.13 ± 0.33
0.26 ± 0.31	0.27 ± 0.35	0.27 ± 0.36	0.12 ± 0.30	0.12 ± 0.30	0.12 ± 0.30
0.20 ± 0.31	0.33 ± 0.36	0.17 ± 0.33	0.13 ± 0.32	0.13 ± 0.33	0.13 ± 0.33
0.21 ± 0.33	0.31 ± 0.41	0.24 ± 0.40	0.13 ± 0.32	0.13 ± 0.32	0.13 ± 0.32
0.40 ± 0.26	0.14 ± 0.33	0.80 ± 0.29	0.03 ± 0.10	0.03 ± 0.10	0.03 ± 0.10
0.29 ± 0.29	0.34 ± 0.32	0.22 ± 0.31	0.12 ± 0.30	0.12 ± 0.31	0.12 ± 0.31
0.13 ± 0.34	0.13 ± 0.32	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.34	0.13 ± 0.32	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.34	0.13 ± 0.32	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.33	0.12 ± 0.30	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.33	0.08 ± 0.23	0.13 ± 0.33	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.33	0.12 ± 0.30	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.33	0.07 ± 0.19	0.13 ± 0.33	0.14 ± 0.33	0.14 ± 0.34	0.14 ± 0.34
0.13 ± 0.33	0.08 ± 0.23	0.13 ± 0.33	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.33	0.12 ± 0.30	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.33	0.07 ± 0.19	0.13 ± 0.33	0.14 ± 0.33	0.14 ± 0.34	0.14 ± 0.34
0.14 ± 0.33	0.13 ± 0.34	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.34	0.13 ± 0.32	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.33	0.07 ± 0.19	0.13 ± 0.33	0.14 ± 0.33	0.14 ± 0.34	0.14 ± 0.34
0.13 ± 0.34	0.14 ± 0.34	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.34	0.13 ± 0.32	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.14 ± 0.33	0.13 ± 0.34	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.09 ± 0.22	0.13 ± 0.34	0.02 ± 0.09	0.86 ± 0.11	0.86 ± 0.11	0.86 ± 0.11
0.07 ± 0.18	0.13 ± 0.33	0.04 ± 0.12	0.68 ± 0.15	0.68 ± 0.15	0.68 ± 0.15
0.13 ± 0.33	0.13 ± 0.34	0.13 ± 0.33	0.20 ± 0.32	0.19 ± 0.32	0.20 ± 0.32
0.13 ± 0.33	0.13 ± 0.33	0.13 ± 0.34	0.16 ± 0.33	0.16 ± 0.33	0.16 ± 0.33
0.13 ± 0.33	0.13 ± 0.34	0.13 ± 0.34	0.14 ± 0.33	0.14 ± 0.33	0.14 ± 0.33
0.11 ± 0.29	0.07 ± 0.19	0.12 ± 0.32	0.18 ± 0.32	0.16 ± 0.33	0.16 ± 0.33
0.11 ± 0.29	0.07 ± 0.19	0.12 ± 0.32	0.18 ± 0.32	0.16 ± 0.33	0.16 ± 0.33
0.09 ± 0.23	0.10 ± 0.27	0.11 ± 0.29	0.24 ± 0.30	0.22 ± 0.31	0.22 ± 0.31
0.14 ± 0.33	0.13 ± 0.34	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.33	0.13 ± 0.34	0.13 ± 0.34	0.14 ± 0.33	0.14 ± 0.33	0.14 ± 0.33
0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.14 ± 0.33	0.22 ± 0.35	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.34	0.13 ± 0.33	0.13 ± 0.33	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.13 ± 0.34	0.13 ± 0.33	0.13 ± 0.33	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.14 ± 0.34	0.24 ± 0.35	0.14 ± 0.34	0.13 ± 0.34	0.13 ± 0.34	0.13 ± 0.34
0.17 ± 0.33	0.31 ± 0.37	0.15 ± 0.33	0.13 ± 0.33	0.13 ± 0.33	0.13 ± 0.33
0.17 ± 0.33	0.31 ± 0.37	0.15 ± 0.33	0.13 ± 0.33	0.13 ± 0.33	0.13 ± 0.33

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6.2.2 **Integral Risk Index**

The Integral Risk Index (IRI) was calculated using the following equation:

$$\text{Integral Risk Index} = \frac{\Sigma\ (\text{Hazard Index x Pollutant Concentration in Soil})}{\text{Number of Pollutants}}$$

The parameter *number of pollutants* allows to compare two or various zones, independently on the number of contaminants assessed. Moreover, the pollutant concentration must be normalized to be comparable.

In the previous study, the IRI of the chemical/petrochemical area of Tarragona was calculated and mapped out.(Nadal et al., 2006) Calculations were based on the concentrations of various inorganic and organic pollutants found in soils in 2002.(Nadal et al., 2004b, 2004c; Schuhmacher et al., 2004) In 2005, a 5-years environmental surveillance program was started in order to evaluate the temporal trends of the pollutant levels in the environment surrounding the same area of Tarragona. In the first survey, 27 soil samples were obtained in 4 different zones: chemical, petrochemical, urban, and unpolluted.(Nadal et al., 2007) The results corresponding to 2002 and 2005 surveys are summarized in Table 6.2. Lognormal distributions were constructed using the mean and standard deviation values corresponding to the 4 sampling areas for each of the surveys. In the present study, the IRI of the baseline study (2002) was again calculated from a probabilistic point of view. Moreover, the results of the 2005 study were used to assess the change of risk after 3 years.

6.3 Results And Discussion

6.3.1 **Hazard Index**

The resulting Kohonen's map after applying SOM to the 11 PBT parameters is depicted in Figure 6.1. The chemicals were grouped according to their similarities in persistence, bioaccumulation, and toxicity. Arsenic and heavy metals, and PCBs were located in the upper-left and upper-right sides of the grid, respectively. PCDD/F homologues appeared on the right of the map. In turn, the high molecular weight PAHs

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were found in the middle of the grid, while the most volatile PAHs were located in the lower-left corner. In turn, the component planes (c-planes) associated to the obtained map is shown in Figure 6.2. The c-planes represent the normalized values (0-1) of the mean and standard deviation for each parameter in a map. The position of each pollutant is the same in both, the Kohonen's map and the c-planes. The PDF of each parameter is then elaborated using the cell value occupied by the chemicals. This probabilistic value of the HI corresponding to each pollutant, extracted from the c-planes, is numerically summarized in Table III. The HI of the 41 evaluated chemicals, grouped in pollutant classes, as well as the percentages of persistence, bioaccumulation, and toxicity, are shown in Table 6.4. In addition, the HI in a descendent order is also depicted in Figure 6.3.

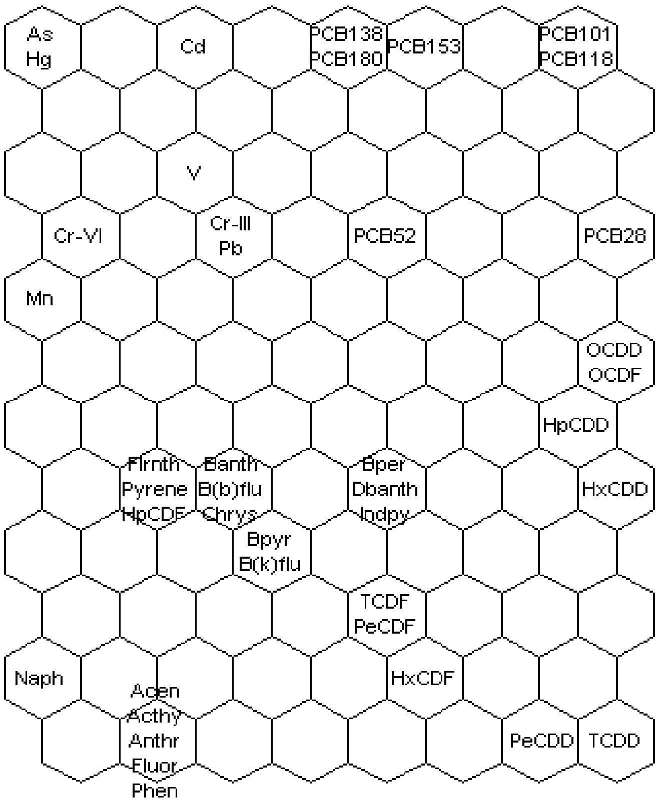

Figure 6.1: Self-organizing map obtained after applying the Probabilistic SOM

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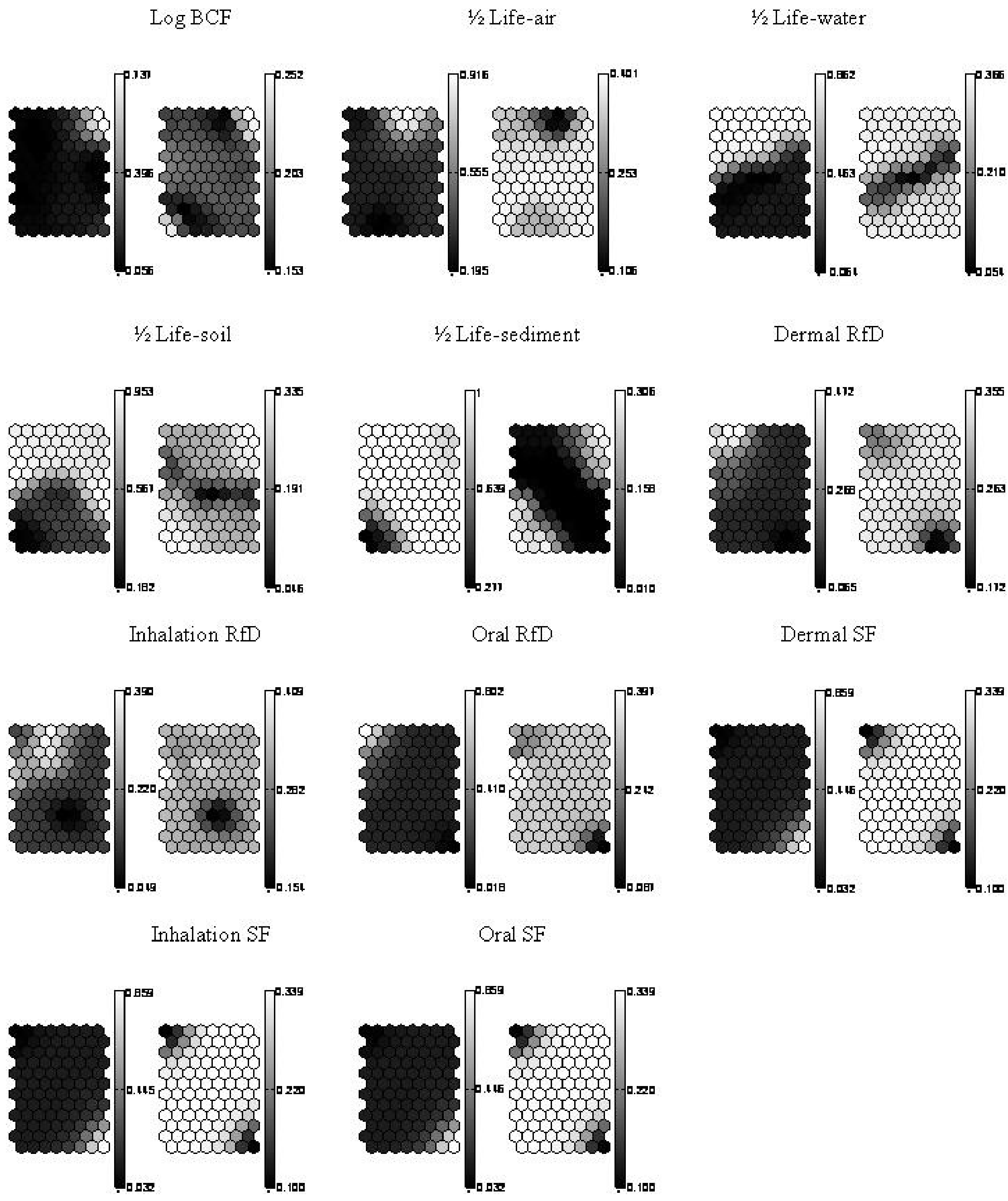

Figure 6. 2: C-planes of mean and standard deviation values for the 11 PBT parameters

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Table 6.4: Hazard Index (HI) of the 41 pollutants under study

	Mean	*St. Dev..*	*Median*	*90th perc.*	*Persistence*	*Bioaccum.*	*Toxicity*
As	3.46	0.53	3.39	4.09	2.27	0.22	0.96
Cd	3.48	0.76	3.36	4.30	2.32	0.20	0.95
Cr-III	3.23	0.88	3.07	4.11	2.31	0.19	0.72
Cr-VI	3.30	0.96	3.13	4.18	2.31	0.20	0.78
Pb	3.21	0.77	3.07	4.07	2.31	0.19	0.72
Mn	3.25	0.91	3.07	4.16	2.28	0.21	0.76
Hg	3.45	0.56	3.38	4.11	2.27	0.22	0.96
V	3.29	0.85	3.14	4.15	2.32	0.18	0.80
Acenaphthene	1.48	0.90	1.29	2.39	0.70	0.24	0.53
Acenaphthylene	1.47	0.87	1.27	2.36	0.70	0.24	0.53
Anthracene	1.46	0.84	1.27	2.35	0.70	0.24	0.53
Benz[a]anthracene	2.06	0.86	1.86	2.86	1.29	0.24	0.52
Benzo[a]pyrene	2.09	0.81	1.89	2.94	1.32	0.28	0.50
Benzo[b]fluoranthene	2.06	0.86	1.86	2.86	1.29	0.24	0.52
Benzo[g,h,i]perylene	2.19	0.86	1.99	3.06	1.34	0.35	0.49
Benzo[k]fluoranthene	2.11	0.78	1.91	2.96	1.32	0.28	0.50
Chrysene	2.06	0.85	1.86	2.84	1.29	0.24	0.52
Dibenz[a,h]anthracene	2.20	0.88	1.99	3.10	1.34	0.35	0.49
Fluoranthene	2.00	0.80	1.82	2.81	1.25	0.20	0.54
Fluorene	1.47	0.89	1.27	2.40	0.70	0.24	0.53
Indeno[1,2,3-cd]pyrene	2.18	0.84	1.98	3.07	1.34	0.35	0.49
Naphthalene	1.45	0.92	1.23	2.39	0.67	0.26	0.53
Phenanthrene	1.49	0.90	1.28	2.42	0.70	0.24	0.53
Pyrene	2.00	0.96	1.80	2.82	1.25	0.20	0.54
TCDD	3.88	0.76	3.72	4.75	1.38	0.61	1.88
PeCDD	3.43	0.76	3.27	4.30	1.39	0.51	1.53
HxCDD	2.66	0.88	2.47	3.47	1.82	0.18	0.65
HpCDD	2.61	0.91	2.41	3.41	1.85	0.17	0.58
OCDD	2.54	0.86	2.36	3.33	1.81	0.17	0.55
TCDF	2.27	0.84	2.08	3.15	1.37	0.37	0.54
PeCDF	2.28	0.83	2.09	3.22	1.37	0.37	0.54
HxCDF	2.40	0.83	2.23	3.30	1.37	0.37	0.66
HpCDF	2.00	0.83	1.82	2.82	1.25	0.20	0.54
OCDF	2.53	0.80	2.34	3.30	1.81	0.17	0.55
PCB-28	3.12	0.91	2.94	4.19	1.88	0.72	0.53
PCB-52	3.32	0.87	3.15	4.29	2.30	0.42	0.60
PCB-101	5.10	1.06	4.96	6.42	2.39	2.18	0.53
PCB-118	3.33	0.86	3.16	4.29	2.39	2.18	0.53
PCB-153	4.08	0.80	3.95	5.05	2.73	0.74	0.60
PCB-138	3.80	0.80	3.66	4.72	2.70	0.43	0.68
PCB-180	3.80	0.81	3.65	4.72	2.70	0.43	0.68

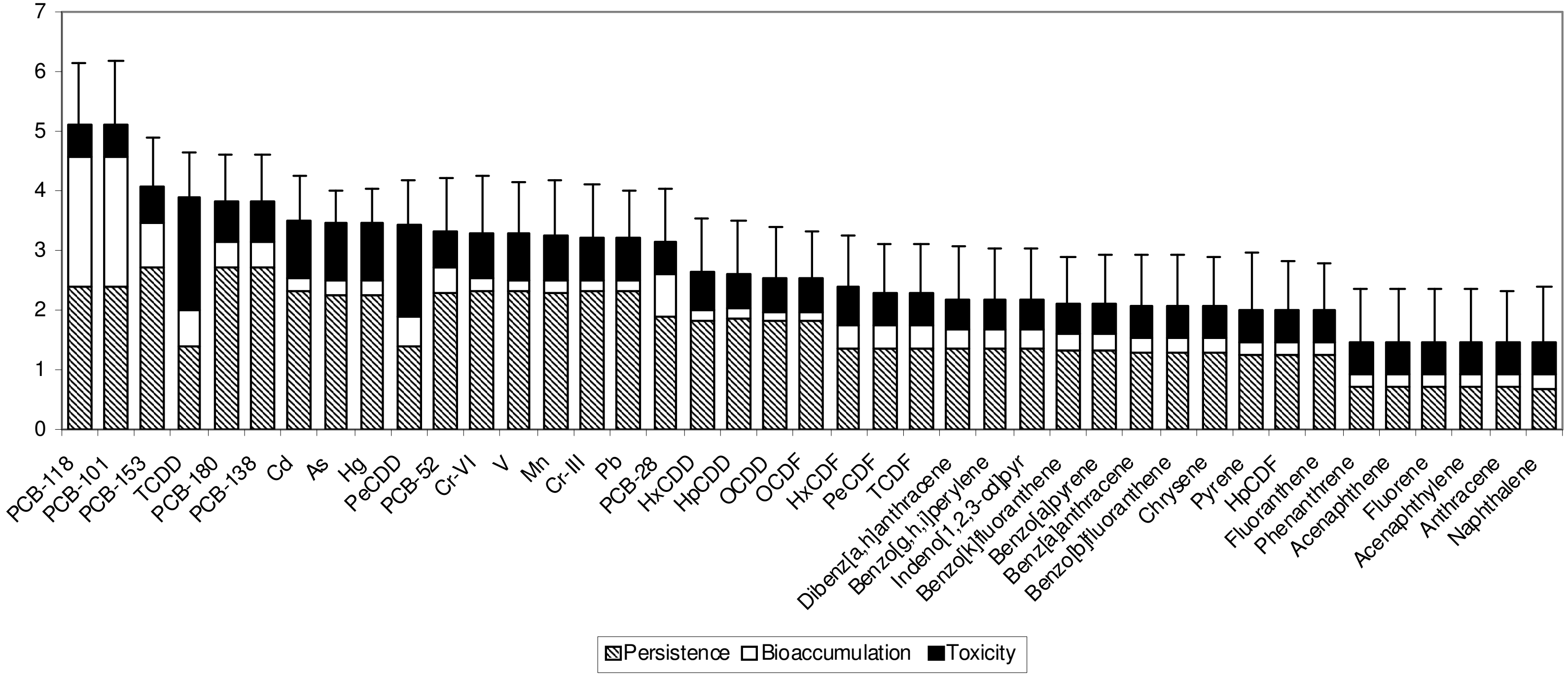

Figure 6.3: Hazard Index of the assessed pollutants ordered following a descendent order and proportion of the PBT variables

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In general terms, PCBs were the pollutants showing the highest hazard. In comparison to the remaining chemicals, PCBs were the most persistent in the environment. Among them, it is important to note the high HI values of PCBs 101 and 118, basically due to their high bioaccumulation factors (1.43·105 and 1.84·105, respectively). In contrast, PCB-28 showed a relatively low HI, which could be due to its low half-lives in air and water.(Sinkkonen & Paasivirta, 2000) In addition to PCBs, TCDD also presented a high HI (3.88), being the fourth in the list. In spite of the relatively lower environmental persistence of this dioxin homologue, TCDD seemed to be much more toxic than PCBs. In fact, TCDD and PeCDD were the only chemicals with a mean toxicity factor higher than 1 (1.88 and 1.53, respectively), which is almost exclusively due to their high carcinogenic slope factors. Although it has been noted that non-carcinogenic effects of PCDD/Fs could be even more important than its potential carcinogenicity,(Greene et al., 2003) no reference dose has been defined by the US EPA yet.(2000) Because of their high half-lives, heavy metals showed a relatively high value of HI. Inorganic elements are essentially non-degradable in the environment. Therefore, they show a very high persistence in environmental compartments.(Mackay et al., 2001) On the other hand, there are important difficulties to obtain reliable data of heavy metals bioaccumulation and bioconcentration in the scientific literature.(Floyd, 2006; McGeer et al., 2003) As a first approach, bioaccumulation factor was extracted from the Kow. Bearing in mind that a Kow cannot be established for inorganic elements and their salts, the bioaccumulation factor in the HI was quite low. Despite the difference was tiny, inorganic elements were divided into two groups in the list of chemicals, according to their toxicity: 1) Cd, As and Hg, and 2) Cr, V, Mn and Pb.

The HI associated to the group of PCDD/Fs ranged from 2.00 to 3.88. Dioxins (PCDDs) seemed to be slightly more hazardous than furans (PCDFs). With the exception of HpCDF, they followed a characteristic tendency: the HI of PCDDs inversely increased with the chlorination degree of the homologue, whereas the most substituted PCDF homologues presented a lower HI. Among the pollutants assessed, PAHs presented the lowest HI value. The 7 PAHs considered as probable human carcinogens by the US EPA were listed first. In recent years, benzo[a,h]anthracene has been catalogued as one of the most toxic PAHs according to the toxic equivalency factors (TEF) associated to them.(Law

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et al., 2002; Nisbet & LaGoy, 1992) Finally, the most volatile PAHs were those presenting the lowest PBT values. Naphthalene was the PAH with a lowest value of HI. In spite of the fact that a dermal RfD has been established, naphthalene is a compound with a very low bioaccumulation potential and a low capacity to persist in the environment.

In our previous investigation, the HI for the same pollutants was calculated using point-values.(Nadal et al., 2006) In general terms, in the deterministic HI the chemicals followed a similar pattern to that observed in the probabilistic development. PCBs and light PAHs were the substances showing the highest and lowest HI values, respectively. However, inorganic elements presented a relatively low HI in contrast to some organic pollutants such as PCDD/Fs and heavy PAHs. In that study,(Nadal et al., 2006) the bioaccumulation factor for the elements was almost negligible. Nevertheless, in the current study, the probabilistic value of bioaccumulation for these inorganic elements increased. Thus, the introduction of probabilistic data instead of deterministic data, allowed to minimize the error linked to the impossibility of obtaining bioconcentration factors for heavy metals.

A sensitivity analysis of the Hazard Index was executed to study the idoneity of the weightings given to the PBT parameters (Figure 6.4). As expected, the BCF showed the highest contribution to variance (28%). The half-lives in air, water, soil and sediments accounted approximately for 43%. However, it should be noted the special low contribution of the half-live in sediments. Most of the analyzed pollutants show a very high level of persistence in sediments, which means they are the most important sink of pollution in the environment. Finally, the sum of RfD and SF (indicators of non-carcinogenic and carcinogenic risks, respectively) accounted for 29%. These percentages of contribution to the variance indicated a good equilibrium among the PBT parameters here considered.

6.3.2 **A case-study: The industrial complex of Tarragona (Catalonia, Spain)**

In 2002, a wide environmental program was started in the chemical/petrochemical area of Tarragona. The levels of several organic (PCDD/Fs, PCBs and PAHs) and inorganic pollutants were determined in soil and vegetation samples. Three years later, a 5-years surveillance campaign was started in order to assess the temporal trend of the same pollutants in the close environment. The scope of the first part of the 2005 study included the determination of heavy metals, PCBs and PAHs in soils. Four zones (chemical, petrochemical, residential, and unpolluted) were sampled in order to evaluate not only temporal trends, but also spatial variations. Although in the 2005 survey no significant differences were noted for the levels of most pollutants with respect to the concentrations found in the 2002 survey, all they did not follow the same tendency.

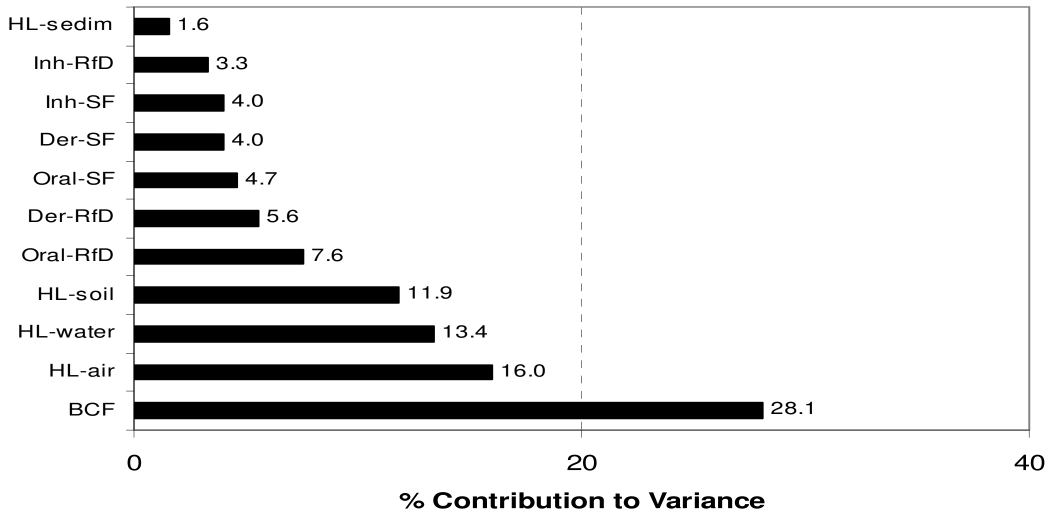

Figure 6.4: Sensitivity analysis of the Hazard Index

From the probabilistic data of both the HI and the soil concentrations of each one of the analyzed substances, the IRI equation was applied to establish the risk generalized change in the 4 zones under evaluation. The PDFs corresponding to the IRI of each area, for the 2002 and 2005 surveys are depicted in Figure 6.5. The temporal trends of risk are shown in Figure 6.6. In the 2005 study, PCDD/Fs were not analyzed. Therefore, the risk of both surveys is not fully comparable. However, the Integral Risk Index in 2002 was also calculated taking into account only the 31 chemical substances analyzed in 2005. The exclusion of the 10 PCDD/F homologues did not mean a notable variation of the risk. The risk was lower in the chemical and residential zones, while it was higher in the unpolluted area. Between 2002 and 2005, an important decrease of the risk was observed in the chemical and urban/residential areas, whereas the risk in the petrochemical zone increased

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(Fig.6). This finding is due to the notable decrease in the levels of PCBs and PAHs in soils close to chemical industries, and in the downtown of various cities.(Nadal et al., 2007) On the other hand, heavy metals did not follow a homogeneous tendency, which can be noted by the fact that the concentration of some elements raised, whereas that of the others decreased. If only the 2005 IRI is taken into account, it can be observed that the integrated risks in the chemical, petrochemical, and urban/residential areas were very similar (1.00, 1.01 and 0.86, respectively). In addition, these values were 2-fold higher than the risk in the zone considered as unpolluted (0.41). However, these risk levels can be only considered from a comparative point of view. Thus, the maximum risk according to the maximum recommended concentration of heavy metals, PCBs and PAHs in soils given by various public administrations(Busquet, 1997; Moss et al., 2001) was 130. It indicates that the current risks in Tarragona derived from the emissions of the anthropogenic activities in the area, are very low. Moreover, the mixture of chemical pollutants does not mean a significant source of health hazard for the local population.

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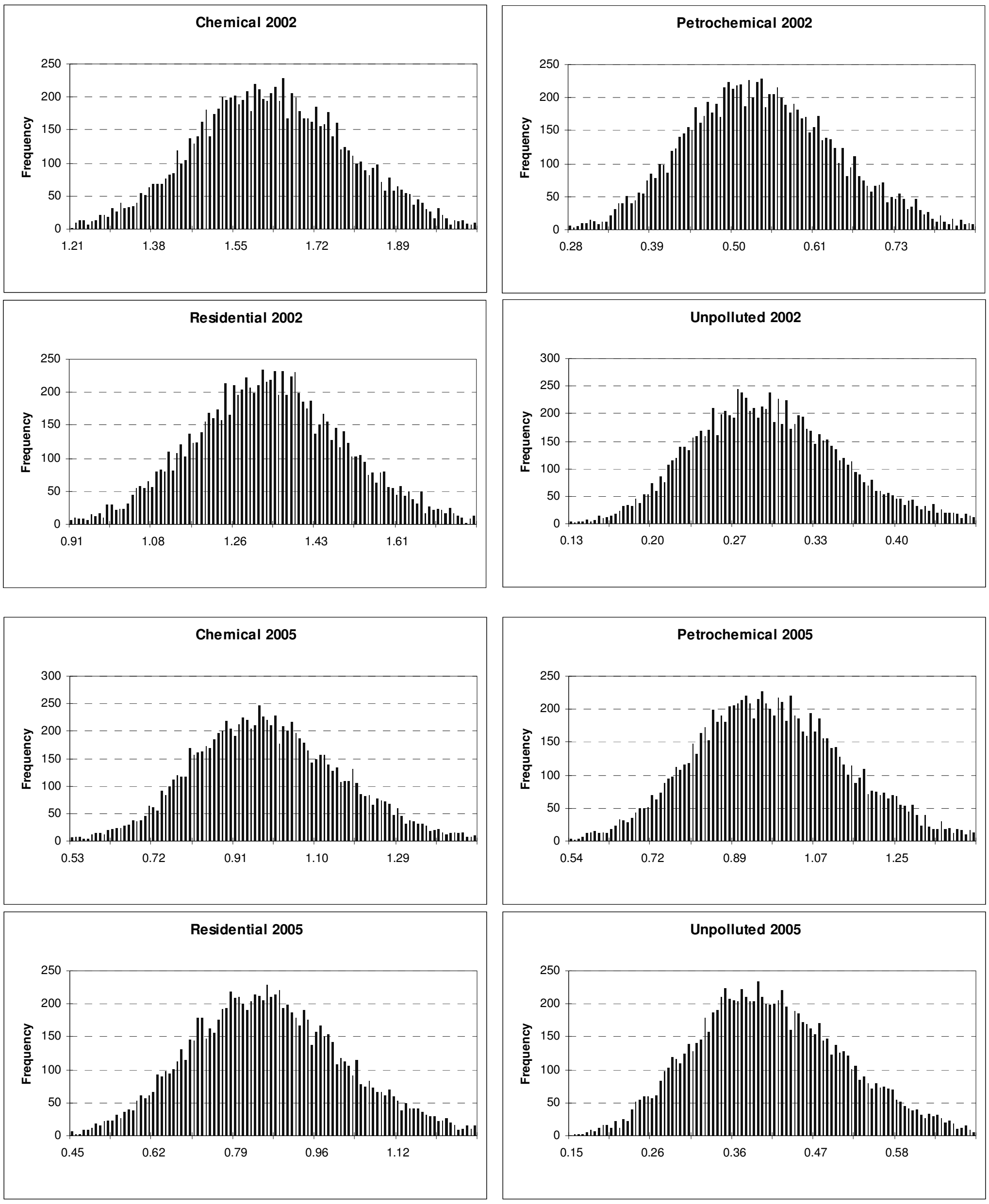

Figure 6.5: Probability density functions of the IRI for 4 areas of Tarragona in 2002 and 2005

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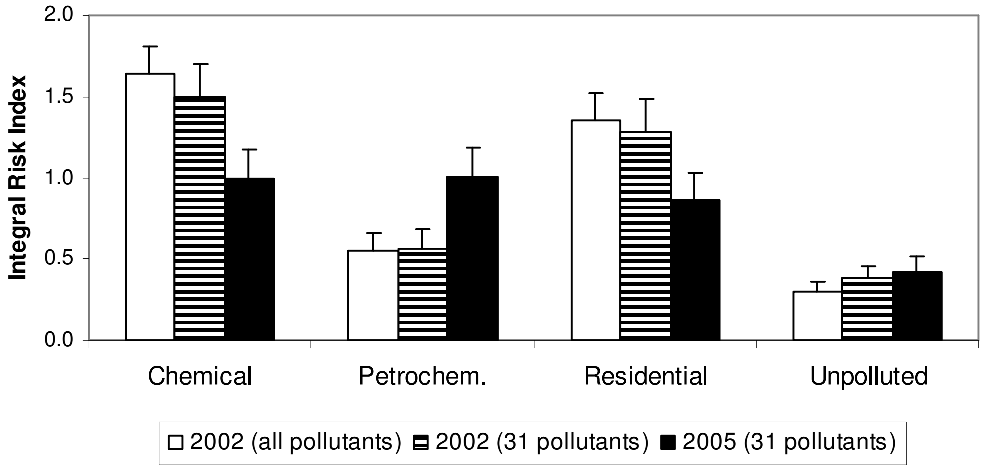

Figure 6. 6: Temporal variation of the Integral Risk Index in 4 areas of Tarragona between 2002 and 2005

6.4 Conclusions and Future Trends

The Neuro-Probabilistic IRI and the associated HI may be useful tools for the environmental decision-making process. This methodology can be highly valuable when allowing the settle-down of new chemical and petrochemical companies, as well as other potentially polluting activities in areas with a strong industrial activity. Moreover, the inclusion of probabilistic aspects makes it to become suitable for human health risk assessment.

In the future, the reliability of the PBT data of all the analyzed substances should be checked. The probabilistic density function associated to them will have to be more precisely determined by adapting continuously updated information regarding the parameters here used. Other probabilistic aspects, which take place in the process, such as considering non-deterministic values of the toxicity equivalency factors (TEF) of PCDD/Fs and PCBs,(Finley et al., 2003) could be also added. Finally, it would be of great importance to use other complementary analysis techniques. In recent years, the implantation of Geographic Information Systems (GIS) has considerably increased.(Lovett et al., 1997; Mayer & Greenberg, 2005; Thayer et al., 2003; Verter & Kara, 2001) In our previous study, the IRI was integrated in a GIS in order to create risk maps. However, given the

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importance of including probability aspects, the possibility to design probabilistic, instead of deterministic, risk maps(Saisana et al., 2004) should be investigated.

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CHAPTER 7

INTEGRATED FUZZY FRAMEWORK TO INCORPORATE UNCERTAINTY IN RISK MANAGEMENT

Abstract

Risk assessment is a complicated systematic process with large inherited uncertainties from system components and process methodologies. Integrated risk assessment of multi-components contamination problem makes the assessment more difficult and full uncertainty. Fuzzy approach widely applicable is useful for handling uncertainty of all kinds no matter what its nature or source. With the growing trend of fuzzy modelling and simulation of environmental problem, there is a need to develop a risk analysis approach which can use the fuzzy number output for characterization of risk. This study has been done to fulfil these needs. Integration of fuzzy system simulation and fuzzy relation analysis allowed incorporating system modelling uncertainty and subjective risk criteria. In this study, an integrated fuzzy relation analysis (IFRA) model is proposed for risk assessment involving multiple criteria. The model is an integrated view on uncertainty techniques based on multi-valued mappings, fuzzy relations and fuzzy analytical hierarchical process. The results obtained from fuzzy system simulation can be used in risk characterisation without aggregation which enables to propagate uncertainty in risk management model. Integration of fuzzy system simulation and fuzzy relation analysis allowed incorporating system modelling uncertainty and subjective risk criteria. The integrated risk can be calculated at different membership level which is useful for comprehensively evaluating risk within an uncertain system containing many factors with complicated relationship. It has been shown that uncertainty can be propagated in complete risk management chain through a broad integration of fuzzy system simulation and fuzzy risk analysis is possible.

Keywords: *Fuzzy modelling; risk analysis; Fuzzy relation analysis; fuzzy analytical hierarchical process.*

7.1. Introduction

The focus and position of risk characterisation within risk assessment has changed over the last decades. Originally risk characterisation was viewed as serving as an intermediary summary phase between risk assessment and risk management, with the purpose of describing the nature, magnitude of risks and associated uncertainty (NRC, 1983). Today, risk characterisation on human health risks is the integration of the first three steps in the risk assessment process, namely hazard identification, dose-response assessment and exposure assessment (Yassy et al., 2001). Further, the increased recognition of the need to protect both man and the environment responds to the perceived need for an integrated and holistic approach to risk assessment (EC, 2003). It is also considered as an integral part of the entire decision-making process and it may reflect analysis and deliberation by all interested parties (NRC, 1996). There has also been lot of development in risk assessment towards a greater emphasis on estimating and describing not just the magnitude and nature of risks but also providing improved descriptions and estimates of associated uncertainties (Williams & Paustenbach, 2002). Today it is commonly accepted that risk management should be more holistic activity involving a better uncertainty propagation approach (Kumar, 2005; Oxley et al., 2004; Refsgaard et al., 2007). The uncertainty assessment is not just something to be added after the completion of the modelling work. Instead uncertainty should be seen as a red thread throughout the modelling study starting from the very beginning, where the identification and characterisation of all uncertainty sources should be performed (Refsgaard et al., 2007). To provide a risk characterisation within reasonable uncertainties, detailed site–specific information forming the basis for hazard identification (agents causing adverse effects), dose – response assessments and exposure assessments is usually needed. Data gaps and uncertainties (important factors in characterising the risk) may, however, in many cases be approached by ‘extrapolation’ of knowledge from one area to another, unless specific research can be directed to solving such problems through. Several approaches to

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uncertainty analysis for systems modelling have been developed (Nilsen & Aven, 2003). However probabilistic uncertainty assessment approach has been most preferred approach due to various reasons (Schuhmacher et al., 2001). It may be the interpretation of Risk definition as probability or likelihood of possible contamination and magnitude or seriousness of consequences or strong basis of classical statistics etc give more confidence in probabilistic approach. However, when applied to diverse problems, probability theory often retains a fundamental assumption about the subject area involved. Specifically, it assumes that there exists a historical run for the observations of events. Also lack of data or imperfect knowledge about the processes may frustrate rigorous probabilistic studies (Kumar, 2005). Another problem with the probability theory is its law of excluded middle [$P(A \cup A^c) = 1$] and contradiction [$P(A \cap A^c) = 0$] (A^c is complement of A).

In recent years, use of fuzzy set approach in environmental application has significantly increased (Abebe et al., 2000; Kumar, 2005; Lauzon & Lence, 2008; Li et al., 2006). For example fuzzy approach is often used as modelling framework in uncertain scenario. For various reason sometime fuzzy approach has been cited as better approach to do uncertainty analysis (Abebe et al., 2000; Dou et al., 1997; Ferson, 2002; Kumar, 2005; Lauzon & Lence, 2008; Li et al., 2007). So many authors have classified uncertainty analysis into two broad categories: probabilistic and possiblistic (or fuzzy)(Blair et al., 2001; Destouni, 1992; Li et al., 2007). However advance studies using fuzzy approach in the environmental risk assessment is still limited. In comparison, many applications to other areas have been reported. In spite of its usefulness in uncertainty analysis, it has not been adopted by environmental risk modellers. One of the reasons is the lack of integrated framework to use fuzzy simulation results in risk management model. It is often a problem to use fuzzy results (which are in form of membership function) in crisp-set based risk management model. The problem becomes more complicated when the risk is produced by multi-contaminants and different factors can affect the level of risk. This complication has discouraged the risk assessment communality to use fuzzy approach in environmental risk management.

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In this study, an integrated fuzzy relation analysis (IFRA) model is proposed for the environmental risk assessment involving multiple criteria. The objective is the integration of system simulation and risk analysis using fuzzy approach which allows incorporation of system modelling uncertainty and subjective risk criteria. In the first part of this paper, the methodology of the proposed Integrated Fuzzy framework has been explained. In the part II, the methodology has been applied to a case study of contaminated soil.

7.2 Integrated Risk Assessment

There is currently a general agreement that risk assessment is best addressed in four stages(EC, 2003), where risk characterisation represents the final integration of the first three steps in the risk assessment process, namely hazard identification, effects assessment and exposure assessment (Figure 1). Hazard is a qualitative term expressing the potential of an environmental agent to harm the health of individuals or populations if the exposure level is high enough and/or if other conditions apply (Yassy et al., 2001). The extent of exposure of receptors to contaminants is one of the fundamental input requirements to any risk characterisation. However there are different units used e.g. concentration, activity concentration or dose/dose rate. Since most effects information describes effects as a function of dose or dose rate, there are strong reasons to quantify exposure primarily as dose rates. It is, however, possible to back–calculate effects benchmarks from dose rate to concentration using dose conversion factors and dosimetric models (USDOE, 2002). Concentration is also an easier concept to understand than dose, and therefore easier to explain to some stakeholders during the screening phase. Ideally, risk characterisation should produce a quantitative estimate of the risk in exposed population or estimates of the potential risk under different plausible exposure scenarios. However it is difficult to provide quantitative description of the exposure. Exposure and effect assessment is a complicated process of different factors which makes risk analysis a function of contaminant concentration and various risk factors. This clearly makes risk analysis a decision analysis problem where the risk characterisation stage attempts to make sense of the available information on exposure and effects and to describe what it means (Williams & Paustenbach, 2002).

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Since the framework presented in Figure 7.1 is a general representation of a complex and varied group of assessments, the sequence may differ among specific assessments or among groups of stressors. For example, sometimes analysis of exposure and effects may be combined with integration of results (i.e. risk characterisation). In other risk assessment schemes, risk characterisation is based on an exposure assessment, which is compared to benchmarks or compliance levels (i.e. effects analysis is not an integral part of the risk assessment)(EC, 2003). Integrating effects analysis will have the advantage that it is easier to ensure that there is sufficient correspondence between the estimated effects profile and the assessment endpoints of concern.

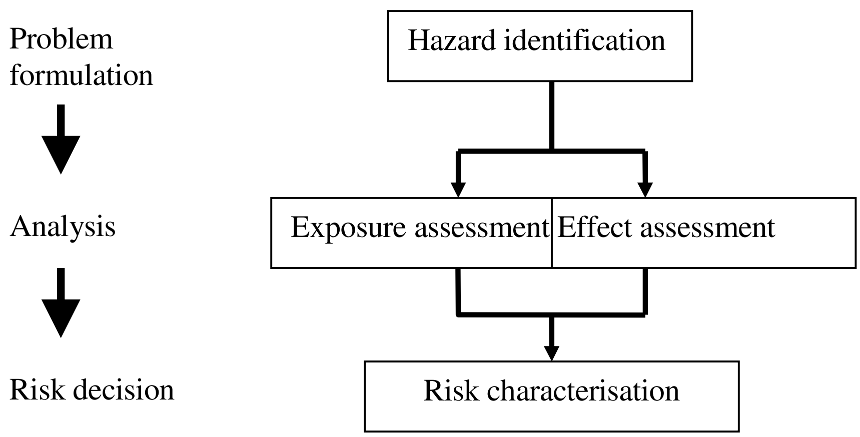

Figure 7.1: A generalised risk assessment framework

In general, there are large similarities between human risk assessment and ERA, since the basic framework adopted in ERA is a direct development from the risk assessment framework originally developed for assessing human health risks (NRC, 1983). Integration of human health and ecological risk assessment is therefore both desirable and feasible. Integration of human health and ecological risk assessment can be done by bottom-up and top-down approaches(Suter, 2004). The bottom-up approach begins with transport, fate and exposure mechanism (physical chemical properties, distribution pathways, contaminant concentration in different media, bioaccumulation, back ground concentration etc) that could be considered as common data needs during problem formulation for both human and ecological risk assessment. The top-down approach in contrast begins with the premise that humans reside in ecosystems, and the changes in the environment imply changes in human health and welfare. Ideally integration should proceed from both directions. However in practice higher value is placed on human life and health risk assessment becomes central objective of risk decision analysis with ecological risk as one of the risk factor(Suter, 2004).

Risk assessments are typically carried out on single substances. Real exposure situations, however, are often more complex with mixtures of contaminants. The most common approach to address multiple exposures is to treat the contribution of each contaminant as additive. The concept of concentration addition is assumed to be valid for contaminants with the same site of action and/or for contaminants with the same mode of action. However, if contaminants have dissimilar action mechanisms and/or different sites of action, independent action of the contaminants is expected. Several methods have been proposed to aggregate the toxicity of multi-contaminants mixtures ranging from non-polar narcotics (general mode of action) to TCDD-equivalents (specific mode of action)(Suter et al., 2003). The most common approach to assess toxicity of mixtures when interaction is known is the Toxicity Unit (TU) approach. TU is given by the sum of the quotients of the effect of each contaminant in the binary mix and alone (i.e. $TU = \sum EC50\_mix/EC50\_alone$). Thus, a TU of 1 indicates additive interaction whereas a $TU>1$ is less than additive (antagonistic) and a $TU<1$ greater than additive (synergistic)(Gallego et al., 2007). Given that the toxicity is additive, the total risk of the mixture can also be assessed as the sum of Risk Quotients (RQs) of each of the contaminants. RQs can be calculated either based on concentrations or on doses, and represents thereby a concentration ratio or dose ratio. Within the European framework for new and existing chemicals (EC, 2003), Predicted Environmental Concentrations (PEC) are compared to Predicted No Effect Concentrations (PNEC) to give a variety of ratios (i.e. $RQ = PEC/PNEC$) for the different environmental compartments considered. The quotient method is widely recognised and easy to use and communicate, which makes it a useful tool in screening and lower tier assessments. However, in higher tier assessments a lot of

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information is lost when deriving deterministic point estimates of exposure and effects. For example, a RQ of 5 may be inferred as a much larger risk than a RQ of 2; however, the RQ value does not quantify the incidence and severity of the adverse effects. Thus, to interpret these concentrations or dose ratios there is a need to calibrate against effects induced. Furthermore, the estimated RQ is influenced by the uncertainties connected with exposure and effects analyses. This means that a high RQ calculated from uncertain data may constitute no larger a risk than a low RQ calculated from more precise data.

7.3 Fuzzy framework of Integrated Risk Assessment

The application of fuzzy sets theory in decision-making problems was become possible when Bellman & Zadeh (1970) and a few years later Zimmermann (1978) introduced fuzzy sets into the field of multiple-criteria analysis. They cleared the way for a new family of methods to deal with problems that had been inaccessible to and unsolvable with standard techniques. More advanced issues in this area incorporates decision-making with interactive and interdependent criteria (Carlsson & Fuller, 1996; Holz & Mosler, 1994; Korvin & Kleyle, 1999), selection of aggregation operators (Calvo et al., 2002; Yager & Kacprzyk, 1997) etc. Risk assessment is not a classical case of decision making process. It involves complex analytical process, so a single decision making method will not be sufficient to cover the whole risk assessment process. Taking clue from decision theory (Neufville, 1990), risk decision can be defined as a process of evaluation with three steps: i) Problem formulation, ii) risk analysis iii) risk decision (Figure 7.1).

7.4 Proposed Integrated Fuzzy Risk Assessment (IFRA) Framework

The Proposed integrated approach to risk management in uncertain scenario includes three components based on fuzzy approach: system modelling and simulation, weight assessment, and risk decision-making (Figure 7.2). In general, modelling results could provide predict concentrations of pollutants and they serve as the bases for further health risk assessment. Integration of exposure and effect into an estimate of risk can be achieved via probabilistic methods or possibility methods. The flow from expert assessment to system modelling is a typical research methodology for many environmental

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subjects and is embedded in this conceptual framework. Here modelling includes the development of different fate and transport models for predicting concentration of contaminants in different media and the development of decision analysis tools for risk decision-making, based on field data, scenario assessment, and system modelling results. The conceptual framework represents a holistic and multidisciplinary approach to environmental risk management, and the three components comprise a work flow for a risk assessment process.

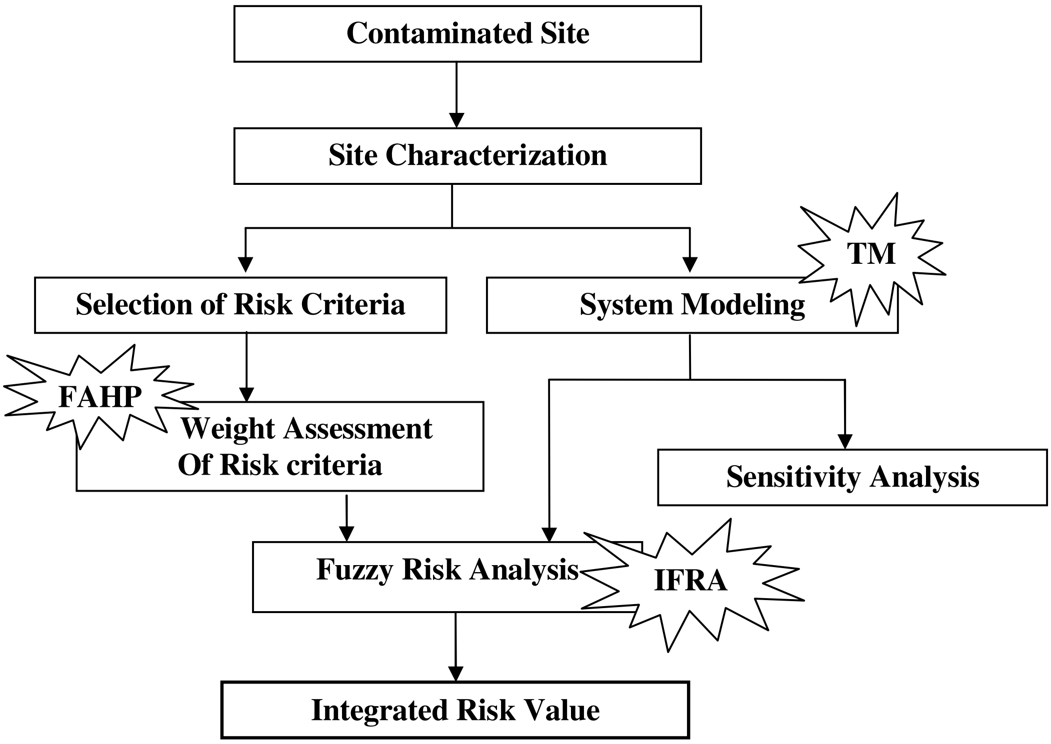

Figure 7.2: General framework of Integrated Fuzzy Relation Analysis Method (FAHP = Fuzzy Analytical Hierarchical Process, TM = Transformation method and IFRA = Integrated Fuzzy Relation Analysis).

7.4.1 **Fuzzy System modelling and simulation**

Basic principal of fuzzy modelling is based on Zadeh's extension principle (Zadeh, 1968). If all input parameters in a mathematical model are known, also the dependent variables are defined with crisp values and if we assume that the input parameters are imprecise and represented by fuzzy numbers, the resulting outputs of the model will also be fuzzy numbers characterised by their membership functions. In this paper Transformation Method (TM) introduced by Hanss (2002) is used. The simulation using TM used in the present study will be next explained. Hanss (2002) has proposed two forms of transformation methods, one general transformation method and other reduced transformation method. These two methods differ in degree of discretisation of particular interval.

Consider fuzzy numbers $\tilde{A}_1, \tilde{A}_2, ..., \tilde{A}n$ are the set of n input parameters defined on the real line R and suppose x_i, where $i = 1,2,\ldots,n$ denotes the element of $\tilde{A}_i$. Now if y is the output of the system which depends on n inputs $x_1, x_2, ..., x_n$ by the mapping $y = f(x_1, x_2, ..., x_n)$, the n input parameters are modelled as fuzzy numbers with a membership function $\mu_A(x)$ of arbitrary shape. Then the solution to the fuzzy number $\tilde{B}$ in y can be obtained by the following steps using transformation method.

6. Using the α-sublevel technique, discretise the range of membership [0,1] into a finite number of values. So an input parameter $\tilde{A}_i$ can be decomposed into a set of m+1 intervals $X_i^{(j)}$, $j = 0,1,...m$. The value of discretisation term, m depends on the degree of accuracy needed in approximation.
7. For each membership level j, find the corresponding intervals for $\tilde{A}$ in $x_i, i = 1, 2, \ldots, n$. These are the supports of the α_j-cuts of $\tilde{A}_1, \tilde{A}_2, ..., \tilde{A}_N$. So if $\left[a_i^{(j)}, b_i^{(j)}\right]$ is the end points interval of i^{th} input parameter and for j^{th} level of membership denoted by $X_i^{(j)}$ then set $\tilde{A}_i = \{X_i^{(0)}, X_i^{(1)}, ..., X_i^{(m)}\}$. When a_i is equal to b_i, the interval reduce to a point i.e. at α-level 1.

Now instead of applying standard interval arithmetic to the interval $X_i^{(j)}$, they are transformed into arrays using combinatorial operation at each α-level.

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8. The intervals are transformed into arrays $\hat{X}_i^{(j)}$ of the following forms:

$$\hat{X}_i^{(j)} = \underbrace{\left(\alpha_i^{(j)}, \beta_i^{(j)}, \alpha_i^{(j)}, \beta_i^{(j)}, \ldots, \alpha_i^{(j)}, \beta_i^{(j)}\right)}_{2^{i-1}\, pairs} \tag{1}$$

with $$\alpha_i^{(j)} = \underbrace{\left(a_i^{(j)}, \ldots a_i^{(j)}\right)}_{2^{n-1}\, elements}, \quad \beta_i^{(j)} = \underbrace{\left(b_i^{(j)}, \ldots b_i^{(j)}\right)}_{2^{n-1}\, elements} \tag{2}$$

where $a_i^{(j)}$ and $b_i^{(j)}$ denote the lower and upper bound of the interval at the membership level μj for the ith uncertain parameter. For each interval level, these arrays combine the interval extrema $a_i^{(j)}$ and $b_i^{(j)}$ in every possible way.

9. Simulation is carried out by evaluating the expression separately at each of the positions of the arrays using the conventional arithmetic for crisp numbers. Thus, if the output $\tilde{B}$ of the system can be expressed in its decomposed and transformed form by the arrays $\hat{B}_i^{(j)}, j = 0,1,\ldots,m$ the kth element ${}^k b_i^{(j)}$ of the array $\hat{B}_i^{(j)}$ is then given by

$${}^k b_i^{(j)} = f\left({}^k \hat{x}_1^{(j)}, {}^k \hat{x}_2^{(j)}, \ldots, {}^k \hat{x}_n^{(j)}\right) \tag{3}$$

where ${}^k \hat{x}_1^{(j)}$ denotes the k^{th} element of the array $\hat{X}_i^{(j)}$.

10. Finally, the fuzzy-valued result $\tilde{B}$ of the problem can be achieved in its decomposed form

$$\tilde{B}^{(j)} = \left[a^{(j)}, b^{(j)}\right], \quad j = 0,1,\ldots,m \tag{4}$$

by retransforming the arrays $\hat{B}_i^{(j)}$ using recursive formulae

$$a^{(j)} = \min_k\left(b^{(j+1)}, {}^k\hat{b}^{(j)}\right), \quad j = 0,1,\ldots,m-1, \tag{5}$$

$$b^{(j)} = \max_k\left(b^{(j+1)}, {}^k\hat{b}^{(j)}\right), \quad j = 0,1,\ldots,m-1, \tag{6}$$

and

$$a^{(m)} = \min_k\left({}^k\hat{b}^{(j)}\right) = \max_k\left({}^k\hat{b}^{(j)}\right) = b^{(m)}. \tag{7}$$

7.4.2 **Weight Assessment of risk criteria**

General weight (W_i) for each pollutant has to be decided according to the relative risk of the pollutants based on different health and ecological risk criteria (EPA, 2005;

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Kumar et al., 2006). The weight has been assigned using Fuzzy Analytical Hierarchical Process (FAHP) proposed by Korvin & Kleyle (1999). FAHP is a systematic approach to multi-criteria decision-making in uncertain environment which involves ranking several alternatives according to their weights. The hierarchical pair-wise comparison is employed to induce the relative weights of alternatives through pair-wise comparison. By means of hierarchy, the importance of the alternatives according to the objective can be viewed. Numerical values in the Decision Matrices (DMs) are fuzzy numbers reflecting uncertainty in the judgement-making process. In applications it is often convenient to work with Triangular Fuzzy Numbers (TFNs) because of their computational simplicity (Giachetti & Young, 1997), and they are useful in promoting representation and information processing in a fuzzy environment. The steps involve in FAHP are quite similar to AHP and have been described next.

1. Arrange the information, (i.e., goal, criteria, and alternatives) into a hierarchical model. In this case the goal is risk weight, criteria are risk factors and alternatives are different contaminants.
2. Use pair-wise assessment to determine the relative importance of each criterion and each alternative. Values are provided as TFNs in the form of a triplet (l, m, u) representing lower, modal, and upper bound of relative importance. Pair-wise assessment specifies which element (criterion or alternative) is more important, preferable, or likely, with respect to its parent node (the goal or the selected criterion).
3. Using triangular fuzzy numbers with the pair-wise comparisons made, the fuzzy comparison matrix $\widetilde{X} = (x_{ij})_{n \times m}$ is constructed. Fuzzy mathematical process that generates relative ratios of measurement, to measure the relative weight from the pair-wise assessments.

The pair-wise comparisons are described by values taken from a pre-defined set of ratio scale values. The ratio comparison between the relative preference of elements indexed i and j on a criterion can be modelled through a fuzzy scale value associated with a degree of fuzziness. Then an element of $\widetilde{X}$, x_{ij} (i.e., a comparison of the ith risk factor with the *j*th risk factors with respect to a specific criterion) is a fuzzy number defined as $x_{ij} = (l_{ij}, m_{ij}, u_{ij})$, where l_{ij}, m_{ij} and u_{ij}, are the lower bound, modal, and upper bound, values for x_{ij}, respectively. By using the fuzzy synthetic extent analysis (Cheng, 1999), the value of fuzzy synthetic extent with respect to the i^{th} criterion $(i = 1,2, ..., n)$ that represents the overall performance (in this case risk) of the j^{th} $(j=1,2,\ldots m)$ decision attribute (in this case contaminant) can be determined by

$$S_i = \sum_{j=1}^{m} x_{ij} \Big/ \sum_{i=1}^{n} \prod_{j=1}^{m} x_{ij} \tag{8}$$

To obtain the estimates for the sets of weight values under each criterion, it is necessary to consider a principle of comparison for fuzzy numbers(Cheng, 1999). For example, for two fuzzy numbers $\tilde{X}_1$ and $\tilde{X}_2$, the degree of possibility of $\tilde{X} \geq \tilde{Y}$ is defined as:

$$V(\tilde{X}_1 \geq \tilde{X}_2) = \sup_{x \geq y} \left[\min(\mu_{\tilde{X}_1}(x), \mu_{\tilde{X}_2}(y)) \right], \tag{9}$$

where *sup* represents supremum (i.e., the least upper bound of a set) and when a pair (x,y) exists such that $x \geq y$ and $\mu_{\tilde{X}_1}(x) = \mu_{\tilde{X}_2}(y) = 1$ it follows that $V(\tilde{X}_1 \geq \tilde{X}_2) = 1$ and $V(\tilde{X}_2 \geq \tilde{X}_1) = 0$. Since $\tilde{X}$ and $\tilde{Y}$ are convex fuzzy numbers defined by the TFNs (l_1, m_1, u_1) and (l_2, m_2, u_2) respectively, it follows that

$$V(\tilde{X}_1 \geq \tilde{X}_2) = 1 \quad m_1 \geq m_2; \tag{10}$$

$$V(\tilde{X}_2 \geq \tilde{X}_1) = hgt(\tilde{X}_1 \cap \tilde{X}_2) = \mu(d), \tag{11}$$

Where *hgt* is the height of fuzzy numbers on the intersection of $\tilde{X}$ & $\tilde{Y}$; *d* is the cross over point's abscissa between the $\mu_{\tilde{X}}$ & $\mu_{\tilde{Y}}$ as shown in Figure 3.

$$\mu(d) = \begin{cases} \dfrac{l_1 - u_2}{(m_2 - u_2) - (m_1 - l_1)} & l_1 \leq u_2; \\ 0 & otherwise. \end{cases} \tag{12}$$

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The degree of possibility for a convex fuzzy number can be obtained from the use equation 11. The degree of possibility for a fuzzy number greater than other fuzzy numbers can be obtained by obtained by max-min operation(Dubois & Prade, 1987). Suppose there are n risk criteria and m pollutants and w_j represents weight of *jth* pollutants aggregated over all risk criteria. Then w_j can be given by:

$$w_j = min(V(\tilde{X}_i \geq \tilde{X}_k / k = 1,2,..n \;\&\; k \neq i)) \quad j = 1,2,...,m \tag{13}$$

And the weight vector is given by:

$$W = (w_1, w_2,..., w_m) \tag{14}$$

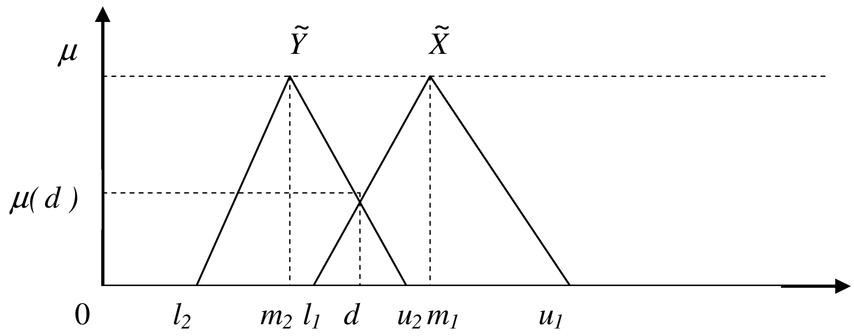

Figure 7.3: Comparison of two fuzzy numbers $\tilde{X}$ and $\tilde{Y}$

Different risk criteria are used to weigh the possible threats of contaminants. These may include risks to population exposed, physical stability of contaminant, chemical characteristics of contaminant, threat to environment, management considerations etc. The criteria whereby acceptability will be judged will obviously depend on the circumstances, and objective of the assessment. The actual set of factors to be considered in any particular case might be fairly simple or highly complex. Even in simple situations, a decision will not necessarily be made on the basis of quantitative criteria. Each criterion can be ranked as TFNs on a numeric scale giving lower, modal and upper bound of rank which can be further used in FAHP weight assessment.

7.4.3 **Integrated Fuzzy Relation Analysis Method**

For the purpose of quantifying uncertainty more effectively and integrating the risk assessment process with system modelling in a fuzzy environment, Integrated Fuzzy

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Relation Analysis (IFRA) has been proposed. The concept of fuzzy relation was first applied to medical diagnosis by (Zadeh, 1968). In a very general setting, the process of fuzzy relation analysis can be conveniently described by pointing out relationships between a collection of pattern features and their class membership vectors. This analysis is useful for multifactorial evaluation and risk assessment under imprecision and uncertainty (Pedrycz, 1990). The axiomatic framework of fuzzy set operation provides a natural setting for constructing multiattribute value functions in order to sort a set of potential actions and make an effective assessment. IFRA method is a generalization and refinement of the interval based methods such as IPFRA proposed by Huang et al. (1999). In IFRA the bounds vary according to the level of confidence one has in the estimation. One can think of a fuzzy number as a nested stack of intervals, each at a different level of presumption or possibility which ranges from zero to one and risk assessment can be performed at each level of possibility.

IFRA method for risk analysis will be explained in the context of multi-contaminants problem in the groundwater. A general framework has been presented in figure 2. Assuming that chronic daily intake and average human life expectancy are constant, the relationship between the risk and the pollutant concentration can be expressed as follows:

$$I = \sum_i C_i \times K_i \, , \tag{15}$$

Where:

I = Integrated Health Risk;

C_i = Concentration of pollutant i in the groundwater (mg/L);

K_i = Constant for the pollutant i $(\text{mg/L})^{-1}$.

Thus, the IFRA modeling computation can be initiated by first defining set U for pollutants and set V for risk levels as follows:

$$U = \{ u_i \mid \forall i \} \tag{16}$$

$$V_i = \{ v_{il} \mid \forall l \} \tag{17}$$

where u_i represents membership grade of pollutant i in the multifactorial space and v_{il} is the criterion for pollutant i at risk level l. Criteria for pollutant at different risk level are

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concentration range which reflects the expected health hazard at that level. This is generally a policy matter and decided by different regulatory agency.

The u_i value can be regarded as a weighting coefficient for pollutant i which can be calculated as follows:

$$u_i = w_i \times \hat{c}_i \tag{18}$$

where w_i is general weighting coefficient for pollutant i, which can be calculated using some multi-attribute decision-aiding model. Here a general weight for each pollutant has been decided according to the relative risk of the pollutants based on different health and ecological risk criteria. This weight was assigned with Fuzzy Analytic Hierarchy Process (FAHP).

And $\hat{C}_i$ is normalized concentration of pollutant i. Normalization (scale to [0, 1]) need to be done to remove the weightage of numeric value during calculation of weighting coefficient.

Pollutants concentration is the output of fuzzy simulation which is a fuzzy number (as explained in section 7.4.1). So with n pollutant under consideration, the pollutants concentration can be represented as fuzzy number discretised over k α-levels which can be decomposed into a set as follows:

$$\tilde{C} = \{ c_{ij}^{\pm} | i = 1,2,...,n;\ j = 0,1,2,...,k \} \tag{19}$$

where $c_{ij}^{\pm}$ denote the lower and upper bound of the i^{th} pollutant concentration at the membership level μ_j.

And normalized concentration $\hat{C}$ can be represented as:

$$\hat{C} = \{ \hat{c}_{ij}^{\pm} | i = 1,2,...,n;\ j = 0,1,2,...,k \} \tag{20}$$

Similarly here $\hat{c}_{ij}^{\pm}$ denote the lower and upper bound of the interval at the membership level μ_j for the i^{th} pollutant.

So following the fuzzy arithmetic principle (Zadeh, 1968), u_i can be calculated as fuzzy set:

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$$\tilde{U} = \{ u_{ij}^{\pm} | i = 1,2,...,n;\ j = 0,1,2,...,k \} \tag{21}$$

Now to evaluate imprecise concentration value of each pollutant versus different risk level, fuzzy relation analysis will be used. A fuzzy subset of C × *V*, which is a binary fuzzy relation from $\tilde{C}$ to *V*, can be characterized through the following membership function:

$$\tilde{R} : \tilde{C} \times V \rightarrow [0,1] \tag{22}$$

Thus, we have fuzzy relation matrix:

$$\tilde{R} = \left\{ {}^{(l)}r_{ij} | i = 1,...,n;\ j = 0,1,...,k; l = 1,2,...m \right\} \tag{23}$$

where ${}^{(l)}r_{ij}^{\pm}$ is the lower-upper bound of membership grade at membership level μ_j of pollutant *i* versus risk level *l*, which is a function of pollutant concentration and risk level criteria.

The membership grade of fuzzy relation at each membership level μ_j between given $c_{ij}^{\pm}$ for fuzzy number $\tilde{C}$ and v_{il} at risk level *l* can be calculated as follows:

Case 1: when $v_{i,l-1} \le c_{ij}^{\pm} \le v_{i,l}$:

$${}^{(l)}r_{ij}^{+} = (c_{ij}^{+} - v_{i,l-1})/(v_{i,l} - v_{i,l-1}), \forall i, j, l \tag{24}$$

$${}^{(l)}r_{ij}^{-} = (c_{ij}^{-} - v_{i,l-1})/(v_{i,l} - v_{i,l-1}), \forall i, j, l \tag{25}$$

Case 2: when $v_{i,l-1} \le c_{ij}^{+} \le v_{i,l}$ and $c_{ij}^{-} \le v_{il-1}$

$${}^{(l)}r_{ij}^{+} = (c_{ij}^{+} - v_{i,l-1})/(v_{i,l} - v_{i,l-1}), \forall i, j, l \tag{26}$$

$${}^{(l)}r_{ij}^{-} = 0, \forall i, j, l, \tag{27}$$

Case 3: when $v_{i,l} \le c_{ij}^{\pm} \le v_{i,l+1}$:

$${}^{(l)}r_{ij}^{+} = (v_{i,l+1} - c_{ij}^{-})/(v_{i,l+1} - v_{i,l}), \forall i, j, l \tag{28}$$

$${}^{(l)}r_{ij}^{-} = (v_{i,l+1} - c_{ij}^{+})/(v_{i,l+1} - v_{i,l}), \forall i, j, l \tag{29}$$

Case 4: when $c_{ij}^{\pm} \le v_{i,l-1}$ or $c_{ij}^{\pm} \ge v_{i,l+1}$:

$${}^{(l)}r_{ij}^{\pm} = 0, \forall i, j, l \tag{30}$$

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Case 5: when $c_{ij}^{-} \leq v_{i,l}$ or $c_{ij}^{+} \geq v_{i,l}$:

$$^{(l)}r_{ij}^{+} = 1, \forall i, j, l \tag{31}$$

$$^{(l)}r_{ij}^{-} = Min\{(c_{ij}^{-} - v_{i,l-1})/(v_{i,l} - v_{i,l-1}), (v_{i,l+1} - c_{ij}^{+})/(v_{i,l+1} - v_{i,l})\}, \forall i, j, l \tag{32}$$

Now we have got $\tilde{R}$ and $\tilde{U}$, from these values the integrated risk level $\tilde{I}$ can be determined as follows:

$$\tilde{I} = \tilde{U} \circ \tilde{R} \tag{33}$$

where $\circ$ cab be a max-min or max-* composition (Zimmermann, 1991).

Let $\tilde{I} = \{ b_j^{\pm} \mid j = 0,1,...,k \}$ (34)

where $b_j^{\pm}$ is integrated risk at membership level $\mu_{j.}$

For the max-min composition, integrated risk at membership level μ_j we have:

$$b_j^{\pm} = \bigvee_{i=1}^{n} (u_{ij}^{\pm} \wedge {}^{(l)}r_{ij}^{\pm}) = max\{min(u_{1j}^{\pm}, {}^{(l)}r_{1j}^{\pm}), min(u_{2j}^{\pm}, {}^{(l)}r_{2j}^{\pm}), ...$$
$$, min(u_{nj}^{\pm}, {}^{(l)}r_{nj}^{\pm})\}, l = 1,2,...,m \tag{35}$$

And for the max-* composition, we have:

$$b_j^{\pm} = \bigvee_{i=1}^{n} (u_{ij}^{\pm} \wedge {}^{(l)}r_{ij}^{\pm}) = max\{(u_{1j}^{\pm} * {}^{(l)}r_{1j}^{\pm}), (u_{2j}^{\pm} * {}^{(l)}r_{2j}^{\pm}), ...$$
$$, (u_{nj}^{\pm} * {}^{(l)}r_{nj}^{\pm})\}, l = 1,2,...,m \tag{36}$$

Thus integrated risk of a system containing several pollutants can be obtained which also integrate different risk criteria in the model. The weightage coefficient calculated from different risk criteria gives a degree of relevance for different pollutant. Fuzzy max-* operation also comply with standard toxicological norm to integrate worst risk scenario.

7.5 Case Study

A hypothetical problem is developed to illustrate integrated fuzzy modelling and risk analysis approach. The study site contains a leaking underground gasoline storage tank. About 600 m away from the tank area, there is a deep bore well used for rural drinking water supply. The recent groundwater monitoring data indicate high concentrations of several chemical stemming from petroleum products. The main contaminants in leaked

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petroleum products are benzene, toluene, ethyl-benzene and xylenes (BTEX). All these compounds are acutely toxic and have noticeable adverse health effects at high concentrations. The BTEX can enter the human body through ingestion of contaminated crops, inhalation of vapour from the soil, intake of contaminated drinking water, and skin exposure. Drinking and bathing in water containing these contaminants can put one at risk of exposure. Since BTEX can evaporate out of water, one can also be exposed by inhaling the vapours that come from drinking water.

7.5.1 **Modelling and Simulation of Contaminant transport**

A multi-phase and multi-component transport problem, with a continuous point source of pollution in a porous media with uniform flow field has been modelled. For this purpose, a finite element generated numerical solution has been used. Such solution generally requires extreme simplifications, but the results can be used for approximate solutions. They are also very useful to illustrate the sensitivity of different parameters in overall uncertainty.

A numerical model consisting of 40x30 nodal grids with a uniform grid spacing of 50 m in both directions was used to simulate the two-dimension solute transport using the following equation (Dou et al., 1997).

$$C_{i,j}^{n+1} = C_{i,j}^{n} + \Delta t\left(\left(\frac{\alpha_L V}{\Delta x^2} + \frac{V}{\Delta x}\right)C_{i-1,j}^{n} - \left(2\frac{\alpha_L V}{\Delta x^2} + 2\frac{\alpha_T V}{\Delta y^2} + \frac{V}{\Delta x}\right)C_{i,j}^{n} + \frac{\alpha_L V}{\Delta x^2}C_{i+1,j}^{n} + \frac{\alpha_T V}{\Delta y^2}C_{i,j-1}^{n} + \frac{\alpha_T V}{\Delta y^2}C_{i,j+1}^{n}\right) + \frac{M_{i,j}\Delta t}{\Delta x \Delta y \varepsilon b} \qquad (36)$$

where $C_{i,j}^{n}$ is the concentration of dissolved chemical (mg/L), V is seepage velocity in the x direction (m/day), α_L and α_T are the longitudinal and transverse dispersion coefficients (m), respectively, b is thickness of aquifer (m), ε is effective porosity, Δt is time increment (day), Δx and Δy are grid spacing in x and y direction respectively (m).

Zero concentration boundaries were placed at the left, upper and lower model boundaries with a constant source placed at 500 m from the surface and 750 m from the left

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boundary. Sample data the contaminated water is collected from 600 m from the pollution point source on the longitudinal section.

For the simulation of numerical model, fuzzy transformation method (Hanss, 2002) has been used (discussed in section 7.4.1).

Characteristics of the uncertain parameters and other data used in the simulation are shown in Table 7.3 and Table 7.4, respectively.

Table 7.1: Triangular fuzzy numbers for uncertain parameters

	Low	Medium	High
V(m/day)	0.3	0.6	1.0
α_L (m)	100	200	300
α_T (m)	20	40	60

Table 7.2: Other crisp input data use in simulation

Parameters	Value
Thickness of flow, b	50 m
Source strength, M	120 kg/day
Effective porosity, p	0.17
Grid distance (Δx)	50 m
Grid distance (Δy)	50 m
Time increment	1 day

The result of the fuzzy simulation (shown in Figure 7.4 and 7.5) along with other system components has been used for risk assessment using IFRA.

7.5.2 **Weight Assessment using (FAHP)**

Five Risk criteria are used to weigh the possible threats of contaminants as listed in table 7.3 (adopted from EPA, 2005). The relative importance of different criteria is assigned using the intensity of importance. Importance is ranked on a scale of one to five. The score 1 represents equal importance, 2 weak importance, 3 good importance, 4 strong importance and 5 very strong importance. It is difficult to map qualitative preferences to point estimates, and hence a degree of uncertainty is associated with some or all pair-wise comparison values in an FAHP problem. Using triangular fuzzy numbers with the pair-wise comparisons made, the fuzzy comparison matrix $X = (x_{ij})_{n \times m}$ has been constructed. Where element of X, x_{ij} is a fuzzy number defined as $x_{ij} = (l_{ij}, m_{ij}, u_{ij})$, where m_{ij}, u_{ij}, and l_{ij} are the modal, upper bound, and lower bound values for x_{ij} respectively. Pair-wise comparision

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between different risk criteria has been shown in table 7.4. In this case study, only the judgements between criteria obtained for the main objective are demonstrated. Subsequently, the judgements between different contaminants (represent Decision Attributes (DAs)) over different Risk criteria are dealt with in an identical manner. In Table 7.6-A &B, pair-wise comparison between contaminants over the risk criteria A and B has been shown. Similarly it has been constructed for other risk criteria.

Table 7.3: Risk factors and decision component

	Factor	Decision components
A	Population exposed	Population size, proximity to contaminants, likelihood of exposure
B	Stability	Mobility of contaminant, site structure, and effectiveness of any institutional or physical controls.
C	Contaminant characteristics	Toxicity and volume.
D	Threat to a significant environment	Endangered species or their critical habitats, sensitive environmental areas.
E	Management Criteria	Remediation technologies, cost function, environmental justice, state involvement, Brownfield/economic redevelopment.

Table 7.4: Pair-wise comparison between Risk Factors (shown in table 7.1) constructed based on the expert opinion

	A	B	C	D	E
A	(1,1,1)	(1,1,1)	(2,3,5)	(2,3,5)	(1,2.25,5)
B	(1,1,1)	(1,1,1)	(2,3,5)	(2,3,5)	(1,2.25,5)
C	(0.2,0.33,0.5)	(0.2,0.33,0.5)	(1,1,1)	(1,1,1)	(0.5,0.75,1)
D	(0.2,0.33,0.5)	(0.2,0.33,0.5)	(1,1,1)	(1,1,1)	(0.5,0.75,1)
E	(0.2,0.44,1)	(0.2,0.44,1)	(1,1.33,2)	(1,1.33,2)	(1,1,1)

Table 7.5: Sum of rows and columns based on different criteria

	Row Sums	Column Sums
A	(7,10.25,17)	(2.6,3.11,4)
B	(7,10.25,17)	(2.6,3.11,4)
C	(2.9, 3.42,4)	(7,9.33,14)
D	(2.9,3.42,4)	(7,9.33,14)
E	(3.4,4.56,7)	(4,7,13)
Sum of columns sums		(23.2,31.89,49)

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Table 7.6: Pair-wise comparison between contaminants over the risk criteria A and B

A	B	T	E	X
B	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
T	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
E	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
X	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)

B	B	T	E	X
B	(1,1,1)	(1,2.5,4)	(2,3,5)	(2,3,5)
T	(1,0.4,0.25)	(1,1,1)	(1,2,3)	(1,2,3)
E	(0.5,0.33,0.2)	(0.5,0.33,0.2)	(1,1,1)	(1,1,1)
X	(1,0.5,0.33)	(1,0.5,0.33)	(1,1,1)	(1,1,1)

The ratio comparison between the relative preference of elements indexed i and j on a criterion can be modelled through a fuzzy scale value associated with a degree of fuzziness.

The first stage of the weight evaluation process is the aggregation of l_{ij}, m_{ij} and u_{ij} values present in the pair-wise comparison matrix for the judgements between criteria (shown in table 7.5). Following the fuzzy synthetic extent concept explained in Cheng (1999), the evaluation with respect to the five criteria in terms of the 1-5 scale can be illustrated as follow.

The associated S_i values can be calculated using equation 8 which have been shown below:

$$S_1 = (7,10.25,17).(\frac{1}{49},\frac{1}{31.89},\frac{1}{23.2}) = (0.143,0.321,0.733);$$

$$S_2 = (7,10.25,17).(\frac{1}{49},\frac{1}{31.89},\frac{1}{23.2}) = (0.143,0.321,0.733);$$

$$S_3 = (2.9,3.42,4).(\frac{1}{49},\frac{1}{31.89},\frac{1}{23.2}) = (0.059,0.107,0.172);$$

$$S_4 = (2.9,3.42,4).(\frac{1}{49},\frac{1}{31.89},\frac{1}{23.2}) = (0.059,0.107,0.172);$$

$$S_5 = (3.4,4.56,7).(\frac{1}{49},\frac{1}{31.89},\frac{1}{23.2}) = (0.069,0.143,0.302);$$

To obtain the estimates for the sets of weight values under each criterion Euations 9-12 have been used.

$V(S_1 \geq S_2) = 1;\ V(S_1 \geq S_3) = 1;\ V(S_1 \geq S_4) = 1;\ V(S_1 \geq S_5) = 1;$

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$V(S_2 \geq S_1) = 1;\; V(S_2 \geq S_3) = 1;\; V(S_2 \geq S_4) = 1;\; V(S_2 \geq S_5) = 1;$

$V(S_3 \geq S_1) = 0.121;\; V(S_3 \geq S_2) = 0.121;\; V(S_3 \geq S_4) = 0.121;\; V(S_3 \geq S_5) = 0.743;$

$V(S_4 \geq S_1) = 0.121;\; V(S_4 \geq S_2) = 0.121;\; V(S_4 \geq S_3) = 0.121;\; V(S_4 \geq S_5) = 0.743;$

$V(S_5 \geq S_1) = 0.471;\; V(S_5 \geq S_2) = 0.471;\; V(S_5 \geq S_3) = 1;\; V(S_5 \geq S_4) = 1;$

The final weight vector is obtained by equation 12. Weight and source strength of different BTEX compounds has been shown in Table 7.8. Weighting coefficient u_i of each pollutant is based on Table 7.8. Risk level criteria for all compounds under study has been shown in Table 7.9 which has been adapted for this case study on the basis of EPA's recommendation of Maximum Contaminant Level (MCL) for drinking water and documentation for Immediately Dangerous to Life or Health Concentrations (IDLHs) (Chau, 2005, Falta et al., 2005, EPA, 2006). Fuzzy subset V has been built based on Table 7.9 and in consultation of expert which denotes the different risk level of pollutants. The membership grade of fuzzy relation between given $c_{ij}^{\pm}$ at membership level μ_j for fuzzy number $\tilde{C}$ and risk level j can be calculated according to conditions set in equations 24-34. And finally the integrated risk level has been determined using equation 35 (equation 36 can also be used).

Table 7.7: The sets of weight values for all fuzzy comparison matrices and the final results obtained

	Weight values for DAs				Criteria Weight
DA	B	T	E	X	
C1	0.25	0.25	0.25	0.25	0.369
C2	0.53075	0.34118	0.06403	0.06403	0.369
C3	0.39669	0.22676	0.3185	0.058055	0.045
C4	0.044739	0.19782	0.36254	0.3949	0.045
C5	0.13388	0.21973	0.3232	0.3232	0.173
Final Results	0.331	0.275	0.202	0.192	1.000

Table 7.8: General weight and source strength of each contaminant

Pollutant	Weight	Source Strength (kg/day)
Benzene	0.331	13.2
Toluene	0.275	31.2
Ethyl Benzene	0.202	13.2
Xylene (o,m,p)	0.192	62.4

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Table 7.9: Risk level criteria for all compounds under study (amount in mg/L)

Risk level	Benzene	Toluene	Ethyl Benzene	Xylene(o,m,p)
Low	0-0.005	0-1	0-0.7	0-10
Moderate	0.005-0.05	1-5	0.7-3	10-20
Moderately High	0.05-1	5-50	3-30	20-100
High	1-50	50-250	30-150	100-400
Very High	50-500	250-500	150-800	400-900
Deadly	>500	>500	>800	>900

7.6 Results and Discussion

Problem of environmental risk is more conceptual rather technical (Christakos, 2003). Common risk assessment process starts with reducing the complicated systems into mathematical models with a conceptual system understanding. The model parameters have lot of associated uncertainty because the state of knowledge is not perfect or near perfect. Assessment of the parameters can be based on expert judgement and sometime expressed as linguistic terms. Crisp set and crisp set based risk assessment frameworks are unable to express different sort of uncertain. Fuzzy logic has been successful in providing coherent framework for uncertainty modelling. In this study, fuzzy technique has been used to provide an integrated modelling and risk assessment framework. The fuzzy transformation method has been used for system modelling. A finite element generated numerical solution for multicomponent transport problem, with a continuous point source of pollution in a porous media with uniform flow field has been used for predicting pollutants concentration in groundwater. Some of the result of the simulations has been shown in Figure 7.4 and 7.5. Figure 7.4 shows membership plot of concentration of different pollutants after 5 years of time period in a well near residencial area.

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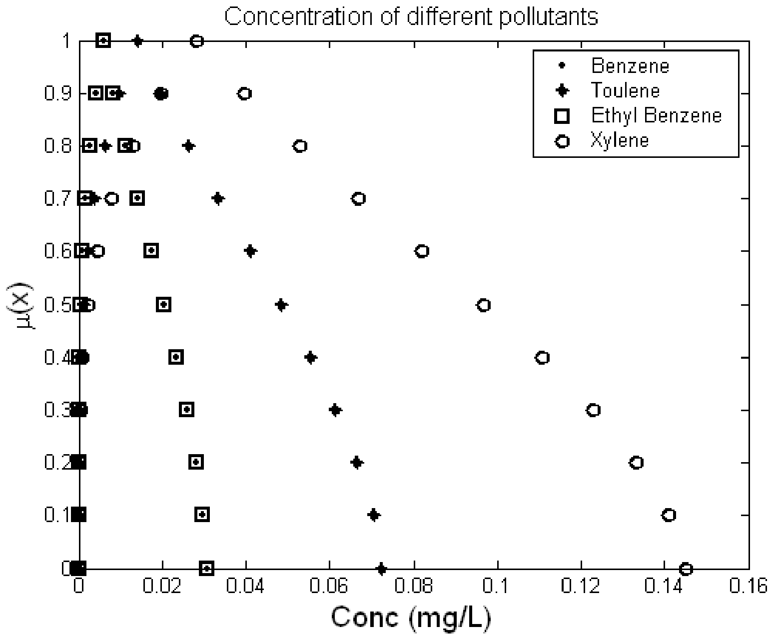

Figure 7.4: Concentration of different pollutants obtained from Fuzzy system simulation.

Figure 7.5 is showing the concentration of solute at different time interval obtained from system simulation for 1000 days time interval. The lower and upper bound of different membership level of fuzzy number, i.e. 0.0, 0.3, 0.5, and 0.8 of α-cuts respectively has been mapped. Concentration graphs are showing clear narrowing of width of the concentration membership function (upper bound minus lower bound) which converges to one line at 1 α-cut. Result has been compared with other fuzzy methods reported by Dou, et al. (1997) in another paper by Kumar and Schuhmacher (2005) (Chapter 3 of this thesis). The width of the concentration membership function obtained from Transformation method is narrower than other comparable fuzzy methods like vertex method in the same case study. The difference in the concentration output is mainly due to interaction of the concentration variable in space and time dimensions. Neglecting this dependency of input variables result in overestimation of the imprecision of solute concentration. A detailed discussion of the effect of fuzzy number dependence can be found in Dou et al. (1995).

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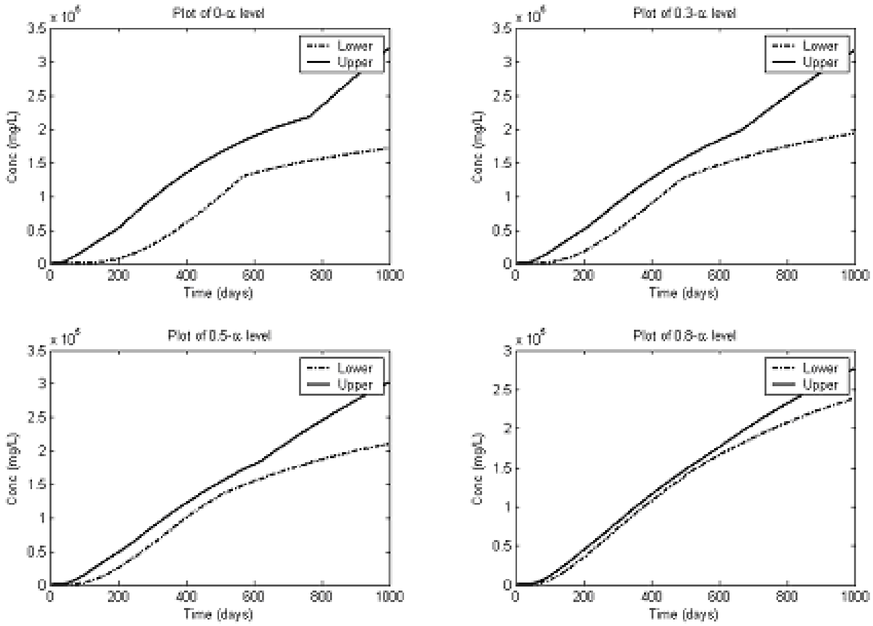

Figure 7.5:Comparison of solute concentration outputs of solute transport at different α-levels obtained from Fuzzy Transformation method

The application of the Fuzzy Analytic Hierarchy Process (FAHP) method has been used for weight assessment of risk criteria. The FAHP provides a productive framework in dealing with complexity by means of a structured hierarchy and in moving from point assessment to environmental-policy evaluation. Apart from exposre parameters, there are many risk criteria are evaluated and integrated in this weight assessment steps. The important consequences of the choice outcome may confer a level of uncertainty on the decision maker, in the form of doubt, procrastination etc. This is one reason for the utilisation of FAHP, with its allowance for imprecision in the judgements made.

From the above steps we obtained fuzzy value of hazard (concentration of BTEX compounds) and weight of risk criteria. We have also estimated risk standards in term of different risk level for the pollutants. Now it needs to be evaluated in logical manner to produce integrated risk. It also needs to quantify uncertainty more effectively from fuzzy output of hazard analysis (quantitative uncertainty) and subjective uncertainty of risk standards (subjective uncertainty). Fuzzy Relation Analysis has been used to provide a systematic framework and effective quantification of uncertainty in integrated risk analysis.

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The result of integrated risk analysis at different membership degree has been shown in Table 10. Degree of membership can be interpreted as confidence level. Uncertainty with the risk prediction is decreasing as level of confidence is increasing. Integrated risk at α-level 0 is 'Low to Moderately High' which become narrower at α-level 0.5 as 'Low to Moderate' which further narrowed to become 'Moderate to moderately high' at α-level 0.8 and 'Moderate' at α-level 1.0. Average risk perception at this contaminated site can be quantified as 'Moderate'. The fuzzy membership of Risk perception in a given context, should be taken as proportional to how similar (in terms of risk) given site risk is (or will be) to some pre-determined prototypical "risk" in the environmental context. Result at different membership level can be interpreted on confidence scale which can be different in different situation. Decision maker have choice to see risk perception at different possiblistic level.

Here we would might go beyond this and suggest an alternate criterion, that the fuzzy membership be proportional to the 'utility' for an appropriately defined decision maker in that context of using different terms for Risk to describe contamination problem (this, for example, would allow us to weigh costs of inappropriate usage of the term). This proposed subjective description makes a lot of sense at management level.

Table 7.10: Integrated Risk at different membership levels

Membership level	Integrated Risk
0	Low to Moderately High
0.1	Low to Moderately High
0.2	Low to Moderately High
0.3	Low to Moderately High
0.4	Low to Moderate
0.5	Low to Moderate
0.6	Low to Moderate
0.7	Low to Moderate
0.8	Moderate to Moderately High
0.9	Moderate to Moderately High
1.0	Moderate

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Advantages of using the IFRA for environmental risk analysis include:

- It is an integrated approach which incorporates effects of different pollutants and different risk criteria within a general framework;
- It can explicitly consider and propagate uncertainties;
- The IFRA can provide a general analysis framework for effectively modelling different kind of uncertainties encountered in risk analysis process;
- It enables the synthesis of quantitative information into qualitative output which is more easily understandable to decision makers and regulators;
- Its modular form is scalable and easily programmable for computer applications and can become a comprehensive risk analysis tool.

The application presented in this paper is a simplified demonstration of the approach. A comprehensive application would require a major effort, including the collaboration of several experts in the various disciplines of knowledge. It still needs to be tested for real case study. One possible limitation of the proposed method may be sensitive to the selection of aggregation operators at different stage of the process (simulation, weight assessment or Fuzzy relation analysis). Different operators can be used for different segments of the model. One possible problem of wrong aggregation operators could be exaggeration and eclipsing. Exaggeration occurs when all parameters have relatively low membership value and the aggregated outcome is unacceptably high. Eclipsing is the opposite phenomenon, where one or more of the parameter is of relatively high value, yet the aggregated value comes out as unacceptably low. Also in the proposed framework the sensitivity analysis should be extended to examine the effects of input scenario and aggregation operators as well. A comprehensive sensitivity analysis will depend on the actual values of the specific case at hand. As the case study presented here is a simplified example, applying such a sensitivity analysis here would be of little value.

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7.7 Conclusion

Common risk assessment approaches based on probabilistic tools such as Monte Carlo are analogous to assessments based on fuzzy logic, however these two methods differ significantly both in approach and interpretation of results. One key advantage of fuzzy logic over Monte Carlo methods is the ability to confront linguistic variables (low, moderate, high, very high). With Monte Carlo methods, we must often force continuous distributions to fit linguistic variables for probabilistic assessments. Fuzzy arithmetic combines outcomes from different sets in a way that is analogous to but different from Monte Carlo methods.

The proposed IFRA approach presents a new model to integrated risk assessment which contributes to the area of environmental risk assessment under uncertainty. Integration of system simulation and risk analysis using fuzzy approach allowed incorporating system modelling uncertainty and subjective and inexact risk criteria. It is useful for comprehensively evaluating risks within a system containing many factors with complicated interrelationships. It can incorporate effects of different pollutants and different remediation techniques within a general framework. Also, the method can effectively reflect uncertainties presented as inexact intervals for a number of modelling inputs. Decisions on activities, practices or interventions that involve contamination of the environment may be informed through the technical assessment procedures but will also be influenced by many other factors, including stakeholder views, which often involve trade-offs. Fuzzy Analytical Hierarchical Process makes it possible to trade-offs between different risk factors and incorporates uncertainty of qualitative decisions. All these factors become integrated in the judgement of acceptability, which – in turn – guides decision-making. A key feature of such decision-making is that the process should be open and transparent, and that all factors considered should be clearly defined such that there is a basis for judgement on the acceptability of the decision.

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CHAPTER 8

GENERAL CONCLUSIONS AND FUTURE DIRECTIONS

The term soft computing describes an array of emerging techniques such as fuzzy logic, probabilistic reasoning, neural networks, and genetic algorithms. All these techniques are essentially heuristic, which provide rational, reasoned out solutions for complex real-world problems. In this study, different soft computing approaches to uncertainty propagation in environmental risk management models have been investigated. The thesis maninly focused on contaminant risk however methods developed can be equily applicable to other area of environment risk. Uncertainty propogation methods are generic and can be used in any system modelling application. Practicability of methods has been shown with application to some real case studies. A brief summary of the work under taken in this study are given as follows:

In the first section of this thesis gives a general introduction and background knowledge on the subject mater. Chapter 2 reviews previous studies on uncertainty propagation in environmental models and different methods used for uncertainty modelling. It also gives background information on fuzzy set and related theories. Review of these efforts provides bases for proposing practical modelling tools for uncertainty modelling in environmental models. Particularly, the existing techniques tackling uncertainties in simulation and risk assessment, such as fuzzy-set and stochastic methods, are examined with their advantages and disadvantages being analysed.

Section two deals with uncertainty propagation methods and consists of two studies. The first study provides comparison of stochastic and fuzzy approaches of uncertainty propagation. A new methodology based on generalized fuzzy α-cut principal and concept of transformation method shows superiority over conventional methods of uncertainty modelling. Transformation method is a special implementation of fuzzy arithmetic based on α-cut principle that avoids the well-known effect of overestimation which usually arises

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from use of interval computation for fuzzy arithmetic. This method has been extended to do sensitivity analysis of uncertain model parameters. A case study of uncertainty analysis of pollutant transport in ground using 2-D transport model has been used to show the utility of this approach. Results are compared with commonly used probabilistic method and normal Fuzzy alpha-cut technique. Based on the structure of the explicit finite-difference equation for solute transport, the transformation method has been applied to solve the fuzzy equation at each node and each time step. Compared to the vertex method which has been reported to overestimate the uncertainty, this method has given comparable or better results and has sorted out the problem of overestimation due to dependencies among uncertain variables at different nodes.

In the second study, a new hybrid-method has been proposed, which allow combined utilization of probabilistic (Latin Hypercube Sampling) and non-probabilistic (fuzzy set theory) approaches for treating model parameter uncertainties in the system model. This method called Fuzzy Latin Hypercube Sampling (FLHS) technique allows the characterization of both uncertainty and variability of one or more input variables. The variability in the random variables of the model is treated using probability density functions (PDFs), while the uncertainty associated with them is treated using fuzzy membership functions for the parameters of these random variables. Thus, means and standard deviations of these PDFs are modelled as fuzzy numbers. This modelling structure gives a generalized framework for uncertainty analysis. This framework of uncertainty analysis encourages the modellers for detailed uncertainty characterization, and at the same time gives enough space to carry out modelling task in case of insufficient information on parameters distribution. If the available information is sufficient for detailed characterization of uncertainty and variability, the method can provide a detailed analysis of uncertainty and variability contribution in the final result. However, in all cases the method can give insight into uncertainty and variability contribution of different parameters of the final result, which would help modeller/decision maker to collect more data or to improve observation of major parameters in order to improve results. The feasibility of the method has been validated analyzing total variance in the calculation of incremental lifetime risks due to polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs) for

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the residents living in the surroundings of a municipal solid waste incinerator (MSWI) in the Basque Country, Spain. The multi-compartmental model and the exposure models are used to do human health risk assessment. Parameters such as ingestion rate, contaminant concentration, exposure frequency and duration, body weight, averaging time, and cancer slope factor are used to estimate the added risk. Traditionally, health risk is calculated characterizing these parameters by either deterministic values or probability density functions.

The third part of thesis consisting two chapters deals with uncertainty management in environmental indices. The first paper focused on the development of an integral risk map of the chemical/petrochemical industrial area using Self-Organizing Maps (SOM). The first step was the creation of a ranking system (Hazard Index) for a number of different inorganic and organic pollutants applying Self-Organizing Maps (SOM) to persistence, bioaccumulation and toxicity properties of the chemicals. Subsequently, an Integral Risk Index was developed taking into account the Hazard Index and the concentrations of all pollutants in soil samples collected in the target area. Finally, a risk map was elaborated by representing the spatial distribution of the Integral Risk Index with a Geographic Information System (GIS). The results of this study show the utility of soft computing approaches to in environmental decision making processes relating to pollutants. The second paper is an improvement over first work. The first work used SOM weight to rank contaminants using their characteristics of persistence, bioaccumulation, and toxicity in order to obtain the Hazard Index (HI). It doesn't consider uncertainty associated with contaminants characteristic values. So in this study a hybrid method of probabilistic SOM is used to calculate Integrated Risk Index. A new approach called Neuro-Probabilistic HI was developed by combining SOM and Monte-Carlo analysis. This new index seems to be an adequate tool to be taken into account in risk assessment processes. In both papers, feasibility of the methods has been validated by applying it to the chemical/petrochemical industrial area of Tarragona (Catalonia, Spain).

The last part of thesis provides a general framework for integrated risk assessment in uncertain situation. In this study, an integrated fuzzy relation analysis (IFRA) model is

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proposed for risk assessment involving multiple criteria. This model offers an integrated view on uncertainty techniques based on multi-valued mappings, fuzzy relations and fuzzy analytical hierarchical process. Integration of fuzzy system simulation and fuzzy relation analysis allowed incorporating system modelling uncertainty and subjective risk criteria. Results obtained from fuzzy system simulation can be used in risk characterisation without aggregation which enables to propagate uncertainty in risk management model. Integrated risk can be calculated at different membership level which is useful for comprehensively evaluating risk within an uncertain system containing many factors with complicated relationship. Decisions on activities, practices or interventions that involve contamination of the environment may be informed through the technical assessment procedures but will also be influenced by many other factors, including stakeholder views, which often involve trade-offs. Fuzzy Analytical Hierarchical process makes it possible to trade-offs between different risk factors and incorporates uncertainty of qualitative decisions. All these factors become integrated in the judgement of acceptability, which – in turn – guides decision-making. A key feature of such decision-making is that the process should be open and transparent, and that all factors considered should be clearly defined such that there is a basis for judgement on the acceptability of the decision. IFRA is useful for comprehensively evaluating risks within a system containing many factors with complicated interrelationships. It can incorporate effects of different pollutants and different remediation techniques within a general framework. Also, the method can effectively reflect uncertainties presented as inexact intervals for a number of modelling inputs. It has been shown that uncertainty can be propagated in a complete risk management chain through a broad integration of fuzzy system simulation and fuzzy risk analysis is possible.

This dissertation research presents a distinguished contribution over traditional methods of uncertainty propagation in risk management by

- Effective quantification of system uncertainties using improved fuzzy logic and hybrid stochastic-fuzzy techniques.

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- Use of Artificial Neural Network (ANN) & Probabilistic-ANN to develop hazard index which can be useful tools for environmental monitoring and decision making process.
- Integrated framework of multi-components risk analysis with explicit uncertainty propagation in the whole process of risk analysis.

The proposed methods could significantly advance methodologies of risk analysis and assessment by effectively addressing critical issues of uncertainty propagation problem. Thus, useful decision analysis tools based on the proposed methods can be developed for resolving different environmental risk management problems.

Recommendation and Future Works

Even though great improvements within the methods of risk assessment have been made during the last decades, the uncertainties in the results are still high, e.g. due to data problems in all parts of risk analysis. These uncertaities will never be reduced compltetely. Hence, an objective environmental risk may exist but will never be exactly quantified. However environmental risk assessment approaches differ concerning the degree of accuracy they are able to achieve. Thus, it is a question which degree of uncertainty in risk assessment one is willining to accept with respect to the objective of the study. The choice of an appropriate uncertainty analysis approach is hence a trade-off between accuracy & effort. In any case the reproach of feigned accuracy should be countered by documenting and if possible quantifying the different type of uncertainties within the risk assessment results. Thereby, the request for a transparent documentation of the uncertainties of risk assessment can be satisfied.

Uncertainty classification and different uncertainty representations offer new research direction to modeler community to further improve the uncertainty analysis approach. In environment risk analysis, an immediate need is to develop a proper methodology (or set of methodlogies for different situations) and guideline to characterize uncertainty and variability associated with different environmental models. Fuzzy

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representation of uncertainty needs further validation to test the degree of satisfaction of compliance guideline. For example different risk compliance guidelines have been developed to compare results from stochastic simulation; similar guidelines should be developed to give general uncertainty estimates in accordance with U-V classification. Recently few researchers have proposed different fuzzy measures (e.g. possibility and necessity measures) to test the degree of satisfaction of the compliance guideline. However it still needs to be tested and adopted by different regulatory bodies before being used by modeler community. In the recent past, many methodologies have been proposed to model second order uncertainty. However, all these emerging modeling techniques are based on different assumption of defining uncertainty and variability. Comparison of these techniques is not straight forward. It needs further research, and then an adequate comparison can be performed. In this study, no attempt has been made to compare FLHS with other evolving techniques but in future if proper comparision measures will be develepoed, it can be possible to make a comparision. Also further research performed in order to develop decision analysis models, which directly use U-V outcomes in decision making process and improve risk estimation, will enhance the framework.

In future works, IFRA can be augmented with other algorithms. One promising technique can be pareto-genetic algorithm. This direction will point us toward handling environmental risk management with optimisation routine. It has the property of presenting the user with a set of solution to choose from rather than a single solution thus facilitating more informed choices.

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CURRICULUM VITAE

Vikas Kumar
Catchment Science Centre, The University of Sheffield, UK.
e-mail: **vikas.kumar@sheffield.ac.uk**

EDUCATION

2003 –	Ph.D.: "*Soft Computing Approaches to Uncertainty Propagation in Environmental Risk Management*" at the Department of Chemical Engineering, University of Rovira i Virgili, Spain.
2003 – 2005	Advanced Diploma (Master) in Chemical and Process Engineering, at the Department of Chemical Engineering, University of Rovira I Virgili, Spain Project: "*Integrated Fuzzy Environmental Modeling and Risk Assessment*"
1999 – 2001	Master in Computer Application at Indian Agricultural Research Institute, New Delhi., India, Thesis Project: "*A Search Engine for small non-commercial site (AgriKhoj)*".
1995 – 1999	B.Sc (Agriculture), Benaras Hindu University, Varanasi, India.

TRAINING AND RESEARCH

2007 - 2008	Marie Curie Early Training at the Catchment Science Centre, The University of Sheffield, UK.
2006	Research Visit, Catchment Science Centre, The University of Sheffield, UK (April – September).
2005 – 2006	Research Visit, Catchment Science Centre, The University of Sheffield, UK (April – September).
2004 – 2006	Teaching Assistant at the Department of Chemical Engineering, University of Rovira I Virgili, Spain.
2003	International PhD School in Formal Languages and Applications, URV, Tarragona, Spain (March – June).
2001 – 2003	Research Associate, at Indian Agriculture and Statistics Research Institute, New Delhi, India, Project: "*Expert System of Extension*".

SCHOLARSHIP AND GRANTS

2007 – 2008	Marie Curie Early Training, at the Catchment Science Centre, The University of Sheffield, UK.
2004 – 2007	Doctorate Scholarship ,URV, Spain.
2006	Mobility Grant (BE2005), GenCat, Spain
2004	Scholarship for Collaboration, Department de Filologies Romàniques, URV, Spain.

2003 – 2004 Predoctoral Scholarship(MECD), URV, Spain.
2001 – 2003 Research Associatship (RA), IASRI, India.
1999 – 2001 Junior Research Scholarship (JRF), ICAR, India.

AWARDS AND HONORS

2002 *Nehru Memorial Gold Medal* for best performance in Master Study at IASRI New Delhi.
1999 Awarded Junior Research Fellowship (JRF) for postgraduate study at IARI, New Delhi, India.
1999 Secured All India rank 3rd in JRF Entrance Examination for admission to the ICAR's Institutes.
1998 Student of the Year awards for Culture activities and Leadership initiative at IAS, BHU, Varanasi, India.

MEMBER OF PROFESIONAL SOCIETY

2005 - Member of International Environmental Modelling and Software Society.
2006 - Member of American Geographical Union (AGU).

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